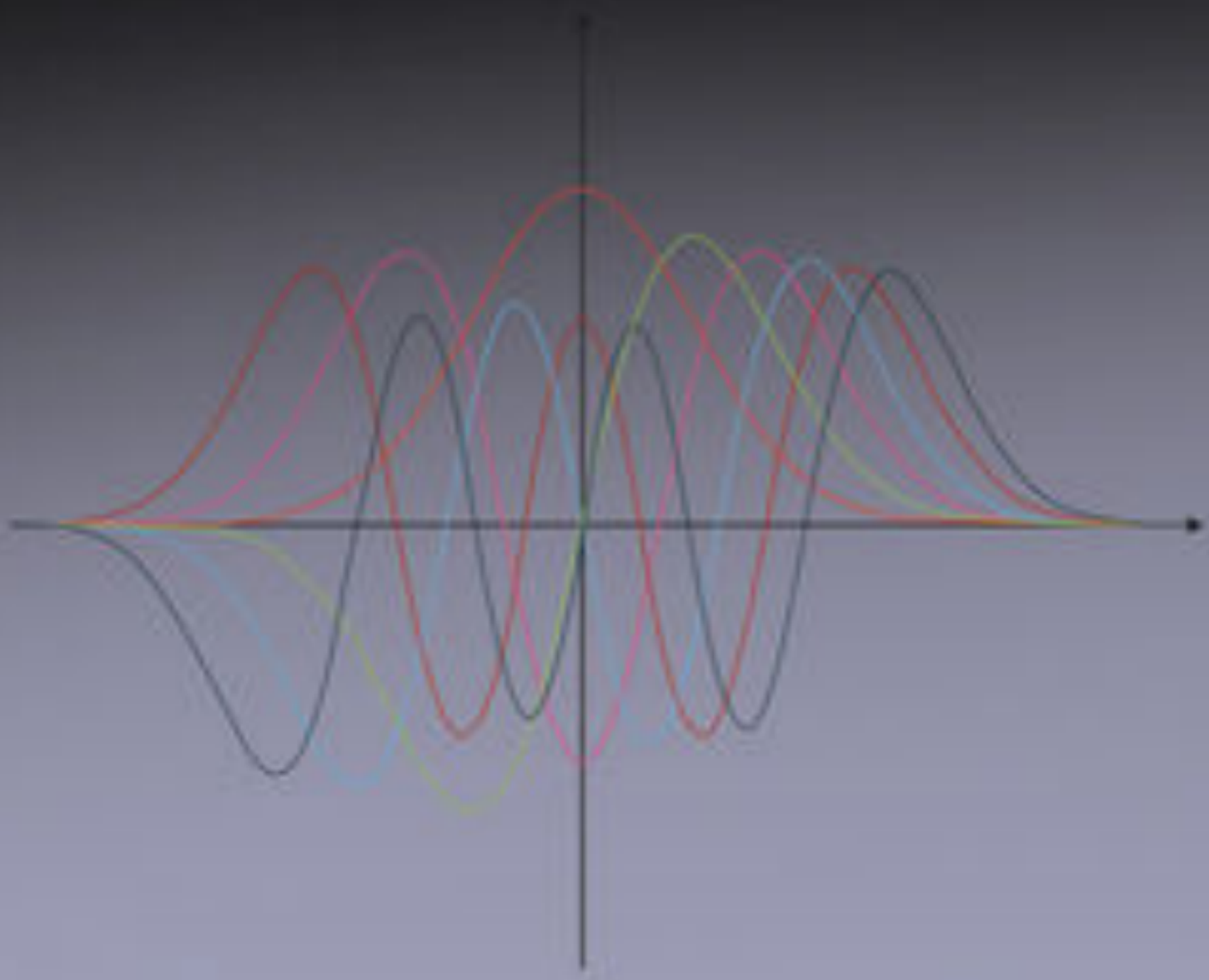
QUANTUM OSCILLATORS

Olivier HENRI-ROUSSEAU Paul BLAISE



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This book is dedicated to
Prof. Andrzej Witkowski of the Jagellonian University of Cracow,
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PREFACE

Quantum oscillators play a fundamental role in many area of physics and chemical physics, especially in infrared spectroscopy. They are encountered in molecular normal modes, or in solid-state physics with phonons, or in the quantum theory of light, with photons. Besides, quantum oscillators have the merit to be more easily exposed than the other physical systems interested by quantum mechanics because of their one-dimensional fundamental nature. However, despite the relative simplicity of quantum oscillators combined with their physical importance, there is a lack of monographs specifically devoted to them. Indeed it would be thereby of interest to dispose of a treatise widely covering the quantum properties of quantum harmonic oscillators at the following levels of increasing difficulty: (i) time-independent properties, (ii) reversible dynamics, (iii) thermal statistical equilibrium, and (iv) irreversible evolution toward equilibrium. And not only harmonic oscillators but also anharmonic ones, as well as single oscillators and anharmonically coupled oscillators.

As a matter of fact, such subjects are dispersed among different books of more or less difficulty and mixed with other physical systems. The aim of the present book is to remove that which would be considered as a lack. This book will start from an undergraduate level of knowledge and then will rise progressively to a graduate one. To allow that, it is divided into seven different parts of increasing conceptual difficulties.

Part I with Chapters 1–4 gives all the basic concepts required to study the different aspects of quantum oscillators. Part II, Chapters 5–8, is devoted to the properties of *single quantum harmonic oscillators*. Moreover, Part III deals with *anharmonicity*, either that of single anharmonic oscillator (Chapter 9) or that of anharmonically coupled harmonic oscillators (Chapter 10). Furthermore, Part IV, Chapters 11–13, treats the *thermal properties* of a large population of harmonic oscillators at statistical equilibrium. Part V concerns different kinds of *quantum normal modes* met either in light (Chapter 14) or in molecules and solids (Chapter 15). Finally, Part VI, Chapter 16, studies the irreversible behavior of *damped quantum oscillators*, whereas Part VII, Chapter 17, applies many of the results of the previous chapters to some *spectroscopic properties* of quantum oscillators. Its now time to be more precise with the contents of these parts.

Chapter 1 summarizes the minimal mathematical properties (specially those of Hilbert spaces and of noncommuting operator algebra) required to understand quantum principles. That is the aim of Chapter 2, which, after giving the postulates of quantum mechanics, treats quantum average values and dispersion, allowing one to get the Heisenberg uncertainty relations, and develops the basic consequences of the time-dependent Schrödinger equation. Then, Chapter 3 goes further by looking at the different representations of quantum mechanics, which makes tractable the

quantum generalities exposed in the previous chapter, and which will be of great help in the further studies of quantum oscillators. These quantum descriptions are *matrix mechanics*, *wave mechanics*, and time-dependent representations, that is, *Schrödinger*, *Heisenberg*, and *interaction pictures*, and finally the *density operator* representation, which may be declined according to matrix mechanics or wave mechanics and also to different time-dependent pictures. Chapter 4 ends Part I, being devoted to three different but important physical models, which will enlighten the further studies of quantum oscillators. They are the *particle-in-a-box model*, which is a simple and didactic introduction to energy quantization that will be met for quantum oscillators, the *two-energy-level model,* which will be used when studying *Fermi resonances* appearing in vibrational spectroscopy, and the *Fermi golden rule*, involving concepts that will be used in the same area of vibrational spectroscopy.

Following Part 1, which deals with the basis required for quantum oscillators studies, Part II enters into the heart of the subject. Chapter 5 focuses attention on the quantum energetic representation of harmonic oscillators by solving their time-independent Schrödinger equation using *ladder operators (Boson operators)*, thus allowing one to determine the *quantized energy levels* and the corresponding *Hamiltonian eigenkets*, and also the action of the ladder operators on these eigenkets. It continues by obtaining the *oscillator excited wavefunctions,* from the corresponding ground state using the action of the ladder operators on the Hamiltonian eigenkets. After this Hamiltonian eigenket representation, Chapter 6 is concerned with *coherent states*, which minimize the Heisenberg uncertainty relations, and *translation operators,* the action of which on Hamiltonian ground states yields coherent states, by studying their properties, which are deeply interconnected, and then used to calculate *Franck–Condon factors* and to diagonalize the Hamiltonian of *driven harmonic oscillators*. Chapter 7 continues Part II by giving proofs of some *Boson operator theorems*, which are applied at its end to find the dynamics of a *driven harmonic oscillator* and which will be widely used in the following. Finally, Chapter 8 closes Part II by treating some more complicated topics such as *phase operators*, *squeezed states*, and *Bogoliubov–Valatin transformation*, which involve products of ladder operators.

The properties of single quantum harmonic oscillators found in Part II allow us to treat anharmonicity in Part III. That is first done in Chapter 9 by studying anharmonic oscillators such as those involving *Morse potentials*, which are more realistic than harmonic potentials for diatomic molecules or *double-well* potentials leading to *quantum tunneling*, and in Chapter 10 by studying several harmonic oscillators involving anharmonic coupling. In this last chapter of Part III, together with *Fermi resonances*, is studied the *strong anharmonic coupling theory* encountered in the quantum theory of weak H-bonded species and allowing the *adiabatic separation* between low- and high-frequency anharmonically coupled oscillators, which is studied in detail. Chapter 10 ends with a study of anharmonic coupling between four oscillators, which is used to model a centrosymmetric cyclic H-bonded dimer.

Parts II and III ignored the thermal properties of single or coupled quantum oscillators, considering them as isolated from the medium, what they may be, harmonic or anharmonic. The aim of Part IV is to address the thermal influence of the medium. Part IV begins this study with a somewhat unusual chapter (Chapter 11) dealing with the dynamics of very large populations of linearly coupled harmonic

oscillators starting from an initial situation where the energy is found only on one of the oscillators. Moreover, having proven the *Boltzmann H-theorem* according to which the entropy increases until statistical equilibrium is attained, Chapter 12 applies the results of Chapter 11 to show how, after some characteristic time has elapsed, the statistical entropy reaches its maximum, in agreement with the Boltzmann theorem, whereas a *coarse-grained energy analysis* of the energy distribution of the oscillators sets reveals a *Boltzmann energy* distribution. Then, applying the principle of entropy maximization at statistical equilibrium, this chapter obtains the *microcanonical* and *canonical* density operators. Finally, Chapter 13 closes Part IV by studying the thermal properties of quantum harmonic oscillators (*thermal average energies*, *heat capacities*, *thermal energy fluctuations*) and ends with the demonstration of the expression of the thermal average of general functions of Boson operators, which contains as a special case the *Bloch theorem*.

Chapter 11 of Part IV studies the dynamics of a large population of coupled quantum harmonic oscillators that, as calculation intermediates, are considered to be *normal modes*, but without taking attention to them due to the dynamics preoccupations. Since normal modes of systems of many degrees of freedom are collective harmonic motions in which all the parts are moving at the same angular frequency and the same phase, it is possible, within classical physics, to extract for such systems the classical normal modes and then to quantize them to get quantum harmonic oscillators to which it is possible to apply all the results of Parts II–IV. This is the purpose of Part V, which starts (Chapter 14) with a study of the quantum normal modes of electromagnetic fields. That may be first performed with obtaining the classical normal modes of the fields by passing for the Maxwell equations in the vacuum, from the geometrical space to the reciprocal one, using Fourier transforms, and then introduce a commutation rule between the conjugate variables of the electromagnetic field, which are the potential vector and the electric field in the reciprocal space. Then, applying the thermal properties of quantum oscillators found in Chapter 13, it is possible to derive the *black-body radiation Planck law* and the *Stefan–Boltzmann law,* and also the ratio of the *Einstein coefficients*. Chapter 15 completes this part devoted to normal modes by determining the classical molecular normal modes and then quantizing them, and so obtaining the normal modes of a one-dimensional solid in the reciprocal space, allowing one, on application of the thermal properties of oscillators, to obtain the Einstein and the Debye results concerning the solids *heat capacity* of solids.

Continuing the work of Part IV devoted to thermal equilibrium, which was applied in Part V to find the thermal statistical properties of normal modes, Part VI, involving only Chapter 16, studies the irreversible behavior of harmonic oscillators, which are damped due to the influence of the medium. This irreversible influence is modeled by considering the medium, acting as a thermal bath, as a very large set of harmonic oscillators of variable angular frequencies, weakly coupled to the damped oscillator, and each constrained to remain in statistical thermal equilibrium. Then, solving within this approach the *Liouville equation*, and after performing the Markov approximation, the *master equations* governing the dynamics of the density operators of driven or undriven harmonic oscillators are obtained. This procedure allows one to derive in a subsequent section the *Fokker–Planck equation* for damped harmonic oscillators. Next, Chapter 16 continues, by aid of an approach similar to that used for the

master equations by deriving the *Langevin equations* governing the time-dependent statistical averages of the Boson operators, and ends, using these Langevin equations, by obtaining the interaction picture time evolution operator of driven damped quantum harmonic oscillators, which allows one to get the corresponding time-dependent density operator, which may be envisaged as a consequence of the corresponding master equation governing the dynamics of damped oscillators.

The book ends with Part VII corresponding to the single Chapter 17, by applying many of the properties of quantum oscillators obtained in Parts II and III (Chapter 10), Part IV (Chapter 13), and Part VI (Chapter 16), to find some important results in vibrational spectroscopy, such as the IR selection rule for quantum harmonic oscillators, and to study using *linear response theory*, and after having proved it, the line shapes of some physical realistic situations involving anharmonically coupled damped quantum harmonic oscillators encountered in the area of H-bonded species.

Clearly, the topics studied in all these parts involve progressive levels of difficulty, varying from undergraduate to graduate.

It may be of interest to list the quantum theoretical tools necessary to treat the different subjects of the book. Essential tools are *kets*, *bras*, *scalar products*, *closure relation*, *linear Hermitian* and *unitary operators*, *commutators* and *eigenvalue equations*, as well as *quantum mechanical fundamentals*. There exist seven postulates, concerning the notions of quantum average values and of the corresponding fluctuations leading to the Heisenberg uncertainty relations. We list the time dependence of the quantum average values leading to the Ehrenfest theorem and to the virial theorem, the different representations of quantum mechanics involving wave mechanics, matrix representation, the different time-dependent representations, that is, the Schrödinger and Heisenberg ones and also the interaction picture, all using the time evolution operators and, finally, the various density operator representations. Furthermore, there are also mathematical tools that are not specific to the subject but necessary to the understanding of some developments and that will be treated in the Appendix (Chapter 18). Among them, some commutator algebra, particularly those dealing with the position and momentum operators, some theorems concerning exponential operators as the Baker–Campbell–Hausdorff relation or the Glauber–Weyl theorem, some information about Fourier transforms and distribution functions, the Lagrange multipliers method, complex results concerning vectorial analysis, and elements dealing with the point-group theory.

On the other hand, as it may be inferred from the presentation of the different parts of the book, the following quantum oscillator properties will be considered: Hamiltonian eigenkets of harmonic oscillators and their corresponding wavefunctions, ladder operators, action of these operators on the Hamiltonian eigenkets, coherent states, translation operators, squeezed states and corresponding squeezing operators, time dependence of the ladder operators, canonical transformations involving ladder operators, normal and antinormal ordering, Bogolyubov transformations, Boltzmann density operators of harmonic oscillators, and thermal quantum average values of operators, specially that of the translation operator leading to the Bloch theorem.

Despite the complexity of the project, our aim is to propose a progressive course where all the demonstrations, whatever their level may be, would present no particular

difficulties, and thus would be readable at various levels ranging from undergraduate to postgraduate levels. In this end, we have applied our teaching experience, which used the Gestalt psychology, according to which the main operational principle of the mind is holistic, the whole being more important than the sum of its parts, that is particularly sensitive with respect to the visual recognition of figures and whole forms instead of just a collection of simple lines and curves: We have observed that this concept is very well verified to those unfamiliar with long equations involving many intricated symbols.

There are different ways to read this book. The first one concerns quantum mechanics, which, since considered from the viewpoint of oscillators, allows one to avoid all the mathematical difficulties related to the techniques for solving the second-order partial differential equations encountered in wave mechanics. The second one gives the elements required to understand the theories dealing with the line shapes met spectroscopy more specially in the area of H-bonded species. The third one may be viewed as a simple introduction to quantization of light. The fourth one may be considered as an introduction to quantum equilibrium statistical properties of oscillators, while the fifth focuses attention on the irreversible behavior of oscillators Finally, the sixth concerns chemists interested in molecular spectroscopy. The chapters may be considered as follows:

Domains	**Chapters**																
Quantum oscillators	1	2	3	4	**5**	6	7		9	10			13	14	15	16	
IR line shape spectra		2	3	4	**5**	6	7		9	10			13		15		17
Theory of light		2	3		**5**	6	7	8					13	14		16	
Statistical equilibrium		2	3		**5**	6	7					12	13				
Irreversibility		2	3		**5**	6	7				11					16	
Molecular spectroscopy	1	2			**5**				9	10							17

The cost to be paid will be the inclusion of many details in the demonstrations, which sometimes appear to the advanced readers to be superfluous. In addition, to make the equations more easily readable we have sometimes used unusual notations combined with the introduction of additive brackets, which would appear to be surprising and unnecessary for those indifferent to the didactic advantages of the Gestalt psychology, which is our option.

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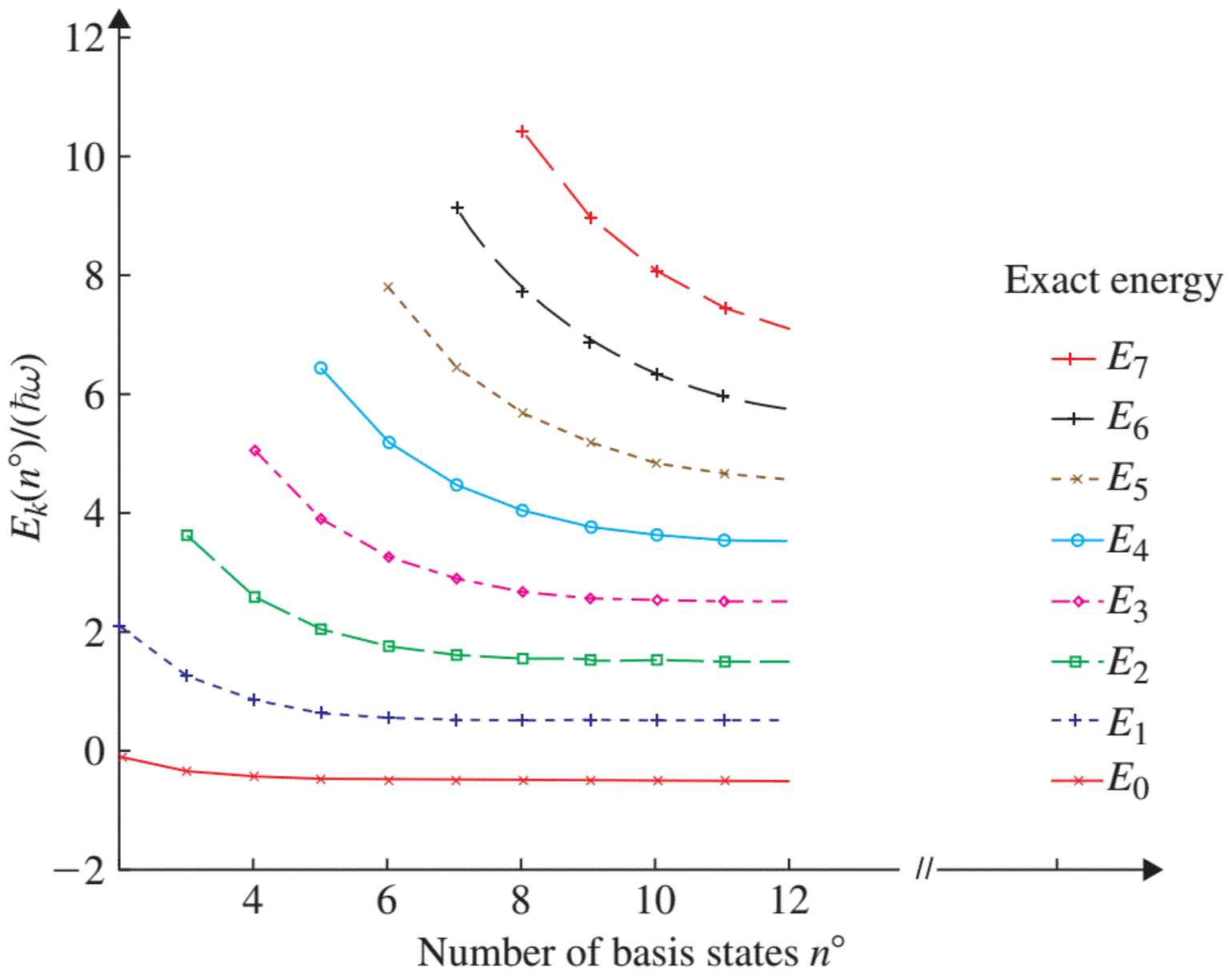


Figure 6.3 Stabilization of the energy of the eight lowest eigenvalues $E_k(n^\circ)/\hbar\omega^\circ$ with respect to n°.

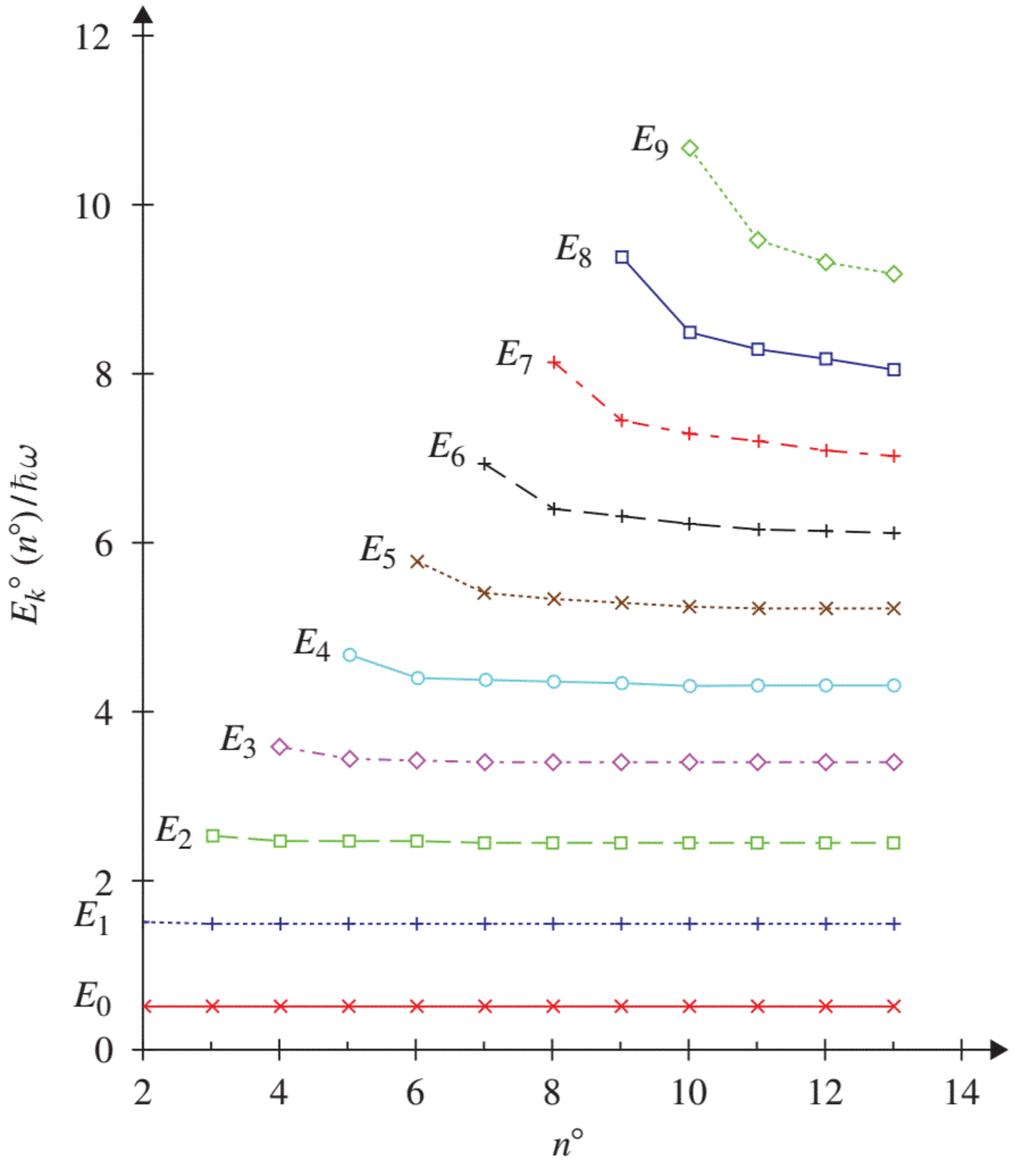


Figure 9.2 Progressive stabilization of the eigenvalues appearing in Eq. (9.50) with the dimension n° of the truncated matrix representation ($\eta = -0.017$).

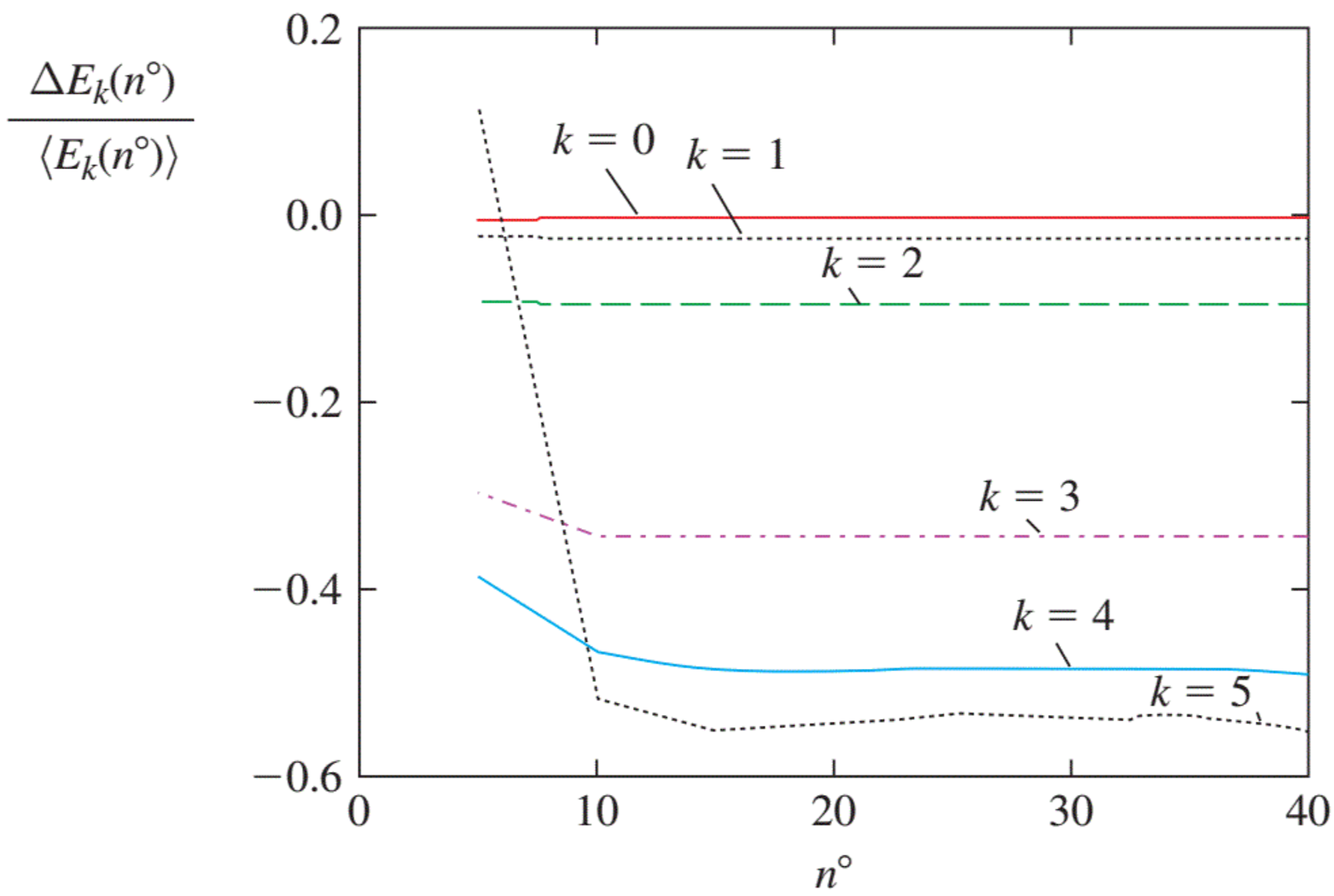


Figure 9.3 Relative dispersion of the difference between the energy levels and the virial theorem.

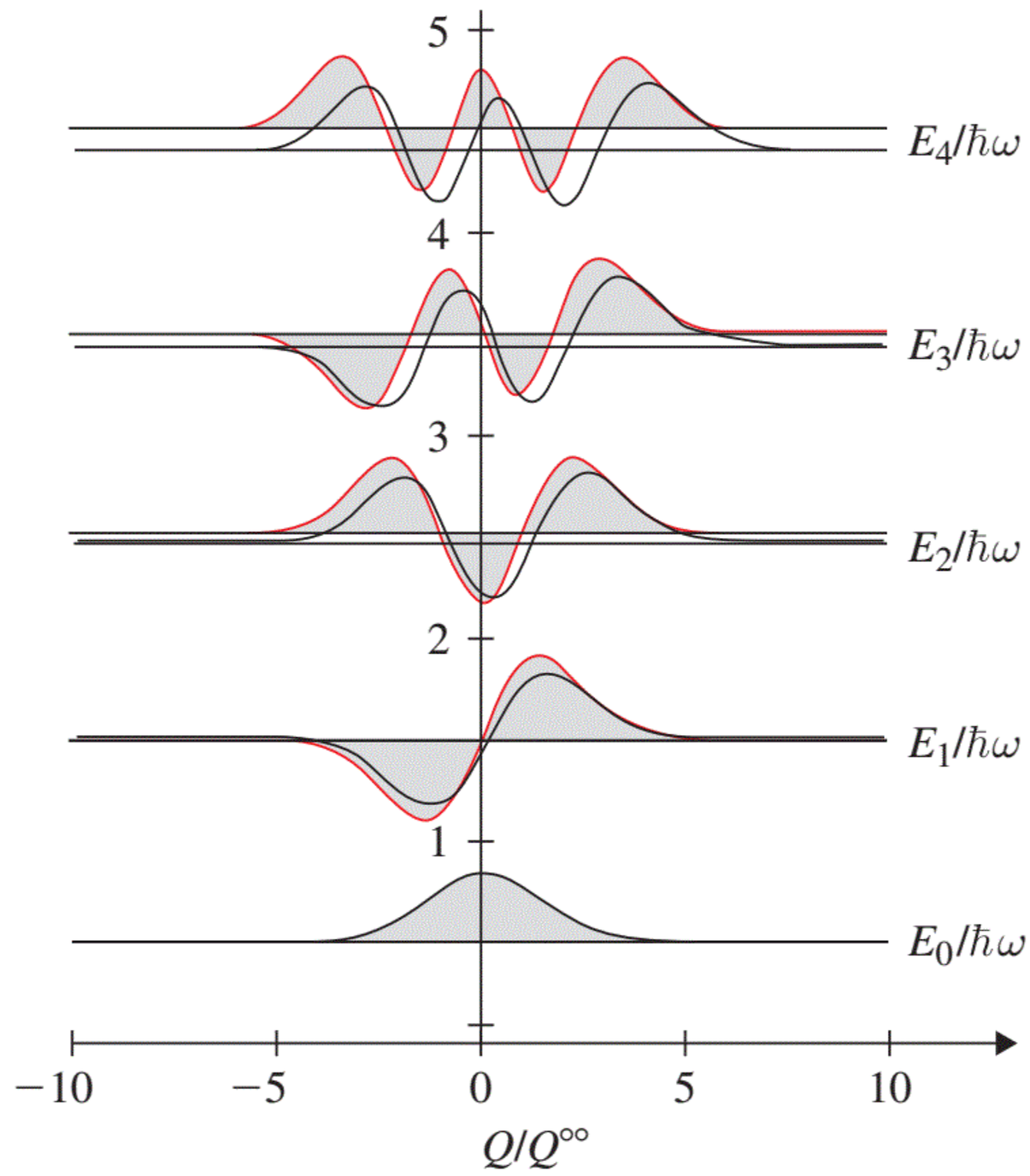


Figure 9.4 Five lowest wavefunctions $\Psi_k(\xi)$ of the Morse Hamiltonian compared to the five symmetric or antisymmetric lowest wavefunctions $\Phi_n(\xi)$ of the harmonic Hamiltonian. The length unit is $Q^{\circ\circ} = \sqrt{h/2mw}$.

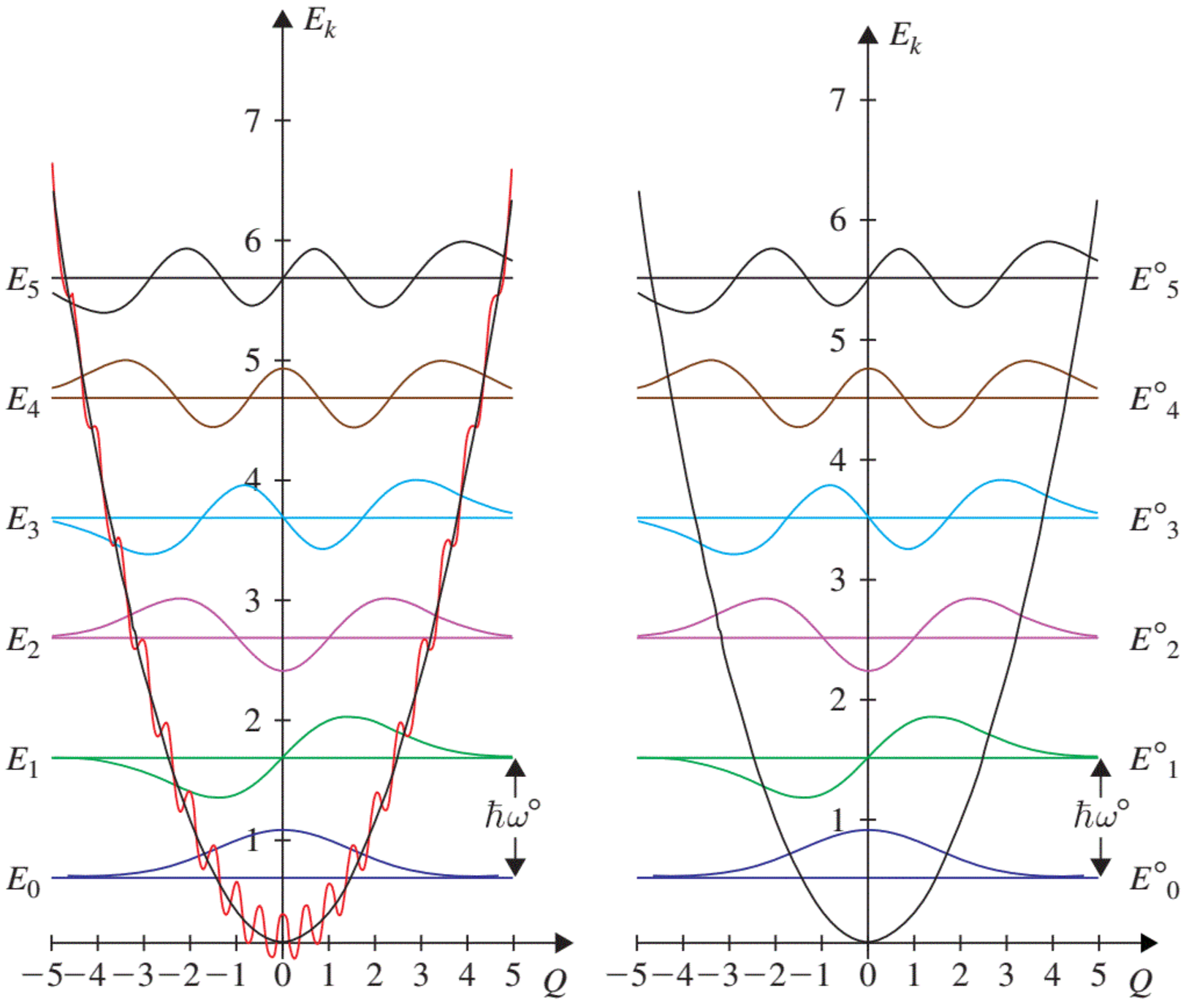


Figure 9.7 Comparison between the energy levels calculated by Eq. (9.100) and the wavefunctions obtained by Eq. (9.101) and the energy levels and the wavefunctions of the harmonic oscillator.

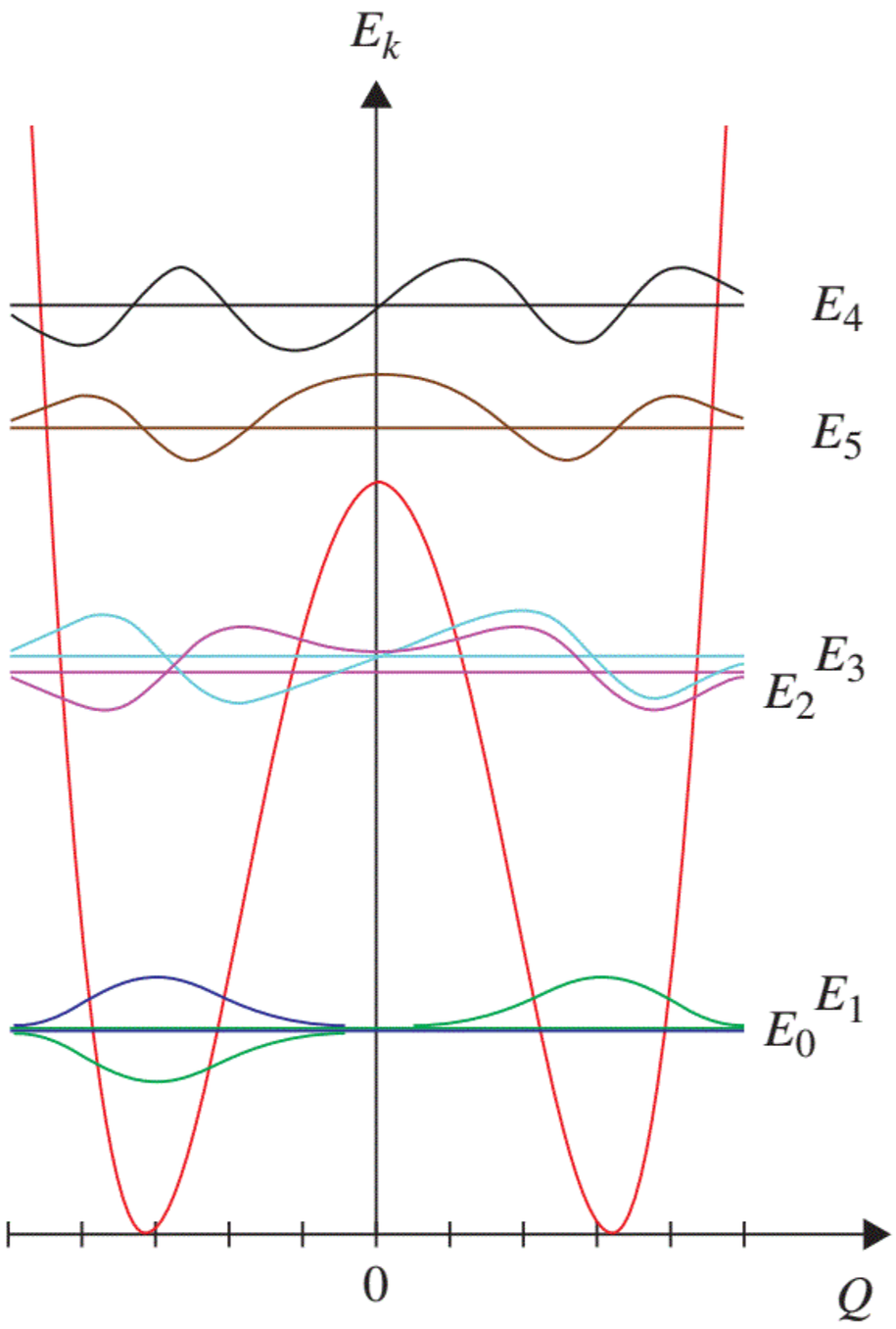


Figure 9.11 Representation of the six lowest wavefunctions and the corresponding energy levels for symmetrical double-well potential.

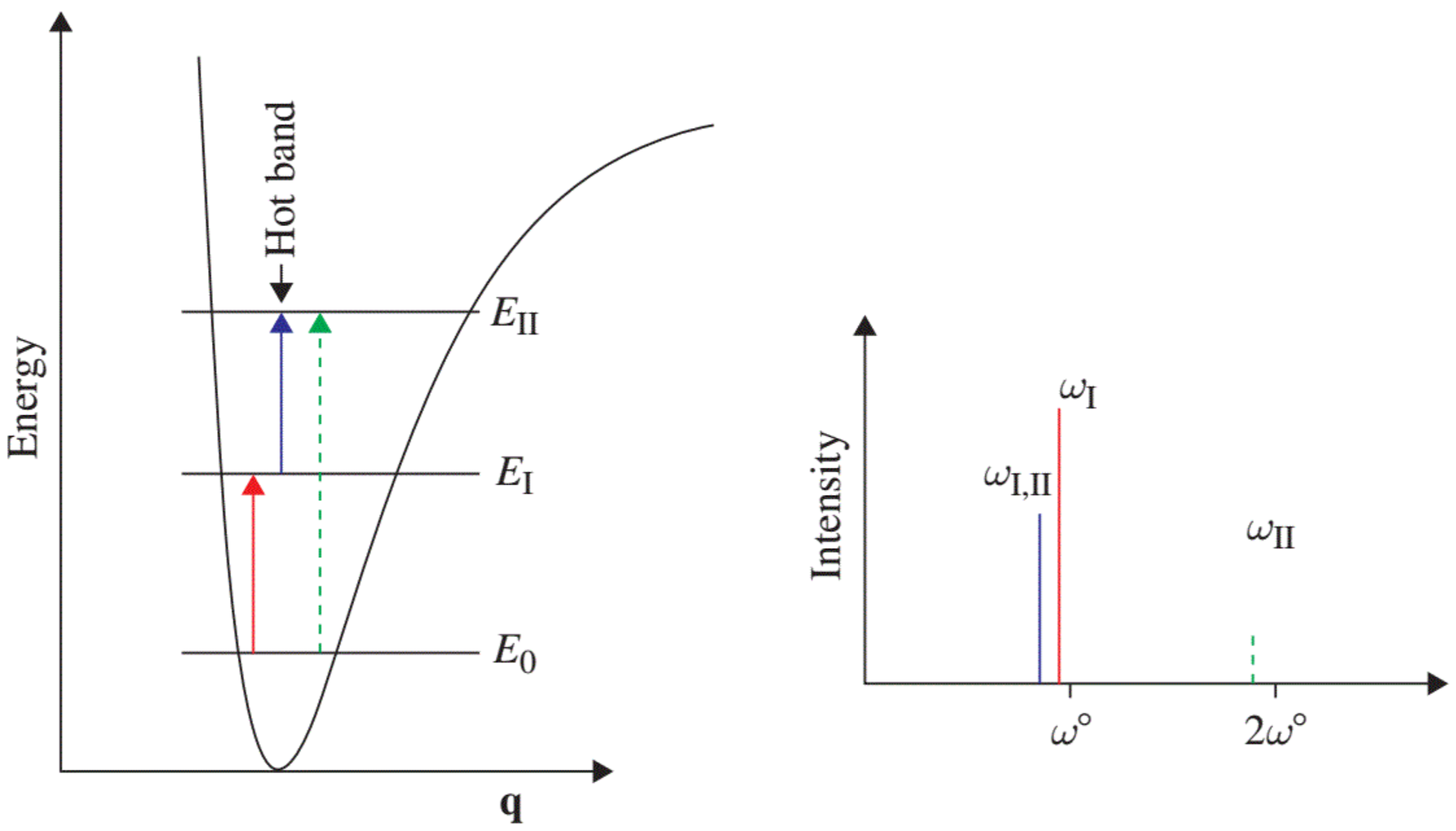


Figure 17.3 Appearance of a hot band in the IR spectrum of a Morse oscillator.

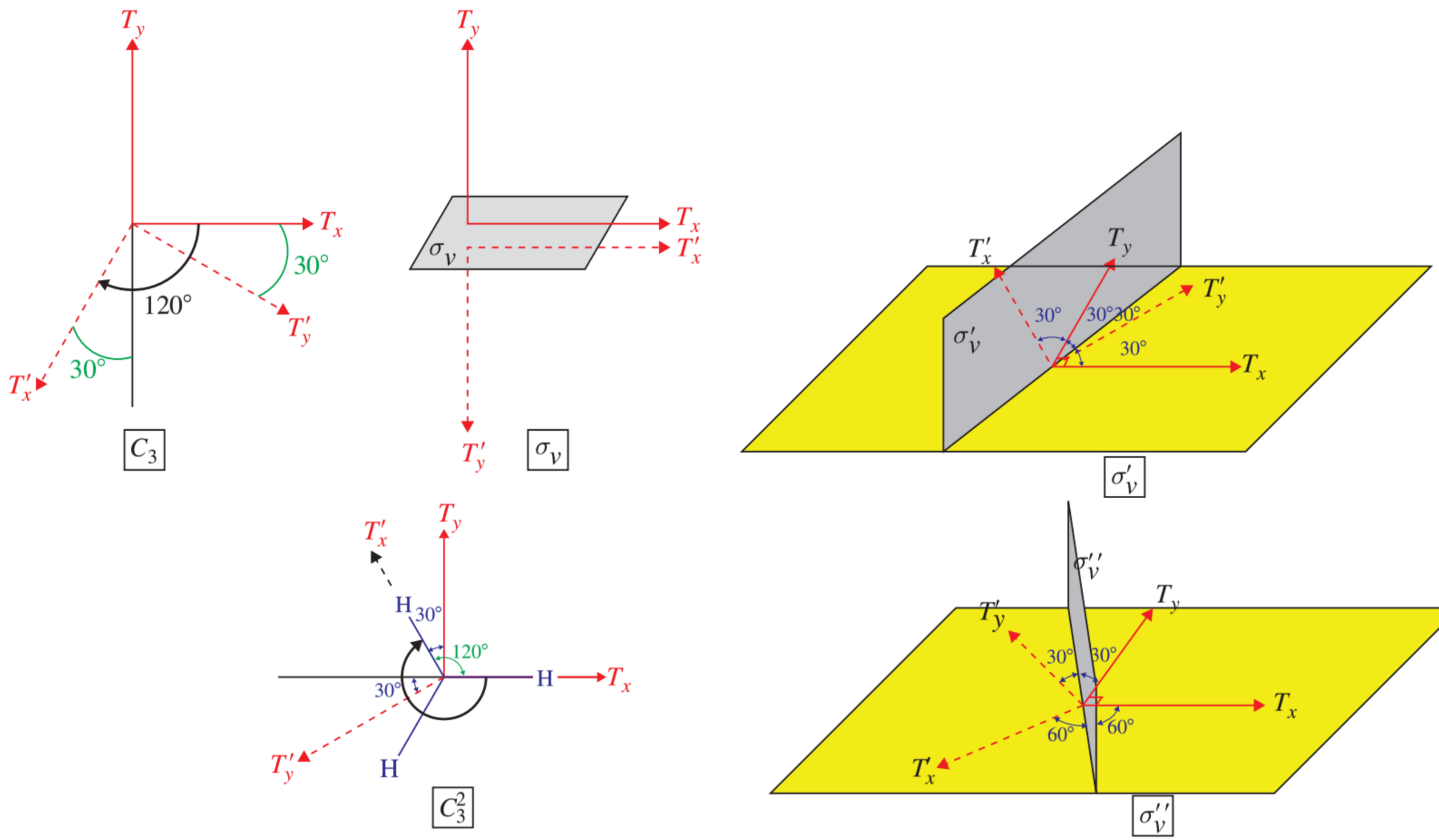


Figure 18.3 The C_{3v} symmetry operations.

PART I

BASIS REQUIRED FOR QUANTUM OSCILLATOR STUDIES

CHAPTER 1

BASIC CONCEPTS REQUIRED FOR QUANTUM MECHANICS

In order to summarize the quantum basis required for the study of oscillators, it is necessary to define some mathematical notions concerning the properties of state spaces, particularly the concepts of linear operators, kets, bras, Hermiticity, eigenvalues, and eigenvectors of linear operators involved in the formulation of the different postulates. The first two sections of this chapter are devoted to this. However, it is possible to pass directly to the third section leaving for later the lecture of the previous one.

1.1 BASIC CONCEPTS OF COMPLEX VECTORIAL SPACES

1.1.1 Kets, bras, and scalar products

Quantum mechanics deals with *state spaces*, that is, vectorial spaces involving complex scalar products that are generally of infinite dimension. Any element of these spaces is named a *ket* and symbolized $|\ldots\rangle|$ by inserting inside it a free notation allowing one to clearly identify this ket; for instance, $|\Psi_k\rangle$[1] or $|n\rangle$.

Since the space of states is vectorial, and if the kets $|\Psi_1\rangle$ and $|\Psi_2\rangle$ belong to the same state space, then the ket $|\Phi\rangle$ defined by the linear superposition

$$|\Phi\rangle = \lambda_1|\Psi_1\rangle + \lambda_2|\Psi_2\rangle$$

where λ_1 and λ_2 are two scalars, belongs also to the same state space.

Now, to some ket $|\Psi\rangle$ of the state space there exists a linear functional that associates with some another ket $|\Phi\rangle$ of this space a complex scalar $A_{\Phi\Psi}$, which is *the scalar product* of $|\Psi\rangle$ by $|\Phi\rangle$. This may be written

$$A_{\Phi\Psi} = \langle\Phi|\Psi\rangle \tag{1.1}$$

[1]All the notations inside the symbol $|\ldots\rangle|$ are designed to distinguish clearly the ket of interest. For instance, some Latin n or Greek Ψ letters lead to the writing $|n\rangle$ or $|\Psi\rangle$, but the notation may be as complex as required; for instance, $|n_l\rangle$ or $|\Psi_k\rangle$, the subscripts allowing to distinguish between two kets $|n_l\rangle$ and $|n_j\rangle$ of the same kind, and in a similar way to kets $|\Psi_k\rangle$ and $|\Psi_j\rangle$. In the following we shall use also as specification notations of the form: $|\{n\}\rangle$, $|(n)\rangle$, $|[n]\rangle$ in order to reserve the notations $|n_l\rangle$ or $|\Psi_k\rangle$ for kets belonging to the same basis.

Quantum Oscillators, First Edition. Olivier Henri-Rousseau and Paul Blaise.
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This linear functional, which is denoted $\langle\Phi|$, is named the *bra*, corresponding to the ket $|\Phi\rangle$. The bras may be viewed as belonging to a state space that is the *dual space* of the state space to which belong the kets, that is, the bras are the Hermitian conjugates of the corresponding kets, namely

$$\langle\Phi| = |\Phi\rangle^\dagger \tag{1.2}$$

where the superscript† denotes the Hermitian conjugation. The scalar products have the following properties:

$$(\langle\lambda_1\Phi_1 + \lambda_2\Phi_2|)|\Psi\rangle = \lambda_1^*\langle\Phi_1|\Psi\rangle + \lambda_2^*\langle\Phi_2|\Psi\rangle$$

$$\langle\Phi|(|\lambda_1\Psi_1 + \lambda_2\Psi_2\rangle) = \lambda_1\langle\Phi|\Psi_1\rangle + \lambda_2\langle\Phi|\Psi_2\rangle$$

$$\langle\Psi_k|\Phi_l\rangle = \langle\Phi_l|\Psi_k\rangle^* \tag{1.3}$$

$$\langle\Psi|\Psi\rangle > 0 \quad \text{if } |\Psi\rangle \neq 0$$

$$\boxed{\langle\Psi|\Psi\rangle = 0 \quad \text{if and only if } |\Psi\rangle = 0} \tag{1.4}$$

In addition, if this scalar product is *normalized*, we have

$$\langle\Psi|\Psi\rangle = 1$$

If the scalar product of two kets $|\Psi\rangle$ and $|\Phi\rangle$ is zero, the two kets $|\Psi\rangle$ and $|\Phi\rangle$ are said to be *orthogonal*:

$$\langle\Psi|\Phi\rangle = 0$$

1.1.2 Linear transformations

Let us consider the action of a linear operator $\mathbf{A}$ on a *ket* $|\xi\rangle$ belonging to the state space. This action leads to another ket $|\Phi\rangle$ according to

$$\mathbf{A}|\xi\rangle = |\Phi\rangle \tag{1.5}$$

Consider now the action of an another linear operator $\mathbf{B}$ acting on the same ket $|\xi\rangle$. Generally, it will yield another ket $|\Psi\rangle$:

$$\mathbf{B}|\xi\rangle = |\Psi\rangle$$

In most situations, the product of two operators $\mathbf{A}$ and $\mathbf{B}$ does not commute, that is,

$$\mathbf{AB} \neq \mathbf{BA}$$

The *commutator* of two operators $\mathbf{A}$ and $\mathbf{B}$ is symbolized[2] by

$$[\mathbf{A}, \mathbf{B}] \equiv \mathbf{AB} - \mathbf{BA}$$

[2]The standard notation for a commutator is […, …] where the comma separates the two operators involved. Since the comma risks being unnoticed, in order to avoid this risk we have chosen to reserve as far as, the notation involving [..,..] to commutators, and to use for other situations notations of the kinds (…) or {…}.

In some situations, a linear operator $\mathbf{A}$ may act on different kets $|\Psi_1\rangle$, $|\Psi_2\rangle$, …, in such a way as it multiplies them by scalars A_1, A_2, …, more generally

$$\mathbf{A}|\Psi_l\rangle = A_l|\Psi_l\rangle \tag{1.6}$$

The kets $|\Psi_l\rangle$ corresponding to these special situations are the *eigenvectors* of the operator $\mathbf{A}$ while the scalars A_l are the corresponding *eigenvalues*. Equation (1.6) is called an *eigenvalue equation*. The scalar A_l is generally complex.

When different eigenvectors exist corresponding to a same eigenvalue, then a *degeneracy* exists, its degree being the number of eigenvectors associated with this same eigenvalue. In the following, we shall not encounter degeneracy except for very special situations so that we shall ignore the particular treatment of this case.

1.1.2.1 Hermitian conjugate of a linear transformation

The Hermitian conjugate of the linear operator $\mathbf{A}$ is $\mathbf{A}^\dagger$. Consider a linear transformation of the form (1.5)

$$\mathbf{A}|\Psi\rangle = |\Phi\rangle \tag{1.7}$$

Its Hermitian conjugate is the bra $\langle\Phi|$:

$$\{\mathbf{A}|\Psi\rangle\}^\dagger = \langle\Phi|$$

Now, the Hermitian conjugate of the linear transformation (1.7) is

$$\boxed{\{\mathbf{A}|\Psi\rangle\}^\dagger = \langle\Psi|\mathbf{A}^\dagger} \tag{1.8}$$

which is equivalent to

$$\langle\Phi| = \langle\Psi|\mathbf{A}^\dagger \tag{1.9}$$

Consider now an eigenvalue equation of the form (1.6)

$$\mathbf{A}|\Psi\rangle = A|\Psi\rangle \tag{1.10}$$

Then, owing to Eq. (1.8), and because the Hermitian conjugate of a scalar is its complex conjugate, the Hermitian conjugate of Eq. (1.10) is

$$\langle\Psi|\mathbf{A}^\dagger = \langle\Psi|A^* \tag{1.11}$$

1.1.3 Basis and closure relation

A set $\{|\Phi_n\rangle\}$ of kets $|\Phi_n\rangle$ of the state space is said to be orthonormal if these states satisfy

$$\boxed{\langle\Phi_n|\Phi_m\rangle = \delta_{nm}} \tag{1.12}$$

where δ_{nm} is the Kronecker symbol given by

$$\delta_{mm} = 1 \qquad \text{and} \qquad \delta_{mn} = 0 \quad \text{if} \quad m \neq n \tag{1.13}$$

Again, such a set $\{|\Phi_n\rangle\}$ forms a basis in the state space, provided all kets $|\Psi_k\rangle$ belonging to this space may be expanded according to

$$|\Psi_k\rangle = \sum_{n=1}^{\infty} C_{nk}|\Phi_n\rangle \tag{1.14}$$

where the C_{nk} are the expansion coefficients, which may be complex.

Now, premultiply both members of Eq. (1.14) by a bra $\langle\Phi_m|$ corresponding to some ket belonging to the basis $\{|\Phi_n\rangle\}$. It reads

$$\langle\Phi_m|\Psi_k\rangle = \langle\Phi_m| \sum_{n=1}^{\infty} C_{nk}|\Phi_n\rangle$$

or

$$\langle\Phi_m|\Psi_k\rangle = \sum_{n=1}^{\infty} C_{nk}\langle\Phi_m|\Phi_n\rangle$$

Therefore, in view of Eq. (1.12), it transforms to

$$\langle\Phi_m|\Psi_k\rangle = \sum_{n=1}^{\infty} C_{nk}\delta_{nm}$$

or, in view of Eq. (1.13),

$$\langle\Phi_m|\Psi_k\rangle = C_{mk} \tag{1.15}$$

Then, introducing Eq. (1.15) into Eq. (1.14) we have

$$|\Psi_k\rangle = \sum_{n=1}^{\infty} \langle\Phi_n|\Psi_k\rangle|\Phi_n\rangle$$

Furthermore, after commuting the scalar product with the ket in the second member of this equation, we have

$$|\Psi_k\rangle = \sum_{n=1}^{\infty} \{|\Phi_n\rangle\langle\Phi_n|\}\,|\Psi_k\rangle \tag{1.16}$$

Now, in order for Eq. (1.16) to be satisfied, whatever may be the ket $|\Psi_k\rangle$ appearing on both sides of this equation, it is necessary that

$$\boxed{\sum_{n=1}^{\infty} |\Phi_n\rangle\langle\Phi_n| = \mathbf{1}} \tag{1.17}$$

Equation (1.17) is known as *the closure relation*. The closure relation (1.17) together with the orthonormality condition (1.12) are the two important properties of a basis, the first being the consequence of the second one.

Now, consider the following operation:

$$\{|\Phi_n\rangle\langle\Phi_n|\}\,|\Psi_k\rangle$$

Then, using the expansion (1.16), this expression reads

$$\{|\Phi_n\rangle\langle\Phi_n|\}|\Psi_k\rangle = \{|\Phi_n\rangle\langle\Phi_n|\}\sum_{m=1}^{\infty} C_{mk}|\Phi_m\rangle$$

or

$$\{|\Phi_n\rangle\langle\Phi_n|\}|\Psi_k\rangle = |\Phi_n\rangle\sum_{m=1}^{\infty} C_{mk}\langle\Phi_n|\Phi_m\rangle$$

and thus, using the orthonormality properties (1.12)

$$\{|\Phi_n\rangle\langle\Phi_n|\}|\Psi_k\rangle = |\Phi_n\rangle\sum_{m=1}^{\infty} C_{mk}\delta_{nm}$$

so that

$$\{|\Phi_n\rangle\langle\Phi_n\}|\Psi_k\rangle = |\Phi_n\rangle C_{nk}$$

Thus, $|\Phi_n\rangle\langle\Phi_n|$ acts on the ket $|\Psi_k\rangle$ as an operator, projecting it on to the state $|\Phi_n\rangle$. Thus it is called a *projector*

1.1.4 Schwarz inequality

Consider a ket $|\Psi\rangle$ that is the superposition of two different kets $|\Phi\rangle$ and $|\xi\rangle$:

$$|\Psi\rangle = |\Phi\rangle + \lambda|\xi\rangle \tag{1.18}$$

where λ is a complex scalar number. The Hermitian conjugate of this equation is

$$\langle\Psi| = \langle\Phi| + \lambda^*\langle\xi| \tag{1.19}$$

Consider now the norm of this ket, which cannot be negative, so that it must be written

$$\langle\Psi|\Psi\rangle \geqslant 0 \tag{1.20}$$

Then, using Eqs. (1.18) and (1.19) the norm becomes

$$\langle\Psi|\Psi\rangle = \langle\Phi|\Phi\rangle + \lambda\langle\Phi|\xi\rangle + \lambda^*\langle\xi|\Phi\rangle + \lambda\lambda^*\langle\xi|\xi\rangle \tag{1.21}$$

Now, suppose that the scalar λ is given by

$$\lambda = -\frac{\langle\xi|\Phi\rangle}{\langle\xi|\xi\rangle} \tag{1.22}$$

Then, according to Eq. (1.3), the complex conjugate of λ is

$$\lambda^* = -\frac{\langle\Phi|\xi\rangle}{\langle\xi|\xi\rangle} \tag{1.23}$$

Again, introducing Eqs. (1.22) and (1.23) in (1.21), one obtains

$$\langle\Psi|\Psi\rangle = \langle\Phi|\Phi\rangle - \frac{\langle\xi|\Phi\rangle}{\langle\xi|\xi\rangle}\langle\Phi|\xi\rangle - \frac{\langle\Phi|\xi\rangle}{\langle\xi|\xi\rangle}\langle\xi|\Phi\rangle + \frac{\langle\xi|\Phi\rangle}{\langle\xi|\xi\rangle}\frac{\langle\Phi|\xi\rangle}{\langle\xi|\xi\rangle}\langle\xi|\xi\rangle \tag{1.24}$$

yielding, after an initial simplification

$$\langle\Psi|\Psi\rangle = \langle\Phi|\Phi\rangle - \frac{\langle\xi|\Phi\rangle}{\langle\xi|\xi\rangle}\langle\Phi|\xi\rangle - \frac{\langle\Phi|\xi\rangle}{\langle\xi|\xi\rangle}\langle\xi|\Phi\rangle + \frac{\langle\xi|\Phi\rangle}{\langle\xi|\xi\rangle}\langle\Phi|\xi\rangle$$

Then, after cancellation of the two last right-hand terms, this last equation becomes

$$\langle\Psi|\Psi\rangle = \langle\Phi|\Phi\rangle - \frac{\langle\xi|\Phi\rangle\langle\Phi|\xi\rangle}{\langle\xi|\xi\rangle}$$

or, in view of the inequality (1.20)

$$\langle\Phi|\Phi\rangle\langle\xi|\xi\rangle - \langle\xi|\Phi\rangle\langle\Phi|\xi\rangle \geqslant 0$$

leading to a result that is known as the *Schwarz inequality*:

$$\langle\Phi|\Phi\rangle\langle\xi|\xi\rangle \geqslant \langle\xi|\Phi\rangle\langle\Phi|\xi\rangle \tag{1.25}$$

1.2 HERMITIAN CONJUGATION

1.2.1 Theorem dealing with Hermitian conjugates

Consider the linear transformation

$$\mathbf{B}|\Psi\rangle = |\xi\rangle \tag{1.26}$$

Again, owing to Eq. (1.8), its Hermitian conjugate is

$$\langle\Psi|\mathbf{B}^\dagger = \langle\xi| \tag{1.27}$$

Then, premultiplying Eq. (1.26) by $\langle\Phi|$ and postmultiplying Eq. (1.27) by $|\Phi\rangle$, one obtains, respectively,

$$\langle\Phi|\mathbf{B}|\Psi\rangle = \langle\Phi|\xi\rangle \tag{1.28}$$

$$\langle\Psi|\mathbf{B}^\dagger|\Phi\rangle = \langle\xi|\Phi\rangle \tag{1.29}$$

Thus, owing to Eq. (1.3), it appears that, in the present situation

$$\langle\Phi|\xi\rangle = \langle\xi|\Phi\rangle^*$$

Thus, Eqs. (1.28) and (1.29) yield

$$\boxed{\langle\Psi|\mathbf{B}^\dagger|\Phi\rangle = \langle\Phi|\mathbf{B}|\Psi\rangle^*} \tag{1.30}$$

1.2.2 Hermitian conjugate of $\mathbf{A}^\dagger$

Consider the Hermitian conjugate $(\mathbf{A}^\dagger)^\dagger$ of the Hermitian conjugate $\mathbf{A}^\dagger$ of the linear operator $\mathbf{A}$. First, we may write that the Hermitian conjugate of the operator $\mathbf{A}$ is a new operator $\mathbf{B}$:

$$\mathbf{B} = \mathbf{A}^\dagger \tag{1.31}$$

Then, the Hermitian conjugate of $\mathbf{A}^\dagger$ is $\mathbf{B}^\dagger$:

$$(\mathbf{A}^\dagger)^\dagger = \mathbf{B}^\dagger \tag{1.32}$$

Now, premultiply the two members of Eq. (1.32) by some bra $\langle\Psi|$ and postmultiply them by some ket $|\Phi\rangle$. Then, one obtains

$$\langle\Psi|(\mathbf{A}^\dagger)^\dagger|\Phi\rangle = \langle\Psi|\mathbf{B}^\dagger|\Phi\rangle$$

Owing to Eq. (1.30), this last expression becomes

$$\langle\Psi|(\mathbf{A}^\dagger)^\dagger|\Phi\rangle = \langle\Phi|\mathbf{B}|\Psi\rangle^*$$

Again, introduce Eq. (1.31) on the right-hand side of this last result. Then, one finds

$$\langle\Psi|(\mathbf{A}^\dagger)^\dagger|\Phi\rangle = \langle\Phi|\mathbf{A}^\dagger|\Psi\rangle^*$$

Moreover, using again theorem (1.30), one gets

$$\langle\Psi|(\mathbf{A}^\dagger)^\dagger|\Phi\rangle = \langle\Psi|\mathbf{A}|\Phi\rangle$$

Finally, since the latter must be true whatever $\langle\Psi|$ and $|\Phi\rangle$ are, it follows that

$$\boxed{(\mathbf{A}^\dagger)^\dagger = \mathbf{A}} \tag{1.33}$$

1.2.3 Successive Hermitian conjugations of a linear transformation

Consider the Hermitian conjugate of a linear transformation (1.8). It is

$$\{\{\mathbf{A}|\Psi\rangle\}^\dagger\}^\dagger = \{\langle\Psi|\mathbf{A}^\dagger\}^\dagger \tag{1.34}$$

Now, let

$$\mathbf{A}|\Psi\rangle = |\Phi\rangle \qquad \text{and} \qquad \langle\Psi|\mathbf{A}^\dagger = \langle\Phi| \tag{1.35}$$

Then, due to this last equation, Eq. (1.34) reads

$$\{\{\mathbf{A}|\Psi\rangle\}^\dagger\}^\dagger = \langle\Phi|^\dagger$$

or, in view of Eq. (1.2)

$$\{\{\mathbf{A}|\Psi\rangle\}^\dagger\}^\dagger = |\Phi\rangle$$

Moreover, due to the first equation of (1.35), we also have

$$\{\{\mathbf{A}|\Psi\rangle\}^\dagger\}^\dagger = \mathbf{A}|\Psi\rangle$$

1.2.4 Hermitian conjugate of $|\xi\rangle\langle\zeta|$

Consider the following operator and its Hermitian conjugate:

$$\mathbf{A} = |\xi\rangle\langle\zeta| \qquad \text{and} \qquad \mathbf{A}^\dagger = \{|\xi\rangle\langle\zeta|\}^\dagger \tag{1.36}$$

What is the relation between $\mathbf{A}$ and $\mathbf{A}^\dagger$? To answer this question, premultiply both the operator and its Hermitian conjugate by the bra $\langle\Phi|$ and postmultiply both of them by the ket $|\Psi\rangle$ leading, respectively, to

$$\langle\Phi|\mathbf{A}|\Psi\rangle = \langle\Phi|\{|\xi\rangle\langle\zeta|\}|\Psi\rangle$$

and

$$\langle\Phi|\mathbf{A}^\dagger|\Psi\rangle = \langle\Phi|\,\{|\xi\rangle\langle\zeta|\}^\dagger\,|\Psi\rangle$$

Now, according to Eq. (1.30), the operator defined by Eq. (1.36) must obey

$$\langle\Phi|\mathbf{A}^\dagger|\Psi\rangle = \langle\Psi|\mathbf{A}|\Phi\rangle^*$$

Thus, in the present situation, due to the expressions (1.36), the latter takes on the form

$$\langle\Phi|\,\{|\xi\rangle\langle\zeta|\}^{\dagger}\,|\Psi\rangle = \{\langle\Psi|\,\{|\xi\rangle\langle\zeta|\}\,|\Phi\rangle\}^{*}$$

After simplifying the notation in the more usual form, we have

$$\langle\Phi|\,\{|\xi\rangle\langle\zeta|\}^{\dagger}\,|\Psi\rangle = \{\langle\Psi|\xi\rangle\langle\zeta|\Phi\rangle\}^{*} \tag{1.37}$$

Again, the two terms of the right-hand side of this last equation are scalars obeying

$$\langle\Psi|\xi\rangle^{*} = \langle\xi|\Psi\rangle \qquad \text{and} \qquad \langle\zeta|\Phi\rangle^{*} = \langle\Phi|\zeta\rangle$$

Thus, Eq. (1.37) transforms to

$$\langle\Phi|\,\{|\xi\rangle\langle\zeta|\}^{\dagger}\,|\Psi\rangle = \langle\xi|\Psi\rangle\langle\Phi|\zeta\rangle$$

Now, the two right scalars appearing on the right-hand side of this last expression do commute, so that

$$\langle\Phi|\,\{|\xi\rangle\langle\zeta|\}^{\dagger}\,|\Psi\rangle = \langle\Phi|\zeta\rangle\langle\xi|\Psi\rangle$$

Finally, since this last equation must be satisfied, whatever $\langle\Psi|$ and $|\Phi\rangle$ are, one obtains the final result

$$\boxed{\{|\xi\rangle\langle\zeta|\}^{\dagger} = |\zeta\rangle\langle\xi|} \tag{1.38}$$

1.2.5 Hermitian conjugate of a product of operators that do not commute

Now, consider two noncommuting linear operators **A** and **B** the product of which is **C**, that is,

$$\mathbf{AB} = \mathbf{C} \qquad \text{and} \qquad [\mathbf{A},\mathbf{B}] \neq 0$$

Then, seek the Hermitian conjugate $(\mathbf{AB})^{\dagger}$ of their product **AB**. Hence, premultiply the product **AB** by the bra $\langle\Psi|$ and postmultiply it by the ket $|\Phi\rangle$. Then, considering the product **AB** as a new operator **C**, and applying the theorem (1.30), that is,

$$\langle\Psi|\mathbf{C}^{\dagger}|\Phi\rangle = \langle\Phi|\mathbf{C}|\Psi\rangle^{*}$$

we have

$$\langle\Psi|(\mathbf{AB})^{\dagger}|\Phi\rangle = \langle\Phi|\mathbf{AB}|\Psi\rangle^{*} \tag{1.39}$$

Now, observe that the action of the operator **B** on the ket $|\Psi\rangle$ and that of the operator **A** on the bra $\langle\Phi|$ are linear transformations of the type

$$\mathbf{B}|\Psi\rangle = |\chi\rangle \qquad \text{and} \qquad \langle\Phi|\mathbf{A} = \langle\mu| \tag{1.40}$$

Then, owing to these linear transformations defining the ket $|\chi\rangle$ and the bra $\langle\mu|$, Eq. (1.39) reads

$$\langle\Psi|(\mathbf{AB})^{\dagger}|\Phi\rangle = \langle\mu|\chi\rangle^{*} \tag{1.41}$$

Again, due to the relation (1.3) defining the scalar product and its complex conjugate, there is

$$\langle \mu | \chi \rangle^* = \langle \chi | \mu \rangle$$

Hence, Eq. (1.41) takes the form

$$\langle \Psi | (\mathbf{AB})^\dagger | \Phi \rangle = \langle \chi | \mu \rangle \tag{1.42}$$

Moreover, the Hermitian conjugate of the linear transformations (1.40) is

$$\langle \Psi | \mathbf{B}^\dagger = \langle \chi | \qquad \text{and} \qquad \mathbf{A}^\dagger | \Phi \rangle = | \mu \rangle$$

Thus, the corresponding scalar product yields

$$\langle \chi | \mu \rangle = \langle \Psi | \mathbf{B}^\dagger \mathbf{A}^\dagger | \Phi \rangle$$

As a consequence, Eq. (1.42) becomes

$$\langle \Psi | (\mathbf{AB})^\dagger | \Phi \rangle = \langle \Psi | \mathbf{B}^\dagger \mathbf{A}^\dagger | \Phi \rangle$$

Of course, this last equation must be true for all $\langle \Psi |$ and $| \Phi \rangle$ so that

$$\boxed{(\mathbf{AB})^\dagger = \mathbf{B}^\dagger \mathbf{A}^\dagger} \tag{1.43}$$

1.2.6 Hermitian conjugate of a general expression involving kets, bra operators, and scalars

We may summarize here the present results obtained previously and that dealt with the Hermitian conjugate in special situations given, respectively, by Eqs. (1.33), (1.38), and (1.43). For operators we have

$$(\mathbf{A}^\dagger)^\dagger = \mathbf{A}; \qquad \{ |\xi\rangle\langle\zeta| \}^\dagger = |\zeta\rangle\langle\xi| \qquad \text{and} \qquad (\mathbf{AB})^\dagger = \mathbf{B}^\dagger \mathbf{A}^\dagger$$

For linear transformations, we have

$$\text{If} \qquad \mathbf{A}|\Psi\rangle = A|\Psi\rangle \quad \text{then} \quad \{\mathbf{A}|\Psi\rangle\}^\dagger = \langle \Psi | \mathbf{A}^\dagger \quad \text{with} \quad \langle \Psi | \mathbf{A}^\dagger = \langle \Psi | A^*$$

Finally, for scalars, we have

$$\langle \Phi | \Psi \rangle = \langle \Psi | \Phi \rangle^* \qquad \text{and} \qquad \langle \Psi | \mathbf{B}^\dagger | \Phi \rangle = \langle \Phi | \mathbf{B} | \Psi \rangle^*$$

Thus, it is possible to deduce general rules allowing one to find the Hermitian conjugate of a general expression involving linear operators kets, bra, and scalars, that is,

1. Replace
   - (a) scalars by their complex conjugates
   - (b) kets by the corresponding bras and vice versa
   - (c) linear operators by their Hermitian conjugates
2. Invert the order of the different terms, recalling that the position of the scalar is irrelevant.

As a first example, consider the following expression, which is a scalar:

$$\langle\Psi|\mathbf{A}|\Psi\rangle = A$$

Since the Hermitian conjugate of $|\Psi\rangle$ is $\langle\Psi|$ and vice versa and since the Hermitian conjugate of the scalar A is its complex conjugate A^*, the Hermitian conjugate of this expression is

$$\langle\Psi|\mathbf{A}^\dagger|\Psi\rangle = A^*$$

Now, consider the following operator:

$$\mathbf{B} = \lambda\langle\Phi|\mathbf{A}|\chi\rangle|\Phi\rangle\langle\mu|$$

Applying the above rules, its Hermitian conjugate is given by

$$\mathbf{B}^\dagger = \lambda^*|\mu\rangle\langle\Phi|\langle\chi|\mathbf{A}^\dagger|\Phi\rangle$$

Finally, consider the operator $\mathbf{C}$, which consists of an exponential of another operator $\mathbf{A}$:

$$\mathbf{C} = e^{i\mathbf{A}} \quad \text{with} \quad i^2 = -1$$

Since the complex conjugate of the scalar i is $-i$, the Hermitian conjugate of the operator $\mathbf{C}$ is

$$\mathbf{C}^\dagger = (e^{i\mathbf{A}})^\dagger = e^{-i\mathbf{A}^\dagger} \tag{1.44}$$

1.3 HERMITICITY AND UNITARITY

1.3.1 Hermitian operators

If certain linear operators $\mathbf{A}$ are equal to their Hermitian conjugate $\mathbf{A}^\dagger$, then they are said to be *Hermitian*:

$$\mathbf{A} = \mathbf{A}^\dagger \tag{1.45}$$

1.3.1.1 Reality of eigenvalues and orthonormality of the eigenvectors In order to show that the eigenvalues of Hermitian operators are real, let us write the eigenvalue equation of a linear operator

$$\mathbf{A}|\Psi_i\rangle = A_i|\Psi_i\rangle \tag{1.46}$$

where A_i is one of the eigenvalues of this operator and $|\Psi_i\rangle$ the corresponding eigenvector. Premultiply the two members of this equation by the bra $\langle\Psi_i|$, conjugate to the ket $|\Psi_i\rangle$:

$$\langle\Psi_i|\mathbf{A}|\Psi_i\rangle = \langle\Psi_i|A_i|\Psi_i\rangle$$

The eigenvalue A_i being a scalar, must commute with the bra so that one may write

$$\langle\Psi_i|\mathbf{A}|\Psi_i\rangle = A_i\langle\Psi_i|\Psi_i\rangle \tag{1.47}$$

Next, assume that the eigenvector $|\Psi_i\rangle$ is normalized, that is,

$$\langle\Psi_i|\Psi_i\rangle = 1$$

Then, Eq. (1.47) simplifies to

$$\langle\Psi_i|\mathbf{A}|\Psi_i\rangle = A_i \tag{1.48}$$

On the other hand, the Hermitian conjugate of this equation is

$$\langle\Psi_i|\mathbf{A}^\dagger|\Psi_i\rangle = A_i^* \tag{1.49}$$

Again, since we have assumed that the linear operator is Hermitian, it obeys Eq. (1.45), so that

$$\langle\Psi_i|\mathbf{A}^\dagger|\Psi_i\rangle = \langle\Psi_i|\mathbf{A}|\Psi_i\rangle$$

Thus, it appears from Eqs. (1.48) and (1.49) that the eigenvalue A_i of the Hermitian operator is equal to its complex conjugate A_i^*, that is, it is real since it obeys

$$A_i = A_i^* \tag{1.50}$$

Thus, we have the following property:

$$\boxed{\text{If} \qquad \mathbf{A} = \mathbf{A}^\dagger \quad \text{then} \quad A_i = A_i^*} \tag{1.51}$$

Now, in order to show that the eigenvectors of an Hermitian operator are orthogonal, let us write the eigenvalue equation of a linear operator for two distinct eigenvalues and eigenvectors:

$$\mathbf{A}|\Psi_i\rangle = A_i|\Psi_i\rangle \qquad \text{and} \qquad \mathbf{A}|\Psi_k\rangle = A_k|\Psi_k\rangle$$

The Hermitian conjugate of the first expression in this eigenvalue equation, is

$$\langle\Psi_i|\mathbf{A}^\dagger = A_i^*\langle\Psi_i|$$

Besides, if we assume that the operator $\mathbf{A}$ is Hermitian, then the eigenvalue A_i is real; then, according to Eq. (1.50), the following results hold:

$$\mathbf{A}|\Psi_k\rangle = A_k|\Psi_k\rangle \qquad \text{and} \qquad \langle\Psi_i|\mathbf{A} = A_i\langle\Psi_i| \quad \text{if } \mathbf{A} = \mathbf{A}^\dagger$$

Now, premultiply the two members of the first eigenvalue equation by the bra $\langle\Psi_i|$, and postmultiply the two members of its Hermitian conjugate by the ket $|\Psi_k\rangle$. Then, after commuting the eigenvalues that are scalars, one obtains the two expressions

$$\langle\Psi_i|\mathbf{A}|\Psi_k\rangle = A_k\langle\Psi_i|\Psi_k\rangle \qquad \text{and} \qquad \langle\Psi_i|\mathbf{A}|\Psi_k\rangle = A_i\langle\Psi_i|\Psi_k\rangle$$

Now, substract the second expression from the first one, that is,

$$\langle\Psi_i|\mathbf{A}|\Psi_k\rangle - \langle\Psi_i|\mathbf{A}|\Psi_k\rangle = (A_k - A_i)\langle\Psi_i|\Psi_k\rangle$$

yielding

$$(A_k - A_i)\langle\Psi_i|\Psi_k\rangle = 0$$

Thus, since we have assumed that the two eigenvalues are different, that is,

$$(A_k - A_i) \neq 0$$

hence it appears that the corresponding eigenvectors of Hermitian operators are orthogonal, leading us to write

$$\boxed{\langle \Psi_i | \Psi_k \rangle = 0 \quad \text{if} \quad \mathbf{A} = \mathbf{A}^\dagger \quad \text{with} \quad \mathbf{A}|\Psi_k\rangle = A_k|\Psi_k\rangle} \tag{1.52}$$

1.3.1.2 Trace and invariance of the trace By definition the trace operation, denoted **tr**, over any operator **C** is[3]

$$\mathbf{tr}\{\mathbf{C}\} = \sum_n \langle \Phi_n | \mathbf{C} | \Phi_n \rangle \tag{1.53}$$

where the $|\Phi_n\rangle$ involved in the infinite sum belong to the basis $\{|\Phi_n\rangle\}$. Next, suppose that the operator **C** is the product of two operators **A** and **B**, which do not commute, that is,

$$\mathbf{C} = \mathbf{AB} \quad \text{with} \quad [\mathbf{A}, \mathbf{B}] \neq 0$$

Then, the trace takes the form

$$\mathbf{tr}\{\mathbf{AB}\} = \sum_n \langle \Phi_n | \mathbf{AB} | \Phi_n \rangle \tag{1.54}$$

Introduce between **A** and **B** the closure relation built up from the basis $\{|\Phi_m\rangle\}$. This procedure leads to a double summation not only over n but also over m:

$$\mathbf{tr}\{\mathbf{AB}\} = \sum_n \sum_m \langle \Phi_n | \mathbf{A} | \Phi_m \rangle \langle \Phi_m | \mathbf{B} | \Phi_n \rangle$$

Since the terms involved in the double summation are scalar, they commute, so that

$$\mathbf{tr}\{\mathbf{AB}\} = \sum_n \sum_m \langle \Phi_m | \mathbf{B} | \Phi_n \rangle \langle \Phi_n | \mathbf{A} | \Phi_m \rangle$$

Then, one may omit between **B** and **A** the closure relation involving the summation over n to give

$$\mathbf{tr}\{\mathbf{AB}\} = \sum_m \langle \Phi_m | \mathbf{BA} | \Phi_m \rangle \tag{1.55}$$

However, owing to the definition (1.53) of the trace, the right-hand side of Eq. (1.56) yields

$$\sum_m \langle \Phi_m | \mathbf{BA} | \Phi_m \rangle = \mathbf{tr}\{\mathbf{BA}\} \tag{1.56}$$

Hence, comparison of Eq. (1.54) and (1.56) shows that

$$\mathbf{tr}\{\mathbf{AB}\} = \mathbf{tr}\{\mathbf{BA}\}$$

so that the trace operation is invariant with respect to a permutation of **A** and **B**.

[3]In order to make clear what is meant by the trace operation, in the following we shall denote it, by **tr**{ } where all the operators involved **A**, **B**… will be inside the notation {…}. For instance, **tr**{**AB**}.

1.3.1.3 Hermitization of the product AB *of Hermitian operators when* $[\mathbf{A},\mathbf{B}] \neq 0$

Consider the product **C** of two linear operators **A** and **B**:

$$\mathbf{C} = \mathbf{AB} \tag{1.57}$$

Again, assume that **A** and **B** are Hermitian operators that do not commute, that is,

$$\mathbf{A} = \mathbf{A}^\dagger \qquad \mathbf{B} = \mathbf{B}^\dagger \qquad [\mathbf{A},\mathbf{B}] \neq 0$$

As we shall see, their product **C** is not Hermitian so that it is necessary to convert it to Hermitian form. To show that the product **C** is not Hermitian let us write with the aid of Eq. (1.43) the Hermitian of **C**:

$$\mathbf{C}^\dagger = (\mathbf{AB})^\dagger = \mathbf{B}^\dagger\mathbf{A}^\dagger$$

Since both operators are Hermitian, it is possible to write

$$\mathbf{C}^\dagger = \mathbf{BA} \quad \text{if} \quad \mathbf{B} = \mathbf{B}^\dagger \qquad \text{and} \qquad \mathbf{A} = \mathbf{A}^\dagger \tag{1.58}$$

Thus, since by hypothesis the two operators do not commute, the comparison of Eqs. (1.57) and (1.58) shows that the product **C** is not Hermitian. Hence, it is necessary to recall that

$$\mathbf{C}^\dagger \neq \mathbf{C} \quad \text{if} \quad [\mathbf{A},\mathbf{B}] \neq 0 \quad \text{when} \quad \mathbf{A} = \mathbf{A}^\dagger \qquad \text{and} \qquad \mathbf{B} = \mathbf{B}^\dagger \tag{1.59}$$

In order to write the product in Hermitian form, we consider the linear combination of **C** and its Hermitian conjugate, namely

$$\mathbf{D} = \tfrac{1}{2}(\mathbf{C} + \mathbf{C}^\dagger)$$

Then, the Hermitian conjugate $\mathbf{D}^\dagger$ of **D** is Hermitian since

$$\mathbf{D}^\dagger = \tfrac{1}{2}(\mathbf{C}^\dagger + \mathbf{C}) = \mathbf{D}$$

As a consequence, it appears that the linear combination of the products **AB** and **BA** is Hermitian. Hence, important property of Hermitization of the product of two Hermitian operators follows, namely

$$\boxed{\mathbf{D} = \tfrac{1}{2}\{\mathbf{AB} + \mathbf{BA}\} = \mathbf{D}^\dagger \quad \text{if} \quad \mathbf{A} = \mathbf{A}^\dagger \qquad \mathbf{B} = \mathbf{B}^\dagger \qquad [\mathbf{A},\mathbf{B}] \neq 0} \tag{1.60}$$

1.3.2 Eigenkets of two commuting Hermitian operators

1.3.2.1 First theorem

Consider two operators **A** and **B** that commute, that is,

$$[\mathbf{A},\mathbf{B}] = 0 \tag{1.61}$$

The eigenvalue equation of **A** is

$$\mathbf{A}|\Psi_i\rangle = A_i|\Psi_i\rangle \tag{1.62}$$

where A_i is the scalar eigenvalue of the operator **A**. Now, consider the action of the product **BA** of the two operators on any eigenket of **A**

$$\mathbf{BA}|\Psi_i\rangle = \mathbf{B}A_i|\Psi_i\rangle = A_i\mathbf{B}|\Psi_i\rangle = A_i|\mathbf{B}\Psi_i\rangle$$

In addition, owing to the nullity of the commutator (1.61), we have

$$\mathbf{BA}|\Psi_i\rangle = \mathbf{AB}|\Psi_i\rangle = \mathbf{A}|\mathbf{B}\Psi_i\rangle \tag{1.63}$$

where $|\mathbf{B}\Psi_i\rangle$ is the ket obtained by the linear transformation of $\mathbf{B}$ over $|\Psi_i\rangle$. Thus, by identification of the two last equations, it appears that

$$\mathbf{A}|\mathbf{B}\Psi_i\rangle = A_i|\mathbf{B}\Psi_i\rangle \tag{1.64}$$

This result shows that when $\mathbf{A}$ and $\mathbf{B}$ commute, and that, according to Eq. (1.62) if $|\Psi_i\rangle$ is an eigenket of $\mathbf{A}$, then, due to Eq. (1.64), $|\mathbf{B}\Psi_i\rangle$ is also an eigenket of $\mathbf{A}$.

In a like manner, if the eigenvalue equation of $\mathbf{B}$ is

$$\mathbf{B}|\Phi_k\rangle = B_k|\Phi_k\rangle$$

then one obtains

$$\mathbf{B}|\mathbf{A}\Phi_k\rangle = B_k|\mathbf{A}\Phi_k\rangle \tag{1.65}$$

showing that when $\mathbf{A}$ and $\mathbf{B}$ commute, if $|\Phi_k\rangle$ is an eigenket of $\mathbf{B}$, $|\mathbf{A}\Phi_k\rangle$ is also an eigenket of $\mathbf{B}$.

1.3.2.2 Second theorem Consider the two following eigenvalue equations of the same linear Hermitian operator $\mathbf{A}$:

$$\mathbf{A}|\Psi_1\rangle = A_1|\Psi_1\rangle \qquad \text{and} \qquad \mathbf{A}|\Psi_2\rangle = A_2|\Psi_2\rangle \tag{1.66}$$

where A_1 and A_2 are two different eigenvalues of $\mathbf{A}$, that is,

$$A_1 - A_2 \neq 0 \tag{1.67}$$

Now, consider another linear operator $\mathbf{B}$, which commutes with $\mathbf{A}$, but which is not necessarily Hermitian, that is,

$$[\mathbf{A}, \mathbf{B}] = 0$$

Then, owing to the nullity of this commutator, we have

$$\langle\Psi_1|[\mathbf{A}, \mathbf{B}]|\Psi_2\rangle = 0 \tag{1.68}$$

Expanding the commutator gives

$$\langle\Psi_1|[\mathbf{A}, \mathbf{B}]|\Psi_2\rangle = \langle\Psi_1|\mathbf{AB}|\Psi_2\rangle - \langle\Psi_1|\mathbf{BA}|\Psi_2\rangle$$

Then, using the first equation of (1.66) or the Hermitian conjugate of the second, one reads

$$\langle\Psi_1|\,[\mathbf{A}, \mathbf{B}]\,|\Psi_2\rangle = (A_1 - A_2)\,\langle\Psi_1|\mathbf{B}|\Psi_2\rangle \tag{1.69}$$

Hence, owing to Eqs. (1.67)–(1.69), it appears that

$$\langle\Psi_1|\mathbf{B}|\Psi_2\rangle = 0 \tag{1.70}$$

Thus, if $|\Psi_1\rangle$ and $|\Psi_2\rangle$ are eigenkets of any Hermitian operator $\mathbf{A}$, then Eq. (1.70) holds for any operator $\mathbf{B}$ that commutes with $\mathbf{A}$.

1.3.3 Eigenvalue equation of an exponential operator

Consider an exponential operator $e^{\xi \mathbf{A}}$, which is a function of the scalar ξ, and another operator $\mathbf{A}$ obeying the eigenvalue equation

$$\mathbf{A}|\Phi_n\rangle = A_n|\Phi_n\rangle \tag{1.71}$$

We search what is the effect of this operator on an eigenstate $|\Phi_n\rangle$. For this purpose, we may expand on the right-hand side of this last equation the exponential operator in Taylor series, to give

$$e^{\xi \mathbf{A}}|\Phi_n\rangle = \sum_k \frac{\xi^k}{k!}\mathbf{A}^k|\Phi_n\rangle \tag{1.72}$$

Now, observe that

$$\mathbf{A}^k|\Phi_n\rangle = \mathbf{A}^{k-1}\mathbf{A}|\Phi_n\rangle$$

or, in view of Eq. (1.71)

$$\mathbf{A}^k|\Phi_n\rangle = \mathbf{A}^{k-1}A_n|\Phi_n\rangle$$

Again, after commuting the scalar A_n with the operator $\mathbf{A}^{k-1}$ written $\mathbf{A}^{k-2}\mathbf{A}$, one obtains

$$\mathbf{A}^k|\Phi_n\rangle = A_n\mathbf{A}^{k-2}\mathbf{A}|\Phi_n\rangle$$

or

$$\mathbf{A}^k|\Phi_n\rangle = A_nA_n\mathbf{A}^{k-2}|\Phi_n\rangle$$

Proceeding in the same way for each power of $\mathbf{A}$, one gets finally

$$\mathbf{A}^k|\Phi_n\rangle = A_n^k|\Phi_n\rangle$$

Then, using this result, Eq. (1.72) becomes

$$e^{\xi \mathbf{A}}|\Phi_n\rangle = \sum_k \frac{\xi^k}{k!}A_n^k|\Phi_n\rangle$$

Again, return to the expansion appearing on the right-hand side of this last equation to the exponential, and one obtains

$$\boxed{e^{\xi \mathbf{A}}|\Phi_n\rangle = e^{\xi A_n}|\Phi_n\rangle} \tag{1.73}$$

1.3.4 Unitary operators

Consider the inverse $\mathbf{U}^{-1}$ of a linear operator $\mathbf{U}$. This inverse is defined by

$$\mathbf{U}\mathbf{U}^{-1} = \mathbf{U}^{-1}\mathbf{U} = \mathbf{1}$$

Next, assume that the inverse $\mathbf{U}^{-1}$ of the linear operator $\mathbf{U}$ is the Hermitian conjugate of $\mathbf{U}$:

$$\mathbf{U}^{-1} = \mathbf{U}^{\dagger}$$

Then the operator $\mathbf{U}$, which is said to be *unitary*, obeys the following relation:

$$\boxed{\mathbf{U}\mathbf{U}^\dagger = \mathbf{U}^\dagger\mathbf{U} = 1 \quad \text{if} \quad \mathbf{U}^{-1} = \mathbf{U}^\dagger} \tag{1.74}$$

As an example of unitary operator, consider the following expression for the linear operator $\mathbf{U}$, which is an exponential of the Hermitian operator $\mathbf{B}$ times a real scalar λ times the imaginary number i:

$$\mathbf{U} = e^{i\lambda\mathbf{B}} \quad \text{with} \quad \mathbf{B} = \mathbf{B}^\dagger \qquad \lambda = \lambda^* \qquad \text{and} \qquad i^2 = -1$$

Then, using Eq. (1.44), the Hermitian conjugate of $\mathbf{U}$ appears to be given by

$$\mathbf{U}^\dagger = e^{-i\lambda\mathbf{B}}$$

On the other hand, it is obvious that the inverse of $\mathbf{U}$ is

$$\mathbf{U}^{-1} = e^{-i\lambda\mathbf{B}}$$

As a consequence, comparison of the two above equations shows that the Hermitian conjugate of $\mathbf{U}$ is its inverse, showing that $\mathbf{U}$ is unitary:

$$\mathbf{U}^\dagger = \mathbf{U}^{-1}$$

1.4 ALGEBRA OPERATORS

Here, we give some important results dealing with the algebra of operators, which are proved in Appendices 1–5. They are

- The commutator involving three noncommuting operators. $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$:

$$\boxed{[\mathbf{A}, \mathbf{BC}] = [\mathbf{A}, \mathbf{B}]\mathbf{C} + \mathbf{B}[\mathbf{A}, \mathbf{C}]} \tag{1.75}$$

- The transformations

$$\boxed{e^{\xi\mathbf{A}}\mathbf{B}e^{-\xi\mathbf{A}} = \mathbf{B} + [\mathbf{A}, \mathbf{B}]\xi + \frac{1}{2}[\mathbf{A}, [\mathbf{A}, \mathbf{B}]]\xi^2 + \frac{1}{3!}[\mathbf{A}, [\mathbf{A}, [\mathbf{A}, \mathbf{B}]]]\xi^3 + \ldots} \tag{1.76}$$

$$\boxed{e^{\xi\mathbf{A}}\mathbf{F}(\mathbf{B})e^{-\xi\mathbf{A}} = \mathbf{F}(e^{\xi\mathbf{A}}\mathbf{B}e^{-\xi\mathbf{A}})} \tag{1.77}$$

  where ξ is a scalar and $\mathbf{A}$ and $\mathbf{B}$ are two independent linear operators that do not depend on ξ and that do not commute.

- the *Glauber* or *Glauber–Weyl relation*

$$\boxed{e^{\xi\mathbf{A}}e^{\xi\mathbf{B}} = e^{(\mathbf{A}+\mathbf{B})\xi}e^{+[\mathbf{A},\mathbf{B}]\xi^2/2} \text{ with } [\mathbf{A}, [\mathbf{A}, \mathbf{B}]] = 0 \quad \text{and} \quad [\mathbf{B}, [\mathbf{A}, \mathbf{B}]] = 0} \tag{1.78}$$

  where ξ is a scalar and may be also written

$$e^{(\mathbf{A}+\mathbf{B})\xi} = e^{\xi\mathbf{A}}e^{\xi\mathbf{B}}e^{-[\mathbf{A},\mathbf{B}]\xi^2/2} = e^{(\mathbf{B}+\mathbf{A})\xi} \tag{1.79}$$

$$e^{(\mathbf{A}+\mathbf{B})\xi} = e^{\xi\mathbf{B}\xi\mathbf{A}}e^{-[\mathbf{B},\mathbf{A}]\xi^2/2} = e^{(\mathbf{B}+\mathbf{A})\xi} \tag{1.80}$$

In the latter equations, the last terms on the right-hand side have been introduced in order to focus attention on the fact that

$$e^{(\mathbf{B}+\mathbf{A})\xi} = e^{(\mathbf{A}+\mathbf{B})\xi}$$

Now, we may summarize the most important results as follows:

Basic equations for quantum mechanics
Linear transformations and their Hermitian conjugates:
$\mathbf{A}\|\Psi\rangle = \|\Phi\rangle \qquad \langle\Psi\|\mathbf{A}^\dagger = \langle\Phi\|$ **Hermitian operators A, unitary operators U, commutators:** $\mathbf{A} = \mathbf{A}^\dagger \qquad \mathbf{U}^{-1} = \mathbf{U}^\dagger \quad \text{with} \quad \mathbf{U}\mathbf{U}^{-1} = \mathbf{U}^{-1}\mathbf{U} = 1 \qquad [\mathbf{A}, \mathbf{B}] = \mathbf{AB} - \mathbf{BA}$
Eigenvalue equations and their Hermitean conjugates:
$\mathbf{A}\|\Psi_i\rangle = A_i\|\Psi_i\rangle \qquad \langle\Psi_i\|\mathbf{A}^\dagger = \langle\Psi_i\|A_i^*$
Eigenvalue equations of Hermitian operators and their Hermitean conjugates:
$\mathbf{A}\|\Psi_i\rangle = A_i\|\Psi_i\rangle \qquad \langle\Psi_i\|\mathbf{A} = \langle\Psi_i\|A_i$ with $\quad \langle\Psi_i\|\Psi_k\rangle = \delta_{ik} \qquad$ and $\qquad \sum \|\Psi_k\rangle\langle\Psi_k\| = 1$
An important relation:
$\langle\Psi\|\mathbf{B}^\dagger\|\Phi\rangle = \langle\Phi\|\mathbf{B}\|\Psi\rangle^*$
Invariance of the trace:
$\sum\langle\Psi_k\|\mathbf{AB}\|\Psi_k\rangle = \sum\langle\Psi_k\|\mathbf{BA}\|\Psi_k\rangle \quad$ even if $\quad [\mathbf{A}, \mathbf{B}] \neq 0$

CHAPTER 2

BASIS FOR QUANTUM APPROACHES OF OSCILLATORS

INTRODUCTION

Using the mathematical basis treated in this chapter, it will be possible to discuss the quantum mechanics tools necessary for the study of the behavior of oscillators. We begin with an exposition of the postulates of quantum mechanics, which will be the purpose of Section 2.1. An important place will be given to the notions of *quantum average values* and to *quantum fluctuations*, allowing one to deduce from quantum principles the *Heisenberg uncertainty relations* according to which it is not possible to simultaneously know with arbitrary accuracy both the position and the momentum of any particle. In a subsequent section, some dynamic aspects will be developed allowing one both to determine the time dependence of the quantum average values and show that the Heisenberg uncertainty relations introduce a limit to the perfect knowledge assumed by classical mechanics. However, the quantum principles lead to the *Ehrenfest equations*, which nearly behave as the Newton equations, save that they are dealing with average values and not with exact ones, as for the classical equations. Related to these dynamic aspects, we shall prove the *energy conservation*, in a quantum averaged form, and the *virial theorem* relating the quantum average value of the kinetic and potential energies to the total energy, which holds also in classical mechanics. The last section will be devoted to some developments dealing with quantum concepts related to the connection between the position and the momentum, which will be used in Chapter 3 to relate quantum mechanics to wave mechanics.

2.1 OSCILLATOR QUANTIZATION AT THE HISTORICAL ORIGIN OF QUANTUM MECHANICS

2.1.1 Ultraviolet catastrophe

Measurements of thermal capacity of solids were discovered at the beginning of the twentieth century to be in contradiction with the principles of statistical physics

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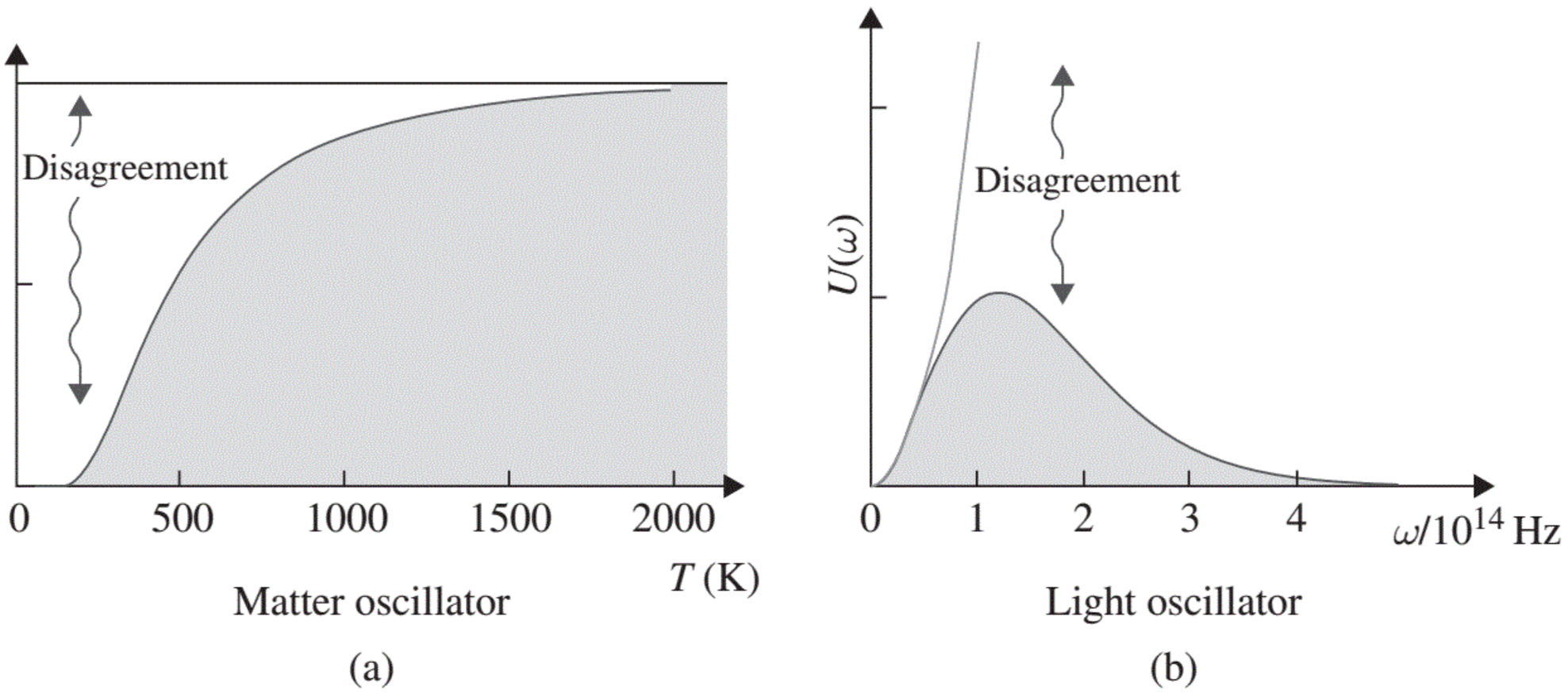


Figure 2.1 Contradiction between experiment (shaded areas) and classical prediction (lines).

based on classical mechanics: The experiments show that these thermal capacities are temperature dependent, whereas the theory assuming that they result from the partial derivative with respect to the temperature of the average oscillation energy of the atoms within the solids predicted that they ought to be constant, due to the equipartition theorem of statistical mechanics applied to classical mechanics, according to which each degree of freedom of vibration of the solid contributes the same energy amount $k_B T$ (where k_B is the Boltzmann constant and T the absolute temperature). See, for instance, Fig. 2.1a. In addition, the study of the frequency distribution of the intensity of the electromagnetic radiations enclosed in a heated cavity at thermal equilibrium (black-body radiations) lead to the results that this intensity narrows to zero as the frequency increases, in utter contradiction with the classical statistical mechanics predictions (applied to Maxwell electromagnetic modes of vibration) by Rayleigh and Jeans, according to which the intensity ought to tend to infinity (*the ultraviolet catastrophe*). See Fig. 2.1b.

2.1.2 Planck, Einstein, and Bohr's old quantum mechanics

To reconcile the ultraviolet catastrophe with physics, Planck (1858–1947) assumed that the walls of the black body responsible for the absorption and emission of ultraviolet light are made of small oscillators of various frequencies, the energy of which cannot vary continuously as in Newtonian mechanics, but is quantized, the energy levels E_n obeying

$$E_n(\text{matter oscillator}) = nh\nu$$

where n is an integer, ν the frequency of the microscopic oscillator, and h *Planck's constant*. With this assumption of the oscillator energy quantization, Planck was able in 1901 to reproduce with great accuracy the experimental results.

Moreover, some time later, Einstein proposed (1905) a theoretical interpretation of the *photoelectric effect*, a recent and unexplained laboratory result: It had been

discovered that an electron can be expelled from a material by a light radiation, when its frequency is greater than a threshold characteristic of the material, the kinetic energy of the emitted electron increasing linearly with the light frequency beyond the threshold. To interpret that Einstein assumed that light, considered at this time by the physicists as of wave nature, has also to be considered as consisting of a grain of light, *the photon*, the energy of which is proportional to the angular frequency ω of the light, the proportionality constant being that introduced by Planck in his theory.

$$E_n(\text{light oscillator}) = n\hbar\omega \quad \text{with} \quad \hbar = \frac{h}{2\pi}$$

A few years later, in 1913, Bohr (1885–1962), a Danish physicist, attacked the problem raised by the absorption and emission of light rays by hydrogen atoms. The frequencies of these lines, which are the same for both processes, were found by Balmer (1825–1898) to obey with a perfect precision an empirical formula, the *Balmer formula*, involving integer numbers. Bohr was able to theoretically reproduce the empirical Balmer formula by assuming that the angular momentum of the electron generated by its circular orbit motion around the proton is quantized, being an integer multiple of Planck's constant already introduced in the Planck and in the Einstein theoretical approaches.

Moreover, Bohr assumed that when the electron moves from one orbit to another, it performs that in a sudden and unrepresentative manner, by emitting or absorbing a quantum of light (photon) of frequency given by the absolute difference between the orbit's energies divided by Planck's constant. In addition, to link his theoretical approach with classical mechanics, Bohr introduced a *correspondence principle*, claiming that when the quantized energy levels of the electronic orbits are higher and higher, the transitions between successive energy levels involve a dynamics that approaches more and more closely the classical circular motion.

2.1.3 Heisenberg and matrix mechanics

All these works of Planck, Einstein, and Bohr called into question the continuous variation of the energy level of atoms since they assumed that energy may change only by small packets, the energy quanta involving the Planck constant. These works aroused passionate debates, some scientists thinking with Bohr that the classical mechanics of Newton would have to be rethought from top to bottom in order to deeply reflect the new realities at the scale of molecules, atoms, and their elementary constituents.

Among these young physicists, Heisenberg (1901–1976) played a pioneering role, building during his thesis in 1924 a new theory. He focused on quantizing the energy of microscopic oscillators proposed by Planck. His ideas were primarily based on two kinds of square noncommutative matrices, one of which was intended to represent the position coordinate and the other one the conjugated momentum. Heisenberg completed this assumption by introducing Planck's constant in these matrices.

Heisenberg justified his assumption of noncommutative matrices representing position coordinates and momentum by the positivist postulate that it is impossible

on the atomic scale to measure the position of a particle without changing instantly ipso facto speed and therefore its momentum. Heisenberg was able, from his noncommutative matrices (recognized as such by Jordan), to find the formulas postulated by Planck for the quantization of the energy of small oscillators belonging to the atomic scale. This work may be regarded as the foundation stone of the new quantum mechanics.

2.1.4 De Broglie and wave mechanics

As seen above, Einstein introduced in his interpretation of the photoelectric effect the necessity to add corpuscular properties to the wave ones assumed for light, following the interference experiments of Young and others. This dual nature of light, Louis de Broglie (1892–1987) has extended it to *matter*, that is, all entities involving mass, which comprise the physical realities around us: At the same time Heisenberg was working on his thesis on the matrix mechanics, de Broglie, starting from intuitions of the Irish physicist Hamilton (1805–1865). proposed a new mechanism applying to the microscopic scale in which a wave is associated with the particle dynamics. In this new mechanics, the wavelength λ (*de Broglie wavelength*) of free particles (particles moving in a straight line in the absence of potential) is equal to Planck's constant divided by the momentum p of the particles (*de Broglie relation*):

$$\lambda = \frac{h}{p}$$

Hence, since the momentum is proportional to the product of mass times velocity, the de Broglie wavelength becomes smaller the greater the mass, so that it becomes negligible when going from the atomic and molecular scales to the human one and, a fortiori, to those of the planets and stars.

In this wave mechanics, the corpuscular properties of matter are linked with the position coordinates, while the wave properties are linked to the momentum through the de Broglie wavelength. That is the origin of the term *wave mechanics* given to this new discipline of physics. One of the famous theoreticians of the time, the Austrian physicist Schrödinger (1887–1961), who initially despised the ideas of the young French physicist de Broglie, thereafter applied them to the hydrogen atom. By solving the partial differential equation governing in wave mechanics the electron behavior of the hydrogen atom, Schrödinger retrieved the results of Bohr concerning the empirical Balmer formula.

Wave mechanics was soon experimentally confirmed by Davisson (1881–1958) and Germer (1896–1971) in connection with diffraction observations on crystals, allowing to verify the validity of the de Broglie relation. In addition the wave particle duality nature became evident via new experiments where particles having crossed separately a dispersion pattern, strike a screen by exhibit an interference pattern, thus suggesting that each isolated particle *interferes with itself*. This phenomenon was observed for light (photons) and also for material particles such as atoms.

2.2 QUANTUM MECHANICS POSTULATES AND NONCOMMUTATIVITY

2.2.1 The principles

2.2.1.1 First postulate At a given time, the physical state of a system is described by a *ket* $|\Psi_j(t)\rangle$ belonging to the *state space*, that is, to a vector space of infinite dimension involving complex scalar products.

2.2.1.2 Second postulate With each classical physical variable A is associated a linear operator $\mathbf{A}$ acting in the state space, which must be *Hermitian* (*observable*), and obeying, therefore,

$$\mathbf{A} = \mathbf{A}^{\dagger}$$

2.2.1.3 Third postulate The possible measurements of an observable $\mathbf{A}$ are given by the *eigenvalues* A_n of this operator, that is

$$\mathbf{A}|\Phi_n\rangle = A_n|\Phi_n\rangle$$

where $|\Phi_n\rangle$ are the corresponding eigenkets of the eigenvectors of $\mathbf{A}$. Owing to the Hermiticity of the observables, their eigenvalues are real:

$$A_n = A_n^*$$

This constraint of Hermiticity on linear operators, which describe the physical variables, avoids the possibility of complex expressions involving an imaginary part in measurements of many physical variables.

2.2.1.4 Fourth postulate The transition of a system from any ket $|\Phi_n\rangle$ to another $|\Psi_j\rangle$ cannot be predicted in a deterministic way but only in a probabilistic one defined by a probability $\mathbb{P}_{nj}$, which may be calculated from the squared modulus of the scalar product of the initial and final kets, that is, by

$$\boxed{\mathbb{P}_{nj} = |\langle\Psi_j|\Phi_n\rangle|^2} \tag{2.1}$$

2.2.1.5 Fifth postulate This postulate concerns situations where the eigenvalues are *degenerate*, which we shall not encounter here. Thus, in order to simplify, we do not give it here.

2.2.1.6 Sixth postulate There are two different equivalent ways to obtain the dynamics of a quantum system. In the first one, the kets and bras are time dependent and the operators are constants. This is the *Schrödinger picture*. In the second one, the kets and bras are constants, and it is the operators that are time dependent. The latter is the *Heisenberg picture*.

The sixth postulate, in the Schrödinger picture, states that the kets describing a physical system evolve with time between two quantum jumps in a deterministic

way, which is given by the following equation named the *time-dependent Schrödinger equation* or more shortly the *Schrödinger equation*:

$$\boxed{i\hbar\frac{\partial}{\partial t}|\Psi_j(t)\rangle = \mathbf{H}|\Psi_j(t)\rangle \quad \text{with} \quad i^2 = -1} \tag{2.2}$$

where $\mathbf{H}$ is the total quantum Hamiltonian describing the system, whereas $\hbar$ is the Planck constant divided by 2π. Note that in Eq. (2.2) the partial derivative with respect to time is sometimes replaced by a time derivative. However, as the ket may be affected by transformations other than that of time, for instance, translations of the origin (vide infra the translation operators), we prefer the partial derivative notation.

2.2.1.7 Seventh postulate The quantum operator $\mathbf{A}$ describing a classical physical variable A may be obtained as follows:

1. Express the classical variable A in terms of the space variables Q_k related to the different freedom degrees k of the system, and of their corresponding conjugate momentum P_k, that is, write $A(P_k, Q_k)$.
2. Associate the Hermitian operators $\mathbf{Q}_i$ and $\mathbf{P}_i$, respectively, to each space variable Q_k and to its corresponding conjugate momentum P_k, in order to pass from the classical expression $A(P_k, Q_k)$ to the corresponding quantum Hermitian operator $\mathbf{A}(\mathbf{P}_k, \mathbf{Q}_k)$, that is,

$$A(P_k, Q_k) \rightarrow \mathbf{A}(\mathbf{P}_k, \mathbf{Q}_k)$$

3. Require that the $\mathbf{Q}_k$ and $\mathbf{P}_k$ operators obey the commutation rule

$$\boxed{[\mathbf{Q}_k, \mathbf{P}_l] = i\hbar\delta_{kl} \quad \text{with} \quad i^2 = -1} \tag{2.3}$$

where $\hbar$ is the Planck constant given by

$$\hbar = \frac{h}{2\pi} = \frac{6.62}{2\pi} \times 10^{-34}\ \mathrm{J \cdot S}$$

Some further information concerning the commutation rules are given in Section 18.5.

The third and fourth postulates lead to the following important remarks:

The third postulate leads one to distinguish, in the measurement of an observable, two different possibilities according to whether or not before any measurement of one of its observables, the system was in an eigenket of the measured operator. This postulate gives directly a response only in the specific situation where the system was in an eigenket of this last one. Owing to Eq. (2.3), noting that the basic physical variables $\mathbf{P}$ and $\mathbf{Q}$ do not commute, different Hermitian operators $\mathbf{A}(\mathbf{P}_k, \mathbf{Q}_k)$ and $\mathbf{B}(\mathbf{P}_l, \mathbf{Q}_l)$, both functions of $\mathbf{P}$ and $\mathbf{Q}$, have no reasons to commute:

$$[\mathbf{A}(\mathbf{P}_k, \mathbf{Q}_k), \mathbf{B}(\mathbf{P}_l, \mathbf{Q}_l)] \neq 0 \tag{2.4}$$

To make clear the discussion, write the eigenvalue equations of these two Hermitian operators:

$$\mathbf{A}(\mathbf{P}_k, \mathbf{Q}_k)|\Phi_v\rangle = A_v|\Phi_v\rangle \qquad \text{and} \qquad \mathbf{B}(\mathbf{P}_k, \mathbf{Q}_k)|\Psi_\mu\rangle = B_\mu|\Psi_\mu\rangle$$

where $|\Phi_\nu\rangle$ and $|\Psi_\mu\rangle$ are, respectively, the eigenkets of $\mathbf{A}(\mathbf{P}_k, \mathbf{Q}_k)$ and $\mathbf{B}(\mathbf{P}_k, \mathbf{Q}_k)$, whereas A_ν and B_μ are the corresponding eigenvalues. Of course, since these operators do not commute, they do not admit the same set of eigenvectors. Moreover, since they are Hermitian, each eigenket of one of these operators may be linearly expanded in the set of eigenkets of the other operator. For instance,

$$|\Psi_\mu\rangle = \sum_\nu a_{\nu\mu}|\Phi_\nu\rangle \quad \text{with} \quad a_{\nu\mu} = \langle\Phi_\nu|\Psi_\mu\rangle \tag{2.5}$$

Now, suppose that at an initial time the system is in one of the eigenstates $|\Psi_\mu\rangle$ of the $\mathbf{B}(\mathbf{P}_k, \mathbf{Q}_k)$ operator. Next, if a measurement of the Hermitian operator $\mathbf{A}(\mathbf{P}_k, \mathbf{Q}_k)$ is performed on this system, then, according to the third postulate, this measurement will yield, for instance, A_η of the different eigenvalues and A_ν of the Hermitian operator $\mathbf{A}(\mathbf{P}_k, \mathbf{Q}_k)$. That implies that, after such a measurement, the system is now in the ket $|\Phi_\eta\rangle$ corresponding to the eigenvalue A_η. It appears, therefore, that measurement of the operator $\mathbf{A}(\mathbf{P}_k, \mathbf{Q}_k)$ of the system, which was initially in the ket $|\Psi_\mu\rangle$, has induced a jump in the ket $|\Phi_\eta\rangle$. Hence, according to the fourth postulate, this jump is not deterministic but occurs with probability

$$\mathbb{P}_{\mu\eta} = |\langle\Psi_\mu|\Phi_\eta\rangle|^2$$

or, compare, Eq. (2.5),

$$\mathbb{P}_{\mu\eta} = \left|\sum_\nu a_{\nu\mu}\langle\Phi_\nu|\Phi_\eta\rangle\right|^2$$

so that due to the orthonormality of the eigenkets of a Hermitian operator $\mathbf{A}(\mathbf{P}_k, \mathbf{Q}_k)$

$$\mathbb{P}_{\mu\eta} = \left|\sum_\nu a_{\nu\mu}\delta_{\eta\nu}\right|^2 = |a_{\mu\eta}|^2$$

Thus, the measurement of $\mathbf{A}(\mathbf{P}_k, \mathbf{Q}_k)$ has induced the abrupt change

$$\sum_\nu a_{\nu\mu}|\Phi_\nu\rangle \to |\Phi_\eta\rangle$$

with the probability equal to the squared absolute value of the coefficients $a_{\mu\eta}$ of the expansion appearing on the left-hand side of this last equation. As a matter of fact, the measurement of $\mathbf{A}(\mathbf{P}_k, \mathbf{Q}_k)$ has induced a reduction of the left-hand-side expansion, which is called the *wave packet reduction*, for historical reasons related to the fact that in wave mechanics the $|\Phi_\nu\rangle$ may be related to different orthogonal wavefunctions (see the discussion in Chapter 3 dealing with wave mechanics).

2.2.2 Classical mechanics as special limit of quantum mechanics

Despite its very formal character, which is far from classical mechanics, quantum mechanics is not without a link with it. As we shall see, it is possible from the postulates of quantum mechanics, to demonstrate the following equations, named the *Ehrenfest equations*, which govern the dynamics of a system:

$$\boxed{\frac{d\langle\mathbf{Q}(t)\rangle_\Psi}{dt} = \frac{\langle\mathbf{P}(t)\rangle_\Psi}{m} \qquad \text{and} \qquad \frac{d\langle\mathbf{P}(t)\rangle_\Psi}{dt} = -\left\langle\frac{\partial\mathbf{V}}{\partial\mathbf{Q}}\right\rangle_\Psi} \tag{2.6}$$

Here, $\langle \mathbf{Q}(t) \rangle_\Psi$, $\langle \mathbf{P}(t) \rangle_\Psi$, and $\langle (\partial \mathbf{V}/\partial \mathbf{Q}) \rangle_\Psi$ are, respectively, the average values of the position, momentum, and potential when the system is in the quantum state characterized by the ket $|\Psi\rangle$. Now, these equations are very similar to Newton's equations:

$$\boxed{\frac{d\vec{Q}(t)}{dt} = \frac{\vec{P}(t)}{m} \qquad \text{and} \qquad \frac{d\vec{P}(t)}{dt} = -\frac{\partial V}{\partial \vec{Q}}} \tag{2.7}$$

Letters with arrow mean vectorial entities in classical mechanics, at the opposite of bold letters appearing above and meaning quantum mechanical operators. However, an important difference exists because the quantum Eqs. (2.6) govern average values, whereas the classical Eqs. (2.7) govern exact ones. Hence, if they are average values $\langle \mathbf{A} \rangle_\Psi$, they indicate that dispersion of the possible values around the average values exists, which may be analyzed using the *variance* $\Delta \mathbf{A}$, namely

$$\Delta \mathbf{A} = \sqrt{\langle \mathbf{A}^2 \rangle_\Psi - \langle \mathbf{A} \rangle_\Psi^2} \tag{2.8}$$

where $\langle \mathbf{A}^2 \rangle_\Psi$ is the average of the square of $\mathbf{A}$. For the position and the momentum, the time-dependent average values are governed by Eqs. (2.6), whereas the corresponding variance are governed by the *Heisenberg uncertainty relation* (which will be demonstrated later). Figure 2.2 shows two situations occurring for the relative variance $\Delta \mathbf{A}/\langle \mathbf{A} \rangle$, the left-hand-side showing a quantum behavior, whereas the right-hand-side exhibits classical behavior.

$$\boxed{(\Delta \mathbf{P}(t))_\Psi (\Delta \mathbf{Q}(t))_\Psi \geqslant \frac{\hbar}{2}} \tag{2.9}$$

The passage from the quantum mechanics to the classical mechanics occurs when

$$\boxed{\frac{(\Delta \mathbf{P}(t))_\Psi}{\langle \mathbf{P}(t) \rangle_\Psi} \to 0} \qquad \text{and} \qquad \boxed{\frac{(\Delta \mathbf{Q}(t))_\Psi}{\langle \mathbf{Q}(t) \rangle_\Psi} \to 0} \tag{2.10}$$

When the size of the system is very small, of the order of the size of molecules or atoms or smaller, the quantum mechanics of Eqs. (2.6) holds. However, when this

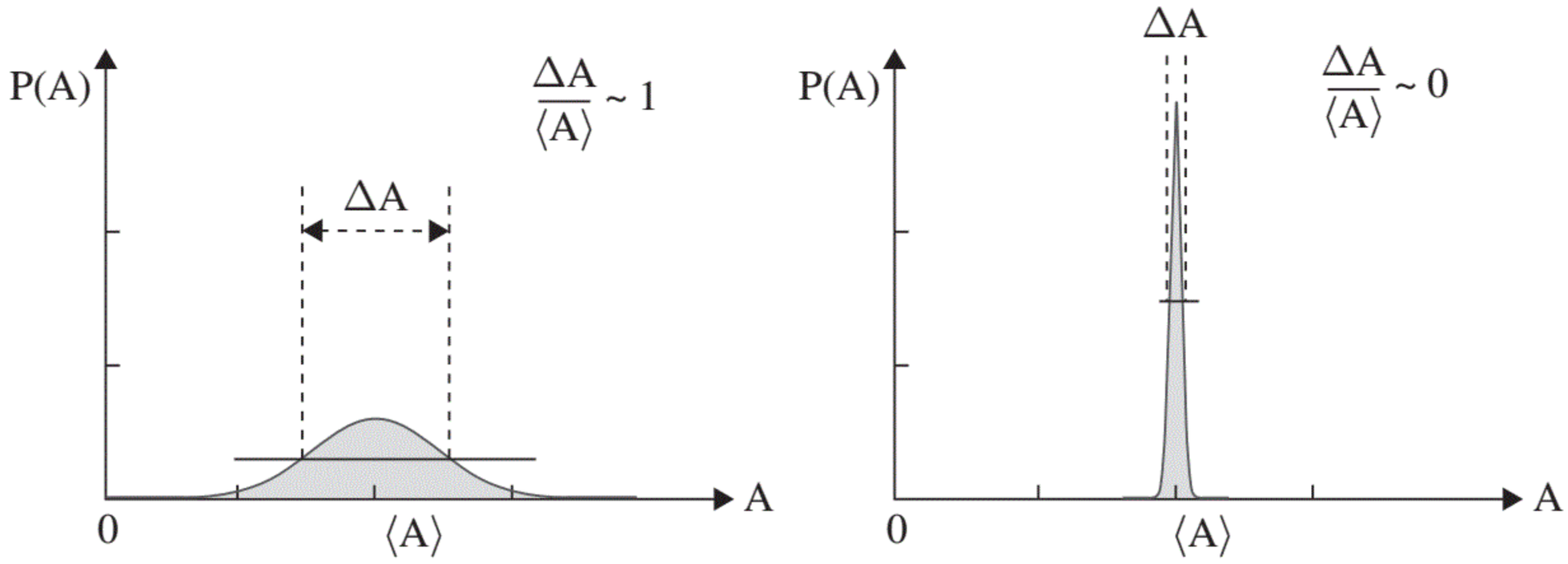


Figure 2.2 Quantum and classical relative variance $\Delta \mathbf{A}/\langle \mathbf{A} \rangle$.

size is progressively increasing, the conditions (2.10) are more and more verified so that the quantum mechanics of Eqs. (2.6) transforms to classical mechanics (2.7).

The specific physical behavior as the size of the system decreases is linked to the basic uncertainty characterizing the fundamental physical variables of small particles manifested via the following probability passage from any state of position to one of momentum, which may be the initial position and the final momentum, or vice versa, through the following relation, which will be demonstrated later

$$\boxed{|\langle\{P\}|\{Q\}\rangle|^2 = \frac{1}{2\pi\hbar}} \tag{2.11}$$

where $|\{Q\}\rangle$ and $|\{P\}\rangle$ are, respectively, the eigenkets of the position $\mathbf{Q}$ and momentum $\mathbf{P}$ operators defined, according to the third postulate by the continuous eigenvalue equation

$$\mathbf{Q}|\{Q\}\rangle = Q|\{Q\}\rangle \qquad \text{and} \qquad \mathbf{P}|\{P\}\rangle = P|\{P\}\rangle$$

where Q and P are, respectively, the eigenvalues of $\mathbf{Q}$ and $\mathbf{P}$, and thus the respective measured values of these operators, when the system is either in $|\{Q\}\rangle$ or in $|\{P\}\rangle$, Eq. (2.11) implies therefore that, after a measurement of the position yielding Q, another measurement of the momentum may lead to all the possible values P, with the same probability, is given by

$$\mathbb{P}_{Q\to P} = \mathbb{P}_{P\to Q} = \frac{1}{2\pi\hbar}$$

The Heisenberg uncertainty relation (2.9) and the jump probability (2.11) are consequence of the fundamental commutator

$$[\mathbf{Q}, \mathbf{P}] = i\hbar \tag{2.12}$$

Thus, the noncommutativity properties of observables, which are very general, play a fundamental role in the knowledge of the possible measurement of a physical variable. In order to appreciate the role played by the Hermitian operators in quantum mechanics, it is necessary to find the expression of the commutators $[\mathbf{Q}, \mathbf{F}(\mathbf{P})]$ and $[\mathbf{P}, \mathbf{F}(\mathbf{Q})]$, which are deeply linked to their behavior. In Appendix 5 are demonstrated some expressions dealing with commutators that are functions of $\mathbf{P}$ and $\mathbf{Q}$, and that result from the basic commutator (2.12). They are the following:

$$\boxed{[\mathbf{Q}, \mathbf{P}^n] = n(i\hbar)\mathbf{P}^{n-1}} \tag{2.13}$$

$$\boxed{[\mathbf{Q}, \mathbf{F}(\mathbf{P})] = (i\hbar)\left(\frac{\partial \mathbf{F}(\mathbf{P})}{\partial \mathbf{P}}\right)} \tag{2.14}$$

$$\boxed{[\mathbf{P}, \mathbf{Q}^n] = -n(i\hbar)\mathbf{Q}^{n-1}}$$

$$\boxed{[\mathbf{P}, \mathbf{F}(\mathbf{Q})] = -(i\hbar)\left(\frac{\partial \mathbf{F}(\mathbf{Q})}{\partial \mathbf{Q}}\right)} \tag{2.15}$$

2.3 HEISENBERG UNCERTAINTY RELATIONS

2.3.1 Mean values

Clearly, according to the third postulate, if a system is in a state $|\Phi_n\rangle$, which is an eigenvector of some Hermitian operator $\mathbf{A}$, the measurement of the physical variable associated to this operator is given by the corresponding real eigenvalue A_n of this operator, that is,

$$\mathbf{A}|\Phi_n\rangle = A_n|\Phi_n\rangle \quad \text{with} \quad \mathbf{A} = \mathbf{A}^\dagger \tag{2.16}$$

However, if the system is described by a state $|\Psi_k\rangle$ that is not an eigenvector of the operator, we have seen that, according to the fourth postulate, there are as many possibilities to get measurements of the physical variable associated to $\mathbf{A}$ as there are eigenvalues of $\mathbf{A}$. Then the only possibility for a measurement of $\mathbf{A}$ is an average value $\langle\mathbf{A}\rangle_{\Psi_k}$ given by

$$\langle\mathbf{A}\rangle_{\Psi_k} = \langle\Psi_k|\mathbf{A}|\Psi_k\rangle \tag{2.17}$$

To show that $\langle\mathbf{A}\rangle_{\Psi_k}$ is an average value, use the closure relation of the eigenkets of the Hermitian operator $\mathbf{A}$:

$$1 = \sum_n |\Phi_n\rangle\langle\Phi_n| \tag{2.18}$$

Then insert it on the right-hand side of Eq. (2.17) just after $\mathbf{A}$:

$$\langle\mathbf{A}\rangle_{\Psi_k} = \langle\Psi_k|\mathbf{A}\left\{\sum_n |\Phi_n\rangle\langle\Phi_n|\right\}|\Psi_k\rangle$$

This last expression reads in the more usual form on commuting the sum

$$\langle\mathbf{A}\rangle_{\Psi_k} = \sum_n \langle\Psi_k|\mathbf{A}|\Phi_n\rangle\langle\Phi_n|\Psi_k\rangle$$

Again, according to the eigenvalue Eq. (2.16), this equation transforms to

$$\langle\mathbf{A}\rangle_{\Psi_k} = \sum_n \langle\Psi_k|A_n|\Phi_n\rangle\langle\Phi_n|\Psi_k\rangle$$

or, on commuting the eigenvalues A_n that are scalars

$$\langle\mathbf{A}\rangle_{\Psi_k} = \sum_n A_n\langle\Psi_k|\Phi_n\rangle\langle\Phi_n|\Psi_k\rangle$$

Moreover, using the fact that the two right-hand-side scalar products are complex conjugates, we have

$$\langle\mathbf{A}\rangle_{\Psi_k} = \sum_n A_n|\langle\Psi_k|\Phi_n\rangle|^2 \tag{2.19}$$

Finally, due to the fourth postulate, the right-hand-side squared modulus is the transition probability to pass from the ket $|\Psi_k\rangle$ in which the system was initially before

the measurement of **A** to the eigenket $|\Phi_n\rangle$ of this operator **A** associated with the eigenvalue A_n to which the measurement of **A** has lead.

$$|\langle\Psi_k|\Phi_n\rangle|^2 = \mathbb{P}_{kn} \tag{2.20}$$

Thus, the left-hand side of Eq. (2.19), which is defined by Eq. (2.17), appears to be given by

$$\boxed{\langle\mathbf{A}\rangle_{\Psi_k} = \sum_n \mathbb{P}_{kn} A_n = \langle\Psi_k|\mathbf{A}|\Psi_k\rangle} \tag{2.21}$$

Examination of this last result shows that $\langle\mathbf{A}\rangle_{\Psi_k}$ has the properties of a statistical average value since it is the sum of the possible values of the observable **A** weighted by their corresponding probabilities.

2.3.2 Variation theorem

It is now possible to prove the variation theorem. The sixth postulate attributes to the Hamiltonian a privileged role. Dealing with the Hamiltonian, there is, in quantum mechanics, a theorem that is of great interest concerning the energy of physical systems. Let us write the eigenvalue equation of the Hamiltonian **H**:

$$\mathbf{H}|\Psi_i\rangle = E_i\,|\Psi_i\rangle \quad \text{with} \quad \langle\Psi_i|\Psi_j\rangle = \delta_{ij} \tag{2.22}$$

where E_i are the eigenvalues and $|\Psi_i\rangle$ the corresponding eigenvectors. Now, consider the average value over any ket $|\Phi_l\rangle$ of the difference between the Hamiltonian and the lowest eigenvalue E_0:

$$\langle\Phi_l|\,(\mathbf{H} - E_0)\,|\Phi_l\rangle = \langle\Phi_l|\,\mathbf{H}|\,\Phi_l\rangle - E_0\langle\Phi_l|\Phi_l\rangle \tag{2.23}$$

Next, assume that the ket $|\Phi_l\rangle$ is given by the following expansion over the eigenkets $|\Psi_i\rangle$ of the Hamiltonian, that is,

$$|\Phi_l\rangle = \sum_j a_{jl}|\Psi_j\rangle \qquad \text{and} \qquad \langle\Phi_l| = \sum_i a_{li}\langle\Psi_i|$$

Then, Eq. (2.23) becomes

$$\langle\Phi_l|\,(\mathbf{H} - E_0)\,|\Phi_l\rangle = \sum_i \sum_j a_{jl}a_{li}\,\{\langle\Psi_i|\,\mathbf{H}\,|\,\Psi_j\rangle - E_0\langle\Psi_i|\Psi_j\rangle\}$$

Furthermore, due to the eigenvalue equation (2.22) by orthogonality properties we have

$$\langle\Phi_l|\,(\mathbf{H} - E_0)|\Phi_l\rangle = \sum_i \sum_j a_{jl}a_{li}(E_j - E_0)\delta_{ij}$$

and thus

$$\langle\Phi_l|\,(\mathbf{H} - E_0)|\Phi_l\rangle = \sum_j |a_{jl}|^2(E_j - E_0) \tag{2.24}$$

Now, observe that, since E_0 is the lowest eigenvalue, the right-hand-side differences are positive in the same way as the squared modulus of the expansion coefficients, that is,

$$(E_j - E_0) \geqslant 0 \qquad \text{and} \qquad |a_{jl}|^2 \geqslant 0$$

Thus, we have from the left-hand side of Eq. (2.24), the following inequality:

$$\langle \Phi_l | (\mathbf{H} - E_0) | \Phi_l \rangle \geqslant 0$$

Since E_0 is a scalar, one then obtains the following fundamental result:

$$\boxed{\langle \Phi_l | \mathbf{H} | \Phi_l \rangle \geqslant E_0} \tag{2.25}$$

Hence, the average value of the Hamiltonian performed over any one ket cannot be smaller than the lowest energy E_0. That gives the possibility to approach E_0 by variational methods if it is not possible to solve exactly the eigenvalue equation (2.22) of the Hamiltonian.

2.3.3 Variance

Now, observe that in probability theory and statistics, the variance ΔA of a random variable is a measurement of the statistical dispersion averaging the squared distance of its possible values from the mean value $\langle A \rangle$. Start from the variance (2.8):

$$\Delta \mathbf{A}_{\Psi_k} = \sqrt{\langle \mathbf{A}^2 \rangle_{\Psi_k} - \langle \mathbf{A} \rangle_{\Psi_k}^2} \tag{2.26}$$

In this last equation, the second term under the square root is given by Eq. (2.21). In order to get the first one, we may begin by using the definition (2.17) of the average of some operator, by taking $\mathbf{A}^2$ in place of $\mathbf{A}$:

$$\langle \mathbf{A}^2 \rangle_{\Psi_k} = \langle \Psi_k | \mathbf{A}^2 | \Psi_k \rangle$$

which may also be written

$$\langle \mathbf{A}^2 \rangle_{\Psi_k} = \langle \Psi_k | \mathbf{A}\mathbf{A} | \Psi_k \rangle \tag{2.27}$$

Again, write the eigenvalue equation of Hermitian operators and the corresponding closure relation:

$$\mathbf{A}|\Phi_n\rangle = A_n|\Phi_n\rangle \qquad \text{and} \qquad \sum_n |\Phi_n\rangle\langle\Phi_n| = 1 \tag{2.28}$$

Then, introduce in Eq. (2.27) between $\mathbf{A}$ and $|\Psi_k\rangle$ this last closure relation

$$\langle \mathbf{A}^2 \rangle_{\Psi_k} = \langle \Psi_k | \mathbf{A}\mathbf{A} \left(\sum_n |\Phi_n\rangle\langle\Phi_n| \right) |\Psi_k\rangle$$

Using the eigenvalue equation appearing in (2.28), one obtains

$$\langle \mathbf{A}^2 \rangle_{\Psi_k} = \sum_n \langle \Psi_k | \mathbf{A} A_n | \Phi_n \rangle \langle \Phi_n | \Psi_k \rangle$$

Next, commuting the scalar A_n, this equation becomes

$$\langle \mathbf{A}^2 \rangle_{\Psi_k} = \sum_n A_n \langle \Psi_k | \mathbf{A} | \Phi_n \rangle \langle \Phi_n | \Psi_k \rangle$$

Again using in turn the eigenvalue equation (2.28), one finds

$$\langle \mathbf{A}^2 \rangle_{\Psi_k} = \sum_n A_n \langle \Psi_k | A_n | \Phi_n \rangle \langle \Phi_n | \Psi_k \rangle$$

or, A_n being a scalar

$$\langle \mathbf{A}^2 \rangle_{\Psi_k} = \sum_n A_n^2 | \langle \Psi_k | \Phi_n \rangle |^2$$

Finally, using the fourth postulate given in the present context by Eq. (2.20) leads to

$$\langle \mathbf{A}^2 \rangle_{\Psi_k} = \sum_n \mathbb{P}_{kn} A_n^2 \quad \text{with} \quad \mathbb{P}_{kn} = | \langle \Psi_k | \Phi_n \rangle |^2$$

Thus, the variance (2.26) takes the form

$$\Delta \mathbf{A}_{\Psi_k} = \sqrt{\left(\sum_n \mathbb{P}_{kn} \, A_n^2 \right) - \left(\sum_n \mathbb{P}_{kn} \, A_n \right)^2}$$

2.3.4 Product of two variances

2.3.4.1 Variances of two different operators before and after some shift

Consider two Hermitian operators **A** and **B**, the commutator of which is obeying

$$[\mathbf{A}, \mathbf{B}] = i\mathbf{C} \quad \text{with} \quad i^2 = -1 \tag{2.29}$$

and

$$\mathbf{A} = \mathbf{A}^\dagger \qquad \mathbf{B} = \mathbf{B}^\dagger \qquad \mathbf{C} = \mathbf{C}^\dagger$$

Again, consider the average values of these operators **A** and **B**, respectively, calculated on some ket $|\Psi\rangle$ that we shall suppose normalized:

$$\langle \mathbf{A} \rangle_\Psi = \langle \Psi | \mathbf{A} | \Psi \rangle \qquad \text{and} \qquad \langle \mathbf{B} \rangle_\Psi = \langle \Psi | \mathbf{B} | \Psi \rangle \quad \text{with} \quad \langle \Psi | \Psi \rangle = 1 \tag{2.30}$$

Next, consider the following transformed operators:

$$\tilde{\mathbf{A}} = \{ \mathbf{A} - \langle \mathbf{A} \rangle_\Psi \} \qquad \tilde{\mathbf{B}} = \{ \mathbf{B} - \langle \mathbf{B} \rangle_\Psi \} \tag{2.31}$$

with average values on $|\Psi\rangle$

$$\langle \tilde{\mathbf{A}} \rangle_\Psi = \langle \Psi | \tilde{\mathbf{A}} | \Psi \rangle \qquad \text{and} \qquad \langle \tilde{\mathbf{B}} \rangle_\Psi = \langle \Psi | \tilde{\mathbf{B}} | \Psi \rangle \tag{2.32}$$

Now, write explicitly the first of the average values (2.32), using the first equation of (2.31):

$$\langle \tilde{\mathbf{A}} \rangle_\Psi = \langle \Psi | \{ \mathbf{A} - \langle \mathbf{A} \rangle_\Psi \} | \Psi \rangle$$

That gives

$$\langle \tilde{\mathbf{A}} \rangle_\Psi = \langle \mathbf{A} \rangle_\Psi - \langle \mathbf{A} \rangle_\Psi \langle \Psi | \Psi \rangle = \{ \langle \mathbf{A} \rangle_\Psi - \langle \mathbf{A} \rangle_\Psi \} = 0 \tag{2.33}$$

where the normalization of $|\Psi\rangle$ has been used. In like manner one may find that $\langle \tilde{\mathbf{B}} \rangle_\Psi$ is zero. Hence, one may write

$$\langle \tilde{\mathbf{A}} \rangle_\Psi = 0 \qquad \text{and} \qquad \langle \tilde{\mathbf{B}} \rangle_\Psi = 0 \tag{2.34}$$

Now, consider the corresponding squares of the variances concerning the two operators (2.31), that is,

$$\Delta\tilde{\mathbf{A}}_\Psi^2 = \{\langle\tilde{\mathbf{A}}^2\rangle_\Psi - \langle\tilde{\mathbf{A}}\rangle_\Psi^2\} \qquad \text{and} \qquad \Delta\tilde{\mathbf{B}}_\Psi^2 = \{\langle\tilde{\mathbf{B}}^2\rangle_\Psi - \langle\tilde{\mathbf{B}}\rangle_\Psi^2\}$$

or, owing to Eq. (2.34)

$$\Delta\tilde{\mathbf{A}}_\Psi^2 = \langle\tilde{\mathbf{A}}^2\rangle_\Psi \qquad \text{and} \qquad \Delta\tilde{\mathbf{B}}_\Psi^2 = \langle\tilde{\mathbf{B}}^2\rangle_\Psi \tag{2.35}$$

Furthermore, the quantum averages over $|\Psi\rangle$ of the operators (2.31) are

$$\langle\tilde{\mathbf{A}}^2\rangle_\Psi = \langle\Psi|\tilde{\mathbf{A}}^2|\Psi\rangle \qquad \text{and} \qquad \langle\tilde{\mathbf{B}}^2\rangle_\Psi = \langle\Psi|\tilde{\mathbf{B}}^2|\Psi\rangle \tag{2.36}$$

Thus, Eq. (2.35) reads

$$\Delta\tilde{\mathbf{A}}_\Psi^2 = \langle\Psi|\tilde{\mathbf{A}}^2|\Psi\rangle \qquad \text{and} \qquad \Delta\tilde{\mathbf{B}}_\Psi^2 = \langle\Psi|\tilde{\mathbf{B}}^2|\Psi\rangle$$

Next, owing to the first equation of (2.31), the first equation of (2.36) transforms, after expanding the squared expression, into

$$\langle\tilde{\mathbf{A}}^2\rangle_\Psi = \langle\Psi|\{\mathbf{A}^2 + \langle\mathbf{A}\rangle_\Psi^2 - 2\mathbf{A}\langle\mathbf{A}\rangle_\Psi\}|\Psi\rangle$$

or

$$\langle\tilde{\mathbf{A}}^2\rangle_\Psi = \langle\Psi|\mathbf{A}^2|\Psi\rangle + \langle\Psi|\langle\mathbf{A}\rangle_\Psi^2|\Psi\rangle - 2\langle\Psi|\mathbf{A}|\Psi\rangle\langle\mathbf{A}\rangle_\Psi$$

Since $|\Psi\rangle$ is normalized and due to the first equation of (2.30), we then have

$$\langle\tilde{\mathbf{A}}^2\rangle_\Psi = \langle\mathbf{A}^2\rangle_\Psi + \langle\mathbf{A}\rangle_\Psi^2 - 2\langle\mathbf{A}\rangle_\Psi\langle\mathbf{A}\rangle_\Psi$$

or

$$\langle\tilde{\mathbf{A}}^2\rangle_\Psi = \langle\mathbf{A}^2\rangle_\Psi - \langle\mathbf{A}\rangle_\Psi^2 \tag{2.37}$$

Now, observe that the right-hand side of Eq. (2.37) is the dispersion of the operator $\mathbf{A}$ averaged on the ket $|\Psi\rangle$:

$$\langle\mathbf{A}^2\rangle_\Psi - \langle\mathbf{A}\rangle_\Psi^2 = \Delta\mathbf{A}_\Psi^2$$

Thus, Eq. (2.37) yields

$$\langle\tilde{\mathbf{A}}^2\rangle_\Psi = \Delta\mathbf{A}_\Psi^2$$

Thus, compare Eq. (2.35), and working in the same way for $\tilde{\mathbf{B}}$ as for $\tilde{\mathbf{A}}$, one obtains, respectively,

$$\boxed{\Delta\tilde{\mathbf{A}}_\Psi^2 = \Delta\mathbf{A}_\Psi^2 \qquad \text{and} \qquad \Delta\tilde{\mathbf{B}}_\Psi^2 = \Delta\mathbf{B}_\Psi^2} \tag{2.38}$$

which we shall use later on.

2.3.4.2 Product of variances of A and B and Heisenberg uncertainty relations

Now, consider the product of the variances of $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{B}}$, over $|\Psi\rangle$. In view of Eqs. (2.30) and (2.35), it is

$$\Delta\tilde{\mathbf{A}}_\Psi^2\Delta\tilde{\mathbf{B}}_\Psi^2 = \langle\Psi|\tilde{\mathbf{A}}^2|\Psi\rangle\langle\Psi|\tilde{\mathbf{B}}^2|\Psi\rangle$$

or

$$\Delta\tilde{\mathbf{A}}_\Psi^2 \Delta\tilde{\mathbf{B}}_\Psi^2 = (\langle\Psi|\tilde{\mathbf{A}})(\tilde{\mathbf{A}}|\Psi\rangle)(\langle\Psi|\tilde{\mathbf{B}})(\tilde{\mathbf{B}}|\Psi\rangle) \tag{2.39}$$

Next, observe that the linear action of the operators $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{B}}$ transforms, respectively, the ket $|\Psi\rangle$ into the new kets $|\Phi\rangle$ and $|\xi\rangle$ according to

$$\tilde{\mathbf{A}}|\Psi\rangle = |\Phi\rangle \qquad \text{and} \qquad \tilde{\mathbf{B}}|\Psi\rangle = |\xi\rangle \tag{2.40}$$

The Hermitian conjugates of these two linear transformations are

$$\langle\Psi|\tilde{\mathbf{A}} = \langle\Phi| \qquad \text{and} \qquad \langle\Psi|\tilde{\mathbf{B}} = \langle\xi| \tag{2.41}$$

Thus, Eq. (2.39) becomes

$$\Delta\tilde{\mathbf{A}}_\Psi^2 \Delta\tilde{\mathbf{B}}_\Psi^2 = \langle\Phi|\Phi\rangle\langle\xi|\xi\rangle \tag{2.42}$$

Now, observe that the Schwarz inequality (1.25) stipulates that

$$\langle\Phi|\Phi\rangle\langle\xi|\xi\rangle \geqslant \langle\xi|\Phi\rangle\langle\Phi|\xi\rangle$$

Hence, the product of uncertainties (2.42) transforms to the following inequality:

$$\Delta\tilde{\mathbf{A}}_\Psi^2 \Delta\tilde{\mathbf{B}}_\Psi^2 \geqslant \langle\xi|\Phi\rangle\langle\Phi|\xi\rangle \tag{2.43}$$

Again, in view of the linear transformations (2.40) and (2.41), the scalar products involved on the right-hand side of this last inequality are given by

$$\langle\Phi|\xi\rangle = \langle\Psi|\tilde{\mathbf{A}}\tilde{\mathbf{B}}|\Psi\rangle \qquad \text{and} \qquad \langle\xi|\Phi\rangle = \langle\Psi|\tilde{\mathbf{B}}\tilde{\mathbf{A}}|\Psi\rangle$$

Thus, the product of uncertainties (2.43) transforms to

$$\Delta\tilde{\mathbf{A}}_\Psi^2 \Delta\tilde{\mathbf{B}}_\Psi^2 \geqslant \langle\Psi|\tilde{\mathbf{A}}\tilde{\mathbf{B}}|\Psi\rangle\langle\Psi|\tilde{\mathbf{B}}\tilde{\mathbf{A}}|\Psi\rangle \tag{2.44}$$

Moreover, keeping in mind Eq. (1.60), and since neither $\tilde{\mathbf{A}}\tilde{\mathbf{B}}$ nor $\tilde{\mathbf{B}}\tilde{\mathbf{A}}$ are Hermitian, it is suitable to express these products in terms of symmetric and antisymmetric combinations according to

$$\tilde{\mathbf{A}}\tilde{\mathbf{B}} = \tfrac{1}{2}(\tilde{\mathbf{A}}\tilde{\mathbf{B}} + \tilde{\mathbf{B}}\tilde{\mathbf{A}}) + \tfrac{1}{2}(\tilde{\mathbf{A}}\tilde{\mathbf{B}} - \tilde{\mathbf{B}}\tilde{\mathbf{A}}) \tag{2.45}$$

Remark that the antisymmetric part is just the commutator of $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{B}}$:

$$(\tilde{\mathbf{A}}\tilde{\mathbf{B}} - \tilde{\mathbf{B}}\tilde{\mathbf{A}}) = [\tilde{\mathbf{A}}, \tilde{\mathbf{B}}]$$

Now, this commutator involving the transformed operators may be expressed in terms of the initial ones using Eq. (2.31), so that

$$[\tilde{\mathbf{A}}, \tilde{\mathbf{B}}] = [(\mathbf{A} - \langle\mathbf{A}\rangle_\Psi), (\mathbf{B} - \langle\mathbf{B}\rangle_\Psi)]$$

Then, since the average values involved in this last equation are scalars, the commutator of the transformed operators appears to be that of the nontransformed ones:

$$[\tilde{\mathbf{A}}, \tilde{\mathbf{B}}] = [\mathbf{A}, \mathbf{B}]$$

Thus, Eq. (2.45) transforms to

$$\tilde{\mathbf{A}}\tilde{\mathbf{B}} = \tfrac{1}{2}(\tilde{\mathbf{A}}\tilde{\mathbf{B}} + \tilde{\mathbf{B}}\tilde{\mathbf{A}}) + \tfrac{1}{2}[\mathbf{A}, \mathbf{B}]$$

Again, owing to the assumption (2.29) we have performed for the commutators of the initial operators $\mathbf{A}$ and $\mathbf{B}$, this last equation leads to

$$\tilde{\mathbf{A}}\tilde{\mathbf{B}} = \tfrac{1}{2}\{\tilde{\mathbf{A}}\tilde{\mathbf{B}} + \tilde{\mathbf{B}}\tilde{\mathbf{A}} + i\mathbf{C}\} \tag{2.46}$$

Now, consider $\tilde{\mathbf{B}}\tilde{\mathbf{A}}$, which reads

$$(\tilde{\mathbf{B}}\tilde{\mathbf{A}} - \tilde{\mathbf{A}}\tilde{\mathbf{B}}) = [\tilde{\mathbf{B}}, \tilde{\mathbf{A}}] = -[\mathbf{A}, \mathbf{B}]$$

Then, due to Eq. (2.29), we have

$$\tilde{\mathbf{B}}\tilde{\mathbf{A}} = \tfrac{1}{2}\{\tilde{\mathbf{A}}\tilde{\mathbf{B}} + \tilde{\mathbf{B}}\tilde{\mathbf{A}} - i\mathbf{C}\} \tag{2.47}$$

As a consequence of Eqs. (2.46) and (2.47), Eq. (2.44) becomes

$$\Delta\tilde{\mathbf{A}}_\Psi^2 \Delta\tilde{\mathbf{B}}_\Psi^2 \geqslant \tfrac{1}{4}\langle\Psi|\{\tilde{\mathbf{A}}\tilde{\mathbf{B}} + \tilde{\mathbf{B}}\tilde{\mathbf{A}} + i\mathbf{C}\}|\Psi\rangle\langle\Psi|\{\tilde{\mathbf{A}}\tilde{\mathbf{B}} + \tilde{\mathbf{B}}\tilde{\mathbf{A}} - i\mathbf{C}\}|\Psi\rangle$$

Thus

$$\Delta\tilde{\mathbf{A}}_\Psi^2 \Delta\tilde{\mathbf{B}}_\Psi^2 \geqslant \tfrac{1}{4}(\langle\Psi|(\tilde{\mathbf{A}}\tilde{\mathbf{B}} + \tilde{\mathbf{B}}\tilde{\mathbf{A}})|\Psi\rangle + i\langle\Psi|\mathbf{C}|\Psi\rangle)(\langle\Psi|(\tilde{\mathbf{A}}\tilde{\mathbf{B}} + \tilde{\mathbf{B}}\tilde{\mathbf{A}})|\Psi\rangle - i\langle\Psi|\mathbf{C}|\Psi\rangle)$$

or

$$\Delta\tilde{\mathbf{A}}_\Psi^2 \Delta\tilde{\mathbf{B}}_\Psi^2 \geqslant \tfrac{1}{4}\{\langle\Psi|(\tilde{\mathbf{A}}\tilde{\mathbf{B}} + \tilde{\mathbf{B}}\tilde{\mathbf{A}})|\Psi\rangle^2 + \langle\Psi|\mathbf{C}|\Psi\rangle^2\} \tag{2.48}$$

Now, as it appears by inspection of this last inequality, each member of the right-hand-side, however small it may be, cannot be negative since it is a squared average value. Moreover, the inequality is also satisfied when one substracts from the smallest right-hand-side term, its first squared term involving the products $\tilde{\mathbf{A}}\tilde{\mathbf{B}}$ and $\tilde{\mathbf{B}}\tilde{\mathbf{A}}$. Hence, if the inequality (2.48) is satisfied, the following one will be a fortiori satisfied:

$$\Delta\tilde{\mathbf{A}}_\Psi^2 \Delta\tilde{\mathbf{B}}_\Psi^2 \geqslant \tfrac{1}{4}\langle\Psi|\mathbf{C}|\Psi\rangle^2$$

Hence, owing to Eq. (2.38), it appears that the same inequality for the dispersions dealing with the initial operators $\mathbf{A}$ and $\mathbf{B}$ exists, so that it reads

$$\Delta\mathbf{A}_\Psi^2 \Delta\mathbf{B}_\Psi^2 \geqslant \tfrac{1}{4}\langle\Psi|\mathbf{C}|\Psi\rangle^2$$

or, in view of Eq. (2.29)

$$\boxed{\Delta\mathbf{A}_\Psi^2 \Delta\mathbf{B}_\Psi^2 \geqslant -i\tfrac{1}{4}\langle\Psi|[\mathbf{A}, \mathbf{B}]|\Psi\rangle^2} \tag{2.49}$$

Now, apply the inequality (2.49) to the coordinate operator $\mathbf{Q}$ and its conjugate momentum $\mathbf{P}$. Then take

$$\mathbf{A} = \mathbf{Q} \qquad \mathbf{B} = \mathbf{P} \quad \text{and} \quad [\mathbf{A}, \mathbf{B}] = [\mathbf{Q}, \mathbf{P}] = i\hbar$$

Besides, due to Eq. (2.29), that is,

$$i\mathbf{C} = [\mathbf{Q}, \mathbf{P}] = i\hbar$$

Then, the inequality (2.49) takes the form

$$\Delta\mathbf{P}_\Psi^2 \Delta\mathbf{Q}_\Psi^2 \geqslant \frac{1}{4}\langle\Psi|\hbar|\Psi\rangle^2 = \left(\frac{\hbar}{2}\right)^2$$

so that the product of variances of the coordinate $\mathbf{Q}$ and its conjugate momentum $\mathbf{P}$ appears, whatever the ket $|\Psi\rangle$ describing the system

$$\boxed{\Delta\mathbf{P}_\Psi \Delta\mathbf{Q}_\Psi \geqslant \frac{\hbar}{2}} \tag{2.50}$$

That is the Heisenberg uncertainty relation. Of course, this relation holds for the three Cartesian coordinates of some particle, so that

$$\boxed{(\Delta P_x)_\Psi (\Delta Q_x)_\Psi \geqslant \frac{\hbar}{2}}$$

$$\boxed{(\Delta P_y)_\Psi (\Delta Q_y)_\Psi \geqslant \frac{\hbar}{2}}$$

$$\boxed{(\Delta P_z)_\Psi (\Delta Q_z)_\Psi \geqslant \frac{\hbar}{2}}$$

An important consequence of these uncertainty relations is that the *trajectory*, which is fundamental in classical mechanics, has no meaning in quantum mechanics. The reason is that, to define the trajectory of some particle, it is necessary to know exactly both its position and momentum at all times. This impossibility of a precise trajectory indicates that two particles of the same kind, such as, for instance, two electrons, or two protons, or two hydrogen atoms, are *indistinguishable* because the only possibility to distinguish them would be their individual trajectories, which is impossible because of the uncertainty relations.

2.4 SCHRÖDINGER PICTURE DYNAMICS

Now, we shall consider some dynamic behaviors appearing in quantum mechanics as a consequence of the Schrödinger equation appearing in the sixth postulate. Recall that according to this equation, the kets and the corresponding bras are time dependent, whereas the operators are constant. Such a time description in which kets and bras are time dependent whereas the operators are constant is called the *Schrödinger picture* (SP) in order to differentiate it from another description named *Heisenberg picture* (HP) in which the operators are changing with time whereas the kets and bras remain constant.

We shall first show that the Schrödinger equation preserves the conservation of the norm that is required from the physical viewpoint. Then, we shall demonstrate some fundamental dynamic equations, and, finally, two theorems, one of which is the Ehrenfest theorem, which resembles the basic Newtonian equations of classical mechanics, the only difference being that the Ehrenfest theorem governs average values instead of exact ones.

2.4.1 Norm conservation and average values time dependence

2.4.1.1 Norm conservation

Consider the Schrödinger equation

$$i\hbar\left(\frac{\partial|\Psi(t)\rangle}{\partial t}\right)=\mathbf{H}|\Psi(t)\rangle \tag{2.51}$$

where $\mathbf{H}$ is the Hamiltonian operator, which is, of course, Hermitian. If it is normalized, the norm of the ket$|\Psi(t^\circ)\rangle$ at time t° is

$$\langle\Psi(t^\circ)|\Psi(t^\circ)\rangle=1$$

Of course, if the norm has to be conserved, it must be given at any time $t\neq t^\circ$ by

$$\langle\Psi(t)|\Psi(t)\rangle=1$$

We shall show that this last equation is in agreement with the Schrödinger equation. For this purpose, we write explicitly the time derivative of the norm

$$\left(\frac{\partial\langle\Psi(t)|\Psi(t)\rangle}{\partial t}\right)=\left(\frac{\partial\langle\Psi(t)|}{\partial t}\right)|\Psi(t)\rangle+\langle\Psi(t)|\left(\frac{\partial|\Psi(t)\rangle}{\partial t}\right) \tag{2.52}$$

To calculate the time derivative of the bra involved on the first right-hand-side term of this last equation, we consider the Hermitian conjugate of Eq. (2.51)

$$-i\hbar\left(\frac{\partial\langle\Psi(t)|}{\partial t}\right)=\langle\Psi(t)|\mathbf{H}^\dagger$$

Then, since the Hamiltonian is Hermitian, that is, $\mathbf{H}^\dagger=\mathbf{H}$, this last equation becomes

$$-i\hbar\left(\frac{\partial\langle\Psi(t)|}{\partial t}\right)=\langle\Psi(t)|\mathbf{H} \tag{2.53}$$

As a consequence of Eqs. (2.51) and (2.53), the time derivative of the norm (2.52) becomes

$$\left(\frac{\partial\langle\Psi(t)|\Psi(t)\rangle}{\partial t}\right)=-\frac{1}{i\hbar}\langle\Psi(t)|\mathbf{H}|\Psi(t)\rangle+\frac{1}{i\hbar}\langle\Psi(t)|\mathbf{H}|\Psi(t)\rangle$$

This last result simplifies to

$$\boxed{\left(\frac{\partial\langle\Psi(t)|\Psi(t)\rangle}{\partial t}\right)=0}$$

showing, as required, that the norm is conserved along the time.

2.4.2 Time evolution of operator average value

2.4.2.1 General expression

We shall now consider how the average value of some operator $\mathbf{A}$ calculated over any ket $|\Psi(t)\rangle$ evolves, which is time dependent because of the Schrödinger equation.

In the Schrödinger time-dependent picture, any operator $\mathbf{A}$ does not depend on time so that the time derivative of the average value of $\mathbf{A}$ over $|\Psi(t)\rangle$ is

$$\left(\frac{\partial\langle\Psi(t)|\mathbf{A}|\Psi(t)\rangle}{\partial t}\right)=\left(\frac{\partial\langle\Psi(t)|}{\partial t}\right)\mathbf{A}|\Psi(t)\rangle+\langle\Psi(t)|\mathbf{A}\left(\frac{\partial|\Psi(t)\rangle}{\partial t}\right) \tag{2.54}$$

Using Eqs. (2.51) and (2.53), this equation transforms to

$$\left(\frac{\partial\langle\Psi(t)|\mathbf{A}|\Psi(t)\rangle}{\partial t}\right) = -\frac{1}{i\hbar}\langle\Psi(t)|\mathbf{H}\mathbf{A}|\Psi(t)\rangle + \frac{1}{i\hbar}\langle\Psi(t)|\mathbf{A}\mathbf{H}|\Psi(t)\rangle$$

or, in term of the commutator of $\mathbf{H}$ and $\mathbf{A}$

$$\left(\frac{\partial\langle\Psi(t)|\mathbf{A}|\Psi(t)\rangle}{\partial t}\right) = \frac{i}{\hbar}\langle\Psi(t)|[\mathbf{H},\mathbf{A}]|\Psi(t)\rangle \tag{2.55}$$

which may be written in the compact form

$$\boxed{\left(\frac{\partial\langle\mathbf{A}(t)\rangle_\Psi}{\partial t}\right) = \frac{i}{\hbar}\langle[\mathbf{H},\mathbf{A}]\rangle_\Psi} \tag{2.56}$$

with

$$\langle\mathbf{A}(t)\rangle_\Psi \equiv \langle\Psi(t)|\mathbf{A}|\Psi(t)\rangle \qquad \langle[\mathbf{H},\mathbf{A}]\rangle_\Psi = \langle\Psi(t)|[\mathbf{H},\mathbf{A}]|\Psi(t)\rangle \tag{2.57}$$

We remark that the notation $\langle\mathbf{A}(t)\rangle_\Psi$ does not imply that $\mathbf{A}$ depends on time but only means that the average value $\langle\mathbf{A}(t)\rangle_\Psi$ of $\mathbf{A}$ depends on time. Besides, observe that, in the Schrödinger time-dependent picture, some physical systems that have to be studied may appear quantum mechanically for one part and classically for another one. In such systems, which are said to be *hemiquantal*, there is then the possibility for any operator $\mathbf{A}$ to present a time dependence through its classical part. Then, Eq. (2.55) has to be generalized into

$$\left(\frac{\partial\langle\Psi(t)|\mathbf{A}(t)|\Psi(t)\rangle}{\partial t}\right) = \frac{i}{\hbar}\langle\Psi(t)|[\mathbf{H},\mathbf{A}(t)]|\Psi(t)\rangle + \langle\Psi(t)|\left(\frac{\partial\mathbf{A}(t)}{\partial t}\right)|\Psi(t)\rangle \tag{2.58}$$

2.4.2.2 Conservation of the total energy and exchange of energies In the special situation where the operator is the Hamiltonian, and what may be the ket $|\Psi(t)\rangle$ describing the system, Eq. (2.56) reads

$$\left(\frac{\partial\langle\mathbf{H}\rangle_\Psi}{\partial t}\right) = \frac{i}{\hbar}\langle[\mathbf{H},\mathbf{H}]\rangle_\Psi = 0 \tag{2.59}$$

Hence, the average value of the total Hamiltonian, that is, the total energy, remains constant whichever ket $|\Psi(t)\rangle$ describes the system.

However, if the total energy is conserved, it is not true for the energies of subsystems from which any physical system is built up. Suppose, for instance, that the total Hamiltonian is the sum of two Hamiltonians, which do not mutually commute:

$$\mathbf{H} = \mathbf{H}_1 + \mathbf{H}_2 \quad \text{with} \quad [\mathbf{H}_1,\mathbf{H}_2] \neq 0$$

Then, the commutators of $\mathbf{H}_1$ and $\mathbf{H}_2$ with $\mathbf{H}$ are

$$[\mathbf{H}_1,\mathbf{H}] = [\mathbf{H}_1,\mathbf{H}_2] \qquad \text{and} \qquad [\mathbf{H}_2,\mathbf{H}] = [\mathbf{H}_2,\mathbf{H}_1] = -[\mathbf{H}_1,\mathbf{H}_2] \tag{2.60}$$

Thus, due to Eqs. (2.56) and (2.60), the time dependences of the averages of the Hamiltonians of the two subsystems obey

$$\left(\frac{\partial\langle\mathbf{H}_1(t)\rangle_\Psi}{\partial t}\right) = \frac{i}{\hbar}\langle[\mathbf{H}_2,\mathbf{H}_1]\rangle_\Psi \tag{2.61}$$

$$\left(\frac{\partial\langle\mathbf{H}_2(t)\rangle_\Psi}{\partial t}\right) = -\frac{i}{\hbar}\langle[\mathbf{H}_2,\mathbf{H}_1]\rangle_\Psi \tag{2.62}$$

We emphasize that in these last equations, they are the average values of $\mathbf{H}_1$ and $\mathbf{H}_2$, which depend on time through $\Psi(t)$, although the operators $\mathbf{H}_1$ and $\mathbf{H}_2$ do not depend on time. Equations (2.61) and (2.62) show that the energy moves back and forth between the two subsystems according to

$$\left(\frac{\partial\langle\mathbf{H}_1(t)\rangle_\Psi}{\partial t}\right) = -\left(\frac{\partial\langle\mathbf{H}_2(t)\rangle_\Psi}{\partial t}\right)$$

in such a way as their sum remains constant according to Eq. (2.59). Of course, if one considers, respectively, in place of $\mathbf{H}_1$ and $\mathbf{H}_2$ the kinetic and potential energies, $\mathbf{T}$ and $\mathbf{V}$ of the system, the Eqs. (2.61) and (2.62) become

$$\left(\frac{\partial\langle\mathbf{T}(t)\rangle_\Psi}{\partial t}\right) = \frac{i}{\hbar}\langle[\mathbf{V},\mathbf{T}]\rangle_\Psi$$

$$\left(\frac{\partial\langle\mathbf{V}(t)\rangle_\Psi}{\partial t}\right) = -\frac{i}{\hbar}\langle[\mathbf{V},\mathbf{T}]\rangle_\Psi$$

so that the kinetic and potential energies exchange themselves with time according to

$$\left(\frac{\partial\langle\mathbf{T}(t)\rangle_\Psi}{\partial t}\right) = -\left(\frac{\partial\langle\mathbf{V}(t)\rangle_\Psi}{\partial t}\right)$$

2.4.2.3 Stationary states By definition, a stationary state is an eigenstate of the Hamiltonian, that is, it obeys the eigenvalue equation

$$\mathbf{H}|\Psi_k(t)\rangle = E_k|\Psi_k(t)\rangle$$

The time-dependent Schrödinger equation is

$$i\hbar\left(\frac{\partial|\Psi_k(t)\rangle}{\partial t}\right) = \mathbf{H}|\Psi_k(t)\rangle$$

For a stationary state, it reads

$$i\hbar\left(\frac{\partial|\Psi_k(t)\rangle}{\partial t}\right) = E_k|\Psi_k(t)\rangle$$

so that, by integration

$$|\Psi_k(t)\rangle = |\Psi_k(0)\rangle e^{-iE_kt/\hbar} \tag{2.63}$$

Now, consider the average value of any operator over a stationary state. At an initial time it is

$$\langle\mathbf{A}(0)\rangle_{\Psi_k} = \langle\Psi_k(0)|\mathbf{A}|\Psi_k(0)\rangle \tag{2.64}$$

At time t, it is given by

$$\langle\mathbf{A}(t)\rangle_{\Psi_k} = \langle\Psi_k(t)|\mathbf{A}|\Psi_k(t)\rangle \tag{2.65}$$

Then, owing to Eq. (2.63) and to its Hermitian conjugate, one has

$$\langle\mathbf{A}(t)\rangle_{\Psi_k} = e^{iE_kt/\hbar}\langle\Psi_k(0)|\mathbf{A}|\Psi_k(0)\rangle e^{-iE_kt/\hbar}$$

and, thus, after simplification

$$\langle \mathbf{A}(t) \rangle_{\Psi_k} = \langle \Psi_k(0) | \mathbf{A} | \Psi_k(0) \rangle \tag{2.66}$$

Comparison of Eqs. (2.64) and (2.66) shows that

$$\left(\frac{\partial \langle \mathbf{A}(t) \rangle_{\Psi_k}}{\partial t} \right) = 0 \quad \text{for any stationary state} \tag{2.67}$$

2.4.3 Ehrenfest equations

Now, we are able to demonstrate the Ehrenfest equations governing the dynamics of the operators $\mathbf{Q}$ and $\mathbf{P}$. Applying Eq. (2.56), one obtains, respectively,

$$\left(\frac{\partial \langle \mathbf{Q}(t) \rangle_{\Psi_k}}{\partial t} \right) = \frac{i}{\hbar} \langle [\mathbf{H}, \mathbf{Q}] \rangle_{\Psi_k} \tag{2.68}$$

$$\left(\frac{\partial \langle \mathbf{P}(t) \rangle_{\Psi_k}}{\partial t} \right) = \frac{i}{\hbar} \langle [\mathbf{H}, \mathbf{P}] \rangle_{\Psi_k} \tag{2.69}$$

When the system involves only forces that are the derivative of a potential, the Hamiltonian $\mathbf{H}(\mathbf{P}, \mathbf{Q})$ is as above the sum of the kinetic $\mathbf{T}(\mathbf{P})$ and potential $\mathbf{V}(\mathbf{Q})$ operators, the first one depending on $\mathbf{P}$ and the last one on $\mathbf{Q}$:

$$\mathbf{H}(\mathbf{P}, \mathbf{Q}) = \mathbf{T}(\mathbf{P}) + \mathbf{V}(\mathbf{Q})$$

For a single particle, the kinetic operator is simply

$$\mathbf{T}(\mathbf{P}) = \frac{\mathbf{P}^2}{2m}$$

Of course, the commutators of the kinetic momentum operators and that of the potential and coordinate operators, are, respectively, zero, that is

$$[\mathbf{T}(\mathbf{P}), \mathbf{P}] = [\mathbf{V}(\mathbf{Q}), \mathbf{Q}] = 0$$

Thus, the commutators of the Hamiltonian with the coordinate and momentum operators are, respectively,

$$[\mathbf{H}, \mathbf{Q}] = \frac{1}{2m} [\mathbf{P}^2, \mathbf{Q}] \tag{2.70}$$

$$[\mathbf{H}, \mathbf{P}] = [\mathbf{V}(\mathbf{Q}), \mathbf{P}] \tag{2.71}$$

Besides, owing to Eqs. (2.14) and (2.15), the commutators appearing on the right-hand sides of these two last equations are, respectively,

$$[\mathbf{P}^2, \mathbf{Q}] = -2i\hbar \mathbf{P}$$

$$[\mathbf{V}(\mathbf{Q}), \mathbf{P}] = i\hbar \left(\frac{\partial \mathbf{V}}{\partial \mathbf{Q}} \right)$$

Then, using for the two commutators (2.70) and (2.71), these two last equations, and introducing them into Eqs. (2.68) and (2.69), one obtains the final results, which

are known as the *Ehrenfest equations*, and which hold whatever the ket $|\Psi_k(t)\rangle$ considered for the calculation:

$$\boxed{\langle \mathbf{P}(t)\rangle_{\Psi_k} = m\left(\frac{d\langle \mathbf{Q}(t)\rangle_{\Psi_k}}{dt}\right)} \tag{2.72}$$

$$\boxed{\frac{\partial}{\partial t}\langle \mathbf{P}(t)\rangle_{\Psi_k} = -\left\langle\left(\frac{\partial \mathbf{V}}{\partial \mathbf{Q}}\right)\right\rangle_{\Psi_k}} \tag{2.73}$$

Thus, the first Ehrenfest equation looks like the Newton equation defining the momentum in terms of the velocity, whereas the second one looks like that relating the time derivative of the momentum (i.e., the acceleration) to the gradient of the potential (i.e., the force). However, the ket $|\Psi_k(t)\rangle$ considered for the calculation can never be simultaneously an eigenket of $\mathbf{P}$ and $\mathbf{Q}$ because

$$[\mathbf{Q}, \mathbf{P}] = i\hbar$$

thus, the uncertainty relations must be retained so that the Ehrenfest equations [(2.72) and (2.73)] have always to be considered mindful of the Heisenberg uncertainty relation:

$$\boxed{(\Delta \mathbf{P})_{\Psi_k}(\Delta \mathbf{Q})_{\Psi_k} \geqslant \frac{\hbar}{2}}$$

2.4.4 Virial theorem

2.4.4.1 Demonstration of the virial theorem Now, we shall prove the virial theorem, which relates the average values of the kinetic and potential operators, when the averages are performed over stationary states $|\Psi_k\rangle$, that is, eigenstates of the Hamiltonian $\mathbf{H}$ obeying the eigenvalue equation

$$\mathbf{H}|\Psi_k\rangle = E_k|\Psi_k\rangle \tag{2.74}$$

Apply Eq. (2.56) to the product $\mathbf{QP}$ of the coordinate and momentum operators $\mathbf{Q}$ and $\mathbf{P}$. Hence

$$i\hbar\left(\frac{\partial\langle \mathbf{QP}\rangle_{\Psi_k}}{\partial t}\right) = \langle[\mathbf{QP}, \mathbf{H}]\rangle_{\Psi_k} \tag{2.75}$$

The Hamiltonian $\mathbf{H}$ may be written, as above, as the sum of the kinetic $\mathbf{T}$ and potential $\mathbf{V}$ operators, the first only a function of $\mathbf{P}$ and the latter of $\mathbf{Q}$.

$$\mathbf{H} = \mathbf{T}(\mathbf{P}) + \mathbf{V}(\mathbf{Q})$$

Of course, as above, the following commutators are zero:

$$[\mathbf{T}(\mathbf{P}), \mathbf{P}] = [\mathbf{V}(\mathbf{Q}), \mathbf{Q}] = 0 \tag{2.76}$$

Thus, the commutator appearing on the right-hand side of Eq. (2.75) reads

$$[\mathbf{QP}, \mathbf{H}] = [\mathbf{QP}, \mathbf{T}(\mathbf{P})] + [\mathbf{QP}, \mathbf{V}(\mathbf{Q})] \tag{2.77}$$

For a single particle, the kinetic operator is

$$\mathbf{T}(\mathbf{P}) = \frac{1}{2m}\mathbf{P}^2 \tag{2.78}$$

Hence, the first commutator appearing on the right-hand side of Eq. (2.77) is

$$[\mathbf{QP}, \mathbf{T}(\mathbf{P})] = \frac{1}{2m}[\mathbf{QP}, \mathbf{P}^2] \tag{2.79}$$

The commutator appearing on the right member of this last equation may be written

$$[\mathbf{QP}, \mathbf{P}^2] = (\mathbf{QP}^2 - \mathbf{P^2Q})\mathbf{P}$$

or

$$[\mathbf{QP}, \mathbf{P}^2] = [\mathbf{Q}, \mathbf{P}^2]\mathbf{P}$$

Thus, in view of Eq. (2.13), it transforms to

$$[\mathbf{QP}, \mathbf{P}^2] = (i\hbar)2\mathbf{P}^2$$

Hence, the commutator (2.79) becomes

$$[\mathbf{QP}, \mathbf{T}(\mathbf{P})] = i\hbar\frac{\mathbf{P}^2}{m} \tag{2.80}$$

Now, consider the second commutator appearing on the right-hand side of Eq. (2.77):

$$[\mathbf{QP}, \mathbf{V}(\mathbf{Q})] = \mathbf{QPV}(\mathbf{Q}) - \mathbf{V}(\mathbf{Q})\mathbf{QP}$$

which, since $\mathbf{Q}$ commutes with $\mathbf{V}(\mathbf{Q})$, transforms to

$$[\mathbf{QP}, \mathbf{V}(\mathbf{Q})] = \mathbf{QPV}(\mathbf{Q}) - \mathbf{QV}(\mathbf{Q})\mathbf{P}$$

so that Eq. (2.76) reads

$$[\mathbf{QP}, \mathbf{V}(\mathbf{Q})] = \mathbf{Q}[\mathbf{P}, \mathbf{V}(\mathbf{Q})]$$

Then, using Eq. (2.15), we have

$$[\mathbf{QP}, \mathbf{V}(\mathbf{Q})] = -(i\hbar)\mathbf{Q}\left(\frac{\partial \mathbf{V}}{\partial \mathbf{Q}}\right) \tag{2.81}$$

Now, using Eqs. (2.80) and (2.81) the commutator (2.77) appears to be given by

$$[\mathbf{QP}, \mathbf{H}] = (i\hbar)\left\{\frac{1}{m}\mathbf{P}^2 - \mathbf{Q}\left(\frac{\partial \mathbf{V}}{\partial \mathbf{Q}}\right)\right\}$$

Moreover, after averaging over $|\Psi_k\rangle$ one obtains

$$\langle[\mathbf{QP}, \mathbf{H}]\rangle_{\Psi_k} = (i\hbar)\left\{\frac{1}{m}\langle\mathbf{P}^2\rangle_{\Psi_k} - \left\langle\mathbf{Q}\left(\frac{\partial \mathbf{V}}{\partial \mathbf{Q}}\right)\right\rangle_{\Psi_k}\right\}$$

Finally, using this result into Eq. (2.75), we have

$$\left(\frac{\partial\langle\mathbf{Q}\,\mathbf{P}\rangle_{\Psi_k}}{\partial t}\right) = 2\left\langle\frac{\mathbf{P}^2}{2m}\right\rangle_{\Psi_k} - \left\langle\mathbf{Q}\left(\frac{\partial \mathbf{V}}{\partial \mathbf{Q}}\right)\right\rangle_{\Psi_k} \tag{2.82}$$

When the ket, over which the average value is performed, is stationary, Eq. (2.67) holds, so that the time dependence of the average value of the correlation between **Q** and **P** is zero:

$$\left(\frac{\partial\langle \mathbf{Q}\,\mathbf{P}\rangle_{\Psi_k}}{\partial t}\right) = 0$$

Hence, for stationary situations, Eq. (2.82) simplifies to

$$2\left\langle\frac{\mathbf{P}^2}{2m}\right\rangle_{\Psi_k} = \left\langle \mathbf{Q}\left(\frac{\partial \mathbf{V}}{\partial \mathbf{Q}}\right)\right\rangle_{\Psi_k} \tag{2.83}$$

Observe that the gradient of the potential may be written as a force **F** according to

$$\left(\frac{\partial \mathbf{V}}{\partial \mathbf{Q}}\right) = -\mathbf{F}$$

so that, Eq. (2.83) yields

$$2\left\langle\frac{\mathbf{P}^2}{2m}\right\rangle_{\Psi_k} = -\langle \mathbf{Q}\,\mathbf{F}\rangle_{\Psi_k} \tag{2.84}$$

This equation may be generalized for many degrees of freedom j. We have

$$2\sum_{j=1}^{N}\left\langle\frac{\mathbf{P}_j^2}{2m}\right\rangle_{\Psi_k} = -\sum_{j=1}^{N}\langle \mathbf{Q}_j\,\mathbf{F}_j\rangle_{\Psi_k}$$

2.4.4.2 Applications of the virial theorem

2.4.4.2.1 Systems involving harmonic potential Now, apply Eq. (2.83) to a quantum harmonic oscillator where the potential obeys

$$\mathbf{V}(\mathbf{Q}) = \tfrac{1}{2}k\mathbf{Q}^2 \tag{2.85}$$

where k is the force constant of the potential, which is a scalar. Then, deriving Eq. (2.85) leads to

$$\left(\frac{\partial \mathbf{V}}{\partial \mathbf{Q}}\right) = k\mathbf{Q}$$

Besides, multiplying both terms by **Q** gives

$$\mathbf{Q}\left(\frac{\partial \mathbf{V}}{\partial \mathbf{Q}}\right) = k\mathbf{Q}^2$$

Again, averaging over the ket $|\Psi_k\rangle$ and in view of Eq. (2.85),

$$\left\langle \mathbf{Q}\left(\frac{\partial \mathbf{V}}{\partial \mathbf{Q}}\right)\right\rangle_{\Psi_k} = 2\langle \mathbf{V}(\mathbf{Q})\rangle_{\Psi_k} \tag{2.86}$$

At last, owing to Eqs. (2.78) and (2.83), Eq. (2.86) yields

$$\langle \mathbf{T}\rangle_{\Psi_k} = \langle \mathbf{V}(\mathbf{Q})\rangle_{\Psi_k}$$

On the other hand, the average value of the Hamiltonian is the sum of the kinetic and potential operators, that is,

$$\langle \mathbf{H} \rangle_{\Psi_k} = \langle \mathbf{T} \rangle_{\Psi_k} + \langle \mathbf{V}(\mathbf{Q}) \rangle_{\Psi_k} \tag{2.87}$$

However, since the average value of the Hamiltonian is performed over one of its eigenstates obeying Eq. (2.74), this is just the corresponding eigenvalue E_k so that Eq. (2.87) gives

$$E_k = \langle \mathbf{T} \rangle_{\Psi_k} + \langle \mathbf{V}(\mathbf{Q}) \rangle_{\Psi_k} \tag{2.88}$$

Hence, one may determine the average value of the kinetic and potential operators from the value of the corresponding energy levels via

$$\langle \mathbf{T} \rangle_{\Psi_k} = \frac{E_k}{2} = \langle \mathbf{V}(\mathbf{Q}) \rangle_{\Psi_k} \tag{2.89}$$

2.4.4.2.2 Systems involving Coulomb potential Now consider, as a second example, a Coulomb potential involving two electrical charges q and q' obeying

$$\mathbf{V}(\mathbf{Q}) = -K\frac{1}{\mathbf{Q}} \quad \text{with} \quad K = \frac{qq'}{4\pi\varepsilon^{\circ}} \tag{2.90}$$

where ε° is the vacuum permittivity, which is a scalar. Then, after deriving $\mathbf{V}$ with respect to $\mathbf{Q}$ and rearranging, it reads

$$\mathbf{Q}\left(\frac{\partial \mathbf{V}}{\partial \mathbf{Q}}\right) = K\frac{1}{\mathbf{Q}}$$

Furthermore, the quantum average over $|\Psi_k\rangle$ leads, by aid of Eq. (2.90), to

$$\left\langle \mathbf{Q}\left(\frac{\partial \mathbf{V}}{\partial \mathbf{Q}}\right) \right\rangle_{\Psi_k} = -\langle \mathbf{V}(\mathbf{Q}) \rangle_{\Psi_k}$$

Now, with Eq. (2.78), the virial theorem (2.83), takes the form

$$2\langle \mathbf{T} \rangle_{\Psi_k} = -\langle \mathbf{V}(\mathbf{Q}) \rangle_{\Psi_k}$$

Of course, since Eqs. (2.87) and (2.88) continue to apply, one may obtain from the expression for the energy levels the corresponding average values of the potential and kinetic operators by aid of

$$\langle \mathbf{V}(\mathbf{Q}) \rangle_{\Psi_k} = 2E_k \qquad \text{and} \qquad \langle \mathbf{T} \rangle_{\Psi_k} = -E_k$$

2.5 POSITION OR MOMENTUM TRANSLATION OPERATORS

2.5.1 Eigenvalue equations of the position and momentum operators

Consider the eigenvalue equation of the coordinate operator $\mathbf{Q}$:

$$\mathbf{Q}|\{Q\}\rangle = Q|\{Q\}\rangle \tag{2.91}$$

The meaning of this eigenvalue equation is that when a system is in an eigenket $|\{Q\}\rangle$[1] of the coordinate operator $\mathbf{Q}$, the measurement of its position is given by the corresponding eigenvalue Q. Of course, since the $\mathbf{Q}$ operator is Hermitian, the Hermitian conjugate of Eq. (2.91) is

$$\langle\{Q\}|\mathbf{Q} = \langle\{Q\}|Q$$

Now, observe that the possible measurements of the Q coordinate are continuous. Thus, the orthormality properties of the $\mathbf{Q}$ operator involving two different kets $|\{Q\}\rangle$ and $|\{Q'\}\rangle$ must be written according to this continuous property. Hence

$$\langle\{Q\}|\{Q'\}\rangle = \delta(Q - Q') \tag{2.92}$$

Furthermore, the eigenvectors of the Hermitian operator $\mathbf{Q}$ form a basis that must be continuous, owing to this continuity of Q. Thus, the usual closure relation (1.17) built up on the eigenvectors, must be replaced by a new one where an infinite integral takes the place of the sum over the eigenkets. That leads to

$$\int_{-\infty}^{+\infty} |\{Q\}\rangle\langle\{Q\}|\, dQ = \mathbf{1}$$

In a similar way, we may write the eigenvalue equation of the momentum operator $\mathbf{P}$ and its Hermitian conjugate

$$\mathbf{P}|\{P\}\rangle = P|\{P\}\rangle \qquad \text{and} \qquad \langle\{P\}|\mathbf{P} = \langle\{P\}|P \tag{2.93}$$

Here, $|\{P\}\rangle$[2] is an eigenket of the momentum operator $\mathbf{P}$ with the eigenvalue P. Besides, owing to the continuity of the eigenvalues of the operator $\mathbf{P}$, that is, of its possible measured values, the orthonormality of the eigenkets of $\mathbf{P}$ and the closure relation are similar to those dealing with $\mathbf{Q}$, that is,

$$\langle\{P\}|\{P'\}\rangle = \delta(P - P') \qquad \text{and} \qquad \int_{-\infty}^{+\infty} |\{P\}\rangle\langle\{P\}|\, dP = \mathbf{1} \tag{2.94}$$

In the following, we shall show that the scalar product of any eigenket of the position operator $\mathbf{Q}$ by some eigenket of its momentum conjugate $\mathbf{P}$ is the same irrespective of the corresponding eigenvalues Q and P:

$$\boxed{\langle\{P\}|\{Q\}\rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left\{-\frac{iPQ}{\hbar}\right\}}$$

which is consistent with the Heisenberg uncertainty relation

$$(\Delta P)_\Psi (\Delta Q)_\Psi \geqslant \frac{\hbar}{2}$$

[1]We shall use for the eigenkets of $\mathbf{Q}$, the notation $|\{Q\}\rangle$ in place of the usual one $|Q\rangle$ in order to make clearer some equations (see later).

[2]In a similar way we shall use for the eigenkets of $\mathbf{P}$, the notation $|\{P\}\rangle$ in place of the usual one $|P\rangle$ in order to make clearer some equations (see later).

and with the basic postulate commutator

$$[\mathbf{Q}, \mathbf{P}] = i\hbar$$

Now, one has to get the expression of the unitary operators, allowing one to translate the origin of the position and momentum operators.

2.5.2 Position operator translation

First, consider the following linear operator:

$$\boxed{\mathbf{A}(\mathbf{P}, Q^\circ) \equiv \mathbf{A}(Q^\circ) = \exp\left\{-\frac{iQ^\circ \mathbf{P}}{\hbar}\right\}} \tag{2.95}$$

where Q° is a real scalar having the dimension of a length, and $\mathbf{P}$ the momentum operator, conjugate to the position operator $\mathbf{Q}$. Its Hermitian conjugate is

$$\mathbf{A}(\mathbf{P}, Q^\circ)^\dagger = \exp\left\{\frac{iQ^\circ \mathbf{P}^\dagger}{\hbar}\right\}$$

Since $\mathbf{P}$ is Hermitian, that is, $\mathbf{P} = \mathbf{P}^\dagger$, this equation transforms to

$$\mathbf{A}(\mathbf{P}, Q^\circ)^\dagger = \exp\left\{\frac{iQ^\circ \mathbf{P}}{\hbar}\right\} \tag{2.96}$$

Thus

$$\mathbf{A}(\mathbf{P}, Q^\circ)^\dagger = \mathbf{A}(\mathbf{P}, Q^\circ)^{-1} \tag{2.97}$$

Now, the operator $\mathbf{A}(\mathbf{P}, Q^\circ)$ is unitary, so that

$$\mathbf{A}(\mathbf{P}, Q^\circ)^\dagger \mathbf{A}(\mathbf{P}, Q^\circ) = 1 \tag{2.98}$$

Now, calculate the commutator of the operator (2.95) with $\mathbf{Q}$. Then, since $\mathbf{A}(Q^\circ, \mathbf{P})$ is a function of $\mathbf{P}$, in view of Eq. (2.14) it takes the form

$$[\mathbf{Q}, \mathbf{A}(\mathbf{P}, Q^\circ)] = i\hbar\left(\frac{\partial \mathbf{A}(\mathbf{P}, Q^\circ)}{\partial \mathbf{P}}\right) \tag{2.99}$$

The right-hand side of this last equation may be obtained differentiating Eq. (2.95) to give

$$\left(\frac{\partial \mathbf{A}(\mathbf{P}, Q^\circ)}{\partial \mathbf{P}}\right) = -\left(\frac{i}{\hbar}\right) Q^\circ \mathbf{A}(\mathbf{P}, Q^\circ)$$

As a consequence, Eq. (2.99) becomes

$$[\mathbf{Q}, \mathbf{A}(\mathbf{P}, Q^\circ)] = Q^\circ \mathbf{A}(\mathbf{P}, Q^\circ) \tag{2.100}$$

Next, writing explicitly the left-hand side of Eq. (2.100) yields

$$\mathbf{Q}\mathbf{A}(Q^\circ) = \mathbf{A}(\mathbf{P}, Q^\circ)\mathbf{Q} + Q^\circ \mathbf{A}(\mathbf{P}, Q^\circ) \tag{2.101}$$

Again, premultiply each member of Eq. (2.101) by the inverse of **A**, that is,

$$\mathbf{A}(\mathbf{P}, Q^\circ)^{-1}\mathbf{Q}\mathbf{A}(\mathbf{P}, Q^\circ) = \mathbf{A}(\mathbf{P}, Q^\circ)^{-1}\mathbf{A}(\mathbf{P}, Q^\circ)\mathbf{Q} + Q^\circ\mathbf{A}(\mathbf{P}, Q^\circ)^{-1}\mathbf{A}(\mathbf{P}, Q^\circ)$$

Then, after simplifying, by aid of Eqs. (2.97) and (2.98), this last expression reduces to

$$\boxed{\mathbf{A}(\mathbf{P}, Q^\circ)^{-1}\mathbf{Q}\mathbf{A}(\mathbf{P}, Q^\circ) = \mathbf{Q} + Q^\circ} \tag{2.102}$$

Thus, Eq. (2.102), which is called *a canonical transformation* on the coordinate operator **Q**, translates the origin of **Q** by the scalar amount Q°. Furthermore, for an infinitesimal scalar displacement dQ°, Eq. (2.102) transforms to

$$\mathbf{A}(\mathbf{P}, dQ^\circ)^{-1}\mathbf{Q}\mathbf{A}(\mathbf{P}, dQ^\circ) = \mathbf{Q} + dQ^\circ \tag{2.103}$$

2.5.3 Momentum operator translation

Now, consider the linear operator $\mathbf{B}(\mathbf{Q}, P^\circ)$:

$$\boxed{\mathbf{B}(\mathbf{Q}, P^\circ) = \exp\left\{\frac{iP^\circ\mathbf{Q}}{\hbar}\right\}} \tag{2.104}$$

where P° is a scalar having the dimension of a momentum and **Q** being the Hermitian coordinate operator. The inspection of its expression shows that the operator $\mathbf{B}(P^\circ)$ is unitary since its inverse $\mathbf{B}(\mathbf{Q}, P^\circ)^{-1}$ is equal to its Hermitian conjugate $\mathbf{B}(\mathbf{Q}, P^\circ)^\dagger$:

$$\mathbf{B}(\mathbf{Q}, P^\circ)^\dagger = \mathbf{B}(\mathbf{Q}, P^\circ)^{-1}$$

Calculate the commutator of this operator with the momentum operator **P**. Since $\mathbf{B}(P^\circ, \mathbf{Q})$ is a function of **Q**, one may use Eq. (2.15), which leads to

$$[\mathbf{P}, \mathbf{B}(\mathbf{Q}, P^\circ)] = -i\hbar\left(\frac{\partial\mathbf{B}(\mathbf{Q}, P^\circ)}{\partial\mathbf{Q}}\right)$$

Differentiating Eq. (2.104), and after identification, one obtains

$$[\mathbf{P}, \mathbf{B}(\mathbf{Q}, P^\circ)] = P^\circ\mathbf{B}(\mathbf{Q}, P^\circ) \tag{2.105}$$

Then, writing explicitly the commutator, Eq. (2.105) reads

$$\mathbf{P}\mathbf{B}(\mathbf{Q}, P^\circ) = \mathbf{B}(\mathbf{Q}, P^\circ)\mathbf{P} + P^\circ\mathbf{B}(\mathbf{Q}, P^\circ) \tag{2.106}$$

Moreover, premultiply this equation by the inverse of **B** to get

$$\mathbf{B}(\mathbf{Q}, P^\circ)^{-1}\mathbf{P}\mathbf{B}(\mathbf{Q}, \mathbf{P}^\circ) = \mathbf{B}(\mathbf{Q}, P^\circ)^{-1}\mathbf{B}(\mathbf{Q}, P^\circ)\mathbf{P} + \mathbf{B}(\mathbf{Q}, P^\circ)^{-1}P^\circ\ \mathbf{B}(\mathbf{Q}, P^\circ) \tag{2.107}$$

On simplification, this expression reduces to

$$\boxed{\mathbf{B}(\mathbf{Q}, P^\circ)^{-1}\mathbf{P}\mathbf{B}(\mathbf{Q}, P^\circ) = \mathbf{P} + P^\circ} \tag{2.108}$$

Clearly, this canonical transformation allows to translate **P** by the scalar amount P°.

2.5.4 Quantum Galilean transformation

One may define the Galilean transformation operator according to

$$\boxed{\mathbf{S}(v) = \exp\left\{\frac{i}{\hbar}(mv\mathbf{Q} - \mathbf{P}vt)\right\}} \tag{2.109}$$

where v is the scalar velocity. Observe that this operator is Hermitian since

$$\mathbf{S}^{\dagger}(v) = \exp\left\{-\frac{i}{\hbar}(mv\mathbf{Q} - \mathbf{P}vt)\right\} = \mathbf{S}^{-1}(v)$$

Using the Glauber theorem (1.78), the operator (2.109) and its inverse take, respectively, the forms

$$\mathbf{S}(v) = \exp\left\{\frac{i}{\hbar}mv\mathbf{Q}\right\}\exp\left\{-\frac{i}{\hbar}\mathbf{P}vt\right\}e^{\zeta}$$

$$\mathbf{S}^{-1}(v) = \exp\left\{\frac{i}{\hbar}\mathbf{P}vt\right\}\exp\left\{-\frac{i}{\hbar}mv\mathbf{Q}\right\}e^{-\zeta}$$

with

$$\zeta = -\frac{1}{2}\left[\frac{i}{\hbar}mv\mathbf{Q}, -\frac{i}{\hbar}\mathbf{P}v\right]$$

Next, perform the following transformation on the position coordinate according to

$$\mathbf{S}(v)^{-1}\mathbf{Q}\mathbf{S}(v) = \exp\left\{\frac{i}{\hbar}\mathbf{P}vt\right\}\exp\left\{-\frac{i}{\hbar}mv\mathbf{Q}\right\}\mathbf{Q}\ \exp\left\{\frac{i}{\hbar}mv\mathbf{Q}\right\}\exp\left\{-\frac{i}{\hbar}\mathbf{P}vt\right\}$$

Hence

$$\mathbf{S}(v)^{-1}\mathbf{Q}\mathbf{S}(v) = \exp\left\{\frac{i}{\hbar}\mathbf{P}vt\right\}\mathbf{Q}\ \exp\left\{-\frac{i}{\hbar}\mathbf{P}vt\right\} \tag{2.110}$$

Next, taking vt in place of P°, and using Eq. (2.108), with the aid of Eq. (2.104), Eq. (2.110) reads

$$\boxed{\mathbf{S}(v)^{-1}\mathbf{Q}\mathbf{S}(v) = \mathbf{Q}-vt} \tag{2.111}$$

On the other hand, the transformation on the $\mathbf{P}$ coordinate involving the unitary operator (2.109) takes the form

$$\mathbf{S}(v)^{-1}\mathbf{P}\mathbf{S}(v) = \exp\left\{\frac{i}{\hbar}\mathbf{P}vt\right\}\exp\left\{-\frac{i}{\hbar}mv\mathbf{Q}\right\}\mathbf{P}\ \exp\left\{\frac{i}{\hbar}mv\mathbf{Q}\right\}\exp\left\{-\frac{i}{\hbar}\mathbf{P}vt\right\}$$

Again, taking mv in place of Q°, and then using Eqs. (2.102) and (2.95), yields

$$\mathbf{S}(v)^{-1}\mathbf{P}\mathbf{S}(v) = \exp\left\{\frac{i}{\hbar}\mathbf{P}vt\right\}(\mathbf{P} + mv)\exp\left\{-\frac{i}{\hbar}\mathbf{P}vt\right\}$$

or, after simplification

$$\boxed{\mathbf{S}(v)^{-1}\mathbf{P}\mathbf{S}(v) = \mathbf{P} + mv} \tag{2.112}$$

Equations (2.111) and (2.112) are the quantum Galilean transformations dealing with the $\mathbf{Q}$ and $\mathbf{P}$ operators

2.5.5 Action of translation operators on the Q eigenkets

Start from Eq. (2.101), that is, omitting the dependence of the translation operator on **P**

$$\mathbf{Q}\mathbf{A}(Q^\circ) = \mathbf{A}(Q^\circ)\mathbf{Q} + Q^\circ\mathbf{A}(Q^\circ) \quad \text{with} \quad \mathbf{A}(Q^\circ) = \exp\left\{-\frac{iQ^\circ\mathbf{P}}{\hbar}\right\} \tag{2.113}$$

where $\mathbf{A}(Q^\circ)$ is the translation operator, Q° a scalar having the dimension of a length, and **Q** and **P** having their usual meaning. Now, postmultiply both members of the first equation appearing in (2.113) by an eigenket $|\{Q\}\rangle$ of the position operator **Q**:

$$\mathbf{Q}\mathbf{A}(Q^\circ)|\{Q\}\rangle = \mathbf{A}(Q^\circ)\mathbf{Q}|\{Q\}\rangle + Q^\circ\mathbf{A}(Q^\circ)|\{Q\}\rangle \tag{2.114}$$

Owing to the eigenvalue equation (2.91), this equation transforms to

$$\mathbf{Q}\mathbf{A}(Q^\circ)|\{Q\}\rangle = \mathbf{A}(Q^\circ)Q|\{Q\}\rangle + Q^\circ\mathbf{A}(Q^\circ)|\{Q\}\rangle$$

or, after commuting the scalar Q, with the translation operator

$$\mathbf{Q}\mathbf{A}(Q^\circ)|\{Q\}\rangle = (Q + Q^\circ)\mathbf{A}(Q^\circ)|\{Q\}\rangle \tag{2.115}$$

Now, using the notation

$$\mathbf{A}(Q^\circ)|\{Q\}\rangle \equiv |\{\mathbf{A}(Q^\circ)Q\}\rangle$$

Eq. (2.115) yields

$$\mathbf{Q}|\{\mathbf{A}(Q^\circ)Q\}\rangle = (Q + Q^\circ)|\{\mathbf{A}(Q^\circ)Q\}\rangle \tag{2.116}$$

On the other hand, the eigenvalue equation Eq. (2.91) reads

$$\mathbf{Q}\,|\{Q + Q^\circ\}\rangle = (Q + Q^\circ)|\{Q + \ Q^\circ\}\rangle \tag{2.117}$$

where $|\{Q + Q^\circ\}\rangle$ is the corresponding eigenvector of **Q**. Then, by comparison of Eqs. (2.115) and (2.117) and ignoring a phase factor without interest, it appears that

$$\boxed{\mathbf{A}(Q^\circ)|\{Q\}\rangle = |\{Q + Q^\circ\}\rangle} \tag{2.118}$$

or, in view of Eq. (2.95)

$$\exp\left\{-\frac{iQ^\circ\mathbf{P}}{\hbar}\right\}|\{Q\}\rangle = |\{Q + Q^\circ\}\rangle \tag{2.119}$$

Of course, since **P** is Hermitian and Q° a real scalar, the Hermitian conjugate of this last expression is

$$\langle\{Q\}|\exp\left\{\frac{iQ^\circ\mathbf{P}}{\hbar}\right\} = \langle\{Q + Q^\circ\}| \tag{2.120}$$

Now, remark that for the infinitesimal transformation (2.103), the translation operator (2.95) may be expanded up to first order in dQ° to give

$$\mathbf{A}(dQ^\circ) = 1 - \frac{i}{\hbar}dQ^\circ\mathbf{P}$$

Next, the action of this infinitesimal translation operator on an eigenket of **Q** takes the form

$$\mathbf{A}(dQ^\circ)|\{Q\}\rangle = \left(1 - \frac{i}{\hbar} dQ^\circ \mathbf{P}\right)|\{Q\}\rangle$$

or, due to Eq. (2.118), with dQ° in place of Q°

$$\mathbf{A}(dQ^\circ)|\{Q\}\rangle = |\{Q + dQ^\circ\}\rangle$$

Thus, by identification of these two last equations, one gets

$$\boxed{|\{Q + dQ^\circ\}\rangle = \left(1 - \frac{i}{\hbar} dQ^\circ \mathbf{P}\right)|\{Q\}\rangle} \tag{2.121}$$

Next, let $|\{0\}_Q\rangle$ be the eigenket of the coordinate operator **Q**, corresponding to the zero eigenvalue

$$\mathbf{Q}|\{0\}_Q\rangle = 0\,|\{0\}_Q\rangle \tag{2.122}$$

Then, Eq. (2.118) reads

$$\mathbf{A}(Q^\circ)|\{0\}_Q\rangle = |\{0 + Q^\circ\}\rangle$$

or

$$\mathbf{A}(Q^\circ)|\{0\}_Q\rangle = |\{Q^\circ\}\rangle \tag{2.123}$$

Again, writing explicitly the translation operator by the aid of Eq. (2.95), and substituting the notation Q° by the more general one Q, without modifying anything, one obtains

$$\boxed{\exp\left\{-\frac{i}{\hbar} Q\mathbf{P}\right\}|\{0\}_Q\rangle = |\{Q\}\rangle} \tag{2.124}$$

On the other hand, recall Eq. (2.106), that is,

$$\mathbf{PB}(P^\circ) = \mathbf{B}(P^\circ)\mathbf{P} + P^\circ \mathbf{B}(P^\circ) \tag{2.125}$$

with

$$\mathbf{B}(P^\circ) = \exp\left\{\frac{iP^\circ \mathbf{Q}}{\hbar}\right\}$$

where $\mathbf{B}(P^\circ)$ is the translation operator and where P° is a scalar having the dimension of an impulsion. Now, postmultiply Eq. (2.125) by an eigenket $|\{P\}\rangle$ of **P**

$$\mathbf{PB}(P^\circ)|\{P\}\rangle = \mathbf{B}(P^\circ)\mathbf{P}|\{P\}\rangle + P^\circ \mathbf{B}(P^\circ)|\{P\}\rangle$$

Then, by an inference very similar to that allowing one to pass from Eq. (2.114) to (2.118), one finds

$$\mathbf{B}(P^\circ)|\{P\}\rangle = |\{P + P^\circ\}\rangle \tag{2.126}$$

Now, consider the eigenvalue equation of the momentum operator corresponding to the zero eigenvalue, that is,

$$\mathbf{P}|\{0\}_P\rangle = 0|\{0\}_P\rangle$$

Then, Eq. (2.126) yields

$$\mathbf{B}(P^\circ)|\{0\}_P\rangle = |\{P^\circ\}\rangle$$

Finally, explicitly writing the translation operator $\mathbf{B}(P^\circ)$, using Eq. (2.104), and taking P in place of P°, and $|\{P\}\rangle$ in place of $|\{P^\circ\}\rangle$, this last equation becomes

$$\boxed{\exp\left\{\frac{iP\mathbf{Q}}{\hbar}\right\}|\{0\}_P\rangle = |\{P\}\rangle} \tag{2.127}$$

2.5.6 Scalar products $\langle\{P\}|\{Q\}\rangle$

We have now to find the expression of the scalar product between an eigenket of $\mathbf{Q}$ and one of $\mathbf{P}$.

2.5.6.1 A first expression

To this aim, premultiply Eq. (2.124) by any bra $\langle\{P\}|$:

$$\langle\{P\}|\{Q\}\rangle = \langle\{P\}|\exp\left\{-\frac{iQ\mathbf{P}}{\hbar}\right\}|\{0\}_Q\rangle$$

Using Eq. (2.93) and the action of the exponential operator on the left bra, which is an eigenbra of the $\mathbf{P}$ operator with the eigenvalue P, one obtains from (2.93)

$$\langle\{P\}|\{Q\}\rangle = \exp\left\{-\frac{iQP}{\hbar}\right\}\langle\{P\}|\{0\}_Q\rangle \tag{2.128}$$

Now, observe that in this last equation, the bra $\langle\{P\}|$ may be obtained via the Hermitian conjugate of Eq. (2.127), that is,

$$\langle\{P\}| = \langle\{0\}_P|\exp\left\{-\frac{iP\mathbf{Q}}{\hbar}\right\}$$

Then, using this expression for the bra $\langle\{P\}|$, Eq. (2.128) transforms to

$$\langle\{P\}|\{Q\}\rangle = \exp\left\{-\frac{iQP}{\hbar}\right\}\left\langle\{0\}_P\left|\exp\left\{-\frac{iP\mathbf{Q}}{\hbar}\right\}\right|\{0\}_Q\right\rangle \tag{2.129}$$

Next, owing to Eq. (2.122), we may remark that the eigenvalue of $\mathbf{Q}$ corresponding to the right-hand-side ket of this last equation, is zero, so that the corresponding eigenvalue equation involving the exponential of $\mathbf{Q}$ reduces to

$$\exp\left\{-\frac{iP\mathbf{Q}}{\hbar}\right\}|\{0\}_Q\rangle = |\{0\}_Q\rangle$$

Thus, the scalar product (2.129) yields

$$\boxed{\langle\{P\}|\{Q\}\rangle = \exp\left\{-\frac{iQP}{\hbar}\right\}\langle\{0\}_P|\{0\}_Q\rangle} \tag{2.130}$$

2.5.6.2 Scalar products involved on the right-hand side of Eq. (2.130) To further utilize Eq. (2.130), we require the following scalar product:

$$\langle\{0\}_P|\{0\}_Q\rangle$$

For this purpose, let us first consider the scalar product $\langle\{P'\}|\{P''\}\rangle$ between two different eigenkets of the momentum operator, which obeys Eq. (2.94), that is,

$$\langle\{P'\}|\{P''\}\rangle = \delta(P' - P'')$$

Introduce between the ket and the bra the closure relation on the eigenkets of the coordinate operator:

$$\langle\{P'\}| \left\{ \int_{-\infty}^{+\infty} |\{Q\}\rangle\langle\{Q\}|\, dQ \right\} |\{P''\}\rangle = \delta(P' - P'')$$

or

$$\int_{-\infty}^{+\infty} \langle\{P'\}|\{Q\}\rangle\langle\{Q\}|\{P''\}\rangle dQ' = \delta(P' - P'')$$

On the other hand, using Eq. (2.130) and its complex conjugate, this last expression yields

$$|\langle\{0\}_P|\{0\}_Q\rangle|^2 \int_{-\infty}^{+\infty} \exp\left\{-\frac{iQP'}{\hbar}\right\} \exp\left\{\frac{iQP''}{\hbar}\right\} dQ = \delta(P' - P'')$$

or

$$|\langle\{0\}_P|\{0\}_Q\rangle|^2 \int_{-\infty}^{+\infty} \exp\left\{-\frac{iQ(P' - P'')}{\hbar}\right\} dQ = \delta(P' - P'') \tag{2.131}$$

Now, observe that according to Eq. (18.60) and keeping in mind the fact that the dimension of P is that of $Q/\hbar$, the integral appearing in Eq. (2.131) reads

$$\int_{-\infty}^{+\infty} \exp\left\{-\frac{iQ(P' - P'')}{\hbar}\right\} dQ = 2\pi\hbar\delta(P' - P'')$$

Thus, Eq. (2.131) simplifies to

$$|\langle\{0\}_P|\{0\}_Q\rangle|^2 = \frac{1}{2\pi\hbar}$$

Therefore, ignoring the unknown phase factor, which is without interest,

$$\langle\{0\}_P|\{0\}_Q\rangle = \sqrt{\frac{1}{2\pi\hbar}}$$

Eq. (2.130) becomes

$$\boxed{\langle\{P\}|\{Q\}\rangle = \sqrt{\frac{1}{2\pi\hbar}} \exp\left\{-\frac{iPQ}{\hbar}\right\}} \tag{2.132}$$

At last, the probability of passage from some ket $|\{Q\}\rangle$ to any ket $|\{P\}\rangle$ or vice versa is, according to the fourth postulate

$$\boxed{|\langle\{P\}|\{Q\}\rangle|^2 = \frac{1}{2\pi\hbar}} \tag{2.133}$$

That shows that whatever the value observed for the position coordinate before a measurement of the momentum, the probability to find after such a measurement some value of the momentum is the same whatever this last value and vice versa. Equation (2.133) may be viewed as the expression of the basic contingency affecting the most simple and fundamental variables appearing in physics through Lagrange's equations.

2.6 CONCLUSION

This chapter has considered the presentation of the principles of quantum mechanics. We have introduced the important concepts of bras and kets describing the quantum states, that of Hermitean operators describing the physical variables, that of the measurement of physical variables through the eigenvalues of the corresponding Hermitian operators, and the notions of quantum average values generally relating kets and Hermitian operators. In discussing the quantum principles, large parts have been devoted to the time-dependent Schrödinger equation and to quantum averages and to their corresponding fluctuations. The quantum principles were shown to lead to a limitation of the knowledge of some physical conjugated variables, which is illustrated by the Heisenberg uncertainty relations, forbidding one to know simultaneously and exactly the position and momentum, however, preserving the main features of Newton's laws of classical mechanics, the cost to be paid to the Heisenberg uncertainty relations being the fact that these laws govern average values of the position and momentum in place of exact ones. Now, to be useful applied to particular situations such as, for instance, oscillators, quantum mechanics requires different equivalent representations such as matrix mechanics, wave mechanics, density operator approach, and also equivalent different time-dependent representations such as the Schrödinger, the Heisenberg, and the interaction pictures. The most important results of this chapter are summarized below:

Basic equations for quantum mechanics
Deterministic and probalistic changes:
$i\hbar\left(\dfrac{\partial\|\Psi(t)\rangle}{\partial t}\right) = \mathbf{H}\|\Psi(t)\rangle \qquad \mathbb{P}_{kl} = \|\langle\Phi_k\|\Psi_l\rangle\|^2$
Average values, dispersions, and their dynamics:
$\langle\mathbf{A}\rangle_\Psi = \langle\Psi\|\mathbf{A}\|\Psi\rangle \qquad \Delta\mathbf{A}_\Psi = \sqrt{\langle\mathbf{A}^2\rangle_\Psi - \langle\mathbf{A}\rangle_\Psi^2}$ $\left(\dfrac{\partial\langle\Psi(t)\|\mathbf{A}\|\Psi(t)\rangle}{\partial t}\right) = \dfrac{i}{\hbar}\langle\Psi(t)\|[\mathbf{H},\mathbf{A}]\|\Psi(t)\rangle$

Eigenvalue equations of the Hermitian operators and their eigenvalues and eigenvectors:

$$\mathbf{A}|\Phi_n\rangle = A_n|\Phi_n\rangle \text{ since } \mathbf{A} = \mathbf{A}^\dagger, \quad A_n = A_n^*, \quad \langle\Phi_n|\Phi_m\rangle = \delta_{nm}, \quad \sum |\Phi_n\rangle\langle\Phi_n| = 1$$

Important relations resulting from the commutation rule $[\mathbf{Q}, \mathbf{P}] = i\hbar$:

$$[\mathbf{Q}, \mathbf{F}(\mathbf{P})] = (i\hbar)\left(\frac{\partial \mathbf{F}(\mathbf{P})}{\partial \mathbf{P}}\right) \qquad [\mathbf{P}, \mathbf{F}(\mathbf{Q})] = -(i\hbar)\left(\frac{\partial \mathbf{F}(\mathbf{Q})}{\partial \mathbf{Q}}\right)$$

$$(e^{iQ^\circ \mathbf{P}/\hbar})\mathbf{Q}\,(e^{-iQ^\circ \mathbf{P}/\hbar}) = \mathbf{Q} + Q^\circ \qquad (e^{-iP^\circ \mathbf{Q}/\hbar})\mathbf{P}(e^{iP^\circ \mathbf{Q}/\hbar}) = \mathbf{P} + P^\circ$$

$$\text{if} \quad \mathbf{Q}|\{Q\}\rangle = Q|\{Q\}\rangle \text{ and } \mathbf{P}|\{P\}\rangle = P|\{P\}\rangle \qquad \langle\{P\}|\{Q\}\rangle$$

$$= \sqrt{\frac{1}{2\pi\hbar}} e^{-iQP/\hbar} \qquad \Delta P_\Psi \; \Delta Q_\Psi \geqslant \hbar$$

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CHAPTER 3

QUANTUM MECHANICS REPRESENTATIONS

INTRODUCTION

In the previous chapter we obtained different simple but important results following from the postulates of quantum mechanics such as the Ehrenfest and the virial theorems, the Heisenberg uncertainty relations, and the scalar products between any eigenket of **Q** and another one of **P**, the modulus of them being the same whatever the corresponding eigenvalues. But, in order to become tractable for the study of concrete situations, it is necessary to adapt the postulates. That is the aim of what is termed different representations of quantum mechanics. Among them there are the *matrix mechanics*, due initially to Heisenberg, Born, Jordan, and Pauli, and the *wave mechanics* of Louis de Broglie and Schrödinger. There are also different time-dependent representations besides those of Schrödinger, that is, the *Heisenberg picture* and the different *interaction pictures*, which deal with time evolution operators. Finally, there are the density operator representations in which the informations dealing with the kets or the wavefunctions are introduced into an operator and which are very useful when working on many-particle systems. All these representations will be studied in the present chapter.

3.1 MATRIX REPRESENTATION

Because the postulates of quantum mechanics concern the state space, which is a vector space, the matrices play a fundamental role in quantum mechanics leading to the fact that there are matrix representations for all theoretical entities involved in the postulates, that is, for kets, bras, linear transformations, eigenvalue equations, and so on. The purpose of the present section is to consider that subject more deeply.

3.1.1 Kets and bras

First, consider the eigenvalue equation of a Hermitian operator **A**:

$$\mathbf{A}|\Phi_l\rangle = A_l|\Phi_l\rangle \quad \text{with} \quad \mathbf{A} = \mathbf{A}^\dagger \qquad \text{and thus} \qquad \langle\Phi_l|\Phi_k\rangle = \delta_{lk}$$

Quantum Oscillators, First Edition. Olivier Henri-Rousseau and Paul Blaise.
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We remember that the eigenvectors $|\Phi_l\rangle$ of $\mathbf{A}$ obey the closure relation

$$\sum_i |\Phi_i\rangle\langle\Phi_i| = 1$$

Then consider a ket $|\Psi_k\rangle$ of the state space that does not belong to the set $\{\Phi_l\}$ of the eigenvectors $|\Phi_l\rangle$, and multiply it by the above closure relation:

$$|\Psi_k\rangle = \mathbf{1}|\Psi_k\rangle = \left\{\sum_i |\Phi_i\rangle\langle\Phi_i|\right\}|\Psi_k\rangle$$

Hence

$$|\Psi_k\rangle = \sum_i \langle\Phi_i|\Psi_k\rangle|\Phi_i\rangle$$

or

$$|\Psi_k\rangle = \sum_i a_{ik}|\Phi_i\rangle \quad \text{with} \quad a_{ik} = \langle\Phi_i|\Psi_k\rangle \tag{3.1}$$

Owing to the convention for matrix notation in which the first index corresponds to the row and the second one to the column, and in view of Eq. (3.1), a ket $|\Psi_k\rangle$ may be represented, in a basis $\{|\Phi_i\rangle\}$, by a column vector, the components of which are the coefficients a_{ik}:

$$|\Psi_k\rangle \Leftrightarrow \begin{pmatrix} a_{1k} \\ a_{2k} \\ \dots \\ a_{ik} \\ \dots \end{pmatrix} \tag{3.2}$$

Next, one may proceed in a similar way for the bra $\langle\Psi_j|$ corresponding to the above ket. Then, the Hermitian conjugate of Eq. (3.1) is

$$\langle\Psi_j| = \sum_i a_{ji}\langle\Phi_i| \quad \text{with} \quad a_{ji} = \langle\Psi_j|\Phi_i\rangle$$

This last result shows that the matrix representation of the bra $\langle\Psi_j|$ is a row vector, the components of which are the expansion coefficients of the above equation:

$$\langle\Psi_j| \quad \Leftrightarrow \quad (a_{j1} \quad a_{j2} \quad \dots \quad a_{ji} \quad \dots) \tag{3.3}$$

Note that the expansion coefficients a_{ik} and a_{ki} are complex conjugates since they are the expressions of the complex conjugate scalar products, tha is,

$$a_{ij} = a_{ji}^* \quad \text{because} \quad \langle\Phi_i|\Psi_j\rangle = \langle\Psi_j|\Phi_i\rangle^*$$

3.1.2 Scalar products

Consider the following expansions of the ket $|\Psi_k\rangle$ and of the bra $\langle\xi_j|$ in the basis $\{|\Phi_i\rangle\}$ obeying

$$\langle\Phi_i|\Phi_l\rangle = \delta_{il} \tag{3.4}$$

$$|\Psi_k\rangle = \sum_i a_{ik}|\Phi_i\rangle \quad \text{with} \quad a_{ik} = \langle\Phi_i|\Psi_k\rangle$$

$$\langle\xi_j| = \sum_l b_{jl}\langle\Phi_l| \quad \text{with} \quad b_{jl} = \langle\xi_j|\Phi_l\rangle$$

Now, the scalar product $\langle\xi_j|\Psi_k\rangle$ reads

$$\langle\xi_j|\Psi_k\rangle = \left\{\sum_l b_{jl}\langle\Phi_l|\right\}\left\{\sum_i a_{ik}|\Phi_i\rangle\right\}$$

or

$$\langle\,\xi_j|\Psi_k\rangle = \sum_l \sum_i b_{jl}a_{ik}\langle\Phi_l|\Phi_i\rangle$$

so that, due to the orthonormality properties (3.4)

$$\langle\xi_j|\Psi_k\rangle = \sum_l b_{jl}a_{lk} \tag{3.5}$$

Owing to the matrix convention according to which the first index refers to the row and the second to the column, expression (3.5) appears to be the matrix product between the jth line and the kth column vectors constructed, respectively, from the set of b_{jl} and a_{lk} coefficients.

$$\langle\xi_j|\Psi_k\rangle \Leftrightarrow (b_{j1} \quad b_{j2} \quad \cdots \quad b_{jl} \quad \cdots)\begin{pmatrix} a_{1k} \\ a_{2k} \\ \cdots \\ a_{lk} \\ \cdots \end{pmatrix}$$

3.1.3 Operators

Consider a linear operator **A**. Premultiply it by the bra $\langle\Phi_i|$ and postmultiply it by the ket $|\Phi_k\rangle$ belonging to the same basis as the ket $|\Phi_l\rangle$, the Hermitian conjugate of which is $\langle\Phi_i|$. The linear operation of **A** on $|\Phi_k\rangle$ gives a new ket $|\Psi_k\rangle$ on which the action of $\langle\Phi_i|$ corresponds to a scalar product, the result of which is the double index scalar A_{ik}:

$$\langle\Phi_i|\mathbf{A}|\Phi_k\rangle = \langle\Phi_i|\Psi_k\rangle = A_{ik} \tag{3.6}$$

The different scalars A_{ik} (which may be obtained by allowing the indexes of the ket and of the bra to run over the different terms of the basis) appear to be the matrix elements of a square matrix the dimension of which is generally infinite. Observe that, owing to Eq. (1.30),

$$\langle\Phi_i|\mathbf{A}|\Phi_k\rangle = \langle\Phi_k|\mathbf{A}^\dagger|\Phi_i\rangle^* \tag{3.7}$$

3.1.3.1 *Hermitian operators*

If the linear operator is Hermitian, that is,

$$\mathbf{A} = \mathbf{A}^{\dagger}$$

then the matrix elements (3.7) simplify to

$$\langle \Phi_i | \mathbf{A} | \Phi_k \rangle = \langle \Phi_k | \mathbf{A} | \Phi_i \rangle^*$$

Hence, from Eq. (3.6), it appears that the matrix elements are complex conjugate with respect to the diagonal part, which is real, so that

$$A_{ik} = A_{ki}^* \quad \text{and thus} \qquad A_{kk} = A_{kk}^* \quad \text{so that} \quad A_{kk} \text{ is real} \tag{3.8}$$

with

$$A_{ki}^* = \langle \Phi_k | \mathbf{A} | \Phi_i \rangle^*$$

A matrix the elements defined by condition (3.8) is a Hermitian matrix.

3.1.3.2 *Unitary operators*

Consider the linear unitary operator $\mathbf{U}$ satisfying

$$\mathbf{U}^{-1} = \mathbf{U}^{\dagger} \quad \text{with} \quad \mathbf{U}^{-1}\mathbf{U} = 1 \tag{3.9}$$

Now, consider a matrix element of this operator

$$U_{ik} = \langle \Phi_i | \mathbf{U} | \Phi_k \rangle$$

and the corresponding matrix elements of its inverse and of its Hermitian conjugate. They must be equal owing to the fact that the inverse of the unitary operator is equal to its Hermitian conjugate. Hence

$$\langle \Phi_i | \mathbf{U}^{-1} | \Phi_k \rangle = \langle \Phi_i | \mathbf{U}^{\dagger} | \Phi_k \rangle \tag{3.10}$$

Of course, owing to the general property (1.30), the following relation for the right-hand-side matrix element of the latter equation exists:

$$\langle \Phi_i | \mathbf{U}^{\dagger} | \Phi_k \rangle = \langle \Phi_k | \mathbf{U} | \Phi_i \rangle^* \tag{3.11}$$

Thus, because of this last equation, Eq. (3.10) becomes

$$\langle \Phi_i | \mathbf{U}^{-1} | \Phi_k \rangle = \langle \Phi_k | \mathbf{U} | \Phi_i \rangle^*$$

Thus, the following general relation between the matrix elements of the unitary operator and those of its inverse exists:

$$\boxed{U_{ik}^{-1} = U_{ki}^*} \tag{3.12}$$

with

$$U_{ki} = \langle \Phi_k | \mathbf{U} | \Phi_i \rangle \qquad U_{ik}^{-1} = \langle \Phi_i | \mathbf{U}^{-1} | \Phi_k \rangle \qquad \text{and} \qquad U_{ki}^* = \langle \Phi_k | \mathbf{U} | \Phi_i \rangle^* \tag{3.13}$$

Next, consider the matrix element built up from the definition of an inverse operator:

$$\langle \Phi_i | \mathbf{U}^{-1}\mathbf{U} | \Phi_k \rangle = \langle \Phi_i | \mathbf{1} | \Phi_k \rangle \tag{3.14}$$

Since the ket $|\Phi_k\rangle$ and the ket $|\Phi_i\rangle$ (which is the Hermitian conjugate of the bra $\langle \Phi_i |$) belong to the same basis, they are orthogonal, that is,

$$\langle \Phi_i | \mathbf{1} | \Phi_k \rangle = \langle \Phi_i | \Phi_k \rangle = \delta_{ik}$$

so that the matrix element (3.14) obeys

$$\langle \Phi_i | \mathbf{U}^{-1} \mathbf{U} | \Phi_k \rangle = \delta_{ik} \tag{3.15}$$

Next, use the closure relation on the basis $\{|\Phi_l\rangle\}$

$$\sum_l |\Phi_l\rangle\langle\Phi_l| = \mathbf{1}$$

By inserting it in Eq. (3.15) between the unitary operator and its inverse, it yields

$$\langle \Phi_i | \mathbf{U}^{-1} \left\{ \sum_l |\Phi_l\rangle\langle\Phi_l| \right\} \mathbf{U} | \Phi_k \rangle = \delta_{ik}$$

Then, using the properties (3.9) of the unitary operator, we have

$$\sum_l \langle \Phi_i | \mathbf{U}^\dagger | \Phi_l \rangle \langle \Phi_l | \mathbf{U} | \Phi_k \rangle = \delta_{ik} \tag{3.16}$$

or, due to Eq. (3.11)

$$\sum_l \langle \Phi_l | \mathbf{U} | \Phi_i \rangle^* \langle \Phi_l | \mathbf{U} | \Phi_k \rangle = \delta_{ik}$$

so that owing to Eq. (3.13)

$$\boxed{\sum_l U_{li}^* U_{lk} = \delta_{ik}}$$

This last expression may be split into two equations, the first of which shows that any column labeled i of some unitary matrix is normalized and that two different columns labeled i and k of such a matrix are orthogonal:

$$\sum_l |U_{li}|^2 = 1 \qquad \text{and} \qquad \sum_l U_{li}^* U_{lk} = 0 \quad \text{if} \quad i \neq k \tag{3.17}$$

All the matrix elements U_{li}, with l running over the elements of the basis, form therefore a column vector so that Eq. (3.17) may be visualized as the orthonormality properties of the column vectors from which the unitary matrix is built up. Now, taking the Hermitian conjugate of Eq. (3.16) and proceeding in a similar way, one would obtain the two following equations, expressing, respectively, that any row i of a unitary matrix is normalized and that two different rows i and k of such a matrix are orthogonal:

$$\sum_l |U_{il}|^2 = 1 \qquad \text{and} \qquad \sum_l U_{il}^* U_{kl} = 0 \quad \text{if} \quad i \neq k$$

Observe that some unitary matrices are real so that, owing to Eq. (3.12), their matrix elements O_{ik} obey

$$O_{ik}^{-1} = O_{ki}$$

For such matrices, which are said to be *orthogonal*, and, owing to Eq. (3.17), their columns obey the simplified orthonormality properties (which are at the origin of their name):

$$\sum_l O_{lk}^2 = 1 \qquad \text{and} \qquad \sum_l O_{li} O_{lk} = 0 \quad \text{if} \quad l \neq k$$

3.1.4 Linear transformations

3.1.4.1 Simple linear transformations Consider the eigenvalue equation of the Hermitian operator **B**:

$$\mathbf{B}|\Phi_l\rangle = B_l|\Phi_l\rangle$$

Since it is Hermitian, its eigenkets $|\Phi_l\rangle$ are orthonormal so that the following basis $\{|\Phi_l\rangle\}$ can be constructed:

$$\sum_i |\Phi_i\rangle\langle\Phi_i| = \mathbf{1} \qquad \text{and} \qquad \langle\Phi_i|\Phi_j\rangle = \delta_{ij} \tag{3.18}$$

Next, consider the following linear transformation involving the linear operator **A**, which does not commute with **B** and which transforms a ket $|\Psi_k\rangle$ into any another one $|\xi_q\rangle$:

$$\mathbf{A}|\Psi_k\rangle = |\xi_q\rangle \quad \text{with} \quad [\mathbf{A}, \mathbf{B}] \neq 0 \tag{3.19}$$

Now, introduce the closure relation appearing in (3.18) in this linear transformation according to

$$\mathbf{A} \sum_i |\Phi_i\rangle\langle\Phi_i|\Psi_k\rangle = |\xi_q\rangle$$

Again, premultiply both sides of this equation by the bra $\langle\Phi_r|$:

$$\boxed{\sum_i \langle\Phi_r|\mathbf{A}|\Phi_i\rangle\langle\Phi_i|\Psi_k\rangle = \langle\Phi_r|\xi_q\rangle}$$

which reads

$$\sum_i A_{ri}\, b_{ik} = a_{rk} \tag{3.20}$$

with, respectively,

$$A_{ri} = \langle\Phi_r|\mathbf{A}|\Phi_i\rangle \qquad b_{ik} = \langle\Phi_i|\Psi_k\rangle \qquad \text{and} \qquad a_{rq} = \langle\Phi_r|\xi_q\rangle$$

Owing to the matrix convention, and within the representation defined by the basis (3.18), Eq. (3.19) appears to be the matrix linear transformation (3.20) through

$$\begin{pmatrix} a_{1q} \\ a_{2q} \\ \cdots \\ a_{lq} \\ \cdots \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1i} & \cdots \\ A_{21} & A_{22} & & & \\ \cdots & & & & \\ A_{r1} & & & & \\ \cdots & & & & \end{pmatrix} \begin{pmatrix} b_{1k} \\ b_{2k} \\ \cdots \\ b_{lk} \\ \cdots \end{pmatrix}$$

3.1.4.2 Inverse transformations Now, we shall consider the inverse of the transformation (3.19). Hence, premultiply both members of this equation by the inverse $\mathbf{A}^{-1}$ of the operator $\mathbf{A}$:

$$\mathbf{A}^{-1}\mathbf{A}|\Psi_k\rangle = \mathbf{A}^{-1}|\xi_q\rangle$$

Then, after simplification, we have

$$|\Psi_k\rangle = \mathbf{A}^{-1}|\xi_q\rangle$$

Now, insert the closure relation (3.18) in the following way:

$$|\Psi_k\rangle = \mathbf{A}^{-1}\sum_i |\Phi_i\rangle\langle\Phi_i|\xi_q\rangle$$

Premultiplying by the bra $\langle\Phi_r|$ reads

$$\langle\Phi_r|\Psi_k\rangle = \sum_i \langle\Phi_r|\mathbf{A}^{-1}|\Phi_i\rangle\langle\Phi_i|\xi_q\rangle$$

leading to the following matrix representation of the inverse linear transformation:

$$\begin{pmatrix} b_{1k} \\ b_{2k} \\ \cdots \\ b_{lk} \\ \cdots \end{pmatrix} = \begin{pmatrix} A_{11}^{-1} & A_{12}^{-1} & \cdots & A_{1i}^{-1} & \cdots \\ A_{21}^{-1} & A_{22}^{-1} & & & \\ \cdots & & & & \\ A_{r1}^{-1} & & & & \\ \cdots & & & & \end{pmatrix} \begin{pmatrix} a_{1q} \\ a_{2q} \\ \cdots \\ a_{iq} \\ \cdots \end{pmatrix}$$

that may be also written

$$b_{rk} = \sum_i A_{ri}^{-1} a_{iq}$$

with

$$a_{iq} = \langle\Phi_i|\xi_q\rangle \qquad \text{and} \qquad A_{ri}^{-1} = \langle\Phi_r|\mathbf{A}^{-1}|\Phi_i\rangle$$

respectively.

3.1.4.3 Unitary transformations Consider a matrix element of a matrix representation of a linear operator $\mathbf{A}$ in some basis $\{|\Psi_k\rangle\}$ defined by the eigenvalue equation of a Hermitian operator $\mathbf{C}$ that does not commute with $\mathbf{A}$:

$$\mathbf{C}|\Psi_k\rangle = C_k|\Psi_k\rangle \quad \text{with} \quad \mathbf{C} = \mathbf{C}^\dagger \qquad \text{and} \qquad [\mathbf{C}, \mathbf{A}] \neq 0$$

$$\sum_k |\Psi_k\rangle\langle\Psi_k| = \mathbf{1} \qquad \text{and} \qquad \langle\Psi_k|\Psi_l\rangle = \delta_{kl} \tag{3.21}$$

This element is

$$\langle\Psi_l|\mathbf{A}|\Psi_k\rangle = A_{lk} \tag{3.22}$$

Now, seek the representation of this operator within a new basis $\{|\Phi_q\rangle\}$ defined by the eigenvalue equation of another Hermitian operator **B**, which commutes neither with **A** nor with **C**:

$$\mathbf{B}|\Phi_q\rangle = B_q|\Phi_q\rangle \quad \text{with} \quad \mathbf{B} = \mathbf{B}^\dagger \qquad \text{and} \qquad [\mathbf{B}, \mathbf{A}] \neq 0$$

$$\sum_q |\Phi_q\rangle\langle\Phi_q| = \mathbf{1} \qquad \text{and} \qquad \langle\Phi_p|\Phi_q\rangle = \delta_{pq} \tag{3.23}$$

To this end, introduce twice the unity operator inside the matrix element (3.22):

$$\langle\Psi_l|\mathbf{A}|\Psi_k\rangle = \langle\Psi_l|\mathbf{1}\,\mathbf{A}\,\mathbf{1}|\Psi_k\rangle$$

Then, using for the unity operator of the closure relation appearing in Eq. (3.23), it reads

$$A_{lk} = \langle\Psi_l|\mathbf{A}|\Psi_k\rangle = \langle\Psi_l| \left\{\sum_q |\Phi_q\rangle\langle\Phi_q|\right\} \mathbf{A} \left\{\sum_p |\Phi_p\rangle\langle\Phi_p|\right\} |\Psi_k\rangle$$

or

$$A_{lk} = \sum_q \sum_p \langle\Psi_l|\Phi_q\rangle\langle\Phi_q|\mathbf{A}|\Phi_p\rangle\langle\Phi_p|\Psi_k\rangle$$

and thus

$$\boxed{A_{lk} = \sum_q \sum_p a_{lq}\tilde{A}_{qp}a_{pk}} \tag{3.24}$$

with

$$a_{lq} = \langle\Psi_l|\Phi_q\rangle \qquad \tilde{A}_{qp} = \langle\Phi_q|\mathbf{A}|\Phi_p\rangle \qquad \text{and} \qquad a_{pk} = \langle\Phi_p|\Psi_k\rangle \tag{3.25}$$

Owing to the matrix notation conventions, Eq. (3.24) appears as the following product of matrices:

$$\begin{pmatrix} A_{11} & A_{12} & & A_{1k} & \cdots \\ A_{21} & A_{22} & & & \\ \vdots & & \cdots & & \\ A_{k1} & A_{k2} & & A_{kk} & \\ & & & & \cdots \end{pmatrix}$$

$$= \begin{pmatrix} a_{11} & a_{12} & \cdots & \cdots & \\ a_{21} & a_{22} & \cdots & \cdots & \\ \cdots & \cdots & & & \\ a_{l1} & a_{l2} & & a_{ll} & \\ & & & & \cdots \end{pmatrix} \begin{pmatrix} \tilde{A}_{11} & \tilde{A}_{12} & & \cdots & \cdots \\ \tilde{A}_{21} & \tilde{A}_{22} & & & \\ \cdots & \cdots & \cdots & & \\ \tilde{A}_{q1} & \tilde{A}_{q2} & & \cdots & \\ & & & & \cdots \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & \cdots & \cdots & \\ a_{21} & a_{22} & \cdots & \cdots & \\ \cdots & \cdots & & & \\ a_{p1} & a_{p2} & & \cdots & \\ & & & & \cdots \end{pmatrix} \tag{3.26}$$

Now, observe that the first and third right-hand-side matrices are unitary, which may be proved by first observing that due to Eq. (3.25), it is always possible to write

$$\sum_q a_{lq} a_{qk} = \sum_q \langle \Psi_l | \Phi_q \rangle \langle \Phi_q | \Psi_k \rangle$$

Again, using the closure relation appearing in Eq. (3.23), and the orthonormality properties (3.21), we have

$$\sum_q a_{lq} a_{qk} = \langle \Psi_l | \Psi_k \rangle = \delta_{lk}$$

On the other hand, the unitary transformation (3.26) may be denoted

$$\boxed{\mathbf{A}} = \boxed{\mathbf{U}}^{-1} \boxed{\tilde{\mathbf{A}}} \boxed{\mathbf{U}}$$

where $\boxed{\mathbf{A}}$ is the matrix representation of the operator $\mathbf{A}$ in the basis (3.21), $\boxed{\tilde{\mathbf{A}}}$ is that of the same operator in the basis (3.23), and $\boxed{\mathbf{U}}$ is the unitary matrix whose elements are given by (3.25).

3.1.4.4 Eigenvalue equations Now, write the eigenvalue equations of a linear operator $\mathbf{A}$:

$$\mathbf{A}|\Psi_k\rangle = A_k|\Psi_k\rangle \tag{3.27}$$

Now, seek the matrix representation of this equation in the basis $\{|\Phi_i\rangle\}$ of the eigenkets of a Hermitian operator $\mathbf{B}$, which does not commute with $\mathbf{A}$:

$$\mathbf{B}|\Phi_q\rangle = B_q|\Phi_q\rangle \quad \text{with} \quad \mathbf{B} = \mathbf{B}^\dagger \qquad \text{and} \qquad [\mathbf{B}, \mathbf{A}] \neq 0$$

$$\sum_q |\Phi_q\rangle\langle\Phi_q| = \mathbf{1} \qquad \text{and} \qquad \langle \Phi_q | \Phi_p \rangle = \delta_{qp} \tag{3.28}$$

Now, introduce this closure relation on both sides of the eigenvalue equation (3.27) according to

$$\mathbf{A} \left\{ \sum_q |\Phi_q\rangle\langle\Phi_q| \right\} |\Psi_k\rangle = A_k \left\{ \sum_q |\Phi_q\rangle\langle\Phi_q| \right\} |\Psi_k\rangle$$

so that

$$\sum_q \mathbf{A}|\Phi_q\rangle\langle\Phi_q|\Psi_k\rangle = \sum_q A_k|\Phi_q\rangle\langle\Phi_q|\Psi_k\rangle$$

Again, premultiply both sides of this last equation by a bra $\langle\Phi_p|$:

$$\langle\Phi_p| \sum_q \mathbf{A}|\Phi_q\rangle\langle\Phi_q|\Psi_k\rangle = \langle\Phi_p| \sum_q A_k|\Phi_q\rangle\langle\Phi_q|\Psi_k\rangle$$

which may be written

$$\sum_q \langle\Phi_p|\mathbf{A}|\Phi_q\rangle\langle\Phi_q|\Psi_k\rangle = \sum_q A_k\langle\Phi_p|\Phi_q\rangle\langle\Phi_q|\Psi_k\rangle$$

which, owing to the orthonormality properties (3.28) of the basis $\{|\Phi_i\rangle\}$, transforms to

$$\sum_q \langle \Phi_p|\mathbf{A}|\Phi_q\rangle\langle\Phi_q|\Psi_k\rangle = \sum_q A_k \delta_{pq}\langle\Phi_q|\Psi_k\rangle$$

or

$$\sum_q \langle \Phi_p|\mathbf{A}|\Phi_q\rangle\langle\Phi_q|\Psi_k\rangle = A_k\langle\Phi_p|\Psi_k\rangle$$

and thus

$$\boxed{\sum_q A_{pq}a_{qk} = A_k a_{pk}} \tag{3.29}$$

with

$$A_{pq} = \langle \Phi_p|\mathbf{A}|\Phi_q\rangle \qquad \text{and} \qquad a_{pk} = \langle\Phi_p|\Psi_k\rangle$$

Equation (3.29) leads to the following matrix representation in the basis (3.28) of the eigenvalue equation (3.27):

$$\begin{pmatrix} A_{11} & A_{12} & & A_{1q} & \cdots \\ A_{21} & A_{22} & & & \\ \cdots & \cdots & \cdots & & \\ A_{q1} & A_{q2} & & A_{qq} & \\ & & & & \cdots \end{pmatrix} \begin{pmatrix} a_{1k} \\ a_{2k} \\ \cdots \\ a_{qk} \\ \cdots \end{pmatrix} = A_k \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & 1 \end{pmatrix} \begin{pmatrix} a_{1k} \\ a_{2k} \\ \cdots \\ a_{pk} \\ \cdots \end{pmatrix} \tag{3.30}$$

3.1.5 Block matrix representation and symmetry

When some symmetry in a system exists, the matrix representation of the Hamiltonian operator takes the form of a block matrix, the study of which is the aim of the present section. As shown in section 18.9, the symmetry operations all have an inverse, so that the operators $\mathbf{S}$ describing them must also have an inverse $\mathbf{S}^{-1}$ obeying

$$\mathbf{S}^{-1}\mathbf{S} = \mathbf{S}\mathbf{S}^{-1} = \mathbf{1} \tag{3.31}$$

Furthermore, since the Hamiltonian operator $\mathbf{H}$ of a system cannot be modified by symmetry operations in the same way as its corresponding classical scalar form, the action of any symmetry operator on it cannot modify it so that one may write

$$\mathbf{S}\mathbf{H} = \mathbf{H} \qquad \text{and} \qquad \mathbf{S}^{-1}\mathbf{H} = \mathbf{H}$$

Hence, the following canonical transformation yields

$$\mathbf{S}^{-1}\mathbf{H}\mathbf{S} = \mathbf{H} \tag{3.32}$$

demonstrating that the symmetry operators $\mathbf{S}$ commute with the Hamiltonians $\mathbf{H}$, that is,

$$[\mathbf{H}, \mathbf{S}] = 0 \tag{3.33}$$

Now, consider a basis $\{|\Phi_l\rangle\}$ yielding a matrix representation of the Hamiltonian. Then, one may form linear combinations $|\Psi_k^{\{g\}}\rangle$ or $|\Psi_j^{\{u\}}\rangle$ of the kets $|\Phi_l\rangle$ belonging

to this basis, which are such that they will be symmetric or antisymmetric with respect to the symmetry operation corresponding to the **S** operator, that is, constructed from the following linear combinations:

$$|\Psi_k^{\{g\}}\rangle = \sum_l \{C_{lk}^{\{g\}}\}|\Phi_l\rangle$$

$$|\Psi_j^{\{u\}}\rangle = \sum_l \{C_{lj}^{\{u\}}\}|\Phi_l\rangle$$

obeying

$$\mathbf{S}^{-1}|\Psi_k^{\{g\}}\rangle = |\Psi_k^{\{g\}}\rangle \qquad \text{and} \qquad \langle\Psi_k^{\{g\}}|\mathbf{S} = \langle\Psi_k^{\{g\}}| \tag{3.34}$$

$$\mathbf{S}^{-1}|\Psi_j^{\{u\}}\rangle = -|\Psi_j^{\{u\}}\rangle \qquad \text{and} \qquad \langle\Psi_j^{\{u\}}|\mathbf{S} = -\langle\Psi_j^{\{u\}}| \tag{3.35}$$

Here the symbols $\{g\}$ (*gerade*) and $\{u\}$ (*ungerade*) have been used to distinguish between the symmetric and antisymmetric linear combinations.

Moreover, consider a matrix element of the Hamiltonian built up from a gerade ket and an ungerade bra. Then, insert the unity operator defined by Eq. (3.31) before and after **H** in such a way that

$$\langle\Psi_j^{\{u\}}|\mathbf{H}|\Psi_k^{\{g\}}\rangle = \langle\Psi_j^{\{u\}}|\mathbf{S}\mathbf{S}^{-1}\mathbf{H}\mathbf{S}\mathbf{S}^{-1}|\Psi_k^{\{g\}}\rangle$$

which, because of Eq. (3.32), simplifies to

$$\langle\Psi_j^{\{u\}}|\mathbf{H}|\Psi_k^{\{g\}}\rangle = \langle\Psi_j^{\{u\}}|\mathbf{S}\mathbf{H}\mathbf{S}^{-1}|\Psi_k^{\{g\}}\rangle$$

a result that, owing to Eqs. (3.34) and (3.35), reads

$$\langle\Psi_j^{\{u\}}|\mathbf{H}|\Psi_k^{\{g\}}\rangle = -\langle\Psi_j^{\{u\}}|\mathbf{H}|\Psi_k^{\{g\}}\rangle$$

so that

$$\boxed{\langle\Psi_j^{\{u\}}|\mathbf{H}|\Psi_k^{\{g\}}\rangle = \langle\Psi_k^{\{g\}}|\mathbf{H}|\Psi_j^{\{u\}}\rangle = 0} \tag{3.36}$$

where, in the last step, has used Eq. (1.30) and the Hermiticity of **H**. Equation (3.36) expresses the fact that the matrix element of a Hamiltonian between two kets of different symmetry is zero.

As an illustration, if, for instance, a subspace spanned by two gerade and two ungerade kets exists, then, according to Eq. (3.36), the matrix representation of the Hamiltonian takes on the following block form:

	$\|\Psi_1^{\{g\}}\rangle$	$\|\Psi_2^{\{g\}}\rangle$	$\|\Psi_1^{\{u\}}\rangle$	$\|\Psi_2^{\{u\}}\rangle$
$\langle\Psi_1^{\{g\}}\|$	$\{H_{11}^{\{g\}}\}$	$\{H_{12}^{\{g\}}\}$	0	0
$\langle\Psi_2^{\{g\}}\|$	$\{H_{21}^{\{g\}}\}$	$\{H_{22}^{\{g\}}\}$	0	0
$\langle\Psi_1^{\{u\}}\|$	0	0	$\{H_{11}^{\{u\}}\}$	$\{H_{12}^{\{u\}}\}$
$\langle\Psi_2^{\{u\}}\|$	0	0	$\{H_{21}^{\{u\}}\}$	$\{H_{22}^{\{u\}}\}$

(3.37)

The interest of the symmetry is to allow size reducing of Hamiltonian matrix representations to be diagonalized.

Now, consider any ket $|\{\xi\}\rangle$ describing the state of a system of the given symmetry characterized by the symmetry operation $\mathbf{S}$, which may be expressed by a linear combination of g and u state, according to

$$|\{\xi_l\}\rangle = \sum_k \{b_{kl}^{\{g\}}\}|\Psi_k^{\{g\}}\rangle + \sum_j \{b_{jl}^{\{u\}}\}|\Psi_j^{\{u\}}\rangle \tag{3.38}$$

Then, due to the first expressions of (3.34) and (3.35), it reads, respectively

$$\tfrac{1}{2}\{1+\mathbf{S}\}|\Psi_k^{\{g\}}\rangle = \tfrac{1}{2}\{|\Psi_k^{\{g\}}\rangle + |\Psi_k^{\{g\}}\rangle\} = |\Psi_k^{\{g\}}\rangle$$

$$\tfrac{1}{2}\{1-\mathbf{S}\}|\Psi_k^{\{u\}}\rangle = \tfrac{1}{2}\{|\Psi_k^{\{u\}}\rangle + |\Psi_k^{\{u\}}\rangle\} = |\Psi_k^{\{u\}}\rangle$$

$$\tfrac{1}{2}\{1-\mathbf{S}\}|\Psi_k^{\{g\}}\rangle = \tfrac{1}{2}\{|\Psi_k^{\{g\}}\rangle - |\Psi_k^{\{g\}}\rangle\} = 0$$

$$\tfrac{1}{2}\{1+\mathbf{S}\}|\Psi_k^{\{u\}}\rangle = \tfrac{1}{2}\{|\Psi_k^{\{u\}}\rangle - |\Psi_k^{\{u\}}\rangle\} = 0$$

As a consequence of these results and of Eq. (3.38), one obtains, respectively

$$\boxed{\frac{1}{2}\{1+\mathbf{S}\}|\{\xi_l\}\rangle = \sum_k \{b_{kl}^{\{g\}}\}|\Psi_k^{\{g\}}\rangle} \tag{3.39}$$

$$\boxed{\frac{1}{2}\{1-\mathbf{S}\}|\{\xi_l\}\rangle = \sum_j \{b_{jl}^{\{u\}}\}|\Psi_j^{\{u\}}\rangle} \tag{3.40}$$

3.2 WAVE MECHANICS

Following the above exposition of the matrix representation of quantum mechanics, we now pass to wave mechanics, that is, to the representation of quantum mechanics in the basis of the eigenkets of the $\mathbf{Q}$ operator, which is sometimes called the *Q representation* of quantum mechanics. The precise foundation of wave mechanics by Louis de Broglie in 1924 was completely independent from that of quantum matrix mechanics by Heisenberg, the deep link between the two approaches being later discovered.

3.2.1 Quantum mechanics in representation $\{|\{Q\}\rangle\}$

In order to introduce wave mechanics, we start from the eigenvalue equation of the coordinate operator $\mathbf{Q}$ and its Hermitian conjugate:

$$\mathbf{Q}|\{Q\}\rangle = Q|\{Q\}\rangle \qquad \text{and} \qquad \langle\{Q\}|\mathbf{Q} = Q\langle\{Q\}| \tag{3.41}$$

together with the closure relation over the eigenstates of $\mathbf{Q}$ and the corresponding orthonormality relations

$$\int_{-\infty}^{+\infty} |\{Q\}\rangle\langle\{Q\}|dQ = \mathbf{1} \qquad \text{and} \qquad \langle\{Q\}|\{Q'\}\rangle = \delta(Q-Q') \tag{3.42}$$

Now, consider the following scalar product of a ket $|\Psi\rangle$ by any eigenket $|\{Q\}\rangle$ of $\mathbf{Q}$ and its complex conjugate, that is,

$$\langle\{Q\}|\Psi\rangle = \Psi(Q) \qquad \text{and} \qquad \langle\Psi|\{Q\}\rangle = \Psi^*(Q) \tag{3.43}$$

Here, the scalar $\Psi(Q)$, which is by definition the *representation* $\{|\{Q\}\rangle\}$ of the ket $|\Psi\rangle$, is named the *wavefunction* associated with this ket at the measured position Q. It is generally complex. The squared modulus of this scalar product is

$$|\langle\{Q\}|\Psi\rangle|^2 = |\Psi(Q)|^2 \tag{3.44}$$

Owing to the fourth postulate, the left-hand side of Eq. (3.44) corresponds to the probability for the system to jump from the ket $|\Psi\rangle$ into the ket $|\{Q\}\rangle$, which is an eigenket of the position operator $\mathbf{Q}$ with the corresponding eigenvalue Q. Thus, on the right-hand side of Eq. (3.44), $|\Psi(Q)|^2$ *is the probability for the system described by the scalar function* $\Psi(Q)$ *to be found at the position* Q.

Now, consider the scalar products of two different kets $|\Psi\rangle$ and $|\Phi\rangle$, and introduce inside the scalar product the closure relation (3.42)

$$\langle\Psi|\Phi\rangle = \langle\Psi| \left\{ \int_{-\infty}^{+\infty} |\{Q\}\rangle\langle\{Q\}| dQ \right\} |\Phi\rangle$$

Since the integration operation commutes with the kets or the bras, the scalar product simply reads

$$\langle\Psi|\Phi\rangle = \int_{-\infty}^{+\infty} \langle\Psi|\{Q\}\rangle\langle\{Q\}|\Phi\rangle dQ$$

Thus, in view of Eq. (3.43), it takes the form

$$\langle\Psi|\Phi\rangle = \int_{-\infty}^{+\infty} \Psi^*(Q)\Phi(Q)\, dQ$$

Next, if the two kets involved in the scalar product belong to a given orthonormal basis, we have

$$\langle\Psi_k|\Psi_l\rangle = \int_{-\infty}^{+\infty} \Psi_k^*(Q)\Psi_l(Q)\, dQ = \delta_{kl} \tag{3.45}$$

When applied to the norm of any ket, Eq. (3.45) reduces to the *normalization* condition

$$\int_{-\infty}^{+\infty} \Psi_k^*(Q)\Psi_k(Q)\, dQ = 1$$

3.2.2 Many-particle systems

The fourth postulate allows one to find the ket of a system formed by many particles, each of them being characterized by their own ket. We illustrate as follows:

Consider the value of the total wavefunction $\Psi_{\text{Tot}}(Q)$ of two particles at any value Q of the position, the individual wavefunction of each particle being,

respectively, $\Phi^{\{1\}}(Q)$ and $\Phi^{\{2\}}(Q)$. The probability to find the two particles at position Q may be obtained by

$$\mathbb{P}_{\text{Tot}}(Q) = |\Psi_{\text{Tot}}(Q)|^2$$

Again, since the probabilities multiply, one has

$$|\Psi_{\text{Tot}}(Q)|^2 = |\Phi^{\{1\}}(Q)|^2 \, |\Phi^{\{2\}}(Q)|^2$$

As a consequence of each wavefunction working within its own state space, the total wavefunction may be written

$$\Psi_{\text{Tot}}(Q)\Psi_{\text{Tot}}(Q)^* = (\Phi^{\{1\}}(Q)\Phi^{\{1\}}(Q)^*)(\Phi^{\{2\}}(Q)\Phi^{\{2\}}(Q)^*)$$

so that

$$\Psi_{\text{Tot}}(Q) = \Phi^{\{1\}}(Q)\Phi^{\{2\}}(Q)$$

Hence, since the probabilities multiply, the meaning of the wavefunction implies that the total wavefunction of a system composed of two particles may be written as the product of the wavefunctions of each particle. By generalization to N particles, we have

$$\boxed{\Psi_{\text{Tot}}(Q) = \prod_{k=1}^{N} \Phi^{\{k\}}(Q)} \tag{3.46}$$

Furthermore, the wavefunctions $\Psi_{\text{Tot}}(Q)$ and $\Phi^{\{k\}}(Q)$ are given, respectively, by the following scalar products:

$$\Psi_{\text{Tot}}(Q) = \langle \{Q\} | \Psi_{\text{Tot}} \rangle$$

$$\Phi^{\{k\}}(Q) = \langle \{Q\} | \Phi^{\{k\}} \rangle$$

Then, Eq. (3.46) leads to

$$\langle \{Q\}| \, \Psi_{\text{Tot}} \rangle = \prod_{k=1}^{N} \langle \{Q\}| \, \Phi^{\{k\}} \rangle$$

This equation may be also written

$$\langle \{Q\}| \, \Psi_{\text{Tot}} \rangle = \langle \{Q\}| \prod_{k=1}^{N} |\Phi^{\{k\}} \rangle$$

Of course, this expression holds what may be the bra involved in the scalar products. Thus, it is possible to write

$$\boxed{|\Psi_{\text{Tot}}\rangle = \prod_{k=1}^{N} |\Phi^{\{k\}}\rangle} \tag{3.47}$$

That shows that the total ket of a system formed by several particles is the product of the kets of the different particles.

3.2.3 Momentum operator in representation $\{|\{Q\}\rangle\}$

In order to get the action of the momentum operator $\mathbf{P}$ on any ket $|\Psi\rangle$ within the $\{Q\}$ representation, introduce between $\mathbf{P}$ and $|\Psi\rangle$ the closure relation on the eigenkets of $\mathbf{P}$:

$$\langle\{Q\}|\mathbf{P}|\Psi\rangle = \langle\{Q\}|\mathbf{P}\left\{\int_{-\infty}^{+\infty}|\{P\}\rangle\langle\{P\}|dP\right\}|\Psi\rangle$$

which due to the eigenvalue equation of $\mathbf{P}$ becomes

$$\langle\{Q\}|\mathbf{P}|\Psi\rangle = \langle\{Q\}|\int_{-\infty}^{+\infty}P|\{P\}\rangle\langle\{P\}|\{\Psi\}\rangle dP$$

or, using

$$\langle\{P\}|\{\Psi\}\rangle = \Psi(P)$$

$$\langle\{Q\}|\mathbf{P}|\Psi\rangle = \int_{-\infty}^{+\infty}P\langle\{Q\}|\{P\}\rangle\Psi(P)dP \tag{3.48}$$

Moreover, observe that we have shown that the scalar product of an eigenket of $\mathbf{Q}$ by another one of $\mathbf{P}$ is given by Eq. (2.132), that is,

$$\langle\{P\}|\{Q\}\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left\{-\frac{iPQ}{\hbar}\right\}$$

so that Eq. (3.48) transforms to

$$\langle\{Q\}|\mathbf{P}|\Psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}P\exp\left\{-\frac{iPQ}{\hbar}\right\}\Psi(P)dP \tag{3.49}$$

Now, using Eq. (18.49), that is,

$$\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}Pf(P)e^{iQP/\hbar}dQ = i\hbar\left(\frac{\partial f(Q)}{\partial Q}\right) \quad \text{with} \quad \Psi(Q) = f(Q)$$

Eq. (3.49) takes the form

$$\boxed{\langle\{Q\}|\mathbf{P}|\Psi\rangle = i\hbar\left(\frac{\partial\Psi(Q)}{\partial Q}\right)} \tag{3.50}$$

This last result shows that in the quantum representation $\{|\{Q\}\rangle\}$, the momentum operator is acting on a wavefunction as a partial derivative with respect to the scalar Q times $\hbar/i$, which may be written formally as

$$\boxed{P = \frac{\hbar}{i}\frac{\partial}{\partial Q} = -i\hbar\frac{\partial}{\partial Q}} \tag{3.51}$$

Of course, in the quantum representation $\{|\{Q\}\rangle\}$, the action of the operator $\mathbf{Q}$ over some ket $|\Psi\rangle$ reads

$$\langle\{Q\}|\mathbf{Q}|\Psi\rangle = Q\langle\{Q\}|\Psi\rangle = Q\Psi(Q) \tag{3.52}$$

Observe that the following commutator reads

$$[Q,P] = \frac{\hbar}{i}\left(Q\frac{\partial}{\partial Q} - \frac{\partial}{\partial Q}Q\right)$$

thereby taking into account the fact that the right-hand side of this last equation is acting on any function. Thus one has to write

$$\frac{\partial}{\partial Q}Q = Q\frac{\partial}{\partial Q} + 1$$

and, after simplification, the above commutator becomes

$$\boxed{[Q,P] = i\hbar}$$

That is the equivalent in the quantum representation $\{|\{Q\}\rangle\}$ of the fundamental commutator given by the last postulate of quantum mechanics:

$$[\mathbf{Q},\mathbf{P}] = i\hbar$$

3.2.4 Time-independent Schrödinger equation

Consider some operator function $\mathbf{F}(\mathbf{Q},\mathbf{P})$ of $\mathbf{P}$ and $\mathbf{Q}$ that may be separately expanded in powers of $\mathbf{P}$ and $\mathbf{Q}$ according to

$$\mathbf{F}(\mathbf{Q},\mathbf{P}) = \sum_n \{C_n\mathbf{P}^n + B_n\mathbf{Q}^n\} \tag{3.53}$$

where C_n and B_n are, respectively, the expansion coefficients that are scalars.

Now, consider matrix elements of this operator:

$$\langle\{Q\}|\mathbf{F}(\mathbf{Q},\mathbf{P})|\Psi\rangle = \sum_n \langle\{Q\}|\{C_n\mathbf{P}^n + B_n\mathbf{Q}^n\}|\Psi\rangle \tag{3.54}$$

Again, owing to Eqs. (3.52), and (3.50), it appears that

$$\langle\{Q\}|\mathbf{Q}^n|\Psi\rangle = Q^n\Psi(Q) \tag{3.55}$$

$$\langle\{Q\}|\mathbf{P}^n|\Psi\rangle = \left(\frac{\hbar}{i}\frac{\partial}{\partial Q}\right)^n \Psi(Q) \tag{3.56}$$

Hence, with Eqs. (3.55) and (3.56), Eq. (3.54) transforms to

$$\langle\{Q\}|\mathbf{F}(\mathbf{Q},\mathbf{P})|\Psi\rangle = \sum_n \left\{C_n\left(\frac{\hbar}{i}\frac{\partial}{\partial Q}\right)^n + B_nQ^n\right\}\Psi(Q) \tag{3.57}$$

When the operator $\mathbf{F}(\mathbf{Q},\mathbf{P})$ is the Hamiltonian $\mathbf{H}(\mathbf{Q},\mathbf{P})$

$$\mathbf{H}(\mathbf{Q},\mathbf{P}) = \mathbf{T}(\mathbf{P}) + \mathbf{V}(\mathbf{Q})$$

with

$$\mathbf{T}(\mathbf{P}) = \frac{\mathbf{P}^2}{2m} \qquad \text{and} \qquad \mathbf{V}(\mathbf{Q}) = \sum_n B_n \mathbf{Q}^n$$

Eq. (3.57) takes the form

$$\langle \{Q\} | \mathbf{H}(\mathbf{Q}, \mathbf{P}) | \Psi \rangle = \hat{H} \Psi(Q) \tag{3.58}$$

with

$$\hat{H} = \hat{T} + \hat{V}(Q) \quad \text{with} \quad \hat{T} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial Q^2} \tag{3.59}$$

and

$$\hat{V}(Q) = B_n Q^n$$

so that

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial Q^2} + \hat{V}(Q) \tag{3.60}$$

This equation is the wave mechanics representation of the Hamiltonian, the eigenvalue equation of which is

$$\hat{H} \Phi_k(Q) = E_k \Phi_k(Q)$$

or

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial Q^2} \Phi_k(Q) + \hat{V}(Q) \Phi_k(Q) = E_k \Phi_k(Q) \tag{3.61}$$

This is the time-independent Schrödinger equation, that is, the wave mechanics representation of the Hamiltonian eigenvalue equation

$$\mathbf{H}(\mathbf{Q}, \mathbf{P}) | \Phi_k \rangle = E_k | \Phi_k \rangle \tag{3.62}$$

3.2.5 Wavefunction boundary conditions

The eigenvalues E_k are the same in both Eqs. (3.61) and (3.62), whereas the connection between the eigenfunction $\Phi_k(Q)$ of H and the eigenket $|\Phi_k\rangle$ of $\mathbf{H}(\mathbf{Q}, \mathbf{P})$ is through the following scalar product:

$$\Phi_k(Q) = \langle \{Q\} | \Phi_k \rangle \tag{3.63}$$

Recall that, the fourth postulate allows one to write

$$|\langle \{Q\} | \Phi_k \rangle|^2 = |\Phi_k(Q)|^2 \equiv \mathbb{P}(Q) \tag{3.64}$$

Observe that $\mathbb{P}(Q)$ may be regarded as the probability density, which is also denoted $\rho(Q)$. Again, since the probabilities $\mathbb{P}(Q)$ must obey

$$\int_{-\infty}^{+\infty} \mathbb{P}(Q) dQ = 1$$

thus Eq. (3.64) implies that the wavefunction $\Phi_k(Q)$ has the normalization property

$$\boxed{\int_{-\infty}^{+\infty} |\Phi_k(Q)|^2 dQ = 1} \tag{3.65}$$

Furthermore, if the wavefunction is not normalized, it may be written as $\tilde{\Phi}_k(Q)$. In order to be square summable, its integral must be finite according to

$$\int_{-\infty}^{+\infty} |\tilde{\Phi}_k(Q)|^2 dQ = k^2 \quad \text{with } k^2 \text{ finite}$$

Then, in order to satisfy Eq. (3.65), one has

$$\Phi_k(Q) = \frac{1}{k}\tilde{\Phi}_k(Q)$$

where $1/k$ is the normalization constant. The normalization condition implies that at infinity the wavefunction must vanish, that is,

$$\boxed{\Phi_k(Q \to \pm\infty) \to 0} \tag{3.66}$$

This is an essential boundary condition for the time-independent Schrödinger equation (3.61). Such a condition leads to quantized eigenvalues and thus to quantized energy levels, not only for the eigenvalue equation (3.61) but also for that (3.62), which is equivalent.

Since the eigenvalue equation (3.61) has the structure of a wave equation, the $\{Q\}$ representation (3.61) of the eigenvalue equation (3.62) of the Hamiltonian may be viewed as a *wave mechanics equation.*

3.2.6 Time-dependent Schrödinger equation

From the Schrödinger equation it is possible, with help from the sixth postulate, to find the linear time-dependent operator that transforms some ket at initial time $|\Psi(0)\rangle$ into the corresponding one $|\Psi(t)\rangle$ at time t.

To get this operator, we start from the Schrödinger equation

$$i\hbar\left(\frac{\partial|\Psi(t)\rangle}{\partial t}\right) = \mathbf{H}|\Psi(t)\rangle$$

In order to solve this equation, premultiply it by some eigenbra of $\mathbf{Q}$ leading to

$$i\hbar\left(\frac{\partial\langle\{Q\}|\Psi(t)\rangle}{\partial t}\right) = \langle\{Q\}|\mathbf{H}|\Psi(t)\rangle$$

or, due to Eq. (3.58),

$$\boxed{i\hbar\left(\frac{\partial\Psi(Q,t)}{\partial t}\right) = \hat{H}\Psi(Q,t)} \tag{3.67}$$

By omitting the Q dependence, after integration between $t = 0$ and t one obtains

$$\ln\left(\frac{\Psi(t)}{\Psi(0)}\right) = -\frac{i}{\hbar}\hat{H}t$$

Passing to the exponential, that reads

$$\frac{\Psi(t)}{\Psi(0)} = e^{-i\hat{H}t/\hbar}$$

or

$$\boxed{\Psi(t) = e^{-i\hat{H}t/\hbar}\Psi(0)} \tag{3.68}$$

3.2.7 Current density and continuity equation

Now, let us define the *current density* operator according to the Hermitian product of the two Hermitian operators $\mathbf{P}|\{Q\}\rangle\langle\{Q\}|$ and $|\{Q\}\rangle\langle\{Q\}|\mathbf{P}$:

$$\mathbf{J} \equiv \frac{1}{2m}\{\mathbf{P}|\{Q\}\rangle\langle\{Q\}| + |\{Q\}\rangle\langle\{Q\}|\mathbf{P}\}$$

Now, consider the diagonal matrix elements of this operator built up from some eigenkets of any Hermitian operator, that is,

$$J = \langle\Psi|\mathbf{J}|\Psi\rangle$$

This representation of the operator is therefore

$$J = \left\{\frac{1}{2m}\langle\Psi|\mathbf{P}|\{Q\}\rangle\langle\{Q\}|\Psi\rangle\right\} + \text{hc}$$

where hc denotes the Hermitian conjugate. Then, using Eq. (3.50) and its Hermitian conjugate, one obtains

$$\boxed{J = -\left(i\frac{\hbar}{2m}\right)\left(\Psi(Q)^*\frac{\partial}{\partial Q}\Psi(Q) - \Psi(Q)\frac{\partial}{\partial Q}\Psi(Q)^*\right)} \tag{3.69}$$

Now, in order to find the continuity equation governing the wavefunction, differentiate the current density (3.69) with respect to Q

$$\left(\frac{\partial J}{\partial Q}\right) = -\left(i\frac{\hbar}{2m}\right)\frac{\partial}{\partial Q}\left(\Psi^*\frac{\partial}{\partial Q}\Psi - \Psi\frac{\partial}{\partial Q}\Psi^*\right) \tag{3.70}$$

One obtains, respectively,

$$\frac{\partial}{\partial Q}\left(\Psi^*\frac{\partial}{\partial Q}\Psi\right) = \left(\frac{\partial}{\partial Q}\Psi^*\frac{\partial}{\partial Q}\Psi + \Psi^*\frac{\partial^2}{\partial Q^2}\Psi\right)$$

$$\frac{\partial}{\partial Q}\left(\Psi\frac{\partial}{\partial Q}\Psi^*\right) = \left(\frac{\partial}{\partial Q}\Psi\frac{\partial}{\partial Q}\Psi^* + \Psi\frac{\partial^2}{\partial Q^2}\Psi^*\right)$$

Thus, Eq. (3.70) transforms to

$$\left(\frac{\partial J}{\partial Q}\right) = -\left(i\frac{\hbar}{2m}\right)\left(\Psi^*\frac{\partial^2}{\partial Q^2}\Psi - \Psi\frac{\partial^2}{\partial Q^2}\Psi^*\right) \tag{3.71}$$

On the other hand, consider the probability density related to the wavefunction

$$\boxed{\rho = \Psi^*\Psi} \tag{3.72}$$

By differentiation with respect to time, we get

$$\left(\frac{\partial \rho}{\partial t}\right) = \left(\frac{\partial \Psi^*}{\partial t}\right)\Psi + \Psi^*\left(\frac{\partial \Psi}{\partial t}\right) \tag{3.73}$$

Besides, the two derivatives of the wavefunction are governed by the time-dependent Schrödinger equation (3.67) and its Hermitian conjugate, that is,

$$i\hbar\left(\frac{\partial \Psi}{\partial t}\right) = H\Psi \qquad \text{and} \qquad -i\hbar\left(\frac{\partial \Psi^*}{\partial t}\right) = \hat{H}\Psi^* \tag{3.74}$$

Moreover, according to Eq. (3.60), the Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial Q^2}\right) + \hat{V}$$

Hence, Eqs. (3.74) lead to

$$i\hbar\left(\frac{\partial \Psi}{\partial t}\right) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial Q^2}\right)\Psi + \hat{V}\Psi \quad \text{and} \quad -i\hbar\left(\frac{\partial \Psi^*}{\partial t}\right) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial Q^2}\right)\Psi^* + \hat{V}\Psi^*$$

These two last equations allow one to transform Eq. (3.73) into

$$\left(\frac{\partial \rho}{\partial t}\right) = -i\left(\frac{\hbar}{2m}\right)\left\{\Psi\frac{\partial^2}{\partial Q^2}\Psi^* - \Psi^*\frac{\partial^2}{\partial Q^2}\Psi\right\}$$

Finally, it appears from comparison with Eq. (3.71) that the following one-dimensional equation is verified:

$$\left(\frac{\partial \rho}{\partial t}\right) = -\left(\frac{\partial J}{\partial Q}\right)$$

By generalization to the three-dimensional equation, one obtains the *continuity equation*

$$\boxed{\left(\frac{\partial \rho}{\partial t}\right) + \mathbf{Div}\ \vec{J} = 0} \tag{3.75}$$

where the arrow indicates a vectorial entity.

3.3 EVOLUTION OPERATORS

As we have seen, when considering the sixth postulate of quantum mechanics dealing with the dynamics involved in quantum mechanics, there are several time-dependent descriptions of quantum mechanics. In the *Schrödinger picture (SP)*, the kets depend on time, whereas the operators do not change with it. However, another time-dependent description, the *Heisenberg picture (HP)* exists, where the operators depend on time whereas the kets remain constant. Finally, many other time-dependent representations of quantum mechanics exist, which are intermediate between the Schrödinger and the Heisenberg pictures, in which both the kets and the operators depend on time in subtle ways. They are named the *interaction pictures*. We shall first consider the *time evolution operator* within the Schrödinger picture.

3.3.1 Schrödinger picture

Starting from the Schrödinger equation defined by the sixth postulate and governing the dynamics of some time-dependent ket $|\Psi(t)\rangle$

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \mathbf{H}|\Psi(t)\rangle \tag{3.76}$$

where $\mathbf{H}$ is the total Hamiltonian of the system. Then, we introduce a linear operator $\mathbf{U}(t)$, the time evolution operator, allowing one to transform the ket $|\Psi(0)\rangle$ at an initial time $t = 0$ into one at time t according to

$$\boxed{|\Psi(t)\rangle = \mathbf{U}(t)|\Psi(0)\rangle} \tag{3.77}$$

with the obvious condition

$$\mathbf{U}(0) = 1$$

Then, time differentiation of Eq. (3.77) yields

$$\frac{\partial}{\partial t}|\Psi(t)\rangle = \left(\frac{\partial \mathbf{U}(t)}{\partial t}\right)|\Psi(0)\rangle \tag{3.78}$$

Again, introduce on the right-hand side of Eq. (3.78)

$$\mathbf{U}(t)^{-1}\mathbf{U}(t) = 1 \tag{3.79}$$

in such a way as to write

$$\frac{\partial}{\partial t}|\Psi(t)\rangle = \left(\frac{\partial \mathbf{U}(t)}{\partial t}\right)\mathbf{U}(t)^{-1}\mathbf{U}(t)|\Psi(0)\rangle$$

leading with the help of Eq. (3.77) and after multiplying by $i\hbar$, to

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = i\hbar\left(\frac{\partial \mathbf{U}(t)}{\partial t}\right)\mathbf{U}(t)^{-1}|\Psi(t)\rangle \tag{3.80}$$

Thus, identification of Eqs. (3.76) and (3.80) yields

$$\mathbf{H}|\Psi(t)\rangle = i\hbar\left(\frac{\partial \mathbf{U}(t)}{\partial t}\right)\mathbf{U}(t)^{-1}|\Psi(t)\rangle$$

Hence, since this latter result holds irrespective of $|\Psi(t)\rangle$, it appears that the following relation between the operators $\mathbf{U}(t)$ and $\mathbf{H}$ exists:

$$\boxed{i\hbar\left(\frac{\partial \mathbf{U}(t)}{\partial t}\right) = \mathbf{H}\mathbf{U}(t)} \tag{3.81}$$

The foregoing partial differential equation reads

$$\frac{d\mathbf{U}(t)}{\mathbf{U}(t)} = -\frac{i}{\hbar}\mathbf{H}\,dt$$

which, by integration yields

$$\ln\frac{\mathbf{U}(t)}{\mathbf{U}(0)} = -\frac{i}{\hbar}\mathbf{H}t$$

or due to the boundary condition (3.79)

$$\boxed{\mathbf{U}(t) = e^{-i\mathbf{H}t/\hbar}} \tag{3.82}$$

Observe that the Hamiltonian $\mathbf{H}$ being Hermitian, the evolution operator $\mathbf{U}(t)$ is unitary since its inverse is equal to its Hermitian conjugate, that is,

$$\mathbf{U}(t)^{-1} = \mathbf{U}(t)^{\dagger} = e^{i\mathbf{H}t/\hbar} \tag{3.83}$$

so that

$$\mathbf{U}(t)^{\dagger}\mathbf{U}(t) = \mathbf{U}(t)^{-1}\mathbf{U}(t) = 1 \tag{3.84}$$

Moreover, due to Eq. (3.82), Eq. (3.77) becomes

$$|\Psi(t)\rangle = (e^{-i\mathbf{H}t/\hbar})|\Psi(0)\rangle \tag{3.85}$$

We remark that Eq. (3.68) is the wave mechanics representation of the quantum relation (3.85).

Sometimes the Hamiltonian may depend on time, so that one has to solve a dynamic equation that is more complicated than (3.81) and of the form

$$i\hbar\left(\frac{\partial \mathbf{U}(t)}{\partial t}\right) = \mathbf{H}(t)\mathbf{U}(t) \tag{3.86}$$

Here, the Hamiltonians at different times do not commute:

$$[\mathbf{H}(t), \mathbf{H}(t')] \neq 0$$

Moreover, it is possible to write formally a solution of Eq. (3.86) in the same way as (3.81) according to

$$\boxed{\mathbf{U}(t) = \hat{\mathbf{P}} \exp\left\{-\frac{i}{\hbar}\int_0^t \mathbf{H}(t')\,dt'\right\}} \tag{3.87}$$

where $\hat{\mathbf{P}}$ is the *Dyson time-ordering operator*.

3.3.2 Heisenberg picture

Now, it is suitable to introduce a new time-independent picture in which (in contrast to the Schrödinger picture where the kets are time dependent and the operators constant) the kets are constant and the operators time dependent. This is the *Heisenberg picture*. For this purpose, we start from the Schrödinger picture equation (2.65) yielding the mean value of some operator $\mathbf{A}$ averaged over the time-dependent states, that is,

$$\langle \mathbf{A}(t)\rangle_{\Psi_k} = \langle \Psi_k(t)^{\mathrm{SP}}|\mathbf{A}^{\mathrm{SP}}|\Psi_k(t)^{\mathrm{SP}}\rangle$$

where the superior index SP indicates that the Schrödinger picture has been used. Next, due to Eq. (3.85) and to its Hermitian conjugate, this average value reads

$$\langle \mathbf{A}(t)\rangle_{\Psi_k} = \langle \Psi_k(0)|(e^{i\mathbf{H}t/\hbar})\mathbf{A}^{\mathrm{SP}}(e^{-i\mathbf{H}t/\hbar})|\Psi_k(0)\rangle$$

which may be written

$$\langle \mathbf{A}(t)\rangle_{\Psi_k} = \langle \Psi_k^{\mathrm{HP}} | \mathbf{A}(t)^{\mathrm{HP}} | \Psi_k^{\mathrm{HP}} \rangle$$

where $|\Psi_k^{\mathrm{HP}}\rangle$ is the time-independent ket in the Heisenberg picture, whereas $\mathbf{A}(t)^{\mathrm{HP}}$ is the time-dependent operator in this same Heisenberg picture given by

$$\boxed{\mathbf{A}(t)^{\mathrm{HP}} = (e^{i\mathbf{H}t/\hbar})\mathbf{A}^{\mathrm{SP}}(e^{-i\mathbf{H}t/\hbar})} \tag{3.88}$$

or, due to Eqs. (3.82) and (3.83), by

$$\boxed{\mathbf{A}(t)^{\mathrm{HP}} = \mathbf{U}(t)^{\dagger}\mathbf{A}^{\mathrm{SP}}\mathbf{U}(t)} \tag{3.89}$$

Since the operator $\mathbf{A}$ in the Schrödinger picture is time independent, the time derivation of each members of Eq. (3.89) gives after writing $\mathbf{A}^{\mathrm{SP}} = \mathbf{A}$

$$\left(\frac{\partial \mathbf{A}(t)^{\mathrm{HP}}}{\partial t}\right) = \left(\frac{\partial \mathbf{U}(t)^{\dagger}}{\partial t}\right)\mathbf{A}\mathbf{U}(t) + \mathbf{U}(t)^{\dagger}\mathbf{A}\left(\frac{\partial \mathbf{U}(t)}{\partial t}\right) \tag{3.90}$$

Besides, since the Hamiltonian $\mathbf{H}$ is Hermitian, note that the derivative with respect to time of the evolution operator (3.82) and that of its Hermitian conjugate (3.83) are, respectively

$$\left(\frac{\partial \mathbf{U}(t)}{\partial t}\right) = -\left(\frac{i}{\hbar}\right)\mathbf{H}\mathbf{U}(t)$$

$$\left(\frac{\partial \mathbf{U}(t)^{\dagger}}{\partial t}\right) = \left(\frac{i}{\hbar}\right)\mathbf{U}(t)^{\dagger}\mathbf{H}$$

Using these two equations, Eq. (3.90) becomes

$$\left(\frac{\partial \mathbf{A}(t)^{\mathrm{HP}}}{\partial t}\right) = \left(\frac{i}{\hbar}\right)\mathbf{U}(t)^{\dagger}\mathbf{H}\mathbf{A}\mathbf{U}(t) - \left(\frac{i}{\hbar}\right)\mathbf{U}(t)^{\dagger}\mathbf{A}\mathbf{H}\mathbf{U}(t) \tag{3.91}$$

Next, using Eq. (3.84), that is,

$$\mathbf{1} = \mathbf{U}(t)\mathbf{U}(t)^{\dagger} \tag{3.92}$$

and, inserting on the right-hand-side term of Eq. (3.91) this unity operator, first between the Hamiltonian $\mathbf{H}$ and the operator $\mathbf{A}$, and then between the operator $\mathbf{A}$ and the Hamiltonian $\mathbf{H}$, one obtains

$$\left(\frac{\partial \mathbf{A}(t)^{\mathrm{HP}}}{\partial t}\right) = \left(\frac{i}{\hbar}\right)\mathbf{U}(t)^{\dagger}\mathbf{H}\{\mathbf{U}(t)\mathbf{U}(t)^{\dagger}\}\mathbf{A}\mathbf{U}(t) - \left(\frac{i}{\hbar}\right)\mathbf{U}(t)^{\dagger}\mathbf{A}\{\mathbf{U}(t)\mathbf{U}(t)^{\dagger}\}\mathbf{H}\mathbf{U}(t)$$

Thus, by changing the position of the brackets, we have

$$\left(\frac{\partial \mathbf{A}(t)^{\mathrm{HP}}}{\partial t}\right) = \left(\frac{i}{\hbar}\right)(\{\mathbf{U}(t)^{\dagger}\mathbf{H}\mathbf{U}(t)\}\{\mathbf{U}(t)^{\dagger}\mathbf{A}\mathbf{U}(t)\} - \{\mathbf{U}(t)^{\dagger}\mathbf{A}\mathbf{U}(t)\}\{\mathbf{U}(t)^{\dagger}\mathbf{H}\mathbf{U}(t)\}) \tag{3.93}$$

Now, observe that, according to Eqs. (3.82) and (3.83),

$$\{\mathbf{U}(t)^{\dagger}\mathbf{H}\mathbf{U}(t)\} = (e^{i\mathbf{H}t/\hbar})\mathbf{H}(e^{-i\mathbf{H}t/\hbar})$$

Again, since the exponential depends on the Hamiltonian, it must commute with it, so that after simplification this unitary transformation reduces to

$$\{\mathbf{U}(t)^{\dagger}\mathbf{H}\mathbf{U}(t)\} = \mathbf{H}$$

Hence, Eq. (3.93) simplifies to

$$i\hbar\left(\frac{\partial \mathbf{A}(t)^{\mathrm{HP}}}{\partial t}\right) = -(\mathbf{H}\{\mathbf{U}(t)^{\dagger}\mathbf{A}\mathbf{U}(t)\} - \{\mathbf{U}(t)^{\dagger}\mathbf{A}\mathbf{U}(t)\}\mathbf{H})$$

Thus, due to the definition (3.89), this equation transforms to the final result, which is the Heisenberg equation governing the dynamics of any operator in the Heisenberg picture:

$$\boxed{i\hbar\left(\frac{\partial \mathbf{A}(t)^{\mathrm{HP}}}{\partial t}\right) = [\mathbf{A}^{\mathrm{HP}}(t), \mathbf{H}]} \tag{3.94}$$

This equation contains the same information as the Schrödinger time-dependent equation in the Schrödinger picture. It may also be of interest to take the average of this equation in a state $|\Psi\rangle$, in postmultiplying both terms of this equation by $|\Psi\rangle$, and premultiplying them by $\langle\Psi|$

$$i\hbar\langle\Psi|\left(\frac{\partial \mathbf{A}(t)^{\mathrm{HP}}}{\partial t}\right)|\Psi\rangle = \langle\Psi|[\mathbf{A}^{\mathrm{HP}}(t), \mathbf{H}]|\Psi\rangle \tag{3.95}$$

This time dependence of the average value in the Heisenberg picture may be compared to that (2.55) we have obtained above in the Schrödinger picture, that is,

$$i\hbar\langle\Psi(t)|\left(\frac{\partial \mathbf{A}}{\partial t}\right)|\Psi(t)\rangle = \langle\Psi(t)|[\mathbf{A}, \mathbf{H}]|\Psi(t)\rangle \tag{3.96}$$

Comparison of the Heisenberg picture (3.95) and Schödinger picture (3.96) shows clearly the exchange of the time dependence between the operator and the kets.

3.3.3 Hamilton equations

Consider the position and momentum operators in the Heisenberg picture. To simplify the notation, we shall write

$$\mathbf{Q}(t)^{\mathrm{HP}} \equiv \mathbf{Q}(t) \qquad \text{and} \qquad \mathbf{P}(t)^{\mathrm{HP}} \equiv \mathbf{P}(t)$$

These operators are given in the Heisenberg picture by

$$\mathbf{Q}(t) = \mathbf{U}(t)^{\dagger}\mathbf{Q}\mathbf{U}(t) \qquad \text{and} \qquad \mathbf{P}(t) = \mathbf{U}(t)^{\dagger}\mathbf{P}\mathbf{U}(t) \tag{3.97}$$

First, verify that the commutators of the two operators remain the same in the Heisenberg picture, where they are time dependent, as in the Schrödinger picture where they are not so. To verify that, use Eq. (3.97) to write explicitly the commutator appearing on the left-hand side, yielding

$$[\mathbf{Q}(t), \mathbf{P}(t)] = \mathbf{U}(t)^{\dagger}\mathbf{Q}\mathbf{U}(t)\mathbf{U}(t)^{\dagger}\mathbf{P}\mathbf{U}(t) - \mathbf{U}(t)^{\dagger}\mathbf{P}\mathbf{U}(t)\mathbf{U}(t)^{\dagger}\mathbf{Q}\mathbf{U}(t)$$

After simplification using Eq. (3.92), we have

$$[\mathbf{Q}(t), \mathbf{P}(t)] = \mathbf{U}(t)^{\dagger}[\mathbf{Q}, \mathbf{P}]\mathbf{U}(t)$$

so that, after using Eq. (3.92), it appears that

$$[\mathbf{Q}(t), \mathbf{P}(t)] = [\mathbf{Q}, \mathbf{P}]$$

or, due to the basic commutator (2.3), of $\mathbf{Q}$ and $\mathbf{P}$

$$[\mathbf{Q}(t), \mathbf{P}(t)] = i\hbar \tag{3.98}$$

Now, from the Heisenberg dynamic equation (3.94), it is possible to obtain the dynamics governing the time dependence of the position operator and its conjugate momentum.

First consider that of the $\mathbf{Q}(t)$ coordinate. Keeping in mind that $\mathbf{Q}(t)$ depends only on time, Eq. (3.94) allows one to write the differential equation

$$i\hbar \left(\frac{d\mathbf{Q}(t)}{dt} \right) = [\mathbf{Q}, \mathbf{H}(\mathbf{Q}, \mathbf{P})] \tag{3.99}$$

Next, use the theorem (2.14), which in the present situation reads as follows:

$$[\mathbf{Q}, \mathbf{H}(\mathbf{Q}, \mathbf{P})] = i\hbar \left(\frac{\partial \mathbf{H}(\mathbf{Q}, \mathbf{P})}{\partial \mathbf{P}} \right)$$

Then, in view of this result, Eq. (3.99) takes the form

$$\left(\frac{d\mathbf{Q}(t)}{dt} \right) = \left(\frac{\partial \mathbf{H}(\mathbf{Q}, \mathbf{P})}{\partial \mathbf{P}} \right) \tag{3.100}$$

Now, consider the Heisenberg equation governing the dynamics of the momentum

$$i\hbar \left(\frac{d\mathbf{P}(t)}{dt} \right) = [\mathbf{P}, \mathbf{H}(\mathbf{Q}, \mathbf{P})] \tag{3.101}$$

Next, in view of Eq. (2.15), the commutator involved in this equation reads

$$[\mathbf{P}, \mathbf{H}(\mathbf{Q}, \mathbf{P})] = -i\hbar \left(\frac{\partial \mathbf{H}(\mathbf{Q}, \mathbf{P})}{\partial \mathbf{Q}} \right)$$

Thus, Eq. (3.101) becomes

$$\left(\frac{d\mathbf{P}(t)}{dt} \right) = -\left(\frac{\partial \mathbf{H}(\mathbf{Q}, \mathbf{P})}{\partial \mathbf{Q}} \right) \tag{3.102}$$

Both Eqs. (3.100) and (3.102), which satisfy the quantum commutator (3.98), are the quantum Hamilton equations of motion, the classical limits of which are the classical Hamilton equations

$$\left(\frac{d\vec{P}}{dt} \right) = -\left(\frac{\partial H}{\partial \vec{Q}} \right) \quad \text{and} \quad \left(\frac{d\vec{Q}}{dt} \right) = \left(\frac{\partial H}{\partial \vec{P}} \right) \quad \text{with} \quad [\vec{Q}, \vec{P}] = 0$$

3.3.4 Interaction picture

Now, consider a new time-dependent picture of quantum mechanics, the *interaction picture (IP)*, which is intermediate between the Schrödinger and Heisenberg pictures. This picture is sometimes more practical than the pure Schrödinger and Heisenberg representations.

3.3.4.1 Operators and kets in the interaction picture Suppose that the Hamiltonian $\mathbf{H}$ of a system may be split into two parts $\mathbf{H}^\circ$ and $\mathbf{V}$

$$\mathbf{H} = \mathbf{H}^\circ + \mathbf{V} \tag{3.103}$$

Now, we may introduce an IP time-dependent ket through an action on a time-dependent ket in the Schrödinger picture by aid of the Hermitian of the time evolution operator obtained from $\mathbf{H}^\circ$

$$\boxed{|\Psi(t)^{\mathrm{IP}}\rangle \equiv (e^{i\mathbf{H}^\circ t/\hbar})|\Psi(t)^{\mathrm{SP}}\rangle} \tag{3.104}$$

$|\Psi(t)^{\mathrm{SP}}\rangle$ is the ket at time t in the Schrödinger representation, whereas $|\Psi(t)^{\mathrm{IP}}\rangle$ is the corresponding ket at the same time t in the interaction picture.

Now, premultiply each member of this last equation by the inverse of the time evolution operator involved in the previous equation.

$$(e^{-i\mathbf{H}^\circ t/\hbar})|\Psi(t)^{\mathrm{IP}}\rangle = (e^{-i\mathbf{H}^\circ t/\hbar})(e^{i\mathbf{H}^\circ t/\hbar})|\Psi(t)^{\mathrm{SP}}\rangle$$

After simplification, which leads to the equation inverse of (3.104) which allows us to pass from the IP to the SP for all kets

$$|\Psi(t)^{\mathrm{SP}}\rangle = (e^{-i\mathbf{H}^\circ t/\hbar})|\Psi(t)^{\mathrm{IP}}\rangle \tag{3.105}$$

Next, take the partial time derivative of Eq. (3.104), that is,

$$\left(\frac{\partial|\Psi(t)^{\mathrm{IP}}\rangle}{\partial t}\right) = (e^{i\mathbf{H}^\circ t/\hbar})\left(\frac{\partial|\Psi(t)^{\mathrm{SP}}\rangle}{\partial t}\right) + \left(\frac{\partial e^{i\mathbf{H}^\circ t/\hbar}}{\partial t}\right)|\Psi(t)^{\mathrm{SP}}\rangle$$

The last partial time derivative appearing on the right-hand side of this equation is

$$\left(\frac{\partial e^{i\mathbf{H}^\circ t/\hbar}}{\partial t}\right) = \left(\frac{i}{\hbar}\right)\mathbf{H}^\circ(e^{i\mathbf{H}^\circ t/\hbar})$$

whereas the first one is given by the time-dependent Schrödinger equation defined by the sixth postulate, that is,

$$\left(\frac{\partial|\Psi(t)^{\mathrm{SP}}\rangle}{\partial t}\right) = \left(\frac{1}{i\hbar}\right)\mathbf{H}|\Psi(t)^{\mathrm{SP}}\rangle$$

Thus, the time derivative of the IP ket becomes

$$i\hbar\left(\frac{\partial|\Psi(t)^{\mathrm{IP}}\rangle}{\partial t}\right) = (e^{i\mathbf{H}^\circ t/\hbar})\mathbf{H}|\Psi(t)^{\mathrm{SP}}\rangle - \mathbf{H}^\circ(e^{i\mathbf{H}^\circ t/\hbar})|\Psi(t)^{\mathrm{SP}}\rangle$$

Next, use for the right-hand-side SP kets, Eq. (3.105), in order to obtain an equation involving only IP kets. Hence

$$i\hbar\left(\frac{\partial|\Psi(t)^{\mathrm{IP}}\rangle}{\partial t}\right) = (e^{i\mathbf{H}^\circ t/\hbar})\mathbf{H}(e^{-i\mathbf{H}^\circ t/\hbar})|\Psi(t)^{\mathrm{IP}}\rangle - \mathbf{H}^\circ|\Psi(t)^{\mathrm{IP}}\rangle \tag{3.106}$$

where we have performed a simplification on the right-hand-side because the Hamiltonian $\mathbf{H}^\circ$ commutes with all function of it, that is,

$$\mathbf{H}^\circ = (e^{i\mathbf{H}^\circ t/\hbar})\mathbf{H}^\circ(e^{-i\mathbf{H}^\circ t/\hbar})$$

Thus, one may use in Eq. (3.106) the right-hand side of this last equation in place of $\mathbf{H}^\circ$, which reads

$$i\hbar\left(\frac{\partial|\Psi(t)^{\mathrm{IP}}\rangle}{\partial t}\right) = (e^{i\mathbf{H}^\circ t/\hbar})\mathbf{H}(e^{-i\mathbf{H}^\circ t/\hbar})|\Psi(t)^{\mathrm{IP}}\rangle - (e^{i\mathbf{H}^\circ t/\hbar})\mathbf{H}^\circ(e^{-i\mathbf{H}^\circ t/\hbar})|\Psi(t)^{\mathrm{IP}}\rangle$$

Then, rearranging, one obtains

$$i\hbar\left(\frac{\partial|\Psi(t)^{\mathrm{IP}}\rangle}{\partial t}\right) = (e^{i\mathbf{H}^\circ t/\hbar})(\mathbf{H}-\mathbf{H}^\circ)(e^{-i\mathbf{H}^\circ t/\hbar})|\Psi(t)^{\mathrm{IP}}\rangle$$

Again, in view of the partition (3.103), the previous expression reduces to

$$i\hbar\left(\frac{\partial|\Psi(t)^{\mathrm{IP}}\rangle}{\partial t}\right) = (e^{i\mathbf{H}^\circ t/\hbar})\mathbf{V}(e^{-i\mathbf{H}^\circ t/\hbar})|\Psi(t)^{\mathrm{IP}}\rangle$$

which may be written

$$\boxed{i\hbar\left(\frac{\partial|\Psi(t)^{\mathrm{IP}}\rangle}{\partial t}\right) = \mathbf{V}(t)^{\mathrm{IP}}|\Psi(t)^{\mathrm{IP}}\rangle} \tag{3.107}$$

where $\mathbf{V}(t)^{\mathrm{IP}}$ is the perturbation $\mathbf{V}$ in the interaction picture, which is given by

$$\boxed{\mathbf{V}(t)^{\mathrm{IP}} = (e^{i\mathbf{H}^\circ t/\hbar})\mathbf{V}(e^{-i\mathbf{H}^\circ t/\hbar})} \tag{3.108}$$

Observe that in the IP both the perturbation operator and the ket are time dependent at the difference of the SP and HP where it is either the ket or the operator, which evolves with time. More generally, under partition (3.103), the IP time dependence of an operator is given by

$$\mathbf{A}(t)^{\mathrm{IP}} = (e^{i\mathbf{H}^\circ t/\hbar})\mathbf{A}(e^{-i\mathbf{H}^\circ t/\hbar})$$

3.3.4.2 Dynamics of IP time evolution operators Now, we may introduce an interaction picture operator $\mathbf{U}(t)^{\mathrm{IP}}$, which transforms any SP ket at initial time t_0 into the corresponding IP ket at time t, according to

$$\boxed{|\Psi(t)^{\mathrm{IP}}\rangle \equiv \mathbf{U}(t-t_0)^{\mathrm{IP}}|\Psi(t_0)^{\mathrm{SP}}\rangle} \tag{3.109}$$

with the stipulation that

$$\mathbf{U}(t_0)^{\mathrm{IP}} = 1 \tag{3.110}$$

Now, observe that Eq. (3.104) may be written

$$|\Psi^{\mathrm{IP}}(t)\rangle \equiv \mathbf{U}^\circ(t-t_0)^{-1}|\Psi^{\mathrm{SP}}(t)\rangle \tag{3.111}$$

where $\mathbf{U}^\circ(t-t_0)$ is the time evolution operator given by

$$\boxed{\mathbf{U}^\circ(t-t_0) = e^{-i\mathbf{H}^\circ(t-t_0)/\hbar}} \tag{3.112}$$

with, of course,

$$\mathbf{U}^\circ(t_0) = 1$$

Moreover, the inverse transformation of Eq. (3.109) may be obtained by premultiplying in it both members of the inverse of the IP time evolution operator. On simplification, we have

$$|\Psi(t_0)^{\mathrm{SP}}\rangle = \mathbf{U}(t-t_0)^{\mathrm{IP}\,-1}|\Psi(t)^{\mathrm{IP}}\rangle \tag{3.113}$$

On the other hand, taking the partial derivative of both terms of Eq. (3.109) reads

$$\left(\frac{\partial|\Psi(t)^{\mathrm{IP}}\rangle}{\partial t}\right) = \left(\frac{\partial \mathbf{U}(t)^{\mathrm{IP}}}{\partial t}\right)|\Psi(t_0)^{\mathrm{SP}}\rangle$$

Thus, in view of Eq. (3.113) allowing to pass from any SP ket at initial time t_0 to the corresponding IP ket at time t, the equation transforms to

$$\left(\frac{\partial|\Psi(t)^{\mathrm{IP}}\rangle}{\partial t}\right) = \left(\frac{\partial \mathbf{U}(t)^{\mathrm{IP}}}{\partial t}\right)\mathbf{U}(t-t_0)^{\mathrm{IP}\,-1}|\Psi(t)^{\mathrm{IP}}\rangle$$

Then, one may replace the left-hand side of this last equation by its expression given by Eq. (3.107). After rearranging, we have

$$\mathbf{V}(t-t_0)^{\mathrm{IP}}|\Psi(t)^{\mathrm{IP}}\rangle = i\hbar\left(\frac{\partial \mathbf{U}(t)^{\mathrm{IP}}}{\partial t}\right)\mathbf{U}(t-t_0)^{\mathrm{IP}\,-1}|\Psi(t)^{\mathrm{IP}}\rangle$$

Then, since this last linear transformation is satisfied irrespective of the IP ket at any time, we have

$$i\hbar\left(\frac{\partial \mathbf{U}(t)^{\mathrm{IP}}}{\partial t}\right)\mathbf{U}(t-t_0)^{\mathrm{IP}\,-1} = \mathbf{V}(t-t_0)^{\mathrm{IP}}$$

Finally, postmultiply both member of this last equation by $\mathbf{U}(t-t_0)^{\mathrm{IP}}$. Hence, after simplification using the operator property

$$\boxed{i\hbar\left(\frac{\partial \mathbf{U}(t)^{\mathrm{IP}}}{\partial t}\right) = \mathbf{V}(t-t_0)^{\mathrm{IP}}\mathbf{U}(t-t_0)^{\mathrm{IP}}} \tag{3.114}$$

which, when $t_0 = 0$ simplifies to

$$i\hbar\left(\frac{\partial \mathbf{U}(t)^{\mathrm{IP}}}{\partial t}\right) = \mathbf{V}(t)^{\mathrm{IP}}\mathbf{U}(t)^{\mathrm{IP}} \tag{3.115}$$

and, due to Eq. (3.110)

$$\mathbf{U}(0)^{\mathrm{IP}} = 1 \tag{3.116}$$

3.3.4.3 Relation between IP and SP time evolution operators Now, observe that the linear transformation, which is inverse of that given by Eq. (3.111), may be obtained by premultiplying both terms by $\mathbf{U}^{\circ}(t)$ and then simplifying the result using $\mathbf{U}^{\circ}(t-t_0)\mathbf{U}^{\circ}(t-t_0)^{-1} = 1$, leading to

$$|\Psi(t)^{\mathrm{SP}}\rangle = \mathbf{U}^{\circ}(t-t_0)|\Psi(t)^{\mathrm{IP}}\rangle \tag{3.117}$$

Then, premultiplying both members of this last equation by $\mathbf{U}^{\circ}(t-t_0)^{-1}$, we have on simplification

$$\mathbf{U}^{\circ}(t-t_0)^{-1}\mathbf{U}^{\circ}(t-t_0) = 1$$

and

$$\mathbf{U}^{\circ}(t-t_0)^{-1}|\Psi(t)^{\mathrm{SP}}\rangle = |\Psi(t)^{\mathrm{IP}}\rangle \tag{3.118}$$

Next, owing to Eq. (3.109) relating the IP ket at time t with the SP one at initial time t_0, the last equation becomes

$$|\Psi(t)^{\mathrm{SP}}\rangle \equiv \mathbf{U}^{\circ}(t-t_0)\mathbf{U}(t-t_0)^{\mathrm{IP}}|\Psi(t_0)^{\mathrm{SP}}\rangle \tag{3.119}$$

Remark that, according to Eq. (3.85), the SP ket at time t is related to the corresponding one on initial time t_0 via

$$|\Psi(t)^{\mathrm{SP}}\rangle \equiv \mathbf{U}(t-t_0)|\Psi(t_0)^{\mathrm{SP}}\rangle \tag{3.120}$$

with

$$\mathbf{U}(t-t_0) = e^{-i\mathbf{H}(t-t_0)/\hbar} \tag{3.121}$$

Thus, comparison of Eqs. (3.119) and (3.120) shows that

$$\boxed{\mathbf{U}(t-t_0) = \mathbf{U}^{\circ}(t-t_0)\mathbf{U}(t-t_0)^{\mathrm{IP}}} \tag{3.122}$$

Equation (3.122) shows that the full time evolution operator $\mathbf{U}(t-t_0)$, which is given by Eq. (3.121), is equal to the unperturbed time evolution operator $\mathbf{U}^{\circ}(t-t_0)$ given by Eq. (3.112) times the IP time evolution operator governed by the partial differential equation (3.114).

3.3.4.4 Perturbation expansion of the time evolution operator We shall now obtain the full time evolution operator $\mathbf{U}(t)$ when it is only easy to find its corresponding unperturbed time evolution operator $\mathbf{U}^{\circ}(t)$. The solution of the problem requires one to get the IP time evolution operator by solution of Eq. (3.115) with the boundary condition (3.116), that is,

$$i\hbar\left(\frac{\partial \mathbf{U}(t)^{\mathrm{IP}}}{\partial t}\right) = \mathbf{V}(t)^{\mathrm{IP}}\mathbf{U}(t)^{\mathrm{IP}} \quad \text{with} \quad \mathbf{U}(0)^{\mathrm{IP}} = 1$$

On integration between $t' = 0$ and $t' = t$, and using the boundary condition, we have

$$\mathbf{U}(t)^{\mathrm{IP}} = 1 + \left(\frac{1}{i\hbar}\right)\int_0^t \mathbf{V}(t')^{\mathrm{IP}}\,\mathbf{U}(t')^{\mathrm{IP}}dt' \tag{3.123}$$

Now, in order to solve the integral equation (3.123), one may write for $\mathbf{U}(t')^{\mathrm{IP}}$ on its right-hand side, an expression that may be obtained from Eq. (3.123), by the replacements $t' \to t$, and $t'' \to t'$, namely

$$\mathbf{U}(t')^{\mathrm{IP}} = 1 + \left(\frac{1}{i\hbar}\right)\int_0^{t'} \mathbf{V}(t'')^{\mathrm{IP}}\,\mathbf{U}\,(t'')^{\mathrm{IP}}dt''$$

Hence, Eq. (3.123) yields

$$\mathbf{U}(t)^{\mathrm{IP}} = 1 + \left(\frac{1}{i\hbar}\right)\int_0^t \mathbf{V}(t')^{\mathrm{IP}}dt' + \left(\frac{1}{i\hbar}\right)^2\int_0^t\int_0^{t'} \mathbf{V}^{\mathrm{IP}}(t')\mathbf{V}^{\mathrm{IP}}(t'')\mathbf{U}^{\mathrm{IP}}(t'')dt'dt'' \tag{3.124}$$

The foregoing equation may be iterated as many times as required. If the perturbation $\mathbf{V}$ is very small with respect to $\mathbf{H}^\circ$, the third term on the right-hand side of this last equation, which is quadratic in $\mathbf{V}$, may be neglected with respect to the second term, which is linear in $\mathbf{V}$, leading to the first-order expansion of the IP time evolution operator given by

$$\mathbf{U}(t)^{\mathrm{IP}} = 1 + \left(\frac{1}{i\hbar}\right)\int_0^t \mathbf{V}(t')^{\mathrm{IP}}dt' \tag{3.125}$$

To simplify, limit the iteration by truncating the IP time evolution operator $\mathbf{U}(t'')^{\mathrm{IP}}$ at time t'' appearing in Eq. (3.124), to the first term unity

$$\mathbf{U}(t'')^{\mathrm{IP}} = 1 + \left(\frac{1}{i\hbar}\right)\int_0^{t''} \mathbf{V}(t''')^{\mathrm{IP}}\mathbf{U}(t''')^{\mathrm{IP}}dt''' \simeq 1$$

That leads to the following second-order perturbative expansion for the IP time evolution operator:

$$\boxed{\mathbf{U}(t)^{\mathrm{IP}} \simeq 1 + \left(\frac{1}{i\hbar}\right)\int_0^t \mathbf{V}(t')^{\mathrm{IP}}dt' + \left(\frac{1}{i\hbar}\right)^2\int_0^t\int_0^{t'} \mathbf{V}^{\mathrm{IP}}(t')\mathbf{V}^{\mathrm{IP}}(t'')dt'dt''}$$

Next, owing to Eqs. (3.108) and (3.112), the IP time evolution operator reads

$$\mathbf{V}(t)^{\mathrm{IP}} = \mathbf{U}^\circ(t)^{-1}\mathbf{V}\mathbf{U}^\circ(t) \tag{3.126}$$

Then, using (3.126) and also Eq. (3.122) allowing to pass from $\mathbf{U}(t)^{\mathrm{IP}}$ to $\mathbf{U}(t)$, the full time evolution operator appears to be given by

$$\begin{aligned}\mathbf{U}(t) \simeq\ & \mathbf{U}^\circ(t) \\ & + \left(\frac{1}{i\hbar}\right)\mathbf{U}^\circ(t)\int_0^t \mathbf{U}^\circ(t')^{-1}\mathbf{V}\mathbf{U}^\circ(t')dt' \\ & + \left(\frac{1}{i\hbar}\right)^2\mathbf{U}^\circ(t)\int_0^t\int_0^{t'} \mathbf{U}^\circ(t')^{-1}\mathbf{V}\mathbf{U}^\circ(t')\mathbf{U}^\circ(t'')^{-1}\mathbf{V}\mathbf{U}^\circ(t'')dt'dt''\end{aligned}$$

This result must be considered, keeping in mind Eqs. (3.82) and (3.112), that is,

$$\mathbf{U}(t) = (e^{-i\mathbf{H}t/\hbar}) \qquad \text{and} \qquad \mathbf{U}^\circ(t) = (e^{-i\mathbf{H}^\circ t/\hbar})$$

3.3.5 Formal expression to make Eq. (3.123) tractable

Observe that the time evolution operators allow one to pass from a ket at initial time $t = 0$ to another at time t.

$$|\Psi(t)\rangle = \mathbf{U}(t)|\Psi(0)\rangle$$

Now, we may replace the initial time $t = 0$ by any time t°. Then, this equation may be written

$$|\Psi(t)\rangle = \mathbf{U}(t, t^\circ)|\Psi(t^\circ)\rangle \tag{3.127}$$

In this equation, the time evolution operator appears to be a conditional operator, which, if the ket is $|\Psi(t^\circ)\rangle$ at time $t = t^\circ$, transforms this ket into $|\Psi(t)\rangle$ at time t. Note that, $\mathbf{U}(t, t^\circ)$ is by definition given by

$$\mathbf{U}(t, t^\circ) = e^{-i(t-t^\circ)\mathbf{H}/\hbar}$$

Next, consider the following time evolution operators:

$$\mathbf{U}(t_2, t_1) = e^{-i(t_2-t_1)\mathbf{H}/\hbar} \qquad \text{and} \qquad \mathbf{U}(t_1, t^\circ) = e^{-i(t_1-t^\circ)\mathbf{H}/\hbar} \tag{3.128}$$

Again, consider the third evolution operator

$$\mathbf{U}(t_2, t^\circ) = e^{-i(t_2-t^\circ)\mathbf{H}/\hbar}$$

Of course, this operator may be written

$$\mathbf{U}(t_2, t^\circ) = e^{-i\{(t_2-t_1)+(t_1-t^\circ)\}\mathbf{H}/\hbar} \tag{3.129}$$

Then, owing to the equation appearing in Eq. (3.128), the time evolution operator (3.129) appears to be

$$\mathbf{U}(t_2, t^\circ) = \mathbf{U}(t_2, t_1)\,\mathbf{U}(t_1, t^\circ) \tag{3.130}$$

It may be observed that Eqs. (3.127) and (3.130) are true for all kinds of time evolution operators, that is, for full, unperturbed, and IP time evolution operators.

Keeping that in mind, we may return to Eq. (3.123).

$$\mathbf{U}^{\text{IP}}(t, t^\circ) = 1 + \left(\frac{1}{i\hbar}\right)\int_{t^\circ}^{t} \mathbf{V}^{\text{IP}}(\tau, t^\circ)\mathbf{U}^{\text{IP}}(\tau, t^\circ)\, d\tau \tag{3.131}$$

Next, by inversion of Eq. (3.122), one obtains

$$\mathbf{U}^{\text{IP}}(t, t^\circ) = \mathbf{U}^\circ(t, t^\circ)^{-1}\mathbf{U}(t, t^\circ)$$

This equation allows to transform Eq. (3.131) into

$$\mathbf{U}^\circ(t, t^\circ)^{-1}\mathbf{U}(t, t^\circ) = 1 + \left(\frac{1}{i\hbar}\right)\int_{t^\circ}^{t} \mathbf{V}^{\text{IP}}(\tau, t^\circ)\mathbf{U}^{\text{IP}}(\tau, t^\circ)\, d\tau \tag{3.132}$$

Next, we may use

$$\mathbf{U}^\circ(t, t^\circ)^{-1}\mathbf{U}^\circ(t, t^\circ) = 1 \tag{3.133}$$

Then, premultiplying the right-hand side of Eq. (3.132) by this last equation leads to

$$\mathbf{U}^\circ(t, t^\circ)^{-1}\mathbf{U}(t, t^\circ) = \mathbf{U}^\circ(t, t^\circ)^{-1}\mathbf{U}^\circ(t, t^\circ)\left(1 + \left(\frac{1}{i\hbar}\right)\int_{t^\circ}^{t} \mathbf{V}^{\text{IP}}(\tau, t^\circ)\mathbf{U}^{\text{IP}}(\tau, t^\circ)\, d\tau\right) \tag{3.134}$$

Next, premultiply both members of this last equation by $\mathbf{U}^{\circ}(t, t^{\circ})$. Then, owing to Eq. (3.133), Eq. (3.134) reduces to

$$\mathbf{U}(t, t^{\circ}) = \mathbf{U}^{\circ}(t, t^{\circ}) \left(1 + \left(\frac{1}{i\hbar} \right) \int_{t^{\circ}}^{t} \mathbf{V}^{\mathrm{IP}}(\tau, t^{\circ}) \mathbf{U}^{\mathrm{IP}}(\tau, t^{\circ})\, d\tau \right)$$

which may be written as

$$\mathbf{U}(t, t^{\circ}) = \mathbf{U}^{\circ}(t, t^{\circ}) + \left(\frac{1}{i\hbar} \right) \int_{t^{\circ}}^{t} \mathbf{U}^{\circ}(t, t^{\circ}) \mathbf{V}^{\mathrm{IP}}(\tau, t^{\circ}) \mathbf{U}^{\mathrm{IP}}(\tau, t^{\circ})\, d\tau \tag{3.135}$$

Now, observe that the unperturbed time evolution operator, just after the integral allowing one to pass from $t = 0$ to t may be viewed as the product:

$$\mathbf{U}^{\circ}(t, t^{\circ}) = [\mathbf{U}^{\circ}(t, \tau) \mathbf{U}^{\circ}(\tau, t^{\circ})]$$

Then, Eq. (3.135) may be written

$$\mathbf{U}(t, t^{\circ}) = \mathbf{U}^{\circ}(t, t^{\circ}) + \left(\frac{1}{i\hbar} \right) \int_{t^{\circ}}^{t} [\mathbf{U}^{\circ}(t, \tau) \mathbf{U}^{\circ}(\tau, t^{\circ})] \{ \mathbf{V}^{\mathrm{IP}}(\tau, t^{\circ}) \} \mathbf{U}^{\mathrm{IP}}(\tau, t^{\circ})\, d\tau$$

Again, for the perturbation Hamiltonian in the interaction picture use Eq. (3.126):

$$\begin{aligned} \mathbf{U}(t, t^{\circ}) &= \mathbf{U}^{\circ}(t, t^{\circ}) \\ &+ \left(\frac{1}{i\hbar} \right) \int_{t^{\circ}}^{t} \mathbf{U}^{\circ}(t, \tau) \mathbf{U}^{\circ}(\tau, t^{\circ}) \mathbf{U}^{\circ}(\tau, t^{\circ})^{-1} \mathbf{V} \mathbf{U}^{\circ}(\tau, t^{\circ}) \mathbf{U}^{\circ}(\tau, t^{\circ})^{-1} \mathbf{U}^{\circ}(\tau, t^{\circ})\, d\tau \end{aligned}$$

Finally, in order to simplify this last result, we may use the property of a time evolution operator and of its inverse in the following way:

$$\mathbf{U}^{\circ}(\tau, t^{\circ}) \mathbf{U}^{\circ}(\tau, t^{\circ})^{-1} = 1 \qquad \text{and} \qquad \mathbf{U}^{\circ}(\tau, t^{\circ})^{-1} \mathbf{U}^{\circ}(\tau, t^{\circ}) = 1$$

That leads to the final result of importance:

$$\boxed{\mathbf{U}(t, t^{\circ}) = \mathbf{U}^{\circ}(t, t^{\circ}) + \left(\frac{1}{i\hbar} \right) \int_{t^{\circ}}^{t} \mathbf{U}^{\circ}(t, \tau) \mathbf{V} \mathbf{U}^{\circ}(\tau, t^{\circ})\, d\tau} \tag{3.136}$$

Note in this last equation the respective places of the times t°, τ, and t,

3.4 DENSITY OPERATORS

After studying the time dependence of quantum mechanics, through the Schrödinger, Heisenberg, and interaction pictures using the time evolution operator, it is now appropriate to introduce the fundamental concept of the *density operator*, which is a very powerful tool in quantum mechanics.

3.4.1 Basic properties

3.4.1.1 Definition By definition, the density operator $\boldsymbol{\rho}$ of a statistical mixture is

$$\boxed{\boldsymbol{\rho} = \sum_i W_i |\Phi_i\rangle\langle\Phi_i|} \tag{3.137}$$

Here the W_i are the probabilities for the states to be occupied, which are therefore real and must obey

$$\sum_i W_i = 1 \qquad \text{and} \qquad 0 \leq W_i \leq 1$$

whereas the kets $|\Phi_i\rangle$ belong to an arbitrary basis in the state space, and thus obey

$$\sum_i |\Phi_i\rangle\langle\Phi_i| = 1 \qquad \text{and} \qquad \langle\Phi_i|\Phi_k\rangle = \delta_{ik} \tag{3.138}$$

Note that for a pure state, all the operations are zero except one, which is equal to unity. Then the density operator expression (3.137) reduces to

$$\rho = |\Phi_i\rangle\langle\Phi_i| \tag{3.139}$$

3.4.1.2 Trace of the density operator Consider now the trace of the density operator. It is in the basis used for its description:

$$\mathbf{tr}\{\boldsymbol{\rho}\} = \sum_k \langle\Phi_k| \left\{ \sum_i W_i |\Phi_i\rangle\langle\Phi_i| \right\} |\Phi_k\rangle$$

Then, since the W_i are scalars, owing to the orthonormality properties of the basis, this last equation transforms to

$$\mathbf{tr}\{\boldsymbol{\rho}\} = \sum_k \sum_i W_i \langle\Phi_k|\Phi_i\rangle\langle\Phi_i|\Phi_k\rangle$$

Again, owing to the orthonormality properties (3.138) of the basis, that reduces to

$$\mathbf{tr}\{\boldsymbol{\rho}\} = \sum_i W_i$$

At last, since the sum of the probabilities W_i is equal to unity, the trace appears to be simply given as

$$\mathbf{tr}\{\boldsymbol{\rho}\} = 1 \tag{3.140}$$

3.4.1.3 Hermiticity of the density operator The Hermitian conjugate of the density operator (3.137) is

$$\boldsymbol{\rho}^\dagger = \left\{ \sum_i W_i |\Phi_i\rangle\langle\Phi_i| \right\}^\dagger \tag{3.141}$$

Again, using the rules of this section governing Hermitian conjugation, the right-hand side of this last equation is

$$\left\{ \sum_i W_i |\Phi_i\rangle\langle\Phi_i| \right\}^\dagger = \sum_i W_i^* |\Phi_i\rangle\langle\Phi_i|$$

or, since the probabilities are real,

$$\left\{\sum_i W_i|\Phi_i\rangle\langle\Phi_i|\right\}^\dagger = \sum_i W_i|\Phi_i\rangle\langle\Phi_i|$$

Hence, Eq. (3.141) becomes

$$\boldsymbol{\rho}^\dagger = \left\{\sum_i W_i|\Phi_i\rangle\langle\Phi_i|\right\} \tag{3.142}$$

Thus, by comparison of Eq. (3.142) with Eq. (3.137), it appears that

$$\boldsymbol{\rho}^\dagger = \boldsymbol{\rho}$$

showing that the density operator is Hermitian.

3.4.1.4 *Inequality governing the density operator in the general case of mixed states*

Consider the square of the density operator, which, owing to Eq. (3.137), reads

$$\boldsymbol{\rho}^2 = \sum_i W_i|\Phi_i\rangle\langle\Phi_i| \sum_k W_k|\Phi_k\rangle\langle\Phi_k|$$

or, since the probabilities W_i are scalars,

$$\boldsymbol{\rho}^2 = \sum_i \sum_k W_i W_k|\Phi_i\rangle\langle\Phi_i|\Phi_k\rangle\langle\Phi_k|$$

so that due to the orthonormality properties (3.138)

$$\boldsymbol{\rho}^2 = \sum_i \sum_k W_i W_k|\Phi_i\rangle\delta_{ik}\langle\Phi_k|$$

and, thus, after simplification using the properties of the Kronecker symbol, it is found that

$$\boldsymbol{\rho}^2 = \sum_i W_i^2|\Phi_i\rangle\langle\Phi_i| \tag{3.143}$$

Moreover, since the probabilities are smaller than unity, their squares obey the inequality

$$W_i^2 < W_i^2$$

and it appears by comparison of Eq. (3.143) with (3.137) that

$$\boldsymbol{\rho}^2 < \boldsymbol{\rho} \tag{3.144}$$

For a pure state verifying Eq. (3.139), the square of the density operator reduces to

$$\boldsymbol{\rho}^2 = |\Phi_i\rangle\langle\Phi_i|\Phi_i\rangle\langle\Phi_i|$$

or, because of the orthonormality properties (3.138), to

$$\boldsymbol{\rho}^2 = |\Phi_i\rangle\langle\Phi_i|$$

so that

$$\boldsymbol{\rho}^2 = \boldsymbol{\rho} \quad \text{(pure state)}$$

3.4.2 Density operator for many particles

Now, consider the density operator of a set of N particles. Then, according to Eq. (3.47), a ket characterizing a whole system is given by the product

$$|\Psi_{k(1),l(2)...f(N)}\rangle = \prod_{(r)}^{(N)} |\Phi_{j(r)}\rangle \tag{3.145}$$

where $|\Phi_{l(r)}\rangle$ is the lth ket $|\Phi_l\rangle$ of the rth particle.

Next, for a pure case, the full density operator $\boldsymbol{\rho}_{\text{Tot}}$ of the set of N particles is given by an expression of the same form as that in Eq. (3.139) in which the ket given by Eq. (3.145) plays the role of $|\Phi_i\rangle$ in Eq. (3.139), that is,

$$\boldsymbol{\rho}_{\text{Tot}} = |\Psi_{k(1)l(2)...f(N)}\rangle\langle\Psi_{k(1)l(2)....f(N)}|$$

or

$$\boldsymbol{\rho}_{\text{Tot}} = \prod_{(r)}^{(N)} |\Phi_{j(r)}\rangle\langle\Phi_{j(r)}| \tag{3.146}$$

Again, for a mixed situation, the generalization to N particles of Eq. (3.137), leads to

$$\boldsymbol{\rho}_{\text{Tot}} = \sum_{k(1)}\sum_{l(2)}\cdots\sum_{f(N)} \mathbb{W}_{k(1)l(2)...f(N)}|\Psi_{k(1)l(2)...f(N)}\rangle\langle\Psi_{k(1)l(2)....f(N)}|$$

where the $\mathbb{W}_{k(1)l(2)...f(N)}$ are the joint probabilities to find the first particle (1) in the kth state $|\Phi_k\rangle$, with the probability $W_{k(1)}$, the second particle (2) in the lth state $|\Phi_l\rangle$ with the probability $W_{l(2)}$, and so on given by

$$\mathbb{W}_{k(1)l(2)...f(N)} = W_{k(1)}\, W_{l(2)}\, \cdots$$

On the other hand, consider a physical system that may be divided into two different subsystems. Then, the *full density operator* of this system may be written as the product of the density operators of the two subsystems:

$$\boldsymbol{\rho}_{\text{Tot}} = \boldsymbol{\rho}_{(1)}\boldsymbol{\rho}_{(2)}$$

By definition, the *reduced density operator* of one of the two subsystems is the partial trace over the subspace spanned by the other subsystem over the full density operator:

$$\boldsymbol{\rho}_{\text{Red}(2)} = \mathbf{tr}_{(1)}\{\boldsymbol{\rho}_{\text{Tot}}\} \qquad \boldsymbol{\rho}_{\text{Red}(1)} = \mathbf{tr}_{(2)}\{\boldsymbol{\rho}_{\text{Tot}}\}$$

3.4.3 Average values

We now show that the average value of an operator $\mathbf{A}$ performed over the density operator of a statistical mixed state is

$$\boxed{\langle\mathbf{A}\rangle_{\boldsymbol{\rho}} = \mathbf{tr}\{\boldsymbol{\rho}\mathbf{A}\}} \tag{3.147}$$

In order to prove this equation, recall that, according to Eqs. (3.137) and (3.140), the density operator obeys

$$\boldsymbol{\rho} = \sum_i W_i|\Phi_i\rangle\langle\Phi_i| \qquad \text{and} \qquad \mathbf{tr}\{\boldsymbol{\rho}\} = 1$$

Then, Eq. (3.147) becomes

$$\langle \mathbf{A} \rangle_{\boldsymbol{\rho}} = \mathbf{tr} \left\{ \sum_i W_i |\Phi_i\rangle\langle\Phi_i| \mathbf{A} \right\}$$

Perform the trace over the basis $\{|\Phi_i\rangle\}$, which reads

$$\langle \mathbf{A} \rangle_{\boldsymbol{\rho}} = \sum_k \sum_i \langle \Phi_k | W_i | \Phi_i \rangle \langle \Phi_i | \mathbf{A} | \Phi_k \rangle$$

Or, since the probabilities W_i are scalars,

$$\langle \mathbf{A} \rangle_{\boldsymbol{\rho}} = \sum_k \sum_i W_i \langle \Phi_k | \Phi_i \rangle \langle \Phi_i | \mathbf{A} | \Phi_k \rangle$$

Finally, owing to the orthonormality properties (3.138) of the basis $\{|\Phi_i\rangle\}$, that simplifies to

$$\langle \mathbf{A} \rangle_{\boldsymbol{\rho}} = \sum_k \sum_i W_i \delta_{ki} \langle \Phi_i | \mathbf{A} | \Phi_k \rangle$$

and thus

$$\langle \mathbf{A} \rangle_{\boldsymbol{\rho}} = \sum_i W_i \langle \Phi_i | \mathbf{A} | \Phi_i \rangle \tag{3.148}$$

Hence, the average of operator $\mathbf{A}$ over density operator $\boldsymbol{\rho}$ is the sum of all the quantum average values of operator $\mathbf{A}$ over the kets $|\Phi_i\rangle$ belonging to the basis $\{|\Phi_i\rangle\}$, times the corresponding probabilities W_i.

Of course, for a pure density state where all the probabilities are zero, except one which is unity, the average value over the density operator (3.148) reduces to the simple quantum average value (2.21), that is,

$$\langle \mathbf{A} \rangle_{\boldsymbol{\rho}} = \langle \Phi_i | \mathbf{A} | \Phi_i \rangle$$

3.4.4 Entropy and density operators

Introduce the statistical entropy function through

$$S = -k_B \langle \ln \boldsymbol{\rho} \rangle_{\boldsymbol{\rho}}$$

where k_B is the Boltzmann constant. Now, keeping in mind that the average of an operator over the density operator is given by Eq. (3.147), the statistical entropy becomes

$$S = -k_B \mathbf{tr} \{ \boldsymbol{\rho} \ln \boldsymbol{\rho} \} \tag{3.149}$$

Again, writing explicitly the trace involved in Eq. (3.149) by performing the trace over the basis $\{|\Phi_i\rangle\}$ obeying Eq. (3.138), that is,

$$\langle \Phi_k | \Phi_l \rangle = \delta_{kl} \tag{3.150}$$

we have

$$S = -k_B \sum_i \langle \Phi_i | \boldsymbol{\rho} \ln \boldsymbol{\rho} | \Phi_i \rangle \tag{3.151}$$

Moreover, since, owing to Eq. (3.137), the density operator of a mixed state expressed in the basis $\{|\Phi_i\rangle\}$ is given by

$$\boldsymbol{\rho} = \sum_k W_k |\Phi_k\rangle\langle\Phi_k|$$

the statistical entropy (3.151) yields

$$S = -\sum_i \sum_k W_k \langle\Phi_i|\Phi_k\rangle\langle\Phi_k| \ln \left\{ \sum_l W_l |\Phi_l\rangle\langle\Phi_l| \right\} |\Phi_i\rangle$$

or, due to the orthonormality properties (3.138)

$$S = -k_B \sum_i W_i \langle\Phi_i| \ln \left\{ \sum_l W_l |\Phi_l\rangle\langle\Phi_l| \right\} |\Phi_i\rangle \tag{3.152}$$

Next, to calculate the operator $\ln \mathbf{A}$ averaged over $|\Phi_i\rangle$, where

$$\mathbf{A} = \sum_l W_l |\Phi_l\rangle\langle\Phi_l|$$

we use the following formal expansion of the logarithm of some function A given by

$$\ln A = \sum_k C_k A^k \tag{3.153}$$

where C_k are the coefficients involved in the expansion of the logarithm. Then, the logarithm involved on the right-hand side of Eq. (3.152) expands as

$$\ln \left\{ \sum_l W_l |\Phi_l\rangle\langle\Phi_l| \right\} = \sum_k C_k \left(\sum_l W_l |\Phi_l\rangle\langle\Phi_l| \right)^k \tag{3.154}$$

Next, observe that, when $k = 2$, it reads

$$\left(\sum_l W_l |\Phi_l\rangle\langle\Phi_l| \right)^2 = \sum_l \sum_s W_l |\Phi_l\rangle\langle\Phi_l| W_s |\Phi_s\rangle\langle\Phi_s|$$

or, since W_s is a scalar,

$$\left(\sum_l W_l |\Phi_l\rangle\langle\Phi_l| \right)^2 = \sum_l \sum_s W_l W_s |\Phi_l\rangle\langle\Phi_l|\Phi_s\rangle\langle\Phi_s|$$

so that, due to the orthonormality property (3.150),

$$\left(\sum_l W_l |\Phi_l\rangle\langle\Phi_l| \right)^2 = \sum_l \sum_s W_l |\Phi_l\rangle W_s \delta_{ls} \langle\Phi_s|$$

After simplification using the orthonormality properties (3.138) of the basis, that simplifies to

$$\left(\sum_l W_l |\Phi_l\rangle\langle\Phi_l| \right)^2 = \sum_l (W_l)^2 (|\Phi_l\rangle\langle\Phi_l|)^2$$

Again, by recurrence one obtains for any value of k

$$\left(\sum_l W_l|\Phi_l\rangle\langle\Phi_l|\right)^k = \sum_l (W_l)^k|\Phi_l\rangle\langle\Phi_l|$$

so that Eq. (3.154) takes the form

$$\ln\left\{\sum_l W_l|\Phi_l\rangle\langle\Phi_l|\right\} = \sum_k C_k \sum_l (W_l)^k|\Phi_l\rangle\langle\Phi_l|$$

Moreover, due to the latter result, the diagonal matrix elements of Eq. (3.154) read

$$\langle\Phi_i|\ln\left\{\sum_l W_l|\Phi_l\rangle\langle\Phi_l|\right\}|\Phi_i\rangle = \sum_k C_k\langle\Phi_i|\sum_l (W_l)^k(|\Phi_l\rangle\langle\Phi_l|)|\Phi_i\rangle \qquad (3.155)$$

or, in view of the orthonormality properties (3.138), one has

$$\langle\Phi_i|(W_l)^k(|\Phi_l\rangle\langle\Phi_l|)|\Phi_i\rangle = (W_l)^k\delta_{il}$$

Hence, after simplification using the property of δ_{il}, Eq. (3.155) becomes

$$\langle\Phi_i|\ln\left\{\sum_l W_l|\Phi_l\rangle\langle\Phi_l|\right\}|\Phi_i\rangle = \sum_k C_k(W_i)^k$$

Hence, according to the formal expression of the expansion (3.153), in which W_l plays now the role of the function A, we have

$$\langle\Phi_i|\ln\left\{\sum_l W_l|\Phi_l\rangle\langle\Phi_l|\right\}|\Phi_i\rangle = \ln W_i$$

Thus, the entropy given by Eq. (3.152) transforms to the simple form

$$\boxed{S = -k_B\sum_i W_i \ln W_i} \qquad (3.156)$$

which is the usual statistical expression of entropy in information theory. Of course, the probabilities may depend on time, so that the statistical entropy depends also on time. Thus, Eq. (3.156) may be written for any time

$$S = -k_B\sum_i W_i(t)\ln W_i(t) \qquad (3.157)$$

3.4.5 Density operator representations

Start from the general expression (3.137) of the density operator $\boldsymbol{\rho}$ of a mixed state, that is,

$$\boldsymbol{\rho} = \sum_i W_i|\Phi_i\rangle\langle\Phi_i| \qquad (3.158)$$

where W_i is the probability for the ket $|\Phi_i\rangle$ to be occupied. This operator may be expressed in the basis $\{|\{Q\}\rangle\}$ of the eigenstates of the position operator as it will be now seen.

3.4.5.1 Position representation For this purpose, write the eigenvalue equation of the position operator $\mathbf{Q}$, that is,

$$\mathbf{Q}|\{Q\}\rangle = Q|\{Q\}\rangle$$

In the basis $\{|\{Q\}\rangle\}$, the matrix elements of the density operator (3.158) read

$$\langle\{Q\}|\boldsymbol{\rho}|\{Q'\}\rangle = \sum_i W_i \langle\{Q\}|\Phi_i\rangle\langle\Phi_i|\{Q'\}\rangle$$

The scalar products involved in this last equation are the wavefunctions given by

$$\langle\{Q\}|\Phi_i\rangle = \Phi_i(Q) \qquad \text{and} \qquad \langle\Phi_i|\{Q'\}\rangle = \Phi_i^*(Q')$$

Hence, the matrix elements, which may be denoted as $\rho(Q, Q')$, become

$$\langle\{Q\}|\boldsymbol{\rho}|\{Q'\}\rangle = \sum_i W_i \Phi_i(Q)\Phi_i^*(Q') \equiv \rho(Q, Q') \tag{3.159}$$

the corresponding diagonal matrix elements denoted $\rho(Q, Q)$ reduce to

$$\langle\{Q\}|\boldsymbol{\rho}|\{Q\}\rangle = \sum_i W_i |\Phi_i(Q)|^2 \equiv \rho(Q, Q) \tag{3.160}$$

3.4.5.2 Momentum representation Now, write the eigenvalue equation of the momentum P as

$$\mathbf{P}|\{P\}\rangle = P|\{P\}\rangle$$

In the basis of the eigenstates of the position operator, the matrix elements of the density operator are, comparing Eq. (3.158),

$$\langle\{P\}|\boldsymbol{\rho}|\{P'\}\rangle = \sum_i W_i \langle\{P\}|\Phi_i\rangle\langle\Phi_i|\{P'\}\rangle$$

The scalar products involved here are the wavefunctions in the momentum representation, that is,

$$\langle\{P\}|\Phi_i\rangle = \Phi_i(P) \qquad \text{and} \qquad \langle\Phi_i|\{P'\}\rangle = \Phi_i^*(P')$$

Thus, the matrix elements $\rho(P, P')$ become

$$\rho(P, P') = \langle\{P\}|\boldsymbol{\rho}|\{P'\}\rangle = \sum_i W_i \Phi_i(P)\Phi_i^*(P') \tag{3.161}$$

the corresponding diagonal matrix elements being

$$\rho(P, P) = \langle\{P\}|\boldsymbol{\rho}|\{P\}\rangle = \sum_i W_i |\Phi_i(P)|^2 \tag{3.162}$$

3.4.5.3 Wigner distribution function Now, consider for one dimension in the position representation the following off-diagonal matrix elements of the density operator:

$$\rho\left(Q + \frac{\eta}{2}, Q - \frac{\eta}{2}\right) = \left\langle\left\{Q + \frac{\eta}{2}\right\}|\boldsymbol{\rho}|\left\{Q - \frac{\eta}{2}\right\}\right\rangle$$

Then it is possible to write from this matrix element the following function:

$$f_w(P,Q) = \int_{-\infty}^{+\infty} \rho\left(Q + \frac{\eta}{2}, Q - \frac{\eta}{2}\right) \exp\left\{\frac{-iP\eta}{\hbar}\right\} d\eta \tag{3.163}$$

Next, multiply both members of this last equation by $\frac{1}{2}\pi\hbar$ and integrate over all the momentum:

$$\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} f_w(P,Q)\,dP = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \rho\left(Q + \frac{\eta}{2}, Q - \frac{\eta}{2}\right) \exp\left\{\frac{-iP\eta}{\hbar}\right\} d\eta dP \tag{3.164}$$

or

$$\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} f_w(P,Q)\,dP = \int_{-\infty}^{+\infty} \rho\left(Q + \frac{\eta}{2}, Q - \frac{\eta}{2}\right) \frac{1}{2\pi\hbar}\left\{\int_{-\infty}^{+\infty} \exp\left\{\frac{-iP\eta}{\hbar}\right\} dP\right\} d\eta \tag{3.165}$$

Next, owing to the distribution theory leading to Eq. (18.60), the last integral of the right-hand part of Eq. (3.165) reads

$$\frac{1}{2\pi\hbar}\left\{\int_{-\infty}^{+\infty} \exp\left\{\frac{-iP\eta}{\hbar}\right\} dP\right\} = \delta(\eta)$$

so that Eq. (3.164) becomes

$$\boxed{\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} f_w(P,Q)\,dP = \int_{-\infty}^{+\infty} \rho\left(Q + \frac{\eta}{2}, Q - \frac{\eta}{2}\right)\delta(\eta)\,d\eta}$$

Therefore, according to the fact that $\delta(\eta)$ is zero, except if $\eta = 0$, for which $\delta(\eta) = 1$, and keeping in mind Eq. (3.160), this last expression reduces to

$$\boxed{\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} f_w(P,Q)\,dP = \rho(Q,Q) = f(Q)} \tag{3.166}$$

The function $f_w(P,Q)$ (3.163), known as the *Wigner distribution function*, may be viewed as corresponding from quantum mechanics to the classical distribution function in the phase space $f(P,Q)$. However, it must be observed that the Wigner distribution function may be negative, that is, impossible for the classical distribution function $f(P,Q)$. This aspect is the cost to be paid by the requirement to save the Heisenberg uncertainty relations, which forbid the simultaneous knowledge of the position and of the momentum.

3.4.6 Dynamics

3.4.6.1 Schrödinger picture At the difference of the other operators, which do not depend on time in the Schrödinger picture, the density operator is time dependent

in this representation because it is built up from the kets and the corresponding bras, which evolve with time according to the time-dependent Schrödinger equation.

3.4.6.1.1 Populations and coherences Start from the general expression (3.137) of the density operator of a mixed state. In the Schrödinger picture, the kets and bras are time dependent, so that at the difference of the other operators of quantum mechanics, the density operators must be time dependent, that is, when time is taken into account, Eq. (3.137) must read

$$\boldsymbol{\rho}(t)^{\mathrm{SP}} = \sum_i W_i |\Phi_i(t)\rangle\langle\Phi_i(t)| \tag{3.167}$$

where the W_i are time-dependent probabilities. Now, consider the eigenvalue equation of a Hermitian operator $\mathbf{A}$

$$\mathbf{A}|\Psi_n\rangle = A_n|\Psi_n\rangle$$

Next, consider a matrix element of the density operator in the basis $\{|\Psi_n\rangle\}$:

$$\boldsymbol{\rho}_{nm}(t)^{\mathrm{SP}} = \langle\Psi_n|\boldsymbol{\rho}(t)^{\mathrm{SP}}|\Psi_m\rangle \tag{3.168}$$

The time-dependent off-diagonal matrix elements of the density operator are known as *coherences*, whereas the diagonal corresponding ones are known as *populations*. Using Eq. (3.167) gives

$$\boldsymbol{\rho}_{nm}(t)^{\mathrm{SP}} = \sum_i W_i \langle\Psi_n|\ \Phi_i(t)\rangle\langle\Phi_i(t)|\Psi_m\rangle$$

This latter result may be also written for the coherences and for the populations, respectively

$$\boldsymbol{\rho}_{nm}(t)^{\mathrm{SP}} = \sum_i W_i C_{ni}(t) C_{im}(t)$$

$$\boldsymbol{\rho}_{nn}(t)^{\mathrm{SP}} = \sum_i W_i |C_{ni}(t)|^2$$

with

$$C_{ni}(t) = \langle\Psi_n|\ \Phi_i(t)\rangle$$

3.4.6.1.2 Liouville equation In order to get the time dependence of the density operator, first start from its expression (3.167) for a mixed state. Since the W_i are time independent, the partial derivative of Eq. (3.167) is

$$\left(\frac{\partial\boldsymbol{\rho}(t)^{\mathrm{SP}}}{\partial t}\right) = \sum_i W_i \left(\frac{\partial|\Phi_i(t)\rangle\langle\Phi_i(t)|}{\partial t}\right) \tag{3.169}$$

The time derivative of the right-hand side of this last equation is, of course,

$$\left(\frac{\partial|\Phi_i(t)\rangle\langle\Phi_i(t)|}{\partial t}\right) = \left(\frac{\partial|\Phi_i(t)\rangle}{\partial t}\right)\langle\Phi_i(t)| + |\Phi_i(t)\rangle\left(\frac{\partial\langle\Phi_i(t)|}{\partial t}\right)$$

Again, recall that thetime-dependent Schrödinger equation and its Hermitian conjugate are

$$i\hbar\left(\frac{\partial|\Phi_i(t)\rangle}{\partial t}\right) = \mathbf{H}|\Phi_i(t)\rangle \qquad \text{and} \qquad -i\hbar\left(\frac{\partial\langle\Phi_i(t)|}{\partial t}\right) = \langle\Phi_i(t)|\mathbf{H}$$

where $\mathbf{H}$ is the Hamiltonian. Thus, Eq. (3.169) becomes

$$i\hbar\left(\frac{\partial\boldsymbol{\rho}(t)^{\mathrm{SP}}}{\partial t}\right) = \sum_i W_i\mathbf{H}|\Phi_i(t)\rangle\langle\Phi_i(t)| - \sum_i W_i|\Phi_i(t)\rangle\langle\Phi_i(t)|\mathbf{H}$$

or, owing to Eq. (3.167) and since W_i commutes with $\mathbf{H}$,

$$i\hbar\left(\frac{\partial\boldsymbol{\rho}(t)^{\mathrm{SP}}}{\partial t}\right) = \mathbf{H}\boldsymbol{\rho}(t)^{\mathrm{SP}} - \boldsymbol{\rho}(t)^{\mathrm{SP}}\mathbf{H}$$

so that

$$\boxed{i\hbar\left(\frac{\partial\boldsymbol{\rho}(t)^{\mathrm{SP}}}{\partial t}\right) = [\mathbf{H}, \boldsymbol{\rho}(t)^{\mathrm{SP}}]} \tag{3.170}$$

that is, the Liouville–Von Neumann equation also called the *Liouville equation* or the *Von Neumann equation*. Note the difference in the sign of the commutator when passing from this equation, which applies to density operator, to that of (3.94) dealing with the observables. The reason is that the density operator is not an observable but is constructed from projectors and thus from kets and bras. The sign difference between Eq. (3.170) governing the time dependence of the density operator and that of (3.95) giving the time dependence of some operators other than the density operator, in the Heisenberg picture, that is,

$$i\hbar\langle\Psi|\left(\frac{\partial\mathbf{A}(t)^{\mathrm{HP}}}{\partial t}\right)|\Psi\rangle = \langle\Psi|[\mathbf{A}^{\mathrm{HP}}(t), \mathbf{H}]|\Psi\rangle$$

3.4.6.1.3 Density operators in statistical equilibrium When an isolated system is not in statistical equilibrium, its total density operator changes with time:

$$\left(\frac{\partial\boldsymbol{\rho}_{\mathrm{Tot}}(t)^{\mathrm{SP}}}{\partial t}\right) \neq 0$$

and will continue to change until the system has attained its statistical equilibrium:

$$\left(\frac{\partial\boldsymbol{\rho}_{\mathrm{Tot}}(t)^{\mathrm{SP}}}{\partial t}\right) = 0$$

In this special situation, it results from Eq. (3.170) that, at equilibrium, it is necessary that

$$[\mathbf{H}, \boldsymbol{\rho}_{\mathrm{Tot}}(t)^{\mathrm{SP}}] = 0$$

3.4.6.1.4 Energy representation of the density operator Owing to the appearance of the Hamiltonian $\mathbf{H}$ on the right-hand side of the Liouville–Von Neumann

Eq. (3.170), it may be of interest to consider the matrix representation of this equation on the basis of the eigenvectors of the Hamiltonian. Thus, write the eigenvalue equation of the Hamiltonian:

$$\mathbf{H}|\Psi_n\rangle = E_n|\Psi_n\rangle \tag{3.171}$$

Then, on the basis $\{|\Psi_n\rangle\}$, the matrix representation of the Liouville Eq. (3.170) takes the form

$$i\hbar\left(\frac{\partial\langle\Psi_n|\boldsymbol{\rho}(t)^{\mathrm{SP}}|\Psi_m\rangle}{\partial t}\right) = \langle\Psi_n|\mathbf{H}\,\boldsymbol{\rho}(t)^{\mathrm{SP}}|\Psi_m\rangle - \langle\Psi_n|\boldsymbol{\rho}(t)^{\mathrm{SP}}\mathbf{H}|\Psi_m\rangle$$

Due to the eigenvalue equation (3.171), this equation transforms to

$$i\hbar\left(\frac{\partial\langle\Psi_n|\boldsymbol{\rho}(t)^{\mathrm{SP}}|\Psi_m\rangle}{\partial t}\right) = E_n\langle\Psi_n|\boldsymbol{\rho}(t)^{\mathrm{SP}}|\Psi_m\rangle - E_m\langle\Psi_n|\boldsymbol{\rho}(t)^{\mathrm{SP}}|\Psi_m\rangle$$

which may also be written using the notations (3.168) for populations and coherences

$$i\hbar\left(\frac{\partial\boldsymbol{\rho}_{nm}(t)^{\mathrm{SP}}}{\partial t}\right) = (E_n - E_m)\boldsymbol{\rho}_{nm}(t)^{\mathrm{SP}} \tag{3.172}$$

Then, by integration of Eq. (3.172), one obtains

$$\boldsymbol{\rho}_{nm}(t)^{\mathrm{SP}} = \boldsymbol{\rho}_{nm}(0)^{\mathrm{SP}}e^{-i(E_n-E_m)t/\hbar} \tag{3.173}$$

Observe that it appears from Eq. (3.173) that the populations (corresponding to $n = m$) remain constant.

3.4.6.1.5 Canonical transformation on the density operator involving the Schrödinger evolution operator Consider the density operator at initial time $t = 0$. Equation (3.167) reads

$$\boldsymbol{\rho}(0)^{\mathrm{SP}} = \sum_i W_i|\Phi_i(0)\rangle\langle\Phi_i(0)| \tag{3.174}$$

At time t, the W_i being constant, the SP density operator becomes

$$\boldsymbol{\rho}(t)^{\mathrm{SP}} = \sum_i |\Phi_i(t)^{\mathrm{SP}}\rangle\langle\Phi_i(t)^{\mathrm{SP}}| \tag{3.175}$$

In the time evolution operator formalism, the time dependence of the kets and of the corresponding bras is given by Eq. (3.77):

$$|\Phi_i(t)^{\mathrm{SP}}\rangle = \mathbf{U}(t)|\Phi_i(0)^{\mathrm{SP}}\rangle \qquad \text{and} \qquad \langle\Phi_i(t)^{\mathrm{SP}}| = \langle\Phi_i(0)^{\mathrm{SP}}|\mathbf{U}(t)^{\dagger} \tag{3.176}$$

where $\mathbf{U}(t)$ is the time evolution operator (3.82) governed by the Hamiltonian of the system, that is,

$$\mathbf{U}(t) = (e^{-i\mathbf{H}t/\hbar}) \qquad \text{and} \qquad \mathbf{U}(t)^{\dagger} = \mathbf{U}(t)^{-1} = (e^{i\mathbf{H}t/\hbar})$$

The time-dependent density operator is therefore

$$\boldsymbol{\rho}(t)^{\mathrm{SP}} = \sum_i \mathbf{U}(t)|\Phi_i(0)\rangle\langle\Phi_i(0)|\mathbf{U}(t)^{\dagger}$$

Hence, in view of Eq. (3.174)

$$\boldsymbol{\rho}(t)^{\mathrm{SP}} = \mathbf{U}(t)\boldsymbol{\rho}(0)\mathbf{U}(t)^{\dagger} = \mathbf{U}(t)\boldsymbol{\rho}(0)\mathbf{U}(t)^{-1} \tag{3.177}$$

or, writing explicitly the time evolution operator

$$\boxed{\boldsymbol{\rho}(t)^{\mathrm{SP}} = (e^{-i\mathbf{H}t/\hbar})\boldsymbol{\rho}(0)^{\mathrm{SP}}(e^{+i\mathbf{H}t/\hbar})} \tag{3.178}$$

Note that in the canonical transformation of (3.177) or (3.178), the signs have changed with respect to those appearing in the time dependence of the Heisenberg picture or observables that, according to Eqs. (3.89) and (3.88), are

$$\mathbf{A}(t)^{\mathrm{HP}} = (e^{i\mathbf{H}t/\hbar})\mathbf{A}(e^{-i\mathbf{H}t/\hbar}) = \mathbf{U}(t)^{\dagger}\mathbf{A}\mathbf{U}(t)$$

3.4.6.2 Interaction picture Liouville equation Suppose that the system that is studied involves a Hamiltonian $\mathbf{H}$ that may be split into an unperturbed part $\mathbf{H}^{\circ}$ and a perturbation $\mathbf{V}$, according to

$$\mathbf{H} = \mathbf{H}^{\circ} + \mathbf{V}$$

Due to the partition of the Hamiltonian, the Liouville–Von Neumann equation (3.170) takes the form

$$i\hbar\left(\frac{\partial\boldsymbol{\rho}(t)^{\mathrm{SP}}}{\partial t}\right) = [\mathbf{H}^{\circ}, \boldsymbol{\rho}(t)^{\mathrm{SP}}] + [\mathbf{V}, \boldsymbol{\rho}(t)^{\mathrm{SP}}] \tag{3.179}$$

Next, keeping in mind that the SP density operator at time t is given by Eq. (3.175),

$$\boldsymbol{\rho}(t)^{\mathrm{SP}} = \sum_i W_i|\Phi_i(t)^{\mathrm{SP}}\rangle\langle\Phi_i(t)^{\mathrm{SP}}|$$

and since the W_i are constant, it is clear that the corresponding IP density operator is given by

$$\boldsymbol{\rho}(t)^{\mathrm{IP}} = \sum_i W_i|\Phi_i(t)^{\mathrm{IP}}\rangle\langle\Phi_i(t)^{\mathrm{IP}}| \tag{3.180}$$

whereas Eq. (3.118) relating the IP and SP kets is

$$|\Psi(t)^{\mathrm{IP}}\rangle = \mathbf{U}^{\circ}(t)^{-1}|\Psi(t)^{\mathrm{SP}}\rangle \tag{3.181}$$

where

$$\mathbf{U}^{\circ}(t) = (e^{-i\mathbf{H}^{\circ}t/\hbar}) \tag{3.182}$$

Hence, due to Eq. (3.181) and to its Hermitian conjugate, the IP density operator (3.180) reads

$$\boxed{\boldsymbol{\rho}(t)^{\mathrm{IP}} \equiv \mathbf{U}^{\circ}(t)^{-1}\boldsymbol{\rho}(t)^{\mathrm{SP}}\mathbf{U}^{\circ}(t)} \tag{3.183}$$

Then, premultiplying this equation by $\mathbf{U}^{\circ}(t)$ and postmultiplying it by its inverse, leads to

$$\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1} = \mathbf{U}^{\circ}(t)\mathbf{U}^{\circ}(t)^{-1}\boldsymbol{\rho}(t)^{\mathrm{SP}}\mathbf{U}^{\circ}(t)\mathbf{U}^{\circ}(t)^{-1}$$

so that, on simplification of the right-hand side, one obtains the relation inverse to (3.183), that is,

$$\boxed{\boldsymbol{\rho}(t)^{\mathrm{SP}} = \mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1}} \tag{3.184}$$

Moreover, due to Eq. (3.184), Eq. (3.179) yields

$$i\hbar\left(\frac{\partial\boldsymbol{\rho}(t)^{\mathrm{SP}}}{\partial t}\right)=[\mathbf{H}^{\circ},\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1}]+[\mathbf{V},\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1}] \tag{3.185}$$

On the other hand, the partial time derivative of Eq. (3.184), reads

$$\begin{aligned}\left(\frac{\partial\boldsymbol{\rho}(t)^{\mathrm{SP}}}{\partial t}\right)=&\left(\frac{\partial\mathbf{U}^{\circ}(t)}{\partial t}\right)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1}+\mathbf{U}^{\circ}(t)\left(\frac{\partial\boldsymbol{\rho}(t)^{\mathrm{IP}}}{\partial t}\right)\mathbf{U}^{\circ}(t)^{-1}\\&+\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\left(\frac{\partial\mathbf{U}^{\circ}(t)^{-1}}{\partial t}\right)\end{aligned} \tag{3.186}$$

Then, by identification of Eqs. (3.185) and (3.186), one obtains

$$\begin{aligned}&[\mathbf{H}^{\circ},\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1}]+[\mathbf{V},\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1}]\\&=i\hbar\left\{\left(\frac{\partial\mathbf{U}^{\circ}(t)}{\partial t}\right)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1}+\mathbf{U}^{\circ}(t)\left(\frac{\partial\boldsymbol{\rho}(t)^{\mathrm{IP}}}{\partial t}\right)\mathbf{U}^{\circ}(t)^{-1}\right.\\&\left.+\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\left(\frac{\partial\mathbf{U}^{\circ}(t)^{-1}}{\partial t}\right)\right\}\end{aligned} \tag{3.187}$$

Moreover, observe that, according to Eq. (3.81), and since $\mathbf{H}^{\circ}$ is Hermitian, the Schrödinger equation governing the dynamics of the unitary evolution operator $\mathbf{U}^{\circ}(t)$ and its Hermitian conjugate is

$$i\hbar\left(\frac{\partial\mathbf{U}^{\circ}(t)}{\partial t}\right)=\mathbf{H}^{\circ}\mathbf{U}^{\circ}(t)\qquad\text{and}\qquad-i\hbar\left(\frac{\partial\mathbf{U}^{\circ}(t)^{-1}}{\partial t}\right)=\mathbf{U}^{\circ}(t)^{-1}\mathbf{H}^{\circ}$$

These equations allow one to write the first and third right-hand-side terms of Eq. (3.187) according to

$$i\hbar\left(\frac{\partial\mathbf{U}^{\circ}(t)}{\partial t}\right)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1}=\mathbf{H}^{\circ}\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ-1}(t)$$

$$i\hbar\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\left(\frac{\partial\mathbf{U}^{\circ}(t)^{-1}}{\partial t}\right)=-\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1}\mathbf{H}^{\circ}$$

Hence, the sum of these two terms appearing in Eq. (3.187) reads

$$i\hbar\left\{\left(\frac{\partial\mathbf{U}^{\circ}(t)}{\partial t}\right)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1}+\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\left(\frac{\partial\mathbf{U}^{\circ}(t)^{-1}}{\partial t}\right)\right\}=[\mathbf{H}^{\circ},\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1}] \tag{3.188}$$

Hence, the left-hand side of Eq. (3.188) is equivalent to the first and third right-hand terms of Eq. (3.187), whereas the right-hand term of Eq. (3.188) is the same as the first commutator appearing on the left-hand side of Eq. (3.187). As a consequence, Eq. (3.187) simplifies to

$$i\hbar\mathbf{U}^{\circ}(t)\left(\frac{\partial\boldsymbol{\rho}(t)^{\mathrm{IP}}}{\partial t}\right)\mathbf{U}^{\circ}(t)^{-1}=[\mathbf{V},\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1}] \tag{3.189}$$

On the other hand, Eq. (3.179) may be transformed using Eq. (3.184) to

$$i\hbar\left(\frac{\partial\boldsymbol{\rho}(t)^{\mathrm{SP}}}{\partial t}\right)=[\mathbf{H}^{\circ},\boldsymbol{\rho}(t)^{\mathrm{SP}}]+[\mathbf{V},\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1}]$$

which, owing to Eq. (3.189), yields

$$\boxed{\left(\frac{\partial \boldsymbol{\rho}(t)^{\mathrm{SP}}}{\partial t}\right) = \frac{1}{i\hbar}[\mathbf{H}^{\circ}, \boldsymbol{\rho}(t)^{\mathrm{SP}}] + \mathbf{U}^{\circ}(t)\left(\frac{\partial \boldsymbol{\rho}(t)^{\mathrm{IP}}}{\partial t}\right)\mathbf{U}^{\circ}(t)^{-1}} \tag{3.190}$$

On the other hand, writing explicitly the right-hand commutator of Eq. (3.189) gives

$$i\hbar\mathbf{U}^{\circ}(t)\left(\frac{\partial \boldsymbol{\rho}(t)^{\mathrm{IP}}}{\partial t}\right)\mathbf{U}^{\circ}(t)^{-1} = \mathbf{V}\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1} - \mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1}\mathbf{V}$$

Then, postmultiplying both members of this last equation by $\mathbf{U}^{\circ}$ and premultiplying them by its inverse, allows us to write

$$i\hbar\mathbf{U}^{\circ}(t)^{-1}\left(\mathbf{U}^{\circ}(t)\left(\frac{\partial \boldsymbol{\rho}(t)^{\mathrm{IP}}}{\partial t}\right)\mathbf{U}^{\circ}(t)^{-1}\right)\mathbf{U}^{\circ}(t)$$

$$= \mathbf{U}^{\circ}(t)^{-1}(\mathbf{V}\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1})\mathbf{U}^{\circ}(t) - \mathbf{U}^{\circ}(t)^{-1}(\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1}\mathbf{V})\,\mathbf{U}^{\circ}(t)$$

or, on simplification

$$i\hbar\left(\frac{\partial \boldsymbol{\rho}(t)^{\mathrm{IP}}}{\partial t}\right) = \mathbf{U}^{\circ}(t)^{-1}\mathbf{V}\mathbf{U}^{\circ}(t)\boldsymbol{\rho}(t)^{\mathrm{IP}} - \boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{U}^{\circ}(t)^{-1}\mathbf{V}\mathbf{U}^{\circ}(t)$$

a result that may be written

$$i\hbar\left(\frac{\partial \boldsymbol{\rho}(t)^{\mathrm{IP}}}{\partial t}\right) = \mathbf{V}(t)^{\mathrm{IP}}\boldsymbol{\rho}(t)^{\mathrm{IP}} - \boldsymbol{\rho}(t)^{\mathrm{IP}}\mathbf{V}(t)^{\mathrm{IP}} \tag{3.191}$$

where $\mathbf{V}^{\mathrm{IP}}(t)$ is given, in agreement to Eq. (3.88), by

$$\mathbf{V}(t)^{\mathrm{IP}} = \mathbf{U}^{\circ}(t)^{-1}\mathbf{V}\mathbf{U}^{\circ}(t) \tag{3.192}$$

Finally, Eq. (3.191) may be expressed in terms of a commutator to give

$$\boxed{i\hbar\left(\frac{\partial \boldsymbol{\rho}(t)^{\mathrm{IP}}}{\partial t}\right) = [\mathbf{V}(t)^{\mathrm{IP}}, \boldsymbol{\rho}(t)^{\mathrm{IP}}]} \tag{3.193}$$

that is, the *IP Liouville–Von Neumann equation* governing the IP density operator, which involves the same sign for the Hamiltonian and density operator commutator as that appearing in the corresponding SP Liouville equation (3.170).

3.4.6.3 Integration of the IP Liouville Equation Formal integration of the IP Liouville–Von Neumann equation from t_0 to t leads to the following integral equation:

$$\boldsymbol{\rho}(t)^{\mathrm{IP}} = \boldsymbol{\rho}(t_0)^{\mathrm{IP}} + \left(\frac{1}{i\hbar}\right)\int_{t_0}^{t}[\mathbf{V}(t'-t_0)^{\mathrm{IP}}, \boldsymbol{\rho}(t'-t_0)^{\mathrm{IP}}]\,dt' \tag{3.194}$$

with, due to Eqs. (3.192) and (3.182),

$$\mathbf{V}(t'-t_0)^{\mathrm{IP}} = e^{i\mathbf{H}^{\circ}(t'-t_0)/\hbar}\mathbf{V}\mathbf{e}^{-i\mathbf{H}^{\circ}(t'-t_0)/\hbar} \tag{3.195}$$

If the potential $\mathbf{V}$ is small with respect to $\mathbf{H}^{\circ}$, the integral equation (3.194) may be solved by successive approximations. For this purpose, observe that the

time-dependent IP time evolution density operator involved in the commutator appearing on the right-hand side of Eq. (3.194) may be found by using an equation similar to Eq. (3.194), that is,

$$\boldsymbol{\rho}(t' - t_0)^{\mathrm{IP}} = \boldsymbol{\rho}(t_0)^{\mathrm{IP}} + \left(\frac{1}{i\hbar}\right) \int_{t_0}^{t'-t_0} [\mathbf{V}(t'' - t_0)^{\mathrm{IP}}, \boldsymbol{\rho}(t'' - t_0)^{\mathrm{IP}}]\, dt''$$

so that Eq. (3.194) becomes

$$[\mathbf{V}(t' - t_0)^{\mathrm{IP}}, \boldsymbol{\rho}(t' - t_0)^{\mathrm{IP}}]$$
$$= [\mathbf{V}(t' - t_0)^{\mathrm{IP}}, \boldsymbol{\rho}(t_0)^{\mathrm{IP}}] + \left(\frac{1}{i\hbar}\right) \int_0^t [\mathbf{V}(t' - t_0)^{\mathrm{IP}}, [\mathbf{V}(t'' - t_0)^{\mathrm{IP}}, \boldsymbol{\rho}(t'' - t_0)^{\mathrm{IP}}]]\, dt''$$

Then, inserting this expression into Eq. (3.194) yields

$$\boldsymbol{\rho}(t)^{\mathrm{IP}} = \boldsymbol{\rho}(t_0)^{\mathrm{IP}} + \left(\frac{1}{i\hbar}\right) \int_{t_0}^{t} [\mathbf{V}(t' - t_0)^{\mathrm{IP}}, \boldsymbol{\rho}(t_0)^{\mathrm{IP}}]\, dt'$$
$$+ \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t} \int_{t_0}^{t'} [\mathbf{V}(t' - t_0)^{\mathrm{IP}}, [\mathbf{V}(t'' - t_0)^{\mathrm{IP}}, \boldsymbol{\rho}(t'' - t_0)^{\mathrm{IP}}]]\, dt'\, dt''$$

Again, by iteration, one obtains

$$\boldsymbol{\rho}(t)^{\mathrm{IP}} = \boldsymbol{\rho}(t_0)^{\mathrm{IP}} + \frac{1}{i\hbar} \int_{t_0}^{t} [\mathbf{V}(t' - t_0)^{\mathrm{IP}}, \boldsymbol{\rho}(t_0)^{\mathrm{IP}}]\, dt' \tag{3.196}$$
$$+ \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t} \int_{t_0}^{t'} [\mathbf{V}(t' - t_0)^{\mathrm{IP}}, [\mathbf{V}(t'' - t_0)^{\mathrm{IP}}, \boldsymbol{\rho}(t_0)^{\mathrm{IP}}]]\, dt'\, dt''$$
$$+ \left(\frac{1}{i\hbar}\right)^3 \int_{t_0}^{t} \int_{t_0}^{t'} \int_{t_0}^{t''} [\mathbf{V}(t' - t_0)^{\mathrm{IP}}, [\mathbf{V}(t'' - t_0)^{\mathrm{IP}}, [\mathbf{V}(t''' - t_0)^{\mathrm{IP}},$$
$$\boldsymbol{\rho}(t''' - t_0)^{\mathrm{IP}}]]]\, dt'\, dt''\, dt'''$$

This operation may be repeated any number of times. However, if the perturbation $\mathbf{V}$ is weak, the treatment may be limited to the second order in the IP perturbation operator so that Eq. (3.196) becomes truncated at the second order in the perturbation according to

$$\boldsymbol{\rho}(t)^{\mathrm{IP}} \simeq \boldsymbol{\rho}(t_0)^{\mathrm{IP}} + \frac{1}{i\hbar} \int_{t_0}^{t} [\mathbf{V}(t' - t_0)^{\mathrm{IP}}, \boldsymbol{\rho}(t_0)^{\mathrm{IP}}]\, dt'$$
$$+ \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t} \int_{t_0}^{t'} [\mathbf{V}(t' - t_0)^{\mathrm{IP}}, [\mathbf{V}(t'' - t_0)^{\mathrm{IP}}, \boldsymbol{\rho}(t_0)^{\mathrm{IP}}]]\, dt'\, dt'' \tag{3.197}$$

Recall that the IP perturbation operator is given by Eq. (3.192) and that, when the expression of the IP density operator has been obtained with the help of Eq. (3.197), one may retrieve the time-dependent density operator using Eq. (3.184).

3.5 CONCLUSION

This chapter, which was devoted to different representations of quantum mechanics, has lead to important useful developments. (i) Matrix representation allowing one to replace the eigenvalue equation of an Hermitian operator to be solved by a corresponding matrix eigenvalue equation susceptible to be easily numerically solved, which is of great interest for the study of quantum anharmonic oscillators. (ii) Wave mechanics, which is the representation of quantum mechanics in geometrical space, is in many situations such as atoms or molecules more tractable than matrix or quantum mechanics. Although there is less interest in quantum oscillators than matrix mechanics, it will remain of some interest in visualizing some results dealing with these oscillators. (iii) Density operator approaches are very powerful when studying many-particle systems, particularly for statistical equilibrium situations leading to thermal equilibrium, and will be widely used when studying thermal properties of quantum oscillators. (iv) Time-dependent representations other than the Schrödinger picture where the time dependence resides in the quantum states, which constitute the Heisenberg picture where the time dependence is contained in the Hermitian operators, and the interaction picture, which is a description intermediate between the Schrödinger and Heisenberg pictures and which will be very useful when studying the irreversible dynamics of quantum oscillators coupled to a thermal bath.

The important results concerning the time-dependent Schrödinger, Heisenberg, and interaction pictures are collected into the two following lists:

Schrödinger and Heisenberg pictures
Schrödinger equation and evolution operator:
$i\hbar\dfrac{\partial}{\partial t}\lvert\Psi(t)^{\mathrm{SP}}\rangle = \mathbf{H}\lvert\Psi(t)^{\mathrm{SP}}\rangle$
Time-dependent ket in the Schrödinger picture:
$\lvert\Psi(t)^{\mathrm{SP}}\rangle = \mathbf{U}(t)^{\mathrm{SP}}\lvert\Psi(0)^{\mathrm{SP}}\rangle$
Time-dependent evolution operator in the Schrödinger picture:
$\mathbf{U}(t)^{\mathrm{SP}} = e^{-i\mathbf{H}t/\hbar}$
Time-dependent operators in the Heisenberg picture:
$\mathbf{A}(t)^{\mathrm{HP}} = \mathbf{U}(t)^{\mathrm{SP}-1}\mathbf{A}(0)\mathbf{U}(t)^{\mathrm{SP}}$

Dynamic equation governing evolution operators in the Schrödinger picture:
$i\hbar\left(\dfrac{\partial \mathbf{U}(t)^{\mathrm{SP}}}{\partial t}\right) = \mathbf{H}\mathbf{U}(t)^{\mathrm{SP}}$
Dynamic equation governing operators in the Heisenberg picture:
$i\hbar\left(\dfrac{\partial \mathbf{A}(t)^{\mathrm{HP}}}{\partial t}\right) = [\mathbf{A}(t)^{\mathrm{HP}}, \mathbf{H}]$

Interaction picture
Hamiltonian partition and corresponding evolution operators:
$\mathbf{H} = \mathbf{H}^{\circ} + \mathbf{V}$ $\mathbf{U}^{\circ}(t) = e^{-i\mathbf{H}^{\circ}t/\hbar}$ and $\mathbf{U}(t) = e^{-i\mathbf{H}t/\hbar}$
Relation between IP and SP evolution operators:
$\mathbf{U}(t)^{\mathrm{SP}} = \mathbf{U}^{\circ}(t)\mathbf{U}(t)^{\mathrm{IP}}$
Time-dependent operators A in the interaction picture:
$\mathbf{A}(t)^{\mathrm{IP}} = \mathbf{U}^{\circ}(t)^{-1}\mathbf{A}\mathbf{U}^{\circ}(t)$
Dynamic equation governing the interaction picture evolution operator:
$i\hbar\left(\dfrac{\partial \mathbf{U}(t)^{\mathrm{IP}}}{\partial t}\right) = \mathbf{V}(t)^{\mathrm{IP}}\mathbf{U}(t)^{\mathrm{IP}}$
Connection between SP and IP time-dependent kets:
$\lvert\Psi(t)^{\mathrm{SP}}\rangle = \mathbf{U}^{\circ}(t)\lvert\Psi(t)^{\mathrm{IP}}\rangle$

Those dealing with density operators are given as follows:

Density operators
Definition of density operators:
$\boldsymbol{\rho} = \sum_i W_i \lvert\Phi_i\rangle\langle\Phi_i\rvert$
Average values performed over density operators:
$\langle\mathbf{A}\rangle_{\boldsymbol{\rho}} = \mathbf{tr}\{\boldsymbol{\rho}\mathbf{A}\}$

Liouville equation in the Schrödinger picture:
$i\hbar\left(\frac{\partial \boldsymbol{\rho}(t)^{\mathrm{SP}}}{\partial t}\right) = [\mathbf{H}, \boldsymbol{\rho}(t)^{\mathrm{SP}}]$
Statistical entropy:
$S = -k_B \mathbf{tr}\{\boldsymbol{\rho} \ln \boldsymbol{\rho}\}$

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CHAPTER 4

SIMPLE MODELS USEFUL FOR QUANTUM OSCILLATOR PHYSICS

INTRODUCTION

Before studing quantum oscillators, which is the principal aim of the present book, it may be useful to apply the information of the previous chapters dealing with the basis of quantum mechanics to three simple models that will be of interest in the future. The first one is the *particle-in-a-box model*, which comprises a single particle enclosed in a box where the potential is zero, this same potential being infinite beyond the box walls. Applying simply the wave mechanics, we shall get quantized energy levels and their associated wavefunctions, the node number of which increases with the energy. It will also be useful to illustrate the quantization of the energy levels and the decrease of the associated wavelength when the energy rises, two concepts we shall meet when discussing the oscillators. The second model to which the present chapter is devoted deals with the interaction between two energy levels, which will be of interest when focusing attention on the local interaction between two excited states of two different oscillators, a situation that occurs in the area of *Fermi resonances*. Finally, the last section treats the probability for a system to pass from one of its stationary energy levels to another if a potential perturbs it. Using a formalism that will later be applied to the interaction of oscillators with the electromagnetic field, it will lead to the important *Fermi golden rule*.

4.1 PARTICLE-IN-A-BOX MODEL

Consider a particle of mass m enclosed in a box of volume $\mathbb{V}$ given by

$$\mathbb{V} = a_x a_y a_z \tag{4.1}$$

dimensions in which the potential is zero while it is infinite outside. Its kinetic energy is

$$\mathbf{T} = \frac{1}{2m}(\mathbf{P}_x^2 + \mathbf{P}_y^2 + \mathbf{P}_z^2)$$

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where the $\mathbf{P}_i^2$ are the components x, y, and z of the momentum. In the wave mechanics representation, the momentum operator obeys Eq. (3.51):

$$P = -i\hbar\frac{\partial}{\partial Q}$$

Thus, the wave mechanics description of the particle-in-a-box kinetic operator reads

$$T = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

where x, y, and z are the components of Q. Furthermore, since the potential is assumed to be zero inside the box, the wave mechanics description of the potential is simply

$$V = 0$$

The Hamiltonian of the system, which is the sum of the kinetic and potential operators, is in the position representation

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

Now, for this three-dimensional (3D) model, the wavefunction of the particle can be written as the product of the wavefunctions along the three independent dimensions, that is,

$$\Psi(x, y, z) = \Psi(x)\Psi(y)\Psi(z) \tag{4.2}$$

Hence, the eigenvalue equation of the Hamiltonian, that is, the time-independent Schrödinger equation, takes the form

$$-\frac{\hbar^2}{2m}\left(\Psi(y)\Psi(z)\frac{\partial^2\Psi(x)}{\partial x^2} + \Psi(x)\Psi(z)\frac{\partial^2\Psi(y)}{\partial y^2} + \Psi(x)\Psi(y)\frac{\partial^2\Psi(z)}{\partial z^2}\right) = E\Psi(x)\Psi(y)\Psi(z) \tag{4.3}$$

where E is the Hamiltonian eigenvalue.

4.1.1 Solving the 3D Schrödinger equation

Now, the Hamiltonian eigenvalue E may be written as the sum of the energies along the three dimensions, that is,

$$E = E_x + E_y + E_z \tag{4.4}$$

Thus, the Schrödinger equation (4.3) splits into three independent and equivalent Schrödinger equations corresponding to the three dimensions of the geometrical space, according to

$$\left(\frac{\partial^2\Psi(x)}{\partial x^2}\right) = -k_x^2\Psi(x) \tag{4.5}$$

$$\left(\frac{\partial^2\Psi(y)}{\partial y^2}\right) = -k_y^2\Psi(y) \tag{4.6}$$

$$\left(\frac{\partial^2 \Psi(z)}{\partial z^2}\right) = -k_z^2 \Psi(z) \tag{4.7}$$

with

$$k_x^2 = \frac{2m}{\hbar^2} E_x \tag{4.8}$$

$$k_y^2 = \frac{2m}{\hbar^2} E_y \tag{4.9}$$

$$k_z^2 = \frac{2m}{\hbar^2} E_z \tag{4.10}$$

Observe that since outside the box the potential is infinite, it is impossible to the particle to get out of the box (Fig. 4.1). Therefore, the probability for the particle to be outside the box is zero, and, thus, since this probability is the squared modulus of the wavefunction, the three wavefunctions satisfy the following boundary conditions, for example, leading for the x component to

$$\Psi(x) = 0 \quad \text{if} \quad -\infty < x \leqslant 0 \qquad \text{and} \qquad a_x \leqslant x < \infty \tag{4.11}$$

$$\Psi(y) = 0 \quad \text{if} \quad -\infty < y \leqslant 0 \qquad \text{and} \qquad a_y \leqslant y < \infty \tag{4.12}$$

$$\Psi(z) = 0 \quad \text{if} \quad -\infty < z \leqslant 0 \qquad \text{and} \qquad a_z \leqslant z < \infty \tag{4.13}$$

It appears, therefore, that the partial differential equations (4.5)–(4.7) to be solved are subject to the boundary conditions (4.11)–(4.13). The general solution of Eq. (4.5) is of the form

$$\Psi(x) = A_x \sin(k_x x) + B_x \cos(k_x x)$$

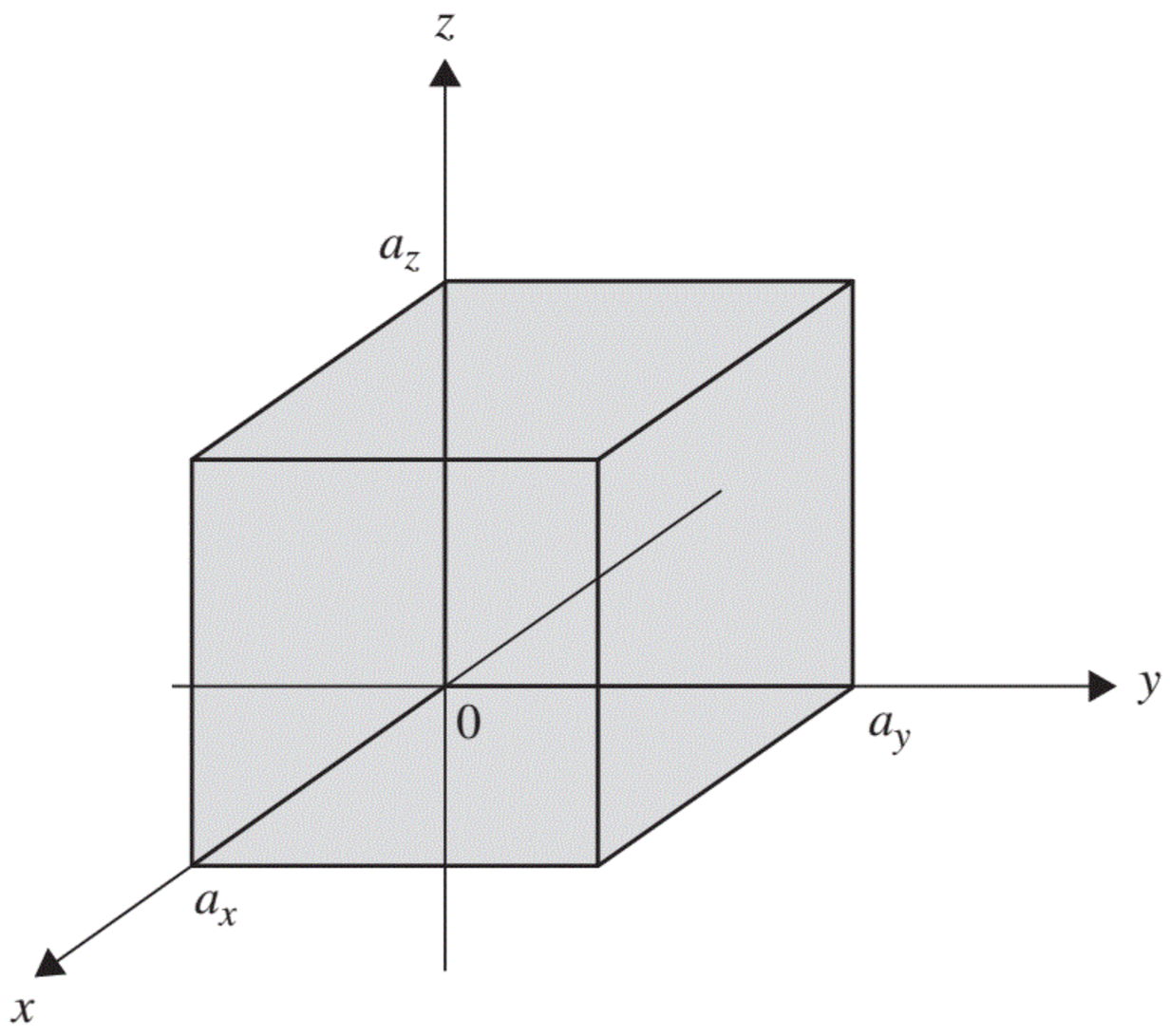


Figure 4.1 Particle-in-a-box model.

where A_x and B_x are two constants. Next, owing to the boundary condition (4.11) implying that, at $x = 0$, $\Psi(0) = 0$, it follows that $B_x = 0$, so that

$$\Psi(x) = A_x \sin(k_x x) \tag{4.14}$$

Now, the same boundary condition (4.11) implying that $x = a$, leads to write $\Psi(a) = 0$ so that, since $A \neq 0$ Eq. (4.14), it is necessary that

$$\sin(k_x a_x) = 0$$

such a condition being verified if

$$k_x a_x = n_x \pi \tag{4.15}$$

where n_x is a number that may take a priori all the integer values between 0 and ∞. That leads one to write the solution (4.14) as

$$\Psi_{n_x}(x) = A_x \sin\left(\frac{n_x \pi}{a_x} x\right) \tag{4.16}$$

In a similar way, one can obtain for the solutions of Eqs. (4.6) and (4.7) subject, respectively, to the boundary conditions (4.12) and (4.13)

$$\Psi_{n_y}(y) = A_y \sin\left(\frac{n_y \pi}{a_y} y\right) \tag{4.17}$$

$$\Psi_{n_z}(z) = A_z \sin\left(\frac{n_z \pi}{a_z} z\right) \tag{4.18}$$

with

$$k_y a_y = n_y \pi \qquad \text{and} \qquad k_z a_z = n_z \pi \tag{4.19}$$

The normalization condition of a wavefunction, which is

$$\int_0^a \Psi_{n_x}(x)^2 \, dx = 1$$

reads for the wavefunction (4.16)

$$A_x^2 \int_0^a \sin^2\left(\frac{n_x \pi}{a_x} x\right) dx = 1 \tag{4.20}$$

Next, using the trigonometric relation

$$\sin^2(z) = \tfrac{1}{2}(1 - \cos 2z)$$

Eq. (4.20) yields

$$A_x^2 \int_0^a \tfrac{1}{2}\left(1 - \cos\left(2\frac{n_x \pi}{a_x} x\right)\right) dx = 1 \tag{4.21}$$

Moreover, due to the fact that

$$\int_0^a \cos\left(2\frac{n_x \pi}{a_x} x\right) dx = 0$$

Eq. (4.21) reduces to

$$\tfrac{1}{2}A_x^2 a_x = 1$$

so that Eq. (4.16) becomes

$$\Psi_{n_x}(x) = \sqrt{\frac{2}{a_x}}\sin\left(\frac{n_x\pi}{a_x}x\right) \tag{4.22}$$

In a similar way, one would obtain for the wavefunctions (4.17) and (4.18),

$$\Psi_{n_y}(y) = \sqrt{\frac{2}{a_y}}\sin\left(\frac{n_y\pi}{a_y}y\right) \tag{4.23}$$

$$\Psi_{n_z}(z) = \sqrt{\frac{2}{a_z}}\sin\left(\frac{n_z\pi}{a_z}z\right) \tag{4.24}$$

4.1.2 3D Wavefunctions and energy levels

Due to Eq. (4.2), and to Eqs. (4.22)–(4.24), the total wavefunction reads

$$\Psi_{n_x,n_y,n_z}(x,y,z) = \frac{2^{3/2}}{\sqrt{\mathbb{V}}}\sin\left(\frac{n_x\pi}{a_x}x\right)\sin\left(\frac{n_y\pi}{a_y}y\right)\sin\left(\frac{n_z\pi}{a_z}z\right) \tag{4.25}$$

where Eq. (4.1) has been used, relating the dimensions a_x, a_y, and a_z of the box to its volume $\mathbb{V}$. Of course, the solutions corresponding to $n_x = 0, n_y = 0$, or $n_z = 0$ are without physical meaning since it would imply erroneously that the wavefunction (4.25) and thus the probability of the particle in all the box would be zero. Thus, all the quantum numbers n_x, n_y, and n_z must be integers, starting from unity.

The wavefunction (4.25) appears to be a product of stationary wavefunctions of the form

$$\Psi_{n_x,n_y,n_z}(x,y,z) = \Psi_{n_x}(x)\Psi_{n_y}(y)\Psi_{n_z}(z)$$

with

$$\Psi_{n_x}(x) = \sqrt{\frac{2}{a_x}}\sin\left(\frac{2\pi}{\lambda_{n_x}}x\right)$$

$$\Psi_{n_y}(y) = \sqrt{\frac{2}{a_y}}\sin\left(\frac{2\pi}{\lambda_{n_y}}y\right)$$

$$\Psi_{n_z}(z) = \sqrt{\frac{2}{a_z}}\sin\left(\frac{2\pi}{\lambda_{n_z}}z\right)$$

and where the λ_{n_x}, λ_{n_y}, and λ_{n_z} are wavelengths obeying

$$\lambda_{n_x} = \left(\frac{2a_x}{n_x}\right) \qquad \lambda_{n_y} = \left(\frac{2a_y}{n_y}\right) \qquad \lambda_{n_z} = \left(\frac{2a_z}{n_z}\right) \tag{4.26}$$

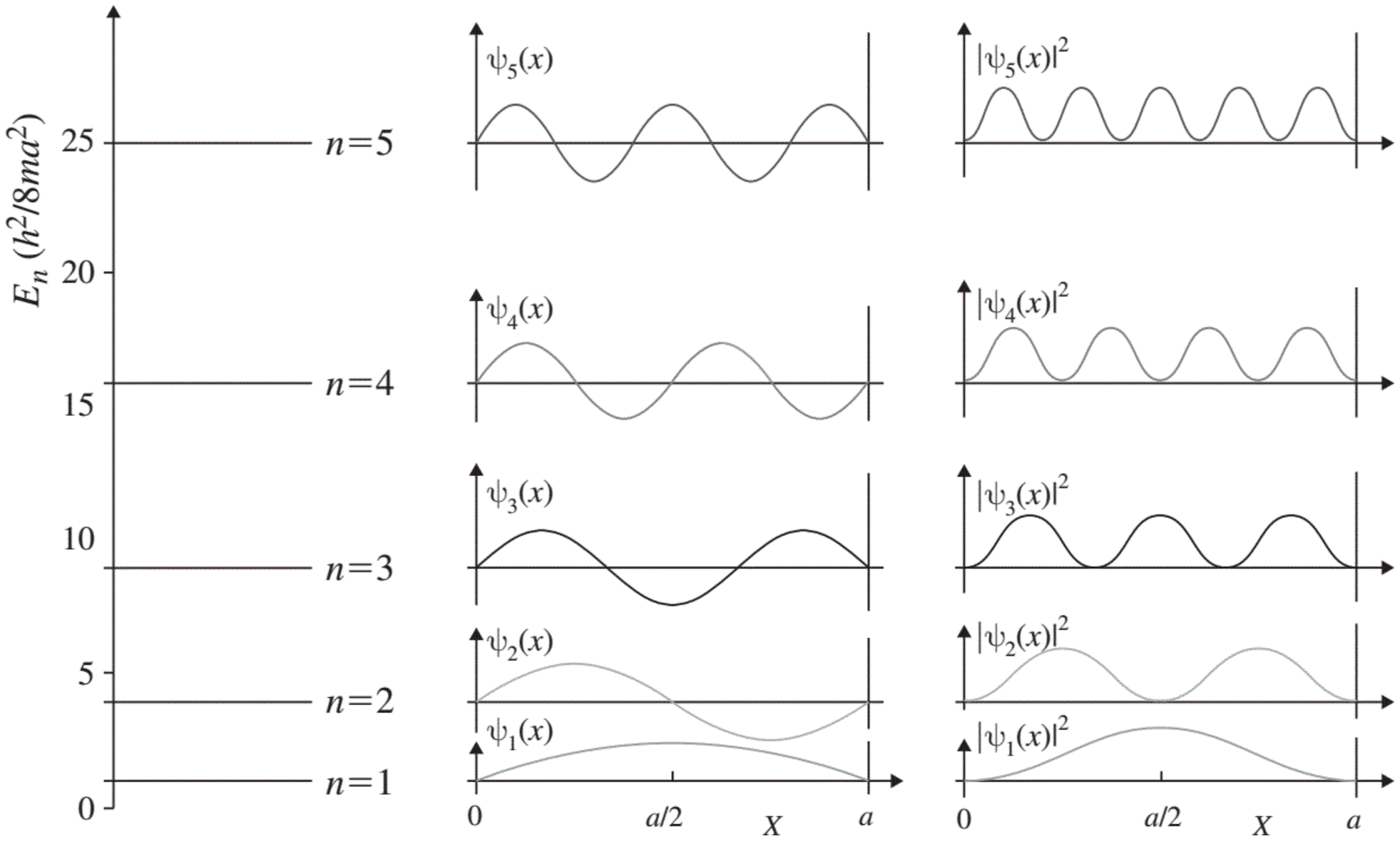


Figure 4.2 One-dimensional particle-in-a-box model. Energy levels and corresponding wavefunctions and probability densities for the four lowest quantum numbers.

In addition, Eqs. (4.8)–(4.10) combined with (4.15)–(4.19) allow us to get following results, with the energies corresponding to the x, y, and z components:

$$E_{n_x} = \left(\frac{\pi^2\hbar^2}{2ma_x^2}\right) n_x^2 \qquad E_{n_y} = \left(\frac{\pi^2\hbar^2}{2ma_y^2}\right) n_y^2 \qquad E_{n_z} = \left(\frac{\pi^2\hbar^2}{2ma_z^2}\right) n_z^2 \tag{4.27}$$

Hence, after passing from $\hbar$ to h, the total energy (4.4) becomes

$$E_{n_x,n_y,n_z} = \frac{h^2}{8m}\left(\frac{n_x^2}{a_x^2} + \frac{n_y^2}{a_y^2} + \frac{n_z^2}{a_z^2}\right) \tag{4.28}$$

It must be emphasized that, since n_x, n_z, and n_z are integers, the energy levels (4.28) are quantized, a result that will be also found later for quantum harmonic oscillators. Figure 4.2, which deals with the x component of the 3D model, gives the dimensionless energy levels and the corresponding wavefunctions for the four lowest quantum number n_x.

Hence, the nodes of the wavefunction are increasing with the quantum number and the corresponding energy level, a situation that will be met later for quantum harmonic oscillators and that is related to the *de Broglie wavelength*, we shall consider some later.

Moreover, when the box is cubic, that is, when

$$a_x = a_y = a_z = a$$

and due to Eq. (4.1), the equation (4.28) giving the energy levels simplifies to

$$E_{n_x,n_y,n_z} = \frac{h^2}{8m}\frac{(n_x^2 + n_y^2 + n_z^2)}{\mathbb{V}^{2/3}} \tag{4.29}$$

Then, in terms of the energy units E°

$$E^\circ = \frac{h^2}{8m\mathbb{V}^{2/3}}$$

and for the two lowest values 1 and 2 of the quantum numbers n_x, n_y, and n_z, the lowest energy levels (4.29) appear to be those given in the tabular expression (4.30):

n_x	n_y	n_z	E_{n_x,n_y,n_z}
1	1	1	1
1	1	2	6
1	2	1	6
2	1	1	6
2	2	1	9
2	1	2	9
1	2	2	9

(4.30)

Inspection of this data shows that different energy levels may have the same energy, that is, they are *degenerate*.

4.1.3 Consequences useful for quantum oscillators

As seen above, the particle-in-a-box model leads to the important result of the energy quantization. However, it leads also to some other interesting consequences, for example, the *de Broglie wavelength* of a quantum particle and a simple understanding of how the energy quantization disappears when the physical dimensions are progressively increasing.

Observe that the energy levels (4.28) are only kinetic in nature since the potential energy is zero inside the box. Thus, they may be written as the sum of the kinetic energies along the three dimensions, that is,

$$E_{n_x,n_y,n_z} = \frac{1}{2m}\left(P_{n_x}^2 + P_{n_y}^2 + P_{n_z}^2\right)$$

Then, by identification of this formal expression with Eq. (4.28), one obtains

$$P_{n_x} = \pm\frac{h}{2a_x}n_x$$

so that, due to Eq. (4.26), it appears that the wavelengths are given by

$$\lambda_{n_x} = \frac{h}{\left|P_{n_x}\right|} \tag{4.31}$$

which is the *Louis de Broglie's relation*, which has been experimentally verified for microscopic particles. Note that Fig. 4.2 reveals that the number of nodes of the wavefunctions are increasing with the quantum number n_x, reflecting the fact that in agreement with Eq. (4.31), the modulus of the momentum raises when the de Broglie wavelength decreases, leading, therefore, to an enhancement of the energy since there is no potential.

In the special case of a cubic box, when one of the quantum numbers is increased by a factor of 1, the others remaining constant, Eq. (4.29) reads

$$E_{n_x+1,n_y,n_z} = \left(\frac{h^2}{8m}\right) \frac{(n_x+1)^2 + n_y^2 + n_z^2}{\mathbb{V}^{2/3}} \tag{4.32}$$

Then, the difference between the two successive energy levels (4.29) and (4.32) yields

$$\Delta E_{n_x,n_x+1} = E_{n_x+1,n_y,n_z} - E_{n_x,n_y,n_z} = \left(\frac{h^2}{8m}\right) \frac{(2n_x+1)}{\mathbb{V}^{2/3}}$$

which, for large quantum numbers, may be approximated as

$$\Delta E_{n_x,n_x+1} = \left(\frac{h^2}{4m}\right) \frac{n_x}{\mathbb{V}^{2/3}} \tag{4.33}$$

This result, which follows from quantum mechanics, holds for microscopic dimensions of atoms or molecules. But there is no reason why it should not also be true for macroscopic systems where the mass (denoted M in place of m) of the particle and the volume in which it is enclosed are those of usual experiences, so that Eq. (4.33) reads

$$\widetilde{\Delta E}_{n_x,n_x+1} = \left(\frac{h^2}{4M}\right) \frac{n_x}{\mathbb{V}^{2/3}} \tag{4.34}$$

As an illustration, when passing from a description of an atomic electron of mass m_e enclosed in a volume $\mathbb{V}$, which is roughly that of the atom of radius a_{at}, to the description of a ball of mass M_B of 1 kg moving in a volume $\mathbb{V}$ around 1 m^3, one has respectively

$$m_e \backsimeq 10^{-30}\,\mathrm{kg} \qquad \text{and} \qquad a_{at} \backsimeq 10^{-10}\,\mathrm{m}$$

$$M_B \backsimeq 1\,\mathrm{kg} \qquad \text{and} \qquad a \backsimeq 1\,\mathrm{m}$$

so that Eq. (4.34) leads to

$$\widetilde{\Delta E}_{n_x,n_x+1} = 10^{-50}\,\Delta E_{n_x,n_x+1} \tag{4.35}$$

In a similar way, when passing from a description of a proton of mass m_p enclosed in a nucleus of volume $\mathbb{V}$, which is roughly that of the third power of the nucleus radius a_{nu}, to that of the Earth of mass M_E moving around the Sun at the distance $a_{\mathrm{Sun}} \backsimeq 10^{11}$ m there are

$$m_p \backsimeq 10^{-27}\,\mathrm{kg} \qquad \text{and} \qquad a_{nu} \backsimeq 10^{-15}\,\mathrm{m}$$

$$M_E \backsimeq 10^{25}\,\mathrm{kg} \qquad \text{and} \qquad a_{\mathrm{Sun}} \backsimeq 10^{11}\,\mathrm{m}$$

so that Eq. (4.34) leads to

$$\widetilde{\Delta E}_{n_x,n_x+1} = 10^{-104}\,\Delta E_{n_x,n_x+1} \tag{4.36}$$

Equations (4.35) and (4.36) illustrate the fact that passing from the microscopic to the macroscopic levels drastically decreases the energy gap between two successive energy levels.

4.2 TWO-ENERGY-LEVEL SYSTEMS

Now, it is time to study the model of two-energy-level systems, which will illustrate the phenomenon called *quantum interference* between kets, which is a simple consequence of the linear properties of quantum mechanics. Such a model will be later applied when studying the interactions dealing with anharmonically coupled oscillators. But, it is suitable to begin the present approach by starting from equations dealing with the more general model of multiple interacting energy levels.

4.2.1 Multiple interacting energy levels

Consider a system the Hamiltonian of which may be split into two parts according to

$$\mathbf{H} = \mathbf{H}^\circ + \mathbf{V} \tag{4.37}$$

Now, suppose that the eigenvalue equation of $\mathbf{H}^\circ$ is known, that is,

$$\mathbf{H}^\circ|\Phi_i\rangle = E_i^\circ|\Phi_i\rangle \tag{4.38}$$

Since $\mathbf{H}^\circ$ is Hermitian, its eigenvectors are orthogonal so that, if they are normalized, they verify

$$\langle\Phi_i|\Phi_j\rangle = \delta_{ij} \tag{4.39}$$

Owing to Eqs. (4.37)–(4.39), and in the basis $\{|\Phi_i\rangle\}$, the diagonal matrix elements of the full Hamiltonian are

$$\langle\Phi_i|\mathbf{H}|\Phi_i\rangle = E_i^\circ + \langle\Phi_i|\mathbf{V}|\Phi_i\rangle \tag{4.40}$$

Now, due to Eq. (4.37), the off-diagonal matrix elements are

$$\langle\Phi_i|\mathbf{H}|\Phi_j\rangle = \langle\Phi_i|(\mathbf{H}^\circ + \mathbf{V})|\Phi_j\rangle$$

In addition, owing to the eigenvalue equation (4.38), there is

$$\langle\Phi_i|\mathbf{H}^\circ|\Phi_j\rangle = \langle\Phi_i|E_j^\circ|\Phi_j\rangle = E_j^\circ\langle\Phi_i|\Phi_j\rangle = E_j^\circ\delta_{ij}$$

so that only part $\mathbf{V}$ of the Hamiltonian (4.37) couples two different eigenkets of $\mathbf{H}^\circ$, according to

$$\langle\Phi_i|\mathbf{H}|\Phi_j\rangle = \langle\Phi_i|\mathbf{V}|\Phi_j\rangle = \beta_{ij}$$

Now, writing

$$\alpha_i = \langle\Phi_i|\mathbf{H}|\Phi_i\rangle \qquad \text{and} \qquad \beta_{ii} = \langle\Phi_i|\mathbf{V}|\Phi_i\rangle \tag{4.41}$$

Eq. (4.40) leads to

$$\alpha_i = E_i^\circ + \beta_{ii}$$

Now, the eigenvalue equation of the full Hamiltonian (4.37) is

$$\mathbf{H}|\Psi_\mu\rangle = E_\mu|\Psi_\mu\rangle \quad \text{with} \quad \langle\Psi_\mu|\Psi_\nu\rangle = \delta_{\mu\nu} \tag{4.42}$$

the matrix representation of this eigenvalue equation in the basis of the eigenkets of $\mathbf{H}^\circ$ being

$$\begin{pmatrix} \alpha_1 & \beta_{12} & \dots & \beta_{1N} \\ \beta_{21} & \alpha_2 & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \beta_{N1} & \dots & \dots & \alpha_N \end{pmatrix} \begin{pmatrix} C_{1\mu} \\ C_{2\mu} \\ \dots \\ C_{N\mu} \end{pmatrix} = E_\mu \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & \dots \\ \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & 1 \end{pmatrix} \begin{pmatrix} C_{1\mu} \\ C_{2\mu} \\ \dots \\ C_{N\mu} \end{pmatrix} \tag{4.43}$$

with

$$C_{\mu i} = \langle \Psi_\mu | \Phi_i \rangle$$

One possibility to obtain the eigenvalues E_μ and the corresponding eigenvectors is to diagonalize the left-hand matrix appearing in Eq. (4.43). However, there is yet another possibility, because this eigenvalue equation may be also written as a system of simultaneous equations:

$$\begin{cases} (\alpha_1 - E_\mu)C_{1\mu} + \beta_{12}C_{2\mu} & + \dots + \beta_{1N}C_{N\mu} & = 0 \\ \beta_{21}C_{1\mu} & + (\alpha_2 - E_\mu)C_{2\mu} + \dots + \dots & = 0 \\ \dots & + \dots & + \dots + \dots & \dots \\ \beta_{N1}C_{1\mu} & + \dots & + \dots + (\alpha_N - E_\mu)C_{N\mu} & = 0 \end{cases}$$

Then, since the coefficients $C_{i\mu}$ cannot be zero, this system of equations is satisfied if the corresponding determinant is zero, that is,

$$\begin{vmatrix} (\alpha_1 - E) & \beta_{12} & \dots & \beta_{1N} \\ \beta_{21} & (\alpha_2 - E) & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \beta_{N1} & \dots & \dots & (\alpha_N - E) \end{vmatrix} = 0 \tag{4.44}$$

where we have omitted the subscript μ for the unknown eigenvalues E_μ.

4.2.2 Energies of two interacting levels

In the special situation of two interacting energy levels α_1 and α_2, and where β_{12} is real and thus equal to β_{21}, the matrix representation of the Hamiltonian reduces to

$$\boxed{\mathbf{H}} = \begin{pmatrix} \alpha_1 & \beta \\ \beta & \alpha_2 \end{pmatrix} \tag{4.45}$$

In order to solve the eigenvalue equation

$$\mathbf{H}|\Psi_\pm\rangle = E_\pm|\Psi_\pm\rangle \tag{4.46}$$

consider the secular equation that, according to Eq. (4.44), reads

$$\begin{vmatrix} \alpha_1 - E & \beta \\ \beta & \alpha_2 - E \end{vmatrix} = 0 \quad \text{with} \quad \beta \equiv \beta_{12} \tag{4.47}$$

Then, expanding the determinant according to the usual rule, that is,

$$(\alpha_1 - E)(\alpha_2 - E) - \beta^2 = 0$$

the following second-order equation in E is obtained

$$E^2 + \alpha_1\alpha_2 - E(\alpha_1 + \alpha_2) - \beta^2 = 0$$

the two roots of which are

$$E_\pm = \frac{(\alpha_1 + \alpha_2) \pm \sqrt{(\alpha_1 + \alpha_2)^2 - 4(\alpha_1\alpha_2 - \beta^2)}}{2}$$

or, after simplification

$$E_\pm = \frac{(\alpha_1 + \alpha_2) \pm \sqrt{(\alpha_1 - \alpha_2)^2 + 4\beta^2}}{2} \tag{4.48}$$

Hence, the difference between the two eigenvalues is

$$E_+ - E_- = \sqrt{(\alpha_1 - \alpha_2)^2 + 4\beta^2} \tag{4.49}$$

On the other hand, the eigenvectors of $\mathbf{H}$ appearing in (4.42), and corresponding to the eigenvalues (4.48), are of the form

$$|\Psi_\pm\rangle = C_{1_\pm}|\Phi_1\rangle + C_{2_\pm}|\Phi_2\rangle \tag{4.50}$$

whereas the orthonormality properties (4.42) of these kets leads to

$$\langle\Psi_-|\Psi_+\rangle = 0 \qquad \text{and} \qquad \langle\Psi_+|\Psi_+\rangle = \langle\Psi_-|\Psi_-\rangle = 1 \tag{4.51}$$

so that, due to Eq. (4.50),

$$(C_{1_-}\langle\Phi_1| + C_{2_-}\langle\Phi_2|)(C_{1_+}|\Phi_1\rangle + C_{2_+}|\Phi_2\rangle) = 0$$

and thus

$$C_{1_-}C_{1_+}\langle\Phi_1|\Phi_1\rangle + C_{2_-}C_{2_+}\langle\Phi_2|\Phi_2\rangle + C_{1_-}C_{2_+}\langle\Phi_1|\Phi_2\rangle + C_{1_+}C_{2_-}\langle\Phi_2|\Phi_1\rangle = 0$$

Then, owing to the orthonormality conditions appearing in Eq. (4.39), this last expression reduces to

$$C_{1_-}C_{1_+} + C_{2_-}C_{2_+} = 0$$

Likewise, the normality conditions appearing in (4.51) lead to

$$C_{1_-}^2 + C_{2_-}^2 = 1 \qquad \text{and} \qquad C_{1_+}^2 + C_{2_+}^2 = 1 \tag{4.52}$$

When the two interacting levels are degenerate, that is, have the same energy, the two eigenvalues (4.48) of the Hamiltonian $\mathbf{H}$ reduce to

$$E_\pm = \alpha \pm \beta \quad \text{when} \quad \alpha_1 = \alpha_2 = \alpha \tag{4.53}$$

Then, in order to get the expansion coefficients of the $\mathbf{H}$ eigenvectors, corresponding to these two eigenvalues, return to Eq. (4.43); however, for the special situation of two interacting levels, that is,

$$\begin{pmatrix} \alpha - E_\pm & \beta \\ \beta & \alpha - E_\pm \end{pmatrix} \begin{pmatrix} C_{1_\pm} \\ C_{2_\pm} \end{pmatrix} = 0 \tag{4.54}$$

which leads to

$$(\alpha - (\alpha \pm \beta))\, C_{1_\pm} = \beta C_{2_\pm}$$

Rearranging, gives, respectively, for the components of the eigenvectors corresponding to the two eigenvalues

$$\frac{C_{1_+}}{C_{2_+}} = 1 \qquad \text{and} \qquad \frac{C_{1_-}}{C_{2_-}} = -1$$

where, of course, the complementary equations (4.52) continue to hold.

4.2.3 Approximate solution far from degeneracy

Now, consider the special situation where

$$|\alpha_1 - \alpha_2| \gg |\beta| \tag{4.55}$$

4.2.3.1 Eigenvalues Before applying this relation, it is convenient to write the eigenvalues (4.48) in the following form:

$$E_\pm = \frac{1}{2}\left[(\alpha_1 + \alpha_2) \pm (\alpha_1 - \alpha_2)\sqrt{1 + \frac{4\beta^2}{(\alpha_1 - \alpha_2)^2}}\right] \tag{4.56}$$

where the square root appears to be of the form

$$\sqrt{1+\varepsilon} \quad \text{with} \quad \varepsilon = \frac{4\beta^2}{(\alpha_1 - \alpha_2)^2} \qquad \text{and} \qquad \varepsilon \ll 1$$

Hence, by expansion of the square root up to first order in ε, one has

$$\sqrt{1+\varepsilon} \simeq 1 + \frac{\varepsilon}{2}$$

Thus, when the condition (4.55) is verified, the eigenvalues are

$$E_\pm = \frac{1}{2}\left[(\alpha_1 + \alpha_2) \pm (\alpha_1 - \alpha_2)\left(1 + \frac{2\beta^2}{(\alpha_1 - \alpha_2)^2}\right)\right]$$

or

$$\boxed{E_+ = \alpha_1 + \frac{\beta^2}{(\alpha_1 - \alpha_2)} \text{ and } E_- = \alpha_2 - \frac{\beta^2}{(\alpha_1 - \alpha_2)}} \tag{4.57}$$

4.2.3.2 Expansion coefficients of the eigenvectors Generally, the following inequalities hold:

$$\alpha_1 < 0, \qquad \alpha_2 < 0, \qquad \beta < 0$$

In order to get the expansion coefficients of the **H** eigenvectors corresponding to the eigenvalues (4.57), it is convenient to return to Eq. (4.54):

$$\begin{pmatrix} \alpha_1 - E_\pm & \beta \\ \beta & \alpha_2 - E_\pm \end{pmatrix}\begin{pmatrix} C_{1_\pm} \\ C_{2_\pm} \end{pmatrix} = 0 \tag{4.58}$$

which yields for the eigenvalue E_+ the following equation:

$$(\alpha_1 - E_+)C_{1+} + \beta C_{2+} = 0$$

so that

$$C_{1+} = -C_{2+}\frac{\beta}{(\alpha_1 - E_+)}$$

Then, inserting the expression of E_+ given by (4.57), one obtains

$$C_{1+} = -C_{2+}\frac{\beta}{\left(\alpha_1 - \left\{\alpha_1 + \dfrac{\beta^2}{\alpha_1 - \alpha_2}\right\}\right)}$$

or

$$C_{1+} = C_{2+}\frac{(\alpha_1 - \alpha_2)}{\beta} \tag{4.59}$$

with the normalization of the **H** eigenkets given, of course, by the last equation of (4.52), that is,

$$C_{1+}^2 + C_{2+}^2 = 1$$

In a similar way, Eq. (4.58) yields for the eigenvalue E_-

$$\beta C_{1-} + (\alpha_2 - E_-)C_{2-} = 0$$

while for E_+ to

$$C_{1-} = -C_{2-}\frac{\beta}{(\alpha_1 - \alpha_2)} \tag{4.60}$$

a result that must be combined to the first normalization condition of (4.52), that is,

$$C_{1-}^2 + C_{2-}^2 = 1$$

4.2.3.3 *Eigenvectors pictorial representation*

Next, suppose that

$$\alpha_1 > \alpha_2 \qquad \text{and} \qquad \beta < 0 \tag{4.61}$$

Then, according to the first inequality, and owing to (4.57), the two eigenvalues obey

$$E_+ > E_-$$

Hence, in view of this new inequality combined with the second one appearing in (4.61), Eqs. (4.59) and (4.60) lead to the following results:

$$\frac{|C_{1+}|}{|C_{2+}|} >> 1 \qquad \text{and} \qquad \frac{|C_{1-}|}{|C_{2-}|} << 1 \tag{4.62}$$

$$\frac{C_{1+}}{C_{2+}} < 0 \qquad \text{and} \qquad \frac{C_{1-}}{C_{2-}} > 0 \tag{4.63}$$

The inequalities (4.61)–(4.63) are illustrated by Fig. 4.3 of the two interacting energy level systems with β negative. Figure 4.3 shows that after an interaction induced by **V**, the energy level E_+ is lowered by the amount $|\beta|$ and the other E_- raised by the same amount, the contribution of the two basic interacting levels being the same for the energy level E_+ and opposite for E_-. That may be viewed as considering the ket associated to E_+ as resulting from a *constructive quantum interference* between the interacting levels and that associated to E_- as following from a *destructive one*.

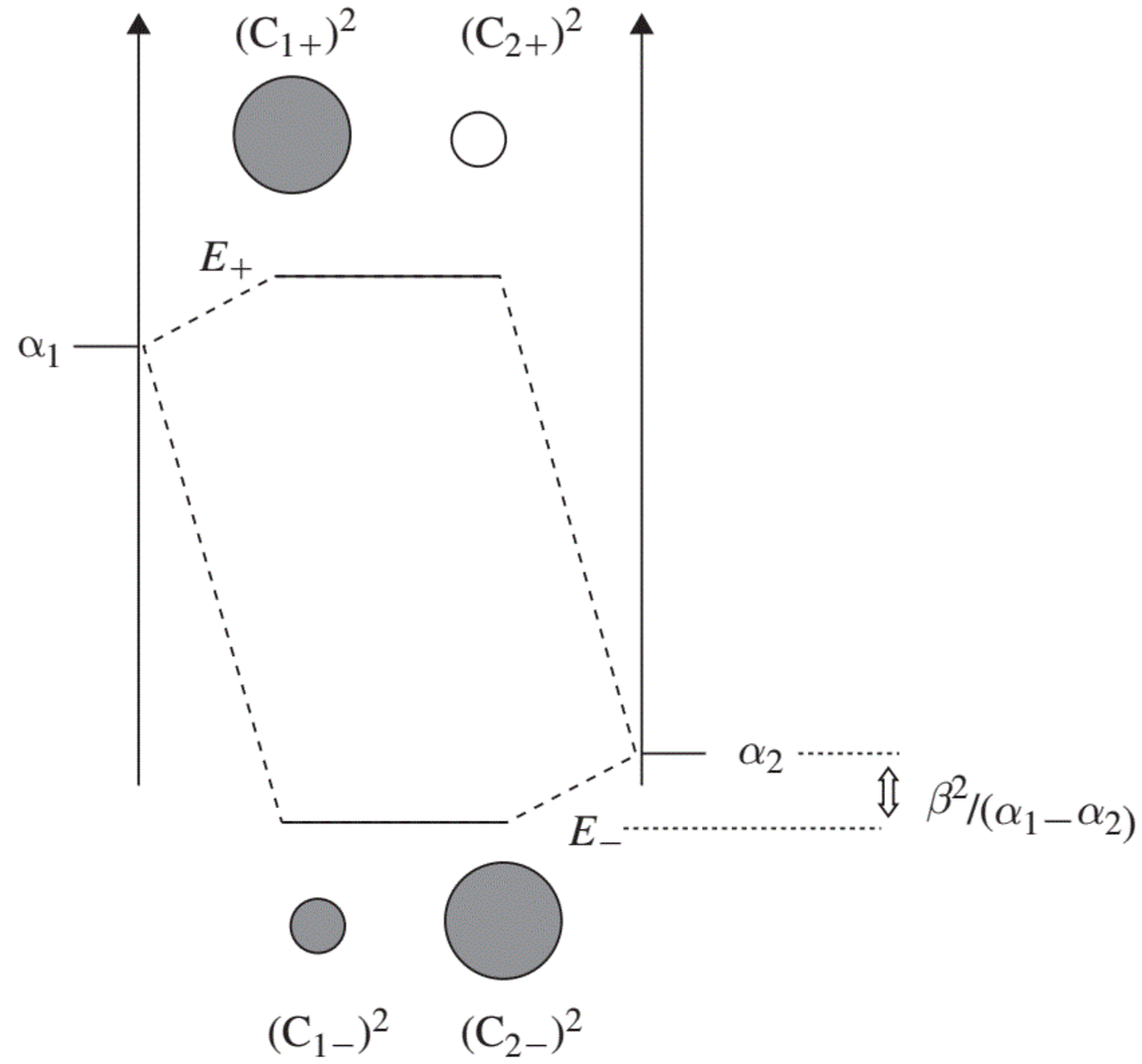


Figure 4.3 Correlation energy levels of two interacting energy levels.

4.2.3.4 Result of second-order perturbation theory In the notation of Eqs. (4.37)–(4.42), the inequality (4.55) and its consequence (4.57) take, respectively, the form

$$|\langle\Phi_i|\mathbf{H}|\Phi_i\rangle - \langle\Phi_j|\mathbf{H}|\Phi_j\rangle| >> \langle\Phi_i|\mathbf{V}|\Phi_j\rangle$$

$$\boxed{\langle\Psi_\pm|\mathbf{H}|\Psi_\pm\rangle \backsimeq \langle\Phi_i|\mathbf{H}|\Phi_i\rangle \pm \frac{\langle\Phi_i|\mathbf{V}|\Phi_j\rangle^2}{\langle\Phi_i|\mathbf{H}|\Phi_i\rangle - \langle\Phi_j|\mathbf{H}|\Phi_j\rangle}} \tag{4.64}$$

with

$$\langle\Psi_\pm|\mathbf{H}|\Psi_\pm\rangle = E_\pm \qquad \langle\Phi_i|\mathbf{H}|\Phi_i\rangle = \alpha_i \qquad \langle\Phi_i|\mathbf{V}|\Phi_j\rangle = \beta$$

Equation (4.64) is the expression for the special case of a two-energy-level system, of *second-order perturbation expansion* of the eigenvalues of the full Hamiltonian **H** in terms of the matrix elements of this Hamiltonian in the basis of the Hamiltonian $\mathbf{H}^\circ$.

4.2.4 Dynamics

In order to get the dynamics of the system, it is convenient to write the Hamiltonian matrix (4.45) in the following form:

$$\boxed{\mathbf{H}} = \begin{pmatrix} \dfrac{\alpha_1+\alpha_2}{2} & 0 \\ 0 & \dfrac{\alpha_1+\alpha_2}{2} \end{pmatrix} + \begin{pmatrix} +\dfrac{\alpha_1-\alpha_2}{2} & \beta \\ \beta & -\dfrac{\alpha_1-\alpha_2}{2} \end{pmatrix} \tag{4.65}$$

or

$$\boxed{\mathbf{H}} = \left(\frac{\alpha_1 + \alpha_2}{2}\right)\boxed{\mathbf{1}} + \left(\frac{\alpha_1 - \alpha_2}{2}\right)\boxed{\mathbf{K}} \tag{4.66}$$

where the last right-hand-side matrix is given by

$$\boxed{\mathbf{K}} = \begin{pmatrix} +1 & \dfrac{2\beta}{\alpha_1 - \alpha_2} \\ \dfrac{2\beta}{\alpha_1 - \alpha_2} & -1 \end{pmatrix} \tag{4.67}$$

According to Section 1.3.2, since the two right-hand-side Hermitian matrices of Eq. (4.66) commute, they admit the same eigenvectors, so that the two following eigenvalue equations, both involving the same eigenkets $|\Psi_\pm\rangle$, are satisfied:

$$\boxed{\mathbf{H}}\,|\Psi_\pm\rangle = E_\pm|\Psi_\pm\rangle \qquad \boxed{\mathbf{K}}\,|\Psi_\pm\rangle = K_\pm|\Psi_\pm\rangle$$

where $E_\pm$ are the Hamiltonian eigenvalues we obtained above, whereas $K_\pm$ are the corresponding eigenvalues of the $\mathbf{K}$ matrix. Hence, due to Eq. (4.66), the eigenvalues of $\boxed{\mathbf{H}}$ read

$$E_\pm = \left(\frac{\alpha_1 + \alpha_2}{2}\right) + \left(\frac{\alpha_1 - \alpha_2}{2}\right)K_\pm \tag{4.68}$$

Next, write the matrix (4.67) as follows:

$$\boxed{\mathbf{K}} = \begin{pmatrix} +1 & \tan\theta \\ \tan\theta & -1 \end{pmatrix}$$

with

$$\tan\theta = \frac{2\beta}{\alpha_1 - \alpha_2} \tag{4.69}$$

Then, since $\boxed{\mathbf{K}}$ and $\boxed{\mathbf{H}}$, which commute, have the same set of eigenvectors $|\Psi_\pm\rangle$, the matricial eigenvalue equation of $\boxed{\mathbf{K}}$ is similar to that for $\boxed{\mathbf{H}}$ given by Eq. (4.58), so that one gets

$$\begin{pmatrix} +1 & \tan\theta \\ \tan\theta & -1 \end{pmatrix}\begin{pmatrix} C_{1_\pm} \\ C_{2_\pm} \end{pmatrix} = K_\pm \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} C_{1_\pm} \\ C_{2_\pm} \end{pmatrix} \tag{4.70}$$

where the $C_{k_\pm}$ are the components of the eigenvectors $|\Psi_\pm\rangle$ given by Eq. (4.50). The corresponding secular determinant, which must be zero, that is,

$$\begin{vmatrix} 1 - K_\pm & \tan\theta \\ \tan\theta & -1 - K_\pm \end{vmatrix} = 0$$

leads by expansion to

$$K_\pm^2 - 1 - \tan^2\theta = 0$$

so that

$$K_\pm^2 = 1 + \tan^2\theta = \frac{\cos^2\theta}{\cos^2\theta} + \frac{\sin^2\theta}{\cos^2\theta} = \frac{1}{\cos^2\theta}$$

and thus

$$K_{\pm} = \pm \frac{1}{\cos\theta} \tag{4.71}$$

Hence, the two Hamiltonian eigenvalues (4.68) read

$$E_{\pm} = \left(\frac{\alpha_1 + \alpha_2}{2}\right) \pm \left(\frac{\alpha_1 - \alpha_2}{2\cos\theta}\right)$$

their difference being

$$E_+ - E_- = \frac{\alpha_1 - \alpha_2}{\cos\theta}$$

so that, by inversion, $\cos\theta$ appears to be

$$\cos\theta = \frac{\alpha_1 - \alpha_2}{E_+ - E_-} \tag{4.72}$$

Now, by insertion of Eq. (4.71) into Eq. (4.70), one gets for the situation corresponding to the E_+ eigenvalue

$$\left(1 - \frac{1}{\cos\theta}\right) C_{1+} + \tan\theta\, C_{2+} = 0$$

which reads

$$(\cos\theta - 1)\, C_{1+} + \sin\theta\, C_{2+} = 0 \tag{4.73}$$

Moreover, keeping in mind the trigonometric relation

$$\frac{1 - \cos 2\theta}{2} = \sin^2\theta \tag{4.74}$$

which reads

$$1 - \cos 2\theta = 2\sin\theta\sin\theta$$

the term multiplying C_{1+} in Eq. (4.73) reads

$$\cos\theta - 1 = -2\sin\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right) \tag{4.75}$$

Furthermore, the trigonometric relation

$$\sin 2\theta = 2\sin\theta\cos\theta$$

yields

$$\sin\theta = 2\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right) \tag{4.76}$$

Hence, using Eqs. (4.75) and (4.76), Eq. (4.73) transforms to

$$-\sin\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right) C_{1+} + \sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right) C_{2+} = 0$$

so that

$$\frac{C_{1+}}{C_{2+}} = \frac{\cos(\theta/2)}{\sin(\theta/2)}$$

Thus, the two expansion coefficients, which are clearly normalized, read

$$C_{1+} = \cos\left(\frac{\theta}{2}\right) \qquad \text{and} \qquad C_{2+} = \sin\left(\frac{\theta}{2}\right)$$

so that Eq. (4.50) yields

$$|\Psi_+\rangle = \cos\left(\frac{\theta}{2}\right)|\Phi_1\rangle + \sin\left(\frac{\theta}{2}\right)|\Phi_2\rangle \tag{4.77}$$

In a similar way one would obtain

$$|\Psi_-\rangle = -\sin\left(\frac{\theta}{2}\right)|\Phi_1\rangle + \cos\left(\frac{\theta}{2}\right)|\Phi_2\rangle \tag{4.78}$$

which may be verified by observing that the two normalized kets (4.77) and (4.78) are orthogonal. Then, multiplying Eq. (4.77) by $\sin(\theta/2)$, and Eq. (4.78) by $\cos(\theta/2)$, one obtains, after summing these results and simplification,

$$|\Phi_2\rangle = \sin\left(\frac{\theta}{2}\right)|\Psi_+\rangle + \cos\left(\frac{\theta}{2}\right)|\Psi_-\rangle \tag{4.79}$$

or, due to Eqs. (4.77) and (4.78),

$$|\Phi_2\rangle = |\Psi_+\rangle\langle\Psi_+|\Phi_2\rangle + |\Psi_-\rangle\langle\Psi_-|\Phi_2\rangle$$

with

$$\langle\Phi_2|\Psi_+\rangle = \langle\Psi_+|\Phi_2\rangle = \sin\left(\frac{\theta}{2}\right) \qquad \text{and} \qquad \langle\Phi_2|\Psi_-\rangle = \langle\Psi_-|\Phi_2\rangle = \cos\left(\frac{\theta}{2}\right) \tag{4.80}$$

In a similar way, after multiplying Eq. (4.77) by $\cos(\theta/2)$, and Eq. (4.78) by $-\sin(\theta/2)$, and adding the results, one obtains,

$$|\Phi_1\rangle = \cos\left(\frac{\theta}{2}\right)|\Psi_+\rangle - \sin\left(\frac{\theta}{2}\right)|\Psi_-\rangle \tag{4.81}$$

4.2.5 Transition probability from $|\Phi_1\rangle$ to $|\Phi_2\rangle$ due to the V perturbation

Suppose that at an initial time the system is in the state

$$|\Psi(0)\rangle = |\Phi_1\rangle \tag{4.82}$$

At time t, this state will transform into $|\Psi(t)\rangle$ given, according to Eq. (3.85), by

$$|\Psi(t)\rangle = (e^{-i\mathbf{H}t/\hbar})|\Psi(0)\rangle$$

or, owing to the initial condition (4.82), by

$$|\Psi(t)\rangle = (e^{-i\mathbf{H}t/\hbar})|\Phi_1\rangle$$

and thus, according to Eq. (4.81), by

$$|\Psi(t)\rangle = \cos\left(\frac{\theta}{2}\right)(e^{-i\mathbf{H}t/\hbar})|\Psi_+\rangle - \sin\left(\frac{\theta}{2}\right)(e^{-i\mathbf{H}t/\hbar})|\Psi_-\rangle$$

Again, owing to the Hamiltonian eigenvalue equation (4.46), this expression reads

$$|\Psi(t)\rangle = \cos\left(\frac{\theta}{2}\right)(e^{-iE_+t/\hbar})|\Psi_+\rangle - \sin\left(\frac{\theta}{2}\right)(e^{-iE_-t/\hbar})|\Psi_-\rangle$$

Next premultiplying both terms of this last equation by the bra $\langle\Phi_2|$ corresponding to the ket (4.79), that is,

$$\langle\Phi_2|\Psi(t)\rangle = \cos\left(\frac{\theta}{2}\right)(e^{-iE_+t/\hbar})\langle\Phi_2|\Psi_+\rangle - \sin\left(\frac{\theta}{2}\right)(e^{-iE_-t/\hbar})\langle\Phi_2|\Psi_-\rangle$$

then, owing to (4.80), it appears that

$$\langle\Phi_2|\Psi(t)\rangle = \sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right)(e^{-iE_+t/\hbar} - e^{-iE_-t/\hbar}) \tag{4.83}$$

Moreover, the probability for the system to jump at time t into the state $|\Phi_2\rangle$ being

$$P_{12}(t) = |\langle\Phi_2|\Psi(t)\rangle|^2$$

becomes with the help of Eq. (4.83)

$$P_{12}(t) = \sin^2\left(\frac{\theta}{2}\right)\cos^2\left(\frac{\theta}{2}\right)(2 - (e^{+i(E_+-E_-)t/\hbar} + e^{-i(E_+-E_-)t/\hbar}))$$

or

$$P_{12}(t) = 2\sin^2\left(\frac{\theta}{2}\right)\cos^2\left(\frac{\theta}{2}\right)\left(1 - \cos\left(\frac{(E_+ - E_-)t}{\hbar}\right)\right) \tag{4.84}$$

Furthermore, by aid of the trigonometric relations

$$\sin^2 x = \left(\frac{1-\cos 2x}{2}\right) \qquad \text{and} \qquad \sin x = 2\sin\left(\frac{x}{2}\right)\cos\left(\frac{x}{2}\right)$$

where x is some variable, we have

$$1 - \cos\left(\frac{(E_+ - E_-)t}{\hbar}\right) = 2\sin^2\left(\frac{(E_+ - E_-)t}{2\hbar}\right)$$

so that Eq. (4.84) may be written

$$P_{12}(t) = \sin^2\theta\sin^2\left(\frac{(E_+ - E_-)\,t}{2\hbar}\right) \tag{4.85}$$

Now, since we do not know $\sin\theta$, but both $\tan\theta$ and $\cos\theta$, which are, respectively, given by Eqs. (4.69) and (4.72), it is suitable to transform this last equation into

$$P_{12}(t) = \cos^2\theta\tan^2\theta\sin^2\left(\frac{(E_+ - E_-)t}{2\hbar}\right)$$

so that, due to Eqs. (4.69) and (4.72), the transition probability transforms to

$$P_{12}(t) = 4\frac{\beta^2}{(E_+ - E_-)^2}\sin^2\left(\frac{(E_+ - E_-)t}{2\hbar}\right)$$

Finally, owing to Eq. (4.49), we have

$$\boxed{P_{12}(t) = \frac{4\beta^2}{(\alpha_1-\alpha_2)^2+4\beta^2}\sin^2\left(\frac{\left(\sqrt{(\alpha_1-\alpha_2)^2+4\beta^2}\right)t}{2\hbar}\right)} \tag{4.86}$$

that is, the *Rabi equation*. Besides, the time-dependent probability $P_{12}(t)$ to jump from $|\Phi_1\rangle$ to $|\Phi_2\rangle$ plus that $P_{11}(t)$ for the system to remain into $|\Phi_1\rangle$ must be unity, one has

$$P_{11}(t) = 1 - P_{12}(t)$$

In the special situation where the two levels are degenerate, Eq. (4.86) reduces to

$$\boxed{P_{12}(t) = \sin^2\left(\frac{\beta t}{\hbar}\right) \quad \text{so that} \quad P_{11}(t) = \cos^2\left(\frac{\beta t}{\hbar}\right) \quad \text{when} \quad \alpha_1 = \alpha_2} \tag{4.87}$$

In the following, many results of this section will be applied to *Fermi resonances*, a physical phenomenon that is met in situations involving anharmonic couplings between molecular oscillators.

4.2.6 Fermi golden rule

In relation with the dynamics of the double energy levels, and to end this chapter, we must now touch on the question of transition probabilities per unit time from one energy level to another one because of a coupling between them, a question that will be of importance when we later study the coupling between molecular oscillators and the electromagnetic field. Thus, consider a system described by a Hamiltonian $\mathbf{H}$ that may be split into two noncommuting parts $\mathbf{H}^\circ$ and $\mathbf{V}$ according to

$$\mathbf{H} = \mathbf{H}^\circ + \mathbf{V} \quad \text{with} \quad [\mathbf{H}^\circ, \mathbf{V}] \neq 0$$

the eigenvalue equation of $\mathbf{H}^\circ$ being

$$\mathbf{H}^\circ |\Psi_k\rangle = E_k |\Psi_k\rangle \tag{4.88}$$

with

$$\langle \Psi_k | \Psi_l \rangle = \delta_{kl} \tag{4.89}$$

We seek the transition probability at time t for the system described by $\mathbf{H}$ to pass from any eigenstate of $\mathbf{H}^\circ$ to another because of the presence of $\mathbf{V}$, that is,

$$|C(l,t|k,0)|^2 = |\langle \Psi_l(t) | \Psi_k(0) \rangle|^2 = \langle \Psi_k(0) | \Psi_l(t) \rangle \langle \Psi_l(t) | \Psi_k(0) \rangle \tag{4.90}$$

Owing to the time-dependent evolution equation, the ket $|\Psi_l(t)\rangle$ evolves with time according to

$$|\Psi_l(t)\rangle = \mathbf{U}(t) |\Psi_l(0)\rangle$$

Now, in the interaction picture, the time evolution operator is given, in terms of the Hamiltonian $\mathbf{H}^\circ$ by Eq. (3.122), that is,

$$\mathbf{U}(t) = (e^{-i\mathbf{H}^\circ t/\hbar}) \mathbf{U}(t)^{\text{IP}}$$

Thus, the transition probability (4.90) becomes

$$|C(l,t|k,0)|^2 = \langle \Psi_k(0) | (e^{-i\mathbf{H}^\circ t/\hbar}) \mathbf{U}(t)^{\text{IP}} | \Psi_l(0) \rangle \langle \Psi_l(0) | \mathbf{U}(t)^{\text{IP}-1} (e^{i\mathbf{H}^\circ \mathbf{t}/\hbar}) | \Psi_l(0) \rangle$$

Again, owing to the eigenvalue equation (4.88), the transition probability transforms to

$$|C(l,t \mid k,0)|^2 = \Psi_k(0) | (e^{-iE_k t/\hbar}) \mathbf{U}(t)^{\text{IP}} | \Psi_l(0) \rangle \langle \Psi_l(0) | \mathbf{U}(t)^{\text{IP}-1} (e^{iE_k t/\hbar}) | \Psi_k(0) \rangle$$

Or, after simplification

$$|C(l,t|k,0)|^2 = |\langle\Psi_k(0)|\mathbf{U}(t)^{\mathrm{IP}}|\Psi_l(0)\rangle|^2 \tag{4.91}$$

Up to first order, the IP time evolution operator is, according to Eq. (3.125), given by

$$\mathbf{U}(t)^{\mathrm{IP}} = 1 + \left(\frac{1}{i\hbar}\right)\int_0^t \mathbf{V}(t')^{\mathrm{IP}}dt'$$

where

$$\mathbf{V}(t)^{\mathrm{IP}} = (e^{i\mathbf{H}^\circ t/\hbar})\mathbf{V}(e^{-i\mathbf{H}^\circ t/\hbar}) \tag{4.92}$$

Thus, Eq. (4.91) becomes

$$|C(l,t|k,0)|^2 = \left|\langle\Psi_k(0)|\left(1 + \left(\frac{1}{i\hbar}\right)\int_0^t \mathbf{V}(t')^{\mathrm{IP}}dt'\right)|\Psi_l(0)\rangle\right|^2$$

Next, using Eq. (4.92) and simplifying by the orthogonality property (4.89), the transition probability takes the form

$$|C(l,t|k,0)|^2 = \left(\frac{1}{\hbar}\right)^2\left|\int_0^t \langle\Psi_k(0)|(e^{i\mathbf{H}^\circ t'/\hbar})\mathbf{V}(e^{-i\mathbf{H}^\circ t'/\hbar})|\Psi_l(0)\rangle dt'\right|^2 \tag{4.93}$$

Again, the eigenvalue equation allows one to transform this result into

$$|C(l,t|k,0)|^2 = \left(\frac{1}{\hbar}\right)^2\left|\int_0^t \langle\Psi_k(0)|(e^{iE_k t'/\hbar})\mathbf{V}(e^{-iE_l t'/\hbar})|\Psi_l(0)\rangle dt'\right|^2$$

or

$$|C(l,t|k,0)|^2 = \left(\frac{1}{\hbar}\right)^2|\langle\Psi_k|\mathbf{V}|\Psi_l\rangle|^2\left|\int_0^t (e^{i\omega_{kl}t'})dt'\right|^2 \tag{4.94}$$

with

$$\omega_{kl} = \frac{(E_k - E_l)}{\hbar} \tag{4.95}$$

where the reference to time $t = 0$ has been omitted. By integration, one has

$$\int_0^t (e^{i\omega_{kl}t'})\,dt' = \frac{1}{i}\left(\frac{e^{i\omega_{kl}t} - 1}{\omega_{kl}}\right) \tag{4.96}$$

In addition, the corresponding absolute value is

$$\left|\int_0^t (e^{i\omega_{kl}t'})\,dt'\right|^2 = \frac{2}{\omega_{kl}^2}(1 - \cos\omega_{kl}t)$$

Moreover, by aid of the usual trigonometric relations

$$(1 - \cos\omega_{kl}t) = 2\sin^2\left(\frac{\omega_{kl}t}{2}\right)$$

Eq. (4.94) becomes

$$|C(l,t|k,0)|^2 = 4|\langle\Psi_k|\mathbf{V}|\Psi_l\rangle|^2\left(\frac{\sin^2(\omega_{kl}t/2)}{(\hbar\omega_{kl})^2}\right) \tag{4.97}$$

This last expression holds for any time, up to first order in $\mathbf{V}$. Now, consider this expression for large times for which it is convenient to write the second right-hand-side term of Eq. (4.97) in the following way:

$$|C(l,t|k,0)|^2 = 4|\langle \Psi_k|\mathbf{V}|\Psi_l\rangle|^2 \left(\frac{\sin^2(xt/2\hbar)}{x^2}\right) \tag{4.98}$$

with

$$x = \hbar\omega_{kl} \tag{4.99}$$

Then, for large time t, Eq. (4.98) reads

$$|C(l,t|k,0)|^2 = |\langle \Psi_k|\mathbf{V}|\Psi_l\rangle|^2 \left(\frac{\sin^2(x/\varepsilon)}{x^2}\right) \tag{4.100}$$

with

$$\frac{t}{2\hbar} = \frac{1}{\varepsilon} \quad \text{with} \quad \varepsilon \to 0 \tag{4.101}$$

Next observe that one of the expressions of the Dirac distribution function is given by Eq. (18.57) of Section 18.6.

$$\delta(x) = \frac{\varepsilon}{\pi}\left(\frac{\sin^2(x/\varepsilon)}{x^2}\right) \quad \text{when} \quad \varepsilon \to 0$$

which, owing to Eqs. (4.99) and (4.100), reads in the present situation

$$\left(\frac{\sin^2(x/\varepsilon)}{x^2}\right) = \frac{\pi t}{2\hbar}\delta(x)$$

so that Eq. (4.100) takes the form

$$|C(l,t|k,0)|^2 = 4|\langle \Psi_k|\mathbf{V}|\Psi_l\rangle|^2 t\frac{\pi}{2\hbar}\delta(x)$$

or, in view of Eqs. (4.95) and (4.99),

$$|C(l,t|k,0)|^2 = \frac{2\pi}{\hbar}|\langle \Psi_k|\mathbf{V}|\Psi_l\rangle|^2 t\delta(E_k - E_l) \tag{4.102}$$

Owing to this result, it is now possible to get the first-order transition probability per unit time, which is by definition

$$W(l,t|k,0) = \left(\frac{\partial|C(l,t|k,0)|^2}{\partial t}\right)$$

That gives what is called the *Fermi golden rule*:

$$\boxed{W(l,t|k,0) = \frac{2\pi}{\hbar}|\langle \Psi_k|\mathbf{V}|\Psi_l\rangle|^2\delta(E_k - E_l)} \tag{4.103}$$

an equation of the form of (4.103) will be met at the end of this book, dealing with molecular spectroscopy, when studying the interaction of molecular oscillators with electromagnetic field through a potential $\mathbf{V}$ involving a coupling of their dipolar moments with the electric field.

4.3 CONCLUSION

This chapter, devoted to some quantum models, has lead to the following important results that will be useful in the subsequent studies of quantum oscillators:

Particle-in-a-box energy and de Broglie relation
$E_{n_x n_y n_z} = \left(\frac{h^2}{8ma^2}\right)(n_x^2 + n_y^2 + n_z^2) \qquad \lambda = \frac{h}{p}$
Second-order perturbation energy:
$\langle \Psi_\pm \vert \mathbf{H} \vert \Psi_\pm \rangle \backsimeq \langle \Phi_i \vert \mathbf{H} \vert \Phi_i \rangle \pm \frac{\langle \Phi_i \vert \mathbf{V} \vert \Phi_j \rangle^2}{\langle \Phi_i \vert \mathbf{H} \vert \Phi_i \rangle - \langle \Phi_j \vert \mathbf{H} \vert \Phi_j \rangle}$
Rabi's relation:
$P_{12}(t) = \frac{4\vert\langle \Phi_1 \vert \mathbf{H} \vert \Phi_2 \rangle\vert^2}{(\langle \Phi_1 \vert \mathbf{H} \vert \Phi_1 \rangle - \langle \Phi_2 \vert \mathbf{H} \vert \Phi_2 \rangle)^2 + 4\vert\langle \Phi_1 \vert \mathbf{H} \vert \Phi_2 \rangle\vert^2} \times \sin^2\left(\frac{\left(\sqrt{(\langle \Phi_1 \vert \mathbf{H} \vert \Phi_1 \rangle - \langle \Phi_2 \vert \mathbf{H} \vert \Phi_2 \rangle)^2 + 4\vert\langle \Phi_1 \vert \mathbf{H} \vert \Phi_2 \rangle\vert^2}\right)t}{2\hbar}\right)$
Fermi's golden rule:
$W(l,t\vert k,0) = \frac{2\pi}{\hbar}\vert\langle \Psi_k \vert \mathbf{V} \vert \Psi_l \rangle\vert^2 \delta(E_k - E_l)$

Among them, the result of the particle-in-a-box model showing that waves associated to quantum states obey the de Broglie wavelength law according to which the number of nodes of the stationary waves increases with energy, a property that is to be obeyed by the energy wavefunctions of quantum oscillators. The other is the quantum interference found in the study of two-energy-state systems, which is met in the study of Fermi resonances, a physical phenomenon appearing in anharmonically coupled molecular oscillators. The latter is the time-dependent amplitude probability for a system to pass from one state to another one due to some coupling with the thermal bath, a result that will be widely used when studying coupling of molecular oscillators with the infrared (IR) electromagnetic field.

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PART II

SINGLE QUANTUM HARMONIC OSCILLATORS

CHAPTER 5

ENERGY REPRESENTATION FOR QUANTUM HARMONIC OSCILLATORS

INTRODUCTION

The present chapter develops the basis of the quantum approach to harmonic oscillators. The dimensionless creation and annihilation operators are first introduced. Using these operators, which are Hermitian self-conjugate, it is possible to solve the eigenvalue equation of the Hamiltonian and thus to get the values of the energy levels of quantum harmonic oscillators. That also permits one to obtain the corresponding orthonormalized eigenkets, thus providing a basis for the study of quantum oscillators. Moreover, in a subsequent section, the relation governing the action of the raising and lowering operators on the eigenkets of the Hamiltonian are derived, leading to the possibility of finding how the Heisenberg uncertainty relations apply to quantum harmonic oscillators, when they are in some eigenkets of their Hamiltonian. The formalism introduced allows them to verify the validity of the virial theorem. Furthermore, a place is reserved to non-Hermitian operators (*Fermion operators*) playing for two-level systems a role analogous to that of creating annihilation operators (*Boson operators*) for quantum oscillators. Another section is devoted to the wave mechanics representation of the eigenkets of the Hamiltonian, which will permit a pictorial description of these kets in terms of wavefunctions, the corresponding number of nodes increasing with the energy. Finally, the time dependence of the creation and annihilation operators is calculated in the Heisenberg picture and applied to get the time dependence of the basic operators and of their mean values averaged over the eigenkets of the oscillator Hamiltonians.

5.1 HAMILTONIAN EIGENKETS AND EIGENVALUES

The most important result dealing with quantum harmonic oscillators is the knowledge of its quantized energy levels E_n, initially introduced by Planck (1901) in order to explain the spectral density of a black body via

$$E_n = n\hbar\omega \quad \text{with} \quad n = 1, 2, \ldots$$

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Later, this assumed expression of the quantized energy levels was weakly modified by Heisenberg (1925) in its matrix mechanics, which showed that they were given by

$$E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega \quad \text{with} \quad n = 0, 1, 2, \ldots$$

From quantum mechanics, the problem is to solve the eigenvalue equation of the Hamiltonian **H**. One possibility is to solve the second-order partial differential equation, which is the wave mechanics picture of this eigenvalue equation, that is, the time-independent Schrödinger equation. Such an approach supposes to have some knowledge about the theory of partial derivative equations. The other possibility is to pass from the position and momentum Hermitian operators involved in the Hamiltonian to two new dimensionless Hermitian self-conjugated operators, the *ladder operators*, which allow an easy resolution of the eigenvalue equation of the Hamiltonian. It is the latter approach that is chosen in the present section.

5.1.1 Hamiltonian in terms of ladder operators

5.1.1.1 Ladder operators Starting from the Hamiltonian **H** of a quantum harmonic oscillator of angular frequency ω and of reduced mass m coupling two masses, m_1 and m_2, that is

$$\mathbf{H} = \left(\frac{\mathbf{P}^2}{2m} + \frac{1}{2}m\omega^2\mathbf{Q}^2\right) \tag{5.1}$$

where **Q** is the position operator and **P** its conjugate momentum obeying the commutation rule

$$[\mathbf{Q}, \mathbf{P}] = i\hbar$$

where the reduced mass m of the oscillator is given by

$$m = \left(\frac{m_1 m_2}{m_1 + m_2}\right) \tag{5.2}$$

In order to solve the eigenvalue equation of this Hamiltonian, it is convenient to work with the following dimensionless non-Hermitian operators, which are mutually Hermitian conjugates (*the ladder operators*):

$$\mathbf{a} = \sqrt{\frac{m\omega}{2\hbar}}\mathbf{Q} + i\sqrt{\frac{1}{2m\hbar\omega}}\mathbf{P} \tag{5.3}$$

$$\mathbf{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\mathbf{Q} - i\sqrt{\frac{1}{2m\hbar\omega}}\mathbf{P} \tag{5.4}$$

Next, we calculate the commutator of these two conjugate Hermitian operators. From Eqs. (5.3) and (5.4), it reads

$$\mathbf{a}\mathbf{a}^\dagger = (\eta\mathbf{Q} + i\zeta\mathbf{P})(\eta\mathbf{Q} - i\zeta\mathbf{P}) = \eta^2\mathbf{Q}^2 + \zeta^2\mathbf{P}^2 + i\zeta\eta[\mathbf{P}, \mathbf{Q}]$$

$$\mathbf{a}^\dagger\mathbf{a} = (\eta\mathbf{Q} - i\zeta\mathbf{P})(\eta\mathbf{Q} + i\zeta\mathbf{P}) = \eta^2\mathbf{Q}^2 + \zeta^2\mathbf{P}^2 - i\zeta\eta[\mathbf{P}, \mathbf{Q}]$$

with

$$\eta = \sqrt{\frac{m\omega}{2\hbar}} \qquad \text{and} \qquad \zeta = \sqrt{\frac{1}{2m\hbar\omega}}$$

Hence, the commutator of $\mathbf{a}$ and $\mathbf{a}^\dagger$ reads

$$\mathbf{a}\mathbf{a}^\dagger - \mathbf{a}^\dagger\mathbf{a} = \mathbf{2}i\zeta\eta[\mathbf{P}, \mathbf{Q}] = \frac{i}{\hbar}[\mathbf{P}, \mathbf{Q}]$$

or, due to the basic commutator (2.3),

$$\boxed{\mathbf{a}\mathbf{a}^\dagger - \mathbf{a}^\dagger\mathbf{a} = [\mathbf{a}, \mathbf{a}^\dagger] = \mathbf{1}} \tag{5.5}$$

Next, by inversion of Eqs. (5.3) and (5.4), one obtains the dependence of $\mathbf{Q}$ and $\mathbf{P}$ operators with respect to $\mathbf{a}$ and $\mathbf{a}^\dagger$, respectively,

$$\boxed{\mathbf{Q} = \sqrt{\frac{\hbar}{2m\omega}}(\mathbf{a}^\dagger + \mathbf{a})} \tag{5.6}$$

$$\boxed{\mathbf{P} = i\sqrt{\frac{m\hbar\omega}{2}}(\mathbf{a}^\dagger - \mathbf{a})} \tag{5.7}$$

For reasons that will be clear later, the ladder operators $\mathbf{a}^\dagger$ and $\mathbf{a}$ are, respectively, often named the *raising* and *lowering* operators or *creation* and *annihilation* operators. Then, the insertion of Eqs. (5.6) and (5.7) into Eq. (5.1) gives

$$\mathbf{H} = \frac{i^2}{2m}\frac{\hbar m\omega}{2}(\mathbf{a}^\dagger - \mathbf{a})^2 + \frac{1}{2}m\omega^2\frac{\hbar}{2m\omega}(\mathbf{a}^\dagger + \mathbf{a})^2$$

or

$$\mathbf{H} = -\frac{\hbar\omega}{4}(\mathbf{a}^\dagger - \mathbf{a})^2 + \frac{\hbar\omega}{4}(\mathbf{a}^\dagger + \mathbf{a})^2$$

Hence,

$$\mathbf{H} = -\frac{\hbar\omega}{4}((\mathbf{a}^\dagger)^2 + (\mathbf{a})^2 - \mathbf{a}^\dagger\mathbf{a} - \mathbf{a}\mathbf{a}^\dagger) + \frac{\hbar\omega}{4}((\mathbf{a}^\dagger)^2 + (\mathbf{a})^2 + \mathbf{a}^\dagger\mathbf{a} + \mathbf{a}\mathbf{a}^\dagger)$$

and, after simplification

$$\mathbf{H} = \frac{\hbar\omega}{2}(\mathbf{a}^\dagger\mathbf{a} + \mathbf{a}\mathbf{a}^\dagger) \tag{5.8}$$

Now, the commutator (5.5) may be written

$$\mathbf{a}\mathbf{a}^\dagger = \mathbf{a}^\dagger\mathbf{a} + 1$$

so that Eq. (5.8) leads to the following fundamental expression for the Hamiltonian of the quantum harmonic oscillator:

$$\boxed{\mathbf{H} = \hbar\omega\left(\mathbf{a}^\dagger\mathbf{a} + \tfrac{1}{2}\right)} \tag{5.9}$$

Observe that this Hamiltonian is Hermitian, as required, since

$$(\mathbf{a}^\dagger\mathbf{a})^\dagger = \mathbf{a}^\dagger\mathbf{a}$$

Now write the Hamiltonian eigenvalue equation to be solved:

$$\mathbf{H}|\{n\}\rangle = E_n|\{n\}\rangle \tag{5.10}$$

where $|\{n\}\rangle$[1] are the eigenvectors and E_n the corresponding eigenvalues, which are real because $\mathbf{H}$ is Hermitian. Besides, since $\mathbf{H}$ is Hermitian, its eigenvectors are orthogonal and, if normalized, satisfy

$$\langle\{n\}|\{m\}\rangle = \delta_{nm} \tag{5.11}$$

5.1.2 Resolution of the Hamiltonian eigenvalue

To solve the eigenvalue equation (5.10), define the following Hermitian operator $\mathbf{N}$, which commutes with the Hamiltonian $\mathbf{H}$, that is,

$$\mathbf{N} = \mathbf{a}^\dagger\mathbf{a} \quad \text{with} \quad [\mathbf{N}, \mathbf{H}] = 0 \qquad \text{and} \qquad \mathbf{N}^\dagger = \mathbf{N} \tag{5.12}$$

5.1.2.1 Commutators [N, a], [N, a†], and eigenvalue equation of N For this purpose, it is necessary to know the commutator $[\mathbf{N}, \mathbf{a}]$ of $\mathbf{N}$ with the annihilation operator $\mathbf{a}$:

$$[\mathbf{N}, \mathbf{a}] = (\mathbf{a}^\dagger\mathbf{a})\mathbf{a} - \mathbf{a}(\mathbf{a}^\dagger\mathbf{a})$$

Now, by changing the position of the second parenthesis, which does not modify anything, the commutator reads

$$[\mathbf{N}, \mathbf{a}] = (\mathbf{a}^\dagger\mathbf{a})\mathbf{a} - (\mathbf{a}\mathbf{a}^\dagger)\mathbf{a} \tag{5.13}$$

In addition, according to Eq. (5.5), that is,

$$\mathbf{a}\mathbf{a}^\dagger = \mathbf{a}^\dagger\mathbf{a} + 1 \tag{5.14}$$

Eq. (5.13) becomes

$$[\mathbf{N}, \mathbf{a}] = \{\mathbf{a}^\dagger\mathbf{a} - (\mathbf{a}^\dagger\mathbf{a} + \mathbf{1})\}\mathbf{a}$$

or

$$\boxed{[\mathbf{N}, \mathbf{a}] = -\mathbf{a} = [\mathbf{a}^\dagger\mathbf{a}, \mathbf{a}]} \tag{5.15}$$

Now, calculate the commutator of $\mathbf{N}$ with the creation operator $\mathbf{a}^\dagger$. We have

$$[\mathbf{N}, \mathbf{a}^\dagger] = (\mathbf{a}^\dagger\mathbf{a})\mathbf{a}^\dagger - \mathbf{a}^\dagger(\mathbf{a}^\dagger\mathbf{a})$$

which, by changing the first parenthesis position, reads

$$[\mathbf{N}, \mathbf{a}^\dagger] = \mathbf{a}^\dagger(\mathbf{a}\mathbf{a}^\dagger) - \mathbf{a}^\dagger(\mathbf{a}^\dagger\mathbf{a})$$

or, due to Eq. (5.14),

$$[\mathbf{N}, \mathbf{a}^\dagger] = \mathbf{a}^\dagger(\mathbf{a}^\dagger\mathbf{a} + \mathbf{1}) - \mathbf{a}^\dagger(\mathbf{a}^\dagger\mathbf{a})$$

[1]We shall use for the writing of the eigenkets of $\mathbf{a}^\dagger\mathbf{a}$ notations such as $|\{n\}\rangle$, $|(n)\rangle$, and $|[n]\rangle$, which are more complex than the usual ones $|n\rangle$, in order to allow one to distinguish easily different eigenkets belonging to different oscillators characterized by different sets of ladder operators $\mathbf{a}^\dagger\mathbf{a}$, $\mathbf{b}^\dagger\mathbf{b}$, and $\mathbf{c}^\dagger\mathbf{c}$. That will appear to be useful in the following chapters.

so that

$$\boxed{[\mathbf{N}, \mathbf{a}^\dagger] = \mathbf{a}^\dagger = [\mathbf{a}^\dagger \mathbf{a}, \mathbf{a}^\dagger]} \tag{5.16}$$

Next, write the eigenvalue equation of $\mathbf{N}$:

$$\boxed{\mathbf{N}|\{n\}\rangle = A_n|\{n\}\rangle} \tag{5.17}$$

where A_n are the eigenvalues of $\mathbf{N}$, which are real because $\mathbf{N}$ is Hermitian, whereas $|\{n\}\rangle$ are the corresponding eigenvectors obeying Eq. (5.11), which must be, therefore, the same as those appearing in Eq. (5.10) because $\mathbf{H}$ and $\mathbf{N}$ commute.

5.1.2.2 Action of N on $|a^k\{n\}\rangle$ To solve the eigenvalue equation (5.17) consider the action of the commutator (5.15) on any eigenket of Eq. (5.17), that is,

$$[\mathbf{N}, \mathbf{a}]|\{n\}\rangle = (\mathbf{Na} - \mathbf{aN})|\{n\}\rangle \tag{5.18}$$

which, due to Eq. (5.15), reads

$$(\mathbf{Na} - \mathbf{aN})|\{n\}\rangle = -\mathbf{a}|\{n\}\rangle$$

and which, owing to Eq. (5.17), transforms to

$$(\mathbf{Na} - \mathbf{a}A_n)|\{n\}\rangle = -\mathbf{a}|\{n\}\rangle$$

Then, rearranging, it yields

$$\mathbf{Na}|\{n\}\rangle = \mathbf{a}A_n|\{n\}\rangle - \mathbf{a}|\{n\}\rangle$$

Since A_n is a scalar that commutes with $\mathbf{a}$, we have

$$\mathbf{Na}|\{n\}\rangle = (A_n - 1)\mathbf{a}|\{n\}\rangle \tag{5.19}$$

Now, observe that the action of $\mathbf{a}$ on the eigenstate $|\{n\}\rangle$ yields a new state, which may be written formally as

$$\mathbf{a}|\{n\}\rangle \equiv |\mathbf{a}\{n\}\rangle \tag{5.20}$$

so that Eq. (5.19) reads

$$\mathbf{N}|\mathbf{a}\{n\}\rangle = (A_n - 1)|\mathbf{a}\{n\}\rangle \tag{5.21}$$

Hence, $(A_n - 1)$ is the eigenvalue of $\mathbf{N}$ corresponding to the ket resulting from the action of $\mathbf{a}$ on $|\{n\}\rangle$.

Again, consider the action of the commutator (5.15); however, let it now act on the ket defined by Eq. (5.20), that is,

$$[\mathbf{N}, \mathbf{a}]|\mathbf{a}\{n\}\rangle = (\mathbf{Na} - \mathbf{aN})|\mathbf{a}\{n\}\rangle$$

Then, proceeding in the same way as for passing from Eq. (5.18) to (5.19), one finds

$$\mathbf{Na}|\mathbf{a}\{n\}\rangle = (A_n - 2)\mathbf{a}|\mathbf{a}\{n\}\rangle \tag{5.22}$$

Moreover, writing

$$\mathbf{a}|\mathbf{a}\{n\}\rangle = |\mathbf{a}^2\{n\}\rangle$$

Eq. (5.22) takes the form

$$\mathbf{N}|\mathbf{a}^2\{n\}\rangle = (A_n - 2)|\mathbf{a}^2\{n\}\rangle \tag{5.23}$$

Hence, from Eqs. (5.21) and (5.23), one obtains by recurrence

$$\boxed{\mathbf{N}|\mathbf{a}^k\{n\}\rangle = (A_n - k)|\mathbf{a}^k\{n\}\rangle \quad \text{with} \quad |\mathbf{a}^k\{n\}\rangle \equiv \mathbf{a}^k|\{n\}\rangle} \tag{5.24}$$

5.1.2.3 Action of N on $|(\mathbf{a}^\dagger)^k\{n\}\rangle$ Now, consider the action of the commutator (5.16) on any eigenket of Eq. (5.17), that is,

$$[\mathbf{N}, \mathbf{a}^\dagger]|\{n\}\rangle = (\mathbf{N}\mathbf{a}^\dagger - \mathbf{a}^\dagger\mathbf{N})|\{n\}\rangle$$

Then, using Eq. (5.16) to express the left-hand-side member of this last expression, one obtains

$$\mathbf{a}^\dagger|\{n\}\rangle = (\mathbf{N}\mathbf{a}^\dagger - \mathbf{a}^\dagger\,\mathbf{N})|\{n\}\rangle$$

Again, using the eigenvalue equation (5.17), one gets

$$\mathbf{a}^\dagger|\{n\}\rangle = (\mathbf{N}\mathbf{a}^\dagger - \mathbf{a}^\dagger A_n)|\{n\}\rangle$$

and thus, after commuting the scalar A_n with the operator $\mathbf{a}^\dagger$, we have

$$\mathbf{N}\mathbf{a}^\dagger|\{n\}\rangle = (A_n + 1)\mathbf{a}^\dagger|\{n\}\rangle$$

or

$$\mathbf{N}|\mathbf{a}^\dagger\{n\}\rangle = (A_n + 1)|\mathbf{a}^\dagger\{n\}\rangle \tag{5.25}$$

with

$$\mathbf{a}^\dagger|\{n\}\rangle \equiv |\mathbf{a}^\dagger\{n\}\rangle$$

Consider again the action of the commutator (5.16) on $|\mathbf{a}^\dagger\{n\}\rangle$:

$$[\mathbf{N}, \mathbf{a}^\dagger]|\mathbf{a}^\dagger\{n\}\rangle = (\mathbf{N}\mathbf{a}^\dagger - \mathbf{a}^\dagger\mathbf{N})|\mathbf{a}^\dagger\{n\}\rangle$$

Then, proceeding as above, one would obtain

$$\mathbf{N}\mathbf{a}^\dagger|\mathbf{a}^\dagger\{n\}\rangle = (A_n + 2)\mathbf{a}^\dagger|\mathbf{a}^\dagger\{n\}\rangle$$

or, changing the notation,

$$\mathbf{N}|(\mathbf{a}^\dagger)^2\{n\}\rangle = (A_n + 2)|(\mathbf{a}^\dagger)^2\{n\}\rangle \tag{5.26}$$

with

$$\mathbf{a}^\dagger|\mathbf{a}^\dagger\{n\}\rangle \equiv |(\mathbf{a}^\dagger)^2\{n\}\rangle \tag{5.27}$$

Hence, from Eqs. (5.25) and (5.26), one gets by recurrence

$$\boxed{\mathbf{N}|(\mathbf{a}^\dagger)^k\{n\}\rangle = (A_n + k)|(\mathbf{a}^\dagger)^k\{n\}\rangle \quad \text{with} \quad |(\mathbf{a}^\dagger)^k\{n\}\rangle = (\mathbf{a}^\dagger)^k|\{n\}\rangle} \tag{5.28}$$

5.1.2.4 Discrete character of the eigenvalues A_n Starting from the assumed eigenvalue equation (5.17), it has been possible to prove Eqs. (5.24) and (5.28). Rewrite them for comparison:

$$\mathbf{N}|\{n\}\rangle = A_n|\{n\}\rangle$$

$$\mathbf{N}|(\mathbf{a})^k\{n\}\rangle = (A_n - k)|(\mathbf{a})^k\{n\}\rangle$$

$$\mathbf{N}|(\mathbf{a}^\dagger)^k\{n\}\rangle = (A_n + k)|(\mathbf{a}^\dagger)^k\{n\}\rangle$$

with

$$|(\mathbf{a})^k\{n\}\rangle \equiv (\mathbf{a})^k|\{n\}\rangle \qquad \text{and} \qquad |(\mathbf{a}^\dagger)^k\{n\}\rangle \equiv (\mathbf{a}^\dagger)^k|\{n\}\rangle \tag{5.29}$$

By inspection of these equations, it appears that

$|\{n\}\rangle$ is an eigenvector of $\mathbf{N}$ with the corresponding eigenvalue A_n.
$|(\mathbf{a})^k\{n\}\rangle$ is an eigenvector of $\mathbf{N}$ with the corresponding eigenvalue $(A_n - k)$.
$|(\mathbf{a}^\dagger)^k\{n\}\rangle$ is an eigenvector of $\mathbf{N}$ with the corresponding eigenvalue $(A_n + k)$.

Hence, $|\{n\}\rangle$, $(\mathbf{a})^k|\{n\}\rangle$, and $(\mathbf{a}^\dagger)^k|\{n\}\rangle$ are eigenvectors of $\mathbf{N}$ with the eigenvalues A_n $(A_n - k)$ and $(A_n + k)$, respectively.

Thus, it may be inferred that the action of the kth power of the $\mathbf{a}$ operator on an eigenvector of $\mathbf{N}$ lowers by k the eigenvalue A_n of $\mathbf{N}$ corresponding to this eigenvector, whereas the action of the kth power of $\mathbf{a}^\dagger$ on the same eigenvector of $\mathbf{N}$ raises by k the eigenvalue A_n. Hence, the eigenvalues of $\mathbf{N}$ obey the relation

$$\boxed{A_n, A_n \pm 1, A_n \pm 2, \ldots} \tag{5.30}$$

5.1.2.5 Impossibility for A_n to be negative Now let us show that A_n cannot be negative. Thus, consider

$$|\mathbf{a}\{n\}\rangle \equiv \mathbf{a}|\{n\}\rangle \tag{5.31}$$

the Hermitian conjugate of which is

$$\langle\{n\}\mathbf{a}^\dagger| \equiv \langle\{n\}|\mathbf{a}^\dagger \tag{5.32}$$

Then, owing to the property of the norm, requiring

$$\langle\{n\}\mathbf{a}^\dagger|\mathbf{a}\{n\}\rangle \geq 0$$

and according to the notations (5.31) and (5.32), we have

$$\langle\{n\}\mathbf{a}^\dagger|\mathbf{a}\{n\}\rangle = \langle\{n\}|\mathbf{a}^\dagger\mathbf{a}|\{n\}\rangle \tag{5.33}$$

Moreover, due to the definition (5.12) of $\mathbf{N}$, Eq. (5.33) transforms to

$$\langle\{n\}\mathbf{a}^\dagger|\mathbf{a}\{n\}\rangle = \langle\{n\}|\mathbf{N}|\{n\}\rangle$$

which, with the help of the eigenvalue equation (5.17), transforms to

$$\langle\{n\}\mathbf{a}^\dagger|\mathbf{a}\{n\}\rangle = \langle\{n\}|A_n|\{n\}\rangle$$

so that A_n being a scalar, is given by

$$A_n = \frac{\langle\{n\}\mathbf{a}^\dagger|\mathbf{a}\{n\}\rangle}{\langle\{n\}|\{n\}\rangle}$$

Now, observe that because the norm cannot be negative one has, respectively,

$$\langle\{n\}\mathbf{a}^\dagger|\mathbf{a}\{n\}\rangle \geq 0 \qquad \text{and} \qquad \langle\{n\}|\{n\}\rangle \geq 0$$

Hence, the eigenvalues of $\mathbf{N}$ cannot be negative

$$\boxed{A_n \geq 0} \tag{5.34}$$

5.1.2.6 Nullity of the lowest eigenvalue Since the eigenvalue A_n cannot be negative, there exists a lowest eigenvalue A_0 to which is associated an eigenvector denoted $|\{0\}\rangle$, leading to write in this special situation the eigenvalue equation (5.17) according to

$$\mathbf{N}|\{0\}\rangle = A_0|\{0\}\rangle$$

Now, the action of $\mathbf{N}$ on the ket resulting from the action of $\mathbf{a}$ on the lowest state $|\{0\}\rangle$ would lead, according to Eq. (5.19), to a new state, eigenvector of $\mathbf{N}$ with a corresponding eigenvalue $(A_0 - 1)$, which is impossible since A_0 was assumed to be the lowest possible eigenvalue:

$$\mathbf{Na}|\{0\}\rangle = \mathbf{N}|\mathbf{a}\{0\}\rangle = (A_0 - 1)|\mathbf{a}\{0\}\rangle \qquad \text{Impossible}$$

Thereby, owing to this impossibility, $|\{0\}\rangle$ must be the fundamental eigenstate of $\mathbf{N}$, leading to write

$$\mathbf{a}|\{0\}\rangle = |\mathbf{a}\{0\}\rangle = 0 \tag{5.35}$$

the Hermitian conjugate of which is

$$\langle\{0\}|\mathbf{a}^\dagger = \langle\{0\}\mathbf{a}^\dagger| = 0$$

Of course, the norm between the states involved in the two above equations is

$$\langle\{0\}\mathbf{a}^\dagger|\mathbf{a}\{0\}\rangle = 0 \tag{5.36}$$

Next, observe that, due to the notations (5.31) and (5.32),

$$\langle\{0\}\mathbf{a}^\dagger|\mathbf{a}\{0\}\rangle \equiv \langle\{0\}|\mathbf{a}^\dagger\mathbf{a}|\{0\}\rangle \tag{5.37}$$

and, due to Eq. (5.12), that

$$\langle\{0\}|\mathbf{a}^\dagger\mathbf{a}|\{0\}\rangle = \langle\{0\}|\mathbf{N}|\{0\}\rangle$$

and, at last, that, owing to Eq. (5.17),

$$\langle\{0\}|\mathbf{N}|\{0\}\rangle = \langle\{0\}|A_0|\{0\}\rangle = A_0\langle\{0\}|\{0\}\rangle \tag{5.38}$$

Again, if $|\{0\}\rangle$ is normalized, that is, if

$$\langle\{0\}|\{0\}\rangle = 1$$

then, in view of Eqs. (5.37) and (5.38), it reads

$$\langle\{0\}\mathbf{a}^\dagger|\mathbf{a}\{0\}\rangle = A_0$$

so that, owing to Eq. (5.36), we have

$$\boxed{A_0 = 0} \tag{5.39}$$

5.1.2.7 Solution of the Hamiltonian eigenvalue equation (5.17) In the above section, we studied the eigenvalue equation (5.17), that is,

$$\mathbf{N}|\{n\}\rangle = A_n|\{n\}\rangle$$

for which it was shown that the eigenvalues A_n obey Eqs. (5.30), (5.34), and (5.39), that is,

$$A_n, A_n \pm 1, A_n \pm 2, \ldots \quad \text{with} \quad A_n \geq 0 \qquad \text{and} \qquad A_0 = 0$$

These results show that A_n is of the form

$$A_n = 0, 1, 2, 3, \ldots$$

Hence, writing explicitly the operator $\mathbf{N}$ by aid of Eq. (5.12) leads to writing the following eigenvalue equation:

$$\boxed{(\mathbf{a}^\dagger\mathbf{a})|\{n\}\rangle = n|\{n\}\rangle \quad \text{with } n \equiv A_n \qquad \text{and} \qquad n = 0, 1, 2, 3, \ldots} \tag{5.40}$$

Since the Hamiltonian of the quantum harmonic oscillator is given by Eq. (5.9), that is,

$$\mathbf{H} = \left(\mathbf{a}^\dagger\mathbf{a} + \tfrac{1}{2}\right)\hbar\omega \tag{5.41}$$

and due to Eq. (5.40), we see that the following eigenvalue equation is satisfied:

$$\boxed{\mathbf{H}|\{n\}\rangle = \hbar\omega\left(n + \tfrac{1}{2}\right)|\{n\}\rangle \quad \text{with} \quad n = 0, 1, 2, 3, \ldots} \tag{5.42}$$

The lowest eigenstate $|\{0\}\rangle$ of the Hamiltonian corresponding to $n = 0$ is called *the ground state*, whereas the corresponding residual energy $\hbar\omega/2$ is called *the zero-point energy* of the oscillator. Now, according to Section 1.3.1, since the Hamiltonian operator (5.9) is Hermitian, its eigenvectors are necessarily orthogonal. Thus, if they have been normalized, they form an orthonormal basis obeying

$$\boxed{\langle\{n\}|\{m\}\rangle = \delta_{nm} \qquad \text{and} \qquad \sum_n |\{n\}\rangle\langle\{n\}| = 1} \tag{5.43}$$

5.1.2.8 Zero-point energy as preserving the Heisenberg uncertainty relations It may be of interest to understand the role of the zero-point energy $\hbar\omega/2$ appearing in Eq. (5.42) in the context of the Heisenberg uncertainty relations (2.9) dealing with the momentum and the position operators:

$$\Delta\mathbf{P}\,\Delta\mathbf{Q} \geqslant \frac{\hbar}{2} \tag{5.44}$$

Now, suppose that the energy of the ground state $|\{0\}\rangle$ is zero. Then, since the harmonic potential energy V of the oscillator cannot be negative because quadratic in the position Q, that is,

$$V = \tfrac{1}{2} M\omega^2 Q^2 \tag{5.45}$$

and because the kinetic energy T, which is quadratic in the momentum P, is necessarily positive, that is,

$$T = \frac{P^2}{2M} > 0 \tag{5.46}$$

our supposition would imply that both the kinetic T and potential V energies ought separately to be zero, that is,

$$T = V = 0 \tag{5.47}$$

However, as a consequence of Eqs. (5.45)–(5.47), it would then appear that

$$P = Q = 0 \tag{5.48}$$

Moreover, if Eq. (5.48) was true, that would in turn imply that P and Q would be known without any uncertainty, that is,

$$\Delta P = \Delta Q = 0$$

in contradiction to the Heisenberg uncertainty relations (5.44).

5.1.3 Action of ladder operators on Hamiltonian eigenkets

The solution of the eigenvalue equation of the Hermitian Hamiltonian has not only the merit that it yields energy levels of the oscillators but also the merit that it provides a basis from which it is possible to obtain matrix representations of all operators dealing with quantum oscillators. Since these operators may be written as functions of the position and momentum operators, they may be also expressed as functions of the raising and lowering operators. Therefore, it appears that the knowledge of the action of these operators on the eigenkets of the Hamiltonian will be of much interest from now on. Thus, the aim of this new section will be to treat this point.

5.1.3.1 Action of a Consider the action of **a** operator on $|\{n\}\rangle$. Keeping in mind Eq. (5.40) according to which $n \equiv A_n$, Eq. (5.21) reads

$$\mathbf{N}|\mathbf{a}\{n\}\rangle = (n-1)|\mathbf{a}\{n\}\rangle \quad \text{with} \quad n = 0, 1, 2, 3, \ldots \tag{5.49}$$

whereas the eigenvalue equation Eq. (5.17) allows one to write

$$\begin{aligned} \mathbf{N}|\{n\}\rangle &= n|\{n\}\rangle \\ \mathbf{N}|\{n-1\}\rangle &= (n-1)|\{n-1\}\rangle \end{aligned} \tag{5.50}$$

Comparison of the eigenvalue equations (5.49) and (5.50) shows that both equations involve the same operator and the same eigenvalues. Moreover, if the eigenvectors

appearing in these eigenvalue equations are not necessarily the same, they must be proportional, so that one may write

$$|\mathbf{a}\{n\}\rangle = \lambda_n |\{n-1\}\rangle$$

where λ_n is a complex scalar. The Hermitian conjugate of this last expression being

$$\langle\{n\}\mathbf{a}^\dagger| = \lambda_n^* \langle\{n-1\}|$$

the corresponding norm is thereby

$$\langle\{n\}\mathbf{a}^\dagger|\mathbf{a}\{n\}\rangle = |\lambda_n|^2 \langle\{n-1\}|\{n-1\}\rangle$$

Next, if the right-hand-side ket is normalized, this last equation reduces to

$$\langle\{n\}\mathbf{a}^\dagger|\mathbf{a}\{n\}\rangle = |\lambda_n|^2 \tag{5.51}$$

On the other hand, Eqs. (5.31) and (5.32) allow one to write the left-hand side of Eq. (5.51) as

$$\langle\{n\}\mathbf{a}^\dagger|\mathbf{a}\{n\}\rangle = \langle\{n\}|\mathbf{a}^\dagger\mathbf{a}|\{n\}\rangle$$

It appears that, due to Eq. (5.40),

$$\langle\{n\}\mathbf{a}^\dagger|\mathbf{a}\{n\}\rangle = n\langle\{n\}|\{n\}\rangle = n \tag{5.52}$$

Therefore, by identification of Eqs. (5.51) and (5.52), we have

$$|\lambda_n|^2 = n$$

so that, ignoring the phase factor (if λ_n would be imaginary), which is of no interest,

$$\lambda_n = \sqrt{n}$$

Thus, one obtains the final result of interest:

$$\boxed{\mathbf{a}|\{n\}\rangle = \sqrt{n}|\{n-1\}\rangle} \tag{5.53}$$

As it appears, the action of operator $\mathbf{a}$ on any eigenstate $|\{n\}\rangle$ of $\mathbf{a}^\dagger\mathbf{a}$ corresponding to the eigenvalue n transforms this state into a new eigenstate $|\{n-1\}\rangle$ of $\mathbf{a}^\dagger\mathbf{a}$ corresponding to the eigenvalue $(n-1)$. This action may be, therefore, viewed as lowering the eigenvalue of $\mathbf{a}^\dagger\mathbf{a}$ by unity and thus the corresponding eigenvector. Hence, $\mathbf{a}$ is called a *lowering operator*. Observe that the Hermitian conjugate of this equation is

$$\langle\{n\}|\mathbf{a}^\dagger = \sqrt{n}\langle\{n-1\}| \tag{5.54}$$

Now, since $|\{0\}\rangle$ is the lowest eigenket of $\mathbf{a}^\dagger\mathbf{a}$, Eqs. (5.53) and (5.54) lead to

$$\mathbf{a}|\{0\}\rangle = \langle\{0\}|\mathbf{a}^\dagger = 0 \tag{5.55}$$

5.1.3.2 Action of $\mathbf{a}^\dagger$ After finding the action of $\mathbf{a}$ on the Hamiltonian eigenkets, then pass to that on its Hermitian conjugate $\mathbf{a}^\dagger$. In view of $A_n = n$, Eq. (5.25) reads

$$\mathbf{N}|\mathbf{a}^\dagger\{n\}\rangle = (n+1)|\mathbf{a}^\dagger\{n\}\rangle \quad \text{with} \quad n = 0, 1, 2, 3, \ldots \tag{5.56}$$

whereas the eigenvalue equation (5.17) reads, respectively,

$$\begin{aligned} \mathbf{N}|\{n\}\rangle &= n|\{n\}\rangle \\ \mathbf{N}|\{n+1\}\rangle &= (n+1)|\{n+1\}\rangle \end{aligned} \tag{5.57}$$

Equation (5.57) is analogous to Eq. (5.56) since the $\mathbf{N}$ operator and the eigenvalues $(n+1)$ are the same in both cases so that the kets appearing in Eqs. (5.56) and (5.57) must be at least proportional to each other, leading one to write

$$|\mathbf{a}^\dagger\{n\}\rangle = \mu_n|\{n+1\}\rangle \tag{5.58}$$

where μ_n is a complex scalar. The corresponding norm is, therefore,

$$\langle\{n\}\mathbf{a}|\mathbf{a}^\dagger\{n\}\rangle = |\mu_n|^2\langle\{n+1\}|\{n+1\}\rangle$$

Again, if the eigenvectors $|\{n+1\}\rangle$ are normalized, this last expression reduces to

$$\langle\{n\}\mathbf{a}|\mathbf{a}^\dagger\{n\}\rangle = |\mu_n|^2 \tag{5.59}$$

In addition, changing the writing with the aid of Eqs. (5.31) and (5.32), the left-hand-side reads

$$\langle\{n\}\mathbf{a}|\mathbf{a}^\dagger\{n\}\rangle = \langle\{n\}|\mathbf{a}\mathbf{a}^\dagger|\{n\}\rangle \tag{5.60}$$

Furthermore, using the commutation rule (5.5), leading to

$$\mathbf{a}\mathbf{a}^\dagger = \mathbf{a}^\dagger\mathbf{a} + 1$$

Eq. (5.60) becomes

$$\langle\{n\}\mathbf{a}|\mathbf{a}^\dagger\{n\}\rangle = \langle\{n\}|(\mathbf{a}^\dagger\mathbf{a} + 1)|\{n\}\rangle \tag{5.61}$$

Moreover, using the eigenvalue equation (5.40), we have

$$(\mathbf{a}^\dagger\mathbf{a} + 1)|\{n\}\rangle = (n+1)|\{n\}\rangle$$

Thus, Eq. (5.61) transforms to

$$\langle\{n\}\mathbf{a}|\mathbf{a}^\dagger\{n\}\rangle = (n+1)\langle\{n\}|\{n\}\rangle$$

or, $|\{n\}\rangle$ being normalized,

$$\langle\{n\}\mathbf{a}|\mathbf{a}^\dagger\{n\}\rangle = n + 1 \tag{5.62}$$

Finally, by identification of Eqs. (5.59) and (5.62)

$$|\mu_n|^2 = n + 1$$

and ignoring an irrelevant phase factor, we have

$$\mu_n = \sqrt{n+1}$$

Hence, from Eq. (5.58), and due to the notations in (5.31) and (5.32), one obtains the final result:

$$\boxed{\mathbf{a}^\dagger|\{n\}\rangle = \sqrt{n+1}|\{n+1\}\rangle} \tag{5.63}$$

the Hermitian conjugate of which is

$$\boxed{\langle\{n\}|\mathbf{a} = \sqrt{n+1}\langle\{n+1\}|} \tag{5.64}$$

Observe that, according to Eq. (5.63), the action of $\mathbf{a}^\dagger$ on any ket $|\{n\}\rangle$ is changed into the raised one $|\{n+1\}\rangle$; hence, this operator is called a *raising operator*.

5.1.3.3 Action of different powers of $a^\dagger$ and a Consider the action of different powers of $\mathbf{a}^\dagger$. The action of $\mathbf{a}^\dagger$ on the lowest state $|\{0\}\rangle$ corresponding to $n=0$, Eq. (5.63) yields

$$\mathbf{a}^\dagger|\{0\}\rangle = |\{1\}\rangle \tag{5.65}$$

In addition, due to Eq. (5.63), the second power of $\mathbf{a}^\dagger$

$$(\mathbf{a}^\dagger)^2|\{0\}\rangle = \mathbf{a}^\dagger\mathbf{a}^\dagger|\{0\}\rangle = \mathbf{a}^\dagger|\{1\}\rangle \tag{5.66}$$

or, using again Eq. (5.63),

$$(\mathbf{a}^\dagger)^2|\{0\}\rangle = \sqrt{1(1+1)}|\{1+1\}\rangle$$

Moreover, the third power of $\mathbf{a}^\dagger$ yields, using Eq. (5.63),

$$(\mathbf{a}^\dagger)^3|\{0\}\rangle = \sqrt{1(1+1)(2+1)}|\{2+1\}\rangle$$

so that, by recurrence, one obtains

$$(\mathbf{a}^\dagger)^n|\{0\}\rangle = \sqrt{n!}|\{n\}\rangle \tag{5.67}$$

the Hermitian conjugate of which is

$$\langle\{0\}|(\mathbf{a})^n = \sqrt{n!}\langle\{n\}| \tag{5.68}$$

Furthermore, by inversion, Eqs. (5.67) and (5.68) read, respectively,

$$|\{n\}\rangle = \frac{(\mathbf{a}^\dagger)^n}{\sqrt{n!}}|\{0\}\rangle \tag{5.69}$$

$$\langle\{n\}| = \langle\{0\}|\frac{(\mathbf{a})^n}{\sqrt{n!}} \tag{5.70}$$

Next, passing to the action of different powers of $\mathbf{a}$ on $|\{n\}\rangle$, Eq. (5.53), allows one to write successively

$$(\mathbf{a})|\{n\}\rangle = \sqrt{n}|\{n-1\}\rangle$$

$$(\mathbf{a})^2|\{n\}\rangle = \sqrt{n}(\mathbf{a})|\{n-1\}\rangle$$

$$(\mathbf{a})^2|\{n\}\rangle = \sqrt{n(n-1)}|\{n-2\}\rangle$$

so that, by recurrence, one gets

$$(\mathbf{a})^l|\{n\}\rangle = \sqrt{n(n-1)\cdots(n-l+1)}|\{n-l\}\rangle \tag{5.71}$$

or

$$\boxed{(\mathbf{a})^l|\{n\}\rangle = \frac{\sqrt{n!}}{\sqrt{(n-l)!}}|\{n-l\}\rangle} \tag{5.72}$$

the Hermitian conjugate of which is

$$\langle\{n\}|(\mathbf{a}^\dagger)^l = \frac{\sqrt{n!}}{\sqrt{(n-l)!}}\langle\{n-l\}| \tag{5.73}$$

In a similar way, one would obtain using Eq. (5.63)

$$(\mathbf{a}^\dagger)^l|\{n\}\rangle = \sqrt{n(n+1)\cdots(n+l)}|\{n+l\}\rangle$$

or

$$\boxed{(\mathbf{a}^\dagger)^l|\{n\}\rangle = \frac{\sqrt{(n+l)!}}{\sqrt{(n)!}}|\{n+l\}\rangle} \tag{5.74}$$

for which the Hermitian conjugate is

$$\langle\{n\}|(\mathbf{a})^l = \frac{\sqrt{(n+l)!}}{\sqrt{(n)!}}\langle\{n+l\}|$$

5.1.4 Matrix representation of ladder operators

Knowledge of the action of the ladder operators on the eigenkets and eigenbras of the Hamiltonian allows one to get the matrix representation of these operators. For this purpose, start from the eigenvalue equation

$$\mathbf{N}|(n)\rangle = n|(n)\rangle \quad \text{with} \quad n = 0, 1, 2, \ldots \tag{5.75}$$

keeping in mind that $\mathbf{N}$ is the Hermitian number occupation operator

$$\mathbf{N} = \mathbf{a}^\dagger\mathbf{a} \qquad \text{and} \qquad \mathbf{N} = \mathbf{N}^\dagger \quad \text{since} \quad (\mathbf{a}^\dagger\mathbf{a})^\dagger = \mathbf{a}^\dagger\mathbf{a} \tag{5.76}$$

whereas $\mathbf{a}$ and $\mathbf{a}^\dagger$ are obeying the commutation rules

$$[\mathbf{a}, \mathbf{a}^\dagger]_- \equiv \mathbf{a}\mathbf{a}^\dagger - \mathbf{a}^\dagger\mathbf{a} = 1 \tag{5.77}$$

$$[\mathbf{a}, \mathbf{a}]_- = [\mathbf{a}^\dagger, \mathbf{a}^\dagger]_- = 0 \tag{5.78}$$

and that the kets form an orthogonal basis so that

$$\langle(n)|(m)\rangle = \delta_{mn} \tag{5.79}$$

Note that the subscript $-$ has been introduced in the expressions for commutators (5.77) and (5.78) in order to distinguish them from the anticommutators, which will appear later. At last, recall Eqs. (5.53) and (5.63), that is,

$$\mathbf{a}|(m)\rangle = \sqrt{m}|(m-1)\rangle \qquad \text{and} \qquad \mathbf{a}^\dagger|(m)\rangle = \sqrt{m+1}|(m+1)\rangle \tag{5.80}$$

Thus, in the basis defined by Eq. (5.79) and using Eq. (5.80), the matrix elements of $\mathbf{a}$ and $\mathbf{a}^\dagger$ read, respectively,

$$\langle (n)|\mathbf{a}|(m)\rangle = \sqrt{m}\langle (n)|(m-1)\rangle = \sqrt{m}\delta_{n,m-1}$$

$$\langle (n)|\mathbf{a}^\dagger|(m)\rangle = \sqrt{m+1}\langle (n)|(m+1)\rangle = \sqrt{m+1}\delta_{n,m+1}$$

As a consequence, the matrix representations of $\mathbf{a}$ and $\mathbf{a}^\dagger$ read, after arbitrary truncation,

$$\boxed{\mathbf{a}} = \begin{pmatrix} 0 & \sqrt{1} & & & \\ & 0 & \sqrt{2} & & \\ & & 0 & \sqrt{3} & \\ & & & 0 & \sqrt{4} \\ & & & & 0 \end{pmatrix} \quad \text{and} \quad \boxed{\mathbf{a}^\dagger} = \begin{pmatrix} 0 & & & & \\ \sqrt{1} & 0 & & & \\ & \sqrt{2} & 0 & & \\ & & \sqrt{3} & 0 & \\ & & & \sqrt{4} & 0 \end{pmatrix} \tag{5.81}$$

Hence, the matrix representation of the occupation number defined by Eq. (5.76) yields

$$\boxed{\mathbf{N}} = \begin{pmatrix} 0 & & & & \\ \sqrt{1} & 0 & & & \\ & \sqrt{2} & 0 & & \\ & & \sqrt{3} & 0 & \\ & & & \sqrt{4} & 0 \end{pmatrix} \begin{pmatrix} 0 & \sqrt{1} & & & \\ & 0 & \sqrt{2} & & \\ & & 0 & \sqrt{3} & \\ & & & 0 & \sqrt{4} \\ & & & & 0 \end{pmatrix}$$

or, after performing the matrix product,

$$\boxed{\mathbf{N}} = \begin{pmatrix} 0 & & & & \\ & 1 & & & \\ & & 2 & & \\ & & & 3 & \\ & & & & 4 \end{pmatrix}$$

That is in agreement with the result obtained by premultiplying Eq. (5.75) by the bra $\langle (m)|$ to give

$$\langle (m)|\mathbf{N}|(n)\rangle = n\langle (m)|(n)\rangle = n\,\delta_{mn}$$

5.1.5 Heisenberg uncertainty relations

As we have said above, Heisenberg provided the first demonstration of the quantized energy levels of harmonic oscillators and was lead to these results through his anticipation of the uncertainty relations. It is, therefore, important to answer the question of the expression of the Heisenberg uncertainty relation when computed over the eigenstates of the quantum harmonic oscillator Hamiltonian. For this purpose, first consider the required average values of $\mathbf{Q}$ and $\mathbf{Q}^2$.

Thus, start from the average value of $\mathbf{Q}$ over the number occupation eigenstates, which, owing to Eq. (5.6), is

$$\langle \{n\}|\mathbf{Q}|\{n\}\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle \{n\}|(\mathbf{a}^\dagger + \mathbf{a})|\{n\}\rangle \tag{5.82}$$

Again, owing to Eq. (5.53), the average value of $\mathbf{a}$ appearing in Eq. (5.82) is zero because of the orthogonality of the eigenkets of the Hamiltonian:

$$\langle\{n\}|\mathbf{a}|\{n\}\rangle = \sqrt{n}\langle\{n\}|\{n-1\}\rangle = 0 \tag{5.83}$$

Of course, the Hermitian conjugate must be also zero:

$$\langle\{n\}|\mathbf{a}^\dagger|\{n\}\rangle = \sqrt{n}\langle\{n-1\}|\{n\}\rangle = 0 \tag{5.84}$$

Therefore, it appears that the average value (5.82) of $\mathbf{Q}$ is zero, that is,

$$\boxed{\langle\{n\}|\mathbf{Q}|\{n\}\rangle = 0} \tag{5.85}$$

Now, owing to Eq. (5.6), the average value of $\mathbf{Q}^2$ reads

$$\langle\{n\}|\mathbf{Q}^2|\{n\}\rangle = \frac{\hbar}{2m\omega}\langle\{n\}|(\mathbf{a}^\dagger + \mathbf{a})^2|\{n\}\rangle \tag{5.86}$$

Moreover, the square appearing on the right-hand-side yields

$$(\mathbf{a}^\dagger + \mathbf{a})^2 = \mathbf{a}^\dagger\mathbf{a}^\dagger + \mathbf{a}\mathbf{a} + \mathbf{a}^\dagger\mathbf{a} + \mathbf{a}\mathbf{a}^\dagger$$

or, due to the commutation rule (5.77), that gives

$$\boxed{(\mathbf{a}^\dagger + \mathbf{a})^2 = (\mathbf{a}^\dagger)^2 + (\mathbf{a})^2 + 2\mathbf{a}^\dagger\mathbf{a} + 1} \tag{5.87}$$

Furthermore, owing to Eq. (5.53), the two successive actions of $\mathbf{a}$ on an eigenstate of the Hamiltonian, lead to

$$\mathbf{a}\mathbf{a}|\{n\}\rangle = \sqrt{n}\mathbf{a}|\{n-1\}\rangle = \sqrt{n}\sqrt{n-1}|\{n-2\}\rangle$$

The average value of $\mathbf{a}\mathbf{a}$ is, therefore, zero, according to the orthogonality of the eigenkets of the Hamiltonian, that is,

$$\langle\{n\}|(\mathbf{a}\mathbf{a})|\{n\}\rangle = \sqrt{n(n-1)}\langle\{n\}|\{n-2\}\rangle = 0 \tag{5.88}$$

Of course, the Hermitian conjugate of this last equation may be obtained by taking for the left-hand-side $\mathbf{a}^\dagger\mathbf{a}^\dagger$ in place of $\mathbf{a}\mathbf{a}$ and permuting, for the right-hand side, the ket and the bra of the scalar product, without changing the real scalar. That is,

$$\langle\{n\}|(\mathbf{a}^\dagger\mathbf{a}^\dagger)|\{n\}\rangle = \sqrt{n(n-1)}\langle\{n-2\}|\{n\}\rangle = 0 \tag{5.89}$$

which is also zero. Finally, in view of Eq. (5.40), the required average value of $\mathbf{a}^\dagger\mathbf{a}$ reads

$$\langle\{n\}|(\mathbf{a}^\dagger\mathbf{a})|\{n\}\rangle = n\langle\{n\}|\{n\}\rangle = n \tag{5.90}$$

Thus, using Eqs. (5.86)–(5.90), one obtains

$$\boxed{\langle\{n\}|\mathbf{Q}^2|\{n\}\rangle = \frac{\hbar}{2m\omega}(2n+1)} \tag{5.91}$$

so that, in view of Eqs. (5.85) and (5.91), the dispersion over $\mathbf{Q}$ appears to be

$$\Delta\mathbf{Q}_{|\{n\}\rangle} = \sqrt{\langle\{n\}|\mathbf{Q}^2|\{n\}\rangle - \langle\{n\}|\mathbf{Q}|\{n\}\rangle^2} = \sqrt{\frac{\hbar}{m\omega}}\sqrt{\left(n+\frac{1}{2}\right)} \tag{5.92}$$

Now, consider the corresponding average value of the momentum, which, according to Eq. (9.35), is

$$\langle\{n\}|\mathbf{P}|\{n\}\rangle = i\sqrt{\frac{\hbar m\omega}{2}}\langle\{n\}|(\mathbf{a}^\dagger - \mathbf{a})|\{n\}\rangle$$

Owing to Eqs. (5.19) and (5.84), it appears to be zero, that is,

$$\boxed{\langle\{n\}|\mathbf{P}|\{n\}\rangle = 0} \tag{5.93}$$

Again, owing to Eq. (9.35), the average value of the square of the momentum is

$$\langle\{n\}|\mathbf{P}^2|\{n\}\rangle = -\frac{\hbar m\omega}{2}\langle\{n\}|(\mathbf{a}^\dagger - \mathbf{a})^2|\{n\}\rangle$$

where, according to the commutation rule, the right-hand-side operator reads

$$(\mathbf{a}^\dagger - \mathbf{a})^2 = \mathbf{a}^\dagger\mathbf{a}^\dagger + \mathbf{a}\mathbf{a} - (2\mathbf{a}^\dagger\mathbf{a} + 1)$$

Hence, by combination of Eqs. (5.88)–(5.90), one gets

$$\boxed{\langle\{n\}|\mathbf{P}^2|\{n\}\rangle = \frac{\hbar m\omega}{2}(2n+1)} \tag{5.94}$$

Thereby, in view of Eqs. (5.93) and (5.94), the dispersion over $\mathbf{P}$ becomes

$$\Delta\mathbf{P}_{|\{n\}\rangle} = \sqrt{\langle\{n\}|\mathbf{P}^2|\{n\}\rangle - \langle\{n\}|\mathbf{P}|\{n\}\rangle^2} = \sqrt{\hbar m\omega}\sqrt{\left(n+\tfrac{1}{2}\right)} \tag{5.95}$$

by combining Eqs. (5.92) and (5.95), one obtains the following expression for the Heisenberg relation as applied to the eigenstates of the Hamiltonian of the harmonic oscillator:

$$\boxed{\Delta\mathbf{Q}_{|\{n\}\rangle}\Delta\mathbf{P}_{|\{n\}\rangle} = \left(n+\tfrac{1}{2}\right)\hbar} \tag{5.96}$$

which is an agreement with the Heisenberg uncertainty relation, which states that

$$\Delta\mathbf{Q}_{|\{n\}\rangle}\Delta\mathbf{P}_{|\{n\}\rangle} \geq \hbar \tag{5.97}$$

5.1.6 Virial theorem

We have seen that the knowledge of the average values of $\mathbf{P}^2$ and $\mathbf{Q}^2$ over the eigenstates of the number occupation operator allowed us to find the uncertainty Heisenberg relation (5.96), which holds for these states. These same average values may also allow us to verify the virial theorem studied in Section 2.4.4. This is the purpose of the present section.

When applied to harmonic oscillators, the virial theorem leads to Eqs. (2.88) and (2.89) from which results the following relation between the average values of the

Hamiltonian and those of the kinetic $\mathbf{T}$ and potential $\mathbf{V}$ operators, what may be the stationary state over which the averages are performed:

$$\langle \mathbf{T} \rangle_{|\Psi\rangle} = \langle \mathbf{V} \rangle_{|\Psi\rangle} = \tfrac{1}{2} \langle \mathbf{H} \rangle_{|\Psi\rangle} \tag{5.98}$$

To verify if our above results of the present chapter are in agreement with this theorem, first consider the average value of the harmonic potential over the states $|\{n\}\rangle$, which, being the eigenstates of the harmonic oscillator Hamiltonian, are therefore stationary:

$$\langle \mathbf{V} \rangle_{|\{n\}\rangle} = \tfrac{1}{2} m\omega^2 \langle \{n\} | \mathbf{Q}^2 | \{n\} \rangle$$

Owing to Eq. (5.91), this takes the form

$$\langle \mathbf{V} \rangle_{|\{n\}\rangle} = \tfrac{1}{2} \hbar\omega \left(n + \tfrac{1}{2} \right) \tag{5.99}$$

On the other hand, the corresponding average value of the kinetic operator is

$$\langle \mathbf{T} \rangle_{|\{n\}\rangle} = \tfrac{1}{2m} \langle \{n\} | \mathbf{P}^2 | \{n\} \rangle$$

or, in view of Eq. (5.94),

$$\langle \mathbf{T} \rangle_{|\{n\}\rangle} = \tfrac{1}{2} \hbar\omega \left(n + \tfrac{1}{2} \right) \tag{5.100}$$

Thus, according to Eq. (5.9), the average value of the harmonic Hamiltonian is

$$\langle \mathbf{H} \rangle_{|\{n\}\rangle} = \hbar\omega \langle \{n\} | \left(\mathbf{a}^\dagger \mathbf{a} + \tfrac{1}{2} \right) | \{n\} \rangle$$

or, due to Eq. (5.90),

$$\langle \mathbf{H} \rangle_{|\{n\}\rangle} = \hbar\omega \left(n + \tfrac{1}{2} \right) \tag{5.101}$$

Hence, as it may be observed, Eqs. (5.99)–(5.101) obey the virial theorem (5.98).

5.1.7 3D Harmonic oscillators

The previous sections dealt with 1D harmonic oscillators. The generalization of 1D results to 3D harmonic oscillators is the aim of the present section.

The kinetic operator $\mathbf{T}$ of a 3D oscillator of reduced mass m is

$$\mathbf{T} = \left(\frac{\mathbf{P}_x^2 + \mathbf{P}_y^2 + \mathbf{P}_z^2}{2m} \right)$$

where the $\mathbf{P}_x$, $\mathbf{P}_y$, and $\mathbf{P}_z$ are, respectively, the x, y, and z Cartesian components of the momentum operator. On the other hand, the potential operator is

$$\mathbf{V} = \tfrac{1}{2} m \left(\omega_x^2 \mathbf{Q}_x^2 + \omega_y^2 \mathbf{Q}_y^2 + \omega_z^2 \mathbf{Q}_z^2 \right)$$

where the $\mathbf{Q}_x$, $\mathbf{Q}_y$, and $\mathbf{Q}_z$ are, respectively, the x, y, and z Cartesian components of the position operator, obeying the commutation rules

$$[\mathbf{Q}_k, \mathbf{P}_l] = i\hbar\, \delta_{kl} \tag{5.102}$$

where k and l run for x, y, and z, whereas the ω_k are the corresponding angular frequencies. Then, the Hamiltonian of the oscillator yields

$$\mathbf{H} = \left(\frac{\mathbf{P}_x^2 + \mathbf{P}_y^2 + \mathbf{P}_z^2}{2m} \right) + \frac{1}{2} m \left(\omega_x^2 \mathbf{Q}_x^2 + \omega_y^2 \mathbf{Q}_y^2 + \omega_z^2 \mathbf{Q}_z^2 \right) \tag{5.103}$$

In a similar way as in Eqs. (5.6) and (5.7), one may express the position and momentum operators in terms of dimensionless non-Hermitian operators according to

$$\mathbf{Q}_k = \sqrt{\frac{\hbar}{2m\omega}}(\mathbf{a}_k^\dagger + \mathbf{a}_k) \tag{5.104}$$

$$\mathbf{P}_k = i\sqrt{\frac{m\hbar\omega}{2}}(\mathbf{a}_k^\dagger - \mathbf{a}_k) \tag{5.105}$$

with the following commutation rule between $\mathbf{a}_k$ and $\mathbf{a}_l^\dagger$ resulting from Eq. (5.102):

$$[\mathbf{a}_k, \mathbf{a}_l^\dagger] = \delta_{kl} \tag{5.106}$$

Again, proceeding as at the beginning of this chapter, the Hamiltonian (5.103) takes the form

$$\mathbf{H} = \mathbf{H}_x + \mathbf{H}_y + \mathbf{H}_z \tag{5.107}$$

with

$$\mathbf{H}_k = \hbar\omega_k \left(\mathbf{a}_k^\dagger \mathbf{a}_k + \tfrac{1}{2}\right) \quad \text{with} \quad k = x, y, z$$

Then, since each term $\mathbf{H}_k$ of the Hamiltonian $\mathbf{H}$ has the same structure as that of Eq. (5.41) of the Hamiltonian of 1D harmonic oscillators, one may write for each Hamiltonian $\mathbf{H}_k$ an eigenvalue equation having the same structure as that of (5.42), that is,

$$\hbar\omega_k \left(\mathbf{a}_k^\dagger \mathbf{a}_k + \tfrac{1}{2}\right) |\{n\}_k\rangle = E_{n_k} |\{n\}_k\rangle \tag{5.108}$$

with, for $k = x, y$, and z,

$$E_{n_k} = \hbar\omega_k \left(n_k + \tfrac{1}{2}\right) \qquad \textit{and} \qquad n_k = 0, 1, 2, 3, \ldots$$

In Eq. (5.108), the $|\{n\}_k\rangle$ are the eigenkets of the $\mathbf{H}_k$ Hamiltonians, whereas the E_{n_k} are the corresponding eigenvalues. Of course, since the Hamiltonians $\mathbf{H}_k$ are Hermitian, their eigenkets are orthonormal:

$$\langle\{n\}_k|\{m\}_k\rangle = \delta_{n_k m_k}$$

and, thereby, form a basis allowing us to write for each dimension the closure relation, that is,

$$\sum_{n_k} |\{n\}_k\rangle\langle\{n\}_k| = 1$$

Now, as for the particle-in-a-box model, the full eigenkets of the 3D Hamiltonian (5.107) must be written as the products of the eigenkets of the 1D Hamiltonians $\mathbf{H}_k$, that is

$$|\Psi_{n_x n_y n_z}\rangle = |\{n\}_x\rangle|\{n\}_y\rangle|\{n\}_z\rangle \tag{5.109}$$

whereas the corresponding eigenvalue of the 3D Hamiltonian must be the sum of the corresponding eigenvalues E_{n_k}, that is,

$$E_{n_x n_y n_z} = \hbar\omega_x \left(n_x + \tfrac{1}{2}\right) + \hbar\omega_y \left(n_y + \tfrac{1}{2}\right) + \hbar\omega_z \left(n_z + \tfrac{1}{2}\right) \tag{5.110}$$

Of course, the eigenkets (5.109) and the eigenvalues (5.110) are related through the eigenvalue equation

$$\mathbf{H}|\{n\}_x\rangle|\{n\}_y\rangle|\{n\}_z\rangle = \left\{\hbar\omega_x\left(n_x+\tfrac{1}{2}\right)+\hbar\omega_y\left(n_y+\tfrac{1}{2}\right)+\hbar\omega_z\left(n_z+\tfrac{1}{2}\right)\right\}|\{n\}_x\rangle|\{n\}_y\rangle|\{n\}_z\rangle$$

Moreover, when the 3D harmonic oscillator is isotropic, the eigenvalue (5.110) reduces to

$$E_{n_x n_y n_z} = \hbar\omega\left((n_x+n_y+n_z)+\tfrac{3}{2}\right) \tag{5.111}$$

Hence, as for the particle-in-a-box model, it appears that degeneracy occurs for all situations having the same value of $(n_x+n_y+n_z)$ verifying Eq. (5.111).

Owing to the equivalence between the three Hamiltonians $\mathbf{H}_x$, $\mathbf{H}_y$, and $\mathbf{H}_z$ and the Hamiltonian of the 1D harmonic oscillator, all that has been proved for 1D oscillators may be transposed to the 3D ones. Using equations similar to Eqs. (5.53) and (5.63), namely,

$$\mathbf{a}_k|\{n\}_k\rangle = \sqrt{n_k}|\{n_k-1\}\rangle$$

$$\mathbf{a}_k^\dagger|\{n\}_k\rangle = \sqrt{n_k+1}|\{n_k+1\}\rangle$$

and by the aid of Eqs. (5.106) and (5.108), it is possible to reproduce for each component of the 3D oscillator the results obtained in the 1D situation, particularly those concerning the Heisenberg uncertainty relations and the virial theorem.

5.2 WAVEFUNCTIONS CORRESPONDING TO HAMILTONIAN EIGENKETS

Although the kets and the corresponding wavefunctions are without direct physical meaning, it may be of interest, for the purpose of physical intuitive investigation, to visualize the forms of the wavefunctions corresponding to the eigenvectors of the Hamiltonian of quantum harmonic oscillators. One of the reasons, which will appear later, is that the number of nodes of these vibrational wavefunctions increases with the corresponding energy in a way that is deeply linked to the de Broglie wavelength rule according to which the kinetic energy increases with the number of nodes of the associated wavelength.

5.2.1 Second-order partial differential equation to be solved

In order to get the expression of the wavefunctions corresponding to the eigenkets of the harmonic Hamiltonian, consider this operator within wave mechanics that reads

$$\hat{H} = \hat{T} + \hat{V}$$

where $\hat{T}$ and $\hat{V}$ are, respectively, the wave mechanical kinetic and potential operators, the first one being given by Eq. (3.51), that is,

$$\hat{T} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial Q^2}$$

and the last one simply by

$$\hat{V} = \tfrac{1}{2} m\omega^2 Q^2$$

According to Eq. (3.60), the Hamiltonian of the harmonic oscillator is, therefore,

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial Q^2} + \frac{1}{2} m\omega^2 Q^2$$

Then, the time-independent Schrödinger equation

$$H\Psi_n(Q) = E_n \Psi_n(Q) \tag{5.112}$$

reads

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2 \Psi_n(Q)}{\partial Q^2}\right) + \frac{1}{2} m\omega^2 Q^2 \Psi_n(Q) = E_n \Psi_n(Q) \tag{5.113}$$

Of course, since the quantum mechanics and the wave mechanics are equivalent, the eigenvalues of the Hamiltonian appearing in Eq. (5.112) are given by Eq. (5.42), that is,

$$E_n = \hbar\omega\left(n + \tfrac{1}{2}\right) \tag{5.114}$$

As a consequence, the eigenvalue equation (5.113) becomes

$$\frac{\hbar^2}{2m}\left(\frac{\partial^2 \Psi_n(Q)}{\partial Q^2}\right) - \left(\frac{m\omega^2}{2} Q^2 - \hbar\omega\left(n + \frac{1}{2}\right)\right)\Psi_n(Q) = 0 \tag{5.115}$$

That is the equation to be solved in order to get the expression of the wavefunction $\Psi_n(Q)$ given by the scalar product

$$\Psi_n(Q) = \langle \{Q\} | \{n\} \rangle$$

its boundary condition being

$$\Psi_n(Q) \to 0 \quad \text{when} \quad Q \to \infty \tag{5.116}$$

Next, perform the following variable change:

$$\xi = \xi^\circ Q \quad \text{with} \quad \xi^\circ = \sqrt{\frac{m\omega}{\hbar}} \tag{5.117}$$

leading to

$$\frac{\partial \xi}{\partial Q} = \xi^\circ \qquad \text{and} \qquad \frac{\partial}{\partial Q} = \frac{\partial}{\partial \xi}\left(\frac{\partial \xi}{\partial Q}\right) = \xi^\circ \frac{\partial}{\partial \xi} \tag{5.118}$$

and thus, using in turn Eq. (5.117), to

$$\frac{\partial^2}{\partial Q^2} = \xi^{\circ 2}\frac{\partial^2}{\partial \xi^2} = \frac{m\omega}{\hbar}\frac{\partial^2}{\partial \xi^2} \tag{5.119}$$

Thereby, using Eqs. (5.117) and (5.119), Eq. (5.115) becomes

$$\frac{\hbar^2}{2m}\frac{m\omega}{\hbar}\left(\frac{\partial^2 \Psi_n(\xi)}{\partial \xi^2}\right) - \left(\frac{m\omega^2}{2}\frac{\hbar}{m\omega}\xi^2 - \left(n + \frac{1}{2}\right)\hbar\omega\right)\Psi_n(\xi) = 0$$

or, after simplifying by $\hbar\omega$

$$\left(\frac{\partial^2\Psi_n(\xi)}{\partial\xi^2}\right) - (\xi^2 - (2n+1))\Psi_n(\xi) = 0 \tag{5.120}$$

with, due to Eq. (5.116), the following boundary condition:

$$\Psi_n(\xi) \to 0 \quad \text{when} \quad \xi \to \infty \tag{5.121}$$

resulting from the fact that the wavefunctions have to be normalized in order to verify that their squared modulus must be a density probability obeying

$$\int_{-\infty}^{+\infty} |\Psi_n(\xi)|^2 d\xi = 1 \tag{5.122}$$

5.2.2 Special solutions of Eq. (5.120)

Now, look at Eq. (5.120) for the lowest state situation corresponding to $n = 0$, that is,

$$\left(\frac{\partial^2\Psi_0(\xi)}{\partial\xi^2}\right) - (\xi^2 - 1)\Psi_0(\xi) = 0 \tag{5.123}$$

with the same boundary condition (5.121). Search for a solution of the form

$$\Psi_0(\xi) = (e^{\pm\xi^2/2}) \tag{5.124}$$

Then, it yields

$$\left(\frac{\partial e^{\pm\xi^2/2}}{\partial\xi}\right) = \pm\xi(e^{\pm\xi^2/2}) \qquad \left(\frac{\partial^2 e^{\pm\xi^2/2}}{\partial\xi^2}\right) = (\xi^2 \pm 1)(e^{\pm\xi^2/2})$$

so that the second partial derivative of the expression (5.124) reads

$$\left(\frac{\partial^2\Psi_0(\xi)}{\partial\xi^2}\right) - (\xi^2 \pm 1)\Psi_0(\xi) = 0 \tag{5.125}$$

Thus, it appears that the two solutions of Eq. (5.123) are verified. But, the boundary condition (5.121) being not compatible with the + solution, the physical solution is necessarily the following one:

$$\Psi_0(\xi) = e^{-\xi^2/2}$$

This last equation is the unnormalized ground-state wavefunction of the Hamiltonian of the harmonic oscillator satisfying Eq. (5.115) with the ground-state energy $\hbar\omega/2$, its normalized form being

$$\Psi_0(\xi) = C_0(e^{-\xi^2/2}) \tag{5.126}$$

where C_0 is the normalization constant of the wavefunction.

The normalization constant C_0 must be such that Eq. (5.122) has to be satisfied. Hence, using Eq. (5.117) in order to return from the dimensionless variable ξ to the dimensioned one Q, the normalization of the ground-state wavefunction (5.126) reads

$$(C_0^2)^{-1} = \int_{-\infty}^{+\infty} \exp\left(-\frac{m\omega}{\hbar}Q^2\right) dQ$$

and, thus, after integration

$$(C_0^2)^{-1} = \sqrt{\frac{\pi\hbar}{m\omega}} \qquad \text{or} \qquad C_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \tag{5.127}$$

5.2.3 Recurrence relation between wavefunctions

Now, in order to pass from the ground-state wavefunction to the excited wavefunctions, use Eq. (5.63), that is,

$$\mathbf{a}^\dagger|\{n\}\rangle = \sqrt{n+1}|\{n+1\}\rangle$$

Then premultiplying both terms by any bra, Hermitian conjugate of some eigenket of the position operator, one obtains

$$\langle\{Q\}|\{n+1\}\rangle = \frac{1}{\sqrt{n+1}}\langle\{Q\}|\mathbf{a}^\dagger|\{n\}\rangle \tag{5.128}$$

or, due to Eq. (5.4), it reads

$$\langle\{Q\}|\{n+1\}\rangle = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{n+1}}\langle\{Q\}|(\xi^\circ\mathbf{Q} - i\zeta^\circ\mathbf{P})|\{n\}\rangle$$

with

$$\xi^\circ = \sqrt{\frac{m\omega}{\hbar}} \qquad \text{and} \qquad \zeta^\circ = \sqrt{\frac{1}{m\hbar\omega}} \tag{5.129}$$

Again, introduce the closure relation over the eigenstates of the position operator:

$$\langle\{Q\}|\{n+1\}\rangle = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{n+1}}\langle\{Q\}|(\xi^\circ\mathbf{Q} - i\zeta^\circ\mathbf{P})\left\{\int_{-\infty}^{+\infty}|\{Q'\}\rangle\langle\{Q'\}|dQ'\right\}|\{n\}\rangle$$

leading to

$$\langle\{Q\}|\{n+1\}\rangle = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{n+1}}\langle\{Q\}|(\xi^\circ\mathbf{Q} - i\zeta^\circ\mathbf{P})\int_{-\infty}^{+\infty}|\{Q'\}\rangle\langle\{Q'\}|\{n\}\rangle dQ'$$

Hence, Eq. (5.128) becomes

$$\Psi_{n+1}(Q) = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{n+1}}\langle\{Q\}|(\xi^\circ\mathbf{Q} - i\zeta^\circ\mathbf{P})\int_{-\infty}^{+\infty}|\{Q'\}\rangle\Psi_n(Q')\,dQ' \tag{5.130}$$

with

$$\Psi_{n+1}(Q) = \langle\{Q\}|\{n+1\}\rangle \qquad \text{and} \qquad \Psi_n(Q') = \langle\{Q'\}|\{n\}\rangle$$

Next, observe that, according to Eqs. (3.50) and (3.52)

$$\langle\{Q\}|\mathbf{P}|\{Q'\}\rangle = -i\hbar\delta(Q-Q')\frac{\partial}{\partial Q}$$

$$\langle\{Q\}|\mathbf{Q}|\{Q'\}\rangle = \delta(Q-Q')Q'$$

As a consequence, using these expressions and the fact that, in wave mechanics, **Q** acts as a scalar Q, Eq. (5.130) transforms to

$$\Psi_{n+1}(Q) = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{n+1}} \left(\xi^\circ Q - \hbar \zeta^\circ \frac{\partial}{\partial Q} \right) \Psi_n(Q) \tag{5.131}$$

Again, in view of Eqs. (5.117) and (5.118) and since [cf., Eq. (5.129)] the following relation between ζ° and ξ° exists

$$\hbar \zeta^\circ = \frac{1}{\xi^\circ}$$

so that Eq. (5.131) takes the final recurrence form

$$\boxed{\Psi_{n+1}(\xi) = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{n+1}} \left(\xi - \frac{\partial}{\partial \xi} \right) \Psi_n(\xi)} \tag{5.132}$$

keeping in mind Eq. (5.117), that is,

$$\xi = \xi^\circ Q$$

5.2.4 Obtaining the lowest wavefunctions

5.2.4.1 First excited wavefunction Now, recall that the ground-state wavefunction (5.126), for reasons that will become apparent, may be formally written

$$\Psi_0(\xi) = C_0 H_0(\xi)(e^{-\xi^2/2}) \tag{5.133}$$

with

$$H_0(\xi) = 1 \tag{5.134}$$

and where C_0 is the normalization constant of the wavefunction. Apply Eq. (5.132) to the ground-state wavefunction (5.133), that is, for $n = 0$

$$\Psi_1(\xi) = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{1}} C_0 \left(\xi - \frac{\partial}{\partial \xi} \right) (e^{-\xi^2/2}) \tag{5.135}$$

The partial derivative with respect to ξ being

$$\frac{\partial}{\partial \xi}(e^{-\xi^2/2}) = -(\xi e^{-\xi^2/2})$$

Eq. (5.135) yields

$$\Psi_1(\xi) = C_1 2(\xi e^{-\xi^2/2}) \tag{5.136}$$

where

$$C_1 = \frac{1}{\sqrt{2}} C_0 = \frac{1}{\sqrt{2}} \left(\frac{m\omega}{\pi \hbar} \right)^{1/4} \tag{5.137}$$

Finally, Eq. (5.136) may be written in a form similar to that of Eq. (5.133):

$$\Psi_1(\xi) = C_1 H_1(\xi) e^{-\xi^2/2} \quad \text{with} \quad H_1(\xi) = 2\xi \tag{5.138}$$

5.2.4.2 Second excited wavefunction Next, in order to get the second excited-state wavefunction, apply Eq. (5.132) to Eq. (5.136), that is

$$\Psi_2(\xi) = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2!}}\left(\xi - \frac{\partial}{\partial\xi}\right)\{C_1 2(\xi e^{-\xi^2/2})\}$$

which reads

$$\Psi_2(\xi) = 2C_2\left(\xi(\xi e^{-\xi^2/2}) - \frac{\partial}{\partial\xi}(\xi e^{-\xi^2/2})\right) \tag{5.139}$$

with, in view of Eq. (5.137),

$$C_2 = \frac{1}{\sqrt{2!}}\left(\frac{1}{\sqrt{2}}\right)C_1 = \frac{1}{\sqrt{2!}}\left(\frac{1}{\sqrt{2}}\right)^2 C_0 \tag{5.140}$$

By derivation one obtains

$$\frac{\partial}{\partial\xi}(\xi e^{-\xi^2/2}) = (1-\xi^2)(e^{-\xi^2/2}) \tag{5.141}$$

so that Eq. (5.139) yields

$$\Psi_2(\xi) = C_2(4\xi^2 - 2)(e^{-\xi^2/2}) \tag{5.142}$$

or

$$\Psi_2(\xi) = C_2 H_2(\xi)(e^{-\xi^2/2}) \quad \text{with} \quad H_2(\xi) = 4\xi^2 - 2 \tag{5.143}$$

5.2.4.3 Third excited wavefunction Again, to get the third excited-state wavefunction, apply Eq. (5.132) a third time to Eq. (5.142), leading to

$$\Psi_3(\xi) = C_3\left(\xi - \frac{\partial}{\partial\xi}\right)\{(4\xi^2 - 2)e^{-\xi^2/2}\} \tag{5.144}$$

with

$$C_3 = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{3!}}C_2 = \frac{1}{\sqrt{3!}}\left(\frac{1}{\sqrt{2}}\right)^3 C_0$$

which transforms to

$$\Psi_3(\xi) = C_3\left((4\xi^3 - 2\xi)(e^{-\xi^2/2}) - \frac{\partial}{\partial\xi}\{(4\xi^2 - 2)(e^{-\xi^2/2})\}\right)$$

Then, obtaining by differentiation

$$\frac{\partial}{\partial\xi}(4\xi^2 - 2)(e^{-\xi^2/2}) = (8\xi - (4\xi^2 - 2)\xi)(e^{-\xi^2/2})$$

the wavefunction becomes

$$\Psi_3(\xi) = C_3(8\xi^3 - 12\xi)(e^{-\xi^2/2}) \tag{5.145}$$

or

$$\Psi_3(\xi) = C_3 H_3(\xi)(e^{-\xi^2/2}) \quad \text{with} \quad H_3(\xi) = 8\xi^3 - 12\xi \tag{5.146}$$

5.2.4.4 nth excited wavefunction Note that the functions $H_k(\xi)$ (5.134), (5.138), (5.143), and (5.146) are the first *Hermite polynomials*. Besides, proceeding in a similar way for the higher excited wavefunctions, one would obtain now

$$\Psi_n(\xi) = C_n H_n(\xi)(e^{-\xi^2/2}) \tag{5.147}$$

with

$$C_n = \frac{1}{\sqrt{n!}}\left(\frac{1}{\sqrt{2}}\right)^n C_0$$

or, in view of Eq. (5.127),

$$C_n = \frac{1}{\sqrt{n!}}\left(\frac{1}{\sqrt{2}}\right)^n \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \tag{5.148}$$

and with, for $n = 4$, 5, and 6,

$$\begin{aligned} H_4(\xi) &= 16\xi^4 - 48\xi^2 + 12 \\ H_5(\xi) &= 32\xi^5 - 160\xi^3 + 120\xi \\ H_6(\xi) &= 64\xi^6 - 480\xi^4 + 720\xi^2 - 120 \end{aligned} \tag{5.149}$$

5.2.4.5 Pictorial representation of the lowest wavefunctions The five lowest wavefunctions and energy levels are pictured in Fig. 5.1a, whereas the corresponding wavefunctions and energy levels of the particle-in-a-box model are shown in Fig. 5.1b.

Observe that, in agreement with Eqs. (5.126), (5.138), (5.143), (5.146), and (5.147), the parity of the wavefunctions $\Psi_n(\xi)$ is alternatively changing, those characterized by *even* quantum numbers n, being *gerade* and the other ones, characterized by *odd* quantum numbers n, being *ungerade*. Observe also that this figure illustrates the node number increase of the wavefunctions when enhancing the quantum number and thus the energy, an evolution that is almost similar to that encountered in the particle-in-a-box model, as may be verified by inspection of Fig. 5.1(b).

5.3 DYNAMICS

In the previous sections we found many important results dealing with static situations of quantum harmonic oscillators. We have now to search the dynamics of these oscillators via the time dependence of the mean values of the basic operators averaged over the eigenkets of the harmonic oscillator Hamiltonian. To get these time dependent average values, it will be suitable to work within the Heisenberg picture (where the operators depend on time whereas the kets remain constant).

5.3.1 Heisenberg equations for oscillator operators

5.3.1.1 Ladder operators Heisenberg equations Look, therefore, at the Heisenberg equation governing the dynamical equation of the lowering operator $\mathbf{a}(t)$, which, according to Eq. (3.94), reads in the present situation

$$i\hbar\left(\frac{d\mathbf{a}(t)}{dt}\right) = [\mathbf{a}(t), \mathbf{H}] \tag{5.150}$$

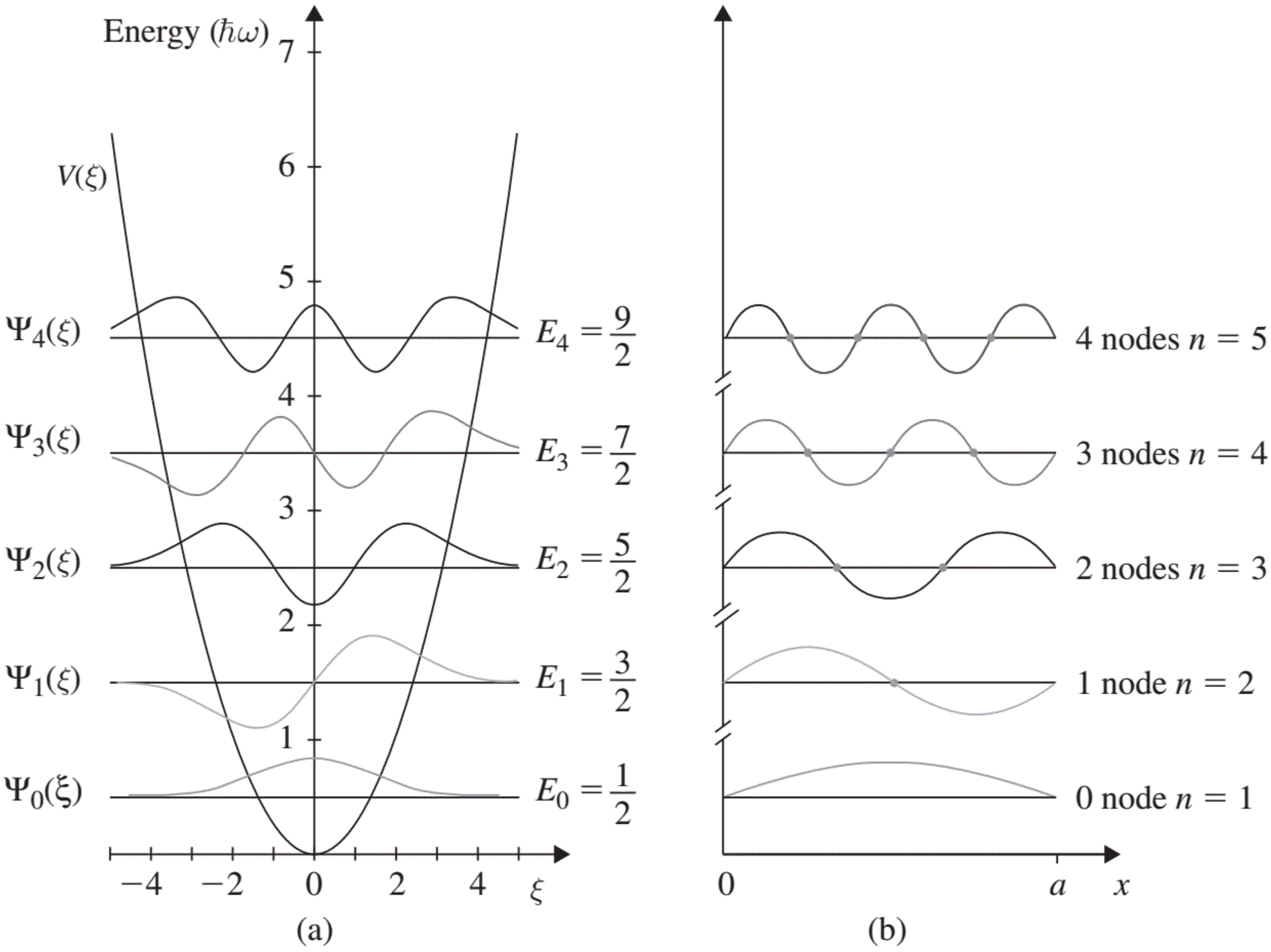


Figure 5.1 Five lowest energy levels and wavefunctions. Comparison between (a) quantum harmonic oscillator and (b) particle-in-a-box model.

which, with the help of Eq. (5.9) defining the Hamiltonian, becomes

$$i\hbar\left(\frac{d\mathbf{a}(t)}{dt}\right) = \hbar\omega\left[\mathbf{a}(t), \left(\mathbf{a}(t)^{\dagger}\mathbf{a}(t) + \frac{1}{2}\right)\right]$$

or

$$i\left(\frac{d\mathbf{a}(t)}{dt}\right) = \omega(\mathbf{a}(t)\mathbf{a}(t)^{\dagger}\mathbf{a}(t) - \mathbf{a}(t)^{\dagger}\mathbf{a}(t)\mathbf{a}(t))$$

and thus

$$\left(\frac{d\mathbf{a}(t)}{dt}\right) = -i\omega[\mathbf{a}(t), \mathbf{a}(t)^{\dagger}]\mathbf{a}(t)$$

Again, the commutation rule (5.5) holds for any time, so that

$$[\mathbf{a}(t), \mathbf{a}(t)^{\dagger}] = 1$$

and thereby

$$\left(\frac{d\mathbf{a}(t)}{dt}\right) = -i\omega\mathbf{a}(t)$$

Hence, after integration, that gives

$$\boxed{\mathbf{a}(t) = \mathbf{a}(0)e^{-i\omega t}} \tag{5.151}$$

the Hermitian conjugate of which being

$$\boxed{\mathbf{a}^\dagger(t) = \mathbf{a}^\dagger(0)e^{i\omega t}} \tag{5.152}$$

Now, observe that when dealing with 3D oscillators, the latter results read

$$\mathbf{a}_k(t) = \mathbf{a}_k(0)e^{-i\omega_k t} \qquad \text{and} \qquad \mathbf{a}_k^\dagger(t) = \mathbf{a}_k^\dagger(0)e^{i\omega_k t}$$

with k standing for the x, y, and z components.

5.3.1.2 Position and momentum Heisenberg equations In view of Eq. (5.6), and owing to Eqs. (5.151) and (5.152), the time dependence of the quantum oscillator position coordinate appears to be

$$\mathbf{Q}(t) = \sqrt{\frac{\hbar}{2m\omega}}(\mathbf{a}^\dagger e^{i\omega t} + \mathbf{a}e^{-i\omega t}) \tag{5.153}$$

Passing then from the imaginary exponentials to the corresponding sine and cosine functions leads to

$$\mathbf{Q}(t) = \sqrt{\frac{\hbar}{2m\omega}}(\mathbf{a}^\dagger \cos\omega t + i\mathbf{a}^\dagger \sin\omega t + \mathbf{a}\cos\omega t - i\mathbf{a}\sin\omega t)$$

or

$$\mathbf{Q}(t) = \sqrt{\frac{\hbar}{2m\omega}}((\mathbf{a}^\dagger + \mathbf{a})\cos\omega t + i(\mathbf{a}^\dagger - \mathbf{a})\sin\omega t) \tag{5.154}$$

so that, due to Eqs. (5.6) and (5.7), we have

$$\boxed{\mathbf{Q}(t) = \mathbf{Q}(0)\cos\omega t + \frac{1}{m\omega}\mathbf{P}(0)\sin\omega t} \tag{5.155}$$

with, respectively,

$$\mathbf{P}(0) = i\sqrt{\frac{\hbar m\omega}{2}}(\mathbf{a}^\dagger - \mathbf{a}) \tag{5.156}$$

$$\mathbf{Q}(0) = \sqrt{\frac{\hbar m\omega}{2}}(\mathbf{a}^\dagger + \mathbf{a}) \tag{5.157}$$

Now, consider the commutator of the position coordinate operators at different times, that is,

$$\begin{aligned}[\mathbf{Q}(t), \mathbf{Q}(t')] &= \frac{\hbar}{2m\omega}((\mathbf{a}^\dagger e^{i\omega t} + \mathbf{a}e^{-i\omega t})(\mathbf{a}^\dagger e^{i\omega t'} + \mathbf{a}e^{-i\omega t'}) - (\mathbf{a}^\dagger e^{i\omega t'} + \mathbf{a}e^{-i\omega t'}) \\ &\quad \times (\mathbf{a}^\dagger e^{i\omega t} + \mathbf{a}e^{-i\omega t}))\end{aligned}$$

which, after performing the products and simplification gets

$$[\mathbf{Q}(t), \mathbf{Q}(t')] = \frac{\hbar}{2m\omega}(\mathbf{a}^\dagger\mathbf{a}(e^{i\omega(t-t')} - e^{-i\omega(t-t')}) + \mathbf{a}\mathbf{a}^\dagger(e^{-i\omega(t-t')} - e^{i\omega(t-t')}))$$

and, thus, after coming back to the sine function, we have

$$[\mathbf{Q}(t), \mathbf{Q}(t')] = \frac{\hbar}{2m\omega}(\mathbf{a}^\dagger \mathbf{a} 2i \sin(\omega(t-t')) - \mathbf{a}\mathbf{a}^\dagger 2i \sin(\omega(t-t')))$$

Then, with the help of the commutation rule (5.5), this last result reduces, after simplification, to

$$\boxed{[\mathbf{Q}(t), \mathbf{Q}(t')] = -i\frac{\hbar}{m\omega}\sin(\omega(t-t'))} \tag{5.158}$$

We emphasizes that this commutator differs from zero, that is,

$$[\mathbf{Q}(t), \mathbf{Q}(t')] \neq 0$$

On the other hand, the time dependence of the momentum, which reads in view of Eq. (5.7)

$$\mathbf{P}(t) = i\sqrt{\frac{\hbar m\omega}{2}}(\mathbf{a}^\dagger e^{i\omega t} - \mathbf{a}e^{-i\omega t}) \tag{5.159}$$

transforms after passing to the trigonometric functions and using Eq. (5.7)

$$\mathbf{P}(t) = i\sqrt{\frac{\hbar m\omega}{2}}((\mathbf{a}^\dagger - \mathbf{a})\cos\omega t + i(\mathbf{a}^\dagger + \mathbf{a})\sin\omega t)$$

so that

$$\mathbf{P}(t) = i\sqrt{\frac{\hbar m\omega}{2}}(\mathbf{a}^\dagger - \mathbf{a})\cos\omega t - \sqrt{\frac{\hbar m\omega}{2}}(\mathbf{a}^\dagger + \mathbf{a})\sin\omega t \tag{5.160}$$

and, therefore, due to Eqs. (5.156) and (5.157), leads to

$$\boxed{\mathbf{P}(t) = \mathbf{P}(0)\cos\omega t - m\omega\mathbf{Q}(0)\sin\omega t} \tag{5.161}$$

Hence, the commutator of $\mathbf{P}$ at different times is not zero.

5.3.2 Time dependence of mean values averaged on Hamiltonian eigenkets

Recall that operators, unlike average values, are not directly connected with experience. Thus, it is now necessary to study the dependence of the average values of the operators defined by Eq. (5.155) or (5.154) and by Eq. (5.160) or (5.161).

5.3.2.1 Average Values of Q(t) and P(t) First, consider the average values of the momentum and position coordinates on the eigenkets of the harmonic Hamiltonian. According to Eq. (5.154), that of the position operator reads

$$\langle\{n\}|\mathbf{Q}(t)|\{n\}\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\langle\{n\}|\mathbf{a}^\dagger|\{n\}\rangle e^{i\omega t} + \langle\{n\}|\mathbf{a}|\{n\}\rangle e^{-i\omega t})$$

Then, keeping in mind Eq. (5.53) and its Hermitian conjugate, that is,

$$\mathbf{a}|\{n\}\rangle = \sqrt{n}|\{n-1\}\rangle \qquad \text{and} \qquad \langle\{n\}|\mathbf{a}^\dagger = \sqrt{n}\langle\{n-1\}|$$

the average value of the position coordinate becomes

$$\langle\{n\}|\mathbf{Q}(t)|\{n\}\rangle = \frac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}(\langle\{n-1\}|\{n\}\rangle e^{i\omega t} + \langle\{n\}|\{n-1\}\rangle e^{-i\omega t})$$

Thus, owing to the orthonormality of the eigenkets of the harmonic oscillator Hamiltonian, we have

$$\langle\{n\}|\mathbf{Q}(t)|\{n\}\rangle = 0 \tag{5.162}$$

Now, proceeding in the same way for the momentum coordinate by the aid of Eq. (5.159), it may be easily shown that

$$\langle\{n\}|\mathbf{P}(t)|\{n\}\rangle = 0 \tag{5.163}$$

Note that the results (5.162) may be also found by the aid of the wave mechanics. In this quantum picture, the left-hand side of Eq. (5.162) reads

$$\langle\{n\}|\mathbf{Q}(t)|\{n\}\rangle = \int_{-\infty}^{+\infty} \Psi_n(Q)Q(t)\Psi_n(Q)\,dQ$$

where

$$\Psi_n(Q) \equiv \langle\{Q\}|\{n\}\rangle$$

Now, since Q commutes with $\Psi_n(Q)$ and irrespective of the time t, which may be omitted, the average value reduces to

$$\langle\{n\}|\mathbf{Q}|\{n\}\rangle = \int_{-\infty}^{+\infty} \Psi_n(Q)^2 Q\,dQ$$

Now, observe that, whatever $\Psi_n(Q)$, the parity of its square is always even, whereas that of Q is odd. Hence, the parity of the integrand, which is the product of that of $\Psi_n(Q)^2$ by that of Q, is always odd, so that the integral involving this integrand must be necessarily zero, the contribution from 0 to $+\infty$ being canceled by that from $-\infty$ to 0, that is,

$$\int_{-\infty}^{+\infty} \Psi_n(Q)^2 Q\,dQ = 0$$

On the other hand, in the Schrödinger picture, Eq. (5.163) takes the form

$$\langle\{n\}(t)|\mathbf{P}|\{n\}(t)\rangle = 0$$

Then, inserting a closure relation over the basis $\{|\{Q\}\rangle\}$ before and after $\mathbf{P}$, it transforms by the aid of Eq. (3.50) into

$$-i\hbar \int_{-\infty}^{+\infty} \Psi_n(Q)^* \frac{\partial}{\partial Q}\Psi_n(Q)\,dQ = 0$$

Of course, Eqs. (5.162) and (5.163) may be immediately extended to the 3D oscillator to give for the three Cartesian components $k = x, y$, and z:

$$\langle\{n\}|\mathbf{Q}_k(t)|\{n\}\rangle = \langle\{n\}|\mathbf{P}_k(t)|\{n\}\rangle = 0$$

5.3.2.2 Average values of V(t) and T(t) Now, consider the time dependence of the average potential energy. In the Heisenberg representation, this average value reads

$$\langle\{n\}|\mathbf{V}(t)|\{n\}\rangle = \tfrac{1}{2}m\omega^2\langle\{n\}|\mathbf{Q}(t)^2|\{n\}\rangle \tag{5.164}$$

Next, the right-hand-side average value may be expressed in terms of the raising and lowering operators by the aid of Eq. (5.153):

$$\langle\{n\}|\mathbf{Q}(t)^2|\{n\}\rangle = \frac{\hbar}{2m\omega}\langle\{n\}|(\mathbf{a}^\dagger e^{i\omega t} + \mathbf{a}e^{-i\omega t})^2|\{n\}\rangle \tag{5.165}$$

By expansion of the square involved on the right-hand side, one finds

$$(\mathbf{a}^\dagger e^{i\omega t} + \mathbf{a}e^{-i\omega t})^2 = (\mathbf{a}^\dagger)^2 e^{2i\omega t} + (\mathbf{a})^2 e^{-2i\omega t} + \mathbf{a}^\dagger\mathbf{a} + \mathbf{a}\mathbf{a}^\dagger \tag{5.166}$$

or, after using the usual commutation rule (5.5) between the raising and lowering operators, Eq. (5.165) becomes

$$\langle\{n\}|\mathbf{Q}(t)^2|\{n\}\rangle = \frac{\hbar}{2m\omega}\langle\{n\}|((\mathbf{a}^\dagger)^2 e^{2i\omega t} + (\mathbf{a})^2 e^{-2i\omega t} + 2\mathbf{a}^\dagger\mathbf{a} + 1)|\{n\}\rangle$$

By inserting this result into Eq. (5.164), the average value of the potential energy is

$$\langle\{n\}|\mathbf{V}(t)|\{n\}\rangle = \tfrac{1}{4}\hbar\omega\langle\{n\}|((\mathbf{a}^\dagger)^2 e^{2i\omega t} + (\mathbf{a})^2 e^{-2i\omega t} + 2\mathbf{a}^\dagger\mathbf{a} + 1)|\{n\}\rangle$$

so that, owing to Eqs. (5.53) and (5.63),

$$\langle\{n\}|(\mathbf{a})^2|\{n\}\rangle = \sqrt{n}\sqrt{n-1}\langle\{n\}|\{n-2\}\rangle = 0$$

$$\langle\{n\}|(\mathbf{a}^\dagger)^2|\{n\}\rangle = \sqrt{n+2}\sqrt{n+1}\langle\{n\}|\{n+2\}\rangle = 0$$

Now, due to Eq. (5.40)

$$\langle\{n\}|(\mathbf{a}^\dagger\mathbf{a})|\{n\}\rangle = n\langle\{n\}|\{n\}\rangle = n$$

Hence, using these equations, the average value of the potential energy becomes

$$\langle\{n\}|\mathbf{V}(t)|\{n\}\rangle = \tfrac{1}{2}\hbar\omega\left(n + \tfrac{1}{2}\right) = const. \tag{5.167}$$

Hence, the average potential energy remains constant throughout time and equal to half the energy when the oscillator is in any eigenstate $|\{n\}\rangle$ of its Hamiltonian as can be directly obtained from the virial theorem.

In a similar way, one would find for the mean kinetic energy averaged over an Hamiltonian eigenket

$$\langle\{n\}|\left(\frac{\mathbf{P}(t)^2}{2m}\right)|\{n\}\rangle = \frac{1}{2}\hbar\omega\left(n + \frac{1}{2}\right) = const. \tag{5.168}$$

with

$$\mathbf{P}(t)^2 = -\frac{\hbar m\omega}{2}(\mathbf{a}^\dagger e^{i\omega t} - \mathbf{a}e^{-i\omega t})^2$$

Of course, results (5.167) and (5.168) may be generalized to the x, y, and z components of 3D harmonic oscillators, leading one to write for each component

$$\langle\{n\}_k|\mathbf{V}_k(t)|\{n\}_k\rangle = \langle\{n\}_k|\left(\frac{\mathbf{P}_k(t)^2}{2m}\right)|\{n\}_k\rangle = \frac{1}{2}\hbar\omega_k\left(n_k + \frac{1}{2}\right)$$

5.4 BOSON AND FERMION OPERATORS

As observed above, the non-Hermitian annihilation and creation operators $\mathbf{a}$ and $\mathbf{a}^\dagger$ are very important in the quantum approach of harmonic oscillators. They are often called *Boson operators* because they are related to the *Bose–Einstein statistics* where the number of particles inside a nondegenerate energy level is arbitrary. On the other hand, in the study of double-energy-level systems one meets non-Hermitian operators $\mathbf{a}_f$ and $\mathbf{a}_f^\dagger$, which play for these simple systems a role presenting analogies with those of $\mathbf{a}$ and $\mathbf{a}^\dagger$ in the quantum oscillators theory. (In all this section, the subscript f refers to Fermions and the corresponding double-energy-level systems.) These new operators are called *Fermion operators* because they are related to the *Fermi–Dirac statistics* where the number of particles inside a nondegenerate energy level can be only either zero or unity. Owing to the importance of Fermion operators description in many double-energy-level system studies, and of their deep analogy with the Boson operators, it is convenient to treat here the Fermion operators.

Consider a two-energy-level system, the Hamiltonian eigenvalue equation of which is

$$\mathbf{H}|(k)_f\rangle = E_k|(k)_f\rangle \quad \text{with} \quad k = 0, 1$$

where E_k are the two eigenvalues, that is, E_0 and E_1, with $E_1 > E_0$, whereas $|(k)_f\rangle$ are the corresponding eigenkets $|(0)_f\rangle$ and $|(1)_f\rangle$ of $\mathbf{H}$, the first one being the ground state and the last one the excited state as illustrated in Fig. 5.2.

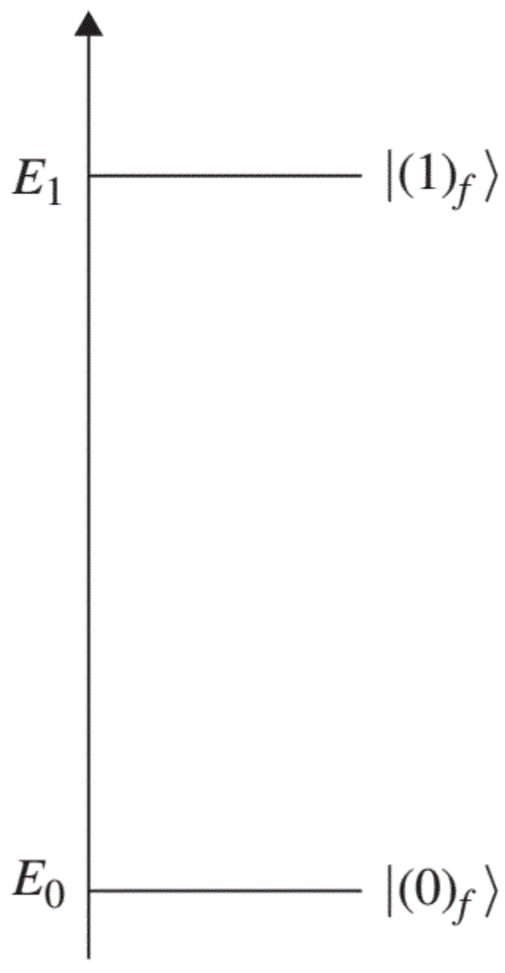


Figure 5.2 Fermion energy levels and corresponding eigenkets.

When normalized and orthogonal, these states read

$$\langle (1)_f | (1)_f \rangle = \langle (0)_f | (0)_f \rangle = 1 \tag{5.169}$$

$$\langle (1)_f | (0)_f \rangle = 0 \tag{5.170}$$

Now, by analogy with the Boson operators $\mathbf{a}^\dagger$ and $\mathbf{a}$, introduce two kinds of non-Hermitian operators $\mathbf{a}_f^\dagger$ and $\mathbf{a}_f$, the *Fermion operators*, obeying the following anticommutation rules:

$$[\mathbf{a}_f, \mathbf{a}_f]_+ = [\mathbf{a}_f^\dagger, \mathbf{a}_f^\dagger]_+ = 0 \tag{5.171}$$

$$[\mathbf{a}_f, \mathbf{a}_f^\dagger]_+ = 1 \tag{5.172}$$

where the anticommutator is defined by

$$[\mathbf{A}, \mathbf{B}]_+ \equiv \mathbf{AB} + \mathbf{BA}$$

The two Fermion operators are assumed to act on the kets $|(1)_f\rangle$ and $|(0)_f\rangle$ according to

$$\mathbf{a}_f |(1)_f\rangle = |(0)_f\rangle \tag{5.173}$$

$$\mathbf{a}_f^\dagger |(0)_f\rangle = |(1)_f\rangle \tag{5.174}$$

$$\mathbf{a}_f |(0)_f\rangle = 0 \tag{5.175}$$

and

$$\mathbf{a}_f^\dagger |(1)_f\rangle = 0 \tag{5.176}$$

Now, by analogy with the Hermitian number occupation operator (5.12) of Boson operators, introduce here the Hermitian operators defined by

$$\mathbf{N}_f = \mathbf{a}_f^\dagger \mathbf{a}_f \quad \text{with} \quad \mathbf{N}_f = \mathbf{N}_f^\dagger \tag{5.177}$$

since

$$(\mathbf{a}_f^\dagger \mathbf{a}_f)^\dagger = \mathbf{a}_f^\dagger \mathbf{a}_f$$

Then, owing to Eq. (5.177), the action of $\mathbf{N}_f$ on the excited state reads

$$\mathbf{N}_f |(1)_f\rangle = \mathbf{a}_f^\dagger \mathbf{a}_f |(1)_f\rangle$$

or, owing to Eq. (5.173),

$$\mathbf{N}_f |(1)_f\rangle = \mathbf{a}_f^\dagger |(0)_f\rangle$$

and thus, due to Eq. (5.174),

$$\mathbf{N}_f |(1)_f\rangle = 1 |(1)_f\rangle \tag{5.178}$$

On the other hand, the action of $\mathbf{N}_f$ on the ground state reads

$$\mathbf{N}_f |(0)_f\rangle = \mathbf{a}_f^\dagger \mathbf{a}_f |(0)_f\rangle$$

which, according to Eq. (5.175), reads

$$\mathbf{N}_f|(0)_f\rangle = 0 \tag{5.179}$$

Equations (5.178) and (5.179) may be viewed as corresponding to the eigenvalue equation (5.75), whereas Eqs. (5.173) and (5.174) may be put into correspondence with Eq. (5.80). Moreover, the anticommutation rules (5.172) and (5.171) dealing with the Fermion operators are in correspondence with the commutation rule of the Boson operators (5.77) and (5.78). Finally, the Hermitian operator $\mathbf{N}_f$ defined by Eq. (5.177) is the *Fermion operator analog* of the number occupation operator $\mathbf{N}$ (5.76) involving Boson operators.

It is now of interest to give matrix representations of the Fermion operators. For this purpose, it is convenient to represent the two orthogonal kets $|(0)_f\rangle$ and $|(1)_f\rangle$, by two orthonormalized column vectors of dimension 2 according to

$$|(0)_f\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad \text{and} \qquad |(1)_f\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{5.180}$$

which satisfy the orthonormality properties, since one obtains, respectively,

$$\langle(1)_f|(1)_f\rangle = (1 \quad 0)\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1$$

$$\langle(0)_f|(0)_f\rangle = (0 \quad 1)\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 1$$

$$\langle(1)_f|(0)_f\rangle = (1 \quad 0)\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0$$

Then, in order to be compatible with Eqs. (5.171)–(5.179), the matrix representations of the two Fermion operators $\mathbf{a}_f$ and $\mathbf{a}_f^\dagger$ of the Hermitian operator $\mathbf{N}_f$ have to be chosen in such a way as

$$\boxed{\mathbf{a}_f} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad \text{and} \qquad \boxed{\mathbf{a}_f^\dagger} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{5.181}$$

These matrix representations, which may be compared to those of the Boson operators $\mathbf{a}$ and $\mathbf{a}^\dagger$ given by Eq. (5.81), satisfy, as required, the anticommutation relation (5.172) because

$$[\mathbf{a}_f, \mathbf{a}_f^\dagger]_+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

leading after matrix multiplication to

$$[\mathbf{a}_f, \mathbf{a}_f^\dagger]_+ = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \boxed{\mathbf{1}}$$

In the same way, the matrix representation of the anticommutator of $\mathbf{a}_f$ with itself, as required by (5.171), reads,

$$[\mathbf{a}_f, \mathbf{a}_f]_+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \boxed{\mathbf{0}}$$

One would find in a similar way that the anticommutator of $\mathbf{a}_f^\dagger$ with itself is also zero as required by (5.171). Moreover, using Eqs. (5.181), the matrix representation of the Hermitian operator $\boxed{\mathbf{N}_f}$ defined by Eq. (5.177) is

$$\boxed{\mathbf{N}_f} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{5.182}$$

Moreover, using Eqs. (5.180) and (5.182), the matrix representation of the action of the operator $\boxed{\mathbf{N}_f}$ on $|(1)_f\rangle$ and $|(0)_f\rangle$, reads

$$\boxed{\mathbf{N}_f}\,|(1)_f\rangle = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{and} \qquad \boxed{\mathbf{N}_f}\,|(0)_f\rangle = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

so it appears that Eqs. (5.178) and (5.179) are satisfied, since the two expressions above yield, respectively,

$$\boxed{\mathbf{N}_f}\,|(1)_f\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |(1)_f\rangle$$

and

$$\boxed{\mathbf{N}_f}\,|(0)_f\rangle = \begin{pmatrix} 0 \\ 0 \end{pmatrix} = 0$$

On the other hand, the matrix representation of the actions of the two Fermion operators $\mathbf{a}_f$ and $\mathbf{a}_f^\dagger$ on the two states, lead, respectively, as required by Eqs. (5.173)–(5.176), to

$$\mathbf{a}_f|(1)_f\rangle = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |(0)_f\rangle$$

$$\mathbf{a}_f|(0)_f\rangle = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} = 0$$

$$\mathbf{a}_f^\dagger|(1)_f\rangle = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} = 0$$

$$\mathbf{a}_f^\dagger|(0)_f\rangle = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |(1)_f\rangle$$

5.5 CONCLUSION

In the present chapter devoted to the study of single isolated quantum harmonic oscillators, we have obtained many important results. Among them, there are the eigenvalues of the Hamiltonian and the action of the raising and lowering operators on the orthonormalized eigenvectors of the Hamiltonian, which constitute a basis in

the state space. We have also considered the time evolution of the average values performed over these kets, of different observables dealing with the oscillators. All these important results, which are convenient to know, are collected in the following list:

Relations between ladder operators and position and momentum operators
$\mathbf{Q}=\sqrt{\frac{\hbar}{2m\omega}}(\mathbf{a}^\dagger+\mathbf{a})$ and $\mathbf{P}=i\sqrt{\frac{m\hbar\omega}{2}}(\mathbf{a}^\dagger-\mathbf{a})$ $[\mathbf{a},\mathbf{a}^\dagger]=1$
Eigenvalue equation of the harmonic Hamiltonian:
$\mathbf{H}=\hbar\omega\left(\mathbf{a}^\dagger\mathbf{a}+\frac{1}{2}\right)$ $\hbar\omega\left(\mathbf{a}^\dagger\mathbf{a}+\frac{1}{2}\right)\lvert\{n\}\rangle=\hbar\omega\left(n+\frac{1}{2}\right)\lvert\{n\}\rangle$ with $n=0,1,2,3,\ldots$ $\langle\{n\}\lvert\{m\}\rangle=\delta_{nm}$
Action of the ladder operators on the harmonic Hamiltonian eigenkets:
$\mathbf{a}\lvert\{n\}\rangle=\sqrt{n}\lvert\{n-1\}\rangle$ and $\mathbf{a}^\dagger\lvert\{n\}\rangle=\sqrt{n+1}\lvert\{n+1\}\rangle$
Time dependence of the Boson operators:
$\mathbf{a}(t)=\mathbf{a}(0)e^{-i\omega t}$ and $\mathbf{a}^\dagger(t)=\mathbf{a}^\dagger(0)e^{i\omega t}$

Finally, the analytical expressions for the vibrational wavefunctions associated with the quantized energy levels exist, which yield some knowledge concerning the corresponding somewhat "esoteric" kets.

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CHAPTER 6

COHERENT STATES AND TRANSLATION OPERATORS

INTRODUCTION

The previous chapter focused essentially on the stationary orthonormal eigenstates of the harmonic oscillator Hamiltonian, which form a basis of the state space. There exist other states dealing with harmonic oscillators that also play a very fundamental role in the area of quantum harmonic oscillators. They are the *coherent states* $|\{\alpha\}\rangle$, which are, by definition, the eigenkets of the lowering operator $\mathbf{a}$. They are of great importance for numerous reasons. The first one is that the coherent states, whatever they are, minimize the Heisenberg uncertainty relations. Another one, which is deeply connected to the first one, is that the harmonic oscillator operators, when averaged on it, lead to behaviors that are more and more classical when the eigenvalue α corresponding to the eigenket $|\{\alpha\}\rangle$ is increasing. In addition, they are good simple examples of how the formalism of quantum mechanics operates. Moreover, since they are the eigenkets of a non-Hermitian operator, they illustrate that, unlike the number occupation operator, they do not necessarily admit real eigenvalues and furthermore are continuous and nonorthogonal. Moreover, they play a fundamental role in the area of the quantum theory of light, the average values of the electric field operators performed on them, being reached via the corresponding classical fields. For all these reasons, coherent states now merit study.

Thus, the present chapter will begin by deducing its definition, the expansion of a coherent state on the eigenkets of the number occupation operator. Then, the scalar product between two coherent states will be calculated. The chapter will continue by proving that the Heisenberg uncertainty relation is always minimal for coherent states. Then, it will be shown that coherent states may be generated by the action of the translation operator. One section concerns the time dependence of coherent states. Thus, it will be possible to obtain the wave representation of coherent states and of their time dependence. In another section, it will be also possible to calculate by the aid of the translation operator, the Franck–Condon factors, that is, the scalar products between any eigenfunction of the harmonic oscillator Hamiltonian and another one that has been translated with respect to the first one. The chapter ends with the quest for the energy levels of driven harmonic oscillators, which are deeply connected to the properties of coherent states and of translation operators. This is the opportunity

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to test numerically approximate approaches of these levels through truncated matrix representations of the driven oscillator Hamiltonian in the basis of the eigenkets of the harmonic oscillator.

6.1 COHERENT-STATE PROPERTIES

6.1.1 Definition and expansion within Hamiltonian eigenkets basis

By definition, coherent states $|\{\alpha\}\rangle$ are the eigenkets of the lowering $\mathbf{a}$ operator, obeying therefore

$$\mathbf{a}|\{\alpha\}\rangle = \alpha|\{\alpha\}\rangle \tag{6.1}$$

where α are the corresponding eigenvalues, the Hermitian conjugate of which is

$$\langle\{\alpha\}|\mathbf{a}^\dagger = \alpha^*\langle\{\alpha\}| \tag{6.2}$$

Observe that, since $\mathbf{a}$ is not Hermitian, its eigenvalues are not necessarily real and different coherent states are not necessarily orthogonal. An important information dealing with coherent states is contained in their expansion over the eigenkets of the occupation number operator, that is, of the harmonic Hamiltonian. Keeping in mind the eigenvalue equation (5.40), that is,

$$\mathbf{a}^\dagger\mathbf{a}|\{n\}\rangle = n|\{n\}\rangle$$

with, of course, since $\mathbf{a}^\dagger\mathbf{a}$ is Hermitian,

$$\mathbf{1} = \sum_{n=0}^{\infty} |\{n\}\rangle\langle\{n\}| \qquad \text{and} \qquad \langle\{m\}|\{n\}\rangle = \delta_{mn} \tag{6.3}$$

In order to get the expansion of a coherent state on this basis $\{|\{n\}\rangle\}$, introduce the unity operator resulting from the closure relation as follows:

$$|\{\alpha\}\rangle = \sum_{n=0}^{\infty} |\{n\}\rangle\langle\{n\}|\{\alpha\}\rangle$$

so that

$$|\{\alpha\}\rangle = \sum_{n=0}^{\infty} C_n(\alpha)|\{n\}\rangle \tag{6.4}$$

where $C_n(\alpha)$ is the scalar product given by

$$C_n(\alpha) = \langle\{n\}|\{\alpha\}\rangle$$

On the other hand, observe that, by action on the left of $\mathbf{a}$ on both sides of Eq. (6.4), one gets

$$\mathbf{a}|\{\alpha\}\rangle = \sum_{n=0}^{\infty} C_n(\alpha)\mathbf{a}|\{n\}\rangle$$

Next, using Eq. (5.53) in order to find the expression of the right-hand side of this last equation, one finds

$$\mathbf{a}|\{\alpha\}\rangle = \sum_{n=0}^{\infty} C_n(\alpha))\sqrt{n}|\{n-1\}\rangle$$

Again, using eigenvalue equation (6.1) we have

$$\alpha|\{\alpha\}\rangle = \sum_{n=0}^{\infty} C_n(\alpha)\sqrt{n}|\{n-1\}\rangle$$

and after using Eq. (6.4) for the left-hand side of this last equation, one gets

$$\alpha \sum_{n=0}^{\infty} C_n(\alpha)|\{n\}\rangle = \sum_{n=0}^{\infty} C_n(\alpha)\sqrt{n}|\{n-1\}\rangle \tag{6.5}$$

Now, observe that the first term involved on the right-hand side of Eq. (6.5) corresponding to $n=0$ is zero since no eigenkets of the harmonic oscillator Hamiltonian under $|\{0\}\rangle$ exist. Thus, performing the following variable change

$$n \to n+1$$

Eq. (6.5) reads

$$\alpha \sum_{n=0}^{\infty} C_n(\alpha)|\{n\}\rangle = \sum_{n=0}^{\infty} C_{n+1}(\alpha)\sqrt{n+1}|\{n\}\rangle$$

Since this last expression must be true for each term of the sum, the following relation must be verified:

$$C_{n+1}(\alpha)\sqrt{n+1} = \alpha C_n(\alpha) \tag{6.6}$$

which yields for $n=0$

$$\sqrt{1}C_1(\alpha) = \alpha C_0(\alpha) \tag{6.7}$$

and for $n=1$

$$\sqrt{2}C_2(\alpha) = \alpha C_1(\alpha)$$

Then, inserting in this last result Eq. (6.7), one obtains

$$C_2(\alpha) = \frac{\alpha^2}{\sqrt{2}} C_0(\alpha) \tag{6.8}$$

Moreover, for $n=2$, Eq. (6.6) gives

$$\sqrt{3}C_3(\alpha) = \alpha C_2(\alpha)$$

which, using Eq. (6.8) leads to

$$C_3(\alpha) = \frac{\alpha^3}{\sqrt{3}\sqrt{2}} C_0(\alpha) \tag{6.9}$$

Hence, one obtains by recurrence from Eqs. (6.7)–(6.9)

$$C_n(\alpha) = \frac{\alpha^n}{\sqrt{n!}} C_0(\alpha) \tag{6.10}$$

Allowing to transform the expansion (6.4) of the coherent state into

$$|\{\alpha\}\rangle = C_0(\alpha) \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |\{n\}\rangle \tag{6.11}$$

Furthermore, in order to find the expression of the unknown coefficient $C_0(\alpha)$, use the Hermitian conjugate of Eq. (6.11), that is,

$$\langle\{\alpha\}| = C_0(\alpha)^* \sum_{m=0}^{\infty} \frac{(\alpha^*)^m}{\sqrt{m!}} \langle\{m\}| \tag{6.12}$$

allowing, with the help of Eq. (6.11), to get the norm of the coherent state

$$\langle\{\alpha\}|\{\alpha\}\rangle = |C_0(\alpha)|^2 \sum_m \sum_n \frac{(\alpha^*)^m (\alpha)^n}{\sqrt{m!}\sqrt{n!}} \langle\{m\}|\{n\}\rangle$$

which, in view of the orthonormality property appearing in (6.3), reduces to

$$\langle\{\alpha\}|\{\alpha\}\rangle = |C_0(\alpha)|^2 \sum_n \frac{|\alpha|^{2n}}{n!} \langle\{n\}|\{n\}\rangle \tag{6.13}$$

Again, owing to Eq. (6.3), and after imposing the coherent state to be normalized, it reads

$$\langle\{\alpha\}|\{\alpha\}\rangle = 1 \qquad \text{and} \qquad \langle\{n\}|\{n\}\rangle = 1$$

so that Eq. (6.13) reduces to

$$|C_0(\alpha)|^2 \sum_n \frac{|\alpha|^{2n}}{n!} = 1$$

which, due to the expansion properties of the exponential, yields

$$|C_0(\alpha)|^2 = e^{-|\alpha|^2} \tag{6.14}$$

At last, passing from the squared absolute value $|C_0(\alpha)|^2$ to the corresponding $C_0(\alpha)$, and after neglecting a phase factor $e^{i\varphi}$ without interest, one obtains

$$C_0(\alpha) = e^{-|\alpha|^2/2} \tag{6.15}$$

so that the recurrence equation (6.10) becomes

$$C_n(\alpha) = e^{-|\alpha|^2/2} \frac{\alpha^n}{\sqrt{n!}}$$

which allows us to transform Eq. (6.4) into

$$\boxed{|\{\alpha\}\rangle = e^{-|\alpha|^2/2} \sum_n \left(\frac{\alpha^n}{\sqrt{n!}} \right) |\{n\}\rangle} \tag{6.16}$$

This 1D result may be generalized to three dimensions, leading, for each x, y, and z components, to coherent states of the form

$$|\{\alpha\}_k\rangle = e^{-|\alpha_k|^2/2} \sum_{n_k} \left(\frac{\alpha_k^{n_k}}{\sqrt{n_k!}} \right) |\{n\}_k\rangle$$

obeying the eigenvalue equations

$$\mathbf{a}_k |\{\alpha\}_k\rangle = \alpha_k |\{\alpha\}_k\rangle$$

6.1.2 Scalar products and closure relations

Since coherent states are the eigenkets of $\mathbf{a}$, which is non-Hermitian, different coherent states being different eigenkets of $\mathbf{a}$, have no reason to be orthogonal, since this property is specific to eigenkets of Hermitian operators. Hence, because of the absence of orthogonality between two coherent states characterized by two different eigenvalues of α, it is necessary to determine their scalar product.

6.1.2.1 Scalar products For this purpose, consider a coherent state $|\{\beta\}\rangle$ obeying an expression of the same form as Eq. (6.1), which reads

$$\mathbf{a}|\{\beta\}\rangle = \beta\, |\{\beta\}\rangle \tag{6.17}$$

where β is the corresponding eigenvalue. The expansion of this new coherent state is of course given by an expression similar to Eq. (6.16), so that its Hermitian conjugate reads as the bra (6.12), that is,

$$\langle\{\beta\}| = e^{-|\beta|^2/2} \sum_m \frac{\beta^{*m}}{\sqrt{m!}} \langle\{m\}|$$

Thereby, the scalar product of $|\{\alpha\}\rangle$, defined by Eq. (6.16) and of $|\{\beta\}\rangle$ given by Eq. (6.17), yields

$$\langle\{\beta\}|\{\alpha\}\rangle = e^{-|\beta|^2/2} e^{-|\alpha|^2/2} \sum_m \sum_n \frac{\alpha^n}{\sqrt{n!}} \frac{\beta^{*m}}{\sqrt{m!}} \langle\{m\}|\{n\}\rangle$$

Next, using the orthonormality properties

$$\langle\{m\}|\{n\}\rangle = \delta_{mn}$$

the above scalar product reduces to

$$\langle\{\beta\}|\{\alpha\}\rangle = e^{-|\beta|^2/2} e^{-|\alpha|^2/2} \sum_n \frac{\left(\alpha\beta^*\right)^n}{n!}$$

or, after passing to exponentials, to

$$\langle\{\beta\}|\{\alpha\}\rangle = \exp\left(-\frac{|\beta|^2 + |\alpha|^2}{2} \right) e^{\alpha\beta^*}$$

and thus

$$\boxed{\langle\{\beta\}|\{\alpha\}\rangle = e^{-|\alpha-\beta|^2/2}} \tag{6.18}$$

6.1.2.2 Closure relations Since coherent states are not orthogonal, they cannot be used to generate a standard discrete closure relation. However, despite this difficulty, it is possible to obtain a continuous closure relation given by

$$I = \frac{1}{\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} |\{\alpha\}\rangle \langle\{\alpha\}| d\,\mathrm{Re}\,(\alpha)\, d\,\mathrm{Im}\,(\alpha) \tag{6.19}$$

In order to prove that Eq. (6.19) is unity, first start from the α complex eigenvalue written as

$$\alpha = \rho e^{i\varphi} \tag{6.20}$$

where ρ and φ are both real, the differentiation of which yields

$$d\alpha = e^{i\varphi}(d\rho + i\rho\, d\varphi)$$

or, after passing to the trigonometric expression,

$$d\alpha = (\cos\varphi + i\sin\varphi)\,(d\rho + i\rho\, d\varphi)$$

and thus

$$d\alpha = d\{\mathrm{Re}\,(\alpha)\} + id\{\mathrm{Im}\,(\alpha)\}$$

where $\mathrm{Re}\,(\alpha)$ and $\mathrm{Im}\,(\alpha)$ are, respectively, the real and imaginary parts of α obeying

$$\begin{pmatrix} d\,\mathrm{Re}\,(\alpha) \\ d\,\mathrm{Im}\,(\alpha) \end{pmatrix} = \begin{pmatrix} \cos\varphi & -\rho\sin\varphi \\ \sin\varphi & +\rho\cos\varphi \end{pmatrix} \begin{pmatrix} d\rho \\ d\varphi \end{pmatrix} \tag{6.21}$$

Next, consider the product of $d\,\mathrm{Re}(\alpha)$ and $d\,\mathrm{Im}(\alpha)$, namely

$$d\,\mathrm{Re}(\alpha)\, d\,\mathrm{Im}(\alpha) = \det(\mathbf{J})\, d\rho\, d\varphi \tag{6.22}$$

where $\mathbf{J}$ is the Jacobian, that is, the determinant corresponding to the matrix involved in Eq. (6.21), that is,

$$\mathbf{J} = \begin{vmatrix} \cos\varphi & -\rho\sin\varphi \\ \sin\varphi & +\rho\cos\varphi \end{vmatrix}$$

Hence, the product (6.22) reads

$$d\,\mathrm{Re}\,(\alpha)\, d\,\mathrm{Im}\,(\alpha) = \rho(\cos^2\varphi + \sin^2\varphi) d\rho\, d\varphi$$

or, after simplifications

$$d\,\mathrm{Re}\,(\alpha)\, d\,\mathrm{Im}\,(\alpha) = \rho\, d\rho\, d\varphi \tag{6.23}$$

Now, in view of Eq. (6.16) and of its Hermitian conjugate, one may write

$$|\{\alpha\}\rangle \langle\{\alpha\}| = e^{-|\alpha|^2} \sum_m \sum_n \frac{\alpha^n}{\sqrt{n!}} \frac{\alpha^{*m}}{\sqrt{m!}} |\{n\}\rangle \langle\{m\}|$$

which, using Eq. (6.20), yields

$$|\{\alpha\}\rangle \langle\{\alpha\}| = e^{-\rho^2} \sum_m \sum_n \frac{\rho^{n+m}}{\sqrt{n!}\sqrt{m!}} e^{i(n-m)\varphi} |\{n\}\rangle\langle\{m\}| \tag{6.24}$$

As a consequence of Eqs. (6.23) and (6.24), the integral I appearing in Eq. (6.19) becomes

$$I = \frac{1}{\pi} \sum_m \sum_n \frac{|\{n\}\rangle \langle\{m\}|}{\sqrt{n!}\sqrt{m!}} \int_0^{+\infty} e^{-\rho^2} \rho^{n+m} \rho \, d\rho \int_0^{2\pi} e^{i(n-m)\varphi} d\varphi \tag{6.25}$$

The last right-hand-side integral has the following solutions:

$$\int_0^{2\pi} e^{i(n-m)\varphi} d\varphi = 2\pi \quad \text{if} \quad n = m$$

$$= \frac{1}{i\,(n-m)} [e^{i(n-m)\varphi}]_0^{2\pi} = 0 \quad \text{if the integers } n \neq m$$

so that

$$\int_0^{2\pi} e^{i(n-m)\varphi} d\varphi = 2\pi\delta_{nm} \tag{6.26}$$

Then, Eq. (6.25) reduces to

$$I = \sum_n I_n \frac{|\{n\}\rangle\langle\{n\}|}{n!} \tag{6.27}$$

with

$$I_n = 2 \int_{-\infty}^{+\infty} e^{-\rho^2} \rho^{2n} \rho \, d\rho \tag{6.28}$$

Again, performing the variable change

$$u = \rho^2$$

the integrals (6.22) yield

$$I_n = \int_0^{+\infty} e^{-u} u^n du = n!$$

Owing to this result, and according to the closure relation appearing in (5.43), the integral (6.27) reduces to

$$I = \pi \sum_n |\{n\}\rangle\langle\{n\}| = \pi$$

Consequently, keeping in mind that, in view of Eqs. (6.20) and (6.23),

$$\rho e^{i\varphi} = \alpha \qquad \text{and} \qquad \rho \, d\rho \, d\varphi = d\text{Re}\,(\alpha)\, d\text{Im}\,(\alpha)$$

it appears that the closure relation over the coherent sates (6.19) is

$$\boxed{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} |\{\alpha\}\rangle\langle\{\alpha\}| \, d\text{Re}\ (\alpha)\, d\text{Im}\,(\alpha) = 1} \tag{6.29}$$

6.2 POISSON DENSITY OPERATOR

Consider a pure density operator of oscillators described by coherent states, which according to Eq. (3.139), reads

$$\rho_\alpha = |\{\alpha\}\rangle\langle\{\alpha\}| \tag{6.30}$$

with

$$\mathbf{a}|\{\alpha\}\rangle = \alpha|\{\alpha\}\rangle \qquad \text{and} \qquad \langle\{\alpha\}|\mathbf{a}^\dagger = \langle\{\alpha\}|\alpha^*$$

and

$$[\mathbf{a}, \mathbf{a}^\dagger] = 1 \qquad \text{and} \qquad \alpha = \alpha^\circ e^{i\varphi} \tag{6.31}$$

Then, owing to Eq. (6.16), Eq. (6.30) becomes

$$\rho_\alpha = e^{-\alpha^{\circ 2}} \sum_m \sum_n \left(\frac{(\alpha)^m}{\sqrt{m!}} \right) |\{m\}\rangle\langle\{n\}| \left(\frac{(\alpha^*)^n}{\sqrt{n!}} \right)$$

or, in view of Eq. (6.31),

$$\rho_\alpha = e^{-\alpha^{\circ 2}} \sum_m \sum_n \left(\frac{(\alpha^\circ)^{m+n}}{\sqrt{m!}\sqrt{n!}} \right) |\{m\}\rangle\langle\{n\}| e^{i(m-n)\varphi} \tag{6.32}$$

Next, performing the average of this density operator over the phase φ according to

$$\bar{\rho}_\alpha = \frac{1}{2\pi} \int_0^{2\pi} \rho_\alpha \, d\varphi$$

Eq. (6.32) transforms to

$$\bar{\rho}_\alpha = e^{-\alpha^{\circ 2}} \sum_m \sum_n \left(\frac{(\alpha^\circ)^{m+n}}{\sqrt{m!}\sqrt{n!}} \right) |\{m\}\rangle\langle\{n\}| \frac{1}{2\pi} \int_0^{2\pi} e^{i(m-n)\varphi} d\varphi$$

which after integration using Eq. (6.26) yields

$$\bar{\boldsymbol{\rho}}_\alpha = e^{-\alpha^{\circ 2}} \sum_m \sum_n \left(\frac{(\alpha^\circ)^{m+n}}{\sqrt{m!}\sqrt{n!}} \right) |\{m\}\rangle\langle\{n\}| \delta_{mn}$$

or

$$\bar{\boldsymbol{\rho}}_\alpha = e^{-\alpha^{\circ 2}} \sum_n \left(\frac{(\alpha^\circ)^{2n}}{n!} \right) |\{n\}\rangle\langle\{n\}| \tag{6.33}$$

Now, observe that this density operator is diagonal in the basis $\{|\{n\}\rangle\}$ and that its diagonal matrix elements are given by the following Poisson distribution:

$$\langle\{n\}|\bar{\boldsymbol{\rho}}_\alpha|\{n\}\rangle = e^{-\alpha^{\circ 2}} \left(\frac{(\alpha^\circ)^{2n}}{n!} \right) \tag{6.34}$$

On the other hand, if the unaveraged density operator (6.32) is not diagonal, its matrix elements are given by

$$\langle\{m\}|\rho_\alpha|\{n\}\rangle = e^{-\alpha^{\circ 2}}\left(\frac{(\alpha^\circ)^{m+n}}{\sqrt{m!}\sqrt{n!}}\right)e^{i(m-n)\varphi} \tag{6.35}$$

Thus, the diagonal matrix elements (6.35) are the same as the diagonal ones (6.34) of the averaged density operator (6.33).

6.3 AVERAGE AND FLUCTUATION OF ENERGY

An important property of coherent states is that these states allow us to easily obtain the mean values of operators averaged on them, whereas another interest is that these mean values exhibit physical properties that are close to those of classical harmonic oscillators. The following sections will thus be devoted to calculate mean values of operators averaged over coherent states, the present one dealing with the average value of the Hamiltonian and of its square, allowing one to find the energy fluctuations within coherent states.

6.3.1 Average Hamiltonian

First, consider the mean value of the harmonic oscillator Hamiltonian averaged over coherent states, that is,

$$\langle\mathbf{H}\rangle_\alpha = \langle\{\alpha\}|\mathbf{H}\,|\{\alpha\}\rangle$$

which becomes in view of Eq. (5.9)

$$\langle\mathbf{H}\rangle_\alpha = \hbar\omega\langle\{\alpha\}|\left(\mathbf{a}^\dagger\mathbf{a}+\tfrac{1}{2}\right)|\{\alpha\}\rangle$$

or

$$\langle\mathbf{H}\rangle_\alpha = \hbar\omega\langle\{\alpha\}|\mathbf{a}^\dagger\mathbf{a}|\{\alpha\}\rangle + \tfrac{1}{2}\hbar\omega\,\langle\{\alpha\}|\{\alpha\}\rangle \tag{6.36}$$

Moreover, in view of Eqs. (6.1) and (6.2), the right-hand-side average value appearing in Eq. (6.36) reads

$$\langle\{\alpha\}|\mathbf{a}^\dagger\mathbf{a}|\{\alpha\}\rangle = \langle\{\alpha\}|\alpha^*\alpha|\{\alpha\}\rangle = \;|\alpha|^2\langle\{\alpha\}|\{\alpha\}\rangle \tag{6.37}$$

so that, if the coherent states are normalized, the average value (6.36) of the energy takes the form

$$\boxed{\langle\mathbf{H}\rangle_\alpha = \hbar\omega\left(|\alpha|^2+\tfrac{1}{2}\right)} \tag{6.38}$$

which may be generalized to 3D oscillators:

$$\langle\mathbf{H}\rangle_\alpha = \hbar\omega_x\;\left(|\alpha_x|^2+\tfrac{1}{2}\right)+\hbar\omega_y\;\left(|\alpha_y|^2+\tfrac{1}{2}\right)+\hbar\omega_z\;\left(|\alpha_z|^2+\tfrac{1}{2}\right)$$

6.3.2 Average squared Hamiltonian

Next, consider the corresponding average value of the squared Hamiltonian, that is,

$$\langle \mathbf{H}^2 \rangle_\alpha = \langle \{\alpha\} | \mathbf{H}^2 | \{\alpha\} \rangle$$

which, by comparing Eq. (5.9), reads

$$\langle \mathbf{H}^2 \rangle_\alpha = (\hbar\omega)^2 \langle \{\alpha\} | \left(\mathbf{a}^\dagger \mathbf{a} + \tfrac{1}{2} \right)^2 | \{\alpha\} \rangle \tag{6.39}$$

or

$$\langle \mathbf{H}^2 \rangle_\alpha = (\hbar\omega)^2 \langle \{\alpha\} | \left(\mathbf{a}^\dagger \mathbf{a} \mathbf{a}^\dagger \mathbf{a} + \mathbf{a}^\dagger \mathbf{a} + \tfrac{1}{4} \right) | \{\alpha\} \rangle \tag{6.40}$$

Again, in view of Eqs. (6.1) and (6.2), the average value of the quadruple product of operators over coherent states takes the form

$$\langle \{\alpha\} | \mathbf{a}^\dagger \mathbf{a} \mathbf{a}^\dagger \mathbf{a} | \{\alpha\} \rangle = \langle \{\alpha\} | \alpha^* \mathbf{a} \mathbf{a}^\dagger \alpha | \{\alpha\} \rangle$$

and thus α being a scalar,

$$\langle \{\alpha\} | \mathbf{a}^\dagger \mathbf{a} \mathbf{a}^\dagger \mathbf{a} | \{\alpha\} \rangle = |\alpha|^2 \langle \{\alpha\} | \mathbf{a} \mathbf{a}^\dagger | \{\alpha\} \rangle \tag{6.41}$$

Furthermore, because of the basic commutator (5.5), the right-hand-side matrix element of Eq. (6.41) becomes

$$\langle \{\alpha\} | \mathbf{a} \mathbf{a}^\dagger | \{\alpha\} \rangle = \langle \{\alpha\} | \left(\mathbf{a}^\dagger \mathbf{a} + \mathbf{1} \right) | \{\alpha\} \rangle$$

and thus using in turn Eqs. (6.1) and (6.2),

$$\langle \{\alpha\} | \mathbf{a} \mathbf{a}^\dagger | \{\alpha\} \rangle = \left(|\alpha|^2 + 1 \right) \langle \{\alpha\} | \{\alpha\} \rangle = |\alpha|^2 + 1$$

so that Eq. (6.41) becomes

$$\langle \{\alpha\} | \mathbf{a}^\dagger \mathbf{a} \mathbf{a}^\dagger \mathbf{a} | \{\alpha\} \rangle = |\alpha|^2 \left(|\alpha|^2 + 1 \right)$$

As a consequence and according to Eqs. (6.40) and (6.37), it yields

$$\langle \{\alpha\} | \left(\mathbf{a}^\dagger \mathbf{a} + \tfrac{1}{2} \right)^2 | \{\alpha\} \rangle = |\alpha|^2 \left(|\alpha|^2 + 1 \right) + |\alpha|^2 + \tfrac{1}{4}$$

so that the average value of the squared Hamiltonian given by Eq. (6.39) becomes

$$\boxed{\langle \mathbf{H}^2 \rangle_\alpha = (\hbar\omega)^2 \left(|\alpha|^4 + 2|\alpha|^2 + \tfrac{1}{4} \right)} \tag{6.42}$$

which for 3D oscillators gives

$$\begin{aligned} \langle \mathbf{H}^2 \rangle_\alpha = {} & (\hbar\omega_x)^2 \left(|\alpha_x|^4 + 2|\alpha_x|^2 + \tfrac{1}{4} \right) + (\hbar\omega_y)^2 \left(|\alpha_y|^4 + 2|\alpha_y|^2 + \tfrac{1}{4} \right) \\ & + (\hbar\omega_z)^2 \left(|\alpha_z|^4 + 2|\alpha_z|^2 + \tfrac{1}{4} \right) \end{aligned}$$

6.3.3 Energy fluctuations

It is now possible to obtain an expression for the relative energy fluctuation of harmonic oscillators within coherent states. The energy fluctuation $\Delta \mathbf{H}_\alpha$ is formally given by

$$\Delta \mathbf{H}_\alpha = \sqrt{\langle \mathbf{H}^2 \rangle_\alpha - \langle \mathbf{H} \rangle_\alpha^2}$$

and, comparing Eqs. (6.38) and (6.42), we have

$$\Delta\mathbf{H}_\alpha = \hbar\omega\sqrt{\left(|\alpha|^4 + 2|\alpha|^2 + \tfrac{1}{4}\right) - \left(|\alpha|^4 + |\alpha|^2 + \tfrac{1}{4}\right)}$$

which reduces to

$$\Delta\mathbf{H}_\alpha = \hbar\omega|\alpha| \tag{6.43}$$

Clearly, the energy fluctuation is not zero because the average value of the Hamiltonian has been performed over a state that is not an eigenstate of this operator.

Now, the relative energy fluctuation reads, with the help of Eqs. (6.38) and (6.43),

$$\left(\frac{\Delta\mathbf{H}_\alpha}{\langle\mathbf{H}\rangle_\alpha}\right) = \frac{|\alpha|}{|\alpha|^2 + \frac{1}{2}}$$

which, when $|\alpha|$ becomes important, simplifies to

$$\left(\frac{\Delta\mathbf{H}_\alpha}{\langle\mathbf{H}\rangle_\alpha}\right) \backsimeq \frac{1}{|\alpha|} \quad \text{when} \quad |\alpha| >> 1$$

which, in turn, vanishes when $|\alpha|$ becomes very large:

$$\boxed{\left(\frac{\Delta\mathbf{H}_\alpha}{\langle\mathbf{H}\rangle_\alpha}\right) \to 0 \quad \text{when} \quad |\alpha| \to \infty}$$

This last result, which holds also for 3D oscillators, narrows the behavior of a classical harmonic oscillator for which the energy is always exact, according to classical mechanics.

6.4 COHERENT STATES AS MINIMIZING HEISENBERG UNCERTAINTY RELATIONS

Coherent states that present such classical asymptotic behavior also minimize the Heisenberg uncertainty relations, which we shall now prove.

6.4.1 Average values of the first and second moments of Q and P

For this purpose, it is necessary to obtain the mean values of the **Q** and **P** operators and of their squares averaged over coherent states.

6.4.1.1 Q and P average values First start from the position operator **Q** averaged over coherent states:

$$\langle\mathbf{Q}\rangle_\alpha = \langle\{\alpha\}|\,\mathbf{Q}\,|\{\alpha\}\rangle$$

which, in view of the expression (5.6) of **Q** in terms of the ladder operators, becomes

$$\langle\mathbf{Q}\rangle_\alpha = \sqrt{\frac{\hbar}{2m\omega}}\langle\{\alpha\}|(\mathbf{a}^\dagger + \mathbf{a})|\{\alpha\}\rangle$$

and due to the eigenvalue equations, (6.1) and (6.2), transforms to

$$\langle \mathbf{Q} \rangle_\alpha = \sqrt{\frac{\hbar}{2m\omega}} \langle \{\alpha\} | (\alpha^* + \alpha) | \{\alpha\} \rangle$$

Moreover, since α and α^* are scalars and when coherent states are normalized, this result reduces to

$$\boxed{\langle \mathbf{Q} \rangle_\alpha = \sqrt{\frac{\hbar}{2m\omega}} \{\alpha^* + \alpha\}} \tag{6.44}$$

Observe that, while the **Q** mean value averaged over Hamiltonian eigenstates is zero, those averaged over the coherent state are not so.

Now, Eq. (5.7) allows us to write the **P** average value over a coherent state, according to

$$\langle \mathbf{P} \rangle_\alpha = \langle \{\alpha\} | \, \mathbf{P} \, | \{\alpha\} \rangle = i \sqrt{\frac{m\hbar\omega}{2}} \langle \{\alpha\} | (\mathbf{a}^\dagger - \mathbf{a}) | \{\alpha\} \rangle$$

which, proceeding in the same way as above using Eqs. (6.1) and (6.2), reads

$$\boxed{\langle \mathbf{P} \rangle_\alpha = i \sqrt{\frac{m\hbar\omega}{2}} \{\alpha^* - \alpha\}} \tag{6.45}$$

6.4.1.2 Q^2 and P^2 average values Now, in order to find the dispersion of **P** and **Q** within a coherent state, one has first to get the mean values of $\mathbf{P}^2$ and $\mathbf{Q}^2$ within these states. Then, with the help of Eq. (5.6) it may be written

$$\langle \mathbf{Q}^2 \rangle_\alpha = \langle \{\alpha\} | \mathbf{Q}^2 | \{\alpha\} \rangle = \frac{\hbar}{2m\omega} \langle \{\alpha\} | (\mathbf{a}^\dagger + \mathbf{a})^2 | \{\alpha\} \rangle$$

or

$$\langle \mathbf{Q}^2 \rangle_\alpha = \frac{\hbar}{2m\omega} \langle \{\alpha\} | \left((\mathbf{a}^\dagger)^2 + (\mathbf{a})^2 + \mathbf{a}^\dagger \mathbf{a} + \mathbf{a}\mathbf{a}^\dagger \right) | \{\alpha\} \rangle$$

which, in view of the commutation rule (5.5), transforms to

$$\langle \mathbf{Q}^2 \rangle_\alpha = \frac{\hbar}{2m\omega} \langle \{\alpha\} | \left(\mathbf{a}^\dagger \mathbf{a}^\dagger + \mathbf{a}\mathbf{a} + 2\mathbf{a}^\dagger \mathbf{a} + 1 \right) | \{\alpha\} \rangle$$

or

$$\langle \mathbf{Q}^2 \rangle_\alpha = \frac{\hbar}{2m\omega} [\langle \{\alpha\} | \mathbf{a}^\dagger \mathbf{a}^\dagger | \{\alpha\} \rangle + \langle \{\alpha\} | \mathbf{a}\mathbf{a} | \{\alpha\} \rangle + 2 \langle \{\alpha\} | \mathbf{a}^\dagger \mathbf{a} | \{\alpha\} \rangle + \langle \{\alpha\} | \{\alpha\} \rangle] \tag{6.46}$$

Next, due to Eq. (6.1) we have

$$\mathbf{a}\mathbf{a} \, | \{\alpha\} \rangle = \mathbf{a} \, \alpha | \{\alpha\} \rangle$$

where

$$\mathbf{a}\mathbf{a} | \{\alpha\} \rangle = \alpha \mathbf{a} \, | \{\alpha\} \rangle = (\alpha)^2 \, | \{\alpha\} \rangle \tag{6.47}$$

the Hermitian conjugate of which is

$$\langle \{\alpha\} | \mathbf{a}^\dagger \mathbf{a}^\dagger = (\alpha^*)^2 \langle \{\alpha\} | \tag{6.48}$$

Hence, comparing Eqs. (6.47) and (6.48), the average value (6.46) becomes

$$\langle \mathbf{Q}^2 \rangle_\alpha = \frac{\hbar}{2m\omega} \left((\alpha^*)^2 + (\alpha)^2 + 2\alpha^* \alpha + 1 \right) \langle \{\alpha\} | \{\alpha\} \rangle$$

Finally, rearranging and assuming normalized coherent states, one obtains

$$\boxed{\langle \mathbf{Q}^2 \rangle_\alpha = \frac{\hbar}{2m\omega} ((\alpha + \alpha^*)^2 + 1)} \tag{6.49}$$

Now, the average value $\langle \mathbf{P}^2 \rangle_\alpha$ reads, in view of Eq. (5.7),

$$\langle \mathbf{P}^2 \rangle_\alpha = \langle \{\alpha\} | \mathbf{P}^2 | \{\alpha\} \rangle = -\frac{m\hbar\omega}{2} \langle \{\alpha\} | (\mathbf{a}^\dagger - \mathbf{a})^2 | \{\alpha\} \rangle$$

which transforms after expanding the right-hand-side term into

$$\langle \mathbf{P}^2 \rangle_\alpha = -\frac{m\hbar\omega}{2} \langle \{\alpha\} | ((\mathbf{a}^\dagger)^2 + (\mathbf{a})^2 - 2\mathbf{a}^\dagger \mathbf{a} - 1) | \{\alpha\} \rangle$$

so that, proceeding in the same way as for $\mathbf{Q}^2$, we have

$$\boxed{\langle \mathbf{P}^2 \rangle_\alpha = -\frac{m\hbar\omega}{2} ((\alpha^* - \alpha)^2 - 1)} \tag{6.50}$$

6.4.2 Heisenberg uncertainty relations

It is now possible to get the dispersion over $\mathbf{Q}$

$$\Delta \mathbf{Q}_\alpha = \sqrt{\langle \mathbf{Q}^2 \rangle_\alpha - \langle \mathbf{Q} \rangle_\alpha^2}$$

which, comparing Eqs. (6.44) and (6.49), reads

$$\Delta \mathbf{Q}_\alpha = \sqrt{\frac{\hbar}{2m\omega}} \tag{6.51}$$

Now, the dispersion over $\mathbf{P}$ is

$$\Delta \mathbf{P}_\alpha = \sqrt{\langle \mathbf{P}^2 \rangle_\alpha - \langle \mathbf{P} \rangle_\alpha^2}$$

which, owing to Eqs. (6.45) and (6.50), becomes

$$\Delta \mathbf{P}_\alpha = \sqrt{\frac{m\hbar\omega}{2}} \tag{6.52}$$

Thus, the product of the uncertainties (6.51) and (6.52) yields, for arbitrary α,

$$\boxed{\Delta \mathbf{Q}_\alpha \Delta \mathbf{P}_\alpha = \frac{\hbar}{2}} \tag{6.53}$$

Thus, this 1D uncertainty relation, which may be generalized to three dimensions, is the minimum compatible with the Heisenberg uncertainty relations.

6.5 DYNAMICS

Owing to the semiclassical properties of the mean values of operators averaged over coherent states, it would be interesting to find if the dynamics of these mean values behave also semiclassically. Since the time dependence of Boson operators is known, it is convenient to perform the dynamic investigations dealing with coherent states within the time-dependent Heisenberg representation instead of the time-dependent Schrödinger one.

6.5.1 Position and momentum time-dependent average values

6.5.1.1 One-dimensional oscillators First, consider the Heisenberg time dependence of the mean value of $\mathbf{Q}(t)$ average over coherent states, which, owing to Eq. (5.153), reads

$$\langle\{\alpha\}|\mathbf{Q}(t)|\{\alpha\}\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\langle\{\alpha\}|\mathbf{a}^{\dagger}(t)|\{\alpha\}\rangle + \langle\{\alpha\}|\mathbf{a}(t)|\{\alpha\}\rangle\right) \tag{6.54}$$

Now, in view of Eqs. (5.151) and (5.152), we have

$$\langle\{\alpha\}|\mathbf{a}(t)|\{\alpha\}\rangle = \langle\{\alpha\}|\mathbf{a}(0)|\{\alpha\}\rangle e^{-i\omega t}$$

$$\langle\{\alpha\}|\mathbf{a}^{\dagger}(t)|\{\alpha\}\rangle = \langle\{\alpha\}|\mathbf{a}^{\dagger}(0)|\{\alpha\}\rangle e^{i\omega t}$$

so that due to (6.1)

$$\langle\{\alpha\}|\mathbf{a}(t)|\{\alpha\}\rangle = \alpha e^{-i\omega t}\langle\{\alpha\}|\{\alpha\}\rangle = \alpha(t)$$

$$\langle\{\alpha\}|\mathbf{a}^{\dagger}(t)|\{\alpha\}\rangle = \alpha e^{i\omega t}\langle\{\alpha\}|\{\alpha\}\rangle = \alpha^{*}(t)$$

with

$$\alpha(t) = \alpha e^{-i\omega t} \tag{6.55}$$

As a consequence, Eq. (6.54) becomes

$$\langle\{\alpha\}|\,\mathbf{Q}(t)|\{\alpha\}\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\alpha^{*}e^{i\omega t} + \alpha e^{-i\omega t})$$

which, if α is real, reduces to

$$\boxed{\langle\{\alpha\}|\mathbf{Q}(t)|\{\alpha\}\rangle = 2\alpha\sqrt{\frac{\hbar}{2m\omega}}\cos\omega t} \tag{6.56}$$

6.5.1.2 Two-dimensional oscillators Now pass from 1D to 2D oscillators for which the time-dependent $\mathbf{Q}(t)$ operator reads

$$\mathbf{Q}(t) = \mathbf{Q}_x(t) + \mathbf{Q}_y(t)$$

Moreover, defining the coherent states dealing with the x and y components using

$$\mathbf{a}_k(t)|\{\alpha\}_k\rangle = \alpha_k(t)|\{\alpha\}_k\rangle \quad \text{with} \quad \mathbf{Q}_k(t) = \sqrt{\frac{\hbar}{2m\omega}}(\mathbf{a}_k^{\dagger}(t) + \mathbf{a}_k(t))$$

where k stands for x or y, the mean values of $\mathbf{Q}_x(t)$ and $\mathbf{Q}_y(t)$ averaged on their corresponding coherent states must be given by expressions similar to that of (6.54), that is,

$$\langle\{\alpha\}_k|\mathbf{Q}_k(t)|\{\alpha\}_k\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\langle\{\alpha\}_k|\mathbf{a}_k^\dagger(t)|\{\alpha\}_k\rangle + \langle\{\alpha\}_k|\mathbf{a}_k(t)|\{\alpha\}_k\rangle)$$

so that, using the eigenvalue equation defining the x and y coherent states, it is obtained

$$\langle\{\alpha\}_k|\mathbf{Q}_k(t)|\{\alpha\}_k\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\langle\{\alpha\}_k|\alpha_k^*(t)|\{\alpha\}_k\rangle + \langle\{\alpha\}_k|\alpha_k(t)|\{\alpha\}_k\rangle\right) \tag{6.57}$$

Next, if, for some reason, dephasing between $\alpha_x(t)$ and $\alpha_y(t)$ exists so that

$$\alpha_x(t) = \alpha e^{-i\omega t} \qquad \text{and} \qquad \alpha_y(t) = \alpha e^{\pm i\pi/2} e^{-i\omega t} \tag{6.58}$$

the two average values (6.57) read, respectively,

$$\langle\{\alpha\}_x|\mathbf{Q}_x(t)|\{\alpha\}_x\rangle = 2\alpha\sqrt{\frac{\hbar}{2m\omega}}\cos(\omega t) \tag{6.59}$$

$$\langle\{\alpha\}_y|\mathbf{Q}_y^\pm(t)|\{\alpha\}_y\rangle = 2\alpha\sqrt{\frac{\hbar}{2m\omega}}\cos\left(\omega t \mp \frac{\pi}{2}\right) \tag{6.60}$$

Hence, for 2D oscillators obeying Eq. (6.58), the mean value of $\mathbf{Q}$ averaged over coherent states, yields

$$\begin{aligned}\langle\{\alpha\}_y|\langle\{\alpha\}_x|\mathbf{Q}^\pm(t)|\{\alpha\}_x\rangle|\{\alpha\}_y\rangle \;=\; &\langle\{\alpha\}_y|\langle\{\alpha\}_x|\mathbf{Q}_x(t)|\{\alpha\}_x\rangle|\{\alpha\}_y\rangle \\ &+\langle\{\alpha\}_x|\langle\{\alpha\}_y|\mathbf{Q}_y^\pm(t)|\{\alpha\}_y\rangle|\{\alpha\}_x\rangle\end{aligned}$$

or, due to Eqs. (6.59) and (6.60) and after simplification,

$$\langle\{\alpha\}_y|\langle\{\alpha\}_x|\mathbf{Q}^\pm(t)|\{\alpha\}_x\rangle|\{\alpha\}_y\rangle = 2\alpha\sqrt{\frac{\hbar}{2m\omega}}(\cos(\omega t) \mp \sin(\omega t)) \tag{6.61}$$

Hence, the two $\pm$ equations (6.61) constitute two inverse polarized circular motions.

Next, using Eq. (5.159), for the averaged momentum, which may be in correspondence with the average value of $\mathbf{Q}(t)$ given by Eq. (6.56), one would obtain

$$\boxed{\langle\{\alpha\}_y|\langle\{\alpha\}_x|\mathbf{P}(t)|\{\alpha\}_x\rangle|\{\alpha\}_y\rangle = -2\alpha\sqrt{\frac{\hbar m\omega}{2}}\sin\omega t} \tag{6.62}$$

6.5.2 Kinetic and potential time-dependent average values

Now, using Eqs. (6.56) and (6.62), giving the average values of $\mathbf{Q}(t)$ and $\mathbf{P}(t)$, it is possible to get the time dependence of the average potential and kinetic energy operators $\mathbf{V}(t)$ and $\mathbf{T}(t)$. For the first one, which is

$$\langle\{\alpha\}|\mathbf{V}(t)|\{\alpha\}\rangle = \tfrac{1}{2}m\omega^2\langle\{\alpha\}|\mathbf{Q}(t)^2|\{\alpha\}\rangle \tag{6.63}$$

the right-hand-side average value may be expressed in terms of the raising and lowering operators from Eq. (5.153), that is,

$$\langle\{\alpha\}|\mathbf{Q}(t)^2|\{\alpha\}\rangle = \frac{\hbar}{2m\omega}\langle\{\alpha\}|\left(\mathbf{a}^\dagger e^{i\omega t} + \mathbf{a}e^{-i\omega t}\right)^2|\{\alpha\}\rangle \tag{6.64}$$

which using Eq. (5.166) and the commutation rule (5.5), Eq. (6.64) reads

$$\langle\{\alpha\}|\mathbf{Q}(t)^2|\{\alpha\}\rangle = \frac{\hbar}{2m\omega}\langle\{\alpha\}|\left(\left(\mathbf{a}^\dagger\right)^2 e^{2i\omega t} + (\mathbf{a})^2 e^{-2i\omega t} + 2\mathbf{a}^\dagger\mathbf{a}+1\right)|\{\alpha\}\rangle$$

so that Eq. (6.63) becomes

$$\langle\{\alpha\}|\mathbf{V}(t)|\{\alpha\}\rangle = \tfrac{1}{4}\hbar\omega\langle\{\alpha\}|(\left(\mathbf{a}^\dagger\right)^2 e^{2i\omega t} + (\mathbf{a})^2 e^{-2i\omega t} + 2\mathbf{a}^\dagger\mathbf{a}+1)|\{\alpha\}\rangle$$

Again, owing to Eq. (6.1) and to the Hermitian conjugate, one obtains, respectively, after a double action of $\mathbf{a}$ on the right and of $\mathbf{a}^\dagger$ on the left,

$$\langle\{\alpha\}|\,(\mathbf{a})^2\,|\{\alpha\}\rangle = \alpha^2\langle\{\alpha\}|\{\alpha\}\rangle = \alpha^2 \tag{6.65}$$

$$\langle\{\alpha\}|\left(\mathbf{a}^\dagger\right)^2|\{\alpha\}\rangle = \alpha^{*2}\langle\{\alpha\}|\{\alpha\}\rangle = \alpha^{*2}$$

Besides, owing to Eq. (6.2) and its Hermitian conjugate, one gets

$$\langle\{\alpha\}|\left(\mathbf{a}^\dagger\mathbf{a}\right)^2|\{\alpha\}\rangle = |\alpha|^2\langle\{\alpha\}|\{\alpha\}\rangle = |\alpha|^2 \tag{6.66}$$

so that, by the aid of these last three equations, the average value of the potential energy becomes

$$\langle\{\alpha\}|\mathbf{V}(t)|\{\alpha\}\rangle = \tfrac{1}{4}\hbar\omega(\alpha^{*2}e^{2i\omega t} + \alpha^2 e^{-2i\omega t} + 2|\alpha|^2 + 1)$$

which, passing to sine and cosine functions, transforms to

$$\langle\{\alpha\}|\mathbf{V}(t)|\{\alpha\}\rangle = \tfrac{1}{4}\hbar\omega((\alpha^2 + \alpha^{*2})\cos 2\omega t\ - i(\alpha^2 - \alpha^{*2})\sin 2\omega t + 2|\alpha|^2 + 1) \tag{6.67}$$

which, in turn, if α is real, reduces to

$$\langle\{\alpha\}|\mathbf{V}(t)|\{\alpha\}\rangle = \tfrac{1}{2}\hbar\omega\left(\alpha^2(\cos 2\omega t + 1) + \tfrac{1}{2}\right) \tag{6.68}$$

On the other hand, the corresponding average value of the kinetic energy, which reads

$$\langle\{\alpha\}|\mathbf{T}(t)|\{\alpha\}\rangle = \frac{1}{2m}\langle\{\alpha\}|\mathbf{P}(t)^2|\{\alpha\}\rangle \tag{6.69}$$

may be found, proceeding in a similar way as for the potential energy by the aid of Eqs. (5.159) and (5.166):

$$\langle\{\alpha\}|\mathbf{T}(t)|\{\alpha\}\rangle = \tfrac{1}{4}\hbar\omega\langle\{\alpha\}|((2\mathbf{a}^\dagger\mathbf{a}+1) - ((\mathbf{a}^\dagger)^2 e^{2i\omega t} + (\mathbf{a})^2 e^{-2i\omega t}))|\{\alpha\}\rangle$$

Thus, in view of Eqs. (6.65) and (6.66), we have

$$\langle\{\alpha\}|\mathbf{T}(t)|\{\alpha\}\rangle = \tfrac{1}{2}\hbar\omega\left(\alpha^2(1 - \cos 2\omega t) + \tfrac{1}{2}\right) \tag{6.70}$$

Observe that, owing to Eqs. (6.67) and (6.70), the average value of the Hamiltonian is a constant given by

$$\langle\{\alpha\}|\mathbf{H}|\{\alpha\}\rangle = \langle\{\alpha\}|\mathbf{T}(t)|\{\alpha\}\rangle + \langle\{\alpha\}|\mathbf{V}(t)|\{\alpha\}\rangle = \hbar\omega(\alpha^2 + \tfrac{1}{2})$$

that is, as required, in agreement with Eq. (6.38). Observe also the difference in the behavior of time dependence of the average values of the kinetic and potential

operators when passing from the eigenstates of the Hamiltonian to the coherent states. Whereas they are constant when the quantum average is performed on the Hamiltonian eigenstates, they become time dependent when passing to coherent states, although coming back and forth in such a way as the average energy remains constant.

6.6 TRANSLATION OPERATORS

The coherent states are deeply connected to the translation operators. As we shall see in this section, the translation operators generate coherent states.

6.6.1 Action of translation operators on ladder operators

To prove this, first seek the action of the translation operator

$$\mathbf{A}(Q^\circ) = \exp\left(-\frac{iQ^\circ \mathbf{P}}{\hbar}\right) \tag{6.71}$$

on the raising and lowering operators. For this, consider the unitary operator given by Eq. (2.95) where $\mathbf{P}$ is the momentum operator and Q° a scalar having the dimension of a length. According to Eq. (2.102) the following canonical transformation holds:

$$\mathbf{A}(Q^\circ)^{-1}\mathbf{Q}\,\mathbf{A}(Q^\circ) = \mathbf{Q} + Q^\circ \tag{6.72}$$

Now, when, expressed in terms of the raising and lowering operators using Eq. (5.7), the translation operator takes the form

$$\mathbf{A}(Q^\circ) = \mathbf{A}(\alpha^\circ) = \exp\left\{-i\frac{Q^\circ}{\hbar} i\sqrt{\frac{\hbar m\omega}{2}}(\mathbf{a}^\dagger - \mathbf{a})\right\} \tag{6.73}$$

or

$$\mathbf{A}(\alpha^\circ) = e^{\alpha^\circ \mathbf{a}^\dagger - \alpha^\circ \mathbf{a}} = e^{-\alpha^\circ \mathbf{a} + \alpha^\circ \mathbf{a}^\dagger} \tag{6.74}$$

with

$$\alpha^\circ = Q^\circ\sqrt{\frac{m\omega}{2\hbar}} \tag{6.75}$$

The second right-hand-side expression in (6.74) has been written to underline the fact that the order of the operators involved in the exponential is irrelevant. Besides, observe that if α° is changed into $-\alpha^\circ$ into Eq. (6.74), this equation transforms to

$$\mathbf{A}(-\alpha^\circ) = e^{-\alpha^\circ \mathbf{a}^\dagger + \alpha^\circ \mathbf{a}} = e^{\alpha^\circ \mathbf{a} - \alpha^\circ \mathbf{a}^\dagger} \tag{6.76}$$

the right-hand side, which is simply the inverse of the translation operator $\mathbf{A}(\alpha^\circ)$ given by Eq. (6.74), so that

$$\mathbf{A}(-\alpha^\circ) = \mathbf{A}(\alpha^\circ)^{-1} \tag{6.77}$$

Now, use Glauber's theorem (1.78) in order to transform the translation operator (6.74) and its inverse (6.76), into products of exponential operators involving only $\mathbf{a}^\dagger$ or $\mathbf{a}$, according to

$$\begin{aligned}
\mathbf{A}(\alpha^\circ) &= (e^{\alpha^\circ \mathbf{a}^\dagger})(e^{-\alpha^\circ \mathbf{a}})e^{[\alpha^\circ \mathbf{a}^\dagger, \alpha^\circ \mathbf{a}]/2} = (e^{-\alpha^\circ \mathbf{a}})(e^{\alpha^\circ \mathbf{a}^\dagger})e^{[\alpha^\circ \mathbf{a}, \alpha^\circ \mathbf{a}^\dagger]/2} \\
\mathbf{A}(\alpha^\circ)^{-1} &= (e^{-\alpha^\circ \mathbf{a}^\dagger})(e^{\alpha^\circ \mathbf{a}})e^{-[\alpha^\circ \mathbf{a}^\dagger, \alpha^\circ \mathbf{a}]/2} = (e^{\alpha^\circ \mathbf{a}})(e^{-\alpha^\circ \mathbf{a}^\dagger})e^{-[\alpha^\circ \mathbf{a}, \alpha^\circ \mathbf{a}^\dagger]/2}
\end{aligned}$$

or, since $[\mathbf{a}^\dagger, \mathbf{a}] = -1$,

$$\boxed{\mathbf{A}(\alpha^\circ) = (e^{\alpha^\circ \mathbf{a}^\dagger})(e^{-\alpha^\circ \mathbf{a}})e^{-\alpha^{\circ 2}/2} = (e^{-\alpha^\circ \mathbf{a}})(e^{\alpha^\circ \mathbf{a}^\dagger})e^{\alpha^{\circ 2}/2}} \tag{6.78}$$

$$\mathbf{A}(\alpha^\circ)^{-1} = (e^{-\alpha^\circ \mathbf{a}^\dagger})(e^{\alpha^\circ \mathbf{a}})e^{\alpha^{\circ 2}/2} = (e^{\alpha^\circ \mathbf{a}})(e^{-\alpha^\circ \mathbf{a}^\dagger})e^{-\alpha^{\circ 2}/2} \tag{6.79}$$

Next, return to the situation where α is real and thus equal to α°. Then, owing to Eqs. (6.75), (6.74) and (6.77), Eq. (6.72) reads

$$\sqrt{\frac{\hbar}{2m\omega}}(e^{-(\alpha^\circ \mathbf{a}^\dagger - \alpha^\circ \mathbf{a})})(\mathbf{a}^\dagger + \mathbf{a})(e^{(\alpha^\circ \mathbf{a}^\dagger - \alpha^\circ \mathbf{a})}) = \sqrt{\frac{\hbar}{2m\omega}}((\mathbf{a}^\dagger + \mathbf{a}) + (\alpha^\circ + \alpha^\circ)) \tag{6.80}$$

or, after simplification and use of Eq. (6.74),

$$\boxed{\mathbf{A}(\alpha^\circ)^{-1}(\mathbf{a}^\dagger + \mathbf{a})\,\mathbf{A}(\alpha^\circ) = (\mathbf{a}^\dagger + \alpha^\circ) + (\mathbf{a} + \alpha^\circ)} \tag{6.81}$$

which, owing to the first expression of (6.78) and (6.79), appears after simplification to be given by

$$(e^{\alpha^\circ \mathbf{a}})(e^{-\alpha^\circ \mathbf{a}^\dagger})(\mathbf{a}^\dagger + \mathbf{a})(e^{\alpha^\circ \mathbf{a}^\dagger})(e^{-\alpha^\circ \mathbf{a}}) = \mathbf{a}^\dagger + \alpha^\circ + \mathbf{a} + \alpha^\circ \tag{6.82}$$

However, the right-hand side of the latter equation may be expressed as

$$\begin{aligned}(e^{\alpha^\circ \mathbf{a}})(e^{-\alpha^\circ \mathbf{a}^\dagger})(\mathbf{a}^\dagger + \mathbf{a})(e^{\alpha^\circ \mathbf{a}^\dagger})(e^{-\alpha^\circ \mathbf{a}}) &= (e^{\alpha^\circ \mathbf{a}})(e^{-\alpha^\circ \mathbf{a}^\dagger}\mathbf{a}^\dagger e^{\alpha^\circ \mathbf{a}^\dagger})(e^{-\alpha^\circ \mathbf{a}}) \\ &\quad + (e^{-\alpha^\circ \mathbf{a}^\dagger})(e^{\alpha^\circ \mathbf{a}}\mathbf{a}e^{-\alpha^\circ \mathbf{a}})(e^{\alpha^\circ \mathbf{a}^\dagger})\end{aligned}$$

Hence, after simplifications, because the function of an operator commutes with this operator, Eq. (6.82) yields

$$(e^{\alpha^\circ \mathbf{a}})(e^{-\alpha^\circ \mathbf{a}^\dagger})(\mathbf{a}^\dagger + \mathbf{a})(e^{\alpha^\circ \mathbf{a}^\dagger})(e^{-\alpha^\circ \mathbf{a}}) = (e^{\alpha^\circ \mathbf{a}})\mathbf{a}^\dagger(e^{-\alpha^\circ \mathbf{a}}) + (e^{-\alpha^\circ \mathbf{a}^\dagger})\mathbf{a}(e^{\alpha^\circ \mathbf{a}^\dagger}) \tag{6.83}$$

As a consequence, due to Eqs. (6.82) and (6.83), it appears that

$$\boxed{(e^{\alpha^\circ \mathbf{a}})\mathbf{a}^\dagger(e^{-\alpha^\circ \mathbf{a}}) = \mathbf{a}^\dagger + \alpha^\circ} \tag{6.84}$$

$$\boxed{(e^{-\alpha^\circ \mathbf{a}^\dagger})\mathbf{a}(e^{\alpha^\circ \mathbf{a}^\dagger}) = \mathbf{a} + \alpha^\circ} \tag{6.85}$$

6.6.2 Action of translation operators on Hamiltonian ground states

Now, study the action of the translation operators given by Eq. (6.78), on the ground state of the Hamiltonian of the quantum harmonic oscillator, which reads

$$\mathbf{A}(\alpha)|\{0\}\rangle = \left\{e^{\frac{-|\alpha|^2}{2}}\right\}(e^{\alpha \mathbf{a}^\dagger})(e^{-\alpha^* \mathbf{a}})|\{0\}\rangle$$

In order to get the action of the exponential operators on $|\{0\}\rangle$, expand the exponential operators as

$$\mathbf{A}(\alpha)|\{0\}\rangle = \left\{e^{\frac{-|\alpha|^2}{2}}\right\}\sum_n \left\{\frac{(\alpha \mathbf{a}^\dagger)^n}{n!}\right\}\sum_m \left\{\frac{(-\alpha^* \mathbf{a})^m}{m!}\right\}|\{0\}\rangle \tag{6.86}$$

Furthermore, due to Eqs. (5.53), that is,

$$\mathbf{a}|\{n\}\rangle = \sqrt{n}|\{n-1\}\rangle \quad \text{leading to} \quad \mathbf{a}|\{0\}\rangle = 0 \tag{6.87}$$

so that

$$\mathbf{a}^n|\{0\}\rangle = \delta_{o\,n}|\{0\}\rangle$$

Eq. (6.86) reduces to

$$\mathbf{A}(\alpha)|\{0\}\rangle = \left\{e^{\frac{-|\alpha|^2}{2}}\right\}\sum_n \left\{\frac{\alpha^n}{n!}(\mathbf{a}^\dagger)^n\right\}|\{0\}\rangle \tag{6.88}$$

or, keeping in mind Eq. (5.67), that is,

$$(\mathbf{a}^\dagger)^n|\{0\}\rangle = \sqrt{n!}|\{n\}\rangle \tag{6.89}$$

Eq. (6.88) transforms to

$$\mathbf{A}(\alpha)|\{0\}\rangle = \left\{e^{\frac{-|\alpha|^2}{2}}\right\}\sum_n \left\{\frac{\alpha^n}{n!}\sqrt{n!}\right\}|\{n\}\rangle$$

or, after simplification,

$$\mathbf{A}(\alpha)|\{0\}\rangle = \left\{e^{\frac{-|\alpha|^2}{2}}\right\}\sum_n \left\{\frac{\alpha^n}{\sqrt{n!}}\right\}|\{n\}\rangle \tag{6.90}$$

Now, since the expansion of coherent states is given by Eq. (6.16), that is,

$$|\{\alpha\}\rangle = \left\{e^{\frac{-|\alpha|^2}{2}}\right\}\sum_n \left\{\frac{\alpha^n}{\sqrt{n!}}\right\}|\{n\}\rangle \tag{6.91}$$

Then, by identification of Eqs. (6.90) and (6.91), it follows that

$$\boxed{\mathbf{A}(\alpha)|\{0\}\rangle = |\{\alpha\}\rangle} \tag{6.92}$$

or, according to Eq. (6.74)

$$\boxed{e^{\alpha\mathbf{a}^\dagger - \alpha^*\mathbf{a}}|\{0\}\rangle = |\{\alpha\}\rangle \quad \text{with} \quad \mathbf{a}|\{\alpha\}\rangle = \alpha|\{\alpha\}\rangle} \tag{6.93}$$

and thus, after using Glauber's theorem (1.79)

$$\boxed{\left\{e^{\frac{-|\alpha|^2}{2}}\right\}(e^{\alpha\mathbf{a}^\dagger})(e^{-\alpha^*\mathbf{a}})|\{0\}\rangle = |\{\alpha\}\rangle} \tag{6.94}$$

Moreover, observe that due to the last equation of (6.87), leading to

$$(e^{-\alpha^*\mathbf{a}})|\{0\}\rangle = \sum_{n=0}^{\infty}\frac{\alpha^{*n}}{n!}(\mathbf{a})^n|\{0\}\rangle = |\{0\}\rangle$$

Eq. (6.94) simplifies to

$$\boxed{\left\{e^{\frac{-|\alpha|^2}{2}}\right\}(e^{\alpha\mathbf{a}^\dagger})|\{0\}\rangle = |\{\alpha\}\rangle} \tag{6.95}$$

6.6.3 Product of translation operators

Now, consider the two following translation operators where ξ and ζ are c-numbers:

$$\mathbf{A}(\xi) = (e^{\xi \mathbf{a}^\dagger - \xi^* \mathbf{a}}) \qquad \mathbf{A}(\zeta) = (e^{\zeta \mathbf{a}^\dagger - \zeta^* \mathbf{a}})$$

Their product

$$\mathbf{A}(\zeta)\mathbf{A}(\xi) = (e^{\zeta \mathbf{a}^\dagger - \zeta^* \mathbf{a}})(e^{\xi \mathbf{a}^\dagger - \xi^* \mathbf{a}})$$

due to the Glauber theorem (1.78), becomes

$$(e^{\zeta \mathbf{a}^\dagger - \zeta^* \mathbf{a}})(e^{\xi \mathbf{a}^\dagger - \xi^* \mathbf{a}}) = (e^{(\zeta \mathbf{a}^\dagger - \zeta^* \mathbf{a}) + (\xi \mathbf{a}^\dagger - \xi^* \mathbf{a})})(e^{[(\xi \mathbf{a}^\dagger - \xi^* \mathbf{a}),\ (\zeta \mathbf{a}^\dagger - \zeta^* \mathbf{a})]/2}) \tag{6.96}$$

Now, since $[\mathbf{a}, \mathbf{a}^\dagger] = 1$, the commutator appearing on the last right-hand-side term is

$$[(\xi \mathbf{a}^\dagger - \xi^* \mathbf{a}), (\zeta \mathbf{a}^\dagger - \zeta^* \mathbf{a})] = -(\xi\zeta^* - \xi^*\zeta)$$

so that Eq. (6.96) yields

$$\boxed{(e^{\zeta \mathbf{a}^\dagger - \zeta^* \mathbf{a}})(e^{\xi \mathbf{a}^\dagger - \xi^* \mathbf{a}}) = (e^{(\xi+\zeta) \mathbf{a}^\dagger - (\xi^*+\zeta^*) \mathbf{a}})(e^{-(\xi\zeta^* - \xi^*\zeta)/2})} \tag{6.97}$$

6.7 COHERENT-STATE WAVEFUNCTIONS

Owing to the quasi-classical behavior of coherent states, it may be of interest to visualize them through their wave mechanics representation, which is the purpose of the present section.

6.7.1 Wavefunctions

According to Eq. (3.43), the wavefunction corresponding to the coherent state is the scalar product

$$\Phi_\alpha(Q) = \langle \{Q\} | \{\alpha\} \rangle \tag{6.98}$$

which, in view of (6.92), reads

$$\Phi_\alpha(Q) = \langle \{Q\} | \mathbf{A}(\alpha) | \{0\} \rangle \tag{6.99}$$

with, according to Eq. (6.74),

$$\mathbf{A}(\alpha) = e^{\alpha \mathbf{a}^\dagger - \alpha^* \mathbf{a}} \tag{6.100}$$

Again, in view of Eqs. (5.3) and (5.4), the argument of the translation operator reads

$$\alpha \mathbf{a}^\dagger - \alpha^* \mathbf{a} = \left(\alpha \sqrt{\frac{m\omega}{2\hbar}} \mathbf{Q} - i\alpha \sqrt{\frac{1}{2m\hbar\omega}} \mathbf{P} \right) - \left(\alpha^* \sqrt{\frac{m\omega}{2\hbar}} \mathbf{Q} + i\alpha^* \sqrt{\frac{1}{2m\hbar\omega}} \mathbf{P} \right)$$

or, after rearranging,

$$\alpha \mathbf{a}^\dagger - \alpha^* \mathbf{a} = (\alpha - \alpha^*) \sqrt{\frac{m\omega}{2\hbar}} \mathbf{Q} - i(\alpha + \alpha^*) \sqrt{\frac{1}{2m\hbar\omega}} \mathbf{P} \tag{6.101}$$

Furthermore, one obtains, respectively, by inversion of Eqs. (6.44) and (6.45)

$$(\alpha - \alpha^*)\sqrt{\frac{m\omega}{2\hbar}} = \frac{i}{\hbar}\langle\{\alpha\}|\mathbf{P}|\{\alpha\}\rangle = \frac{i}{\hbar}\langle\mathbf{P}\rangle_\alpha \tag{6.102}$$

$$(\alpha + \alpha^*)\sqrt{\frac{1}{2m\hbar\omega}} = \frac{1}{\hbar}\langle\{\alpha\}|\mathbf{Q}|\{\alpha\}\rangle = \frac{1}{\hbar}\langle\mathbf{Q}\rangle_\alpha \tag{6.103}$$

Therefore, owing to Eqs. (6.101)–(6.103), the translation operator (6.100) takes the form

$$\mathbf{A}(\alpha) = e^{i(\langle\mathbf{P}\rangle_\alpha\mathbf{Q} - \langle\mathbf{Q}\rangle_\alpha\mathbf{P})/\hbar}$$

which by the aid of Glauber's theorem (1.78) transforms to

$$\mathbf{A}(\alpha) = (\mathbf{e}^{-i\langle\mathbf{Q}\rangle_\alpha\mathbf{P}/\hbar})(e^{i\langle\mathbf{P}\rangle_\alpha\mathbf{Q}/\hbar})(e^{-\zeta}) \tag{6.104}$$

In the preceding equation, ζ is given by

$$\zeta = \frac{1}{2\hbar^2}\langle\mathbf{P}\rangle_\alpha\langle\mathbf{Q}\rangle_\alpha[\mathbf{Q},\mathbf{P}]$$

which due to $[\mathbf{Q},\mathbf{P}] = i\hbar$ reads

$$\zeta = \frac{i}{2\hbar}\langle\mathbf{P}\rangle_\alpha\langle\mathbf{Q}\rangle_\alpha$$

Or, because of Eqs. (6.102) and (6.103) leads by inversion to

$$\langle\mathbf{Q}\rangle_\alpha = \sqrt{\frac{\hbar}{2m\omega}}\{\alpha^* + \alpha\} \qquad \text{and} \qquad \langle\mathbf{P}\rangle_\alpha = i\sqrt{\frac{\hbar m\omega}{2}}\{\alpha^* - \alpha\}$$

so that we have

$$\zeta = -\tfrac{1}{4}\{\alpha^{*2} - \alpha^2\} \tag{6.105}$$

Here, it is possible to get an explicit expression for the coherent state wavefunction (6.99) corresponding to the coherent state, that is,

$$\Phi_\alpha(Q) = \langle\{Q\}|\{\alpha\}\rangle = \langle\{Q\}|\mathbf{A}(\alpha)|\{0\}\rangle$$

which due to Eqs. (6.104) and (6.105) takes the form

$$\Phi_\alpha(Q) = \langle\{Q\}|(e^{-i\langle\mathbf{Q}\rangle_\alpha\mathbf{P}/\hbar})(e^{i\langle\mathbf{P}\rangle_\alpha\mathbf{Q}/\hbar})|\{0\}\rangle(e^{1/4\{\alpha^{*2}-\alpha^2\}}) \tag{6.106}$$

Now, observe that Eq. (2.119) allows us to write

$$(e^{i\langle\mathbf{Q}\rangle_\alpha\mathbf{P}/\hbar})|\{Q\}\rangle = |\{Q - \langle\mathbf{Q}\rangle_\alpha\}\rangle$$

the Hermitian conjugate of this last equation of which is

$$\langle\{Q\}|(e^{-i\langle\mathbf{Q}\rangle_\alpha\mathbf{P}/\hbar}) = \langle\{Q - \langle\mathbf{Q}\rangle_\alpha\}| \tag{6.107}$$

so that the coherent state wavefunction (6.106) takes the form

$$\Phi_\alpha(Q) = \langle\{Q - \langle\mathbf{Q}\rangle_\alpha\}|(e^{i\langle\mathbf{P}\rangle_\alpha\mathbf{Q}/\hbar})|\{0\}\rangle(e^{1/4\{\alpha^{*2}-\alpha^2\}}) \tag{6.108}$$

In Eq. (6.108), the exponential operator is acting on the left on an eigenbra of the position operator $\mathbf{Q}$ and of all operators functions of $\mathbf{Q}$. Hence, the following eigenvalue equation is verified

$$\langle\{Q - \langle\mathbf{Q}\rangle_\alpha\}|(e^{i\langle\mathbf{P}\rangle_\alpha\mathbf{Q}/\hbar}) = \langle\{Q - \langle\mathbf{Q}\rangle_\alpha\}|(e^{i\langle\mathbf{P}\rangle_\alpha(Q-\langle\mathbf{Q}\rangle_\alpha)/\hbar})$$

so that Eq. (6.108) transforms to

$$\Phi_\alpha(Q) = \langle\{Q - \langle\mathbf{Q}\rangle_\alpha\}|\{0\}\rangle(e^{i\langle\mathbf{P}\rangle_\alpha(Q-\langle\mathbf{Q}\rangle_\alpha)/\hbar})(e^1/4\{\alpha^{*2} - \alpha^2\}) \tag{6.109}$$

On the other hand, since the ground-state wavefunction of the quantum harmonic oscillator Hamiltonian is

$$\Psi_0(Q) = \langle\{Q\}|\{0\}\rangle$$

the scalar product involved in Eq. (6.109) is nothing but the displaced ground-state wavefunction, the origin of which has been displaced by the amount $\langle\mathbf{Q}\rangle_\alpha$, that is,

$$\langle\{Q - \langle\mathbf{Q}\rangle_\alpha\}|\{0\}\rangle = \Psi_0(Q - \langle\mathbf{Q}\rangle_\alpha) \tag{6.110}$$

Now, keeping in mind that the ground-state wavefunction may be obtained using Eqs. (5.126) and (5.127), leading to

$$\Psi_0(Q) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}Q^2\right)$$

the translated wavefunction (6.110) becomes

$$\Psi_0(Q - \langle\mathbf{Q}\rangle_\alpha) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \exp\left[-\frac{m\omega}{2\hbar}(Q - \langle\mathbf{Q}\rangle_\alpha)^2\right] \tag{6.111}$$

Finally, in view of Eq. (6.111), and using the expression (6.51) of the uncertainty $\Delta\mathbf{Q}$ performed over a coherent state, Eq. (6.109) becomes

$$\boxed{\Phi_\alpha(Q) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \exp\left(-\left(\frac{Q - \langle\mathbf{Q}\rangle_\alpha}{2\Delta Q_\alpha}\right)^2\right) \exp\left(\tfrac{i}{\hbar}\langle\mathbf{P}\rangle_\alpha(Q - \langle\mathbf{Q}\rangle_\alpha)\right) \exp\left(\tfrac{1}{4}\{\alpha^{*2} - \alpha^2\}\right)} \tag{6.112}$$

with

$$\langle\mathbf{P}\rangle_\alpha = \langle\{\alpha\}|\mathbf{P}|\{\alpha\}\rangle] \qquad \text{and} \qquad \Delta Q_\alpha = \sqrt{\frac{\hbar}{2m\omega}}$$

Note that Eq. (6.112) may be shortly written in a narrowing form encountered in *wavelet* theory, that is,

$$\Phi_\alpha(Q) = Ke^{-(Q/Q^\circ)^2} e^{i\lambda Q}$$

where K, Q°, and λ are constants that may be obtained when passing from Eq. (6.112) to this expression.

6.7.2 Time-dependent coherent-state wavefunctions

It has been shown above that the wave mechanics representation of the coherent state is given by Eq. (6.112). Now, we require its time dependence, and for this purpose

we transform Eq. (6.112) involving the average values of $\langle \mathbf{Q} \rangle_\alpha$ and $\langle \mathbf{P} \rangle_\alpha$ by taking in place of them the corresponding time-dependent average values $\langle \mathbf{Q}(t) \rangle_\alpha$ and $\langle \mathbf{P}(t) \rangle_\alpha$, leading us to write

$$\Phi_\alpha(Q,t) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \exp\left[-\left(\frac{Q - \langle \mathbf{Q}(t) \rangle_\alpha}{2\Delta Q_\alpha}\right)^2\right] \exp\left[\frac{i}{\hbar}\langle \mathbf{P}(t) \rangle_\alpha (Q - \langle \mathbf{Q}(t) \rangle_\alpha)\right]$$
$$\times (\exp 1/4\{\alpha(t)^{*2} - \alpha(t)^2\}) \tag{6.113}$$

where $\alpha(t)$ is now given by Eq. (6.55). Next, in the Schrödinger picture, and due to Eqs. (6.56) and (6.62), the time-dependent average values involved in Eq. (6.113) are given by

$$\langle \mathbf{Q}(t) \rangle_\alpha = \langle \{\alpha\} | \mathbf{Q}(t) | \{\alpha\} \rangle = \alpha \sqrt{\frac{2\hbar}{m\omega}} \cos \omega t$$

$$\langle \mathbf{P}(t) \rangle_\alpha = \langle \{\alpha\} | \mathbf{P}(t) | \{\alpha\} \rangle = -\alpha \sqrt{2\hbar m\omega} \sin \omega t$$

so that the coherent-state wavefunction (6.113) reads

$$\Phi_\alpha(Q,t) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \exp\left[-\frac{m\omega}{2\hbar}(Q - \alpha\sqrt{\tfrac{2\hbar}{m\omega}} \cos \omega t)^2\right]$$
$$\times \exp\left[-\frac{i}{\hbar}\alpha\sqrt{2\hbar m\omega} \sin \omega t_\alpha \left(Q - \alpha\sqrt{\tfrac{2\hbar}{m\omega}} \cos \omega t\right)\right] \left(\exp\left(i\frac{\alpha^2}{2} \sin 2\omega t\right)\right) \tag{6.114}$$

where α stands for the eigenvalue of the coherent state at initial time. Figure 6.1 reports the time dependence of the corresponding modulus $|\Phi_\alpha(Q,t)|^2$:

$$|\Phi_\alpha(Q,t)|^2 = \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \exp\left[-\frac{m\omega}{\hbar}(Q - \alpha\sqrt{\tfrac{2\hbar}{m\omega}} \cos \omega t)^2\right] \tag{6.115}$$

Inspection of this figure shows that the coherent state initially localized on the right-hand side of the equilibrium position moves back and forth around this position without spreading.

6.8 FRANCK–CONDON FACTORS

One has sometimes to compute the overlap integral (*Franck–Condon factors)* between the eigenfunctions of two oscillator Hamiltonians, the harmonic potentials of which are displaced, and thus not orthogonal, as illustrated in Fig. 6.2. Franck–Condon factors are met, for instance, in the area of electronic molecular spectroscopy where the subbands of the electronic line shapes correspond to transitions between vibrational states of the ground and first excited electronic states, the latter being displaced. They are also found in theories dealing with IR line shapes of weak H-bonded species.

As we have seen above, the energy wavefunctions of the quantum harmonic oscillator are given by the following scalar product:

$$\Psi_n(Q) = \langle \{Q\} | \{n\} \rangle \tag{6.116}$$

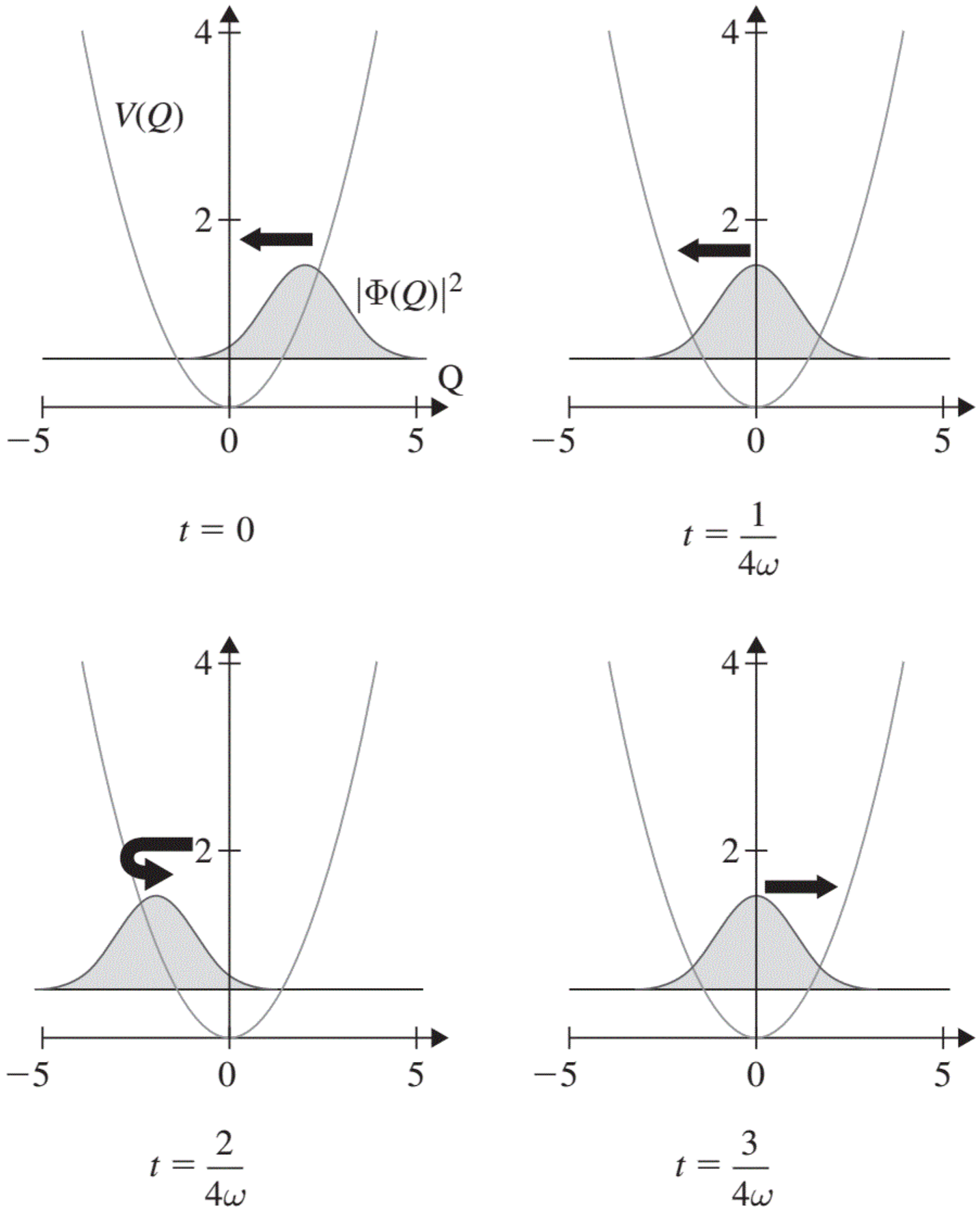


Figure 6.1 Time evolution of the probability density (6.115) of a coherent-state wavefunction, with Q expressed in $\sqrt{\frac{\hbar}{2m\omega}}$ small units, t small in ω^{-1} small units, and $\alpha = 1$,

where $|\{n\}\rangle$ is an eigenket of the number occupation operator. Now, we have shown that the action of the translation operator on an eigenket of the position operator is given by Eq. (2.118), that is,

$$\mathbf{A}(Q^\circ)|\{Q\}\rangle = |\{Q + Q^\circ\}\rangle \tag{6.117}$$

Since the translation operator is unitary, so that its inverse is its Hermitian conjugate, the Hermitian conjugate of Eq. (6.117) is

$$\langle\{Q\}|\mathbf{A}(Q^\circ)^{-1} = \langle\{Q + Q^\circ\}| \tag{6.118}$$

On the other hand, the wavefunction $\{\Psi_m(Q + Q^\circ)\}$ displaced by the amount Q° with respect to that $\Psi_n(Q)$ defined by Eq. (6.116) is given by the scalar product

$$\{\Psi_m(Q + Q^\circ)\} = \langle\{Q + Q^\circ\}|\{m\}\rangle$$

or, in view of Eq. (6.118)

$$\{\Psi_m(Q + Q^\circ)\} = \langle\{Q\}|\mathbf{A}(Q^\circ)^{-1}|\{m\}\rangle \tag{6.119}$$

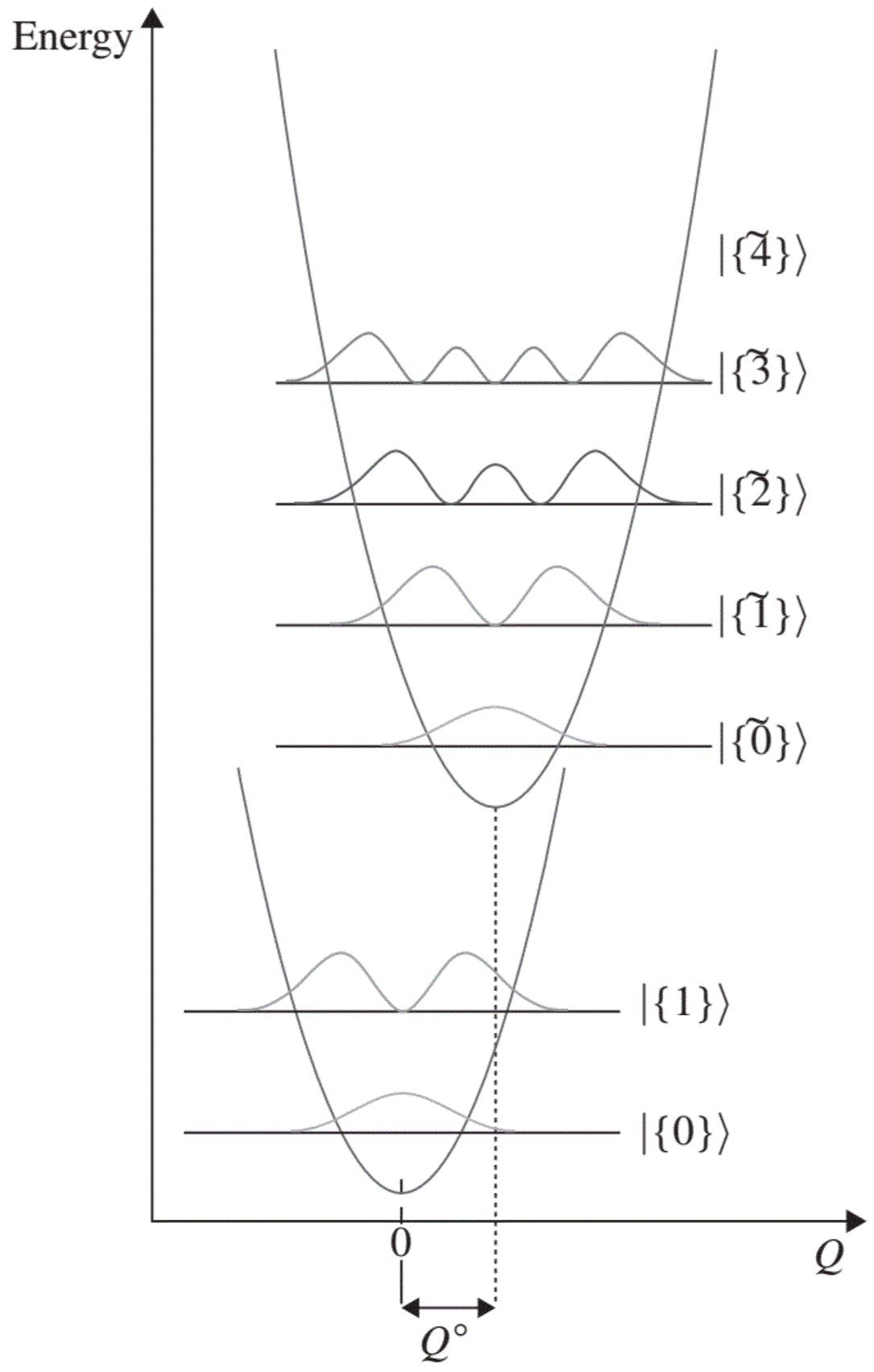


Figure 6.2 Displaced oscillator wavefunctions generating Franck–Condon factors.

Now, look at the Franck–Condon factors, that is, the following overlap integrals

$$\boxed{S_{nm}(Q^\circ) = \int_{-\infty}^{\infty} \{\Psi_n(Q)^*\}\{\Psi_m(Q+Q^\circ)\}dQ} \tag{6.120}$$

which, in view of Eqs. (6.116) and (6.119), take the form

$$S_{nm}(Q^\circ) = \int_{-\infty}^{\infty} \langle\{n\}|\{Q\}\rangle\langle\{Q\}|\mathbf{A}(Q^\circ)^{-1}|\{m\}\rangle\, dQ$$

a result that may be simplified using the closure relation involving the eigenstates of the position operator, that is,

$$\int_{-\infty}^{\infty} |\{Q\}\rangle\langle\{Q\}|\, dQ = 1$$

Thus

$$S_{nm}(Q^\circ) = \langle\{n\}|\mathbf{A}(Q^\circ)^{-1}|\{m\}\rangle \tag{6.121}$$

Next, pass to Boson operators for the translation operators appearing in Eq. (6.121). Then, in view of Eq. (6.74), we have

$$\boxed{S_{nm}(\alpha^\circ) = \langle\{n\}|\ (e^{-\alpha^\circ(\mathbf{a}^\dagger - \mathbf{a})})\ |\{m\}\rangle} \tag{6.122}$$

$$\boxed{S_{nm}(\alpha^\circ) \equiv S_{nm}(Q^\circ) \quad \text{with} \quad \alpha^\circ = Q^\circ\sqrt{\frac{m\omega}{2\hbar}}} \tag{6.123}$$

In order to calculate the Franck–Condon factors, it is convenient to use for the inverse translation operator appearing in Eq. (6.121), the expression (6.79) leading to

$$S_{nm}(\alpha^\circ) = e^{\alpha^{\circ 2}/2}\langle\{n\}|(e^{\alpha^\circ \mathbf{a}})(e^{-\alpha^\circ \mathbf{a}^\dagger})\ |\{m\}\rangle \tag{6.124}$$

or

$$S_{nm}(\alpha^\circ) = e^{\alpha^{\circ 2}/2}\langle\{A\}_n|\{B\}_m\rangle \tag{6.125}$$

with

$$|\{B\}_m\rangle = (e^{-\alpha^\circ \mathbf{a}^\dagger})\ |\{m\}\rangle \qquad \text{and} \qquad \langle\{A\}_n| = \langle\{n\}|(e^{\alpha^\circ \mathbf{a}}) \tag{6.126}$$

We must now compute the scalar product appearing on the right-hand side of Eq. (6.125), and then find in a first place the expression of the ket defined by Eq. (6.126). To obtain it, first expand the exponential appearing on the right-hand side of Eq. (6.126), according to

$$|\{B\}_m\rangle = \sum_k \left(\frac{(-1)^k \alpha^{\circ k}(\mathbf{a}^\dagger)^k}{k!}\right)|\{m\}\rangle \tag{6.127}$$

which, due to Eq. (6.89), is

$$|\{m\}\rangle = \left(\frac{(\mathbf{a}^\dagger)^m}{\sqrt{m!}}\right)|\{0\}\rangle \tag{6.128}$$

Hence, Eq. (6.127) transforms to

$$|\{B\}_m\rangle = \sum_k \left(\frac{(-1)^k \alpha^{\circ k}(\mathbf{a}^\dagger)^{k+m}}{k!\sqrt{m!}}\right)|\{0\}\rangle \tag{6.129}$$

Again, using Eq. (6.128), we have

$$(\mathbf{a}^\dagger)^{k+m}|\{0\}\rangle = \sqrt{(k+m)!}|\{k+m\}\rangle$$

so that Eq. (6.129) becomes

$$|\{B\}_m\rangle = \sum_k \left(\frac{(-1)^k \alpha^{\circ k}\sqrt{(k+m)!}}{k!\sqrt{m!}}\right)|\{k+m\}\rangle \tag{6.130}$$

Now, save that the minus sign is changed into a plus sign, the bra appearing on the right-hand side of Eq. (6.125) is the Hermitian conjugate of Eq. (6.126), so that it is

given by an expression similar to that of (6.130), except for the presence of the power of (-1). Hence, α° being real, this bra appears to be

$$\langle\{A\}_n| = \sum_l \left(\frac{\alpha^{\circ l}\sqrt{(l+n)!}}{l!\sqrt{n!}} \right) \langle\{l+n\}| \tag{6.131}$$

Thus, as a consequence of Eqs. (6.130) and (6.131), the Franck–Condon factors (6.125) take the form

$$S_{nm}(\alpha^\circ) = e^{\alpha^{\circ 2}/2} \sum_k \sum_l \left(\frac{(-1)^k \alpha^{\circ k+l}\sqrt{(l+n)!}\sqrt{(k+m)!}}{l!\sqrt{n!}k!\sqrt{m!}} \right) \langle\{l+n\}|\{k+m\}\rangle \tag{6.132}$$

Finally, due to

$$\langle\{l+n\}|\{k+m\}\rangle = \delta_{l,k+m-n}$$

Eq. (6.132) reduces to

$$\boxed{S_{nm}(\alpha^\circ) = e^{\alpha^{\circ 2}/2} \sum_{k=n-m} \left(\frac{(-1)^k \alpha^{\circ 2k+m-n}\,(k+m)!}{(k+m-n)!\sqrt{n!}k!\sqrt{m!}} \right) \quad \text{with} \quad n \geq m} \tag{6.133}$$

with a similar expression for the situation where $m > n$ in which m is changed into n and vice versa.

6.9 DRIVEN HARMONIC OSCILLATORS

Using the work in the present chapter, it is now possible to find the energy levels of driven harmonic oscillators, the Hamiltonian of which is

$$\mathbf{H}_{\mathrm{Dr}} = \left(\frac{\mathbf{P}^2}{2M} + \frac{1}{2}M\omega^2\mathbf{Q}^2 \right) + b\mathbf{Q}$$

Passing to Boson operators by the aid of Eqs. (5.6), (5.7), and (5.9), this Hamiltonian becomes

$$\mathbf{H}_{\mathrm{Dr}} = \hbar\omega\left(\mathbf{a}^\dagger\mathbf{a} + \tfrac{1}{2}\right) + \alpha^\circ\hbar\omega(\mathbf{a}^\dagger + \mathbf{a}) \tag{6.134}$$

with

$$\alpha^\circ = \frac{b}{\omega}\sqrt{\frac{1}{2M\hbar\omega}}$$

6.9.1 Diagonalization of driven Hamiltonians by aid of translation operators

6.9.1.1 Canonical transformations involving translation operators In order to diagonalize the Hamiltonian operator (6.134), consider the matrix elements of this operator in the basis of the eigenstates of the quantum harmonic oscillator:

$$\langle\{n\}|\mathbf{H}_{\mathrm{Dr}}|\{m\}\rangle = \langle\{n\}|\{\left(\mathbf{a}^\dagger\mathbf{a} + \tfrac{1}{2}\right) + \alpha^\circ(\mathbf{a}^\dagger + \mathbf{a})\}|\{m\}\rangle\hbar\omega \tag{6.135}$$

Next, insert the unity operator built up from the translation operator through

$$\mathbf{1} = \mathbf{A}(\alpha^\circ)^{-1}\mathbf{A}(\alpha^\circ)$$

with

$$\mathbf{A}(\alpha^\circ) = e^{\alpha^\circ \mathbf{a}^\dagger - \alpha^\circ \mathbf{a}} \tag{6.136}$$

in such a way as to write

$$\begin{aligned}\langle\{n\}|\mathbf{A}(\alpha^\circ)^{-1}\mathbf{A}(\alpha^\circ)\mathbf{H}_{\mathrm{Dr}}\mathbf{A}(\alpha^\circ)^{-1}\mathbf{A}(\alpha^\circ)|\{m\}\rangle \\ = \langle\{n\}|\mathbf{A}(\alpha^\circ)^{-1}\mathbf{A}(\alpha^\circ) \\ \times\left\{\left(\mathbf{a}^\dagger\mathbf{a}+\tfrac{1}{2}\right)+\alpha^\circ(\mathbf{a}^\dagger+\mathbf{a})\right\}\mathbf{A}(\alpha^\circ)^{-1}\mathbf{A}(\alpha^\circ)|\{m\}\rangle\hbar\omega \qquad (6.137)\end{aligned}$$

Now, observe that the action of the translation operator transforms the eigenstates of the harmonic Hamiltonian into new displaced ones according to

$$\mathbf{A}(\alpha^\circ)|\{n\}\rangle = |\{\tilde{n}\}\rangle \tag{6.138}$$

$$\langle\{n\}|\mathbf{A}(\alpha^\circ)^{-1} = \langle\{\tilde{n}\}| \tag{6.139}$$

In order to get the expression of the real oscillator wavefunction corresponding to the transformed ket (6.138) observe that, due to Eq. (6.116), the wavefunction corresponding to the states $|\{n\}\rangle$ is given by

$$\Psi_n(Q) = \langle\{Q\}|\{n\}\rangle = \langle\{n\}|\{Q\}\rangle$$

whereas the wavefunction corresponding to the bra $\langle\{\tilde{n}\}|$ appearing in Eq. (6.139), and resulting from the action of the translation operator (involving a real α°), is

$$\Psi_{\tilde{n}}(Q) = \langle\{Q\}|\{\tilde{n}\}\rangle$$

or, due to Eq. (6.139),

$$\Psi_{\tilde{n}}(Q) = \langle\{Q\}|\mathbf{A}(\alpha^\circ)^{-1}|\{n\}\rangle$$

and thus, owing to Eqs. (6.75) and (6.77),

$$\Psi_{\tilde{n}}(Q) = \langle\{Q\}|\mathbf{A}(-Q^\circ)|\{n\}\rangle \tag{6.140}$$

with

$$\alpha^\circ = Q^\circ\sqrt{\frac{m\omega}{2\hbar}}$$

Next, due to Eq. (6.117) leading to

$$\mathbf{A}(-Q^\circ)|\{Q\}\rangle = |\{Q - Q^\circ\}\rangle$$

Eq. (6.140) reads

$$\Psi_{\tilde{n}}(Q) = \langle\{Q - Q^\circ\}|\{n\}\rangle$$

or

$$\Psi_{\tilde{n}}(Q) = \Psi_n(Q - Q^\circ)$$

with

$$\Psi_n(Q - Q^\circ) = \langle \{Q - Q^\circ\} | \{n\} \rangle$$

In a similar way, one would obtain

$$\Psi_{\tilde{m}}(Q) = \Psi_m(Q - Q^\circ) = \langle \{Q - Q^\circ\} | \{m\} \rangle$$

Now, in the context of the transformed states (6.138) and (6.139) corresponding to the wavefunction $\Psi_n(Q - Q^\circ)$, which is displaced by the amount $-Q^\circ$, let us introduce the following transformed Hamiltonian:

$$\tilde{\mathbf{H}}_{\mathrm{Dr}} = \mathbf{A}(\alpha^\circ)\mathbf{H}_{\mathrm{Dr}}\mathbf{A}(\alpha^\circ)^{-1} \tag{6.141}$$

6.9.1.2 Hamiltonian diagonalization by the canonical transformation Then, owing to Eqs. (6.137) and (6.141), the matrix elements of the transformed Hamiltonian $\tilde{\mathbf{H}}_{\mathrm{Dr}}$ take the form

$$\begin{aligned}\langle \{\tilde{n}\} | \tilde{\mathbf{H}}_{\mathrm{Dr}} | \{\tilde{m}\} \rangle = {} & \tfrac{1}{2}\hbar\omega + \langle \{\tilde{n}\} | \mathbf{A}(\alpha^\circ)\mathbf{a}^\dagger\mathbf{a}\, \mathbf{A}(\alpha^\circ)^{-1} | \{\tilde{m}\} \rangle \hbar\omega \\ & + \alpha^\circ \langle \{\tilde{n}\} | \mathbf{A}(\alpha^\circ)(\mathbf{a}^\dagger + \mathbf{a})\mathbf{A}(\alpha^\circ)^{-1} | \{\tilde{m}\} \rangle \hbar\omega \end{aligned} \tag{6.142}$$

Moreover, observe that, according to Eq. (6.81), one has

$$\mathbf{A}(\alpha^\circ)\mathbf{a}^\dagger\mathbf{A}(\alpha^\circ)^{-1} = \mathbf{a}^\dagger - \alpha^\circ \tag{6.143}$$

$$\mathbf{A}(\alpha^\circ)\mathbf{a}\mathbf{A}(\alpha^\circ)^{-1} = \mathbf{a} - \alpha^\circ \tag{6.144}$$

Now, in order to get the result of the canonical transformation on $\mathbf{a}^\dagger\mathbf{a}$ appearing in Eq. (6.142), insert between $\mathbf{a}^\dagger$ and $\mathbf{a}$ the unity operator built up from the unitary translation operator, as follows:

$$\mathbf{A}(\alpha^\circ)\mathbf{a}^\dagger\mathbf{a}\mathbf{A}(\alpha^\circ)^{-1} = \mathbf{A}(\alpha^\circ)\mathbf{a}^\dagger\mathbf{A}(\alpha^\circ)^{-1}\mathbf{A}(\alpha^\circ)\, \mathbf{a}\, \mathbf{A}(\alpha^\circ)^{-1}$$

Then, in view of Eqs. (6.143) and (6.144), we have

$$\mathbf{A}(\alpha^\circ)\mathbf{a}^\dagger\mathbf{a}\mathbf{A}(\alpha^\circ)^{-1} = (\mathbf{a}^\dagger - \alpha^\circ)(\mathbf{a} - \alpha^\circ)$$

Hence, owing to this result and to Eqs. (6.143) and (6.144), the sum of the transformed operators appearing on the right-hand side of Eq. (6.142) yields

$$\begin{aligned}& \mathbf{A}(\alpha^\circ)\mathbf{a}^\dagger\mathbf{a}\, \mathbf{A}(\alpha^\circ)^{-1} + \mathbf{A}(\alpha^\circ)(\mathbf{a}^\dagger + \mathbf{a})\mathbf{A}(\alpha^\circ)^{-1} \\ & = \mathbf{a}^\dagger\mathbf{a} - \alpha^\circ(\mathbf{a}^\dagger + \mathbf{a}) + \alpha^{\circ 2} + \alpha^\circ(\mathbf{a}^\dagger + \mathbf{a}) - 2\alpha^{\circ 2}\end{aligned}$$

or, after simplification

$$\mathbf{A}(\alpha^\circ)(\mathbf{a}^\dagger\mathbf{a} + \alpha^\circ(\mathbf{a}^\dagger + \mathbf{a}))\mathbf{A}(\alpha^\circ)^{-1} = \mathbf{a}^\dagger\mathbf{a} - \alpha^{\circ 2}$$

Therefore, according to these results and to Eqs. (6.138) and (6.139), Eq. (6.142) reduces to

$$\langle \{\tilde{n}\} | \tilde{\mathbf{H}}_{\mathrm{Dr}} | \{\tilde{m}\} \rangle = \langle \{\tilde{n}\} | \left(\mathbf{a}^\dagger\mathbf{a} + \tfrac{1}{2} - \alpha^{\circ 2} \right) | \{\tilde{m}\} \rangle \hbar\omega$$

or, due to Eq. (5.40),

$$\langle \{\tilde{n}\} | \tilde{\mathbf{H}}_{\mathrm{Dr}} | \{\tilde{m}\} \rangle = \left\{ \left(\tilde{n} + \tfrac{1}{2} \right) - \alpha^{\circ 2} \right\} \hbar\omega \delta_{\tilde{m}\tilde{n}} \tag{6.145}$$

Therefore, since, according to Eq. (6.145), the Hamiltonian $\tilde{\mathbf{H}}_{\mathrm{Dr}}$ is diagonal in the basis $\{|\{\tilde{n}\}\rangle\}$ obtained from that $\{|\{n\}\rangle\}$ through the canonical transformation (6.138), it appears that the following eigenvalue equation has been solved:

$$\tilde{\mathbf{H}}_{\mathrm{Dr}}|\{\tilde{n}\}\rangle = E_{\tilde{n}}\,|\{\tilde{n}\}\rangle$$

with the eigenvalues

$$E_{\tilde{n}} = \left\{\left(\tilde{n} + \tfrac{1}{2}\right) - \alpha^{\circ 2}\right\}\hbar\omega$$

6.9.2 Diagonalization of the Hamiltonian matrix representation

Besides the above canonical diagonalization of the driven harmonic oscillator Hamiltonian (6.134), it is also possible to diagonalize the matrix representation (6.135) of this Hamiltonian.

6.9.2.1 Matrix elements of the driven Hamiltonian in the basis of the harmonic Hamiltonian Consider Eq. (6.135):

$$\langle\{n\}|\mathbf{H}_{\mathrm{Dr}}|\{m\}\rangle = \langle\{n\}|\left(\mathbf{a}^{\dagger}\mathbf{a} + \alpha^{\circ}(\mathbf{a}^{\dagger} + \mathbf{a}) + \tfrac{1}{2}\right)|\{m\}\rangle\hbar\omega$$

Next, in view of Eq. (5.40), we have

$$\langle\{n\}|\mathbf{H}_{\mathrm{Dr}}|\{\,m\}\rangle = \alpha^{\circ}\langle\{n\}|(\mathbf{a}^{\dagger} + \mathbf{a})|\{m\}\rangle\hbar\omega + \left(m + \tfrac{1}{2}\right)\langle\{n\}|\{m\}\rangle\hbar\omega \tag{6.146}$$

Now, keeping in mind Eq. (5.40), allowing one to write

$$\mathbf{a}|\{m\}\rangle = \sqrt{m}|\{m-1\}\rangle \qquad \text{and} \qquad \langle\{n\}|\mathbf{a}^{\dagger} = \sqrt{n}\langle\{n-1\}|$$

the matrix elements (6.146) read

$$\begin{aligned}\langle\{n\}|\mathbf{H}_{\mathrm{Dr}}|\{m\}\rangle \;=\; & \alpha^{\circ}(\sqrt{n}\,\langle\{n-1\}|\{m\}\rangle\hbar\omega + \sqrt{m}\,\langle\{n\}|\{m-1\}\rangle) \\ & +(m+\tfrac{1}{2})\langle\{n\}|\{m\}\rangle\hbar\omega \end{aligned} \tag{6.147}$$

which are zero because of the orthonormality properties of the eigenstates of the quantum harmonic Hamiltonian, except the following cases:

$$\langle\{n\}|\mathbf{H}_{\mathrm{Dr}}|\{n\}\rangle = \hbar\omega\left(n + \tfrac{1}{2}\right) \tag{6.148}$$

$$\langle\{n\}|\mathbf{H}_{\mathrm{Dr}}|\{n-1\}\rangle = \alpha^{\circ}\hbar\omega(\sqrt{n} + \sqrt{n-1}) \tag{6.149}$$

with, since the matrix is Hermitian,

$$\langle\{n-1\}|\mathbf{H}_{\mathrm{Dr}}|\{n\}\rangle = \langle\{n\}|\mathbf{H}_{\mathrm{Dr}}|\{n-1\}\rangle \tag{6.150}$$

6.9.2.2 Truncation and diagonalization of the matrix representation The matrix elements involved in the matrix representation of the Hamiltonian (6.134) may be computed using Eqs. (6.148)–(6.150). This Hamiltonian matrix may be built up by starting from the ground-state $|\{0\}\rangle$ and then increasing progressively the quantum number n associated with the kets $|\{n\}\rangle$ and with the bras $\langle\{n\}|$. Now, since the kets and bras appearing in Eq. (6.147) belong to a basis that is infinite, the matrix representation must also be infinite. Thus, in order to be numerically diagonalized, the Hamiltonian matrix (6.135) of the Hamiltonian (6.134) must be truncated beyond some value n° of

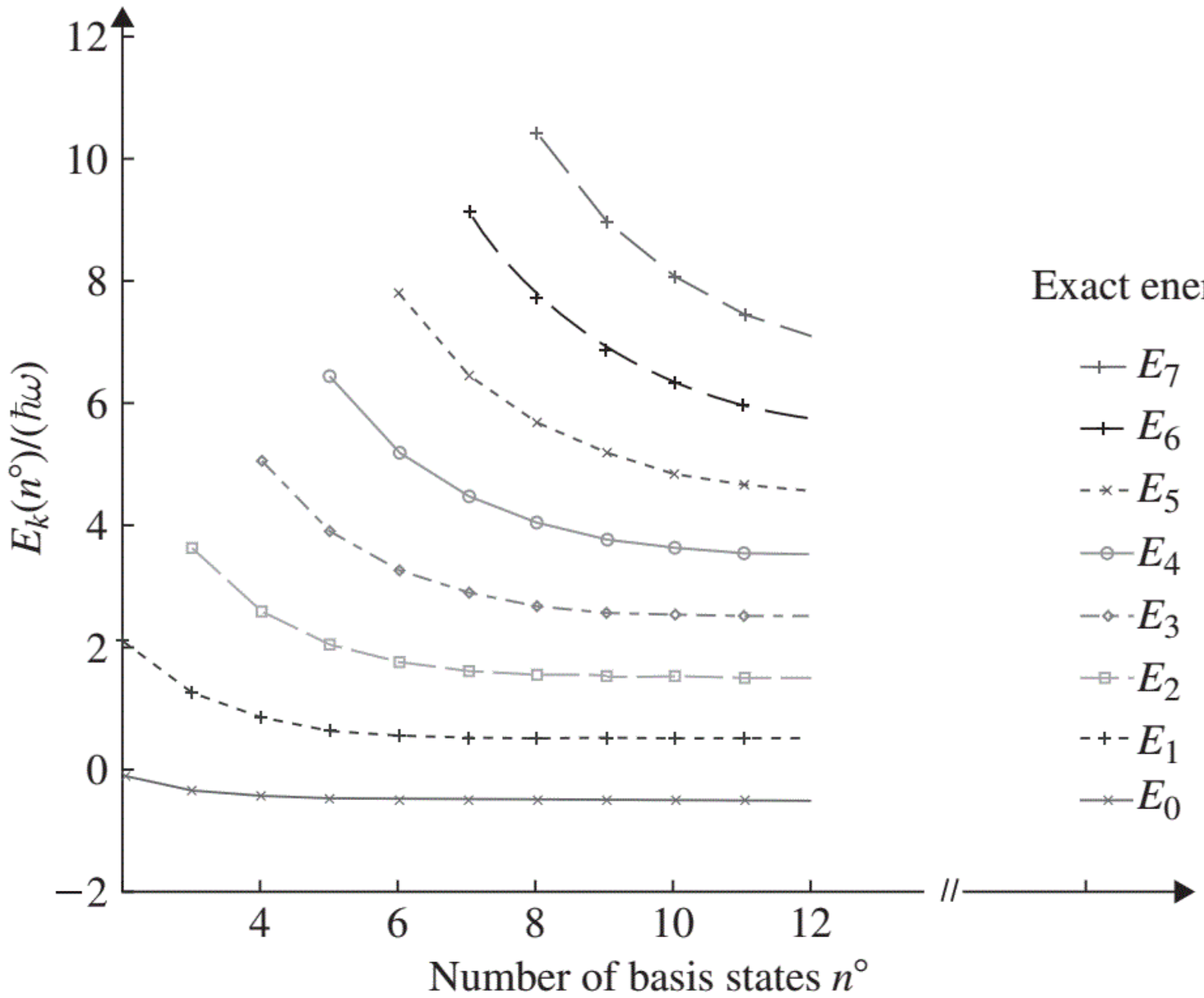


Figure 6.3 Stabilization of the energy of the eight lowest eigenvalues $E_k(n^\circ)/\hbar\omega^\circ$ with respect to n°. (See color insert.)

the quantum number n, leading, therefore, to a finite square $(n^\circ + 1) \times (n^\circ + 1)$ matrix involving the parameters $\hbar\omega$ and α°. The diagonalization of this truncated matrix leads to approximate solutions $E_k(n^\circ)$ of the exact eigenvalue equation

$$\mathbf{H}|\Psi_k(n^\circ)\rangle = E_k|\Psi_k(n^\circ)\rangle$$

Figure 6.3 shows the dependence of the eight lowest eigenvalues $E_k(n^\circ)$ on n° when $\alpha^\circ = 1$.

Inspection of the figure shows that when n° is progressively increased, the lowest eigenvalues $E_k(n^\circ)$ decrease progressively and then stabilize toward their exact values obtained by the aid of Eq. (6.145). Such a result manifests the ability to satisfactorily obtain the eigenvalues of a Hamiltonian by diagonalizing its truncated matrix representations by increasing progressively its dimensions until energy level stabilization occurs. That will be later applied to get the energy levels of anharmonic oscillators for which the direct diagonalization of the Hamiltonian is very difficult or impossible to perform. Now, it may be of interest to observe that, as required from the variation theorem (2.25), the energy of the ground state is lowered when improving the accuracy of the corresponding eigenfunction by increasing the dimension of the truncated basis.

6.10 CONCLUSION

In this chapter, devoted to coherent states assumed to be eigenstates of the lowering operator, the following results have been obtained: (i) the expansion of the coherent states over the eigenstates of the harmonic oscillator Hamiltonian, (ii) the fact that they minimize the Heisenberg uncertainty relations, (iii) the fact that they may

be generated by the action of the translation operator on these eigenkets, and (iv) their wave mechanics representation. In addition, using the translation operator, it has been possible to get the overlap (Franck–Condon factors) between two mutually translated eigenstates of the harmonic Hamiltonian. Moreover, it has been shown how to diagonalize the Hamiltonian of a driven harmonic oscillator by aid of a canonical transformation involving translation operators. Finally, this result allows one to verify the accuracy of the energy levels obtained by diagonalizations of truncated matrix representations of the driven harmonic oscillator Hamiltonian, opening therefore a possibility to obtain numerically the energy levels of anharmonic oscillators for which no analytical expression is available. The most important results of this chapter are listed as follows:

Definition of coherent states
$\mathbf{a}\|\{\alpha\}\rangle = \alpha\|\{\alpha\}\rangle \quad \text{and} \quad \langle\{\alpha\}\|\mathbf{a}^\dagger = \alpha^*\langle\{\alpha\}\|$
Coherent-state expansion in terms of the $\mathbf{a}^\dagger\mathbf{a}$ eigenkets:
$\|\{\alpha\}\rangle = e^{-\|\alpha\|^2/2}\sum_n \left(\frac{\alpha^n}{\sqrt{n!}}\right)\|\{n\}\rangle$
Scalar product between two coherent states:
$\langle\{\beta\}\|\{\alpha\}\rangle = e^{-\|\alpha-\beta\|^2/2}$
Closure relations over coherent states:
$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\|\{\alpha\}\rangle\langle\{\alpha\}\|d\,\mathrm{Re}(\alpha)d\,\mathrm{Im}(\alpha) = 1$
Translation operators:
$\mathbf{A}(\alpha^\circ) = e^{\alpha^\circ\mathbf{a}^\dagger - \alpha^\circ\mathbf{a}} = e^{-\alpha^\circ\mathbf{a} + \alpha^\circ\mathbf{a}^\dagger}$
Generation of coherent states by action of the translation operator:
$\|\{\alpha\}\rangle = \mathbf{A}(\alpha^\circ)\|\{0\}\rangle$

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CHAPTER 7

BOSON OPERATOR THEOREMS

INTRODUCTION

In Chapter 5, some important properties of the ladder operators were found, particularly their action on the eigenkets of the number occupation operator. However, many other theorems dealing with the Boson operators, which are also important when working for not only a single quantum harmonic oscillator but in the context of anharmonic oscillators or sets of coupled harmonic oscillators, exist. The aim of the present chapter is to treat these theorems. This chapter deals with by canonical transformations involving the ladder operators. Then, we consider the normal and antinormal ordering formalism that allows one to pass from equations dealing with noncommuting ladder operators to equations involving only scalars, which are easier to solve and then, after solution, to return to the operator equations that are themselves the solutions of the starting operator equations. A final section illustrates this formalism by applying the procedure to the calculation of time evolution operators of driven quantum harmonic oscillators.

7.1 CANONICAL TRANSFORMATIONS

Here, we shall prove theorems dealing with different canonical transformations on functions of Boson operators, involving operators that are also functions of these Boson operators.

7.1.1 Transformations involving translation operators

Start from the Baker–Campbell–Hausdorff relation given by Eq. (1.77):

$$(e^{\xi \mathbf{A}})\{\mathbf{f}(\mathbf{B})\}(e^{-\xi \mathbf{A}}) = \{\mathbf{f}(e^{\xi \mathbf{A}}\mathbf{B}e^{-\xi \mathbf{A}})\} \tag{7.1}$$

where ξ is a c-number, whereas $\mathbf{f}$, $\mathbf{A}$, and $\mathbf{B}$ are linear operators. Now, apply this relation to the situation where $\mathbf{A}$ is the Boson operator $\mathbf{a}$ and where $\mathbf{f}(\mathbf{B})$ is a function of both $\mathbf{a}$ and its Hermitian conjugate $\mathbf{a}^\dagger$, that is,

$$\mathbf{A} = \mathbf{a} \qquad \text{and} \qquad \mathbf{f}(\mathbf{B}) = \mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)$$

Then, Eq. (7.1) takes the form

$$(e^{\xi \mathbf{a}})\{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}(e^{-\xi \mathbf{a}}) = \{\mathbf{f}((e^{\xi \mathbf{a}}\mathbf{a}e^{-\xi \mathbf{a}}), (e^{\xi \mathbf{a}}\mathbf{a}^\dagger e^{-\xi \mathbf{a}}))\} \tag{7.2}$$

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Now, since any function of a single operator commutes with this operator, the following relation is verified:

$$(e^{\xi \mathbf{a}})\,\mathbf{a}\,(e^{-\xi \mathbf{a}}) = \mathbf{a} \tag{7.3}$$

whereas, due to Eq. (6.84)

$$(e^{\xi \mathbf{a}})\,\mathbf{a}^\dagger (e^{-\xi \mathbf{a}}) = \mathbf{a}^\dagger + \xi \tag{7.4}$$

Thus, owing to Eqs. (7.3) and (7.4), Eq. (7.2) transforms to

$$\boxed{(e^{\xi \mathbf{a}})\{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}(e^{-\xi \mathbf{a}}) = \{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger + \xi)\}} \tag{7.5}$$

Now, apply Eq. (7.1) to another special situation by changing ξ into $-\xi^*$ and taking

$$\mathbf{A} = \mathbf{a}^\dagger \qquad \text{and} \qquad \{\mathbf{f}(\mathbf{B})\} = \{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}$$

Then, Eq. (7.1) reads

$$(e^{-\xi^* \mathbf{a}^\dagger})\{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}(e^{\xi^* \mathbf{a}^\dagger}) = \{\mathbf{f}(e^{-\xi^* \mathbf{a}^\dagger} \mathbf{a} e^{\xi^* \mathbf{a}^\dagger}, e^{-\xi^* \mathbf{a}^\dagger} a^\dagger e^{\xi^* \mathbf{a}^\dagger})\} \tag{7.6}$$

Of course, for the same reasons as those used to obtain Eq. (7.3), one has

$$(e^{-\xi^* \mathbf{a}^\dagger})\,\mathbf{a}^\dagger (e^{\xi^* \mathbf{a}^\dagger}) = \mathbf{a}^\dagger$$

Besides, according to Eq. (6.85), we have

$$(e^{-\xi^* \mathbf{a}^\dagger})\,\mathbf{a} (e^{\xi^* \mathbf{a}^\dagger}) = \mathbf{a} + \xi^*$$

Thus, the canonical transformation (7.6) reads

$$\boxed{(e^{-\xi^* \mathbf{a}^\dagger})\{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}(e^{\xi^* \mathbf{a}^\dagger}) = \{\mathbf{f}(\mathbf{a} + \xi^*, \mathbf{a}^\dagger)\}} \tag{7.7}$$

Next, consider the general transformation

$$(e^{-\xi^* \mathbf{a}^\dagger})(e^{\xi \mathbf{a}})\{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}(e^{-\xi \mathbf{a}})(e^{\xi^* \mathbf{a}^\dagger}) \equiv (e^{-\xi^* \mathbf{a}^\dagger})\{(e^{\xi \mathbf{a}})\{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}(e^{-\xi \mathbf{a}})\}(e^{\xi^* \mathbf{a}^\dagger})$$

which, due to Eq. (7.5), reads

$$(e^{-\xi^* \mathbf{a}^\dagger})(e^{\xi \mathbf{a}})\{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}(e^{-\xi \mathbf{a}})(e^{\xi^* \mathbf{a}^\dagger}) = (e^{-\xi^* \mathbf{a}^\dagger})\{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger + \xi)\}(e^{\xi^* \mathbf{a}^\dagger})$$

and owing to Eq. (7.7) transforms to

$$\boxed{(e^{-\xi^* \mathbf{a}^\dagger})(e^{\xi \mathbf{a}})\{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}(e^{-\xi \mathbf{a}})(e^{\xi^* \mathbf{a}^\dagger}) = \{\mathbf{f}(\mathbf{a} + \xi^*, \mathbf{a}^\dagger + \xi)\}} \tag{7.8}$$

Hence, using the Glauber theorem (1.79), we have

$$(e^{[\mathbf{a}^\dagger, \mathbf{a}]|\xi|^2/2})(e^{-\xi^* \mathbf{a}^\dagger + \xi \mathbf{a}})\{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}(e^{\xi^* \mathbf{a}^\dagger - \xi \mathbf{a}})(e^{-[\mathbf{a}^\dagger, \mathbf{a}]|\xi|^2/2}) = \{\mathbf{f}(\mathbf{a} + \xi^*, \mathbf{a}^\dagger + \xi)\}$$

or, after simplification,

$$(e^{-\xi^* \mathbf{a}^\dagger + \xi \mathbf{a}})\{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}(e^{\xi^* \mathbf{a}^\dagger - \xi \mathbf{a}}) = \{\mathbf{f}(\mathbf{a} + \xi^*, \mathbf{a}^\dagger + \xi)\}$$

so that, noting the definition of the translation operator (6.74),

$$\boxed{\mathbf{A}(\xi)^{-1}\{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}\mathbf{A}(\xi) = \{\mathbf{f}(\mathbf{a} + \xi^*, \mathbf{a}^\dagger + \xi)\}} \tag{7.9}$$

with

$$\mathbf{A}(\xi) = (e^{\xi^* \mathbf{a}^\dagger - \xi \mathbf{a}}) \tag{7.10}$$

7.1.2 Transformations involving number occupation operator exponentials

7.1.2.1 Transformations of the ladder operators Now, consider the following canonical transformation in which ξ is a c-number:

$$\mathbf{g}(\xi) = (e^{\xi \mathbf{a}^\dagger \mathbf{a}})\mathbf{a}(e^{-\xi \mathbf{a}^\dagger \mathbf{a}}) \tag{7.11}$$

which for $\xi = 0$ reads

$$\mathbf{g}(0) = \mathbf{a} \tag{7.12}$$

The derivative of (7.11) with respect to ξ yields

$$\left(\frac{d\mathbf{g}(\xi)}{d\xi}\right) = \left(\frac{d}{d\xi} e^{\xi \mathbf{a}^\dagger \mathbf{a}}\right) \mathbf{a}(e^{-\xi \mathbf{a}^\dagger \mathbf{a}}) + (e^{\xi \mathbf{a}^\dagger \mathbf{a}})\, \mathbf{a} \left(\frac{d}{d\xi} e^{-\xi \mathbf{a}^\dagger \mathbf{a}}\right)$$

or

$$\left(\frac{d\mathbf{g}(\xi)}{d\xi}\right) = (\mathbf{a}^\dagger \mathbf{a}\, e^{\xi \mathbf{a}^\dagger \mathbf{a}})\, \mathbf{a}\, (e^{-\xi \mathbf{a}^\dagger \mathbf{a}}) - (e^{\xi \mathbf{a}^\dagger \mathbf{a}})\, \mathbf{a}\, (\mathbf{a}^\dagger \mathbf{a}\, e^{-\xi \mathbf{a}^\dagger \mathbf{a}}) \tag{7.13}$$

Again, since $\mathbf{a}^\dagger \mathbf{a}$ commutes with all functions of the product $\mathbf{a}^\dagger \mathbf{a}$, the first right-hand-side term of Eq. (7.13) becomes

$$(\mathbf{a}^\dagger \mathbf{a}\, e^{\xi \mathbf{a}^\dagger \mathbf{a}})\mathbf{a}(e^{-\xi \mathbf{a}^\dagger \mathbf{a}}) = (e^{\xi \mathbf{a}^\dagger \mathbf{a}} \mathbf{a}^\dagger \mathbf{a})\, \mathbf{a}\, (e^{-\xi \mathbf{a}^\dagger \mathbf{a}})$$

so that eq. (7.13) transforms to

$$\left(\frac{d\mathbf{g}(\xi)}{d\xi}\right) = (e^{\xi \mathbf{a}^\dagger \mathbf{a}})(\mathbf{a}^\dagger \mathbf{a}\mathbf{a} - \mathbf{a}\mathbf{a}^\dagger \mathbf{a})(e^{-\xi \mathbf{a}^\dagger \mathbf{a}})$$

or

$$\left(\frac{d\mathbf{g}(\xi)}{d\xi}\right) = (e^{\xi \mathbf{a}^\dagger \mathbf{a}})[\mathbf{a}^\dagger, \mathbf{a}]\, \mathbf{a}\, (e^{-\xi \mathbf{a}^\dagger \mathbf{a}}) \tag{7.14}$$

Again, using $[\mathbf{a}, \mathbf{a}^\dagger] = 1$, Eq. (7.14) transforms to

$$\left(\frac{d\mathbf{g}(\xi)}{d\xi}\right) = -(e^{\xi \mathbf{a}^\dagger \mathbf{a}})\, \mathbf{a}\, (e^{-\xi \mathbf{a}^\dagger \mathbf{a}})$$

and, in view of Eq. (7.11), into

$$\left(\frac{d\mathbf{g}(\xi)}{d\xi}\right) = -\mathbf{g}(\xi) \tag{7.15}$$

Next, by derivation of both terms of Eq. (7.15) with respect to ξ, that is,

$$\left(\frac{d^2\mathbf{g}(\xi)}{d\xi^2}\right) = -\left(\frac{d\, \mathbf{g}(\xi)}{d\xi}\right)$$

and, due to Eq. (7.15), it reads

$$\left(\frac{d^2\mathbf{g}(\xi)}{d\xi^2}\right) = \mathbf{g}(\xi)$$

Again, by recurrence, one obtains

$$\left(\frac{d^n\mathbf{g}(\xi)}{d\xi^n}\right) = (-1)^n \mathbf{g}(\xi) \tag{7.16}$$

Now, at $\xi = 0$, and in view of Eq. (7.12), the nth derivative given by Eq. (7.16) reduces to

$$\left(\frac{d^n \mathbf{g}(\xi)}{d\xi^n}\right)_{\xi=0} = (-1)^n \mathbf{a} \tag{7.17}$$

Next, write the Taylor expansion of the function (7.11) around $\xi = 0$, that is,

$$\mathbf{g}(\xi) = \mathbf{g}(0) + \left(\frac{d\mathbf{g}(\xi)}{d\xi}\right)_{\xi=0} \xi + \frac{1}{2}\left(\frac{d^2\mathbf{g}(\xi)}{d\xi^2}\right)_{\xi=0} \xi^2 + \frac{1}{3!}\left(\frac{d^3\mathbf{g}(\xi)}{d\xi^3}\right)_{\xi=0} \xi^3 \ldots$$

Hence, comparing Eqs. (7.12) and (7.17), this expansion takes the form

$$\mathbf{g}(\xi) = \mathbf{a}\left(1 - \xi + \frac{1}{2}\xi^2 - \frac{1}{3!}\xi^3 \ldots..\right)$$

or, passing from the expansion to its corresponding exponential expression,

$$\mathbf{g}(\xi) = \mathbf{a}(e^{-\xi})$$

so that, due to Eq. (7.11), we have

$$\boxed{(e^{\xi \mathbf{a}^\dagger \mathbf{a}})\, \mathbf{a}\, (e^{-\xi \mathbf{a}^\dagger \mathbf{a}}) = \mathbf{a}\, (e^{-\xi})} \tag{7.18}$$

Moreover, by a similar inference as that allowing to pass from Eq. (7.11) to Eq. (7.18), we have

$$\boxed{(e^{\xi \mathbf{a}^\dagger \mathbf{a}})\, \mathbf{a}^\dagger (e^{-\xi \mathbf{a}^\dagger \mathbf{a}}) = \mathbf{a}^\dagger (e^{\xi})} \tag{7.19}$$

Apply Eqs. (7.18) and (7.19) to reproduce the results of the integration of the Heisenberg equation governing the dynamics of the ladder operators, keeping in mind Eq. (3.88) governing the time dependence of an operator $\mathbf{A}$ in the Heisenberg picture, that is,

$$\mathbf{A}(t)^{\mathrm{HP}} = (e^{i\mathbf{H}t/\hbar})\mathbf{A}(e^{-i\mathbf{H}t/\hbar})$$

which reads for the Boson operator $\mathbf{a}$, and when the Hamiltonian $\mathbf{H}$ is that of a harmonic oscillator

$$\mathbf{a}(t)^{\mathrm{HP}} = (e^{i\omega t \mathbf{a}^\dagger \mathbf{a}})\, \mathbf{a}\, (e^{-i\omega t \mathbf{a}^\dagger \mathbf{a}}) \tag{7.20}$$

Then, applying Eqs. (7.18) and (7.19) to the situation where $\xi = i\omega t$, it yields

$$(e^{i\omega t \mathbf{a}^\dagger \mathbf{a}})\, \mathbf{a}\, (e^{-i\omega t \mathbf{a}^\dagger \mathbf{a}}) = \mathbf{a}\, (e^{-i\omega t}) \tag{7.21}$$

$$(e^{i\omega t \mathbf{a}^\dagger \mathbf{a}})\, \mathbf{a}^\dagger (e^{i\omega t \mathbf{a}^\dagger \mathbf{a}}) = \mathbf{a}^\dagger (e^{i\omega t}) \tag{7.22}$$

so that Eq. (7.20) reads

$$\mathbf{a}(t)^{\mathrm{HP}} = \mathbf{a} e^{-i\omega t}$$

the Hermitian conjugate of which is

$$\mathbf{a}^\dagger(t)^{\mathrm{HP}} = \mathbf{a}^\dagger e^{i\omega t}$$

One may verify that these results are equivalent to those of (5.151) and (5.152) obtained by integration of the Heisenberg equation (3.94).

7.1.2.2 Transformations on functions of the ladder operators Now, consider the following transformation:

$$(e^{\xi \mathbf{a}^\dagger \mathbf{a}})\{\mathbf{f}(\mathbf{a})\}(e^{-\xi \mathbf{a}^\dagger \mathbf{a}}) \tag{7.23}$$

where $\mathbf{f}(\mathbf{a})$ is a function of $\mathbf{a}$ that may be expanded according to

$$\{\mathbf{f}(\mathbf{a})\} = \sum_n \{C_n\}(\mathbf{a})^n \tag{7.24}$$

where the $\{C_n\}$ are the scalar coefficients of the expansion. The latter expansion may be transformed using the following unity operator:

$$\mathbf{1} = (e^{-\xi \mathbf{a}^\dagger \mathbf{a}})(e^{\xi \mathbf{a}^\dagger \mathbf{a}}) \tag{7.25}$$

according to

$$\{\mathbf{f}(\mathbf{a})\} = \sum_n \{C_n\}\{\mathbf{a1a}\cdots\mathbf{1a}\}_n$$

so that Eq. (7.24) reads

$$\{\mathbf{f}(\mathbf{a})\} = \sum_n \{C_n\}\{\mathbf{a}(e^{-\xi \mathbf{a}^\dagger \mathbf{a}})(e^{\xi \mathbf{a}^\dagger \mathbf{a}})\mathbf{a}\cdots(e^{-\xi \mathbf{a}^\dagger \mathbf{a}})(e^{\xi \mathbf{a}^\dagger \mathbf{a}})\mathbf{a}\}_n$$

Then, the transformation (7.23) becomes

$$(e^{\xi \mathbf{a}^\dagger \mathbf{a}})\{\mathbf{f}(\mathbf{a})\}e^{(-\xi \mathbf{a}^\dagger \mathbf{a})} = \sum_n \{C_n\}\{(e^{\xi \mathbf{a}^\dagger \mathbf{a}}\mathbf{a}e^{-\xi \mathbf{a}^\dagger \mathbf{a}})(e^{\xi \mathbf{a}^\dagger \mathbf{a}}\mathbf{a}e^{-\xi \mathbf{a}^\dagger \mathbf{a}})\cdots(e^{\xi \mathbf{a}^\dagger \mathbf{a}}\mathbf{a}e^{-\xi \mathbf{a}^\dagger \mathbf{a}})\}_n$$

Again, using Eq. (7.18), we have

$$(e^{\xi \mathbf{a}^\dagger \mathbf{a}})\{\mathbf{f}(\mathbf{a})\}(e^{-\xi \mathbf{a}^\dagger \mathbf{a}}) = \sum_n \{C_n\}(\mathbf{a}e^{-\xi})^n$$

Thus, comparing (7.24), one obtains

$$(e^{\xi \mathbf{a}^\dagger \mathbf{a}})\{\mathbf{f}(\mathbf{a})\}(e^{-\xi \mathbf{a}^\dagger \mathbf{a}}) = \{\mathbf{f}(\mathbf{a}e^{-\xi})\} \tag{7.26}$$

In a similar way, one would find

$$(e^{\xi \mathbf{a}^\dagger \mathbf{a}})\{\mathbf{f}(\mathbf{a}^\dagger)\}(e^{-\xi \mathbf{a}^\dagger \mathbf{a}}) = \{\mathbf{f}(\mathbf{a}^\dagger e^{\xi})\} \tag{7.27}$$

Now, consider a function of both $\mathbf{a}^\dagger$ and $\mathbf{a}$, defined by the following expansion:

$$\mathbf{f}\{(\mathbf{a}^\dagger, \mathbf{a})\} = \sum_{l,m,\ldots,r,\ldots,s,\ldots,u} \{C_{l,m,\ldots,r,\ldots,s,\ldots,u}\}\{(\mathbf{a}^\dagger)^l(\mathbf{a})^m\cdots(\mathbf{a})^r\cdots(\mathbf{a}^\dagger)^s\cdots(\mathbf{a}^\dagger)^u\} \tag{7.28}$$

where the $\{C_{l,m,\ldots,r\ldots,s\ldots,u}\}$ are the scalar coefficients of the expansion. Then, consider the following transformation over this function:

$$\{\mathbf{F}(\mathbf{a}^\dagger, \mathbf{a})\} = (e^{\xi \mathbf{a}^\dagger \mathbf{a}})\{\mathbf{f}(\mathbf{a}^\dagger, \mathbf{a})\}(e^{-\xi \mathbf{a}^\dagger \mathbf{a}}) \tag{7.29}$$

Next, insert in the following way into the right-hand side of Eq. (7.29), the unity operator Eq. (7.25):

$$\{\mathbf{F}(\mathbf{a}^\dagger,\mathbf{a})\} = \sum_{l,m,\ldots,r,\ldots,s,\ldots,u} \{C_{l,m,\ldots,r,\ldots,s,\ldots,u}\} \times (e^{\xi\mathbf{a}^\dagger\mathbf{a}})(\mathbf{a}^\dagger)^l(e^{-\xi\mathbf{a}^\dagger\mathbf{a}}e^{\xi\mathbf{a}^\dagger\mathbf{a}})(\mathbf{a})^m(e^{-\xi\mathbf{a}^\dagger\mathbf{a}}e^{\xi\mathbf{a}^\dagger\mathbf{a}}) \cdots (\mathbf{a})^r \cdots (\mathbf{a}^\dagger)^s \cdots (e^{-\xi\mathbf{a}^\dagger\mathbf{a}}e^{\xi\mathbf{a}^\dagger\mathbf{a}})(\mathbf{a}^\dagger)^u(e^{-\xi\mathbf{a}^\dagger\mathbf{a}})$$

Then, using Eqs. (7.26) and (7.27), we have

$$\{\mathbf{F}(\mathbf{a}^\dagger,\mathbf{a})\} = \sum_{l,m,\ldots,r\ldots,s\ldots,u} \{C_{l,m,\ldots,r\ldots,s\ldots,u}\}$$

Hence, comparing Eqs. (7.29) and Eq.(7.28), we have

$$(e^{\xi\mathbf{a}^\dagger\mathbf{a}})\{\mathbf{f}(\mathbf{a}^\dagger,\mathbf{a})\}(e^{-\xi\mathbf{a}^\dagger\mathbf{a}}) = \{\mathbf{f}(\mathbf{a}^\dagger e^{\xi},\mathbf{a}e^{-\xi})\} \tag{7.30}$$

so that, when $\xi = i\omega t$, one obtains

$$\boxed{(e^{i\omega t\mathbf{a}^\dagger\mathbf{a}})\{\mathbf{f}(\mathbf{a}^\dagger,\mathbf{a})\}(e^{-i\omega t\mathbf{a}^\dagger\mathbf{a}}) = \{\mathbf{f}(\mathbf{a}^\dagger e^{i\omega t},\mathbf{a}e^{-i\omega t})\}} \tag{7.31}$$

7.2 NORMAL AND ANTINORMAL ORDERING FORMALISM

We shall now deal with a formalism that allows us to transform an equation involving the noncommuting Boson operators into new scalar ones involving partial derivatives, which may be solved, the obtained solutions being inversely converted into expressions involving the ladder operators, which are the solutions of the above operator equations we want to solve. This formalism concerns what is called, the *normal and antinormal ordering*.

7.2.1 Normal and antinormal ordering

To introduce this formalism, start from the very simple operator

$$\{\mathbf{f}(\mathbf{a},\mathbf{a}^\dagger)\} = \mathbf{a}\mathbf{a}^\dagger \tag{7.32}$$

which, due to the commutation rule $[\mathbf{a},\mathbf{a}^\dagger] = 1$, and thus to $\mathbf{a}\mathbf{a}^\dagger = \mathbf{a}^\dagger\mathbf{a} + 1$, reads

$$\{\mathbf{f}(\mathbf{a},\mathbf{a}^\dagger)\} = \mathbf{a}^\dagger\mathbf{a} + 1 \tag{7.33}$$

In the latter equation, the raising operator $\mathbf{a}^\dagger$ is before the lowering $\mathbf{a}$, at the opposite of the situation given by Eq. (7.32). In case (7.33), the operators $\mathbf{a}^\dagger$ and $\mathbf{a}$ are said to be in *normal form*, whereas in case (7.32), they are said to be in *antinormal* form. The following notations are used, respectively, for the two equivalent normal $\{n\}$ and antinormal $\{a\}$ expressions:

$$\{\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \mathbf{a}^\dagger\mathbf{a} + 1 \qquad \text{and} \qquad \{\mathbf{f}^{\{a\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \mathbf{a}\mathbf{a}^\dagger$$

Of course, since the two expressions are equivalent, one must write

$$\{\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \{\mathbf{f}^{\{a\}}(\mathbf{a},\mathbf{a}^\dagger)\}$$

Now consider a very general operator $\mathbf{f}(\mathbf{a},\mathbf{a}^\dagger)$, which is some function of the operators $\mathbf{a}$ and $\mathbf{a}^\dagger$, susceptible to be expanded according to

$$\{\mathbf{f}(\mathbf{a},\mathbf{a}^\dagger)\} = \sum_{l,m,\ldots,r,\ldots,s,\ldots,u} \{C_{l,m,\ldots,r,\ldots,s,\ldots,u}\}(\mathbf{a}^\dagger)^l(\mathbf{a})^m\cdots(\mathbf{a})^r\cdots(\mathbf{a}^\dagger)^s\cdots(\mathbf{a}^\dagger)^u \quad (7.34)$$

where $\{C_{l,m,\ldots,r,\ldots,s,\ldots,u}\}$ are the expansion coefficients. Then, it is possible by systematic aid of $\mathbf{a}\mathbf{a}^\dagger = \mathbf{a}^\dagger\mathbf{a} + 1$ resulting from the commutation rule $[\mathbf{a},\mathbf{a}^\dagger] = 1$ to write this operator (7.34) either in normal or in antinormal form, according to

$$\{\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \sum_{rs}\{f^n_{rs}\}(\mathbf{a}^\dagger)^r(\mathbf{a})^s \quad (7.35)$$

$$\{\mathbf{f}^{\{a\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \sum_{sr}\{f^a_{sr}\}(\mathbf{a})^s(\mathbf{a}^\dagger)^r \quad (7.36)$$

Here, f^n_{rs} and f^a_{sr} are, respectively, the expansion coefficients of the normal and antinormal form of the operator (7.34). Of course, as above, the three expressions (7.34)–(7.36) being equivalent, one may write

$$\{\mathbf{f}(\mathbf{a},\mathbf{a}^\dagger)\} = \{\mathbf{f}^{\{a\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \{\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger\}) \quad (7.37)$$

7.2.2 Normal and antinormal ordering operators

Now, consider two linear operators $\hat{\mathbf{N}}$ and $\hat{\mathbf{A}}$, the inverses of which are $\hat{\mathbf{N}}^{-1}$ and $\hat{\mathbf{A}}^{-1}$.

$$\hat{\mathbf{N}}\hat{\mathbf{N}}^{-1} = \hat{\mathbf{N}}^{-1}\hat{\mathbf{N}} = 1 \quad (7.38)$$

$$\hat{\mathbf{A}}\hat{\mathbf{A}}^{-1} = \hat{\mathbf{A}}^{-1}\hat{\mathbf{A}} = 1 \quad (7.39)$$

Then, assume that $\hat{\mathbf{N}}^{-1}$ and $\hat{\mathbf{A}}^{-1}$ allow one to transform, respectively, the normal and antinormal series expansion (7.35) and (7.36) of Boson operators, to the corresponding series expansion of scalars in which the $\mathbf{a}$ and $\mathbf{a}^\dagger$ operators have been transformed, respectively, into the scalars α and α^*:

$$\hat{\mathbf{N}}^{-1}\{\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \{f^{\{n\}}(\alpha,\alpha^*)\} \quad (7.40)$$

$$\hat{\mathbf{A}}^{-1}\{\mathbf{f}^{\{a\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \{f^{\{a\}}(\alpha,\alpha^*)\} \quad (7.41)$$

with, respectively,

$$\{f^{\{n\}}(\alpha^*,\alpha)\} = \sum_{rs}\{\{f^n_{rs}\}(\alpha^*)^r(\alpha)^s\} \quad (7.42)$$

$$\{f^{\{a\}}(\alpha^*,\alpha)\} = \sum_{sr}\{\{f^a_{sr}\}(\alpha)^s(\alpha^*)^r\} \quad (7.43)$$

Premultiply Eqs. (7.40) and (7.41) by $\hat{\mathbf{N}}$ and $\hat{\mathbf{A}}$, respectively,

$$\hat{\mathbf{N}}\hat{\mathbf{N}}^{-1}\{\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \hat{\mathbf{N}}\{f^{\{n\}}(\alpha,\alpha^*)\}$$

$$\hat{\mathbf{A}}\hat{\mathbf{A}}^{-1}\{\mathbf{f}^{\{a\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \hat{\mathbf{A}}\{f^{\{a\}}(\alpha,\alpha^*)\}$$

Then, using Eqs. (7.38) and (7.39), one obtains

$$\boxed{\{\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \hat{\mathbf{N}}\{f^{\{n\}}(\alpha,\alpha^*)\}} \qquad \text{and} \qquad \boxed{\{\mathbf{f}^{\{a\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \hat{\mathbf{A}}\{f^{\{a\}}(\alpha,\alpha^*)\}} \tag{7.44}$$

showing that the linear operators $\hat{\mathbf{N}}$ and $\hat{\mathbf{A}}$ transform the scalar functions (7.42) and (7.43) into the corresponding normal and antinormal operators (7.35) and (7.36).

7.2.3 Commutators of Boson operators with functions of Boson operators

Now, before continuing the study of normal and antinormal formalism, it is necessary to get some commutators of Boson operators with functions of them, and for this purpose consider the following expression:

$$[(\mathbf{a}^\dagger)^2, \mathbf{a}] = \mathbf{a}^\dagger\mathbf{a}^\dagger\mathbf{a} - \mathbf{a}\mathbf{a}^\dagger\mathbf{a}^\dagger \tag{7.45}$$

Then, in view of the commutation rule $\mathbf{a}\mathbf{a}^\dagger - \mathbf{a}^\dagger\mathbf{a} = 1$, the last right-hand side of Eq. (7.45) transforms to

$$(\mathbf{a}\mathbf{a}^\dagger)\mathbf{a}^\dagger = (\mathbf{a}^\dagger\mathbf{a} + 1)\mathbf{a}^\dagger$$

so that Eq. (7.45) reads

$$[(\mathbf{a}^\dagger)^2, \mathbf{a}] = \mathbf{a}^\dagger\mathbf{a}^\dagger\mathbf{a} - \mathbf{a}^\dagger\mathbf{a}\mathbf{a}^\dagger - \mathbf{a}^\dagger \tag{7.46}$$

or, factorizing,

$$[(\mathbf{a}^\dagger)^2, \mathbf{a}] = \mathbf{a}^\dagger(\mathbf{a}^\dagger\mathbf{a} - \mathbf{a}\mathbf{a}^\dagger) - \mathbf{a}^\dagger$$

Hence, using in turn the commutation rule of Bosons, leads to

$$[(\mathbf{a}^\dagger)^2, \mathbf{a}] = -2\mathbf{a}^\dagger \tag{7.47}$$

Hence, one obtains by derivation

$$2\mathbf{a}^\dagger = \left(\frac{\partial(\mathbf{a}^\dagger)^2}{\partial\mathbf{a}^\dagger}\right)$$

so that Eq. (7.47) reads

$$\boxed{[(\mathbf{a}^\dagger)^2, \mathbf{a}] = -\left(\frac{\partial(\mathbf{a}^\dagger)^2}{\partial\mathbf{a}^\dagger}\right)} \tag{7.48}$$

Next, consider the commutator of $\mathbf{a}$ with the third power of its Hermitian conjugate:

$$[(\mathbf{a}^\dagger)^3, \mathbf{a}] = [\mathbf{a}^\dagger(\mathbf{a}^\dagger)^2, \mathbf{a}] \tag{7.49}$$

Again, recall that according to Eq. (1.75), the following relation holds between commutators of operators $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$:

$$[\mathbf{B}\mathbf{C}, \mathbf{A}] = [\mathbf{B}, \mathbf{A}]\mathbf{C} + \mathbf{B}[\mathbf{C}, \mathbf{A}] \tag{7.50}$$

Then, in order to apply this theorem to Eq. (7.49), take

$$\mathbf{B} = \mathbf{a}^\dagger, \qquad \mathbf{C} = (\mathbf{a}^\dagger)^2 \qquad \mathbf{A} = \mathbf{a}$$

so that, by application of theorem (7.50), we have

$$[\mathbf{B}, \mathbf{A}] = [\mathbf{a}^\dagger, \mathbf{a}] = -1$$

and

$$[\mathbf{C}, \mathbf{A}] = [(\mathbf{a}^\dagger)^2, \mathbf{a}]$$

which, due to (7.47), yields

$$[\mathbf{C}, \mathbf{A}] = -2\mathbf{a}^\dagger$$

Thus, Eq. (7.49), reads

$$[(\mathbf{a}^\dagger)^3, \mathbf{a}] = -(\mathbf{a}^\dagger)^2 \quad -2(\mathbf{a}^\dagger)^2 \quad = -3(\mathbf{a}^\dagger)^2$$

The latter result may be also expressed in terms of the derivative of the third power of $\mathbf{a}^\dagger$ with respect to $\mathbf{a}^\dagger$:

$$[(\mathbf{a}^\dagger)^3, \mathbf{a}] = -\left(\frac{\partial(\mathbf{a}^\dagger)^3}{\partial \mathbf{a}^\dagger}\right) \tag{7.51}$$

Moreover, one obtains by recurrence of Eqs. (7.48) and (7.51)

$$\boxed{[(\mathbf{a}^\dagger)^n, \mathbf{a}] = -\left(\frac{\partial(\mathbf{a}^\dagger)^n}{\partial \mathbf{a}^\dagger}\right)} \tag{7.52}$$

In order to obtain the Hermitian conjugate of this expression, first write it explicitly according to

$$(\mathbf{a}^\dagger)^n \mathbf{a} - \mathbf{a}(\mathbf{a}^\dagger)^n = -\left(\frac{\partial(\mathbf{a}^\dagger)^n}{\partial \mathbf{a}^\dagger}\right)$$

Next, to get the full Hermitian conjugate of the latter expression, take the Hermitian conjugate of each term and then invert the result, so that

$$\mathbf{a}^\dagger(\mathbf{a})^n - (\mathbf{a})^n \mathbf{a}^\dagger = -\left(\frac{\partial(\mathbf{a})^n}{\partial \mathbf{a}}\right) \tag{7.53}$$

and thus

$$\boxed{[(\mathbf{a})^n, \mathbf{a}^\dagger] = \left(\frac{\partial(\mathbf{a})^n}{\partial \mathbf{a}}\right)} \tag{7.54}$$

Furthermore, consider the following equation involving commutators:

$$[\mathbf{a}^\dagger, \{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}] = [\mathbf{a}^\dagger, \{\mathbf{f}^{\{a\}}(\mathbf{a}, \mathbf{a}^\dagger)\}]$$

which holds because of Eq. (7.37) expressing the equivalence between any function of the Boson operators and its antinormal order form. Owing to Eq. (7.36), this commutator takes the form

$$[\mathbf{a}^\dagger, \{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}] = \sum_{rs} \{f_{rs}^a\} [\mathbf{a}^\dagger, (\mathbf{a})^r (\mathbf{a}^\dagger)^s] \tag{7.55}$$

which, using Eqs. (7.50) and (7.55), becomes

$$[\mathbf{a}^\dagger, \{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}] = \sum_{rs} \{f_{rs}^a\} ([\mathbf{a}^\dagger, (\mathbf{a})^r](\mathbf{a}^\dagger)^s + (\mathbf{a})^r [\mathbf{a}^\dagger, (\mathbf{a}^\dagger)^s]) \tag{7.56}$$

Now, we remark that in the latter expression, the second right-hand-side commutator is zero, so that this equation reduces to

$$[\mathbf{a}^\dagger, \{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}] = \sum_{rs} \{f_{rs}^a\} [\mathbf{a}^\dagger, (\mathbf{a})^r](\mathbf{a}^\dagger)^s \tag{7.57}$$

Moreover, writing r in place of n, Eq. (7.53), we have

$$[\mathbf{a}^\dagger, (\mathbf{a})^r] = -r(\mathbf{a})^{r-1}$$

so that Eq. (7.57) simplifies to

$$[\mathbf{a}^\dagger, \{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}] = -\sum_{rs} \{f_{rs}^a\} r(\mathbf{a})^{r-1} (\mathbf{a}^\dagger)^s \tag{7.58}$$

Moreover, observe that, owing to Eq. (7.36) the right-hand side of this last equation is just the partial derivative with respect to $\mathbf{a}$ of the antinormal ordered expression of the function of Boson operators. Hence, the commutator (7.58) becomes

$$[\mathbf{a}^\dagger, \{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}] = -\left(\frac{\partial \mathbf{f}^{\{a\}}(\mathbf{a}, \mathbf{a}^\dagger)}{\partial \mathbf{a}} \right)$$

and, thus, owing to Eq. (7.37),

$$[\mathbf{a}^\dagger, \{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}] = -\left(\frac{\partial \mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)}{\partial \mathbf{a}} \right) \tag{7.59}$$

In a similar way, one would obtain

$$[\mathbf{a}, \{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}] = \left(\frac{\partial \mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)}{\partial \mathbf{a}^\dagger} \right) \tag{7.60}$$

7.2.4 Average values over coherent states

Now, consider the following operator written in order form:

$$\{\mathbf{f}^{\{n\}}(\mathbf{a}, \mathbf{a}^\dagger)\} = \sum_{rs} \{f_{rs}^n\} (\mathbf{a}^\dagger)^r (\mathbf{a})^s$$

Then, according to Eq. (7.35), its average value over a coherent state is

$$\langle \{\alpha\} | \{\mathbf{f}^{\{n\}}(\mathbf{a}, \mathbf{a}^\dagger)\} | \{\alpha\} \rangle = \sum_{rs} \{f_{rs}^n\} \langle \{\alpha\} | (\mathbf{a}^\dagger)^r (\mathbf{a})^s | \{\alpha\} \rangle$$

Next, keeping in mind the definitions (6.1) and (6.2) of coherent states

$$\mathbf{a} | \{\alpha\} \rangle = \alpha | \{\alpha\} \rangle \qquad \text{and} \qquad \langle \{\alpha\} | \mathbf{a}^\dagger = \langle \{\alpha\} | \alpha^* \tag{7.61}$$

and applying them to the above average value, one finds

$$\langle \{\alpha\} | \{\mathbf{f}^{\{n\}}(\mathbf{a}, \mathbf{a}^\dagger)\} | \{\alpha\} \rangle = \sum_{rs} \{f_{rs}^n\} \langle \{\alpha\} | (\alpha^*)^r (\alpha)^s | \{\alpha\} \rangle$$

or

$$\langle \{\alpha\} | \mathbf{f}^{\{n\}}(\mathbf{a}, \mathbf{a}^\dagger) | \{\alpha\} \rangle = \sum_{rs} \{f_{rs}^n\} (\alpha^*)^r (\alpha)^s \langle \{\alpha\} | \{\alpha\} \rangle$$

so that if the coherent state is normalized,

$$\langle\{\alpha\}|\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)|\{\alpha\}\rangle = \sum_{rs}\{f_{rs}^n\}(\alpha^*)^r(\alpha)^s$$

Therefore, owing to Eq. (7.42), we have

$$\boxed{\langle\{\alpha\}|\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)|\{\alpha\}\rangle = f^{\{n\}}(\alpha^*,\alpha)} \tag{7.62}$$

which, due to Eq. (7.37), reads also

$$\boxed{\langle\{\alpha\}|\mathbf{f}(\mathbf{a},\mathbf{a}^\dagger)|\{\alpha\}\rangle = f^{\{n\}}(\alpha^*,\alpha)} \tag{7.63}$$

The latter equation shows that the average value of an arbitrary operator function of Boson operators performed on a coherent state is the scalar function defined by Eq. (7.42).

7.2.5 Expression of $|\{\alpha\}\rangle\langle\{\alpha\}|\mathbf{a}$ and of its Hermitian conjugate

Start from the first equation of Eq. (7.61), that is,

$$\mathbf{a}|\{\alpha\}\rangle = \alpha|\{\alpha\}\rangle \tag{7.64}$$

Then, postmultiply both sides of this equation by the bra $\langle\{\alpha\}|$, and one obtains

$$\mathbf{a}|\{\alpha\}\rangle\langle\{\alpha\}| = \alpha|\{\alpha\}\rangle\langle\{\alpha\}| \tag{7.65}$$

Now, the question must be posed: What is the result of the following expression?

$$|\{\alpha\}\rangle\langle\{\alpha\}|\mathbf{a} = ?$$

To answer, write the coherent state in terms of the action of the translation operator on the ground state of the Hamiltonian of the harmonic oscillator by the aid of Eq. (6.94), that is,

$$|\{\alpha\}\rangle = (e^{-|\alpha|^2/2})(e^{\alpha\mathbf{a}^\dagger})(e^{-\alpha^*\mathbf{a}})|\{0\}\rangle \tag{7.66}$$

the Hermitian conjugate of which is

$$\langle\{\alpha\}| = \langle\{0\}|(e^{-\alpha\mathbf{a}^\dagger})(e^{\alpha^*\mathbf{a}})(e^{-|\alpha|^2/2}) \tag{7.67}$$

Then, using the two above equations, we have

$$|\{\alpha\}\rangle\langle\{\alpha\}| = (e^{-|\alpha|^2/2})(e^{\alpha\mathbf{a}^\dagger})(e^{-\alpha^*\mathbf{a}})|\{0\}\rangle\langle\{0\}|(e^{-\alpha\mathbf{a}^\dagger})(e^{\alpha^*\mathbf{a}})(e^{-|\alpha|^2/2}) \tag{7.68}$$

an expression which may be simplified in the following way. First, observe that, by expansion of $\exp\{-\alpha^*\mathbf{a}\}$, it is possible to write

$$(e^{-\alpha^*\mathbf{a}})|\{0\}\rangle = \left\{1+\alpha^*\mathbf{a}+\frac{(\alpha^*\mathbf{a})^2}{2!}+\frac{(\alpha^*\mathbf{a})^3}{3!}+\cdots\right\}|\{0\}\rangle \tag{7.69}$$

Then, due to Eq. (5.35), that is,

$$\mathbf{a}|\{0\}\rangle = 0$$

and thus

$$\mathbf{a}^n|\{0\}\rangle = 0 \quad \text{except if} \quad n = 0$$

Eq. (7.69) simplifies to

$$(e^{-\alpha^*\mathbf{a}})|\{0\}\rangle = |\{0\}\rangle \tag{7.70}$$

the Hermitian conjugate of which is

$$\langle\{0\}|(e^{-\alpha\mathbf{a}^\dagger}) = \langle\{0\}| \tag{7.71}$$

As a consequence of Eqs. (7.70) and (7.71), Eq. (7.68) simplifies to

$$|\{\alpha\}\rangle\langle\{\alpha\}| = (e^{-|\alpha|^2/2})(e^{\alpha\mathbf{a}^\dagger})|\{0\}\rangle\langle\{0\}|(e^{\alpha^*\mathbf{a}})(e^{-|\alpha|^2/2})$$

Next, postmultiplying both right- and left-hand-side terms of this last equation by $\mathbf{a}$ and after rearranging, using

$$e^{-|\alpha|^2/2}e^{-|\alpha|^2/2} = e^{-\alpha\alpha^*} \tag{7.72}$$

one obtains

$$|\{\alpha\}\rangle\langle\{\alpha\}|\mathbf{a} = (e^{-\alpha\alpha^*})(e^{\alpha\mathbf{a}^\dagger})|\{0\}\rangle\langle\{0\}|(e^{\alpha^*\mathbf{a}})\mathbf{a} \tag{7.73}$$

Moreover, due to the expression of the following partial derivative

$$\left(\frac{\partial e^{\alpha^*\mathbf{a}}}{\partial\alpha^*}\right) = (e^{\alpha^*\mathbf{a}})\mathbf{a}$$

Eq. (7.73) transforms to

$$|\{\alpha\}\rangle\langle\{\alpha\}|\mathbf{a} = (e^{-\alpha\alpha^*})(e^{\alpha\mathbf{a}^\dagger})|\{0\}\rangle\langle\{0\}|\left(\frac{\partial e^{\alpha^*\mathbf{a}}}{\partial\alpha^*}\right) \tag{7.74}$$

Again, the partial derivative of the exponential operator with respect to α^* commutes with the bra, the ket, and the operator $e^{\alpha\mathbf{a}^\dagger}$, which do not depend on α, thus allowing one to transform Eq. (7.74) into

$$|\{\alpha\}\rangle\langle\{\alpha\}|\mathbf{a} = (e^{-\alpha\alpha^*})\left(\frac{\partial}{\partial\alpha^*}\{(e^{\alpha\mathbf{a}^\dagger})|\{0\}\rangle\langle\{0\}|(e^{\alpha^*\mathbf{a}})\}\right) \tag{7.75}$$

Furthermore, denoting

$$\{\mathbf{f}(\alpha^*\mathbf{a}, \alpha\mathbf{a}^\dagger)\} = (e^{\alpha\mathbf{a}^\dagger})|\{0\}\rangle\langle\{0\}|(e^{\alpha^*\mathbf{a}}) \tag{7.76}$$

Eq. (7.75) reads

$$|\{\alpha\}\rangle\langle\{\alpha\}|\mathbf{a} = e^{-\alpha\alpha^*}\left(\frac{\partial\mathbf{f}(\alpha^*\mathbf{a}, \alpha\mathbf{a}^\dagger)}{\partial\alpha^*}\right) \tag{7.77}$$

Now, observe that the following relation is verified:

$$\left(\frac{\partial e^{-\alpha\alpha^*}\mathbf{f}(\alpha^*\mathbf{a}, \alpha\mathbf{a}^\dagger)}{\partial\alpha^*}\right) = -\alpha(e^{-\alpha\alpha^*})\{\mathbf{f}(\alpha^*\mathbf{a}, \alpha\mathbf{a}^\dagger)\} + (e^{-\alpha\alpha^*})\left(\frac{\partial\mathbf{f}(\alpha^*\mathbf{a}, \alpha\mathbf{a}^\dagger)}{\partial\alpha^*}\right)$$

Then, rearranging gives

$$(e^{-\alpha\alpha^*})\left(\frac{\partial\mathbf{f}(\alpha^*\mathbf{a}, \alpha\mathbf{a}^\dagger)}{\partial\alpha^*}\right) = \left(\frac{\partial}{\partial\alpha^*} + \alpha\right)\{(e^{-\alpha\alpha^*})\{\mathbf{f}(\alpha^*\mathbf{a}, \alpha\mathbf{a}^\dagger)\}\} \tag{7.78}$$

As a consequence of Eq. (7.78), Eq. (7.77) transforms with the help of Eq. (7.76) into

$$|\{\alpha\}\rangle\langle\{\alpha\}|\mathbf{a} = \left(\frac{\partial}{\partial\alpha^*} + \alpha\right)\{(e^{-\alpha\alpha^*})(e^{\alpha\mathbf{a}^\dagger})|\{0\}\rangle\ \langle\{0\}|(e^{\alpha^*\mathbf{a}})\}$$

or, owing to Eq. (7.72)

$$|\{\alpha\}\rangle\langle\{\alpha\}|\mathbf{a} = \left(\frac{\partial}{\partial\alpha^*} + \alpha\right)\{(e^{-|\alpha|^2})(e^{\alpha\mathbf{a}^\dagger})|\{0\}\rangle\ \langle\{0\}|(e^{\alpha^*\mathbf{a}})\}$$

Then after rearranging the exponential involving the scalar $|\alpha|^2$, we have

$$|\{\alpha\}\rangle\langle\{\alpha\}|\mathbf{a} = \left(\frac{\partial}{\partial\alpha^*} + \alpha\right)\{(e^{-|\alpha|^2/2})(e^{\alpha\mathbf{a}^\dagger})|\{0\}\rangle\ \langle\{0\}|(e^{\alpha^*\mathbf{a}})(e^{-|\alpha|^2/2})\}$$

Again, in view of Eq. (7.71), it may be written in the more complex form

$$|\{\alpha\}\rangle\langle\{\alpha\}|\mathbf{a} = \left(\frac{\partial}{\partial\alpha^*} + \alpha\right)\{(e^{-|\alpha|^2/2})(e^{\alpha\mathbf{a}^\dagger})(e^{-\alpha^*\mathbf{a}})|\{0\}\rangle\ \langle\{0\}|(e^{-\alpha\mathbf{a}^\dagger})(e^{\alpha^*\mathbf{a}})(e^{-|\alpha|^2/2})\}$$

Finally, using Eqs. (7.66) and (7.67), one obtains the result

$$\boxed{|\{\alpha\}\rangle\langle\{\alpha\}|\mathbf{a} = \left(\frac{\partial}{\partial\alpha^*} + \alpha\right)\{|\{\alpha\}\rangle\langle\{\alpha\}|\}} \tag{7.79}$$

the Hermitian conjugate of which is

$$\boxed{\mathbf{a}^\dagger|\{\alpha\}\rangle\langle\{\alpha\}| = \left(\frac{\partial}{\partial\alpha} + \alpha^*\right)\{|\{\alpha\}\rangle\langle\{\alpha\}|\}}$$

7.2.6 Theorems dealing with normal and antinormal ordering

7.2.6.1 Normal ordering Consider the following normal ordered expansion of any operator function of Boson operators

$$\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger) = \sum_{l,m,\ldots,r,\ldots,s,\ldots,u} \{C_{l,m,\ldots,r,\ldots,s,\ldots,u}\}(\mathbf{a}^\dagger)^l(\mathbf{a})^m \cdots (\mathbf{a})^r \cdots (\mathbf{a}^\dagger)^s \cdots (\mathbf{a}^\dagger)^u$$

$$\boxed{|\{\alpha\}\rangle\langle\{\alpha\}|\mathbf{a} = \left(\frac{\partial}{\partial\alpha^*} + \alpha\right)\{|\{\alpha\}\rangle\langle\{\alpha\}|\}} \tag{7.80}$$

Now, consider the average value of this operator over a coherent state allowing one to write via Eqs. (7.62), that is,

$$\langle\{\alpha\}|\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)|\{\alpha\}\rangle = \{f(\alpha, \alpha^*)\}$$

Moreover, introduce after the operator of the left-hand side of Eq. (7.63), a closure relation over some basis $\{|\Psi_k\rangle\}$

$$f^{\{n\}}(\alpha, \alpha^*) = \sum_k \langle\{\alpha\}|\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)|\Psi_k\rangle\langle\Psi_k|\{\alpha\}\rangle$$

which, on commuting the scalar products with the matrix elements, transforms to

$$\{f^{\{n\}}(\alpha, \alpha^*)\} = \sum_k \langle\Psi_k|\{\alpha\}\rangle\langle\{\alpha\}|\mathbf{f}(a, \mathbf{a}^\dagger)|\Psi_k\rangle$$

so that the right-hand side of this last equation may be written formally as the trace over an arbitrary basis $\{|\Psi_k\rangle\}$ according to

$$\{f^{\{n\}}(\alpha,\alpha^*)\} = \mathbf{tr}\{|\{\alpha\}\rangle\langle\{\alpha\}|\mathbf{f}(\mathbf{a},\mathbf{a}^\dagger)\}$$

Next, owing to Eq. (7.80), this average value reads

$$\{f^{\{n\}}(\alpha,\alpha^*)\} = \sum_{l,m,\ldots,r,\ldots,s,\ldots,u} \{C_{l,m,\ldots,r,\ldots,s,\ldots,u}\}\mathbf{tr}\{|\{\alpha\}\rangle\langle\{\alpha\}|(\mathbf{a}^\dagger)^l(\mathbf{a})^m\cdots(\mathbf{a})^r\cdots(\mathbf{a}^\dagger)^s\cdots(\mathbf{a}^\dagger)^u\} \tag{7.81}$$

Now, the Hermitian conjugate of Eq. (7.65) is

$$|\{\alpha\}\rangle\langle\{\alpha\}|\mathbf{a}^\dagger = \alpha^*|\{\alpha\}\rangle\langle\{\alpha\}| \tag{7.82}$$

whereas Eq. (7.79) reads

$$|\{\alpha\}\rangle\langle\{\alpha\}|\mathbf{a} = \left(\alpha + \frac{\partial}{\partial\alpha^*}\right)|\{\alpha\}\rangle\langle\{\alpha\}| \tag{7.83}$$

so that, by iteration of Eqs. (7.82) and (7.83), we have

$$|\{\alpha\}\rangle\langle\{\alpha\}|(\mathbf{a}^\dagger)^r = (\alpha^*)^r|\{\alpha\}\rangle\langle\{\alpha\}| \tag{7.84}$$

$$|\{\alpha\}\rangle\langle\{\alpha\}|(\mathbf{a})^s = \left(\alpha + \frac{\partial}{\partial\alpha^*}\right)^s|\{\alpha\}\rangle\langle\{\alpha\}| \tag{7.85}$$

Hence, Eq. (7.81) transforms to

$$f\{^{\{n\}}(\alpha,\alpha^*)\} = \sum_{l,m,\ldots,r,\ldots,s,\ldots,u} \{C_{l,m,\ldots,r,\ldots,s,\ldots,u}\} \times \mathbf{tr}\left\{(\alpha^*)^l\left(\alpha + \frac{\partial}{\partial\alpha^*}\right)^m\cdots\left(\alpha + \frac{\partial}{\partial\alpha^*}\right)^r\cdots(\alpha^*)^s\cdots(\alpha^*)^u|\{\alpha\}\rangle\langle\{\alpha\}|\right\}$$

Now, writing explicitly the trace, and using the fact that the bras $\langle\Psi_k|$ commute with the α and α^* and the partial derivative with respect to α^*, that gives

$$\{f^{\{n\}}(\alpha,\alpha^*)\} = \sum_{l,m,\ldots,r,\ldots,s,\ldots,u} \{C_{l,m,\ldots,r,\ldots,s,\ldots,u}\}\sum_k \times\left\{(\alpha^*)^l\left(\alpha + \frac{\partial}{\partial\alpha^*}\right)^m\cdots\left(\alpha + \frac{\partial}{\partial\alpha^*}\right)^r\cdots(\alpha^*)^s\cdots(\alpha^*)^u\right\} \times\langle\Psi_k|\{\alpha\}\rangle\langle\{\alpha\}|\Psi_k\rangle \tag{7.86}$$

Moreover, since

$$\sum_k\langle\Psi_k|\{\alpha\}\rangle\langle\{\alpha\}|\Psi_k\rangle = \sum_k|\langle\Psi_k|\{\alpha\}\rangle|^2 = 1$$

Eq. (7.86) reduces to

$$\{f^{\{n\}}(\alpha,\alpha^*)\} = f\left(\alpha + \frac{\partial}{\partial\alpha^*},\alpha^*\right) \tag{7.87}$$

with

$$\left\{f\left(\alpha+\frac{\partial}{\partial\alpha^*},\alpha^*\right)\right\}=\sum_{l,m,\ldots,r,\ldots,s,\ldots,u}\{C_{l,m,\ldots,r,\ldots,s,\ldots,u}\}\times\left\{(\alpha^*)^l\left(\alpha+\frac{\partial}{\partial\alpha^*}\right)^m\cdots\left(\alpha+\frac{\partial}{\partial\alpha^*}\right)^r\cdots(\alpha^*)^s\cdots(\alpha^*)^u\right\}$$

Moreover, premultiply both terms of Eq. (7.87) by the ordering operator $\hat{\mathbf{N}}$, that is,

$$\hat{\mathbf{N}}\{f^{\{n\}}(\alpha^*,\alpha)\}=\hat{\mathbf{N}}\left\{f\left(\alpha+\frac{\partial}{\partial\alpha^*}\alpha^*\right)\right\}$$

Then, owing to the first equation of (7.44), one obtains the important result

$$\boxed{\{\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)\}=\hat{\mathbf{N}}\left\{f\left(\alpha+\frac{\partial}{\partial\alpha^*},\alpha^*\right)\right\}}\tag{7.88}$$

7.2.6.2 Theorem dealing with antinormal ordering Consider the following antinormal ordered expansion of a function of Boson operators:

$$\{\mathbf{f}^{\{a\}}(\mathbf{a},\mathbf{a}^\dagger)\}=\sum_{s,r}\{f^a_{sr}\}(\mathbf{a})^s(\mathbf{a}^\dagger)^r\tag{7.89}$$

Then, using the closure relation (6.19) on coherent states, that is,

$$\frac{1}{\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}|\{\alpha\}\rangle\langle\{\alpha\}|d\{\mathrm{Re}(\alpha)\}d\{\mathrm{Im}(\alpha)\}=1$$

Eq. (7.89) reads

$$\{\mathbf{f}^{\{a\}}(\mathbf{a},\mathbf{a}^\dagger)\}=\frac{1}{\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\sum_{s,r}\{f^a_{sr}\}(\mathbf{a})^s|\{\alpha\}\rangle\langle\{\alpha\}|\,(\mathbf{a}^\dagger)^r d\{\mathrm{Re}(\alpha)\}d\{\mathrm{Im}(\alpha)\}$$

Again, keeping in mind the properties of the coherent state, that is,

$$(\mathbf{a})|\{\alpha\}\rangle=(\alpha)|\{\alpha\}\rangle\qquad\text{and}\qquad\langle\{\alpha\}|(\mathbf{a}^\dagger)=\langle\{\alpha\}|\,(\alpha^*)$$

and leading by iteration

$$(\mathbf{a})^s|\{\alpha\}\rangle=(\alpha)^s|\{\alpha\}\rangle\qquad\text{and}\qquad\langle\{\alpha\}|(\mathbf{a}^\dagger)^r=\langle\{\alpha\}|(\alpha^*)^r$$

the previous equation becomes

$$\{\mathbf{f}^{\{a\}}(\mathbf{a},\mathbf{a}^\dagger)\}=\frac{1}{\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\sum_{s,r}\{f^a_{sr}\}(\alpha)^s(\alpha^*)^r|\{\alpha\}\rangle\langle\{\alpha\}|\,d\{\mathrm{Re}(\alpha)\}d\{\mathrm{Im}(\alpha)\}\tag{7.90}$$

Finally, due to Eq. (7.43), that is,

$$\sum_{s,r}\{f^a_{sr}\}(\alpha)^s(\alpha^*)^r=f^{\{a\}}(\alpha^*,\alpha)$$

Eq. (7.90) yields

$$\boxed{\{\mathbf{f}^{\{a\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \frac{1}{\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f^{\{a\}}(\alpha^*,\alpha)|\{\alpha\}\rangle\langle\{\alpha\}\,|d\{\mathrm{Re}(\alpha)\}d\{\mathrm{Im}(\alpha)\}}$$

7.2.7 Generalization of theorems dealing with normal ordering

We start from the partial derivative with respect to $\mathbf{a}^\dagger$ of the normal ordered expansion (7.35), that is,

$$\left(\frac{\partial\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)}{\partial\mathbf{a}^\dagger}\right) = \frac{\partial}{\partial\mathbf{a}^\dagger}\left(\sum_{r,s}\{f_{rs}^n\}(\mathbf{a}^\dagger)^r(\mathbf{a})^s\right)$$

which reads

$$\left(\frac{\partial\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)}{\partial\mathbf{a}^\dagger}\right) = \sum_{r,s}\{f_{rs}^n\}r(\mathbf{a}^\dagger)^{r-1}(\mathbf{a})^s \tag{7.91}$$

then, owing to the first equation of (7.44), the right-hand side of Eq. (7.91) becomes

$$\sum_{rs}\{f_{rs}^n\}r(\mathbf{a}^\dagger)^{r-1}(\mathbf{a})^s = \hat{\mathbf{N}}\left\{\sum_{r,s}\{f_{rs}^n\}r(\alpha^*)^{r-1}(\alpha)^s\right\}$$

so that Eq. (7.91) yields

$$\left(\frac{\partial\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)}{\partial\mathbf{a}^\dagger}\right) = \hat{\mathbf{N}}\left\{\sum_{r,s}\{f_{rs}^n\}r(\alpha^*)^{r-1}(\alpha)^s\right\}$$

a result that may also be expressed as

$$\left(\frac{\partial\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)}{\partial\mathbf{a}^\dagger}\right) = \hat{\mathbf{N}}\left\{\frac{\partial}{\partial\alpha^*}\sum_{r,s}\{f_{rs}^n\}(\alpha^*)^r(\alpha)^s\right\}$$

or, owing to Eq. (7.42), as

$$\left(\frac{\partial\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)}{\partial\mathbf{a}^\dagger}\right) = \hat{\mathbf{N}}\left\{\left(\frac{\partial}{\partial\alpha^*}f^n(\alpha^*,\alpha)\right)\right\} \tag{7.92}$$

Recall the commutator given by Eq. (7.60), that is,

$$\{\mathbf{a},\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \left(\frac{\partial\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)}{\partial\mathbf{a}^\dagger}\right)$$

allows one to write

$$\{\mathbf{a}\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \{\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)\mathbf{a}\} + \left(\frac{\partial\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)}{\partial\mathbf{a}^\dagger}\right) \tag{7.93}$$

Now, observe that the first right-hand-side term of this last equation, which appears to be in normal order, may be viewed as the result of the action of the normal order operator according to

$$\{\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)\mathbf{a}\} = \hat{\mathbf{N}}\{f^{\{n\}}(\alpha^*,\alpha)\alpha\} = \hat{\mathbf{N}}\{\alpha f^{\{n\}}(\alpha^*,\alpha)\}$$

Now, the last right-hand-side term of Eq. (7.93) is given by Eq. (7.92), so that Eq. (7.93) may be written

$$\{\mathbf{af}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \hat{\mathbf{N}}\{\alpha f^{\{n\}}(\alpha^*,\alpha)\} + \hat{\mathbf{N}}\left\{\frac{\partial f^{\{n\}}(\alpha^*,\alpha)}{\partial\alpha^*}\right\}$$

or

$$\{\mathbf{af}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \hat{\mathbf{N}}\left\{\left(\alpha + \frac{\partial}{\partial\alpha^*}\right) f^{\{n\}}(\alpha^*,\alpha)\right\} \tag{7.94}$$

By generalization of Eq. (7.94), one now obtains

$$(\mathbf{a})^m\{\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \hat{\mathbf{N}}\left\{\left(\alpha + \frac{\partial}{\partial\alpha^*}\right)^m \{f^{\{n\}}(\alpha^*,\alpha)\}\right\} \tag{7.95}$$

which, due to Eq. (7.37), reads

$$(\mathbf{a})^m\{\mathbf{f}(\mathbf{a},\mathbf{a}^\dagger)\} = \hat{\mathbf{N}}\left\{\left(\alpha + \frac{\partial}{\partial\alpha^*}\right)^m \{f^{\{n\}}(\alpha^*,\alpha)\}\right\} \tag{7.96}$$

Next, multiplying both the right- and left-hand sides of Eq. (7.96) by $\hat{\mathbf{N}}^{-1}$, that is,

$$\hat{\mathbf{N}}^{-1}(\mathbf{a})^m\{\mathbf{f}(\mathbf{a},\mathbf{a}^\dagger)\} = \hat{\mathbf{N}}^{-1}\hat{\mathbf{N}}\left\{\left(\alpha + \frac{\partial}{\partial\alpha^*}\right)^m \{f^{\{n\}}(\alpha^*,\alpha)\}\right\}$$

yields after simplification, with the help of Eq. (7.38)

$$\boxed{\hat{\mathbf{N}}^{-1}\,(\mathbf{a})^m\,\{\mathbf{f}(\mathbf{a},\mathbf{a}^\dagger)\} = \left(\alpha + \frac{\partial}{\partial\alpha^*}\right)^m \{f^{\{n\}}(\alpha^*,\alpha)\}} \tag{7.97}$$

On the other hand, it is clear that the following relation is satisfied since the Boson operator $\mathbf{a}^\dagger$ is in front of the function of the normal ordered expression $\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)$ of the Boson operators:

$$\boxed{(\mathbf{a}^\dagger)^k\{\mathbf{f}^{\{n\}}(\mathbf{a},\mathbf{a}^\dagger)\} = \hat{\mathbf{N}}\{(\alpha^*)^k\{f^{\{n\}}(\alpha^*,\alpha)\}\}} \tag{7.98}$$

Then, proceeding in the same way as for passing from Eq. (7.96) to Eq. (7.97), one obtains

$$\boxed{\hat{\mathbf{N}}^{-1}\{(\mathbf{a}^\dagger)^k\{\mathbf{f}(\mathbf{a},\mathbf{a}^\dagger)\}\} = (\alpha^*)^k\{f^{\{n\}}(\alpha^*,\alpha)\}} \tag{7.99}$$

Now, consider an operator equation dealing with Boson operators of the form

$$\{\mathbf{F}(\mathbf{a},\mathbf{a}^\dagger)\} = \{(\mathbf{a}^\dagger)^k(\mathbf{a})^m\mathbf{f}(\mathbf{a},\mathbf{a}^\dagger)\}$$

The question now is what may be in the scalar language an expression of the form

$$\hat{\mathbf{N}}^{-1}\{\mathbf{F}(\mathbf{a},\mathbf{a}^\dagger)\} = \hat{\mathbf{N}}^{-1}\{(\mathbf{a}^\dagger)^k(\mathbf{a})^m\mathbf{f}(\mathbf{a},\mathbf{a}^\dagger)\} \tag{7.100}$$

Owing to Eq. (7.95), it takes the form

$$\hat{\mathbf{N}}^{-1}\{\mathbf{F}(\mathbf{a},\mathbf{a}^\dagger)\} = \hat{\mathbf{N}}^{-1}\left\{(\mathbf{a}^\dagger)^k\hat{\mathbf{N}}\left\{\left(\alpha + \frac{\partial}{\partial\alpha^*}\right)^m \{f^{\{n\}}(\alpha,\alpha^*)\}\right\}\right\} \tag{7.101}$$

However, due to Eq. (7.40) and to the equivalence between $\mathbf{F}(\mathbf{a}, \mathbf{a}^\dagger)$ and $\mathbf{F}^{\{n\}}(\mathbf{a}, \mathbf{a}^\dagger)$, we may write

$$\hat{\mathbf{N}}^{-1}\{\mathbf{F}(\mathbf{a}, \mathbf{a}^\dagger)\} = \hat{\mathbf{N}}^{-1}\{\mathbf{F}^{\{n\}}(\mathbf{a}, \mathbf{a}^\dagger)\} = \{F^{\{n\}}(\alpha, \alpha^*)\}$$

it yields

$$\hat{\mathbf{N}}^{-1}\{(\mathbf{a}^\dagger)^k\{\ldots\}\} = (\alpha^*)^k\hat{\mathbf{N}}^{-1}\{\ldots\}$$

Hence, since $(\mathbf{a}^\dagger)^k$ is in front of $\{\ldots\}$, it appears that Eq. (7.101) leads to

$$\{F^{\{n\}}(\alpha, \alpha^*)\} = (\alpha^*)^k\hat{\mathbf{N}}^{-1}\hat{\mathbf{N}}\left\{\left(\alpha + \frac{\partial}{\partial\alpha^*}\right)^m \{f^{\{n\}}(\alpha, \alpha^*)\}\right\} \tag{7.102}$$

so that, due to Eq. (7.38), Eq. (7.102) simplifies to

$$\boxed{\{F^{\{n\}}(\alpha, \alpha^*)\} = (\alpha^*)^k \left(\alpha + \frac{\partial}{\partial\alpha^*}\right)^m \{f^{\{n\}}(\alpha, \alpha^*)\}} \tag{7.103}$$

7.2.8 Another theorem of interest

Consider the following linear transformation on the ground state of $\mathbf{a}^\dagger\mathbf{a}$:

$$(e^{x\mathbf{a}^\dagger\mathbf{a}})(e^{y\mathbf{a}^\dagger})|\{0\}\rangle$$

where x and y are complex scalars. Insert between the last operator and the ket the unity operator built up from the first operator, that is,

$$(e^{-x\mathbf{a}^\dagger\mathbf{a}})(e^{x\mathbf{a}^\dagger\mathbf{a}}) = 1$$

Hence

$$(e^{x\mathbf{a}^\dagger\mathbf{a}})(e^{y\mathbf{a}^\dagger})|\{0\}\rangle = (e^{x\mathbf{a}^\dagger\mathbf{a}})(e^{y\mathbf{a}^\dagger})(e^{-x\mathbf{a}^\dagger\mathbf{a}})(e^{x\mathbf{a}^\dagger\mathbf{a}})|\{0\}\rangle \tag{7.104}$$

Next, in view of Eq. (7.27) and taking

$$\mathbf{f}(\mathbf{a}^\dagger) = (e^{y\mathbf{a}^\dagger})$$

Eq. (7.104) reads

$$(e^{x\mathbf{a}^\dagger\mathbf{a}})(e^{y\mathbf{a}^\dagger})(e^{-x\mathbf{a}^\dagger\mathbf{a}}) = (e^{y\mathbf{a}^\dagger e^x})$$

Thus, Eq. (7.104) becomes

$$(e^{x\mathbf{a}^\dagger\mathbf{a}})(e^{y\mathbf{a}^\dagger})|\{0\}\rangle = (e^{y\mathbf{a}^\dagger e^x})(e^{x\mathbf{a}^\dagger\mathbf{a}})|\{0\}\rangle$$

However, since $|\{0\}\rangle$ is the ground state of $\mathbf{a}^\dagger\mathbf{a}$, with corresponding zero eigenvalue, the series expansion of the exponential of $\mathbf{a}^\dagger\mathbf{a}$ on the ground state is zero except for the first term of the expansion, i.e.

$$(e^{x\mathbf{a}^\dagger\mathbf{a}})|\{0\}\rangle = \left(1 + x\mathbf{a}^\dagger\mathbf{a} + \frac{x^2(\mathbf{a}^\dagger\mathbf{a})^2}{2!} + \cdots\right)|\{0\}\rangle = |\{0\}\rangle \tag{7.105}$$

Hence, Eq. (7.105) leads to the final result

$$\boxed{(e^{x\mathbf{a}^\dagger\mathbf{a}})(e^{y\mathbf{a}^\dagger})|\{0\}\rangle = (e^{y\mathbf{a}^\dagger e^x})|\{0\}\rangle} \tag{7.106}$$

7.3 TIME EVOLUTION OPERATOR OF DRIVEN HARMONIC OSCILLATORS

With the help of the theorems proved above, it is now possible to study the dynamics of driven quantum harmonic oscillators. For this purpose start from their Hamiltonian, which reads

$$\mathbf{H} = \left(\frac{\mathbf{P}^2}{2M} + \frac{1}{2} M \Omega^2 \mathbf{Q}^2 \right) + b\mathbf{Q}$$

Then, the dynamics of this system is governed by the time evolution operator, a solution of the Schrödinger equation

$$i\hbar \left(\frac{\partial \mathbf{U}(t)}{\partial t} \right) = \mathbf{H}\, \mathbf{U}(t) \quad \text{with} \quad \mathbf{U}(0) = 1$$

Next, in order to solve this equation, it is suitable to work within the interaction picture and thus to make the following partition:

$$\mathbf{H} = \mathbf{H}^\circ + b\mathbf{Q}$$

with

$$\mathbf{H}^\circ = \left(\frac{\mathbf{P}^2}{2M} + \frac{1}{2} M \Omega^2 \mathbf{Q}^2 \right) \tag{7.107}$$

Recall that the time evolution operator $\mathbf{U}(t)$ is related to the IP time evolution operator $\mathbf{U}(t)^{\mathrm{IP}}$ through Eq. (3.122)

$$\mathbf{U}(t) = \mathbf{U}^\circ(t)\mathbf{U}(t)^{\mathrm{IP}} \tag{7.108}$$

with

$$\mathbf{U}^\circ(t) = (e^{-i\mathbf{H}^\circ t/\hbar}) \tag{7.109}$$

Hence, according to Eq. (3.114), the IP time evolution operator obeys the IP Schrödinger equation

$$i\hbar \left(\frac{\partial \mathbf{U}(t)^{\mathrm{IP}}}{\partial t} \right) = b\mathbf{Q}(t)^{\mathrm{IP}} \mathbf{U}(t)^{\mathrm{IP}} \tag{7.110}$$

with the boundary condition

$$\mathbf{U}(0)^{\mathrm{IP}} = 1 \tag{7.111}$$

Next, due to Eq. (3.108), the interaction picture coordinate $\mathbf{Q}(t)^{\mathrm{IP}}$ appearing in Eq. (7.110) is given by

$$\mathbf{Q}(t)^{\mathrm{IP}} = \mathbf{U}^\circ(t)^{-1} \mathbf{Q}(0) \mathbf{U}^\circ(t) \tag{7.112}$$

Moreover, the iteration solution of the integral equation Eq. (7.110) is of the form of (3.124), however, up to infinite order

$$\mathbf{U}(t)^{\mathrm{IP}} \equiv 1 + \left(\frac{b}{i\hbar} \right) \int_0^t \mathbf{Q}(t')^{\mathrm{IP}} dt' + \left(\frac{b}{i\hbar} \right)^2 \int_0^t \mathbf{Q}(t')^{\mathrm{IP}} dt' \int_0^{t'} \mathbf{Q}(t'')^{\mathrm{IP}} dt'' + \cdots$$

a solution that may be written formally as

$$\mathbf{U}(t)^{\mathrm{IP}} = \widehat{\mathbf{P}}\left\{\exp\left(-ib\int_0^t \mathbf{Q}(t')^{\mathrm{IP}}dt'\right)\right\} \tag{7.113}$$

where $\widehat{\mathbf{P}}$ is the Dyson time-ordering operator met in Eq. (3.87). Recall that, owing to Eq. (5.158), the position operators $\mathbf{Q}(t)^{\mathrm{IP}}$ and $\mathbf{Q}(t')^{\mathrm{IP}}$ at different times given by Eq. (7.112) do not commute. Next, passing to Boson operators by the aid of Eqs. (5.6) and (5.7), using Eqs. (5.9) and (7.107), and finally, after neglecting the zero-point energy which is irrelevant for the present purpose, the unperturbed time evolution operator (7.109) reads

$$\mathbf{U}^{\circ}(t) = (e^{-i\mathbf{a}^{\dagger}\mathbf{a}\Omega t}) \tag{7.114}$$

whereas the IP time evolution operator (7.110) becomes

$$i\left(\frac{\partial \mathbf{U}(\mathbf{a},\mathbf{a}^{\dagger},t)^{\mathrm{IP}}}{\partial t}\right) = \alpha^{\circ}\Omega(\mathbf{a}^{\dagger}(t)^{\mathrm{IP}} + \mathbf{a}(t)^{\mathrm{IP}})\mathbf{U}(\mathbf{a},\mathbf{a}^{\dagger},t)^{\mathrm{IP}} \tag{7.115}$$

with

$$\alpha^{\circ} = \frac{b}{\Omega}\sqrt{\frac{\hbar}{2M\Omega}} \tag{7.116}$$

In Eq. (7.115), the IP time-dependent Boson operator is given by

$$\mathbf{a}(t)^{\mathrm{IP}} = \mathbf{U}^{\circ}(t)^{-1}\mathbf{a}\mathbf{U}^{\circ}(t)$$

or in view of Eq. (7.114)

$$\mathbf{a}(t)^{\mathrm{IP}} = (e^{i\mathbf{a}^{\dagger}\mathbf{a}\Omega t})\mathbf{a}(e^{-i\mathbf{a}^{\dagger}\mathbf{a}\Omega t})$$

and thus, according to Eq. (7.21)

$$\mathbf{a}(t)^{\mathrm{IP}} = \mathbf{a}e^{-i\Omega t} \tag{7.117}$$

so that Eq. (7.112) reads

$$\mathbf{Q}(t)^{\mathrm{IP}} = \sqrt{\frac{\hbar}{2M\Omega}}(\mathbf{a}^{\dagger}e^{i\Omega t} + \mathbf{a}e^{-i\Omega t}) \tag{7.118}$$

Therefore, Eq. (7.115) becomes

$$i\left(\frac{\partial \mathbf{U}(\mathbf{a},\mathbf{a}^{\dagger},t)^{\mathrm{IP}}}{\partial t}\right) = \alpha^{\circ}\Omega\,(\mathbf{a}^{\dagger}e^{i\Omega t} + \mathbf{a}e^{-i\Omega t})\{\mathbf{U}(\mathbf{a},\mathbf{a}^{\dagger},t)^{\mathrm{IP}}\} \tag{7.119}$$

Now, solve the differential equation (7.119) by the aid of the normal ordering procedure according to which it is possible to pass from operators that are functions of the noncommutative Boson operators to scalars. That is possible using the inverse of the $\hat{\mathbf{N}}$ operator and of Eqs. (7.97) and (7.99) to get

$$\hat{\mathbf{N}}^{-1}\{\mathbf{a}^{\dagger}\{\mathbf{U}(\mathbf{a},\mathbf{a}^{\dagger},t)^{\mathrm{IP}}\}\} = \alpha^{*}\{U^{\{n\}}(\alpha,\alpha^{*},t)\} \tag{7.120}$$

$$\hat{\mathbf{N}}^{-1}\{\mathbf{a}\{\mathbf{U}(\mathbf{a},\mathbf{a}^{\dagger},t)^{\mathrm{IP}}\}\} = \left(\alpha + \frac{\partial}{\partial\alpha^{*}}\right)\{U^{\{n\}}(\alpha,\alpha^{*},t)\} \tag{7.121}$$

$$\hat{\mathbf{N}}^{-1}\left\{\frac{\partial \mathbf{U}(\mathbf{a},\mathbf{a}^{\dagger},t)^{\mathrm{IP}}}{\partial t}\right\}=\left(\frac{\partial U^{\{n\}}(\alpha,\alpha^{*},t)}{\partial t}\right) \tag{7.122}$$

Thus, it is possible to pass from the partial derivative Eq. (7.119) to

$$i\left(\frac{\partial U^{\{n\}}(\alpha,\alpha^{*},t)}{\partial t}\right)=\alpha^{\circ}\ \Omega\left(\alpha^{*}e^{i\Omega t}+\left(\alpha+\frac{\partial}{\partial\alpha^{*}}\right)e^{-i\Omega t}\right)\{U^{\{n\}}(\alpha,\alpha^{*},t)\} \tag{7.123}$$

with, corresponding to Eq. (7.111), the boundary condition

$$\{U^{\{n\}}(\alpha,\alpha^{*},0)\}=1 \tag{7.124}$$

Now, in order to solve the partial derivative equation (7.123), let us write

$$\{U^{\{n\}}(\alpha,\alpha^{*},t)\}=e^{G(t)} \tag{7.125}$$

Next, in terms of the new scalar function $G(t)$, the partial derivatives of $U^{\{n\}}(\alpha,\alpha^{*},t)$ with respect to the scalars t and α^{*} are, respectively,

$$\left(\frac{\partial U^{\{n\}}(\alpha,\alpha^{*},t)}{\partial t}\right)=\left(\frac{\partial G(t)}{\partial t}\right)U^{\{n\}}(\alpha,\alpha^{*},t)$$

$$\left(\frac{\partial U^{\{n\}}(\alpha,\alpha^{*},t)}{\partial \alpha^{*}}\right)=\left(\frac{\partial G(t)}{\partial \alpha^{*}}\right)U^{\{n\}}(\alpha,\alpha^{*},t)$$

Thus, owing to these equations, and after simplification by $U^{\{n\}}(\alpha,\alpha^{*},t)$, Eq. (7.123) becomes

$$i\left(\frac{\partial G(t)}{\partial t}\right)=\alpha^{\circ}\Omega\left\{e^{i\Omega t}\alpha^{*}+e^{-i\Omega t}\alpha+e^{-i\Omega t}\left(\frac{\partial G(t)}{\partial \alpha^{*}}\right)\right\} \tag{7.126}$$

Again, assume for the intermediate function $G(t)$ appearing in Eq. (7.125), an expression of the form

$$G(t)=A(t)+B(t)\alpha+C(t)\alpha^{*} \tag{7.127}$$

Here, $A(t)$, $B(t)$, and $C(t)$ are unknown functions to be found, which, due to Eqs. (7.124) and (7.125), must satisfy at the initial time

$$A(0)=B(0)=C(0)=1$$

Then, in terms of these new functions, the partial derivatives involved in (7.126) are, respectively,

$$\left(\frac{\partial G(t)}{\partial \alpha^{*}}\right)=C(t)$$

$$\left(\frac{\partial G(t)}{\partial t}\right)=\left(\frac{\partial A(t)}{\partial t}\right)+\left(\frac{\partial B(t)}{\partial t}\right)\alpha+\left(\frac{\partial C(t)}{\partial t}\right)\alpha^{*}$$

so that Eq. (7.126) becomes

$$i\left(\frac{\partial A(t)}{\partial t}+\frac{\partial B(t)}{\partial t}\alpha+\frac{\partial C(t)}{\partial t}\alpha^{*}\right)=\alpha^{\circ}\Omega\{e^{i\Omega t}\alpha^{*}+e^{-i\Omega t}\alpha+e^{-i\Omega t}C(t)\}$$

which, by identification, leads to

$$i\left(\frac{\partial A(t)}{\partial t}\right) = \alpha^{\circ}\Omega e^{-i\Omega t}C(t)$$

$$i\left(\frac{\partial B(t)}{\partial t}\right) = \alpha^{\circ}\Omega e^{-i\Omega t}$$

$$i\left(\frac{\partial C(t)}{\partial t}\right) = \alpha^{\circ}\Omega e^{i\Omega t}$$

Solving these equations yields, respectively, to

$$C(t) = -\alpha^{\circ}(e^{i\Omega t} - 1) \tag{7.128}$$

$$B(t) = \alpha^{\circ}(e^{-i\Omega t} - 1) \tag{7.129}$$

$$A(t) = i\alpha^{\circ 2}\Omega t + \alpha^{\circ}B(t) \tag{7.130}$$

Thus, in view of Eqs. (7.128)–(7.130), Eq. (7.127) becomes

$$G(t) = i\alpha^{\circ 2}\Omega t + \alpha^{\circ 2}(e^{-i\Omega t} - 1) + \alpha^{\circ}(e^{-i\Omega t} - 1)\alpha - \alpha^{\circ}(e^{i\Omega t} - 1)\alpha^{*}$$

so that Eq. (7.125) reads

$$\{U^{(n)}(\alpha, \alpha^{*}, t)\} = (e^{i\alpha^{\circ 2}\Omega t})e^{\Phi^{\circ}(t)\alpha^{\circ 2}}e^{-\Phi^{\circ}(t)^{*}\alpha^{*}}e^{\Phi^{\circ}(t)\alpha} \tag{7.131}$$

with

$$\Phi^{\circ}(t) \equiv \alpha^{\circ}(e^{-i\Omega t} - 1) \tag{7.132}$$

Now, by the aid of Eq. (7.131), it is possible to return to the time evolution operator, using the normal ordering operator $\hat{\mathbf{N}}$ prompting one to write

$$\hat{\mathbf{N}}\{U^{(n)}(\alpha, \alpha^{*}, t)\} = (e^{i\alpha^{\circ 2}\Omega t})e^{\Phi^{\circ}(t)\alpha^{\circ 2}}\hat{\mathbf{N}}\{e^{-\Phi^{\circ}(t)^{*}\alpha^{*}}e^{\Phi^{\circ}(t)\alpha}\} \tag{7.133}$$

Then, according to the first equation of (7.44), we have

$$\hat{\mathbf{N}}\{U^{\{n\}}(\alpha, \alpha^{*}, t)\} = \{\mathbf{U}(\mathbf{a}^{\dagger}, \mathbf{a}, t)^{\mathrm{IP}}\} \tag{7.134}$$

$$\hat{\mathbf{N}}\{e^{-\Phi^{\circ}(t)^{*}\alpha^{*}}e^{\Phi^{\circ}(t)\alpha}\} = (e^{-\Phi^{\circ}(t)^{*}\mathbf{a}^{\dagger}})(e^{\Phi^{\circ}(t)\mathbf{a}}) \tag{7.135}$$

Hence, from Eqs. (7.133)–(7.135), Eq. (7.131) allows us to obtain the IP time evolution operator in the form

$$\{\mathbf{U}(\mathbf{a}, \mathbf{a}^{\dagger}, t)^{\mathrm{IP}}\} = (e^{i\alpha^{\circ 2}\Omega t})e^{\alpha^{\circ}\Phi^{\circ}(t)}(e^{-\Phi^{\circ}(t)^{*}\mathbf{a}^{\dagger}})(e^{\Phi^{\circ}(t)\mathbf{a}}) \tag{7.136}$$

Next, use the Glauber–Weyl theorem (1.79) to transform the right-hand-side product of exponential operators

$$(e^{-\Phi^{\circ}(t)^{*}\mathbf{a}^{\dagger}})(e^{\Phi^{\circ}(t)\mathbf{a}}) = e^{-[\Phi^{\circ}(t)^{*}\mathbf{a}^{\dagger}, \Phi^{\circ}(t)\mathbf{a}]/2}(e^{-\Phi^{\circ}(t)^{*}\mathbf{a}^{\dagger} + \Phi^{\circ}(t)\mathbf{a}}) \tag{7.137}$$

The commutator appearing on the right-hand side is

$$[\Phi^{\circ}(t)^{*}\mathbf{a}^{\dagger}, \Phi^{\circ}(t)\mathbf{a}] = |\Phi^{\circ}(t)|^{2}[\mathbf{a}^{\dagger}, \mathbf{a}] = -|\Phi^{\circ}(t)|^{2}$$

Consequently, Eq. (7.137) becomes

$$(e^{-\Phi^\circ(t)^*\mathbf{a}^\dagger})(e^{\Phi^\circ(t)\mathbf{a}}) = e^{|\Phi^\circ(t)|^2/2}(e^{-\Phi^\circ(t)^*\mathbf{a}^\dagger+\Phi^\circ(t)\mathbf{a}})$$

Hence, Eq. (7.136) takes the form

$$\mathbf{U}(\mathbf{a},\mathbf{a}^\dagger,t)^{\mathrm{IP}} = (e^{i\alpha^{\circ 2}\Omega t})e^{\alpha^\circ\Phi^\circ(t)+|\Phi^\circ(t)|^2/2}(e^{-\Phi^\circ(t)^*\mathbf{a}^\dagger+\Phi^\circ(t)\mathbf{a}}) \tag{7.138}$$

Again, owing to Eq. (7.132), it appears that

$$\left\{\alpha^\circ\Phi^\circ(t)+\tfrac{1}{2}|\Phi^\circ(t)|^2\right\} = \alpha^{\circ 2}((e^{-i\Omega t}-1)+\tfrac{1}{2}(2-e^{i\Omega t}-e^{-i\Omega t}))$$

or

$$\left\{\alpha^\circ\Phi^\circ(t)+\tfrac{1}{2}|\Phi^\circ(t)|^2\right\} = \alpha^{\circ 2}\left(e^{-i\Omega t}-\tfrac{1}{2}e^{i\Omega t}-\tfrac{1}{2}e^{-i\Omega t}\right)$$

and

$$\left\{\alpha^\circ\Phi^\circ(t)+\tfrac{1}{2}|\Phi^\circ(t)|^2\right\} = -i\alpha^{\circ 2}\sin\Omega t$$

so that Eq. (7.138) transforms to

$$\mathbf{U}(\mathbf{a},\mathbf{a}^\dagger,t)^{\mathrm{IP}} = (e^{i\alpha^{\circ 2}\Omega t})(e^{-i\alpha^{\circ 2}\sin\Omega t})(e^{-\Phi^\circ(t)^*\mathbf{a}^\dagger+\Phi^\circ(t)\mathbf{a}}) \tag{7.139}$$

As a consequence, owing to Eqs. (7.114) and (7.139), the full time evolution operator (7.108) takes the form

$$\boxed{\mathbf{U}(t) = (e^{i\alpha^{\circ 2}\Omega t})(e^{-i\alpha^{\circ 2}\sin\Omega t})(e^{-i\mathbf{a}^\dagger\mathbf{a}\Omega t})(e^{-\Phi^\circ(t)^*\mathbf{a}^\dagger+\Phi^\circ(t)\mathbf{a}})} \tag{7.140}$$

Now, in view of Eqs. (7.108), (7.113), and (7.114), it appears that this equation may be also written, after simplification, as

$$\boxed{\widehat{\mathbf{P}}\left\{\exp\left(-ib\int_0^t \mathbf{Q}(t')^{\mathrm{IP}}dt'\right)\right\} = (e^{i\alpha^{\circ 2}\Omega t})(e^{-i\alpha^{\circ 2}\sin\Omega t})(e^{-\Phi^\circ(t)^*\mathbf{a}^\dagger+\Phi^\circ(t)\mathbf{a}})} \tag{7.141}$$

or, due to Eq. (7.118), for the inverse of Eq. (7.141)

$$\widehat{\mathbf{P}}\left\{\exp\left(i\alpha^\circ\int_0^t s[\mathbf{a}^\dagger e^{i\Omega t'}+\mathbf{a}e^{-i\Omega t'}]dt'\right)\right\} = (e^{-i\alpha^{\circ 2}\Omega t})(e^{i\alpha^{\circ 2}\sin\Omega t})(e^{\Phi^\circ(t)^*\mathbf{a}^\dagger-\Phi^\circ(t)\mathbf{a}}) \tag{7.142}$$

7.4 CONCLUSION

This chapter dealt with the theoretical properties of the ladder operators, more elaborate than those found in Chapter 5, and has lead to theorems allowing us to make canonical transformations concerning these operators, particularly those involving translation operators and the other time evolution operators. It has also given the most important results concerning normal and antinormal ordering formalism, allowing one to transform quantum equations dealing with noncommuting ladder operators, to

scalar equivalent ones having the form of partial differential equations. All the results gained in this chapter will be widely used, particularly when studying the reversible or irreversible dynamics of quantum oscillators, more specially the following ones:

Canonical transformations on ladder operators
Involving the translation operator:
$(e^{-\xi^* \mathbf{a}^\dagger + \xi \mathbf{a}})\{\mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}(e^{\xi^* \mathbf{a}^\dagger - \xi \mathbf{a}}) = \{\mathbf{f}(\mathbf{a} + \xi^*, \mathbf{a}^\dagger + \xi)\}$
Involving the Hamiltonian:
$(e^{\xi \mathbf{a}^\dagger \mathbf{a}})\{\mathbf{f}(\mathbf{a}^\dagger, \mathbf{a})\}(e^{-\xi \mathbf{a}^\dagger \mathbf{a}}) = \{\mathbf{f}(\mathbf{a}^\dagger e^{\xi}, \mathbf{a} e^{-\xi})\}$ $\boxed{(e^{i\omega t \mathbf{a}^\dagger \mathbf{a}})\{\mathbf{f}(\mathbf{a}^\dagger, \mathbf{a})\}(e^{-i\omega t \mathbf{a}^\dagger \mathbf{a}}) = \{\mathbf{f}(\mathbf{a}^\dagger e^{i\omega t}, \mathbf{a} e^{-i\omega t})\}}$
Normal ordering formalism
Operator to be transformed:
$\{\mathbf{F}(\mathbf{a}, \mathbf{a}^\dagger)\} = \{(\mathbf{a}^\dagger)^k (\mathbf{a})^m \mathbf{f}(\mathbf{a}, \mathbf{a}^\dagger)\}$
Passage from an operator to its corresponding scalar:
$\hat{\mathbf{N}}^{-1}\{\mathbf{F}(\mathbf{a}, \mathbf{a}^\dagger)\} = \{F^{\{n\}}(\alpha, \alpha^*)\}$
The corresponding scalar expression:
$\boxed{F^{\{n\}}(\alpha, \alpha^*)\} = (\alpha^*)^k \left(\alpha + \frac{\partial}{\partial \alpha^*}\right)^m \{f^{\{n\}}(\alpha, \alpha^*)\}}$

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CHAPTER 8

PHASE OPERATORS AND SQUEEZED STATES

INTRODUCTION

In the present chapter, we study new operators, states, and theorems concerning harmonic oscillators that are less usual than those previously studied. Up to now, in the study of quantum oscillators, we have not yet encountered the concept of *phase*, which is usual in the area of classical oscillators. The corresponding quantum phase may be treated using the *phase operator*, which is the object of the first section of this chapter, where it will be applied to situations in which the quantum harmonic oscillator is described by coherent states. Now, other quantum states exist that resemble coherent states, although they are more complex. They are the *squeezed states*. One of their characteristic properties leads to uncertainty relations, which evoke phase properties because they involve time-dependent oscillatory momentum and position uncertainties coming back and forth. These squeezed states will be comprehensively treated in the second section of this chapter, which ends with a study of the *Bogolioubov–Valatin* transformation allowing one to diagonalize some Hamiltonians involving the product of Boson operators of the same forms as those appearing in squeezed states.

8.1 PHASE OPERATORS

We begin with *phase operators* evoking the phases appearing in the physics of classical oscillators.

8.1.1 Phase operators in the basis of harmonic Hamiltonian eigenkets

For this purpose, define a new operator Φ through the raising and lowering operators according to the following equations:

$$\mathbf{a} = \sqrt{\mathbf{a}^\dagger \mathbf{a} + 1}(e^{i\Phi})$$

$$\mathbf{a}^\dagger = (e^{-i\Phi})\sqrt{\mathbf{a}^\dagger \mathbf{a} + 1}$$

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which read by inversion

$$(e^{i\Phi}) = \left(\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\right)\mathbf{a} \tag{8.1}$$

$$(e^{-i\Phi}) = \mathbf{a}^\dagger\left(\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\right) \tag{8.2}$$

Now, we prove that the operators appearing on the left-hand side of these two last equations are unitary. Thus, take the product of Eq. (8.1) by Eq. (8.2):

$$(e^{i\Phi})(e^{-i\Phi}) = \left(\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\right)\mathbf{a}\mathbf{a}^\dagger\left(\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\right)$$

which, owing to the commutation rule (5.5), yields

$$(e^{i\Phi})(e^{-i\Phi}) = \left(\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\right)(\mathbf{a}^\dagger\mathbf{a}+1)\left(\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\right) \tag{8.3}$$

Now, one may write the last two terms of the right-hand side of this equation as

$$(\mathbf{a}^\dagger\mathbf{a}+1)\left(\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\right) = \sqrt{\mathbf{a}^\dagger\mathbf{a}+1}\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}\left(\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\right)$$

or

$$(\mathbf{a}^\dagger\mathbf{a}+1)\left(\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\right) = \sqrt{\mathbf{a}^\dagger\mathbf{a}+1}$$

so that Eq. (8.3) becomes

$$(e^{i\Phi})(e^{-i\Phi}) = \left(\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\right)\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}$$

which reduces to

$$(e^{i\Phi})(e^{-i\Phi}) = 1 \tag{8.4}$$

Moreover, the action of the operator (8.1) on an eigenstate of the harmonic oscillator Hamiltonian yields

$$(e^{i\Phi})|\{n\}\rangle = \frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\mathbf{a}\,|\{n\}\rangle$$

and, owing to Eq. (5.53),

$$(e^{i\Phi})|\{n\}\rangle = \frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\sqrt{n}|\{n-1\}\rangle \tag{8.5}$$

Again, write the following formal expansion of the square root

$$\frac{1}{\sqrt{y}} = \sum_k C_k y^k \tag{8.6}$$

where an explicit expression of the expansion coefficients C_k need not be given. Applying this expansion to $y = \mathbf{a}^\dagger\mathbf{a}+1$ reads

$$\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}} = \sum_k C_k(\mathbf{a}^\dagger\mathbf{a}+1)^k \quad \text{with} \quad k = 0, 1, \ldots$$

or, after postmultiplying by $|\{n\}\rangle$

$$\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}|\{n\}\rangle = \sum_k C_k(\mathbf{a}^\dagger\mathbf{a}+1)^k|\{n\}\rangle \tag{8.7}$$

Then, due to Eq. (5.42), this last expression transforms to

$$\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}|\{n\}\rangle = \sum_k C_k(n+1)^k|\{n\}\rangle \tag{8.8}$$

Furthermore, applying in turn Eq. (8.6) with $y = n+1$, that is,

$$\sum_k C_k(n+1)^k = \frac{1}{\sqrt{n+1}}$$

Eq. (8.8) becomes

$$\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}|\{n\}\rangle = \frac{1}{\sqrt{n+1}}|\{n\}\rangle$$

or, changing $n+1$ into n, and thus n into $n-1$

$$\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}|\{n-1\}\rangle = \frac{1}{\sqrt{n}}|\{n-1\}\rangle \tag{8.9}$$

Now, recall Eq. (8.5), that is,

$$(e^{i\Phi})|\{n\}\rangle = \frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\sqrt{n}|\{n-1\}\rangle \tag{8.10}$$

which, in view of Eq. (8.9) transforms after simplification into

$$(e^{i\Phi})|\{n\}\rangle = |\{n-1\}\rangle \tag{8.11}$$

In a similar way, one obtains for the corresponding operator defined by Eq. (8.2)

$$(e^{-i\Phi})|\{n\}\rangle = |\{n+1\}\rangle \tag{8.12}$$

Hence, as a consequence of Eqs. (8.11) and (8.12), and owing to the orthonormality of the eigenstates of the harmonic oscillator, the matrix elements of the operators (8.1) and (8.2) satisfy

$$\langle\{m\}|e^{i\Phi}|\{n\}\rangle = \langle\{m\}|\{n-1\}\rangle = \delta_{m,n-1} \tag{8.13}$$

$$\langle\{m\}|e^{-i\Phi}|\{n\}\rangle = \langle\{m\}|\{n+1\}\rangle = \delta_{m,n+1} \tag{8.14}$$

Now, introduce the following operators

$$\cos\Phi = \tfrac{1}{2}(e^{i\Phi}+e^{-i\Phi}) \tag{8.15}$$

$$\sin\Phi = \tfrac{1}{2i}(e^{i\Phi}-e^{-i\Phi}) \tag{8.16}$$

Then, in the basis of the eigenstates of the harmonic oscillator, the matrix elements of the first operator read

$$\langle\{m\}|\cos\Phi|\{n\}\rangle = \tfrac{1}{2}\{\langle\{m\}|e^{i\Phi}|\{n\}\rangle + \langle\{m\}|e^{-i\Phi}|\{n\}\rangle\}$$

or, owing to Eqs. (8.13) and (8.14), we have

$$\langle\{m\}|\cos\Phi|\{n\}\rangle = \tfrac{1}{2}(\delta_{m,n-1} + \delta_{m,n+1})$$

In a similar way, we have

$$\langle\{m\}|\sin\Phi|\{n\}\rangle = \tfrac{1}{2i}(\delta_{m,n-1} - \delta_{m,n+1})$$

As a consequence of these two last equations, it appears that the diagonal elements of these operators are zero, that is,

$$\langle\{n\}|\cos\Phi|\{n\}\rangle = \langle\{n\}|\sin\Phi|\{n\}\rangle = 0 \tag{8.17}$$

Moreover, consider the matrix elements of $\cos^2\Phi$, which, due to Eq. (8.15), read

$$\langle\{m\}|\cos^2\Phi|\{n\}\rangle = \tfrac{1}{4}\{\langle\{m\}|(e^{2i\Phi} + e^{-2i\Phi})|\{n\}\rangle + \langle\{m\}|2|\{n\}\rangle\} \tag{8.18}$$

However, since

$$(e^{2i\Phi})|\{n\}\rangle = (e^{i\Phi})(e^{i\Phi})|\{n\}\rangle$$

and, in view of Eq. (8.11), it appears that

$$(e^{2i\Phi})|\{n\}\rangle = (e^{i\Phi})|\{n-1\}\rangle$$

or, using in turn Eq. (8.11)

$$(e^{2i\Phi})|\{n\}\rangle = |\{n-2\}\rangle \tag{8.19}$$

In a similar way, using Eq. (8.12), we have

$$(e^{-2i\Phi})|\{n\}\rangle = |\{n+2\}\rangle \tag{8.20}$$

Then, Eqs. (8.19) and (8.20) allow to transform Eq. (8.18) into

$$\langle\{m\}|\cos^2\Phi|\{n\}\rangle = \tfrac{1}{4}\langle\{m\}|(|\{n-2\}\rangle + |\{n+2\}\rangle) + \tfrac{1}{2}\delta_{mn}$$

or, using the orthonormality properties of the states involved in this expression, it reduces to

$$\langle\{m\}|\cos^2\Phi|\{n\}\rangle = \tfrac{1}{4}(\delta_{m,n-2} + \delta_{m,n+2}) + \tfrac{1}{2}\delta_{mn} \tag{8.21}$$

In like manner

$$\langle\{m\}|\sin^2\Phi|\{n\}\rangle = -\tfrac{1}{4}(\delta_{m,n-2} + \delta_{m,n+2}) - \tfrac{1}{2}\delta_{mn} \tag{8.22}$$

Hence, the diagonal elements of Eqs. (8.21) and (8.22), reduce simply to

$$\langle\{n\}|\cos^2\Phi|\{n\}\rangle = \langle\{n\}|\sin^2\Phi|\{n\}\rangle = \tfrac{1}{2} \tag{8.23}$$

Moreover, the dispersions of $\cos\Phi$ and $\sin\Phi$ in the states $|\{n\}\rangle$, which are, respectively, given by

$$(\Delta\cos\Phi)_{|n\rangle} = \sqrt{\langle\{n\}|\cos^2\Phi|\{n\}\rangle - \langle\{n\}|\cos\Phi|\{n\}\rangle^2}$$

$$(\Delta\sin\Phi)_{|n\rangle} = \sqrt{\langle\{n\}|\sin^2\Phi|\{n\}\rangle - \langle\{n\}|\sin\Phi|\{n\}\rangle^2}$$

read, due to Eqs. (8.17) and (8.23),

$$(\Delta\cos\Phi)_{|n\rangle} = (\Delta\sin\Phi)_{|n\rangle} = \sqrt{\tfrac{1}{2}}$$

which indicates a random dispersion of the phase.

8.1.2 Commutation rule involving the phase operators

Now, seek the commutator of $\mathbf{a}^\dagger\mathbf{a}$ with the operator defined by Eq. (8.1), that is,

$$[\mathbf{a}^\dagger\mathbf{a},(e^{i\Phi})] = \mathbf{a}^\dagger\mathbf{a}\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\mathbf{a} - \frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\mathbf{a}\mathbf{a}^\dagger\mathbf{a} \tag{8.24}$$

Because $\mathbf{a}^\dagger\mathbf{a}$ commutes with all its powers, and in view of the expression of the commutator (5.5) of $\mathbf{a}^\dagger$ and $\mathbf{a}$, Eq. (8.24) reduces to

$$[\mathbf{a}^\dagger\mathbf{a},(e^{i\Phi})] = \frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\mathbf{a}^\dagger\mathbf{a}\mathbf{a} - \frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}(\mathbf{a}^\dagger\mathbf{a}+1)\mathbf{a}$$

or, factorizing and rearranging,

$$[\mathbf{a}^\dagger\mathbf{a},(e^{i\Phi})] = -\frac{1}{\sqrt{\mathbf{a}^\dagger\mathbf{a}+1}}\mathbf{a}$$

and after simplification and use of Eq. (8.1),

$$[\mathbf{a}^\dagger\mathbf{a},(e^{i\Phi})] = -(e^{i\Phi}) \tag{8.25}$$

Similarly

$$[\mathbf{a}^\dagger\mathbf{a},(e^{-i\Phi})] = (e^{-i\Phi}) \tag{8.26}$$

Hence, due to Eqs. (8.15) and (8.16), Eqs. (8.25) and (8.26) lead to

$$[\mathbf{a}^\dagger\mathbf{a}, \cos\Phi] = -i\sin\Phi \tag{8.27}$$

$$[\mathbf{a}^\dagger\mathbf{a}, \sin\Phi] = i\cos\Phi \tag{8.28}$$

It is now possible to get the product of the uncertainties over $\mathbf{a}^\dagger\mathbf{a}$ and $\cos\Phi$ or $\sin\Phi$. Keeping in mind that the product of uncertainties of two operators $\mathbf{A}$ and $\mathbf{B}$ calculated over kets $|\Psi\rangle$ is given by Eq. (2.49), that is,

$$(\Delta A_\Psi)^2(\Delta B_\Psi)^2 \geq -\tfrac{1}{4}\langle\Psi|[\mathbf{A},\mathbf{B}]|\Psi\rangle^2$$

and taking $\mathbf{A} = \mathbf{a}^\dagger\mathbf{a}$ and $\mathbf{B} = \cos\Phi$ or $\sin\Phi$, Eqs. (8.27) and (8.28) allow us to get the uncertainty relations, which read in the present situation

$$(\Delta\mathbf{a}^\dagger\mathbf{a})^2_\Psi(\Delta\cos\Phi)^2_\Psi \geq \tfrac{1}{4}\langle\Psi|\sin\Phi|\Psi\rangle^2$$

$$(\Delta\mathbf{a}^\dagger\mathbf{a})^2_\Psi(\Delta\sin\Phi)^2_\Psi \geq \tfrac{1}{4}\langle\Psi|\cos\Phi|\Psi\rangle^2$$

or

$$(\Delta\mathbf{a}^\dagger\mathbf{a})_\Psi(\Delta\cos\Phi)_\Psi \geq \tfrac{1}{2}|\langle\Psi|\sin\Phi|\Psi\rangle|$$

$$(\Delta\mathbf{a}^\dagger\mathbf{a})_\Psi(\Delta\sin\Phi)_\Psi \geq \tfrac{1}{2}|\langle\Psi|\cos\Phi|\Psi\rangle|$$

8.1.3 Phase operators within coherent-state picture

8.1.3.1 Diagonal matrix elements of cos Φ Consider now the average value of the operator cos Φ performed over a coherent-state picture:

$$\langle\{\alpha\}|\cos\Phi|\{\alpha\}\rangle = \tfrac{1}{2}(\langle\{\alpha\}|e^{i\Phi}|\{\alpha\}\rangle + \langle\{\alpha\}|e^{-i\Phi}|\{\alpha\}\rangle) \tag{8.29}$$

Keeping in mind the expansion of a coherent state on the eigenstates of the harmonic oscillator Hamiltonian given by Eq. (6.16), that is,

$$|\{\alpha\}\rangle = e^{-|\alpha|^2/2}\sum_n\left(\frac{(\alpha)^n}{\sqrt{n!}}\right)|\{n\}\rangle \tag{8.30}$$

$$\langle\{\alpha\}| = e^{-|\alpha|^2/2}\sum_m\left(\frac{(\alpha^*)^m}{\sqrt{m!}}\right)\langle\{m\}| \tag{8.31}$$

Eq. (8.29) reads

$$\langle\{\alpha\}|\cos\Phi|\{\alpha\}\rangle = \frac{1}{2}e^{-|\alpha|^2}\sum_n\sum_m\left(\frac{(\alpha^*)^m}{\sqrt{m!}}\frac{(\alpha)^n}{\sqrt{n!}}\right)(\langle\{m\}|e^{i\Phi}|\{n\}\rangle + \langle\{m\}|e^{-i\Phi}|\{n\}\rangle)$$

so that, passing from the imaginary exponentials to the corresponding cosine function, and due to Eqs. (8.13) and (8.14), we have

$$\langle\{\alpha\}|\cos\Phi|\{\alpha\}\rangle = \frac{1}{2}e^{-|\alpha|^2}\sum_n\sum_m\left(\frac{(\alpha^*)^m}{\sqrt{m!}}\frac{(\alpha)^n}{\sqrt{n!}}\right)(\delta_{m,n-1} + \delta_{m,n+1})$$

or

$$\langle\{\alpha\}|\cos\Phi|\{\alpha\}\rangle = \frac{1}{2}e^{-|\alpha|^2}\sum_n\left(\frac{(\alpha^*)^{n-1}}{\sqrt{(n-1)!}}\frac{(\alpha)^n}{\sqrt{n!}} + \frac{(\alpha^*)^{n+1}}{\sqrt{(n+1)!}}\frac{(\alpha)^n}{\sqrt{n!}}\right)$$

Since $(n-1)!$ cannot start from $n=0$, the summation must be redefined in the terms where $(n-1)!$ appears, by changing n into $n+1$, leading to

$$\langle\{\alpha\}|\cos\Phi|\{\alpha\}\rangle = \frac{1}{2}e^{-|\alpha|^2}\sum_n\left(\frac{(\alpha^*)^n}{\sqrt{n!}}\frac{(\alpha)^{n+1}}{\sqrt{(n+1)!}} + \frac{(\alpha^*)^{n+1}}{\sqrt{(n+1)!}}\frac{(\alpha)^n}{\sqrt{n!}}\right)$$

or

$$\langle\{\alpha\}|\cos\Phi|\{\alpha\}\rangle = \frac{1}{2}e^{-|\alpha|^2}\sum_n\left(\frac{|\alpha|^{2n}}{\sqrt{n!}}\frac{(\alpha+\alpha^*)}{\sqrt{(n+1)!}}\right) \tag{8.32}$$

Next, writing

$$\alpha = |\alpha|e^{i\theta} \tag{8.33}$$

Eq. (8.32) yields

$$\langle\{\alpha\}|\cos\Phi|\{\alpha\}\rangle = e^{-|\alpha|^2}\cos\theta\sum_n\left(\frac{|\alpha|^{2n+1}}{\sqrt{n!}\sqrt{(n+1)!}}\right)$$

or, using $(n+1)! = (n+1)n!$

$$\langle\{\alpha\}|\cos\Phi|\{\alpha\}\rangle = e^{-|\alpha|^2}\cos\theta\sum_n\left(\frac{|\alpha|^{2n+1}}{n!\sqrt{n+1}}\right)$$

8.1.3.2 Diagonal matrix element of $\cos^2\Phi$ Now, consider the average value of $\cos^2\Phi$ over a coherent state that, owing to Eq. (8.15), reads

$$\langle\{\alpha\}|\cos^2\Phi|\{\alpha\}\rangle = \tfrac{1}{4}\langle\{\alpha\}|(e^{i\Phi}+e^{-i\Phi})^2|\{\alpha\}\rangle$$

or, after expansion of the right-hand-side squared term, and using Eq. (8.4), we have

$$\langle\{\alpha\}|\cos^2\Phi|\{\alpha\}\rangle = \tfrac{1}{4}[\langle\{\alpha\}|(e^{2i\Phi}+e^{-2i\Phi})|\{\alpha\}\rangle + 2\langle\{\alpha\}|\{\alpha\}\rangle]$$

Next, assuming that the coherent states are normalized, and after using Eqs. (8.30) and (8.31), these matrix elements become

$$\langle\{\alpha\}|\cos^2\Phi|\{\alpha\}\rangle = \frac{1}{2}+\frac{1}{4}e^{-|\alpha|^2}\sum_n\sum_m\left(\frac{(\alpha^*)^m}{\sqrt{m!}}\frac{(\alpha)^n}{\sqrt{n!}}\right)[\langle\{m\}|(e^{2i\Phi}+e^{-2i\Phi})|\{n\}\rangle] \tag{8.34}$$

or, due to Eqs. (8.19) and (8.20), the equation above becomes

$$\langle\{\alpha\}|\cos^2\Phi|\{\alpha\}\rangle = \frac{1}{2}+\frac{1}{4}e^{-|\alpha|^2}\sum_n\sum_m\left(\frac{(\alpha^*)^m}{\sqrt{m!}}\frac{(\alpha)^n}{\sqrt{n!}}\right)\langle\{m\}|(|\{n-2\}\rangle+|\{n+2\}\rangle)$$

and, thus, after using the orthonormality properties,

$$\langle\{\alpha\}|\cos^2\Phi|\{\alpha\}\rangle = \frac{1}{2}+\frac{1}{4}e^{-|\alpha|^2}\sum_n\sum_m\left(\frac{(\alpha^*)^m}{\sqrt{m!}}\frac{(\alpha)^n}{\sqrt{n!}}\right)(\delta_{m,n-2}+\delta_{m,n+2})$$

or

$$\langle\{\alpha\}|\cos^2\Phi|\{\alpha\}\rangle = \frac{1}{2}+\frac{1}{4}e^{-|\alpha|^2}\sum_n\left(\frac{(\alpha^*)^{n-2}}{\sqrt{(n-2)!}}\frac{(\alpha)^n}{\sqrt{n!}}+\frac{(\alpha^*)^{n+2}}{\sqrt{(n+2)!}}\frac{(\alpha)^n}{\sqrt{n!}}\right) \tag{8.35}$$

Moreover, as above, shift the index in the sum containing $(n-2)!$ by changing n into $n+2$, so that Eq. (8.35) reads

$$\langle\{\alpha\}|\cos^2\Phi|\{\alpha\}\rangle = \frac{1}{2}+\frac{1}{4}e^{-|\alpha|^2}\sum_n\frac{(\alpha^*)^n(\alpha)^{n+2}+(\alpha^*)^{n+2}(\alpha)^n}{\sqrt{n!}\sqrt{(n+2)!}}$$

or, using Eq. (8.33),

$$\langle\{\alpha\}|\cos^2\Phi|\{\alpha\}\rangle = \frac{1}{2}+\frac{1}{2}e^{-|\alpha|^2}|\alpha|^2\cos(2\theta)\sum_n\left(\frac{|\alpha|^{2n}}{\sqrt{n!}\sqrt{(n+2)!}}\right)$$

so that, using finally $(n+2)!=(n+2)(n+1)n!$, we have

$$\langle\{\alpha\}|\cos^2\Phi|\{\alpha\}\rangle = \frac{1}{2}+e^{-|\alpha|^2}|\alpha|^2\left(\cos^2\theta-\frac{1}{2}\right)\sum_n\left(\frac{|\alpha|^{2n}}{n!\sqrt{(n+2)(n+1)}}\right)$$

8.2 SQUEEZED STATES

We have often encountered coherent states that may be viewed as the result of the action of the translation operator

$$\mathbf{A}(\alpha)=\exp\{\alpha\mathbf{a}^\dagger-\alpha\mathbf{a}\}$$

on any eigenstate $|\{n\}\rangle$ of the harmonic oscillator Hamiltonian, and we have found that, whatever they may be, these states minimize the Heisenberg uncertainty relations.

8.2.1 Canonical transformations on ladder operators using squeezing operators

However, other interesting states exist that may be considered as generalization of coherent states, the *squeezed states*, which may be obtained by the action on the kets $|\{n\}\rangle$ of the following operator:

$$\mathbf{S}(z) = \exp\left\{\tfrac{1}{2}(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2)\right\} \tag{8.36}$$

the Hermitian conjugate of which is

$$\mathbf{S}(z)^\dagger = \exp\left\{\tfrac{1}{2}(z^*\mathbf{a}^2 - z\mathbf{a}^{\dagger 2})\right\} = \exp\left\{-\tfrac{1}{2}(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2)\right\}$$

whereas its inverse is

$$\mathbf{S}(z)^{-1} = \exp\left\{-\tfrac{1}{2}(z\mathbf{a}^{\dagger\,2} - z^*\mathbf{a}^2)\right\} = \mathbf{S}(-z) \tag{8.37}$$

that implies that the operator (8.36) is unitary since obeying

$$\mathbf{S}(z)^\dagger = \mathbf{S}(z)^{-1} \tag{8.38}$$

Next, consider the following canonical transformation:

$$\mathbf{S}(z)\mathbf{a}\mathbf{S}(z)^{-1} = \exp\left\{\tfrac{1}{2}(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2)\right\}\mathbf{a}\exp\left\{-\tfrac{1}{2}(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2)\right\} \tag{8.39}$$

To perform this transformation, one may use the Baker–Campbell–Hausdorff formula (1.76):

$$e^{\xi\mathbf{A}}\mathbf{B}e^{-\xi\mathbf{A}} = \mathbf{B} + [\mathbf{A},\mathbf{B}]\xi + \frac{1}{2}[\mathbf{A},[\mathbf{A},\mathbf{B}]]\xi^2 + \frac{1}{3!}[\mathbf{A},[\mathbf{A},[\mathbf{A},\mathbf{B}]]]\xi^3 + \cdots$$

where $\mathbf{A}$ and $\mathbf{B}$ are two linear operators and ξ a scalar. If one defines the operator $\mathbf{D}$ as

$$\mathbf{D} = \xi\mathbf{A}$$

the Baker–Campbell–Hausdorff relation reads

$$\boxed{e^{\mathbf{D}}\mathbf{B}e^{-\mathbf{D}} = \mathbf{B} + [\mathbf{D},\mathbf{B}] + \frac{1}{2}[\mathbf{D},[\mathbf{D},\mathbf{B}]] + \frac{1}{3!}[\mathbf{D},[\mathbf{D},[\mathbf{D},\mathbf{B}]]] + \cdots} \tag{8.40}$$

Hence, setting in Eq. (8.40)

$$\mathbf{B} = \mathbf{a} \qquad \text{and} \qquad \mathbf{D} = \tfrac{1}{2}(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2)$$

Eq. (8.39) takes the form

$$\begin{aligned}\mathbf{S}(z)\mathbf{a}\mathbf{S}(z)^{-1} = \mathbf{a} &+ \frac{1}{2}[(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}),\mathbf{a}] \\ &+ \frac{1}{2!}\frac{1}{4}[(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}),[(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}),\mathbf{a}]] \\ &+ \frac{1}{3!}\frac{1}{8}[(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a})[(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}),[(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}),\mathbf{a}]]] + \cdots\end{aligned} \tag{8.41}$$

The first commutator appearing in this equation simplifies to

$$[(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), \mathbf{a}] = z[\mathbf{a}^{\dagger 2}, \mathbf{a}] \tag{8.42}$$

Now, keeping in mind that the right-hand-side commutator is given by Eq. (7.47), that is,

$$[\mathbf{a}^{\dagger 2}, \mathbf{a}] = -2\mathbf{a}^\dagger \tag{8.43}$$

the left-hand-side commutator of Eq. (8.42) yields

$$\boxed{[(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}), \mathbf{a}] = -2z\mathbf{a}^\dagger} \tag{8.44}$$

Therefore, the double commutator appearing in Eq. (8.41) reads

$$\begin{aligned}[(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), [(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), \mathbf{a}]] &= [(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), -2z\mathbf{a}^\dagger] \\ &= [(-z^*\mathbf{a}^2), -2z\mathbf{a}^\dagger] = 2|z|^2[\mathbf{a}^2, \mathbf{a}^\dagger]\end{aligned} \tag{8.45}$$

Now, the right-hand-side commutator of Eq. (8.45) is

$$[\mathbf{a}^2, \mathbf{a}^\dagger] = \mathbf{a}\mathbf{a}\mathbf{a}^\dagger - \mathbf{a}^\dagger\mathbf{a}\mathbf{a} = \mathbf{a}(\mathbf{a}^\dagger\mathbf{a} + 1) - \mathbf{a}^\dagger\mathbf{a}\mathbf{a}$$

or

$$[\mathbf{a}^2, \mathbf{a}^\dagger] = (\mathbf{a}\mathbf{a}^\dagger - \mathbf{a}^\dagger\mathbf{a})\mathbf{a} + \mathbf{a} = 2\mathbf{a} \tag{8.46}$$

so that, the double commutator (8.45) becomes

$$\boxed{[(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), [(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), \mathbf{a}]] = 4|z|^2\mathbf{a}} \tag{8.47}$$

Again, due to Eq. (8.47), the triple commutator appearing in Eq. (8.41) reads

$$\begin{aligned}&[(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}), [(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), [(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}), \mathbf{a}]]] \\ &\quad = [(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), 4|z|^2\mathbf{a}] = 4|z|^2 z[\mathbf{a}^{\dagger 2}, \mathbf{a}]\end{aligned}$$

or, using in turn Eq. (8.43)

$$[(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}), [(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), [(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}), \mathbf{a}]]] = -8z|z|^2\mathbf{a}^\dagger \tag{8.48}$$

Moreover, according to Eq. (8.48), the quadruple commutator of Eq. (8.41) takes the form

$$\begin{aligned}&[(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), [(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), [(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), [(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), \mathbf{a}]]]] \\ &\quad = [(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), -8z|z|^2\mathbf{a}^\dagger] = 8|z|^4[\mathbf{a}^2, \mathbf{a}^\dagger]\end{aligned}$$

so that, owing to Eq. (8.46), it becomes

$$\boxed{[(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), [(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), [(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), [(z\mathbf{a}^{\dagger 2} - z^*\mathbf{a}^2), \mathbf{a}]]]] = 16|z|^4\mathbf{a}} \tag{8.49}$$

At last, collecting the results from (8.44), (8.47), (8.48), and (8.49), the canonical transformation (8.41) appears to be

$$\mathbf{S}(z)\mathbf{a}\mathbf{S}(z)^{-1} = \mathbf{a}\left(1 + \frac{1}{2!}|z|^2 + \frac{1}{4!}|z|^4\right) - \mathbf{a}^\dagger\left(z + \frac{1}{3!}z|z|^2 + \frac{1}{5!}z|z|^4\right)$$

or

$$\mathbf{S}(z)\mathbf{a}\mathbf{S}(z)^{-1} = \mathbf{a}\left(1+\frac{1}{2!}|z|^2+\frac{1}{4!}|z|^4+\cdots\right) - \mathbf{a}^\dagger\frac{z}{|z|}\left(|z|+\frac{1}{3!}|z|^3+\frac{1}{5!}|z|^5+\cdots\right) \tag{8.50}$$

Next, due to the following expansions of the hyperbolic sine and cosine functions,

$$\cosh z = 1+\frac{z^2}{2!}+\frac{z^4}{4!}+\cdots$$

$$\sinh z = z+\frac{z^3}{3!}+\frac{z^5}{5!}+\cdots$$

where

$$\cosh z = \left(\frac{e^z+e^{-z}}{2}\right) \qquad \text{and} \qquad \sinh z = \left(\frac{e^z-e^{-z}}{2}\right) \tag{8.51}$$

it appears that the canonical transformation (8.50) reduces to the compact expression

$$\boxed{\mathbf{S}(z)\mathbf{a}\mathbf{S}(z)^{-1} = \mathbf{a}\cosh|z| - \frac{z}{|z|}\mathbf{a}^\dagger\sinh|z|} \tag{8.52}$$

Again, changing z to $-z$, and using Eqs. (8.36) and (8.38), Eq. (8.52) yields

$$\boxed{\mathbf{S}(z)^{-1}\mathbf{a}\mathbf{S}(z) = \mathbf{a}\cosh|z| + \frac{z}{|z|}\mathbf{a}^\dagger\sinh|z|} \tag{8.53}$$

Observe that the Hermitian conjugate of this equation is

$$(\mathbf{S}(z)^{-1}\mathbf{a}\mathbf{S}(z))^\dagger = \mathbf{a}^\dagger\cosh|z| + \mathbf{a}\frac{z}{|z|}|z| \tag{8.54}$$

its left-hand side being

$$(\mathbf{S}(z)^{-1}\mathbf{a}\mathbf{S}(z))^\dagger = (\mathbf{S}(z))^\dagger\mathbf{a}^\dagger(\mathbf{S}(z)^{-1})^\dagger$$

or, since the operator $\mathbf{S}(z)$ is unitary,

$$(\mathbf{S}(z)^{-1}\mathbf{a}\mathbf{S}(z))^\dagger = \mathbf{S}(z)^{-1}\mathbf{a}^\dagger\mathbf{S}(z) \tag{8.55}$$

so that identifying Eqs. (8.54) and (8.55) leads to

$$\boxed{\mathbf{S}(z)^{-1}\mathbf{a}^\dagger\mathbf{S}(z) = \mathbf{a}^\dagger\cosh|z| + \frac{z}{|z|}\mathbf{a}\sinh|z|} \tag{8.56}$$

8.2.2 Uncertainty relations for squeezed state

8.2.2.1 Squeezed state Introduce the squeezed states according to

$$|\{z(t),\alpha(t)\}\rangle = \mathbf{U}^\circ(t)^{-1}\mathbf{A}(\alpha^\circ)\mathbf{S}(|z|)|\{0\}\rangle \tag{8.57}$$

Here $|\{0\}\rangle$ is the ground state of the harmonic Hamiltonian, whereas $\mathbf{S}(|z|)$ is the squeezing operator defined by Eq. (8.36), and $\mathbf{A}(\alpha^\circ)$ the translation operator defined by Eq. (6.74), $\mathbf{U}^\circ(t)$ being the time evolution operator constructed from $\mathbf{a}^\dagger\mathbf{a}$, that is,

$$\mathbf{S}(|z|) = (e^{(|z|\mathbf{a}^{\dagger 2}-|z|\mathbf{a}^2)/2})$$

$$\mathbf{A}(\alpha^\circ) = (e^{\alpha^\circ \mathbf{a}^\dagger - \alpha^\circ \mathbf{a}})$$

$$\mathbf{U}^\circ(t) = e^{-i\omega t \mathbf{a}^\dagger \mathbf{a}}$$

Hence, Eq. (8.57) becomes

$$|\{z(t), \alpha(t)\}\rangle = (e^{i\omega t \mathbf{a}^\dagger \mathbf{a}})\,(e^{\alpha^\circ \mathbf{a}^\dagger - \alpha^\circ \mathbf{a}})\,(e^{(|z|\mathbf{a}^{\dagger 2} - |z|\mathbf{a}^2/2)})|\{0\}\rangle$$

Now, insert between the translation and the squeezing operators and between the squeezing operator and the ground-state eigenket, the unity operator built up from the time evolution operator, that is,

$$(e^{-i\omega t \mathbf{a}^\dagger \mathbf{a}})\,(e^{i\omega t \mathbf{a}^\dagger \mathbf{a}}) = 1$$

We have

$$\begin{aligned}|\{z(t), \alpha(t)\}\rangle \;=\; & (e^{i\omega t \mathbf{a}^\dagger \mathbf{a}})\, e^{\alpha^\circ \mathbf{a}^\dagger - \alpha^\circ \mathbf{a}}\,(e^{-i\omega t \mathbf{a}^\dagger \mathbf{a}})\,(e^{i\omega t \mathbf{a}^\dagger \mathbf{a}}) \\ & \times e^{(|z|\mathbf{a}^{\dagger 2} - |z|\mathbf{a}^2)/2}\,(e^{-i\omega t \mathbf{a}^\dagger \mathbf{a}})\,(e^{i\omega t \mathbf{a}^\dagger \mathbf{a}})|\{0\}\rangle \qquad (8.58)\end{aligned}$$

Next, keeping in mind Eq. (7.31),

$$(e^{i\omega t \mathbf{a}^\dagger \mathbf{a}})\,\mathbf{f}(\mathbf{a}^\dagger, \mathbf{a})\,(e^{-i\omega t \mathbf{a}^\dagger \mathbf{a}}) = \{\mathbf{f}(\mathbf{a}^\dagger e^{i\omega t}, \mathbf{a}\, e^{-i\omega t})\}$$

and applying this expression, we have

$$(e^{i\omega t \mathbf{a}^\dagger \mathbf{a}})\,(e^{\alpha^\circ \mathbf{a}^\dagger - \alpha^\circ \mathbf{a}})\,(e^{-i\omega t \mathbf{a}^\dagger \mathbf{a}}) = e^{\alpha^*(t)\mathbf{a}^\dagger - \alpha(t)\mathbf{a}} = \{\mathbf{A}(\alpha(t))\} \qquad (8.59)$$

$$(e^{i\omega t \mathbf{a}^\dagger \mathbf{a}})\{e^{(|z|\mathbf{a}^{\dagger 2} - |z|\mathbf{a}^2)/2}\}\,(e^{-i\omega t \mathbf{a}^\dagger \mathbf{a}}) = \{e^{(z^*(t)\mathbf{a}^{\dagger 2} - z(t)\mathbf{a}^2)/2}\} = \{\mathbf{S}(z(t))\} \qquad (8.60)$$

where

$$\alpha(t) = \alpha^\circ e^{-i\omega t} \qquad \text{and} \qquad z(t) = |z|e^{-2i\omega t} \qquad (8.61)$$

Now, expansion of the exponential operator appearing in Eq. (8.58) suggests writing the two last terms of the right-hand side of this equation as

$$(e^{i\omega t \mathbf{a}^\dagger \mathbf{a}})|\{0\}\rangle = \left(1 + i\omega t \mathbf{a}^\dagger \mathbf{a} + \frac{(i\omega t \mathbf{a}^\dagger \mathbf{a})^2}{2!} + \cdots\right)|\{0\}\rangle \qquad (8.62)$$

so that keeping in mind that the action of $\mathbf{a}^\dagger \mathbf{a}$ on its ground state $|\{0\}\rangle$ is zero, that is,

$$\mathbf{a}^\dagger \mathbf{a}|\{0\}\rangle = 0|\{0\}\rangle$$

Then, it appears that all terms involved in the sum of Eq. (8.62) are zero, except that corresponding to $n = 0$, which acts on the ground state as the unity operator, so that

$$(e^{i\omega t \mathbf{a}^\dagger \mathbf{a}})|\{0\}\rangle = |\{0\}\rangle \qquad (8.63)$$

Hence, owing to Eqs. (8.59), (8.60), and (8.63), Eq. (8.58) becomes

$$\boxed{|\{z(t), \alpha(t)\}\rangle = \mathbf{A}(\alpha(t))\mathbf{S}(z(t))|\{0\}\rangle} \qquad (8.64)$$

8.2.3 Ladder operator functions averaged over squeezed states

8.2.3.1 Average values of $a^\dagger$ and a Now, consider the time-dependent mean value of $\mathbf{a}^\dagger$ averaged over the squeezed state (8.57), that is,

$$\langle \mathbf{a}(t)^\dagger \rangle_{z,\alpha} = \langle \{z(t), \alpha(t)\} | \mathbf{a}^\dagger | \{z(t), \alpha(t)\} \rangle \tag{8.65}$$

which, due to Eq. (8.64), takes the form

$$\langle \mathbf{a}(t)^\dagger \rangle_{z,\alpha} = \langle \{0\} | \mathbf{S}(z(t))^{-1} \mathbf{A}(\alpha(t))^{-1}\, \mathbf{a}^\dagger \mathbf{A}(\alpha(t)) \mathbf{S}(z(t)) | \{0\} \rangle \tag{8.66}$$

Next, keeping in mind Eq. (6.81), which implies that the action of the time-dependent translation operator on the Boson operators gives

$$\mathbf{A}(\alpha(t))^{-1} \mathbf{a}^\dagger \mathbf{A}(\alpha(t)) = \mathbf{a}^\dagger + \alpha(t)^*$$

$$\mathbf{A}(\alpha(t))^{-1} \mathbf{a} \mathbf{A}(\alpha(t)) = \mathbf{a} + \alpha(t) \tag{8.67}$$

Using also the fact,

$$\mathbf{S}(z(t))^{-1} (\mathbf{a}^\dagger + \alpha(t)^*) \mathbf{S}(z(t)) = \alpha(t)^* + \mathbf{S}(z(t))^{-1} \mathbf{a}^\dagger \mathbf{S}(z(t))$$

and taking into account Eq. (8.56), it appears that

$$\mathbf{S}(z(t))^{-1} \mathbf{A}(\alpha(t))^{-1} \mathbf{a}^\dagger \mathbf{A}(\alpha(t)) \mathbf{S}(z(t)) = \mathbf{a}^\dagger \cosh|z| + \mathbf{a} \frac{z(t)}{|z|} \sinh|z| + \alpha(t)^* \tag{8.68}$$

so that Eq. (8.66) becomes

$$\langle \mathbf{a}(t)^\dagger \rangle_{z,\alpha} = \langle \{0\} | \mathbf{a}^\dagger \cosh|z| | \{0\} \rangle + \langle \{0\} |\, \mathbf{a}\, (e^{-2i\omega t}) \sinh|z| | \{0\} \rangle + \alpha(t)^*$$

Finally, in view of Eq. (8.61), and using

$$\mathbf{a}|\{0\}\rangle = 0 \qquad \text{and} \qquad \langle \{0\} | \mathbf{a}^\dagger = 0$$

we have

$$\boxed{\langle \mathbf{a}(t)^\dagger \rangle_{z,\alpha} = \alpha(t)^* = \alpha^\circ e^{i\omega t}} \tag{8.69}$$

the Hermitian conjugate of which is

$$\langle \mathbf{a}(t) \rangle_{z,\alpha} = \alpha(t) = \alpha^\circ e^{-i\omega t} \tag{8.70}$$

8.2.3.2 Average values of $(a^\dagger)^2$ and $(a)^2$ Moreover, the average value of the square of $\mathbf{a}(t)^\dagger$ defined by

$$\langle (\mathbf{a}(t)^\dagger)^2 \rangle_{z,\alpha} = \langle \{z(t), \alpha(t)\} | (\mathbf{a}^\dagger)^2 | \{z(t), \alpha(t)\} \rangle \tag{8.71}$$

yields, with the help of Eq. (8.64),

$$\langle (\mathbf{a}(t)^\dagger)^2 \rangle_{z,\alpha} = \langle \{0\} | \mathbf{S}(z(t))^{-1} \mathbf{A}(\alpha(t))^{-1} \mathbf{a}^\dagger \mathbf{a}^\dagger \mathbf{A}(\alpha(t)) \mathbf{S}(z(t)) | \{0\} \rangle$$

Again, insert the following unity operator:

$$1 = (\mathbf{A}(\alpha(t)) \mathbf{S}(z(t)) \mathbf{S}(z(t))^{-1} \mathbf{A}(\alpha(t))^{-1}) \tag{8.72}$$

between the two raising operators, as follows:

$$\begin{aligned}\langle(\mathbf{a}(t)^\dagger)^2\rangle_{z,\alpha} = \langle\{0\}|\mathbf{S}(z(t))^{-1}\mathbf{A}(\alpha(t))^{-1}\mathbf{a}^\dagger \\ \times(\mathbf{A}(\alpha(t))\mathbf{S}(z(t))\mathbf{S}(z(t))^{-1}\mathbf{A}(\alpha(t))^{-1})\mathbf{a}^\dagger\mathbf{A}(\alpha(t))\mathbf{S}(z(t))|\{0\}\rangle\end{aligned}$$

leading to

$$\langle(\mathbf{a}(t)^\dagger)^2\rangle_{z,\alpha} = \langle\{0\}|(\mathbf{S}(z(t))^{-1}\mathbf{A}(\alpha(t))^{-1}\mathbf{a}^\dagger\mathbf{A}(\alpha(t))\mathbf{S}(z(t)))^2|\{0\}\rangle$$

and thus, using Eq. (8.68),

$$\langle(\mathbf{a}(t)^\dagger)^2\rangle_{z,\alpha} = \langle\{0\}|(\mathbf{a}^\dagger\cosh|z| + (e^{-2i\omega t})\mathbf{a}\sinh|z| + \alpha(t)^*)^2|\{0\}\rangle$$

Again, performing the square involved on the right-hand-side average value yields

$$\begin{aligned}\langle(\mathbf{a}(t)^\dagger)^2\rangle_{z,\alpha} = \langle\{0\}|\{(\mathbf{a}^\dagger)^2\cosh^2|z| + (e^{4i\omega t})(\mathbf{a})^2\sinh^2|z| \\ + (2\mathbf{a}^\dagger\mathbf{a}+1)\sinh|z|e^{2i\omega t}\cosh|z|\}|\{0\}\rangle \\ + 2\alpha(t)^*\langle\{0\}|(\cosh|z|\mathbf{a}^\dagger + 2e^{2i\omega t}\mathbf{a}\sinh|z|)|\{0\}\rangle + \alpha(t)^{*2}\end{aligned}$$

or, after simplifications, due to

$$\mathbf{a}^\dagger\mathbf{a}|\{0\}\rangle = 0$$

$$\langle\{0\}|(\mathbf{a}^\dagger)^2|\{0\}\rangle = \langle\{0\}|(\mathbf{a})^2|\{0\}\rangle = 0$$

$$\boxed{\langle(\mathbf{a}(t)^\dagger)^2\rangle_{z,\alpha} = (e^{-2i\omega t})\sinh|z|\cosh|z| + \alpha^{\circ 2}(e^{2i\omega t})} \tag{8.73}$$

the Hermitian conjugate of which reads

$$\boxed{\langle(\mathbf{a}(t))^2\rangle_{z,\alpha} = (e^{2i\omega t})\sinh|z|\cosh|z| + \alpha^{\circ 2}(e^{-2i\omega t})} \tag{8.74}$$

8.2.3.3 Average value of $\mathbf{a}^\dagger\mathbf{a}$ Finally, consider the average value of the occupation number $\mathbf{a}^\dagger\mathbf{a}$:

$$\langle(\mathbf{a}^\dagger\mathbf{a})\rangle_{z,\alpha} = \langle\{z(t),\alpha(t)\}|\mathbf{a}^\dagger\mathbf{a}|\{z(t),\alpha(t)\}\rangle \tag{8.75}$$

Then, insert in the following way, between the two Boson operators, the unity operator (8.72):

$$\begin{aligned}\langle(\mathbf{a}^\dagger\mathbf{a})\rangle_{z,\alpha} = \langle\{0\}|(\mathbf{S}(z(t))^{-1}\mathbf{A}(\alpha(t))^{-1}\mathbf{a}^\dagger\mathbf{A}(\alpha(t))\mathbf{S}(z(t))) \\ \times(\mathbf{S}(z(t))^{-1}\mathbf{A}(\alpha(t))^{-1}\mathbf{a}\mathbf{A}(\alpha(t))\mathbf{S}(z(t)))|\{0\}\rangle\end{aligned} \tag{8.76}$$

Hence, using Eq. (8.68), Eq. (8.76) yields

$$\langle(\mathbf{a}^\dagger\mathbf{a})\rangle_{z,\alpha} = \langle\{0\}|(\mathbf{a}^\dagger\cosh|z| + \mathbf{a}(e^{-2i\omega t})\sinh|z| + \alpha^\circ(e^{i\omega t}))\times\mathrm{hc}|\{0\}\rangle$$

where hc is the Hermitian conjugate

$$\mathrm{hc} = \mathbf{a}\cosh|z| + \mathbf{a}^\dagger(e^{2i\omega t})\sinh|z| + \alpha^\circ(e^{-i\omega t})$$

The product involved in the right-hand-side term reads

$$\begin{aligned}(\mathbf{a}^\dagger \cosh|z| + \mathbf{a}e^{-2i\omega t}\sinh|z| + \alpha^\circ(e^{i\omega t}))\times \text{hc}\\ = |\alpha|^2 + \alpha^\circ(e^{-i\omega t})(\mathbf{a}^\dagger\cosh|z| + \mathbf{a}(e^{-2i\omega t})\sinh|z|)\\ + \mathbf{a}^\dagger\mathbf{a}\cosh^2|z| + (2\mathbf{a}^\dagger\mathbf{a}+1)\sinh^2|z|\\ + ((e^{-2i\omega t})(\mathbf{a})^2 + (e^{2i\omega t})(\mathbf{a}^\dagger)^2)\cosh|z|\sinh|z|\\ + \alpha^\circ(e^{i\omega t})(\mathbf{a}\cosh(|z|) + \mathbf{a}^\dagger(e^{2i\omega t})\sinh|z|)\end{aligned}$$

so that Eq. (8.76) appears to be simply

$$\boxed{\langle(\mathbf{a}^\dagger\mathbf{a})\rangle_{z,\alpha} = |\alpha|^2 + \sinh^2|z|} \tag{8.77}$$

Therefore, the mean value of the oscillator Hamiltonian (5.9) averaged over the squeezed states is given by

$$\langle\mathbf{H}\rangle_{z,\alpha} = \hbar\omega\langle\{z(t),\alpha(t)\}|\left(\mathbf{a}^\dagger\mathbf{a} + \tfrac{1}{2}\right)|\{z(t),\alpha(t)\}\rangle$$

which reads, after using Eq. (8.77),

$$\langle\mathbf{H}\rangle_{z,\alpha} = \hbar\omega\left(|\alpha|^2 + \sinh^2|z| + \tfrac{1}{2}\right)$$

8.2.4 Uncertainty relations for squeezed states

8.2.4.1 Average values of Q and P operators It is now possible, using Eqs. (8.69) and (8.70), to get the expression for the corresponding average value of the position operator **Q** and of its conjugate momentum **P**. First, begin with **Q** leading to

$$\langle\mathbf{Q}(t)\rangle_{z,\alpha} = \langle\{z(t),\alpha(t)\}|\mathbf{Q}|\{z(t),\alpha(t)\}\rangle$$

which, according to Eq. (5.6), reads

$$\langle\mathbf{Q}(t)\rangle_{z,\alpha} = \sqrt{\frac{\hbar}{2m\omega}}(\langle\{z(t),\alpha(t)\}|\mathbf{a}^\dagger|\{z(t),\alpha(t)\}\rangle + \langle\{z(t),\alpha(t)\}|\mathbf{a}|\{z(t),\alpha(t)\}\rangle) \tag{8.78}$$

or, due to the definition equation (8.65) and to its Hermitian conjugate,

$$\langle\mathbf{Q}(t)\rangle_{z,\alpha} = \sqrt{\frac{\hbar}{2m\omega}}(\langle\mathbf{a}(t)^\dagger\rangle_{z,\alpha} + \langle\mathbf{a}(t)\rangle_{z,\alpha})$$

and in view of Eqs. (8.69) and (8.70), it yields

$$\boxed{\langle\mathbf{Q}(t)\rangle_{z,\alpha} = 2\alpha^\circ\sqrt{\frac{\hbar}{2m\omega}}\cos\omega t} \tag{8.79}$$

On the other hand, the corresponding average value of the momentum **P**

$$\langle\mathbf{P}(t)\rangle_{z,\alpha} = \langle\{z(t),\alpha(t)\}|\mathbf{P}|\{z(t),\alpha(t)\}\rangle$$

reads, according to Eqs. (5.7) and (8.65),

$$\langle\mathbf{P}(t)\rangle_{z,\alpha} = i\sqrt{\frac{m\hbar\omega}{2}}(\langle\mathbf{a}(t)^\dagger\rangle_{z,\alpha} - \langle\mathbf{a}(t)\rangle_{z,\alpha})$$

so that, in view of Eqs. (8.69) and (8.70), we have

$$\boxed{\langle \mathbf{P}(t)\rangle_{z,\alpha} = 2\alpha^{\circ}\sqrt{\frac{m\hbar\omega}{2}}\sin\omega t} \tag{8.80}$$

8.2.4.2 Mean value of Q^2 and corresponding fluctuation Now consider the following average value of the squared position operator

$$\langle \mathbf{Q}(t)^2\rangle_{z,\alpha} = \langle\{z(t),\alpha(t)\}|\mathbf{Q}^2|\{z(t),\alpha(t)\}\rangle$$

Then, using Eq. (8.57), and the fact that the squeezing and translation operators are unitary, it becomes

$$\langle \mathbf{Q}(t)^2\rangle_{z,\alpha} = \frac{\hbar}{2m\omega}\langle\{0\}|\mathbf{S}(z(t))^{-1}\mathbf{A}(\alpha(t))^{-1}((\mathbf{a}^{\dagger})^2+(\mathbf{a})^2+2\mathbf{a}^{\dagger}\mathbf{a}+1)\mathbf{A}(\alpha(t))\mathbf{S}(z(t))|\{0\}\rangle$$

or, due to Eq. (8.71) and its Hermitian conjugate, and also to Eq. (8.75)

$$\langle \mathbf{Q}(t)^2\rangle_{z,\alpha} = \frac{\hbar}{2m\omega}(\langle(\mathbf{a}^{\dagger}(t))^2\rangle_{z,\alpha} + \langle(\mathbf{a}(t))^2\rangle_{z,\alpha} + 2\langle(\mathbf{a}^{\dagger}\mathbf{a}(t))\rangle_{z,\alpha} + 1)$$

so that, with Eqs. (8.73), (8.74), and (8.77), we have

$$\begin{aligned}\langle \mathbf{Q}(t)^2\rangle_{z,\alpha} = \frac{\hbar}{2m\omega}&((\alpha(t)^{*2} + \alpha(t)^2) + 2\cos 2\omega t \sinh|z|\cosh|z| \\ &+ 2|\alpha(t)|^2 + 2\sinh^2|z| + 1)\end{aligned} \tag{8.81}$$

Next, using the trigonometric formulas

$$\cos 2\omega t = \cos^2\omega t - \sin^2\omega t \tag{8.82}$$

the product of hyperbolic sine and cosine functions leads to

$$\sinh|z|\cosh|z| = \frac{e^{|z|}-e^{-|z|}}{2}\frac{e^{|z|}+e^{-|z|}}{2} = \frac{e^{2|z|}-e^{-2|z|}}{4}$$

$$2\sinh(|z|)\cosh(|z|) = \sinh(2|z|) \tag{8.83}$$

$$2\sinh^2(|z|) = 2\left(\frac{e^{|z|}-e^{-|z|}}{2}\right)^2 = \frac{e^{2|z|}+e^{-2|z|}-2}{2}$$

$$2\sinh^2|z| = \cosh 2|z| - 1 \tag{8.84}$$

Then, Eq. (8.81) reduces to

$$\langle \mathbf{Q}(t)^2\rangle_{z,\alpha} = \frac{\hbar}{2m\omega}\{(\alpha^*(t)+\alpha(t))^2 + (\cos^2\omega t - \sin^2\omega t)\sinh 2|z| + \cosh 2|z|\}$$

which may be also written as

$$\begin{aligned}\langle \mathbf{Q}(t)^2\rangle_{z,\alpha} = \frac{\hbar}{2m\omega}&\{(\alpha^*(t)+\alpha(t))^2 + (\cos^2\omega t - \sin^2\omega t)\sinh 2|z| \\ &+ (\cos^2\omega t + \sin^2\omega t)\cosh 2|z|\}\end{aligned}$$

or

$$\langle \mathbf{Q}(t)^2 \rangle_{z,\alpha} = \frac{\hbar}{2m\omega} \left\{ (\alpha^*(t) + \alpha(t))^2 + (\cos^2 \omega t - \sin^2 \omega t) \frac{e^{2|z|} - e^{-2|z|}}{2} + (\cos^2 \omega t + \sin^2 \omega t) \frac{e^{2|z|} + e^{-2|z|}}{2} \right\}$$

and thus

$$\boxed{\langle \mathbf{Q}(t)^2 \rangle_{z,\alpha} = \frac{\hbar}{2m\omega} \{ (\alpha^*(t) + \alpha(t))^2 + e^{2|z|} \cos^2 \omega t + e^{-2|z|} \sin^2 \omega t \}} \tag{8.85}$$

Hence, according to Eqs. (8.79) and (8.85), the fluctuation of the coordinate operator defined by

$$\Delta \mathbf{Q}_{z,\alpha}(t) = \sqrt{\langle \mathbf{Q}(t)^2 \rangle_{z,\alpha} - \langle \mathbf{Q}(t) \rangle_{z,\alpha}^2}$$

reads

$$\boxed{\Delta \mathbf{Q}_{z,\alpha}(t) = \sqrt{\frac{\hbar}{2m\omega}} \sqrt{e^{2|z|} \cos^2 \omega t + e^{-2|z|} \sin^2 \omega t}} \tag{8.86}$$

On the other hand, the following average value of the squared momentum operator

$$\langle \mathbf{P}(t)^2 \rangle_{z,\alpha} = \langle \{ z(t), \alpha(t) \} | \mathbf{P}^2 | \{ z(t), \alpha(t) \} \rangle \tag{8.87}$$

reads, in view of Eqs. (5.7), (8.57), (8.71), and (8.75),

$$\langle \mathbf{P}(t)^2 \rangle_{z,\alpha} = -\frac{\hbar m\omega}{2} \{ \langle (\mathbf{a}^\dagger(t))^2 \rangle_{z,\alpha} + \langle (\mathbf{a}(t))^2 \rangle_{z,\alpha} - (2 \langle \mathbf{a}^\dagger \mathbf{a} \rangle_{z,\alpha} + 1) \}$$

or, using Eqs. (8.73), (8.74), and (8.77),

$$\langle \mathbf{P}(t)^2 \rangle_{z,\alpha} = -\frac{\hbar m\omega}{2} \{ (\alpha(t)^{*2} + \alpha(t)^2) + 2 \cos 2\omega t \sinh |z| \cosh |z| - (2|\alpha(t)|^2 + 2 \sinh^2 |z| + 1) \}$$

which can be rearranged by the aid of Eqs. (8.82)–(8.84), according to

$$\boxed{\langle \mathbf{P}(t)^2 \rangle_{z,\alpha} = \frac{\hbar m\omega}{2} \{ (\alpha^*(t) - \alpha(t))^2 + e^{-2|z|} \cos^2 \omega t - e^{2|z|} \sin^2 \omega t \}} \tag{8.88}$$

Moreover, owing to Eqs. (8.80) and (8.88), the fluctuation of the momentum

$$\Delta \mathbf{P}_{z,\alpha}(t) = \sqrt{\langle \mathbf{P}(t)^2 \rangle_{z,\alpha} - \langle \mathbf{P}(t) \rangle_{z,\alpha}^2}$$

takes the form

$$\boxed{\Delta \mathbf{P}_{z,\alpha}(t) = \sqrt{\frac{\hbar m\omega}{2}} \sqrt{e^{-2|z|} \cos^2 \omega t + e^{2|z|} \sin^2 \omega t}} \tag{8.89}$$

so that multiplying this result by Eq. (8.86) leads to the following uncertainty relation:

$$\boxed{\Delta \mathbf{P}_{z,\alpha}(t) \Delta \mathbf{Q}_{z,\alpha}(t) = \frac{\hbar}{2} (e^{-2|z|} \cos^2 \omega t + e^{2|z|} \sin^2 \omega t)} \tag{8.90}$$

8.3 BOGOLIUBOV–VALATIN TRANSFORMATION

We shall end the present chapter with the products of Boson operators of the form $\mathbf{a}^\dagger\mathbf{a}^\dagger$ and $\mathbf{a}\,\mathbf{a}$, with the *Bogolioubov–Valatin* transformation allowing one to diagonalize the following Hamiltonian:

$$\mathbf{H} = \hbar\omega_1\mathbf{a}_1^\dagger\mathbf{a}_1 + \hbar\omega_2\mathbf{a}_2^\dagger\mathbf{a}_2 + \hbar\omega_{12}(\mathbf{a}_1^\dagger\mathbf{a}_2^\dagger + \mathbf{a}_1\mathbf{a}_2) \tag{8.91}$$

where ω_1 and ω_2 are the angular frequencies of the two oscillators, $\hbar\omega_{12}$ is the energetic coupling parameter, where $\mathbf{a}_1$, $\mathbf{a}_1^\dagger$ and $\mathbf{a}_2$, $\mathbf{a}_2^\dagger$ are ladder operators satisfying the commutation rule

$$[\mathbf{a}_i, \mathbf{a}_j^\dagger] = \delta_{ij} \tag{8.92}$$

We attempt to diagonalize this Hamiltonian so that it will read

$$\mathbf{H} = E^\circ + \hbar\Omega_1\mathbf{b}_1^\dagger\mathbf{b}_1 + \hbar\Omega_2\mathbf{b}_2^\dagger\mathbf{b}_2 \tag{8.93}$$

where $\mathbf{b}_i$ and $\mathbf{b}_i^\dagger$ are new Boson operators satisfying the commutation relation

$$[\mathbf{b}_i, \mathbf{b}_j^\dagger] = \delta_{ij} \tag{8.94}$$

and where the Ω_i are the angular frequencies of the decoupled oscillators, whereas E° is some reference energy.

The diagonalization of the Hamiltonian (8.91) into (8.93) may be performed through the linear Bogolioubov–Valatin transformation

$$\mathbf{b}_1 = \mathbf{a}_1\cosh\varphi + \mathbf{a}_2^\dagger\sinh\varphi \qquad \mathbf{b}_1^\dagger = \mathbf{a}_1^\dagger\cosh\varphi + \mathbf{a}_2\sinh\varphi \tag{8.95}$$

$$\mathbf{b}_2 = \mathbf{a}_1^\dagger\sinh\varphi - \mathbf{a}_2\cosh\varphi \qquad \mathbf{b}_2^\dagger = \mathbf{a}_1\sinh\varphi - \mathbf{a}_2^\dagger\cosh\varphi \tag{8.96}$$

In order to determine the transformation parameter φ, suppose that the commutator of $\mathbf{b}_1$ with the Hamiltonian (8.91) is equal to that of $\mathbf{b}_1^\dagger\mathbf{b}_1$ with the Hamiltonian (8.93). In this context, observe that, owing to Eq. (8.94), the commutator of $\mathbf{b}_1$ with the Hamiltonian (8.93) is simply

$$[\mathbf{b}_1, \mathbf{H}] = \hbar\Omega_1[\mathbf{b}_1, \mathbf{b}_1^\dagger\mathbf{b}_1] = \hbar\Omega_1\mathbf{b}_1$$

or, using the first equation appearing in (8.95), we have

$$\boxed{[\mathbf{b}_1, \mathbf{H}] = (\mathbf{a}_1\cosh\varphi + \mathbf{a}_2^\dagger\sinh\varphi)\hbar\Omega_1} \tag{8.97}$$

On the other hand, according to the first equation of (8.95), the commutator of $\mathbf{b}_1$ with the Hamiltonian (8.91), reads

$$[\mathbf{b}_1, \mathbf{H}] = [(\mathbf{a}_1\cosh\varphi + \mathbf{a}_2^\dagger\sinh\varphi), (\hbar\omega_1\mathbf{a}_1^\dagger\mathbf{a}_1 + \hbar\omega_2\mathbf{a}_2^\dagger\mathbf{a}_2 + \hbar\omega_{12}(\mathbf{a}_1^\dagger\mathbf{a}_2^\dagger + \mathbf{a}_1\mathbf{a}_2))]$$

or

$$\begin{aligned}[\mathbf{b}_1, \mathbf{H}] = {} & [\mathbf{a}_1, (\hbar\omega_1\mathbf{a}_1^\dagger\mathbf{a}_1 + \hbar\omega_2\mathbf{a}_2^\dagger\mathbf{a}_2 + \hbar\omega_{12}(\mathbf{a}_1^\dagger\mathbf{a}_2^\dagger + \mathbf{a}_1\mathbf{a}_2))]\cosh\varphi \\ & + [\mathbf{a}_2^\dagger, (\hbar\omega_1\mathbf{a}_1^\dagger\mathbf{a}_1 + \hbar\omega_2\mathbf{a}_2^\dagger\mathbf{a}_2) + \hbar\omega_{12}(\mathbf{a}_1^\dagger\mathbf{a}_2^\dagger + \mathbf{a}_1\mathbf{a}_2)]\sinh\varphi \end{aligned} \tag{8.98}$$

Again, owing to the commutation rules (8.92), and applying Eqs. (5.15) and (5.16), it appears that

$$[\mathbf{a}_1, \mathbf{a}_1^\dagger \mathbf{a}_1] = \mathbf{a}_1 \qquad \text{and} \qquad [\mathbf{a}_1, \mathbf{a}_1^\dagger \mathbf{a}_2^\dagger] = \mathbf{a}_2^\dagger$$

$$[\mathbf{a}_2^\dagger, \mathbf{a}_2^\dagger \mathbf{a}_2] = \mathbf{a}_2^\dagger \qquad \text{and} \qquad [\mathbf{a}_2^\dagger, \mathbf{a}_1 \mathbf{a}_2] = -\mathbf{a}_1$$

Thereby, Eq. (8.98) transforms to

$$\boxed{[\mathbf{b}_1, \mathbf{H}] = \mathbf{a}_1(\hbar\omega_1 \cosh\varphi - \hbar\omega_{12} \sinh\varphi) + \mathbf{a}_2^\dagger(\hbar\omega_{12} \cosh\varphi - \hbar\omega_2 \sinh\varphi)} \tag{8.99}$$

Then, equating the two commutators (8.97) and (8.99)yields

$$\begin{aligned}\hbar\Omega_1(\mathbf{a}_1 \cosh\varphi + \mathbf{a}_2^\dagger \sinh\varphi) = {} & \mathbf{a}_1(\hbar\omega_1 \cosh\varphi - \hbar\omega_{12} \sinh\varphi) \\ & + \mathbf{a}_2^\dagger(\hbar\omega_{12} \cosh\varphi - \hbar\omega_2 \sinh\varphi)\end{aligned}$$

or, after identification, since the Boson operators cannot be zero

$$(\Omega_1 - \omega_1)\cosh\varphi + \omega_{12} \sinh\varphi = 0 \tag{8.100}$$

$$-\omega_{12} \cosh\varphi + (\Omega_1 + \omega_2)\sinh\varphi = 0 \tag{8.101}$$

Now, since the coefficients $\cosh\varphi$ and $\sinh\varphi$ are different from zero, the set of equations (8.100) and (8.101) is satisfied if

$$\begin{vmatrix} (\Omega_1 - \omega_1) & \omega_{12} \\ -\omega_{12} & (\Omega_1 + \omega_2) \end{vmatrix} = 0$$

or, after expansion of the determinant,

$$\Omega_1^2 - \Omega_1(\omega_1 - \omega_2) + (\omega_{12}^2 - \omega_1\omega_2) = 0$$

In the two solutions of this equation

$$\Omega_1 = \tfrac{1}{2}((\omega_1 - \omega_2) \pm \sqrt{(\omega_1 + \omega_2)^2 - 4\omega_{12}^2})$$

the one that must be selected is that allowing Ω_1 in Eq. (8.91) to be equal to ω_1 when the coupling ω_{12} is zero, that is,

$$\boxed{\Omega_1 = \tfrac{1}{2}((\omega_1 - \omega_2) + \sqrt{(\omega_1 + \omega_2)^2 - 4\omega_{12}^2})} \tag{8.102}$$

Moreover, according to Eq. (8.100), the ratio of the coefficients $\sinh\varphi$ and $\cosh\varphi$ reads

$$\frac{\sinh\varphi}{\cosh\varphi} = \tanh\varphi = \frac{\omega_1 - \Omega_1}{\omega_{12}}$$

In like manner for the commutator of $\mathbf{b}_2$ with the Hamiltonian $\mathbf{H}$ given, using Eq. (8.91) or (8.93), and with the help of the first equation of (8.96), one obtains for the second angular frequency appearing in Eq. (8.93)

$$\boxed{\Omega_2 = \tfrac{1}{2}((\omega_2 - \omega_1) + \sqrt{(\omega_1 + \omega_2)^2 - 4\omega_{12}^2})} \tag{8.103}$$

Finally, it is possible to get the expression of E° appearing in Eq. (8.93) by transforming this equation using Eqs. (8.95) and (8.96), that is,

$$\mathbf{H} = E^\circ + \hbar\Omega_1((\mathbf{a}_1^\dagger \cosh\varphi + \mathbf{a}_2 \sinh\varphi)(\mathbf{a}_1 \cosh\varphi + \mathbf{a}_2^\dagger \sinh\varphi))$$
$$+ \hbar\Omega_2((\mathbf{a}_1 \sinh\varphi - \mathbf{a}_2^\dagger \cosh\varphi)(\mathbf{a}_1^\dagger \sinh\varphi - \mathbf{a}_2 \cosh\varphi))$$

or, due to the commutation rules (8.92), one obtains

$$\mathbf{H} = E^\circ + \hbar\Omega_1(\mathbf{a}_1^\dagger\mathbf{a}_1 \cosh^2\varphi + (\mathbf{a}_2^\dagger\mathbf{a}_2 + 1)\sinh^2\varphi + (\mathbf{a}_1^\dagger\mathbf{a}_2^\dagger + \mathbf{a}_1\mathbf{a}_2)\sinh\varphi\cosh\varphi)$$
$$+ \hbar\Omega_2((\mathbf{a}_1^\dagger\mathbf{a}_1 + 1)\sinh^2\varphi + \mathbf{a}_2^\dagger\mathbf{a}_2 \cosh^2\varphi - (\mathbf{a}_1^\dagger\mathbf{a}_2^\dagger + \mathbf{a}_1\mathbf{a}_2)\sinh\varphi\cosh\varphi)$$

a result that simplifies to

$$\mathbf{H} = E^\circ + (\hbar\Omega_1 + \hbar\Omega_2)\sinh^2\varphi + \hbar\Omega_1(\cosh^2\varphi + \sinh^2\varphi)\mathbf{a}_1^\dagger\mathbf{a}_1$$
$$+ \hbar\Omega_2(\cosh^2\varphi + \sinh^2\varphi)\mathbf{a}_2^\dagger\mathbf{a}_2$$
$$+ (\hbar\Omega_1 - \hbar\Omega_2)\sinh\varphi\cosh\varphi(\mathbf{a}_1^\dagger\mathbf{a}_2^\dagger + \mathbf{a}_1\mathbf{a}_2)$$

Finally, equating this last expression to that of $\mathbf{H}$ given by Eq. (8.91), leads for the coefficients of $\mathbf{a}_1^\dagger\mathbf{a}_1$, $\mathbf{a}_2^\dagger\mathbf{a}_2$, $\mathbf{a}_1^\dagger\mathbf{a}_2^\dagger$, and $\mathbf{a}_1\mathbf{a}_2$ the following results:

$$\hbar\omega_k = \hbar\Omega_k(\cosh^2\varphi + \sinh^2\varphi) \quad \text{with} \quad k = 1, 2$$

$$\hbar\omega_{12} = (\hbar\Omega_1 - \hbar\Omega_2)\sinh\varphi\cosh\varphi$$

and also to the conclusion that

$$\boxed{E^\circ + (\hbar\Omega_1 + \hbar\Omega_2)\sinh^2\varphi = 0} \tag{8.104}$$

a result allowing one to get E° appearing in the diagonal Hamiltonian (8.93).

8.4 CONCLUSION

This chapter was devoted to various questions related to the notion of phase for quantum oscillators, which is not without connection with the squeezed states susceptible to be obtained through the action of squeezing operators having the structure of translation operators in which the ladder operators have been replaced by their squared expression. It ended by the Bogoliubov–Valatin transformation allowing one to diagonalize the Hamiltonian of coupled oscillators via terms quadratic in the raising and lowering operators. Even though many results will not be used later, they are nevertheless important in many studies lying beyond the scope of the present work particularly in quantum optics.

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PART III

ANHARMONICITY

CHAPTER 9

ANHARMONIC OSCILLATORS

INTRODUCTION

In a previous chapter, we studied the general properties of single-degree-of-freedom quantum harmonic oscillators for which it was possible to solve the Hamiltonian eigenvalue equation and thus to get the energy levels. The calculation was also made for the driven harmonic oscillator by diagonalization of its Hamiltonian through canonical transformations, using the translation operators. Then, it was seen that it is possible to reproduce numerically the exact Hamiltonian eigenvalues obtained by this last procedure, after diagonalization of the truncated matrix representation of the driven Hamiltonian in the basis of the eigenkets of the harmonic oscillator Hamiltonian.

The aim of the present chapter is to find the energy levels of various anharmonic oscillators of interest for which it is not possible to diagonalize the Hamiltonian, using this numerical procedure for the driven harmonic oscillator. We shall first study the energy levels of oscillators for which the harmonic potential is perturbed by a cubic term. Second, we shall consider oscillators in a Morse potential, a physical model that applies to the vibrational behavior of diatomic molecules. Finally, we shall consider particles in a double-well potential, a model that applies to the inversion of ammonia for which tunneling may proceed through the barrier potential between the two wells. However, before commencing these studies, it may be of interest to find how quantum mechanics predicts the form of the anharmonic potentials in which the nuclei of diatomic molecules move.

9.1 MODEL FOR DIATOMIC MOLECULE POTENTIALS

For this purpose, we shall introduce in this section a very crude model applying to the H_2^+ molecular ion, which is the most simple diatomic molecule, since it involves only one electron and two protons. We shall attempt to simplify the notations, using the centimeter–gram–second (cgs) system.

The average kinetic energy $\langle T \rangle$ of the electron belonging to the molecular ion H_2^+ may be approximated by that of the *1D particle-in-a-box* model for which,

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according to Eq. (4.28), the 1D energy levels are given by

$$E_{n_x} = n_x^2 \frac{h^2}{8ma_x^2} \quad \text{with} \quad n_x = 1, 2, \ldots$$

where m is the mass of the particle and a_x the dimension of the 1D box. We shall assume that this kinetic energy is given by the 1D ground state of this model, that is,

$$\langle T \rangle = \frac{h^2}{8ma_x^2}$$

Moreover, in the present situation, the dimension a_x of the box may be viewed roughly as the distance R between the two protons.

For the electronic ground state, this leads us to write the average kinetic energy $\langle T \rangle$:

$$\langle T \rangle = \frac{A_T}{R^2} \quad \text{with} \quad A_T = \frac{h^2}{8m} \tag{9.1}$$

where m is now the mass of the single electron.

On the other hand, the average Coulombic potential energy $\langle V \rangle$ of the ion is the sum of the average attraction energies $\langle V_1 \rangle$ and $\langle V_2 \rangle$ between the single electron and the two protons and of the repulsion energy between the two protons, which is inversely proportional to R, that is,

$$\langle V \rangle = \langle V_1 \rangle + \langle V_2 \rangle + \frac{e^2}{R} \tag{9.2}$$

where e is the elementary electrical charge. The two average attraction energies $\langle V_1 \rangle$ and $\langle V_2 \rangle$ must be the same for symmetry reasons. For each of them, one may roughly assume that they are proportional to the inverse of the average distance between the electron and the nuclei, and more crudely that this average distance is proportional to half the distance R, leading us to write

$$\langle V_1 \rangle = \langle V_2 \rangle = -\frac{e^2}{R/2}$$

Hence, the average potential energy (9.2) becomes

$$\langle V \rangle = -4\frac{e^2}{R} + \frac{e^2}{R}$$

or

$$\langle V \rangle = -\frac{A_V}{R} \quad \text{with} \quad A_V = 3e^2 \tag{9.3}$$

Then, for this crude linear model, the electronic energy $\langle E \rangle$ of the molecular ion is simply the sum of $\langle T \rangle$ and $\langle V \rangle$, given, respectively, by Eqs. (9.1) and (9.3):

$$\langle E \rangle = \left\{ \frac{A_T}{R^2} - \frac{A_V}{R} \right\} \tag{9.4}$$

The evolution of E with respect to R given by Eq. (9.4) is reproduced in Fig. 9.1.

Inspection of this figure shows, as expected, a minimum of the energy function (9.4), which appears to be the result of a compromise between the positive

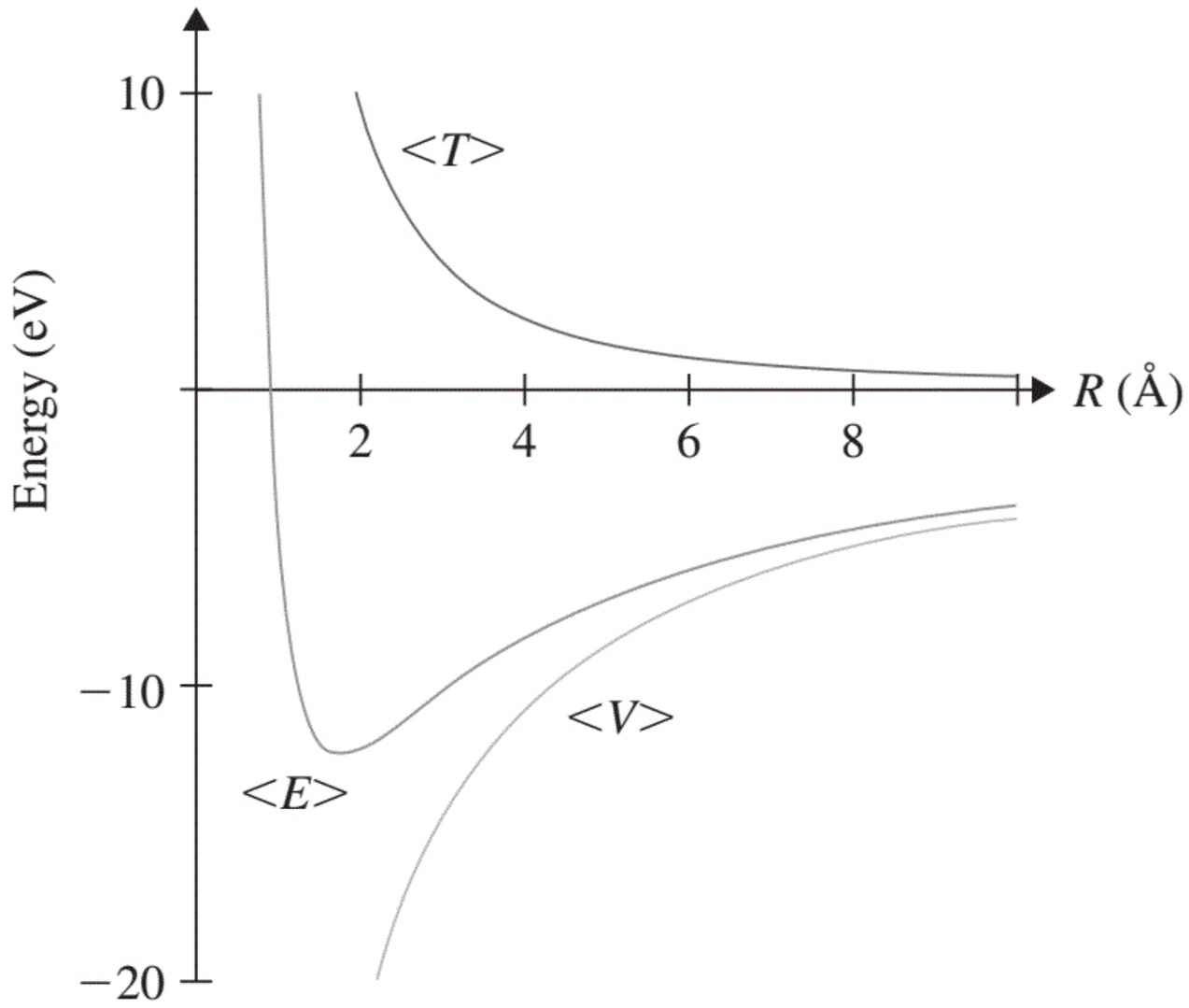


Figure 9.1 Total energy of the molecular ion H_2^+ as a compromise between a repulsive electronic kinetic energy and an attractive potential energy. Energies are in electron volts and distances in Ångström.

kinetic energy, which is decreasing in R, and the negative potential energy, which is correlatively increasing.

By Taylor expansion of the energy $\langle E \rangle$, denoted $E(R)$ near its minimum, corresponding to the internuclear distance $R = R^\circ$ of the energy curve yields

$$E(R) = (E)_{R^\circ} + \left(\frac{\partial E}{\partial R}\right)_{R=R^\circ} (R - R^\circ) + \frac{1}{2!}\left(\frac{\partial^2 E}{\partial R^2}\right)_{R=R^\circ} (R - R^\circ)^2 + \frac{1}{3!}\left(\frac{\partial^3 E}{\partial R^3}\right)_{R=R^\circ} (R - R^\circ)^3 + \frac{1}{4!}\left(\frac{\partial^4 E}{\partial R^4}\right)_{R=R^\circ} (R - R^\circ)^4 + \cdots \quad (9.5)$$

Of course, at the minimum of the energy function, the first derivative is zero, that is,

$$\left(\frac{\partial E}{\partial R}\right)_{R_e} = 0 \quad (9.6)$$

Hence, taking as energy reference

$$(E)_{R_e} = 0 \quad \text{at} \quad R = R_e$$

and near the minimum, the Taylor expansion (9.5) reads

$$E(R) = \frac{1}{2!} k_e (R - R_e)^2 + \frac{1}{3!} g_e (R - R_e)^3 + \frac{1}{4!} j_e (R - R_e)^4 + \cdots \quad (9.7)$$

with, respectively,

$$k_e = \left(\frac{\partial^2 E}{\partial R^2}\right)_{R=R_e} \tag{9.8}$$

$$g_e = \left(\frac{\partial^3 E}{\partial R^3}\right)_{R=R_e} \tag{9.9}$$

$$j_e = \left(\frac{\partial^4 E}{\partial R^4}\right)_{R=R_e} \tag{9.10}$$

In order to get the equilibrium distance R_e, we differentiate the energy function $E(R)$ (9.4) with respect to R:

$$\left(\frac{\partial E}{\partial R}\right) = -\frac{2A_T}{R^3} + \frac{A_V}{R^2} \tag{9.11}$$

Thus, for the equilibrium distance R_e for which Eq. (9.6) is verified, Eq. (9.11) yields

$$-\frac{2A_T}{R_e^3} + \frac{A_V}{R_e^2} = 0$$

so that the equilibrium distance appears to be given by

$$R_e = 2\frac{A_T}{A_V} \tag{9.12}$$

or, owing to Eqs. (9.1) and (9.3),

$$R_e = \left(\frac{h^2}{12me^2}\right) \tag{9.13}$$

and so, inserting numerical values,

$$R_e = 1.73 \times 10^{-8}\,\text{cm} = 1.73\,\text{Å}$$

Now, due to Eq. (9.13) and owing to Eqs. (9.8) and (9.11), the constant k_e reads

$$k_e = \frac{6A_T}{R_e^4} - \frac{2A_V}{R_e^3}$$

or, using Eq. (9.12) for R_e,

$$k_e = 6\left\{A_T\left(\frac{A_V}{2A_T}\right)^4 - A_V\left(\frac{A_V}{2A_T}\right)^3\right\}$$

and, after rearranging and simplifying

$$k_e = \frac{1}{8}\left(\frac{(A_V)^4}{(A_T)^3}\right) \tag{9.14}$$

In a similar way, one may obtain for the constants g_e and j_e defined by Eq. (9.9) and (9.10) the following result:

$$g_e = -\frac{3}{8}\left(\frac{(A_V)^5}{(A_T)^4}\right) \tag{9.15}$$

$$j_e = \frac{9}{8}\left(\frac{(A_V)^6}{(A_T)^5}\right) \tag{9.16}$$

Now, introduce the well-known dimensionless *fine structure constant* α and the *Compton wavelength* λ_c defined, respectively, in the CGS system by

$$\alpha = \frac{e^2}{\hbar c} = 2\pi \frac{e^2}{hc} = \frac{1}{137} \tag{9.17}$$

$$\lambda_c = \left(\frac{h}{mc}\right) = 2.43 \times 10^{-10}\,\text{cm} \quad \text{with } c\text{, the light velocity} \tag{9.18}$$

so that

$$\left(\frac{\lambda_c}{\alpha}\right) = \frac{h}{mc}\frac{\hbar c}{2\pi e^2} = \frac{h^2}{2\pi m e^2} \tag{9.19}$$

Then, due to Eq. (9.19), the equilibrium distance (9.13) may be approximated by

$$R_e = \frac{\pi}{6}\frac{\lambda_c}{\alpha} \backsimeq 0.5\left(\frac{\lambda_c}{\alpha}\right) \tag{9.20}$$

Proceeding in a similar way for k_e, g_e, and j_e, defined by Eqs. (9.14)–(9.16), we have

$$k_e = 3.33\alpha^2(mc^2)\left(\frac{\alpha}{\lambda_c}\right)^2 \backsimeq 3\alpha^2(mc^2)\left(\frac{\alpha}{\lambda_c}\right)^2 > 0 \tag{9.21}$$

$$g_e = 38.11\alpha^2(mc^2)\left(\frac{\alpha}{\lambda_c}\right)^3 \backsimeq -3 \times 12\alpha^2(mc^2)\left(\frac{\alpha}{\lambda_c}\right)^3 < 0 \tag{9.22}$$

$$j_e = 436.78\alpha^2(mc^2)\left(\frac{\alpha}{\lambda_c}\right)^4 \backsimeq 3 \times (12)^2\alpha^2(mc^2)\left(\frac{\alpha}{\lambda_c}\right)^4 < 0 \tag{9.23}$$

Hence, the Taylor expansion of the energy (9.7) yields

$$E(R) \backsimeq 3\alpha^2(mc^2)\left\{\frac{1}{2}\left(\frac{\alpha}{\lambda_c}\right)^2(R-R_e)^2 - \frac{12}{3!}\left(\frac{\alpha}{\lambda_c}\right)^3(R-R_e)^3 + \frac{(12)^2}{4!}\left(\frac{\alpha}{\lambda_c}\right)^4(R-R_e)^4\right\} \tag{9.24}$$

Again, owing to Eq. (9.20), which reads,

$$\frac{\alpha}{\lambda_c} = \frac{1}{2R_e}$$

and after making the approximation $\frac{5}{4} \backsimeq 1$, the expansion (9.24) may be approached by

$$E(R) \backsimeq 3\alpha^2(mc^2) \times \left(\frac{1}{2}\right)^3\left\{\left(\frac{(R-R_e)}{R_e}\right)^2 - 2\left(\frac{(R-R_e)}{R_e}\right)^3 + 3\left(\frac{(R-R_e)}{R_e}\right)^4\right\} \tag{9.25}$$

Next, near the equilibrium distance R_e, where

$$\frac{(R-R_e)}{R_e} << 1$$

then it reads

$$3\left(\frac{(R-R_e)}{R_e}\right)^4 << 2\left(\frac{(R-R_e)}{R_e}\right)^3 << \left(\frac{(R-R_e)}{R_e}\right)^2$$

so that the Taylor expansion (9.7) may be approximated by the first quadratic term, that is, by

$$E(R) = \tfrac{1}{2}k_e(R-R_e)^2 \tag{9.26}$$

from which the following force may be obtained through:

$$F(R) = -\left(\frac{\partial E(R)}{\partial R}\right) \backsimeq -k_e(R-R_e) \tag{9.27}$$

Equation (9.27) now allows one to write the classical dynamics equation

$$M\left(\frac{d^2(R-R_e)}{dt^2}\right) = -k_e(R-R_e)$$

where M is the reduced mass of the two protons. The solution of the latter equation is, of course,

$$(R(t)-R_e) = (R(0)-R_e)\cos(\omega t+\varphi)$$

where φ is some phase, and ω is an angular frequency given by

$$\boxed{\omega = \sqrt{\frac{k_e}{M}}} \tag{9.28}$$

Hence, due to this expression of ω, the electronic energy (9.26) of the molecular ion may be written

$$E(R) = \tfrac{1}{2}M\omega^2(R-R_e)^2 \tag{9.29}$$

This electronic energy $E(R)$ may be viewed as a potential in which the two protons of the molecular ion are allowed to oscillate with angular frequency ω. Then, according to quantum mechanics, one has to write in place of $E(R)$ given by Eq. (9.29) the following potential operator $\mathbf{V}(\mathbf{Q})$:

$$\mathbf{V}(\mathbf{Q}) = \tfrac{1}{2}M\omega^2\mathbf{Q}^2$$

where $\mathbf{Q}$ is the quantum position operator corresponding to the classical elongation Q given by

$$Q = R - R_e$$

Thus, in view of Eq. (9.21), the angular frequency (9.28) takes the form

$$\omega \backsimeq \alpha^2\left(\frac{c}{\lambda_c}\right)\sqrt{3\frac{m}{M}} \tag{9.30}$$

Moreover, observe that the ratio of the electron and proton masses m/M is about 10^3 so that, using Eqs. (9.17) and (9.18) for α and λ_c and for c its numerical value $3\times10^{10}\,\mathrm{cm\cdot s^{-1}}$, this angular frequency appears to be

$$\omega \backsimeq 3.6\times10^{14}\,\mathrm{rad\cdot s^{-1}}$$

Again, passing to vibrational frequency ν, one obtains a value that is in the infrared area:

$$\nu = \frac{\omega}{2\pi} \backsimeq 5 \times 10^{13}\,\text{Hz} \tag{9.31}$$

Now, return to the expansion of the potential energy (9.25). If one limits oneself to the quadratic term, the potential becomes harmonic and that used in the previous chapters dealing with quantum harmonic oscillator. Now, if one likes to go further in the potential energy expansion, the largest correction to incorporate is cubic in the elongation and thus in the $\mathbf{Q}$ operator. The next section is devoted to treating quantum anharmonic oscillators involving such potentials.

9.2 HARMONIC OSCILLATOR PERTURBED BY A Q^3 POTENTIAL

For this purpose, consider the following Hamiltonian:

$$\mathbf{H} = \frac{\mathbf{P}^2}{2M} + \mathbf{V}_{\text{Cub}}(\mathbf{Q}) \tag{9.32}$$

Here $\mathbf{Q}$, $\mathbf{P}$, and M are, respectively, the position and momentum operators and the reduced mass of the oscillator, whereas $\mathbf{V}_{\text{Cub}}(\mathbf{Q})$ is the cubic anharmonic potential

$$\mathbf{V}_{\text{Cub}}(\mathbf{Q}) = \tfrac{1}{2}M\omega^2\mathbf{Q}^2 + \xi\mathbf{Q}^3 \quad \text{with} \quad \xi = \frac{g_e}{3!} < 0 \tag{9.33}$$

where ξ is the dimensionless anharmonic cubic parameter related to the g_e coefficient of the expansion (9.7), which is negative, according to Eq. (9.22). Now consider the raising and lowering operators using Eqs. (5.6) and (5.7), that is,

$$\mathbf{Q} = \sqrt{\frac{\hbar}{2M\omega}}(\mathbf{a}^\dagger + \mathbf{a}) \tag{9.34}$$

$$\mathbf{P} = i\sqrt{\frac{M\hbar\omega}{2}}(\mathbf{a}^\dagger - \mathbf{a}) \tag{9.35}$$

Then, the Hamiltonian (9.32) becomes

$$\mathbf{H} = \hbar\omega\left\{\left(\mathbf{a}^\dagger\,\mathbf{a} + \tfrac{1}{2}\right) + \eta(\mathbf{a}^\dagger + \mathbf{a})^3\right\} \tag{9.36}$$

with

$$\eta = \xi\left(\frac{\hbar}{2M\omega}\right)^{3/2} < 0 \tag{9.37}$$

9.2.1 Matrix representation of the anharmonic Hamiltonian in the basis of the harmonic Hamiltonian eigenkets

Now, consider the basis in which $\mathbf{a}^\dagger\mathbf{a}$ is diagonal, that is,

$$\mathbf{a}^\dagger\mathbf{a}|\{n\}\rangle = n|\{n\}\rangle \quad \text{with} \quad \langle\{m\}|\{n\}\rangle = \delta_{mn} \tag{9.38}$$

In this basis, the matrix representation of the full Hamiltonian is

$$\langle\{m\}|\mathbf{H}|\{n\}\rangle = \hbar\omega\langle\{m\}|\left\{\left(\mathbf{a}^\dagger\,\mathbf{a}+\tfrac{1}{2}\right)+\eta(\mathbf{a}^\dagger+\mathbf{a})^3\right\}|\{n\}\rangle$$

Then, in view of the orthonormality properties appearing in (9.38), it reduces to

$$\langle\{m\}|\mathbf{H}|\{n\}\rangle = \hbar\omega\left\{\left(n+\tfrac{1}{2}\right)\delta_{mn}+\eta\langle\{m\}|(\mathbf{a}^\dagger+\mathbf{a})^3|\{n\}\rangle\right\} \tag{9.39}$$

Again, the matrix elements of the cubic perturbation terms appearing in Eq. (9.39) are

$$\begin{aligned}
&\langle\{m\}|(\mathbf{a}^\dagger+\mathbf{a})^3|\{n\}\rangle \\
&\quad=\langle\{m\}|\mathbf{a}^\dagger\mathbf{a}^\dagger\mathbf{a}^\dagger|\{n\}\rangle+\langle\{m\}|\mathbf{a}^\dagger\mathbf{a}\mathbf{a}|\{n\}\rangle+\langle\{m\}|\mathbf{a}^\dagger\mathbf{a}^\dagger\mathbf{a}|\{n\}\rangle \qquad (9.40)\\
&\qquad+\langle\{m\}|\mathbf{a}^\dagger\mathbf{a}\mathbf{a}^\dagger|\{n\}\rangle+\langle\{m\}|\mathbf{a}\mathbf{a}^\dagger\mathbf{a}^\dagger|\{n\}\rangle \\
&\qquad+\langle\{m\}|\mathbf{a}\mathbf{a}\mathbf{a}|\{n\}\rangle+\langle\{m\}|\mathbf{a}\mathbf{a}^\dagger\mathbf{a}|\{n\}\rangle+\langle\{m\}|\mathbf{a}\mathbf{a}\mathbf{a}^\dagger|\{n\}\rangle
\end{aligned}$$

Next, keeping in mind Eqs. (5.53) and (5.63), that is,

$$\mathbf{a}^\dagger|\{n\}\rangle=\sqrt{n+1}|\{n+1\}\rangle \qquad \text{and} \qquad \mathbf{a}|\{n\}\rangle=\sqrt{n}|\{n-1\}\rangle$$

and after using the orthornormality properties (9.38), the following expressions are obtained for the various matrix elements (9.40):

$$\begin{aligned}
\langle\{m\}|\mathbf{a}^\dagger\mathbf{a}^\dagger\mathbf{a}^\dagger|\{n\}\rangle &= \sqrt{(n+1)(n+2)(n+3)}\delta_{m,n+3} && (9.41)\\
\langle\{m\}|\mathbf{a}^\dagger\mathbf{a}\mathbf{a}|\{n\}\rangle &= (n-1)\sqrt{n}\delta_{m,n-1} && (9.42)\\
\langle\{m\}|\mathbf{a}^\dagger\mathbf{a}^\dagger\mathbf{a}|\{n\}\rangle &= n\sqrt{n+1}\delta_{m,n+1} && (9.43)\\
\langle\{m\}|\mathbf{a}^\dagger\mathbf{a}\mathbf{a}^\dagger|\{n\}\rangle &= (n+1)\sqrt{n+1}\delta_{m,n+1} && (9.44)\\
\langle\{m\}|\mathbf{a}\mathbf{a}^\dagger\mathbf{a}^\dagger|\{n\}\rangle &= \sqrt{n+1}(n+2)\delta_{m,n+1} && (9.45)\\
\langle\{m\}|\mathbf{a}\mathbf{a}\mathbf{a}|\{n\}\rangle &= \sqrt{n}\sqrt{(n-1)(n-2)}\delta_{m,n-3} && (9.46)\\
\langle\{m\}|\mathbf{a}\mathbf{a}^\dagger\mathbf{a}|\{n\}\rangle &= n\sqrt{n}\delta_{m,n-1} && (9.47)\\
\langle\{m\}|\mathbf{a}\mathbf{a}\mathbf{a}^\dagger|\{n\}\rangle &= (n+1)\sqrt{n}\delta_{m,n-1} && (9.48)
\end{aligned}$$

9.2.2 Diagonalization of the truncated matrix representations of the Hamiltonian

The matrix elements involved in the matrix representation (9.39) of the Hamiltonian may be computed using Eq. (9.40) by the aid of Eqs. (9.41)–(9.48). This may be accomplished by starting from the ground state $|\{0\}\rangle$ and increasing progressively the quantum number associated to the ket $|\{n\}\rangle$. Since the basis appearing in Eq. (9.38) is infinite, the matrix representation must be also infinite. Thus, in order to be numerically diagonalized, the matrix representation (9.39) must be truncated after some value n° of the quantum number n characterizing $|\{n\}\rangle$. Then, we get a finite square $(n^\circ+1)\times(n^\circ+1)$ Hamiltonian matrix in the basis $\{|\{n\}\rangle\}$ expressed in terms of $\hbar\omega$

and η. For example, when $\eta = 0.017$ and for a truncation corresponding to $n^\circ = 9$, the matrix representation reads as follows:

$$\boxed{\frac{\mathbf{H}}{\hbar\omega}} = \begin{array}{|r|r|r|r|r|r|r|r|r|r|}
\hline
\mathbf{0.500} & -0.051 & & -0.042 & & & & & & \\ \hline
-0.051 & \mathbf{1.500} & -0.144 & & -0.083 & & & & & \\ \hline
 & -0.144 & \mathbf{2.500} & -0.265 & & -0.132 & & & & \\ \hline
-0.042 & & -0.265 & \mathbf{3.500} & -0.408 & & -0.186 & & & \\ \hline
 & -0.083 & & -0.408 & \mathbf{4.500} & -0.570 & & -0.246 & & \\ \hline
 & & -0.132 & & -0.570 & \mathbf{5.500} & -0.750 & & -0.312 & \\ \hline
 & & & -0.186 & & -0.750 & \mathbf{6.500} & -0.945 & & -0.382 \\ \hline
 & & & & -0.246 & & -0.945 & \mathbf{7.500} & -1.154 & \\ \hline
 & & & & & -10.312 & & -1.154 & \mathbf{8.500} & -1.377 \\ \hline
 & & & & & & -0.382 & & -1.377 & \mathbf{9.500} \\ \hline
\end{array} \tag{9.49}$$

A truncated matrix such as (9.49) may be diagonalized by standard procedures leading to approximate numerical solutions of the eigenvalue equation

$$\mathbf{H}|\Psi_k(n^\circ)\rangle = E_k(n^\circ)|\Psi_k(n^\circ)\rangle \tag{9.50}$$

Here the $E_k(n^\circ)$ are the n°-dependent approximate eigenvalues of (9.49), whereas the $|\Psi_k(n^\circ)\rangle$ are the corresponding n°-dependent approximate eigenvectors, given by

$$|\Psi_k(n^\circ)\rangle = \sum_n C_{nk}(n^\circ)|\{n\}\rangle \tag{9.51}$$

where the $C_{nk}(n^\circ)$ are components of the orthogonal matrix allowing one to diagonalize the matrix (9.49) of dimension n°. Of course, the eigenvalues $E_k(n^\circ)$ and the eigenvectors $|\Psi_k(n^\circ)\rangle$, which are, respectively, the approximate eigenvalues and eigenkets of the Hamiltonian (9.36), may be assumed to change with the dimension n° of the truncated matrix representation of this Hamiltonian in such a way as to stabilize themselves as for the driven harmonic oscillator.

Recall that we have previously studied this driven harmonic oscillator by two different methods. In the first one the Hamiltonian operator was diagonalized using a canonical transformation so that its eigenvalues, that is, the energy levels and the corresponding eigenkets were obtained exactly. In the last one, a matrix representation of the Hamiltonian was performed in the basis of the eigenkets of the harmonic Hamiltonian, and then the truncated matrices of increasing dimension n° were diagonalized, leading to approximate energy levels that progressively decrease to converge toward the exact eigenvalues obtained by the first method, when n° was progressively increased.

Figure 9.2 shows that, as for the driven harmonic oscillator, the approximate energy levels $E_k(n^\circ)$ obtained by diagonalization of the matrix representation of the full Hamiltonian (for $\eta = -0.017$) stabilize indeed when the dimension n° of the truncated matrix is progressively increased.

Hence, the stabilized energy levels may be considered as satisfactorily fitting the exact energy levels.

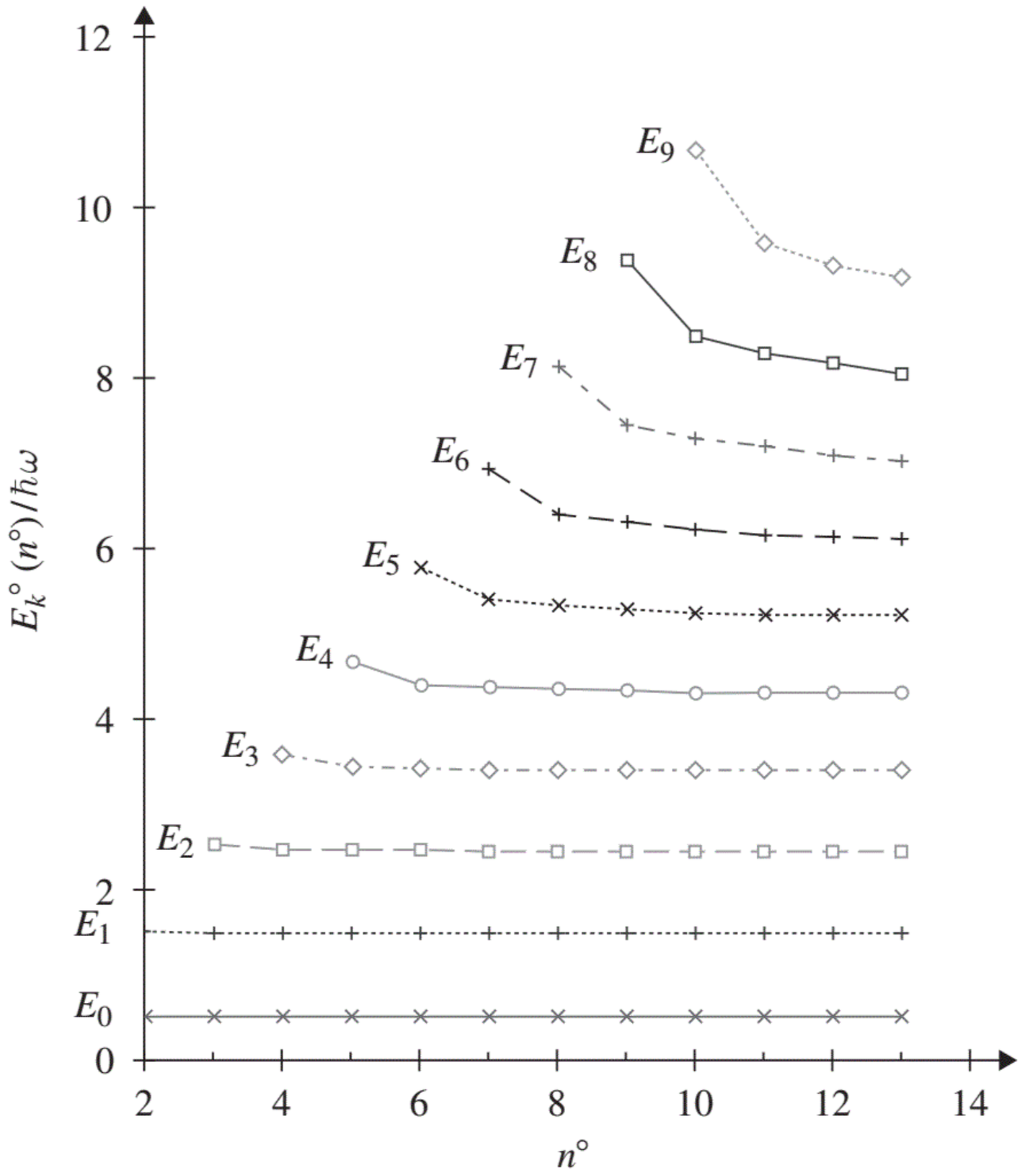


Figure 9.2 Progressive stabilization of the eigenvalues appearing in Eq. (9.50) with the dimension n° of the truncated matrix representation ($\eta = -0.017$). (See color insert.)

9.2.3 Accuracy criterion of the approximate method using the virial theorem

It has been shown above that the virial theorem allows one to write the following expression for the average value of the kinetic operator $\mathbf{T}$:

$$2\langle\Psi_k(n^\circ)|\mathbf{T}|\Psi_k(n^\circ)\rangle = \langle\Psi_k(n^\circ)|\mathbf{Q}\left(\frac{\partial\mathbf{V}(\mathbf{Q})}{\partial\mathbf{Q}}\right)|\Psi_k(n^\circ)\rangle \tag{9.52}$$

where $\mathbf{Q}$ is the coordinate operator and $\mathbf{V}(\mathbf{Q})$ the potential operator. This expression holds if the averages of the operators are performed over a stationary state $|\Psi_k\rangle$. In our study of the present anharmonic oscillator, we are interested in the eigenvalues and the corresponding eigenvectors of the Hamiltonian. Actually, these eigenvectors are stationary states, so that the average values performed on them ought to satisfy Eq. (9.52), if they were exact. But they are only approximate so that it may be of interest to show how Eq. (9.52) is approximately satisfied.

Keeping in mind Eq. (9.33), that is,

$$\mathbf{V}_{\text{Cub}}(\mathbf{Q}) = \tfrac{1}{2}M\omega^2\mathbf{Q}^2 + \xi\mathbf{Q}^3 \tag{9.53}$$

the partial derivative of the potential appearing in Eq. (9.52) yields

$$\left(\frac{\partial \mathbf{V}_{\text{Cub}}(\mathbf{Q})}{\partial \mathbf{Q}}\right) = M\omega^2\mathbf{Q} + 3\xi\mathbf{Q}^2$$

and thus

$$\mathbf{Q}\left(\frac{\partial \mathbf{V}_{\text{Cub}}(\mathbf{Q})}{\partial \mathbf{Q}}\right) = M\omega^2\mathbf{Q}^2 + 2\xi\mathbf{Q}^3 + \xi\mathbf{Q}^3$$

or

$$\mathbf{Q}\left(\frac{\partial \mathbf{V}_{\text{Cub}}(\mathbf{Q})}{\partial \mathbf{Q}}\right) = 2\mathbf{V}_{\text{Cub}}(\mathbf{Q}) + \xi\mathbf{Q}^3$$

Hence, Eq. (9.52) reads

$$\langle\Psi_k(n^\circ)|\mathbf{T}|\Psi_k(n^\circ)\rangle = \langle\Psi_k(n^\circ)|\mathbf{V}_{\text{Cub}}(\mathbf{Q})|\Psi_k(n^\circ)\rangle + \tfrac{1}{2}\xi\langle\Psi_k(n^\circ)|\mathbf{Q}^3|\Psi_k(n^\circ)\rangle \quad (9.54)$$

Moreover, the corresponding average value of the Hamiltonian (9.32), that is,

$$\langle\Psi_k(n^\circ)|\mathbf{H}|\Psi_k(n^\circ)\rangle = \langle\mathbf{T}\rangle_{\Psi_k} + \langle\Psi_k(n^\circ)|\mathbf{V}_{\text{Cub}}(\mathbf{Q})|\Psi_k(n^\circ)\rangle$$

appears, due to Eq. (9.54), to be given by

$$\langle\Psi_k(n^\circ)|\mathbf{H}|\Psi_k(n^\circ)\rangle = 2\langle\Psi_k(n^\circ)|\mathbf{V}_{\text{Cub}}(\mathbf{Q})|\Psi_k(n^\circ)\rangle + \tfrac{1}{2}\xi\langle\Psi_k(n^\circ)|\mathbf{Q}^3|\Psi_k(n^\circ)\rangle \quad (9.55)$$

On the other hand, in view of Eq. (9.50), it may be also given by

$$\langle\Psi_k(n^\circ)|\mathbf{H}|\Psi_k(n^\circ)\rangle = E_k(n^\circ) \quad (9.56)$$

Hence, a good test for the accuracy of the approximate kets $|\Psi_k(n^\circ)\rangle$ may be the differences $\Delta E_k(n^\circ)$ between Eqs. (9.56) and (9.55), which ought to be zero if the kets were the exact eigenvectors of the Hamiltonian.

$$\Delta E_k(n^\circ) = E_k(n^\circ) - \{2\langle\Psi_k(n^\circ)|\mathbf{V}_{\text{Cub}}(\mathbf{Q})|\Psi_k(n^\circ)\rangle + \tfrac{1}{2}\xi\langle\Psi_k(n^\circ)|\mathbf{Q}^3|\Psi_k(n^\circ)\rangle\}$$

Then using Eqs. (9.51) and (9.53), the virial theorem leads to

$$\Delta E_k(n^\circ) = E_k(n^\circ) - \sum_n\sum_m C_{nk}(n^\circ)C_{km}(n^\circ) \times \left\{M\omega^2\langle\{m\}|(\mathbf{Q}^2)|\{n\}\rangle + \tfrac{5}{2}\xi\langle\{m\}|(\mathbf{Q}^3)|\{n\}\rangle\right\}$$

Passing to Boson operators for the cubic term yields

$$\Delta E_k(n^\circ) = E_k(n^\circ) - \sum_n\sum_m C_{nk}\,(n^\circ)C_{km}(n^\circ) \times \left\{M\omega^2\langle\{m\}|\mathbf{Q}^2|\{n\}\rangle + \frac{5}{2}\xi\left(\frac{\hbar}{2M\omega}\right)^{3/2}\langle\{m\}|(\mathbf{a}^\dagger + \mathbf{a})^3|\{n\}\rangle\right\} \quad (9.57)$$

or in dimensionless units, given by (9.37), that is,

$$\xi = \eta\hbar\omega\left(\frac{2M\omega}{\hbar}\right)^{3/2}$$

$$\Delta E_k(n^\circ) = E_k(n^\circ) - \sum_n \sum_m C_{nk}(n^\circ)C_{km}(n^\circ)\hbar\omega \times \left\{\frac{1}{2}\langle\{m\}|(\mathbf{a}^\dagger + \mathbf{a})^2|\{n\}\rangle + \frac{5}{2}\eta\langle\{m\}|(\mathbf{a}^\dagger + \mathbf{a})^3|\{n\}\rangle\right\}$$

Of course, the matrix elements that are cubic with respect to the Boson operators may also be obtained by the aid of Eqs. (9.40) and (9.48). On the other hand, according to Eq. (5.87), those that are quadratic in $(\mathbf{a}^\dagger + \mathbf{a})$ are given by

$$\langle\{m\}|(\mathbf{a}^\dagger + \mathbf{a})^2|\{n\}\rangle = \langle\{m\}|((\mathbf{a}^\dagger)^2 + (\mathbf{a})^2 + 2\mathbf{a}^\dagger\mathbf{a} + 1)|\{n\}\rangle \tag{9.58}$$

and thus, due to Eqs. (5.53) and (5.63),

$$\langle\{m\}|(\mathbf{a}^\dagger + \mathbf{a})^2|\{n\}\rangle = (2n+1)\delta_{mn} + \sqrt{n+1}\sqrt{n+2}\delta_{m,n+2} + \sqrt{n}\sqrt{n-2}\delta_{m,n-2} \tag{9.59}$$

Hence, the verification that the virial theorem is satisfied may be performed by considering the energy difference between $\Delta E_k(n^\circ)/E_k(n^\circ)$ and zero, the smaller being this term and the best accurate being the kets $|\Psi_k(n^\circ)\rangle$ and the corresponding energy levels $E_k(n^\circ)$. In Fig. 9.3, we show the evolution of the relative dispersion $\Delta E_k(n^\circ)/E_k(n^\circ)$ as a function of n°, for the six lowest energy levels.

This criteria for accuracy of the absolute dispersion appears to be more drastic than stabilization of the energy as n° is raised. The graph in Fig. 9.3 shows that even if the energy is stabilized with respect to an enhancement of the number of basis terms, the virial theorem is less and less satisfied.

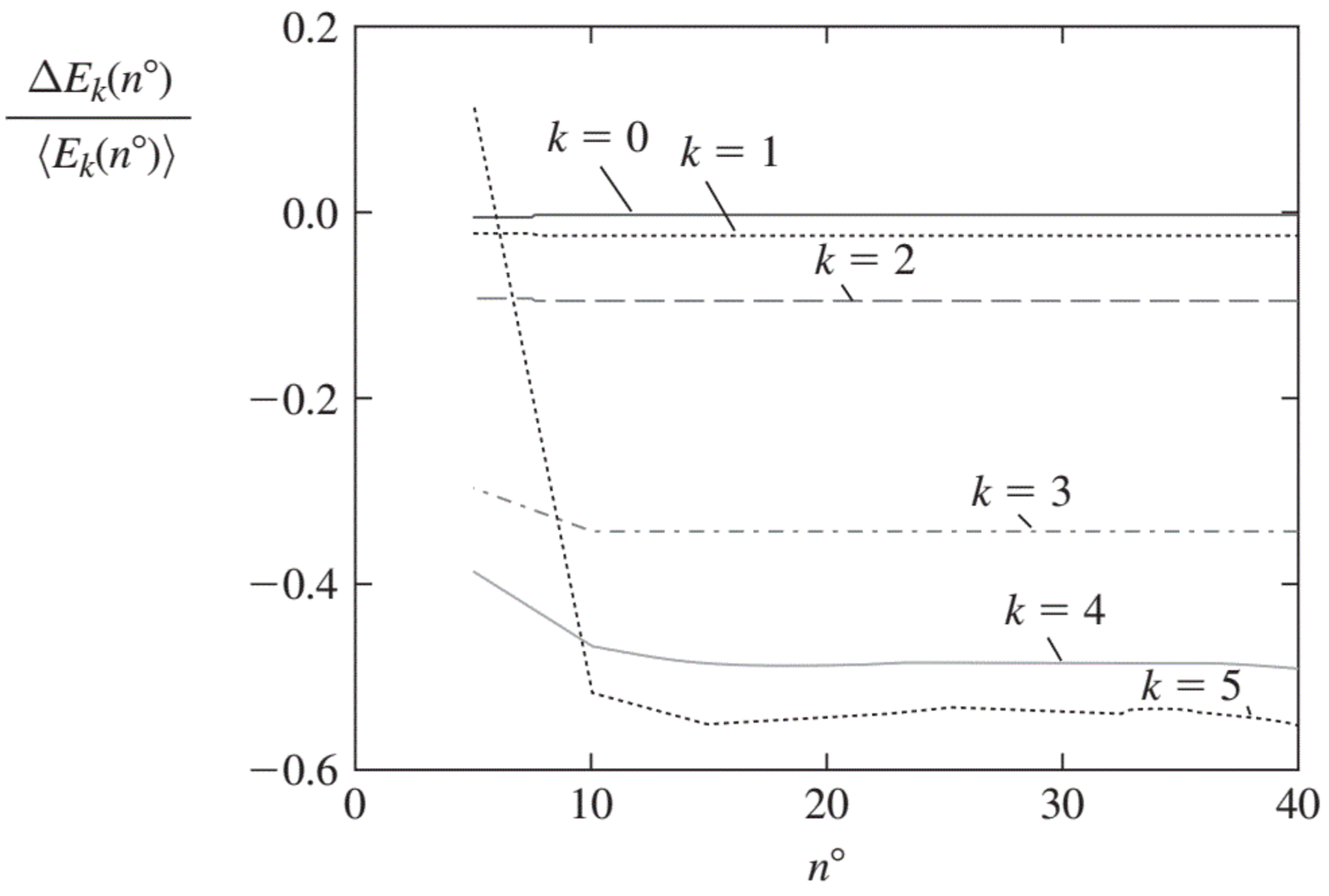


Figure 9.3 Relative dispersion of the difference between the energy levels and the virial theorem. (See color insert.)

9.3 MORSE OSCILLATOR

In the previous section, we approximated the Morse potential for diatomic nuclei by introducing in the harmonic potential the greatest correction, which is cubic with respect to the elongation. However, to be more rigorous it is necessary to take explicitly into account the Morse potential as a whole. For this purpose, one may use the following expression, which is *stricto sensu* what is called a *Morse potential*, to describe the Morse potential operator $\mathbf{V}_{\text{Morse}}$

$$\mathbf{V}_{\text{Morse}} = D_e(1 - e^{-\beta\mathbf{Q}})^2 \tag{9.60}$$

Here, $\mathbf{Q}$ is the position coordinate operator, D_e is the dissociation energy of the diatomic molecule, whereas β is a parameter that is function of the force constant k_e of the oscillator near the equilibrium geometry and of D_e

$$\beta = \left(\frac{k_e}{2D_e}\right)^{1/2}$$

The Hamiltonian governing the vibration of this diatomic molecule is described by

$$\mathbf{H} = \frac{\mathbf{P}^2}{2m} + \mathbf{V}_{\text{Morse}} \tag{9.61}$$

9.3.1 Analytical solution of the Hamiltonian eigenvalue equation

In the wave mechanics picture, the time-independent Schrödinger equation obtained from the Hamiltonian (9.61) is

$$-\frac{\hbar^2}{2M}\left(\frac{\partial^2\Psi_n(Q)}{\partial Q^2}\right) + D_e(1 - e^{-\beta\mathbf{Q}})^2\Psi_n(Q) = E_n\Psi_n(Q) \tag{9.62}$$

where $\Psi_n(Q)$ are the eigenfunctions and E_n the corresponding eigenvalues. Without solving the Schrödinger equation (9.62), the wavefunctions $\Psi_n(Q)$ are found to be[1]

$$\Psi_n(Q) = \left(\frac{2d\beta}{N_n}\right)^{1/2} \exp\{-de^{-\beta Q}\}(2de^{-\beta Q})^{(2d-2n-1)/2}\mathbb{L}_{2d-n-1}^{2d-2n-1}(2de^{-\beta Q}) \tag{9.63}$$

where $\mathbb{L}_{2d-n-1}^{2d-2n-1}(2de^{-\beta Q})$ are the associated Laguerre polynomials given by

$$\mathbb{L}_{2d-n-1}^{2d-2n-1}\left(2de^{-\beta Q}\right) = \sum_{k=0}^{n}(-1)^{k+1}\frac{\{(2d-n-1)!\}^2}{(n-k)!(2d+k-2n-1)!k!}(2de^{-\beta Q})^k$$

$$d = \frac{(2MD_e)^{1/2}}{\beta\hbar}$$

whereas N_n are the normalization constant

$$N_n = ((2d-n-1)!)^2\sum_{s=0}^{n}\frac{(2d-2n+s-2)!}{s!}$$

[1]See, for instance, Mu Sang Lee, L. A. Carreira, and D. A. Berkowitz, *Bull. Korean. Chem. Soc.*, **7** (1986): 6–7.

Of course, since the Hamiltonian (9.62) is Hermitian, the eigenfunctions form an orthonormal basis and thus obey

$$\int \Psi_m(Q)\Psi_n(Q)\,dQ = \delta_{mn}$$

Also, the corresponding energy levels E_n are[2]

$$E_n = \hbar\omega^\circ\left(n+\frac{1}{2}\right) - \frac{(\hbar\omega^\circ)^2}{4D_e}\left(n+\frac{1}{2}\right)^2 \tag{9.64}$$

Now, the analytical solutions (9.63) and (9.64) are exact with respect to the model to which they apply, they are unfortunately not easy to handle as a basis for matrix representations of Hamiltonians of more complex systems in which the Morse potential plays a role. This is the reason why an analytical solution of the Schrödinger equation (9.62) is not given here, and why we shall consider the numerical diagonalization of Hamiltonians involving the Morse potential, susceptible to be generalized to other anharmonic Hamiltonians.

9.3.2 Matrix elements of the Morse potential within the harmonic Hamiltonian eigenkets

9.3.2.1 Morse potential in terms of the ladder operators First, find the expression relating β to the force constant k_e and to the dissociation energy D_e. For this purpose, calculate the second derivative of the potential (9.60) in equilibrium geometry, that is, at the minimum of the Morse curve taken as the origin for the elongation operator $\mathbf{Q}$:

$$\left(\frac{\partial^2 \mathbf{V}_{\text{Morse}}}{\partial \mathbf{Q}^2}\right)_{\mathbf{Q}=0} = 2\beta^2 D_e \tag{9.65}$$

Now, the force constant k_e is by definition the second derivative of the potential at its minimum:

$$k_e = \left(\frac{\partial^2 \mathbf{V}_{\text{Morse}}}{\partial \mathbf{Q}^2}\right)_{\mathbf{Q}=0} \tag{9.66}$$

Thus, after identification of Eqs. (9.65) and (9.66), the β parameter appears to be given by

$$\beta = \sqrt{\frac{k_e}{2D_e}} \tag{9.67}$$

On the other hand, the force constant of a harmonic potential characterized by the angular frequency ω and the reduced mass M is

$$k_e = M\omega^2 \tag{9.68}$$

[2]P. M. Morse, *Phys. Rev.*, **34** (1929): 57–64.

Hence, if this harmonic potential is to be that which reduces the Morse potential at its minimum, Eq. (9.67) transforms using Eq. (9.60) into

$$\beta = \omega\sqrt{\frac{M}{2D_e}}$$

Then, in order to make explicit the Hamiltonian of the harmonic oscillator in the expression (9.61) of the Morse Hamiltonian, it is convenient to write Eq. (9.61) as

$$\mathbf{H} = \frac{\mathbf{P}^2}{2m} + \{\mathbf{V}_{\text{Harm}} - \mathbf{V}_{\text{Harm}}\} + \mathbf{V}_{\text{Morse}} \tag{9.69}$$

with

$$\{\mathbf{V}_{\text{Harm}}\} = \tfrac{1}{2}M\omega^2\mathbf{Q}^2 \tag{9.70}$$

leading to

$$\mathbf{H} = \left(\frac{\mathbf{P}^2}{2M} + \frac{1}{2}M\omega^2\mathbf{Q}^2\right) + (\mathbf{V}_{\text{Morse}} - \mathbf{V}_{\text{Harm}})$$

Next, pass to Boson operators by the aid of Eqs. (9.34) and (9.35). Then, the Morse potential operator (9.60) takes the form

$$\mathbf{V}_{\text{Morse}} = D_e(1 - 2e^{-\beta^\circ(\mathbf{a}^\dagger+\mathbf{a})} + e^{-2\beta^\circ(\mathbf{a}^\dagger+\mathbf{a})}) \tag{9.71}$$

where

$$\beta^\circ = \beta\sqrt{\frac{\hbar}{2M\omega}} = \frac{1}{2}\sqrt{\frac{\hbar\omega}{D_e}} \tag{9.72}$$

whereas the harmonic potential operator (9.70) reads

$$\mathbf{V}_{\text{Harm}} = \frac{\hbar\omega}{4}(\mathbf{a}^\dagger + \mathbf{a})^2 \tag{9.73}$$

Moreover, expansions of the square on the right-hand side give, using the commutation rule $[\mathbf{a}, \mathbf{a}^\dagger] = 1$,

$$\mathbf{V}_{\text{Harm}} = \frac{\hbar\omega}{4}((\mathbf{a}^\dagger)^2 + (\mathbf{a})^2) + \frac{\hbar\omega}{2}\left(\mathbf{a}^\dagger\mathbf{a} + \frac{1}{2}\right) \tag{9.74}$$

Finally, the sum of the potential (9.74) and of the kinetic energy operator, that is, the Hamiltonian of a harmonic oscillator yields, according to Eqs. (5.6) and (5.7),

$$\left(\frac{\mathbf{P}^2}{2M} + \frac{1}{2}M\omega^2\mathbf{Q}^2\right) = \hbar\omega\left(\mathbf{a}^\dagger\mathbf{a} + \frac{1}{2}\right) \tag{9.75}$$

As a consequence of Eqs. (9.71), (9.74), and (9.75), the full Hamiltonian (9.69) transforms to

$$\mathbf{H} = \hbar\omega\left\{\tfrac{1}{2}\left(\mathbf{a}^\dagger\mathbf{a} + \tfrac{1}{2}\right) - \tfrac{1}{4}((\mathbf{a}^\dagger)^2 + (\mathbf{a})^2) + \zeta(1 - 2e^{-\beta^\circ(\mathbf{a}^\dagger+\mathbf{a})} + e^{-2\beta^\circ(\mathbf{a}^\dagger+\mathbf{a})})\right\}$$

with

$$\zeta = \frac{D_e}{\hbar\omega}$$

This may be also written in the condensed form:

$$\mathbf{H} = \hbar\omega \left\{ \tfrac{1}{2}\left(\mathbf{a}^\dagger \mathbf{a} + \tfrac{1}{2}\right) - \tfrac{1}{4}((\mathbf{a}^\dagger)^2 + (\mathbf{a})^2) + \zeta(1 - 2\mathbf{F}(\beta^\circ) + \mathbf{F}(2\beta^\circ)) \right\} \tag{9.76}$$

with

$$\mathbf{F}(\beta^\circ) = e^{-\beta^\circ(\mathbf{a}^\dagger + \mathbf{a})} \qquad \text{and} \qquad \mathbf{F}(2\beta^\circ) = e^{-2\beta^\circ(\mathbf{a}^\dagger + \mathbf{a})}$$

Moreover, using the Glauber–Weyl theorem (1.79), the latter operator reads

$$\mathbf{F}(\beta^\circ) = e^{-\beta^\circ \mathbf{a}^\dagger} e^{-\beta^\circ \mathbf{a}} (e^{-\beta^{\circ 2}[\mathbf{a}^\dagger, \mathbf{a}]/2})$$

which, owing to the commutation rule $\left[\mathbf{a}, \mathbf{a}^\dagger\right] = 1$, it transforms to

$$\mathbf{F}(\beta^\circ) = e^{-\beta^\circ \mathbf{a}^\dagger} e^{-\beta^\circ \mathbf{a}} (e^{\beta^{\circ 2}/2})$$

Finally, expanding the exponentials involving the Boson operators according to

$$\mathbf{F}(\beta^\circ) = (e^{\beta^{\circ 2}/2}) \sum_{k=0}^{\infty} \frac{(-1)^k \beta^{\circ k} (\mathbf{a}^\dagger)^k}{k!} \sum_{l=0}^{\infty} \frac{(-1)^l \beta^{\circ l} (\mathbf{a})^l}{l!}$$

leads to

$$\mathbf{F}(\beta^\circ) = (e^{\beta^{\circ 2}/2}) \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{(-1)^{k+l} \beta^{\circ k+l}}{k!l!} (\mathbf{a}^\dagger)^k (\mathbf{a})^l \tag{9.77}$$

9.3.2.2 Matrix elements of the Morse Hamiltonian Next, consider the matrix elements of the full Hamiltonian (9.76) in the basis $\{|\{n\}\rangle\}$ of the eigenkets of $\mathbf{a}^\dagger \mathbf{a}$:

$$\mathbf{a}^\dagger \mathbf{a} |\{n\}\rangle = n |\{n\}\rangle \quad \text{with} \quad \langle\{n\}|\{n\}\rangle = \delta_{mn} \tag{9.78}$$

They are

$$\begin{aligned} \hbar\omega \langle\{m\}|\mathbf{H}|\{n\}\rangle \; = \; & \tfrac{1}{4} + \tfrac{1}{2}\langle\{m\}|(\mathbf{a}^\dagger \mathbf{a})|\{n\}\rangle - \tfrac{1}{4}\langle\{m\}|(\mathbf{a}^\dagger)^2|\{n\}\rangle - \tfrac{1}{4}\langle\{m\}|(\mathbf{a})^2|\{n\}\rangle \\ & + \zeta(1 - 2\langle\{m\}|\mathbf{F}(\beta^\circ)|\{n\}\rangle + \langle\{m\}|\mathbf{F}(2\beta^\circ)|\{n\}\rangle) \end{aligned} \tag{9.79}$$

Owing to Eq. (5.42), the first-right-hand-side matrix elements of Eq. (9.79) are

$$\langle\{m\}|(\mathbf{a}^\dagger \mathbf{a})|\{n\}\rangle = n \, \delta_{mn} \tag{9.80}$$

Then, one obtains, respectively, by the aid of Eqs. (5.53) and (5.63) for the two matrix elements of the squared Boson operators appearing in Eq. (9.79)

$$\langle\{m\}|(\mathbf{a}^\dagger)^2|\{n\}\rangle = \sqrt{(n+1)(n+2)}\delta_{m,n+2} \tag{9.81}$$

$$\langle\{m\}|(\mathbf{a})^2|\{n\}\rangle = \sqrt{(m+1)(m+2)}\delta_{m+2,n} \tag{9.82}$$

Now, consider the matrix elements of the operator $\mathbf{F}(\beta^\circ)$ (9.77), that is,

$$\langle\{m\}|\mathbf{F}(\beta^\circ)|\{n\}\rangle = (e^{\beta^{\circ 2}/2}) \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{(-1)^{k+l} (\beta^\circ)^{k+l}}{k!l!} \langle\{m\}|(\mathbf{a}^\dagger)^k (\mathbf{a})^l|\{n\}\rangle \tag{9.83}$$

Owing to Eqs. (5.72) and (5.73), the matrix elements involved on the right-hand side of (9.83) are given by

$$\langle\{m\}|(\mathbf{a}^\dagger)^k (\mathbf{a})^l|\{n\}\rangle = \frac{\sqrt{m!}}{\sqrt{(m-k)!}} \frac{\sqrt{n!}}{\sqrt{(n-l)!}} \langle\{m-k\}|\{n-l\}\rangle$$

or, using the orthornormality properties appearing in Eq. (9.78),

$$\langle\{m\}|\mathbf{a}^{\dagger k}\mathbf{a}^{l}|\{n\}\rangle = \frac{\sqrt{m!}}{\sqrt{(m-k)!}}\frac{\sqrt{n!}}{\sqrt{(n-l)!}}\{\delta(n-l,m-k)\}$$

so that the matrix element (9.83) takes the form

$$\langle\{m\}|\mathbf{F}(\beta^\circ)|\{n\}\rangle = e^{\beta^{\circ 2}/2}\sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\frac{(-1)^{k+l}\beta^{\circ k+l}}{k!l!}\frac{\sqrt{m!}}{\sqrt{(m-k)!}}\frac{\sqrt{n!}}{\sqrt{(n-l)!}}\{\delta(n-l,m-k)\} \tag{9.84}$$

Now, because

$$\{\delta(n-l,m-k)\} = 1 \quad \text{if} \quad l = n-m+k$$

and

$$\{\delta(n-l,m-k)\} = 0 \quad \text{otherwise}$$

Eq. (9.84) leads, respectively, according to whether $m \geq n$ or $m < n$, to

$$\langle\{m\}|\mathbf{F}(\beta^\circ)|\{n\}\rangle = e^{1/2\beta^{\circ 2}}\sum_{k=n-m}^{m}\frac{(-1)^{(n-m+2k)}\beta^{\circ(n-m+2k)}}{k!(n-m+k)!}\frac{\sqrt{m!}\sqrt{n!}}{(m-k)!} \quad \text{if} \quad m \geq n \tag{9.85}$$

and a similar expression for $n > m$ in which n and m have to be permuted.

Of course, the matrix elements $\langle\{m\}|\mathbf{F}(2\beta^\circ)|\{n\}\rangle$ appearing in Eq. (9.79) may be obtained by the aid of Eq. (9.85) in which the argument β° has been replaced by $2\beta^\circ$.

9.3.3 Diagonalization of the truncated Hamiltonian matrix representation

It is now possible to construct various truncated matrix representations (9.79) of the full Hamiltonian (9.61) by the aid of Eqs. (9.76), (9.80), (9.81), (9.82), and (9.85), the dimension n° of which being progressively increased, and then to numerically diagonalize them. This procedure leads to numerical approximations of the eigenvalue equation of the full Hamiltonian:

$$\mathbf{H}|\Psi_k(n^\circ)\rangle = E_k(n^\circ)|\Psi_k(n^\circ)\rangle$$

$$|\Psi_k(n^\circ)\rangle = \sum_{n=0}^{N-1} C_{nk}(n^\circ)|\{n\}\rangle \tag{9.86}$$

where $E_k(n^\circ)$ are the approximate eigenvalue functions of n°, whereas $|\Psi_k(n^\circ)\rangle$ are the corresponding eigenvectors, the components of which in the basis $\{|\{n\}\rangle\}$ are $C_{nk}(n^\circ)$. As previously for the driven harmonic oscillator and for the anharmonic oscillator involving a cubic potential, the approximate eigenvalues E_k of the Hamiltonian matrix are progressively stabilized.

As an illustration we reproduce the result of a numerical calculation where the dissociation energy of the Morse potential is $D_e = 50\,\hbar\omega$. The 10 lowest energy levels

$E_k(n^\circ)$ expressed in units $\hbar\omega$ are given in (9.87) and compared to the eigenvalues of the harmonic Hamiltonians:

	E_0	E_1	E_2	E_3	E_4	E_5	E_6	E_7	E_8	E_9
Morse	0.499	1.489	2.469	3.489	4.309	5.349	6.289	7.219	8.139	9.049
Harm	0.500	1.500	2.500	3.500	4.500	5.500	6.500	7.500	8.500	9.500

(9.87)

Inspection of (9.87) shows that the energy levels of the Morse Hamiltonian are more and more lowered with respect to those of the harmonic Hamiltonian when the energy levels are raising, the explanation lying in the fact that there is more place for the atoms to move inside the potential when passing from the harmonic to the Morse potential, which induces a lowering of the average kinetic energy according to the particle-in-a-box model.

On the other hand the 10 first components C_{nk} (n°) of the eigenvectors $|\Psi_k(n^\circ)\rangle$ corresponding to the 10 lowest energy levels E_k are given in (9.88):

	$\|\Psi_0\rangle$	$\|\Psi_1\rangle$	$\|\Psi_2\rangle$	$\|\Psi_3\rangle$	$\|\Psi_4\rangle$	$\|\Psi_5\rangle$	$\|\Psi_6\rangle$	$\|\Psi_7\rangle$	$\|\Psi_8\rangle$	$\|\Psi_9\rangle$
C_{0k}	−0.998	−0.053	0.001	0.013	0.005	0.001	0.001	−0.000	0.000	−0.000
C_{1k}	−0.053	0.987	−0.149	−0.012	−0.026	−0.015	−0.005	0.002	−0.001	0.001
C_{2k}	−0.003	0.148	0.950	0.268	0.039	0.041	0.029	−0.013	0.006	−0.003
C_{3k}	−0.015	0.016	0.266	−0.872	−0.393	−0.086	−0.059	0.048	−0.026	0.012
C_{4k}	−0.002	0.030	0.046	−0.388	0.742	0.507	0.155	−0.084	0.071	−0.045
C_{5k}	−0.000	0.007	0.051	−0.095	0.497	−0.555	−0.585	0.241	−0.119	0.097
C_{6k}	−0.000	0.001	0.019	−0.080	0.162	−0.570	0.320	−0.606	0.333	−0.165
C_{7k}	−0.000	0.001	0.005	−0.039	0.117	−0.239	0.586	0.058	−0.549	0.410
C_{8k}	0.000	0.000	0.003	−0.012	0.069	−0.164	0.314	0.529	−0.199	−0.409
C_{9k}	0.000	0.000	0.001	−0.007	0.027	−0.109	0.216	0.369	0.396	−0.406

(9.88)

Inspection of (9.88) shows that the 5 lowest eigenvectors have only components on the 10 lowest eigenstates $|\{n\}\rangle$ of the harmonic oscillator Hamiltonian. This result allows one to get numerical representations of the 5 lowest wavefunctions $\Psi_k(Q)$ corresponding to these 5 lowest eigenvectors $|\Psi_k\rangle$ defined by

$$\Psi_k(Q, n^\circ) = \langle\{Q\}|\Psi_k(n^\circ)\rangle \quad \text{with} \quad \mathbf{Q}|\{Q\}\rangle = Q|\{Q\}\rangle$$

Owing to Eq. (9.86) these wavefunctions are given by

$$\Psi_k(Q, n^\circ) = \langle\{Q\}| \sum_{n=0} C_{nk}(n^\circ)|\{n\}\rangle$$

or

$$\Psi_k(Q, n^\circ) = \sum_{n=0}^{4} C_{nk}(n^\circ)\Phi_n(Q) \tag{9.89}$$

where the $\Phi_n(Q)$ are the wavefunctions of the harmonic oscillators defined by

$$\Phi_n(Q, n^\circ) = \langle\{Q\}|\{n\}\rangle$$

Now, it has been seen above that, in dimensionless position, coordinate ξ is given by Eq. (5.117), that is,

$$\xi = \sqrt{\frac{m\omega}{\hbar}} Q$$

the wavefunctions of the harmonic oscillator Hamiltonian are given by Eq. (5.147):

$$\Phi_n(\xi) = K_n H_n(\xi) e^{-\xi^2/2} \tag{9.90}$$

The coefficients K_n are given by Eq. (5.148):

$$K_n = \frac{1}{\sqrt{n!}} \left(\frac{1}{\sqrt{2}}\right)^n \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \tag{9.91}$$

whereas $H_n(\xi)$ are the Hermite polynomials, the five lowest of which being, respectively, given by Eqs. (5.134), (5.138), (5.143), (5.146), and (5.149)

$$H_0(\xi) = 1 \qquad H_1(\xi) = 2\xi \qquad H_2(\xi) = 4\xi^2 - 2 \tag{9.92}$$

$$H_3(\xi) = 8\xi^3 - 12\xi \qquad H_4(\xi) = 16\xi^4 - 48\xi^2 + 12 \tag{9.93}$$

Equations (9.89) and (9.90)–(9.93) allow one to get pictorial representations of the wavefunctions of the Morse oscillator using the values of the expansion coefficients C_{nk} appearing in (9.88), as shown in Fig. 9.4.

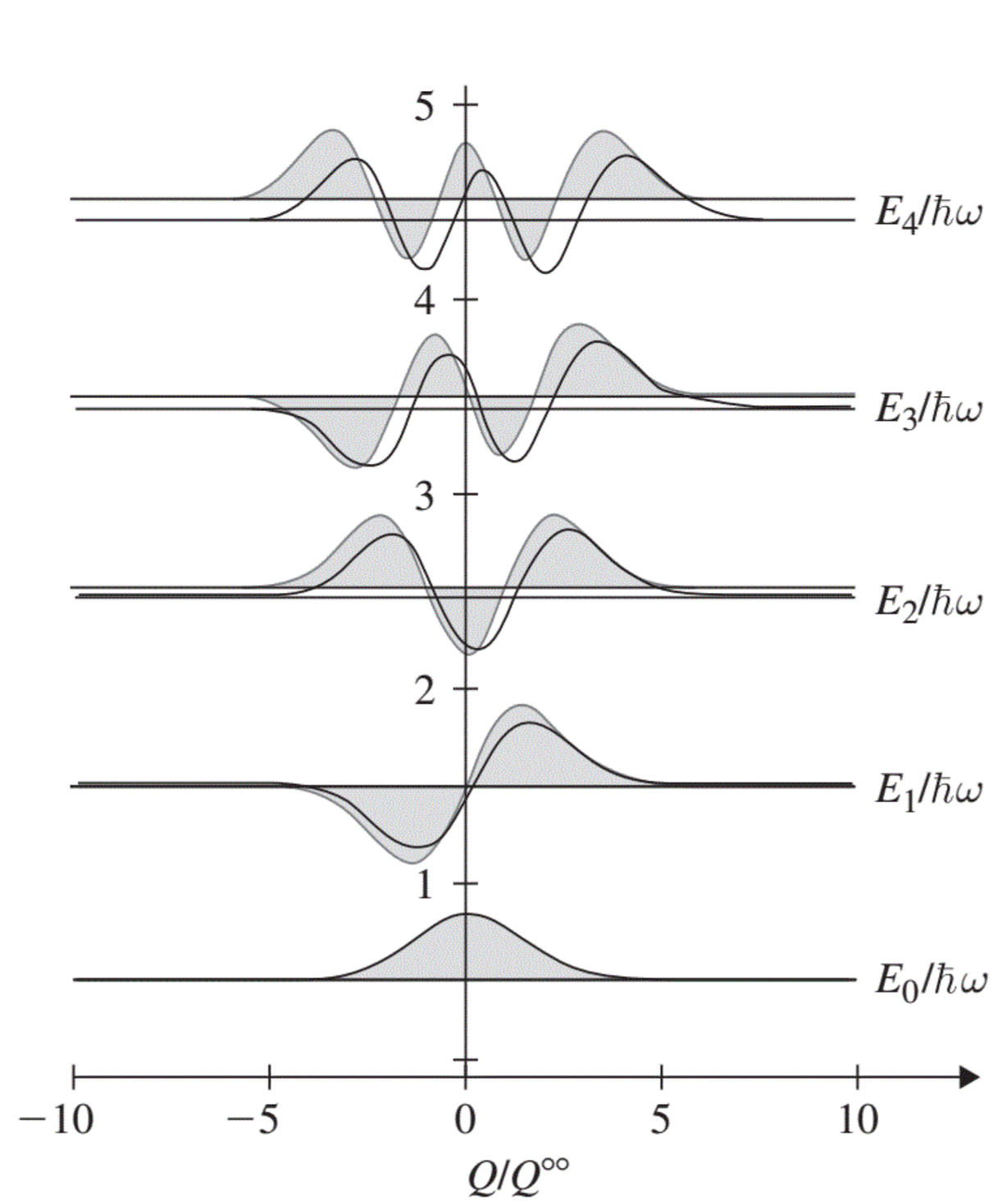


Figure 9.4 Five lowest wavefunctions $\Psi_k(\xi)$ of the Morse Hamiltonian compared to the five symmetric or antisymmetric lowest wavefunctions $\Phi_n(\xi)$ of the harmonic Hamiltonian. The length unit is $Q^{\circ\circ} = \sqrt{h/2m\omega}$. (See color insert.)

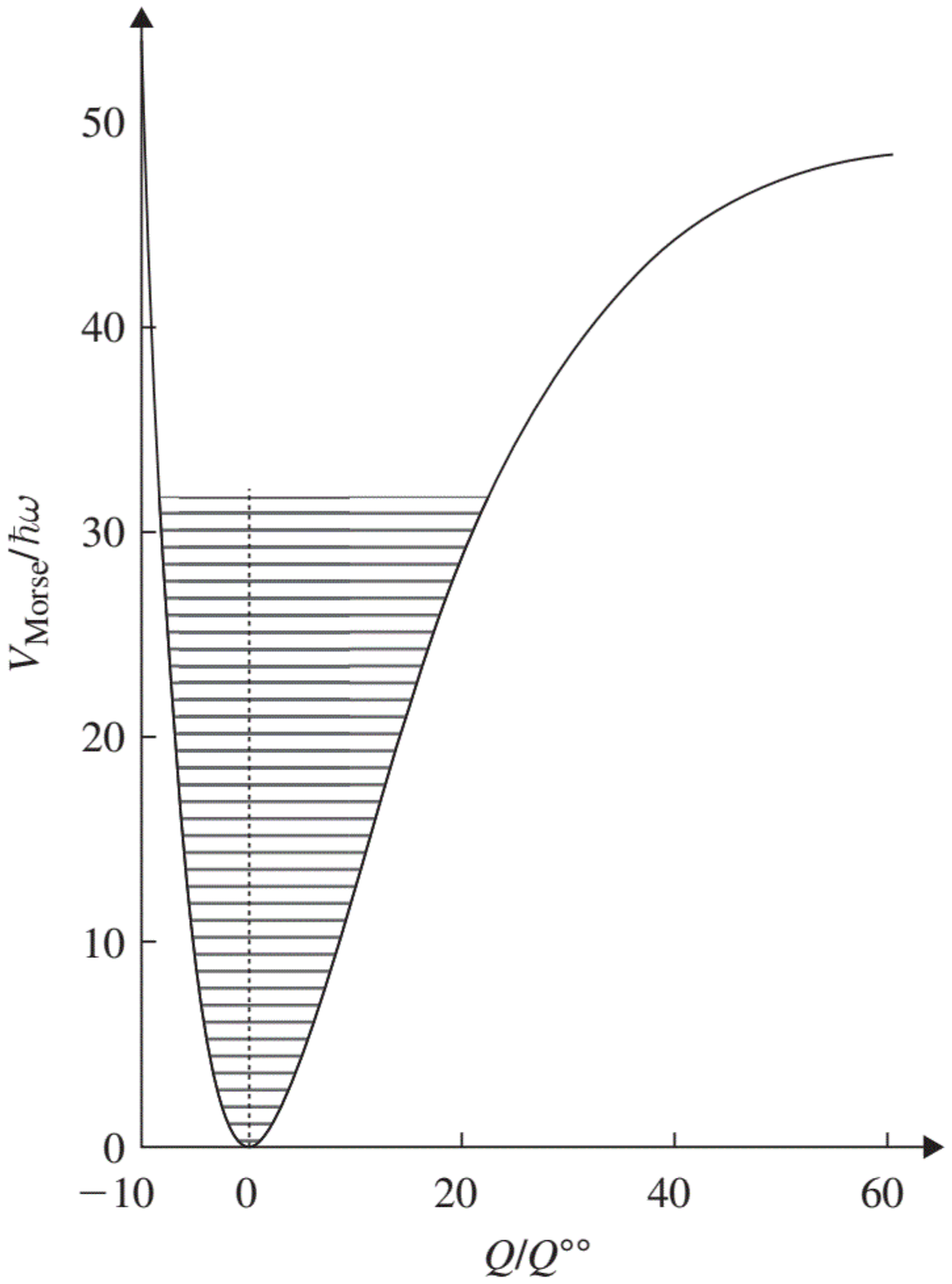


Figure 9.5 The 40 lowest energy levels of the Morse oscillator. The length unit is $Q^{\circ\circ} = \sqrt{\hbar/2m\omega}$.

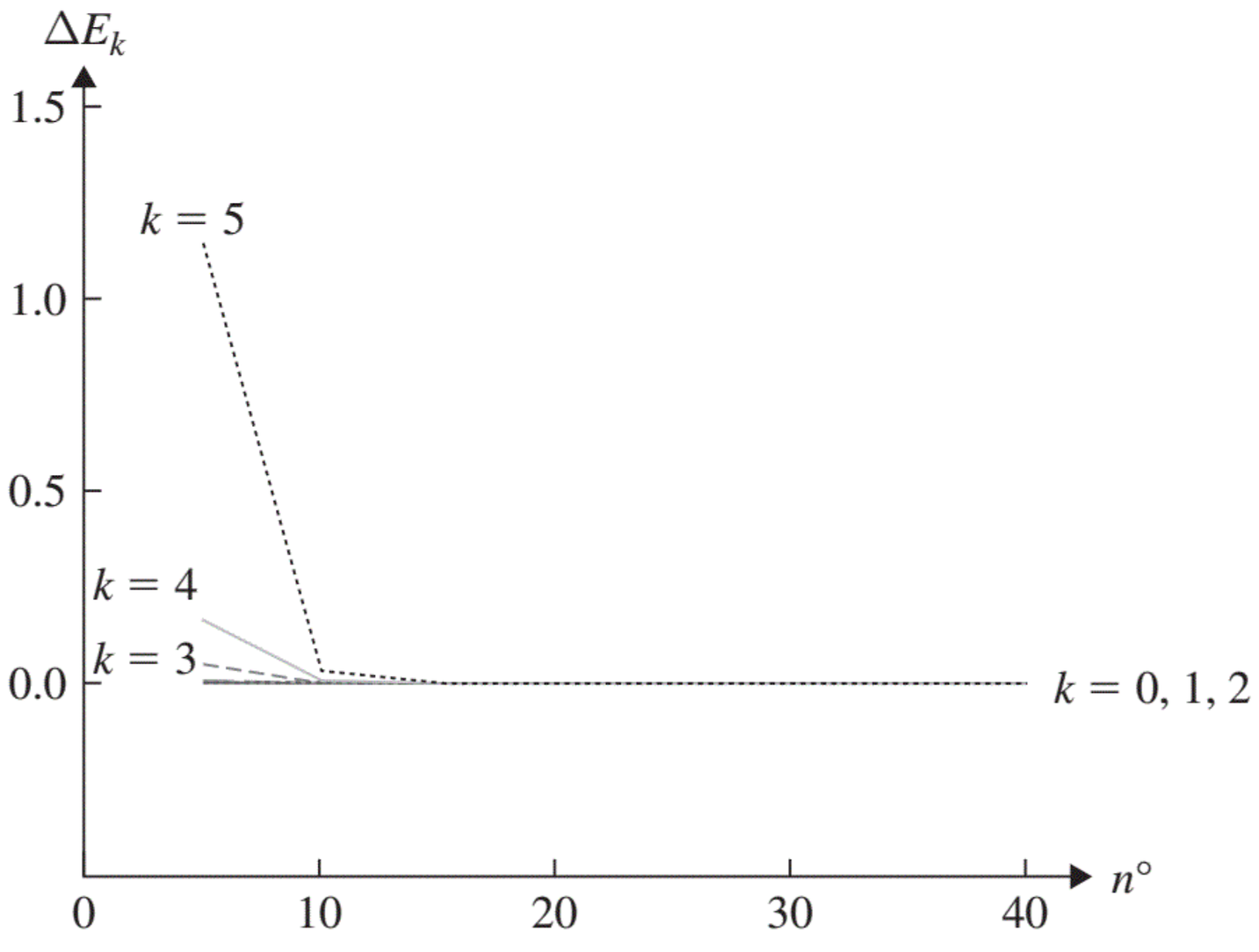


Figure 9.6 Energy gap between the numerical and exact eigenvalues for a Morse oscillator.

Finally, it may be convenient to reproduce the 40 lowest energy levels. That is illustrated in Fig. 9.5, which illustrates a situation that would roughly apply, for instance, to the deuterium molecule D_2.

Also, it would be of interest to compare these numerical eigenvalues $E_k(n^\circ)$ obtained by diagonalization of the Hamiltonian (9.76) with the analytical E_k° obtained with Eq. (9.64). In Fig. 9.6 we show, as a function of the number of basis states n° of the numerical procedure, the gap $\Delta E_k(n^\circ)$ between the numerical eigenvalues and the exact analytical ones, defined by

$$\Delta E_k(n^\circ) = E_k(n^\circ) - E_k^\circ$$

9.4 QUADRATIC POTENTIALS PERTURBED BY COSINE FUNCTIONS

In situations dealing with the biophysics of proteins, modulated harmonic potentials are encountered that may be modeled by potentials that, translated in quantum mechanics, read

$$\mathbf{V}(\mathbf{Q}) = \frac{1}{2}m\omega^2\mathbf{Q}^2 + A\cos\left(\frac{k\mathbf{Q}}{\hbar}\right)$$

where A and k are parameters characterizing the system. The Hamiltonian $\mathbf{H}$ corresponding to such a potential is then

$$\mathbf{H} = \frac{\mathbf{p}^2}{2m} + \mathbf{V}(\mathbf{Q}) \tag{9.94}$$

Passing to Boson operators, the Hamiltonian (9.94) reads

$$\mathbf{H} = \hbar\omega\left\{\left(\mathbf{a}^\dagger\mathbf{a}+\tfrac{1}{2}\right) + \alpha\cos(\beta(\mathbf{a}^\dagger + \mathbf{a}))\right\}$$

or

$$\mathbf{H} = \hbar\omega\left\{\left(\mathbf{a}^\dagger\mathbf{a}+\tfrac{1}{2}\right) + \frac{\alpha}{2}(e^{i\beta(\mathbf{a}^\dagger+\mathbf{a})} + e^{-i\beta(\mathbf{a}^\dagger+\mathbf{a})})\right\} \tag{9.95}$$

with

$$\alpha = \frac{A}{\hbar\omega} \qquad \text{and} \qquad \beta = \frac{k}{\hbar}\sqrt{\frac{\hbar}{2m\omega}}$$

Now, to get the energy levels of the system, we have to diagonalize the matrix representation of the Hamiltonian (9.95) in the basis where $\mathbf{a}^\dagger\mathbf{a}$ is diagonal and calculate the matrix elements $\langle\{m\}|\mathbf{H}|\{n\}\rangle$ of this expression. The matrix elements of the Hamiltonian (9.95) are of the form

$$\begin{aligned}\langle\{m\}|\mathbf{H}|\{n\}\rangle \;=\; \hbar\omega\Big(&\langle\{m\}|\left(\mathbf{a}^\dagger\mathbf{a}+\tfrac{1}{2}\right)|\{n\}\rangle \\ &+ \frac{\alpha}{2}\{\langle\{m\}|(e^{i\beta(\mathbf{a}^\dagger+\mathbf{a})})|\{n\}\rangle + \langle\{m\}|(e^{-i\beta(\mathbf{a}^\dagger+\mathbf{a})})|\{n\}\rangle\}\Big)\end{aligned} \tag{9.96}$$

Again, using the Glauber theorem (1.79), the exponential operators of the right-hand side of the latter equation become

$$(e^{\pm i\beta(\mathbf{a}^\dagger+\mathbf{a})}) = (e^{-(\pm i\beta)^2[\mathbf{a}^\dagger,\mathbf{a}]/2})(e^{\pm i\beta\mathbf{a}^\dagger})(e^{\pm i\beta\mathbf{a}})$$

and thus, due to $[\mathbf{a}^\dagger, \mathbf{a}] = -1$

$$(e^{\pm i\beta(\mathbf{a}^\dagger+\mathbf{a})}) = (e^{-\beta^2/2})(e^{\pm i\beta\mathbf{a}^\dagger})(e^{\pm i\beta\mathbf{a}})$$

Again, after expanding the two last exponentials, the corresponding matrix elements read

$$\langle\{m\}|(e^{\pm i\beta(\mathbf{a}^\dagger+\mathbf{a})})|\{n\}\rangle = (e^{-\beta^2/2})\sum_{k=0}\sum_{l}\frac{(\pm i)^{k+l}\beta^{k+l}}{k!l!}\langle\{m\}|(\mathbf{a}^\dagger)^k(\mathbf{a})^l|\{n\}\rangle \quad (9.97)$$

Then, using Eq. (5.72), and its Hermitian conjugate (5.73), that is,

$$(\mathbf{a})^l|\{n\}\rangle = \frac{\sqrt{n!}}{\sqrt{(n-l)!}}|\{n-l\}\rangle \qquad \text{and} \qquad \langle\{m\}|(\mathbf{a}^\dagger)^k = \langle\{m-k\}|\frac{\sqrt{m!}}{\sqrt{(m-k)!}}$$

Eq. (9.97) yields

$$\langle\{m\}|(e^{\pm i\beta(\mathbf{a}^\dagger+\mathbf{a})})|\{n\}\rangle$$
$$= (e^{-\beta^2/2})\sum_{k}\sum_{l}\frac{(\pm i)^{k+l}\beta^{k+l}}{k!l!}\frac{\sqrt{m!}}{\sqrt{(m-k)!}}\frac{\sqrt{n!}}{\sqrt{(n-l)!}}\langle\{m-k\}|\{n-l\}\rangle$$

or due to the orthogonality properties

$$\langle\{m\}|(e^{\pm i\beta(\mathbf{a}^\dagger+\mathbf{a})})|\{n\}\rangle$$
$$= (e^{-\beta^2/2})\sum_{k}\sum_{l}\frac{(\pm i)^{k+l}\beta^{k+l}}{k!l!}\frac{\sqrt{m!}}{\sqrt{(m-k)!}}\frac{\sqrt{n!}}{\sqrt{(n-l)!}}\{\delta_{m-k,n-l}\} \quad (9.98)$$

and thus after simplification because

$$\{\delta_{m-k,n-l}\} = 0 \quad \text{except if} \quad l = n-m+k$$

$$\langle\{m\}|(e^{\pm i\beta(\mathbf{a}^\dagger+\mathbf{a})})|\{n\}\rangle = (e^{-\beta^2/2})\sum_{k}\frac{(\pm i)^{2k+n-m}\beta^{2k+n-m}}{k!(k+n-m)!}\frac{\sqrt{m!}\sqrt{n!}}{(m-k)!} \quad (9.99)$$

Take care that in Eq. (9.99) the forms of the factorials imply that in the sum over k, this variable runs from $k = (m-n)$ to m if $m \geqslant n$, and from $k = (n-m)$ to n if $m < n$.

Then, numerical diagonalizations of the truncated Hamiltonian matrix representation (9.96), the dimension n° of which is progressively increased, have to be performed until the required stabilization of the energy levels $E_k(n^\circ)$ with respect to the dimension of the basis has been attained. Of course, the stabilized energy levels $E_k(n^\circ)$ and the corresponding eigenkets $|\Psi_k(n^\circ)\rangle$ obey the formal eigenvalue equation

$$\mathbf{H}|\Psi_k(n^\circ)\rangle = E_k(n^\circ)|\Psi_k(n^\circ)\rangle \quad \text{with} \quad |\Psi_k(n^\circ)\rangle = \sum_n\{C_{nk}(n^\circ)\}|\{n\}\rangle \quad (9.100)$$

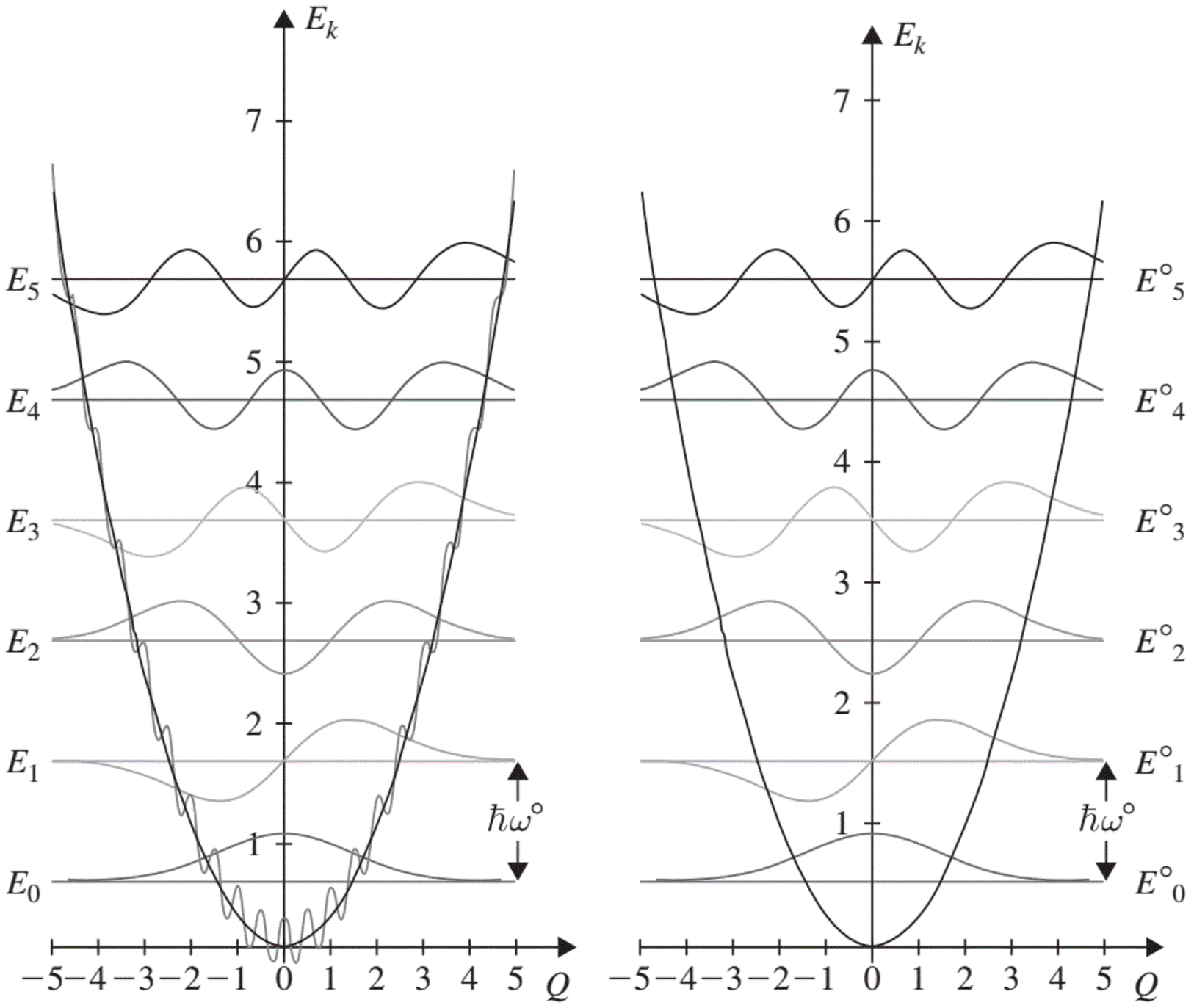


Figure 9.7 Comparison between the energy levels calculated by Eq. (9.100) and the wavefunctions obtained by Eq. (9.101) and the energy levels and the wavefunctions of the harmonic oscillator. (See color insert.)

the wavefunctions $\Psi_k(Q, n^\circ)$ corresponding to the kets $|\Psi_k(n^\circ)\rangle$ being given by

$$\{\Psi_k(Q, n^\circ)\} = \langle\{Q\}|\Psi_k(n^\circ)\rangle = \sum_n \{C_{nk}(n^\circ)\}\langle\{Q\}|\{n\}\rangle = \sum_n \{C_{nk}(n^\circ)\}\Phi_n(Q) \tag{9.101}$$

Figure 9.7 gives a modulated potential and the corresponding energy levels obtained.

As may be noted, the form of the potential practically does not affect the energy spacing of the levels, which remains close to that of the harmonic oscillator and does not sensitively modify the corresponding wavefunctions.

9.5 DOUBLE-WELL POTENTIAL AND TUNNELING EFFECT

Many situations dealing with molecules involve double-well potentials in which the nuclei of atoms are moving. For example, consider the gaseous NH_3 ammonia molecule. This tetrahedral molecule is pyramidal, shaped with the three hydrogen atoms forming the base and the nitrogen atom at the top, as shown in Fig. 9.8.

The nitrogen atom sees a double-well potential with one well on either side of the plane defined by the hydrogen atoms, as shown in Fig. 9.9.

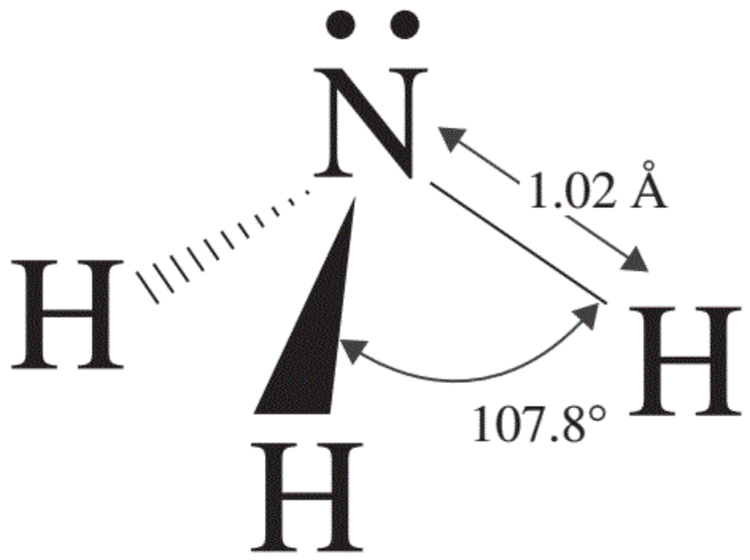


Figure 9.8 Ammonia molecule.

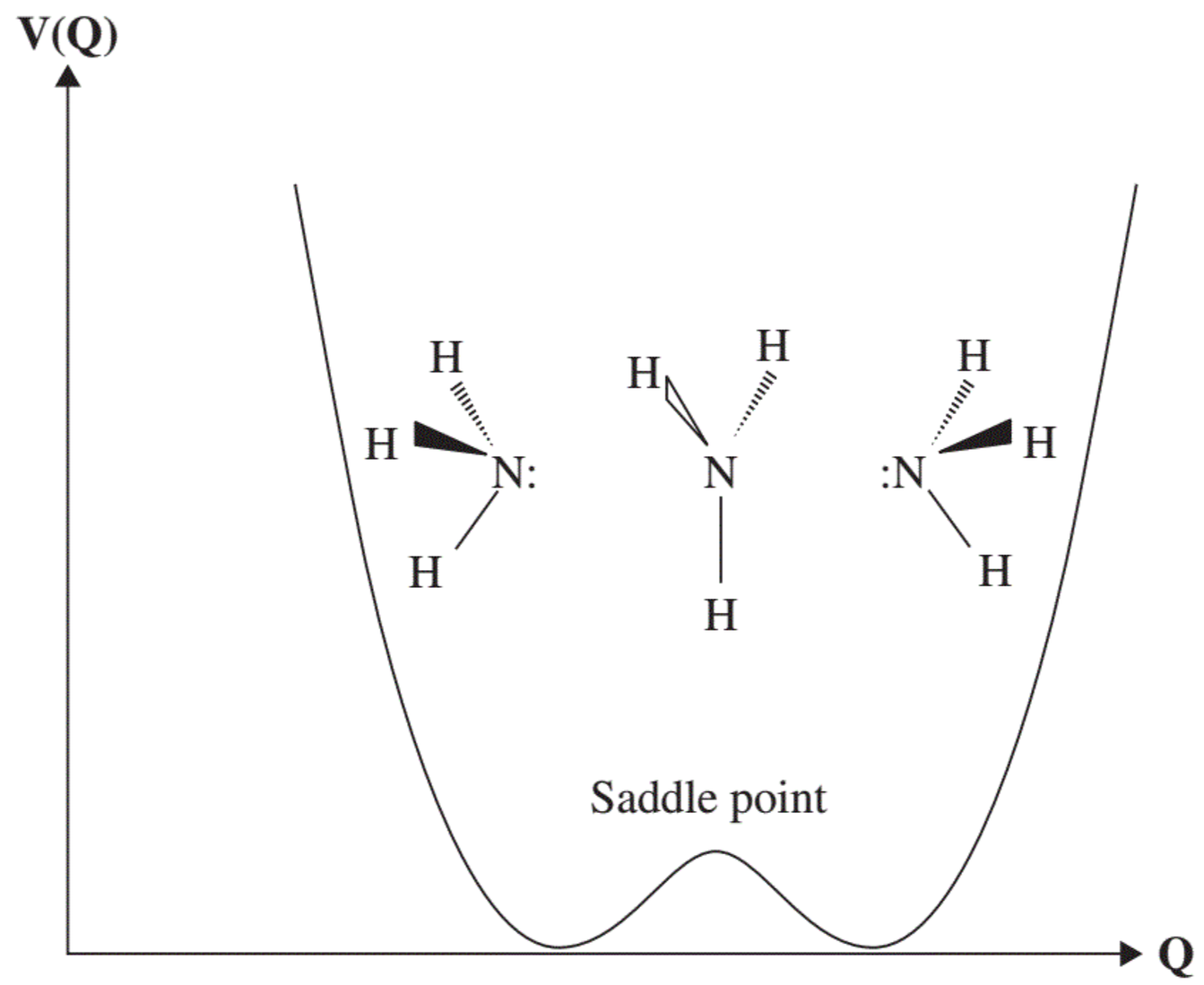


Figure 9.9 Double-well ammonia potential.

9.5.1 Hamiltonians in terms of the ladder operators

For generality, we shall consider an asymmetric double-well potential. The Hamiltonian $\mathbf{H}$ of a factitious particle of mass M moving in this potential is the sum of its kinetic operator and of the corresponding potential one $\mathbf{V}_{\text{wells}}(\mathbf{Q})$:

$$\mathbf{H} = \frac{\mathbf{P}^2}{2M} + \mathbf{V}_{\text{wells}}(\mathbf{Q}) \tag{9.102}$$

In order to have a suitable expression for this double-well asymmetric potential, one may choose to describe it by a quartic potential $\mathbf{Q}^4$ perturbed by a quadratic potential $\mathbf{Q}^2$ such as

$$\mathbf{V}_{\text{wells}}(\mathbf{Q}) = A\mathbf{Q}^4 - B\,(\mathbf{Q}-C)^2 \tag{9.103}$$

Here A, B, and C are parameters characterizing the asymmetric potential function, A having the dimension of an energy per the fourth power of a length, B of an energy per squared length, and C that of a length.

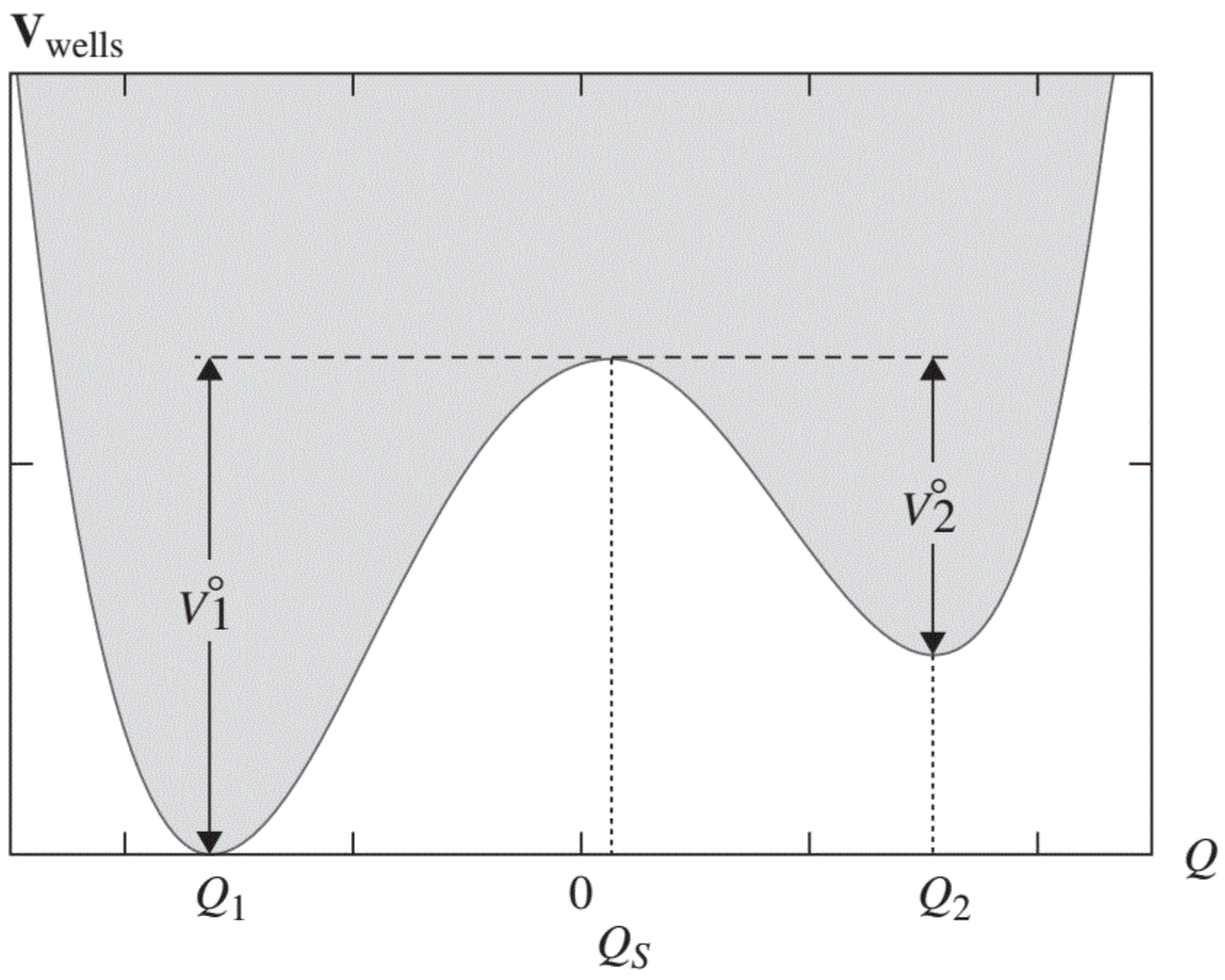


Figure 9.10 Example of double-well potential $V(Q)$ defined by Eq. (9.103) in terms of the geometric parameters V_1°, V_2°, Q_S, Q_1 and Q_2 defined in the text.

Figure 9.10 illustrates an asymmetric double-well potential (9.103) in which are shown the coordinates of the two minima Q_1 and Q_2 and the Q_S of the saddle point and also the energy barriers V_1° and V_2° separating the two energy minima from the energy maximum.

Owing to Eq. (9.103), the Hamiltonian (9.102) takes the form

$$\mathbf{H} = \frac{\mathbf{P}^2}{2M} + A\mathbf{Q}^4 - B(\mathbf{Q}-C)^2 \tag{9.104}$$

where M is the reduced mass of interest. Adding and substracting the harmonic potential $\frac{1}{2}M\omega^{\circ 2}\mathbf{Q}^2$ where ω° is some reference angular frequency yields

$$\mathbf{H} = \left(\frac{\mathbf{P}^2}{2M} + \frac{1}{2}M\omega^{\circ 2}\mathbf{Q}^2\right) - \frac{1}{2}M\omega^{\circ 2}\mathbf{Q}^2 + A\mathbf{Q}^4 - B(\mathbf{Q}-C)^2 \tag{9.105}$$

Now, from A, B, and C, we define the following dimensionless parameters:

$$\xi = \frac{A}{\hbar\omega^\circ}\left(\frac{\hbar}{2M\omega^\circ}\right)^2 \qquad \beta = \frac{B}{\hbar\omega^\circ}\left(\frac{\hbar}{2M\omega^\circ}\right) \qquad \eta = C\sqrt{\frac{2M\omega^\circ}{\hbar}}$$

hence Eq. (9.105) becomes

$$\mathbf{H} = \hbar\omega^\circ\left\{\left(\mathbf{a}^\dagger\mathbf{a}+\tfrac{1}{2}\right) - \tfrac{1}{4}(\mathbf{a}^\dagger + \mathbf{a})^2 + \xi(\mathbf{a}^\dagger + \mathbf{a})^4 - \beta((\mathbf{a}^\dagger + \mathbf{a}) - \eta)^2\right\}$$

or

$$\mathbf{H} = \hbar\omega^\circ\left\{\left(\mathbf{a}^\dagger\mathbf{a}+\tfrac{1}{2}\right) - \left(\beta - \tfrac{1}{4}\right)(\mathbf{a}^\dagger + \mathbf{a})^2 + \xi(\mathbf{a}^\dagger + \mathbf{a})^4 + 2\beta\eta(\mathbf{a}^\dagger + \mathbf{a}) - \beta\eta^2\right\} \tag{9.106}$$

9.5.2 Hamiltonian matrix elements

To obtain the energy levels, the matrix representation of the Hamiltonian **H** (9.106) has to be diagonalized in the basis of the eigenkets of $\mathbf{a}^\dagger\mathbf{a}$. This requires expressions for the matrix elements:

$$\begin{aligned}\langle\{n\}|\mathbf{H}|\{m\}\rangle \;=\; & \hbar\omega^\circ\langle\{n\}|\left(\mathbf{a}^\dagger\mathbf{a}+\tfrac{1}{2}\right)|\{m\}\rangle \\ & -\hbar\omega^\circ\left(\beta-\tfrac{1}{4}\right)\langle\{n\}|(\mathbf{a}^\dagger+\mathbf{a})^2|\{m\}\rangle+\hbar\omega^\circ\xi\langle\{n\}|(\mathbf{a}^\dagger+\mathbf{a})^4|\{m\}\rangle \\ & +2\hbar\omega^\circ\beta\eta\langle\{n\}|(\mathbf{a}^\dagger+\mathbf{a})|\{m\}\rangle\;-\hbar\omega^\circ\beta\eta^2 \end{aligned} \tag{9.107}$$

Due to the commutation rule of Boson operators, the matrix elements of $(\mathbf{a}^\dagger+\mathbf{a})^2$ are by Eq. (9.59)

$$\langle\{n\}|(\mathbf{a}^\dagger+\mathbf{a})^2|\{m\}\rangle=\sqrt{m+1}\sqrt{m+2}\delta_{n,m+2}+\sqrt{m}\sqrt{m-1}\delta_{n,m-2}+(2m+1)\delta_{nm} \tag{9.108}$$

Now, from the usual commutation rules $[\mathbf{a},\mathbf{a}^\dagger]=1$, development of $(\mathbf{a}^\dagger+\mathbf{a})^4$ yields

$$\begin{aligned}(\mathbf{a}^\dagger+\mathbf{a})^4 \;=\; & (4\mathbf{a}^\dagger\mathbf{a}+1)+4(\mathbf{a}^\dagger\mathbf{a})^2+(\mathbf{a}^\dagger)^4+(\mathbf{a})^4 \\ & +((\mathbf{a}^\dagger)^2(\mathbf{a})^2+(\mathbf{a})^2(\mathbf{a}^\dagger)^2)+\mathbf{2}((\mathbf{a}^\dagger)^2+(\mathbf{a})^2)(\mathbf{a}^\dagger\mathbf{a}) \\ & +\mathbf{2}(\mathbf{a}^\dagger\mathbf{a}+1)((\mathbf{a}^\dagger)^2+(\mathbf{a})^2)\end{aligned} \tag{9.109}$$

Then, Eq. (5.71) and its Hermitian conjugate allow one to find the following results:

$$\langle\{n\}|(\mathbf{a}^\dagger)^4|\{m\}\rangle=\sqrt{(m+1)(m+2)(m+3)(m+4)}\,\delta_{n,m+4}$$

Moreover, due to Eqs. (5.53) and (5.54)

$$(\mathbf{a})^2|\{m\}\rangle=\sqrt{m(m-1)}|\{m-2\}\rangle$$

the Hermitian conjugate of which is, after taking n in place of m,

$$\langle\{n\}|(\mathbf{a}^\dagger)^2=\sqrt{n(n-1)}\langle\{n-2\}|$$

Hence, it follows that

$$\langle\{n\}|(\mathbf{a}^\dagger)^2(\mathbf{a})^2|\{m\}\rangle=\sqrt{n(n-1)}\sqrt{m(m-1)}\langle\{n-2\}|\{m-2\}\rangle$$

so that, after simplification, it reads

$$\langle\{n\}|(\mathbf{a}^\dagger)^2(\mathbf{a})^2|\{m\}\rangle=\sqrt{n(n-1)}\sqrt{m(m-1)}\,\delta_{nm} \tag{9.110}$$

On the other hand, one has, respectively,

$$\begin{aligned}\mathbf{a}|\{m\}\rangle \;&=\; \sqrt{m}|\{m-1\}\rangle \\ \langle\{n\}|(\mathbf{a}^\dagger)^3 \;&=\; \sqrt{(n)(n-1)(n-2)}\langle\{n-3\}|\end{aligned}$$

so that

$$\langle\{n\}|(\mathbf{a}^\dagger)^3\mathbf{a}|\{m\}\rangle=\sqrt{(m)(n)(n-1)(n-2)}\langle\{n-3\}|\{m-1\}\rangle=\delta_{n-3,m-1}$$

and thus

$$\langle\{n\}|(\mathbf{a}^\dagger)^3\mathbf{a}|\{m\}\rangle = \sqrt{(m)(n)(n-1)(n-2)}\,\delta_{n-2,m} \tag{9.111}$$

Again, keeping in mind that the matrix elements (1.30) of a real non-Hermitian operator $\mathbf{B}$ obey

$$\langle\{n\}|\mathbf{B}|\{m\}\rangle = \langle\{m\}|\mathbf{B}^\dagger|\{n\}\rangle^* = \langle\{m\}|\mathbf{B}^\dagger|\{n\}\rangle \tag{9.112}$$

it follows, respectively, from Eqs. (9.110) and (9.111) that

$$\begin{aligned}\langle\{m\}|(\mathbf{a})^2(\mathbf{a}^\dagger)^2|\{n\}\rangle &= \sqrt{n(n-1)}\sqrt{m(m-1)}\,\delta_{nm}\\ \langle\{n\}|\mathbf{a}(\mathbf{a}^\dagger)^3|\{m\}\rangle &= \sqrt{(m)(n)(n-1)(n-2)}\,\delta_{n-2,m}\end{aligned}$$

Hence, the matrix elements (9.109) read

$$\begin{aligned}\langle\{n\}|(\mathbf{a}^\dagger+\mathbf{a})^4|\{m\}\rangle = {} & 3(2m^2+2m+1)\,\delta_{nm} + (2(2m+3)\sqrt{m+1}\sqrt{m+2})\,\delta_{n,m+2}\\ & + (\sqrt{(m+1)(m+2)(m+3)(m+4)})\,\delta_{n,m+4}\\ & + \sqrt{(m)(m-1)(m-2)(m-3)}\,\delta_{n,m-4}\\ & + (2(2m-1)\sqrt{(m)(m-1)})\,\delta_{n,m-2}\end{aligned} \tag{9.113}$$

Thus, it is possible, using Eqs. (9.107)–(9.113) to build up the matrix representation of the Hamiltonian (9.106) and then to diagonalize different truncated matrix representations of this Hamiltonian, the dimensions of which have to be progressively increased until stabilization of the lowest eigenvalues occurs.

9.5.3 Tunneling in symmetric double-well potentials

It is now possible to consider the tunneling effect, which may occur through the potential barrier of a double-wells potential. For this purpose, consider the two lowest eigenstates of the Hamiltonian (9.102) obtained by diagonalization of the matrix representation (9.107) of dimension n°, which obey the eigenvalue equations

$$\mathbf{H}|\Psi_k(n^\circ)\rangle = E_k(n^\circ)|\Psi_k(n^\circ)\rangle \quad \text{with} \quad k = 0, 1 \tag{9.114}$$

The diagonalization of the matrix representation of this Hamiltonian gives, respectively, for the two lowest quasi-degenerate eigenvalues (in $\hbar\omega^\circ$ units with three decimals)

$$E_0(n^\circ) = 1.357 \qquad \text{and} \qquad E_1(n^\circ) = \ 1.357$$

whereas it gives for the two corresponding eigenvectors

$$|\Psi_k(n^\circ)\rangle = \sum_n C_{nk}(n^\circ)|\{n\}\rangle \quad \text{with} \quad C_{nk}(n^\circ) = \langle\{n\}|\Psi_k(n^\circ)\rangle \tag{9.115}$$

and for the expansion coefficients $C_{nk}(n^\circ)$ the following tabular data in (9.116) in which we restrict the number of component eigenstates to 20:

n	$\langle\{n\}\|\Psi_0\rangle$	$\langle\{n\}\|\Psi_1\rangle$	n	$\langle\{n\}\|\Psi_0\rangle$	$\langle\{n\}\|\Psi_1\rangle$
0	0.305	0.000	10	0.035	0.000
1	0.000	0.598	11	0.000	0.038
2	0.786	0.000	12	0.011	0.000
3	0.000	0.760	13	0.000	−0.011
4	0.526	0.000	14	−0.014	0.000
5	0.000	0.212	15	0.000	−0.004
6	−0.037	0.000	16	0.004	0.000
7	0.000	−0.135	17	0.000	0.005
8	−0.102	0.000	18	0.000	0.000
9	0.000	−0.020	19	0.000	−0.002

(9.116)

Next, introduce the wavefunctions corresponding to the kets (9.115) by premultiplying Eq. (9.115) by the bra $\langle\{Q\}|$ to give

$$\Psi_k(Q, n^\circ) = \sum_n C_{nk}(n^\circ)\Phi_n(Q, n^\circ) \tag{9.117}$$

with

$$\Psi_k(Q, n^\circ) = \langle\{Q\}|\Psi_k(n^\circ)\rangle \qquad \text{and} \qquad \Phi_n(Q, n^\circ) = \langle\{Q\}|\{n\}\rangle \tag{9.118}$$

In addition, recall that the wavefunctions $\Phi_n(Q)$ corresponding to the eigenkets of the harmonic oscillator Hamiltonian may be expressed in terms of $H_n(\alpha Q)$ and given by Eq. (5.147), that is,

$$\Phi_n(Q, n^\circ) = K_n(e^{-\alpha^2 Q^2/2})H_n(\alpha Q) \tag{9.119}$$

where $H_n(\alpha Q)$ are the Hermite polynomials and where α and K_n are, respectively, given by

$$\alpha = \sqrt{\frac{M\omega^\circ}{\hbar}} \qquad \text{and} \qquad K_n = \left(\frac{\alpha}{\sqrt{\pi}2^n n!}\right)^{1/2}$$

Then, using the expansion coefficients $C_{nk}(n^\circ)$ given in (9.116), and resulting from the diagonalization of the matrix representation (9.107), Eqs. (9.117) and (9.119) allow one to obtain the wavefunctions corresponding to the eigenstates of the Hamiltonian $\mathbf{H}(\mathbf{a}, \mathbf{a}^\dagger)$. Figure 9.11 gives the picture of the six lowest wavefunctions and their corresponding energy levels for any symmetric double-well potential. Inspection of the figure shows that the four energy levels lying below the barrier are split, E_0 and E_1 being quasi-degenerate, whereas the two others $E_2(n^\circ)$ and $E_3(n^\circ)$ involve a large splitting. It shows also that the wavefunctions $\Psi_2(Q, n^\circ)$ and $\Psi_3(Q, n^\circ)$ corresponding to the energy levels $E_2(n^\circ)$ and $E_3(n^\circ)$ represent residual amplitudes inside the potential barrier, a region that would be forbidden for the particle from the viewpoint of classical mechanics. This penetration of the particle through the energy barrier is a manifestation of what is called the *tunneling effect*.

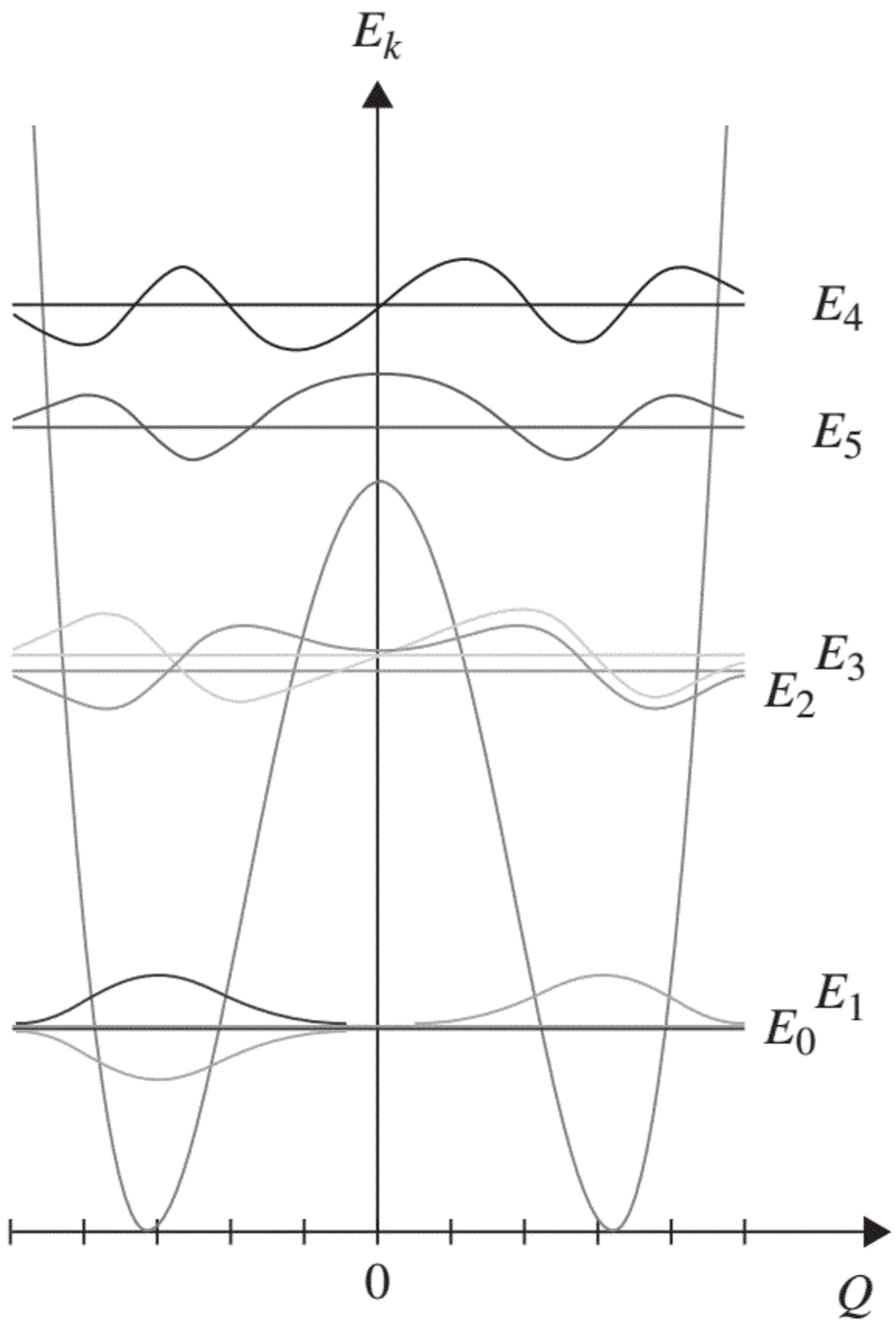


Figure 9.11 Representation of the six lowest wavefunctions and the corresponding energy levels for symmetrical double-well potential. (See color insert.)

In addition, Fig. 9.12 deals with the influence on tunneling of the asymmetry parameter η of the double-well potential. Inspection of this figure shows that increasing the values of the dimensionless asymmetry parameter η of the potential induces drastic changes in the wavefunctions corresponding to the energy levels lying below the barrier, since their delocalizations are strongly vanishing as soon as the asymmetry is slightly increasing.

In may be of interest to study the precise behavior of the particle when tunneling is occurring. The best way would be to deal with that involving $\Psi_2(Q)$ and $\Psi_3(Q)$ appearing in Fig. 9.11 and in which n° has been omitted. But, although the tunneling effect is weaker for the levels E_0 and E_1 than for those E_2 and E_3, it is, however, simpler to use $\Psi_0(Q)$ and $\Psi_1(Q)$ because of their great simplicity, allowing a better visual picture. Thus, to get such a picture, assume that, at an initial time, the system is described by either $\Theta_+(Q,0)$ or $\Theta_-(Q,0)$, which are combinations of the wavefunctions $\Psi_0(Q,0)$ and $\Psi_1(Q,0)$ at initial time $t=0$:

$$\Theta_\pm(Q,0) = \frac{1}{\sqrt{2}}(\Psi_0(Q,0) \pm \Psi_1(Q,0)) \tag{9.120}$$

Figure 9.13 gives a schematic representation of the two wavefunctions involved in the expansions (9.120), which according to (9.116) are given by

$$\begin{aligned}\Psi_0(Q,0) = {} & 0.30\Phi_0(Q) + 0.79\Phi_2(Q) + 0.53\Phi_4(Q) - 0.04\Phi_6(Q) - 0.10\Phi_8(Q) \\ & + 0.03\Phi_{10}(Q)\end{aligned}$$

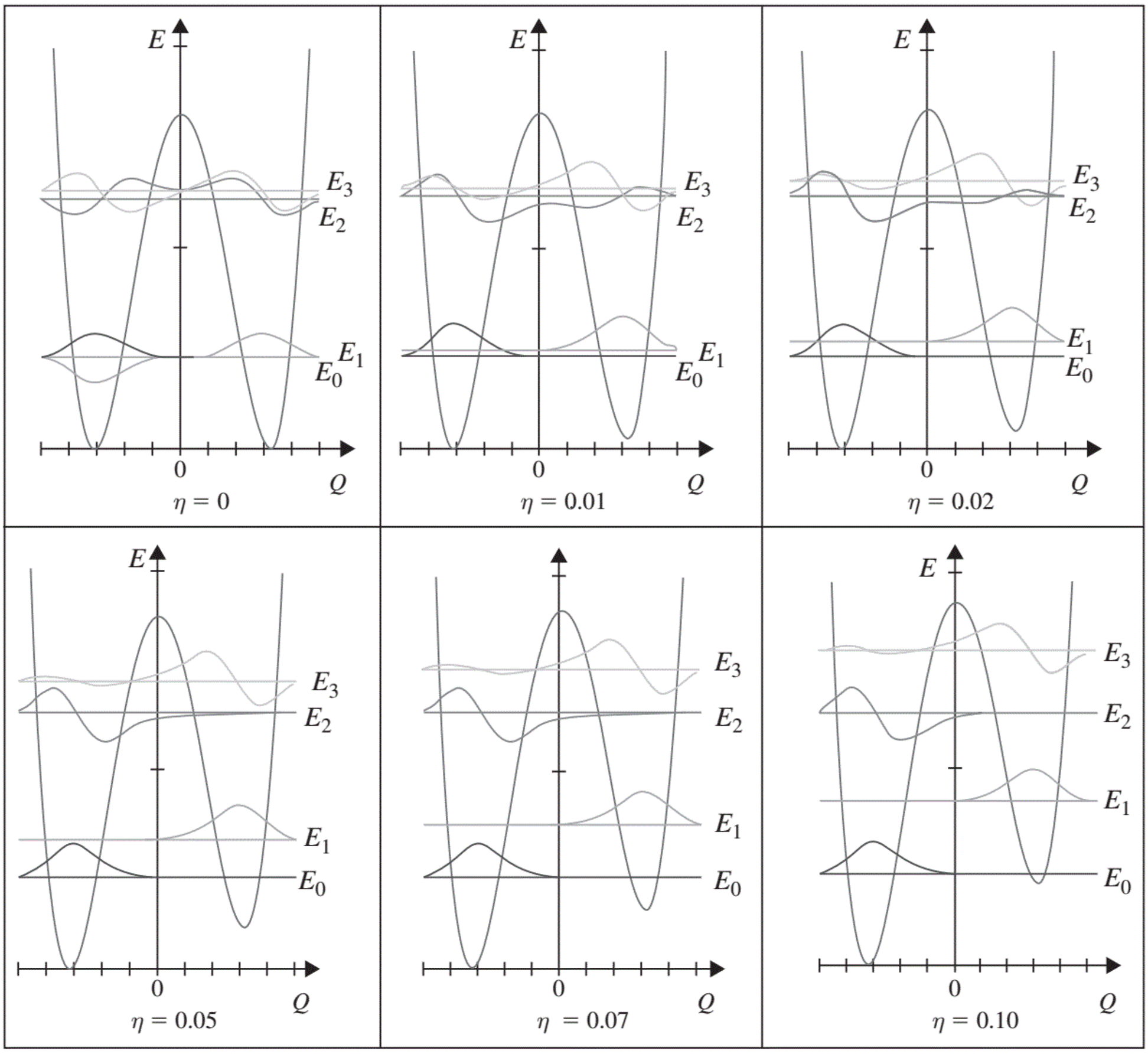


Figure 9.12 Influence of the double-well potential asymmetry on the eigenstates of the double-well potential Hamiltonian.

$$\Psi_1(Q,0) = 0.60\Phi_1(Q) + 0.76\Phi_3(Q) + 0.21\Phi_5(Q) - 0.013\Phi_7(Q) - 0.02\Phi_9(Q) + 0.04\Phi_{11}(Q)$$

Thus, $\Theta_+(Q,0)$ and $\Theta_-(Q,0)$ are each localized on one of the two potential minima.

Next, at time t, the linear combination (9.120) reads

$$\{\Theta_\pm(Q,t)\} = \frac{1}{\sqrt{2}}(\{\Psi_0(Q,t)\} \pm \{\Psi_1(Q,t)\}) \tag{9.121}$$

where the two time-dependent wavefunctions $\Psi_0(Q,t)$ and $\Psi_1(Q,t)$ are solutions of the Schrödinger equations:

$$i\hbar\left(\frac{\partial\Psi_k(Q,t)}{\partial Q}\right) = \mathbf{H}\{\Psi_k(Q,t)\} \quad \text{with} \quad k = 0,1$$

Since, according to Eq. (9.114), the Hamiltonian $\mathbf{H}$ here acts on some of its eigenstates, the corresponding eigenvalues are the energy levels E_K with $K = 0, 1$, so that

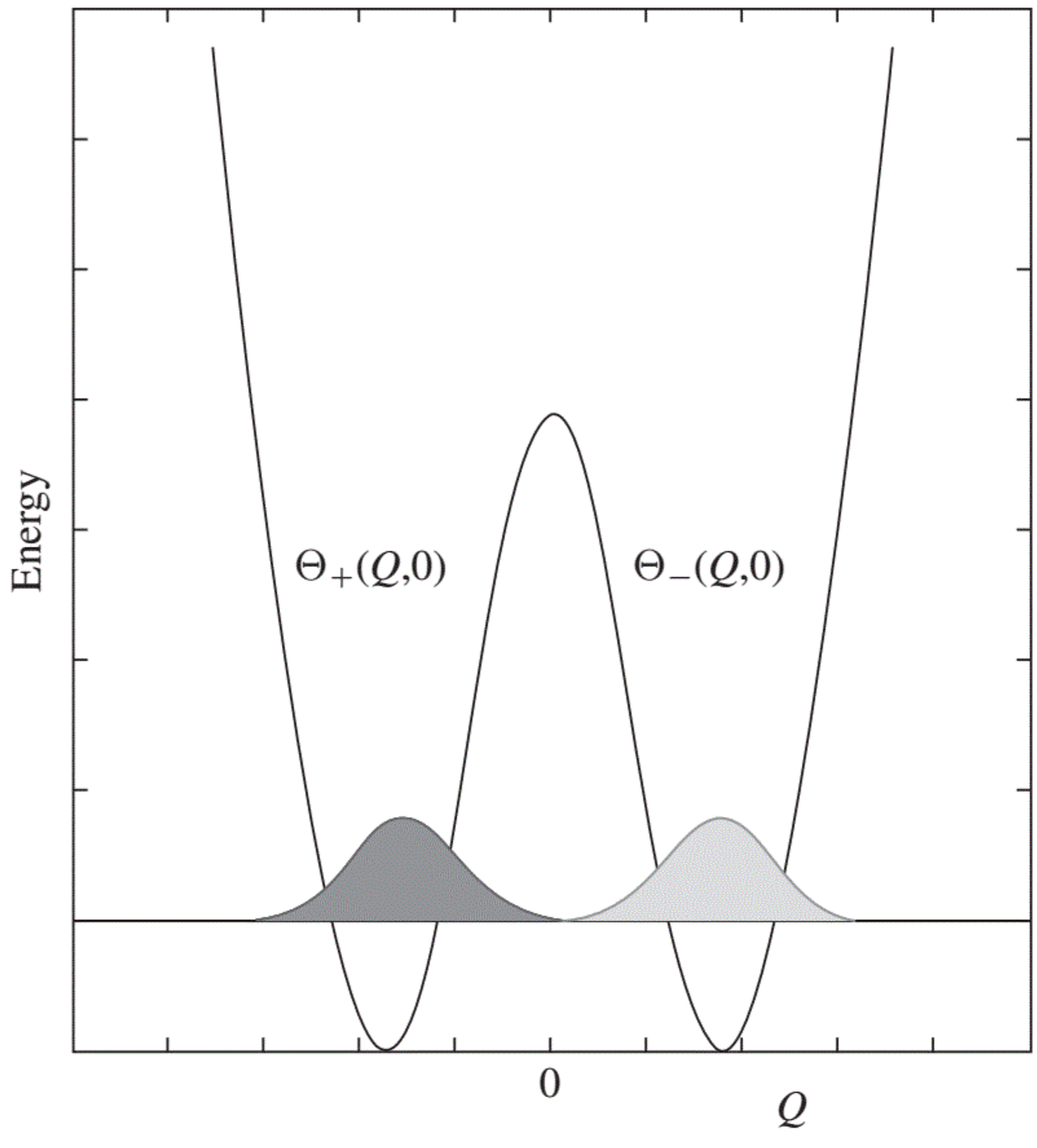


Figure 9.13 Schematic representation of the two wavefunctions (9.120).

the two time-dependent Schrödinger equations become

$$i\hbar\left(\frac{\partial\Psi_k(Q,t)}{\partial Q}\right) = E_k\{\Psi_k(Q,t)\} \quad \text{with} \quad k = 0,1$$

the integration of which leads to

$$\{\Psi_k(Q,t)\} = \{\Psi_k(Q,0)\}e^{-iE_kt/\hbar} \quad \text{with} \quad k = 0,1 \tag{9.122}$$

Hence, at time t the linear combinations of the two time-dependent wavefunctions (9.121) take the form

$$\{\Theta_\pm(Q,t)\} = \frac{1}{\sqrt{2}}(\{\Psi_0(Q,0)\}e^{-iE_0t/\hbar} \pm \{\Psi_1(Q,0)\}e^{-iE_1t/\hbar})$$

so that the corresponding squared modulus read

$$|\Theta_+(Q,t)|^2 = \{\Psi_0(Q,0)\}^2 + \{\Psi_1(Q,0)\}^2 + \{\Psi_0(Q,0)\}\{\Psi_1(Q,0)\}\cos\omega_{01}t \tag{9.123}$$

$$|\Theta_-(Q,t)|^2 = \{\Psi_0(Q,0)\}^2 + \{\Psi_1(Q,0)\}^2 - \{\Psi_0(Q,0)\}\{\Psi_1(Q,0)\}\sin\omega_{01}t \tag{9.124}$$

with

$$\omega_{01} = \hbar/(E_0 - E_1)$$

Figure 9.14 gives some changes with time of Eq. (9.124), that is, of the probability to find the system at any position Q within the double-well potential.

Inspection shows that this density probability oscillates from one side to the other of the double well at the angular frequency ω_{01}. Hence, the system tunnels back

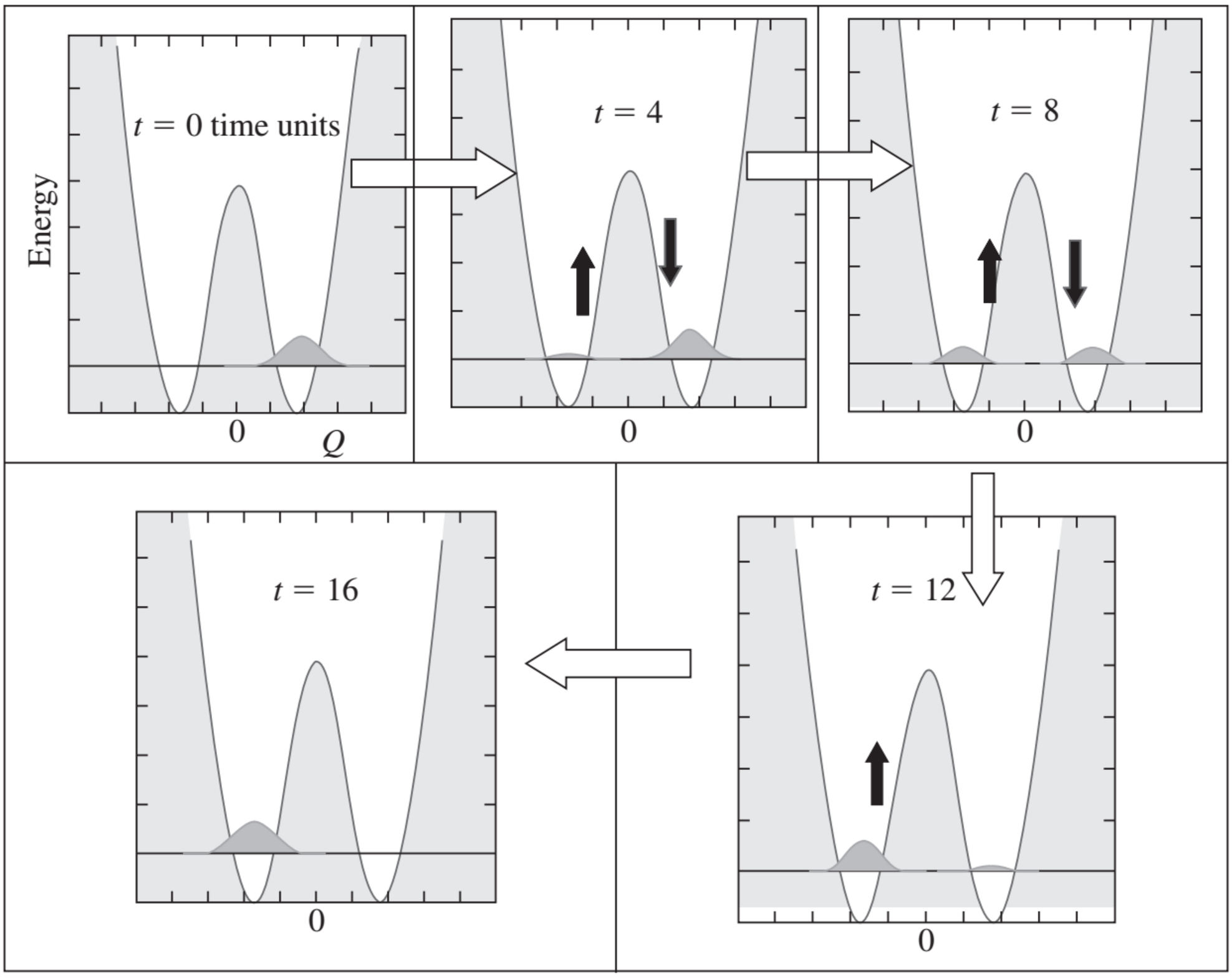


Figure 9.14 Probability density (9.124) for different times t expressed in units ω^{-1}.

and forth through the barrier potential. In a similar way, one would obtain, for the two *gerade* g and *ungerade* u levels corresponding to the energy levels E_2 and E_3, the following results:

$$|\Theta_g(Q,t)|^2 = \{\Psi_2(Q,0)\}^2 + \{\Psi_3(Q,0)\}^2 + \{\Psi_2(Q,0)\}\{\Psi_3(Q,0)\}\cos\omega_{23}t$$

$$|\Theta_u(Q,t)|^2 = \{\Psi_2(Q,0)\}^2 + \{\Psi_3(Q,0)\}^2 - \{\Psi_2(Q,0)\}\{\Psi_3(Q,0)\}\sin\omega_{23}t$$

with

$$\omega_{23} = \hbar/(E_2 - E_3)$$

In such a situation, the pictorial representation of the time evolution of the wavepacket would be more complex, the tunneling effect occurring with an angular frequency larger than for Eq. (9.124) since it appears from Fig. 9.11 that

$$\omega_{23} > \omega_{01}$$

the oscillations would of course remain.

9.6 CONCLUSION

This chapter has shown how to treat the energy levels of quantum anharmonic oscillators for which it is not generally possible to solve the Hamiltonian eigenvalue equation. That was performed by numerically diagonalizing the matrix representations of the different Hamiltonians in the basis of the eigenkets of the harmonic oscillator Hamiltonian, a method the accuracy of which had been satisfactorily tested in a previous chapter on the driven harmonic oscillator and which was tested in the present chapter on anharmonic oscillators involving a cubic term perturbing the harmonic potential with the help of the virial theorem, and on anharmonic oscillators involving Morse potentials, by comparison with the analytical solutions, which exist for this model. The numerical calculations involving anharmonic potentials, which did not modify sensitively the harmonic potential, lead one to conclude that the anharmonic perturbation does not modify drastically the energy levels, whereas those dealing with double-well potentials reveal the possibility of tunneling through the potential barrier separating the two wells, when the potential is symmetric.

BIBLIOGRAPHY

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