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Two Soluble Models of an Antiferromagnetic Chain

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Two genuinely quantum mechanical models for an antiferromagnetic linear chain with nearest neighbor interactions are constructed and solved exactly, in the sense that the ground state, all the elementary excitations and the free energy are found. A general formalism for calculating the instantaneous correlation between any two spins is developed and applied to the investigation of short- and long-range order. Both models show nonvanishing long-range order in the ground state for a range of values of a certain parameter λ which is analogous to an anisotropy parameter in the Heisenberg model. A detailed comparison with the Heisenberg model suggests that the latter has no long-range order in the isotropic case but finite long-range order for any finite amount of anisotropy. The unreliability of variational methods for determining long-range order is emphasized. It is also shown that for spin $\frac{1}{2}$ systems having rather general isotropic Heisenberg interactions favoring an antiferromagnetic ordering, the ground state is nondegenerate and there is no energy gap above the ground state in the energy spectrum of the total system.

I. INTRODUCTION

For an infinite chain of spins interacting with nearest neighbors via a Heisenberg interaction, the exact energy eigenstates were found, in principle, many years ago by Bethe (*1*) and the ground-state energy was found somewhat later by Hulthén (*2*). The problem has nevertheless occasioned a persistent theoretical interest. This is because the exact method of Bethe does not seem capable of generalization to the more interesting cases of two and three dimensions. The aim has generally been to construct approximate methods that give accurate results in one dimension, as determined by a comparison with the known exact results, but which can be generalized to two or three dimensions with some degree of confidence and simplicity. Unfortunately, the crucial test for any approximate method is how well it describes the long-range order; but it is precisely this test which has been impossible, because the long-range order has never been calculated exactly by the method of Bethe.

There is, in fact, still considerable doubt about the nature of the long-range order in one or more dimensions. On the one hand, spin wave methods used by Anderson (*3*) and Kubo (*4*) have predicted long-range order in two or three dimensions, although Anderson (but not Kubo) predicts no long-range order in one dimension. Variational methods of Kasteleijn (*5*) generalized to two and

three dimensions by Taketa and Nakamura (*6*), and of Marshall (*7*), all related to a variational method of Hulthén (*2*), indicate no long-range order in one, two, and three dimensions for the completely isotropic interaction. On the other hand, they all predict the onset of long-range order for a certain critical amount of anisotropy—the same amount at which a kink is predicted for the short-range order. Exact calculations by Orbach (*8*) on the anisotropic case, generalizing the method of Bethe, show the kink to be spurious for the one-dimensional case, but throw no further light on the long-range order. Walker (*9*) has observed that the ground-state energy calculated by Orbach has a power series expansion around the limiting case of the completely anisotropic interaction (Ising limit) which seems to give a good representation of the ground-state energy even for the isotropic case, although he observes that a similar expansion for the long-range order suggests the long-range order might vanish when the anisotropy falls below a certain critical value. Ruijgrok and Rodriguez (*10*) have developed a variational method for the one-dimensional case which gives a good value for the ground-state energy, significantly better than previous variational methods, and which also predicts finite long-range order. Davis (*11*) has performed a perturbation theoretic calculation which indicates, to the order to which it has been carried, a long-range order in any number of dimensions even for the isotropic case.

There are two questions raised by all these investigations. First, can a purely isotropic Heisenberg interaction between nearest neighbors produce long-range order in any number of dimensions? Second, if such an ordering tendency exists in, say, two or three dimensions, will it also exist in only one dimension, or would the absence of order in one dimension prove nothing at all about order in two or three dimensions?

The purpose of the present paper is to gain further insight into the effects of anisotropy in one dimension. Two models will be constructed which can be solved exactly in considerable detail and which bear a reasonably close resemblance to the Heisenberg model. The investigation of the first of these models strongly suggests that the isotropic Heisenberg model has no long-range order but that such order exists for any finite amount of anisotropy. Both models emphasize the subtle nature of long-range order and the insufficiency of variational methods as a reliable approach to this question. The question of the relation of these results to two- and three-dimensional cases is left completely open.

In Section II we consider the first of these models, the "XY model." It is shown that the Hamiltonian can be expressed as a quadratic form in creation and annihilation operators for fermions, and this quadratic form can be diagonalized, thereby giving the complete set of states, excitation energies, and partition sum. In terms of these operators, general expressions for the order between any two spins are derived involving a kind of Green function, G_{ij}, which can be explicitly

evaluated. The general relation between the order and G_{ij} is equally valid for the Heisenberg model, but G_{ij} itself is then not explicitly calculable. The short-, intermediate-, and long-range order are calculated for various situations, and it is shown that only for the isotropic case does the long-range order vanish. The model is compared with the Heisenberg model for one special case from which reasonable surmises may be made about the latter.

In Section III we consider the "Heisenberg-Ising model" in a similar way. Although the excited states and statistical mechanics are considerably more complicated, the conclusions about long-range order are much the same. An application of the method of Ruijgrok and Rodriguez to this model emphasizes the care with which one must interpret the results of variational calculations with regard to the ground-state energy.

II. THE XY MODEL

A. Formulation

The first model consists of N spin $\frac{1}{2}$'s (N even) arranged in a row and having only nearest neighbor interactions. It is

$$H_\gamma = \sum_i [(1+\gamma) S^x{}_i S^x{}_{i+1} + (1-\gamma) S^y{}_i S^y{}_{i+1}], \tag{2.1}$$

where γ is a parameter characterizing the degree of anisotropy in the xy-plane. $S^x{}_i$, $S^y{}_i$ and $S^z{}_i$ may be represented by the usual Pauli spin matrices ($\hbar = 1$):

$$S^x{}_i = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \qquad S^y{}_i = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \qquad S^z{}_i = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Because the Hamiltonian only involves the x- and y- components of the spin operators, we call this model the XY model.

The ends of the chain may be treated in at least two different but physically reasonable ways:

(i) as free ends, in which case the range of the summation index is $1 \leqq i \leqq N-1$, a situation that is convenient for discussing the long-range order;

(ii) as a cyclic chain, in which case $1 \leqq i \leqq N$ and $S^x{}_{N+1} \equiv S^x{}_1$, $S^y{}_{N+1} \equiv S^y{}_1$. This problem, or a slight variation of it (see below), is most convenient for for calculating interesting physical quantities other than the long-range order.

The XY model is exactly soluble for all values of γ, although we shall consider only the range $-1 \leqq \gamma \leqq 1$. Furthermore, it is strikingly similar to the generalized Heisenberg model described by the Hamiltonian

$$H_\gamma = \sum_i [(1+\gamma) S^x{}_i S^x{}_{i+1} + (1-\gamma)(S^y{}_i S^y{}_{i+1} + S^z{}_i S^z{}_{i+1})]. \tag{2.1'}$$

As $\gamma \to 1$ both models tend to the Ising model in which the x-components of spin are completely order and the y- and z-components are completely disordered. For $|\gamma| \neq 1$ both models are genuinely quantum mechanical because

different components of $\mathbf{S}_i$ appearing in H do not commute. The effect of the "transverse terms" (those multiplied by $1 - \gamma$ in either Hamiltonian) in both models is to oppose the ordering of the x-components but to favor the ordering of the y-components (and, in the Heisenberg model, of the z-components, too). Hitherto, it has not been clear for the Heisenberg model just how strong these two effects are: for any particular positive value of γ, do the transverse terms either establish any long-range order among the y- and z-components or destroy the long-range order of the x-components (which would imply absence of long-range order for the y- and z-components as well)? For the XY model, as we shall see, the transverse terms do neither until the limiting case $\gamma = 0$, when they succeed in destroying the order of the x-components. This result is highly suggestive for the Heisenberg model, a subject we discuss in detail in Section II F.

To solve the XY model, we first introduce the raising and lowering operators

$$a_i^\dagger = S^x{}_i + iS^y{}_i \quad \text{and} \quad a_i = S^x{}_i - iS^y{}_i \tag{2.2a}$$

in terms of which the Pauli spin operators are

$$S^x{}_i = (a_i^\dagger + a_i)/2; \qquad S^y{}_i = (a_i^\dagger - a_i)/2i; \qquad S^z{}_i = a_i^\dagger a_i - \tfrac{1}{2} \tag{2.2b}$$

and the Hamiltonian is

$$H_\gamma = \tfrac{1}{2}\sum_i [(a_i^\dagger a_{i+1} + \gamma a_i^\dagger a_{i+1}^\dagger) + \text{h.c.}]. \tag{2.3}$$

These operators partly resemble Fermi operators in that

$$\{a_i , a_i^\dagger\} = 1; \qquad a_i^2 = (a_i^\dagger)^2 = 0; \tag{2.4a}$$

and they partly resemble Bose operators in that

$$[a_i^\dagger, a_j] = [a_i^\dagger, a_j^\dagger] = [a_i , a_j] = 0, \qquad i \neq j. \tag{2.4b}$$

It is therefore not possible to diagonalize the quadratic form appearing in (2.3) directly with a canonical transformation; principal axis transformations of the a's and $a^\dagger$'s do not preserve this mixed set of canonical rules. However, it is possible to transform to a new set of variables that are strictly Fermi operators and in terms of which the Hamiltonian is just as simple.[1] Let

[1] This transformation from a set of Pauli spin operators to a set of fermion creation and annihilation operators dates back at least as far as the classical paper on second quantization of fermion fields by Jordan and Wigner (*12*). It is described in that context, for example, by Kramers (*12*). It was used as the basis for approximate calculations of the ground-state energy of the isotropic Heisenberg model independently by Meyer (*12*), and by Rodriguez (*12*). The more sophisticated variational calculation of an approximate ground-state energy and long-range order by Ruijgrok and Rodriguez (*10*) is also based on this transformation. A somewhat different procedure, based on the same idea of converting nearest neighbor pairs of "paulions" to nearest neighbor pairs of fermions, was applied to precisely $H_{\gamma=0}$ by Nambu (*12*). The spirit of our paper is, however, entirely different from the work of the previous

$$c_i \equiv \exp\left[\pi i \sum_1^{i-1} a_j^\dagger a_j\right] a_i \tag{2.5a}$$

and

$$c_i^\dagger \equiv a_i^\dagger \exp\left[-\pi i \sum_1^{i-1} a_j^\dagger a_j\right]. \tag{2.5b}$$

Then

$$c_i^\dagger c_i = a_i^\dagger a_i\,, \tag{2.6}$$

so that the inverse transformation is simply

$$a_i^\dagger = \exp\left[-\pi i \sum_1^{i-1} c_j^\dagger c_j\right] c_i\,, \tag{2.7a}$$

$$a_i^\dagger = c_i^\dagger \exp\left[\pi i \sum_1^{i-1} c_j^\dagger c_j\right]. \tag{2.7b}$$

The c's and $c^\dagger$'s are Fermi operators:

$$\{c_i\,, c_j^\dagger\} = \delta_{ij}\,, \tag{2.8a}$$

$$\{c_i\,, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0. \tag{2.8b}$$

Because $c_j^\dagger c_j$ is an occupation number having values 0 or 1,

$$\exp(\pi i c_j^\dagger c_j) = \exp(-\pi i c_j^\dagger c_j). \tag{2.9}$$

Furthermore, for $i = 1, 2, \ldots, N-1$,

$$a_i^\dagger a_{i+1} = c_i^\dagger c_{i+1} \tag{2.10a}$$

and

$$a_i^\dagger a_{i+1}^\dagger = c_i^\dagger c_{i+1}^\dagger, \tag{2.10b}$$

so that, for the case of free ends, the Hamiltonian is

$$H_\gamma = \tfrac{1}{2} \sum_1^{N-1} [(c_i^\dagger c_{i+1} + \gamma c_i^\dagger c_{i+1}^\dagger) + \text{h.c.}]. \tag{2.11}$$

For the cyclic chain, we need also

$$a_N^\dagger a_1 = -c_N^\dagger c_1 \exp(i\pi\mathfrak{N}) \neq c_N^\dagger c_1 \tag{2.12a}$$

and

$$a_N^\dagger a_1^\dagger = -c_N^\dagger c_1^\dagger \exp(i\pi\mathfrak{N}) \neq c_N^\dagger c_1^\dagger, \tag{2.12b}$$

authors, and the results are rather more extensive. Because the cases of particular interest ($\gamma \neq 0$, free ends) contain complications not previously encountered, we present here a detailed exposition of the mathematical tricks needed for the ultimate solution.

where

$$\mathfrak{N} \equiv \sum_1^N c_j^\dagger c_j = \sum_1^N (S^z{}_j + \tfrac{1}{2}). \tag{2.13}$$

The Hamiltonian is

$$\begin{aligned} H_\gamma = \tfrac{1}{2} \sum_1^N [(c_i^\dagger c_{i+1} + \gamma c_i^\dagger c_{i+1}^\dagger) + \text{h.c.}] \\ - \tfrac{1}{2}[(c_N^\dagger c_1 + \gamma c_N^\dagger c_1^\dagger) + \text{h.c.}]\,(\exp(i\pi\mathfrak{N}) + 1). \end{aligned} \tag{2.11'}$$

That is, in terms of the Fermi operators c_i and $c_i^\dagger$, H_γ no longer has a simple cyclic structure. For large systems we may neglect the correction term proportional to $\exp(i\pi\mathfrak{N}) + 1$ in which case we call it the "c-cyclic" problem (the original problem being the "a-cyclic" problem). Actually it is not difficult to solve the a-cyclic problem exactly, but we shall first consider the simpler c-cyclic one.

In all cases, the Hamiltonian is a simple quadratic form in Fermi operators and can be exactly diagonalized. The particular simplicity of H_γ depends on the fact that the spins can be arranged in a definite order, that interactions occur only between neighboring spins in this ordering, and that the z-components of spin do not enter. If the interactions were to extend to nth nearest neighbors, H_γ would involve a polynomial of order $2n$ in the c's. In two-dimensional models, it can be readily seen that any ordering and nontrivial scheme of interactions must lead to a Hamiltonian involving a polynomial roughly of order $2N$ for a system of N^2 spins. Thus we are making maximum use of the nearest neighbor character of the interactions and the one-dimensionality of the system.

B. Ground-State Energy, Elementary Excitations, and Free Energy

The diagonalization of quadratic forms such as occur in (2.11) or (2.11') is discussed in Appendix A. The Hamiltonian is reduced to the diagonal form

$$H_\gamma = \sum_k \Lambda_k \eta_k^\dagger \eta_k + \text{constant} \tag{2.14}$$

by the linear transformation

$$\eta_k = \sum_i \frac{\phi_{ki} + \psi_{ki}}{2} c_i + \frac{\phi_{ki} - \psi_{ki}}{2} c_i^\dagger, \tag{2.15a}$$

$$\eta_k^\dagger = \sum_i \frac{\phi_{ki} + \psi_{ki}}{2} c_i^\dagger + \frac{\phi_{ki} - \psi_{ki}}{2} c_i, \tag{2.15b}$$

where ϕ_k and ψ_k, considered as N-component vectors, are real solutions to certain matrix equations. For the c-cyclic problem, the relevant matrices

$$\mathbf{A} = \frac{1}{2}\begin{pmatrix} 0 & 1 & & & & & 1 \\ 1 & 0 & 1 & & & & \\ & \cdot & \cdot & \cdot & & \mathbf{0} & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & \mathbf{0} & & & 1 & 0 & 1 \\ 1 & & & & & 1 & 0 \end{pmatrix}, \tag{2.16a}$$

$$\mathbf{B} = \frac{1}{2}\gamma\begin{pmatrix} 0 & 1 & & & & & -1 \\ -1 & 0 & 1 & & & & \\ & \cdot & \cdot & \cdot & & \mathbf{0} & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & \mathbf{0} & & & -1 & 0 & 1 \\ 1 & & & & & -1 & 0 \end{pmatrix}, \tag{2.16b}$$

$(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B}) =$

$$\frac{1}{4}\begin{pmatrix} 2(1+\gamma^2) & 0 & 1-\gamma^2 & \cdot & \cdot & \cdot & 1-\gamma^2 & 0 \\ 0 & 2(1+\gamma^2) & 0 & 1-\gamma^2 & & & & 1-\gamma^2 \\ 1-\gamma^2 & 0 & 2(1+\gamma^2) & 0 & 1-\gamma^2 & & \mathbf{0} & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \\ \cdot & & \cdot & \cdot & \cdot & \cdot & \cdot & \\ \cdot & \mathbf{0} & & 1-\gamma^2 & 0 & 2(1+\gamma^2) & 0 & 1-\gamma^2 \\ 1-\gamma^2 & & & & 1-\gamma^2 & 0 & 2(1+\gamma^2) & 0 \\ 0 & 1-\gamma^2 & & & & 1-\gamma^2 & 0 & 2(1+\gamma^2) \end{pmatrix}. \tag{2.16c}$$

The vectors are the real solutions of the eigenvalue equation

$$\phi_k(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B}) = \Lambda_k^2\phi_k\,. \tag{2.17}$$

A complete set of solutions is

$$\phi_{kj} = \begin{matrix} (2/N)^{\frac{1}{2}} \sin kj \\ (2/N)^{\frac{1}{2}} \cos kj \end{matrix} \tag{2.18a}$$

belonging to the set of eigenvalues

$$\Lambda_k^2 = 1 - (1 - \gamma^2)\sin^2 k, \tag{2.18b}$$

where

$$k = 2\pi m/N, \qquad m = -\tfrac{1}{2}N, \cdots, 0, 1, \cdots, \tfrac{1}{2}N - 1. \quad (2.18c)$$

In (2.18a) we take the upper solution for ϕ_{kj} if $k > 0$, the lower solution if $k \leqq 0$. For $\Lambda_k \neq 0$, $(A - 7a)$ gives

$$\psi_{kj} = \Lambda_k^{-1} (\cos k\, \phi_{kj} + \gamma \sin k\, \phi_{-kj}), \quad (2.18d)$$

while if $\Lambda_k = 0$

$$\psi_{kj} = \pm \phi_{kj}. \quad (2.18d')$$

$\Lambda_k = 0$ is an eigenvalue only if $\gamma = 0$ and $N/4$ is an integer. To simplify the discussion, let us assume that $N/4$ is not an integer and therefore that $\Lambda_k \neq 0$.

The sign of Λ_k being arbitrary, we shall take it always to be positive. This corresponds to a particle-hole picture for the η-particles, where the ground state has no elementary fermions and the elementary fermion excitations both above and below the Fermi surface have positive energies.[2] Λ_k is shown in Fig. 1 for the isotropic and extreme anisotropic (Ising) cases and for one intermediate case. Remark that only for the isotropic case is there no energy gap.

The ground state Ψ_0 is the state with no elementary excitations:

$$\eta_k \Psi_0 = 0, \quad \text{all } k. \quad (2.19)$$

The ground-state energy, according to (A-12) is

$$E_0 = -\tfrac{1}{2} \sum_k \Lambda_k. \quad (2.20)$$

In the limit $N \to \infty$, the sum can be replaced by an integral giving

$$\begin{aligned} E_0/N &= -(1/4\pi) \int_{-\pi}^{\pi} dk\, [1 - (1 - \gamma^2) \sin^2 k]^{\frac{1}{2}} \\ &= -(1/\pi)\mathcal{E}(1 - \gamma^2), \end{aligned} \quad (2.21)$$

where $\mathcal{E}(k^2)$ is one of the complete elliptic integrals (*13*). E_0/N goes smoothly between the limiting cases

$$E_0/N = -1/\pi, \quad \text{isotropic case}, \quad \gamma = 0, \quad (2.22a)$$

and

$$E_0/N = -\tfrac{1}{2}, \quad \text{Ising case}, \quad \gamma = 1. \quad (2.22b)$$

[2] The "Fermi surface" consists of the points $k = \pm\pi/2$. The alternate picture in which all excitations are "particles" (in the isotropic case, a "particle" is an up spin) would be obtained by letting Λ_k have the sign of $\cos k$. The Fermi sea would then be defined by $|\, k\, | > \pi/2$. The particle-hole picture is preferred because it somewhat simplifies the algebra.

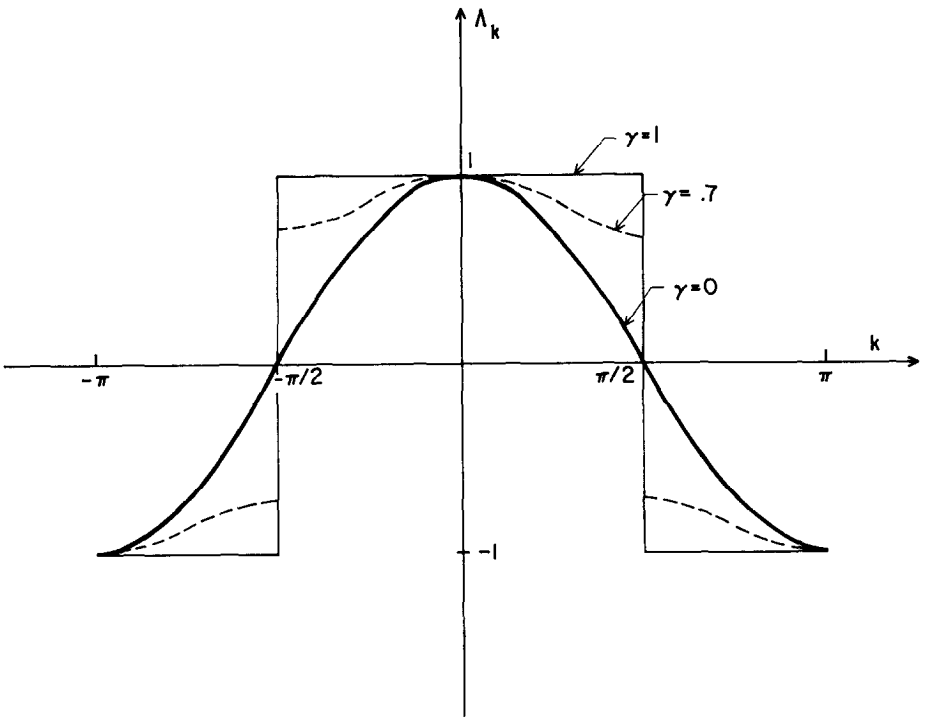

FIG. 1. Energy of elementary excitations in XY model as function of wave vector for three different degrees of anisotropy.

At this point let us remark on the simplification resulting from the consideration of the c-cyclic rather than the a-cyclic problem. According to (2.11′), the Hamiltonian for the a-cyclic problem is complicated by the presence of the term

$$-\tfrac{1}{2}[(c_N^\dagger c_1 + \gamma c_N^\dagger c_1^\dagger) + \text{h.c.}]\,(\exp(i\pi\mathfrak{N}) + 1).$$

Although $\mathfrak{N}$ is not invariant under the transformation (2.15), its evenness or oddness is invariant, so that $\exp(i\pi\mathfrak{N})$ is invariant. Now in the ground state of the c-cyclic problem, and in all states with an even number of excitations, the number of c-particles is odd (assuming $N/4$ is not an integer, the k's are occupied symmetrically around $k = 0$, except that $k = \pi$ but not $k = -\pi$ is occupied). Therefore, the additional term gives zero acting on such states and they remain eigenstates of the a-cyclic problem. States with an odd number of excitations, on the other hand, have $\mathfrak{N}$ even, giving the additional term

$$-\tfrac{1}{2}(c_N^\dagger c_1 + \gamma c_N^\dagger c_1 + \text{h.c.})$$

in the Hamiltonian. This has the effect of making changes of order $1/N$ in the

k's, ϕ_k's, and ψ_k's, all of which can be exactly calculated and are negligible in the calculation of real physical quantities. Strictly speaking though, the elementary excitations are not independent for the a-cyclic problem because of this dependence on the evenness or oddness of the total number of excitations present, and this is why we have preferred to consider the c-cyclic problem.

The free energy is the grand potential of such a system of noninteracting fermions with zero chemical potential ($\beta = 1/kT$):

$$F_\gamma/N = -kT\left[\ln 2 + \frac{2}{\pi}\int_0^{\pi/2} dk \ln\cosh\left(\tfrac{1}{2}\beta\Lambda_k\right)\right]. \tag{2.23}$$

In the isotropic limit we obtain

$$F_{\text{isotrop.}}/N = -kT\left[\ln 2 + \frac{2}{\pi}\int_0^{\pi/2} dk \ln\cosh\left(\tfrac{1}{2}\beta\cos k\right)\right]; \tag{2.24a}$$

while in the Ising limit, we obtain the classical result,

$$F_{\text{Ising}}/N = -kT(\ln 2 + \ln\cosh\tfrac{1}{2}\beta). \tag{2.24b}$$

Neither case exhibits any singular behavior as a function of temperature, a result to be expected in view of the one-dimensional nature of the model.

C. Short- and Long-Range Order in the Ground State

The long-range order for the Heisenberg model is often defined in terms of two sublattices (in the case of the linear chain, the sublattices of all even sites and of all odd sites). It is taken to be the preponderance of spins up to spins down on one of the sublattices, or of spins up on one sublattice to spins up on the other. Because of the invariance of the Hamiltonian under translations by any number of sites and also under 180° rotations about the x-, y-, and z-axes in spin space, it is clear that for a nondegenerate stationary state such a definition of long-range order must give zero, even if by any reasonable definition the state were ordered. That the ground state is nondegenerate is shown in Appendix B. The completely ferromagnetic states can have long-range order by this definition only because they are so highly degenerate. The definition has nevertheless been useful because the approximate states considered have not always had the full symmetry of the Hamiltonian. A much better measure of the long-range order is the quantity

$$\rho_{lm} = \langle\Psi_0 \mid \mathbf{S}_l\cdot\mathbf{S}_m \mid \Psi_0\rangle. \tag{2.25}$$

This is the contraction at $t = 0$, of the time-dependent spin correlation tensor

$$\varrho_{lm}(t) = \langle\Psi_0 \mid \mathbf{S}_l(0)\mathbf{S}_m(t) \mid \Psi_0\rangle \tag{2.26}$$

which enters in the calculation of any process, such as neutron scattering, con-

ceived to measure the order directly. Because of the nature of the model, we wish to calculate separately the various contributions to this order parameter:

$$\rho^x_{lm} = \langle\Psi_0 \mid S^x{}_l S^x{}_m \mid \Psi_0\rangle = \tfrac{1}{4}\langle\Psi_0 \mid (a_l^\dagger + a_l)(a_m^\dagger + a_m) \mid \Psi_0\rangle, \tag{2.27a}$$

$$\rho^y_{lm} = \langle\Psi_0 \mid S^y{}_l S^y{}_m \mid \Psi_0\rangle = \tfrac{1}{4}\langle\Psi_0 \mid (a_l^\dagger - a_l)(a_m^\dagger - a_m) \mid \Psi_0\rangle, \tag{2.27b}$$

$$\rho^z_{lm} = \langle\Psi_0 \mid S^z{}_l S^z{}_m \mid \Psi_0\rangle = \langle\Psi_0 \mid (a_l^\dagger a_l - \tfrac{1}{2})(a_m^\dagger a_m - \tfrac{1}{2}) \mid \Psi_0\rangle. \tag{2.27c}$$

We shall derive general expressions which reduce the calculation of these contributions to quadratures.

Consider ρ^x_{lm} in terms of the c's and $c^\dagger$'s:

$$\begin{aligned}\rho^x_{lm} &= \tfrac{1}{4}\left\langle \Psi_0 \left| (c_l^\dagger + c_l) \exp\left(\pi i \sum_l^{m-1} c_i^\dagger c_i\right)(c_m^\dagger + c_m) \right| \Psi_0 \right\rangle \\ &= \tfrac{1}{4}\left\langle \Psi_0 \left| (c_l^\dagger - c_l) \exp\left(\pi i \sum_{l+1}^{m-1} c_i^\dagger c_i\right)(c_m^\dagger + c_m) \right| \Psi_0 \right\rangle.\end{aligned} \tag{2.28}$$

Now observe that

$$\exp(\pi i c_i^\dagger c_i) = (c_i^\dagger + c_i)(c_i^\dagger - c_i), \tag{2.29a}$$

a result that is readily verified in the representation diagonalizing $c_i^\dagger c_i$. Defining

$$A_i = c_i^\dagger + c_i \quad \text{and} \quad B_i = c_i^\dagger - c_i, \tag{2.30}$$

we have

$$\rho^x_{lm} = \tfrac{1}{4}\langle\Psi_0 \mid B_l A_{l+1} B_{l+1} \cdots A_{m-1} B_{m-1} A_m \mid \Psi_0\rangle. \tag{2.31a}$$

In a similar way, using

$$\exp(\pi i c_i^\dagger c_i) = -(c_i^\dagger - c_i)(c_i^\dagger + c_i), \tag{2.29b}$$

we have

$$\rho^y_{lm} = (-1)^{m-l}\tfrac{1}{4}\langle\Psi_0 \mid A_l B_{l+1} A_{l+1} \cdots B_{m-1} A_{m-1} B_m \mid \Psi_0\rangle. \tag{2.31b}$$

Finally, because

$$a_i^\dagger a_i - \tfrac{1}{2} = -\tfrac{1}{2}(a_i^\dagger + a_i)(a_i^\dagger - a_i) = -\tfrac{1}{2}(c_i^\dagger + c_i)(c_i^\dagger - c_i), \tag{2.29c}$$

we have

$$\rho^z_{lm} = \tfrac{1}{4}\langle\Psi_0 \mid A_l B_l A_m B_m \mid \Psi_0\rangle. \tag{2.31c}$$

To evaluate expectation values such as appear in (2.31a, b, c), we make use of the well-known Wick Theorem[3] in quantum field theory, which allows us to express the vacuum expectation value of a product of operators, all of which

[3] See Wick (*14*) or subsequent books on quantum field theory.

obey anticommutation rules, in terms of so-called contractions of pairs, i.e., vacuum expectation values of products of just two operators. Explicitly, if $\mathcal{O}_1, \cdots, \mathcal{O}_{2n}$ are a set of such operators, then

$$\langle \Psi_0 \mid \mathcal{O}_1 \cdots \mathcal{O}_{2n} \mid \Psi_0 \rangle = \sum_{\text{all pairings}} (-1)^{p'} \prod_{\text{all pairs}} (\text{contraction of the pair}),$$

where the contraction $\langle \mathcal{O}_i \mathcal{O}_j \rangle$ is defined to be $\langle \Psi_0 \mid \mathcal{O}_i \mathcal{O}_j \mid \Psi_0 \rangle$, and where p' is the signature of the permutation, for a given pairing, necessary to bring operators of the same pair next to one another from the original order.

A particular simplification occurs in evaluating (2.31a, b, c) because certain kinds of contractions vanish. In fact, the basic contractions that arise are readily calculated:

$$\langle A_i A_j \rangle = \sum_k \phi_{ki} \phi_{kj} = \delta_{ij}, \tag{2.32a}$$

$$\langle B_i B_j \rangle = -\sum_k \psi_{ki} \psi_{kj} = -\delta_{ij}, \tag{2.32b}$$

$$\langle B_i A_j \rangle = -\langle A_j B_i \rangle = -\sum_k \psi_{ki} \phi_{kj} \equiv G_{ij}. \tag{2.32c}$$

Because $\langle A_i A_i \rangle$ and $\langle B_i B_i \rangle$ never occur, only pairings in which all contractions are of the type $\langle B_i A_j \rangle$ contribute in (2.31a, b, c).

The most straightforward pairing contributing to ρ^x_{lm} is

$$\langle B_l A_{l+1} \rangle \langle B_{l+1} A_{l+2} \rangle \cdots \langle B_{m-1} A_m \rangle.$$

All other pairings can be obtained from this one by permuting the A's among themselves with the B's fixed. Because the number of crossings of B's by A's is then always even, the sign associated with a given permutation is $(-1)^{p'}$, where p' is the signature of the permutation of the A's. Thus

$$\begin{aligned} \rho^x_{lm} &= \tfrac{1}{4} \sum_P (-1)^{p'} G_{l,P(l+1)} \cdots G_{m-1,P(m)} \\ &= \tfrac{1}{4} \begin{vmatrix} G_{l,l+1} & G_{l,l+2} & \cdots & G_{lm} \\ \vdots & & & \vdots \\ G_{m-1,l+1} & \cdots & & G_{m-1,m} \end{vmatrix}. \end{aligned} \tag{2.33a}$$

Similarly, because $A_l B_{l+1} = -B_{l+1} A_l$, etc.

$$\rho^y_{lm} = \tfrac{1}{4} \begin{vmatrix} G_{l+1,l} & G_{l+1,l+1} & \cdots & G_{l+1,m-1} \\ \vdots & & & \vdots \\ G_{ml} & \cdots & & G_{m,m-1} \end{vmatrix}. \tag{2.33b}$$

Thus, both ρ^x_{lm} and ρ^y_{lm} are particular subdeterminants of $\det \mathbf{G}$. ρ^z_{lm} is immediately calculable from (2.31c) and Wick's theorem. For $l < m$,

$$\begin{aligned} \rho^z_{lm} &= \tfrac{1}{4}(\langle A_l B_l \rangle \langle A_m B_m \rangle - \langle A_l B_m \rangle \langle A_m B_l \rangle) \\ &= \tfrac{1}{4}(G_{ll} G_{mm} - G_{ml} G_{lm}). \end{aligned} \tag{2.33c}$$

Let us now consider the detailed properties of the G_{ij}'s. First observe that G_{ij}, considered as an element of an $N \times N$ matrix is just

$$G_{ij} = -(\psi^T \phi)_{ij}, \tag{2.34}$$

where ϕ and ψ are the matrices ϕ_{ki} and ψ_{ki}. It is immediately obvious that $\mathbf{G}$ is unitary because ϕ and ψ are unitary:

$$\mathbf{G}\mathbf{G}^T = \psi^T \phi \phi^T \psi = \psi^T \psi = \mathbf{1}. \tag{2.35}$$

The determinant of $\mathbf{G}$ is thus ± 1. The actual sign, which will be needed in the following section, is readily calculated:

$$\det \mathbf{G} = \det(-\psi^T \phi) = (-1)^N \det \psi^T \phi.$$

But from (A-7a)

$$(\psi^T)_{ik} = ((\mathbf{A} - \mathbf{B})^T \phi^T \Lambda^{-1})_{ik},$$

where

$$(\mathbf{\Lambda})_{kk'} = \Lambda_k \delta_{kk'}.$$

Thus, using $\det \phi = \pm 1$, we obtain

$$\det \mathbf{G} = (-1)^N \det \mathbf{\Lambda}^{-1} \det(\mathbf{A} - \mathbf{B}).$$

Now $\det \mathbf{\Lambda}^{-1} > 0$, because $\Lambda_k > 0$ for all k. Thus

$$\det \mathbf{G} = (-1)^N \det(\mathbf{A} - \mathbf{B}) / |\det(\mathbf{A} - \mathbf{B})|. \tag{2.36}$$

A second important property of G_{ij} is that, for the cyclic problem,

$$G_{ij} = G_{i-j} \equiv G_r, \tag{2.37}$$

a result which can be proved either from the invariance properties of the cyclic Hamiltonian or from direct evaluation of the sums in (2.32c).

To calculate G_r explicitly we consider the limit $N \to \infty$ with r fixed. It is shown in Appendix C that

$$G_r = -[\tfrac{1}{2}(1 + \gamma)L_{r+1} + \tfrac{1}{2}(1 - \gamma)L_{r-1}], \qquad r \text{ odd},$$

and

$$G_r = 0, \qquad r \text{ even}, \tag{2.38a}$$

where

$$L_r(\gamma) = (2/\pi) \int_0^{\pi/2} dk \cos kr \, [1 - (1 - \gamma^2) \sin^2 k]^{-\frac{1}{2}} = L_{-r}(\gamma). \tag{2.38b}$$

It is thus evident that $\gamma \to -\gamma$ is equivalent to $r \to -r$. In the isotropic limit

($\gamma = 0$), (2.38), reduces to

$$G_r = (-1)^{\frac{1}{2}(r+1)} 2/\pi r, \qquad r \text{ odd},$$

and

$$G_r = 0, \qquad r \text{ even}. \tag{2.39a}$$

In the extreme anisotropic limit ($\gamma = 1$)

$$G_{-1} = -1,$$

and

$$G_r = 0, \qquad r \neq -1. \tag{2.39b}$$

In the general anisotropic case, G_r is not so simply evaluated. The special cases of G_1 and G_{-1} (all that are needed for the nearest neighbor order in the cyclic chain) can be expressed in terms of the complete elliptic integrals (*13*) $\mathfrak{K}(k^2)$ and $\mathfrak{D}(k^2)$

$$G_{\pm 1} = -(2/\pi)[\mathfrak{K}(1 - \gamma^2) - (1 \pm \gamma)\mathfrak{D}(1 - \gamma^1)]. \tag{2.40}$$

The asymptotic behavior of G_r for $r \to \infty$, crucial for the long-range order, can be obtained by repeated integrations by parts. Assuming $\gamma \neq 0$ and r even, one finds for L_r

$$L_r(\gamma) = \frac{1}{r^4}[f^{(\mathrm{III})}(0) - (-1)^{\frac{1}{2}r} f^{(\mathrm{III})}(\pi/2)]$$

$$- \frac{1}{r^6}\left[f^{(\mathrm{IV})}(0) - (-1)^{\frac{1}{2}r} f^{(\mathrm{IV})}(\pi/2) + \int_0^{\pi/2} dk\, f^{(\mathrm{VI})}(k) \cos kr\right],$$

where

$$f(k) = (2/\pi)[1 - (1 - \gamma^2)\sin^2 k]^{-\frac{1}{2}}. \tag{2.41}$$[4]

Thus for sufficiently large odd r

$$G_r \sim -\frac{1}{r^4}[f^{(\mathrm{III})}(0) + 2\gamma(-1)^{\frac{1}{2}(r-1)} f^{(\mathrm{III})}(\pi/2)] + O(1/r^6)$$

or

$$|G_r| < A/r^4 \quad \text{for} \quad |r| > r_0, \tag{2.42}$$

where A and r_0 are constants depending on γ but not on r. For general values of r, the following series for L_r (r even) is convenient:

$$L_r(\gamma) = (-1)^{\frac{1}{2}r} \frac{2}{1+\gamma}\left[g_0 g_{r/2} - \frac{1}{\pi}\ln(1 - \lambda^2) - \sum_1^\infty \lambda^{2l}\left(\frac{1}{\pi l} - g_l g_{l+\frac{1}{2}r}\right)\right] \tag{2.43a}$$

[4] This behavior is found because $f'(0) = f'(\pi/2) = 0$, which is true only if $\gamma \neq 0$.

where

$$\lambda = (1 - \gamma)/(1 + \gamma) \tag{2.43b}$$

and

$$g_l = 2^{-2l}\binom{2l}{l} \underset{l\to\infty}{\sim} (\pi l)^{-\frac{1}{2}}. \tag{2.43c}$$

This series is readily obtained using the relations

$$[1 - (1 - \gamma^2)\sin^2 k]^{\frac{1}{2}} = [2/(1 + \gamma)] \sum_0^\infty (-\lambda)^m P_m(\cos 2k),$$

$$P_m(\cos 2k) = \sum_{l=0}^{m} g_l g_{m-l} \cos[(m - 2l)2k],$$

and

$$g_l \sim (\pi l)^{-\frac{1}{2}}.$$

Actual numerical evaluation for $\lambda^2 = \frac{2}{3}$ or $\gamma = 0.10102$ gives Table I. It should be remarked that L_r, G_r, the various contributions to the order parameter, and the ground-state energy are all nonanalytic functions of γ at the point $\gamma = 0$, although they are analytic at $\gamma = \pm 1$. This is, of course, the reason for the different asymptotic behavior of G_r for $\gamma = 0$ and $\gamma \neq 0$. This suggests that a perturbation treatment should converge if the totally anisotropic case is considered as the zeroth order Hamiltonian, a result observed by Walker (*9*) for the full anisotropic Heisenberg model of the antiferromagnetic chain.

We now investigate the short-, intermediate-, and long-range order for the

TABLE I

QUANTITIES USEFUL IN CALCULATING ORDER BETWEEN DIFFERENT SPINS FOR THE XY MODEL WITH $\gamma = 0.10102$

r	$\frac{1}{2}(1+\gamma)L_{r-1}$	G_r	G_{-r}
1	1.2917	−0.4560	−0.8029
3	−0.5986	0.1047	0.2850
5	0.3841	−0.0455	−0.1652
7	−0.2680	0.0242	0.1091
9	0.1946	−0.0143	−0.0765
11	−0.1446	0.0089	0.0555
13	0.1092	−0.0058	−0.0412
15	−0.0833	0.0039	0.0310
17	0.0641	−0.0027	−0.0236
19	−0.0497		

cyclic case. The various contributions to the short-range order are readily calculated:

$$\rho_{i,i+1}^{x} \equiv \rho_1^{x} = \tfrac{1}{4}G_{-1}$$
$$= -(2\pi)^{-1}[\mathfrak{K}(1-\gamma^2) - (1-\gamma)\mathfrak{D}(1-\gamma^2)], \tag{2.44a}$$
$$\rho_{i,i+1}^{y} \equiv \rho_1^{y} = \tfrac{1}{4}G_1$$
$$= -(2\pi)^{-1}[\mathfrak{K}(1-\gamma^2) - (1+\gamma)\mathfrak{D}(1-\gamma^2)], \tag{2.44b}$$
$$\rho_{i,i+1}^{z} \equiv \rho_1^{z} = -\tfrac{1}{4}G_1G_{-1}$$
$$= -\pi^{-2}[(\mathfrak{K}(1-\gamma^2) - \mathfrak{D}(1-\gamma^2))^2 - \gamma^2(\mathfrak{D}(1-\gamma^2))^2]. \tag{2.44c}$$

We plot these parameters and the total order $\rho_1 \equiv \rho_1^{x} + \rho_1^{y} + \rho_1^{z}$ as functions of γ in Fig. 2.

For the intermediate-range order one must fall back on a numerical evalua-

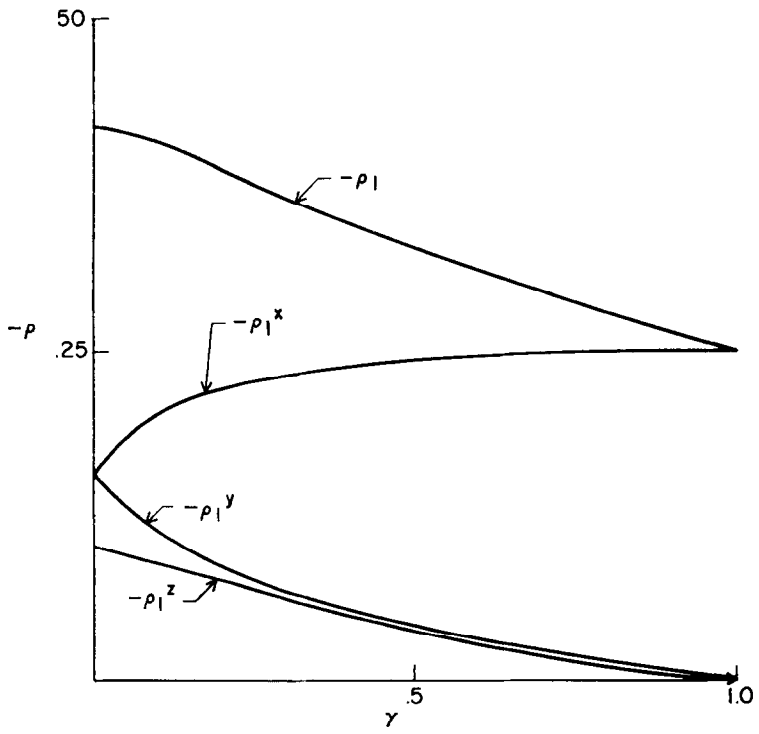

FIG. 2. Various contributions to the short-range order as functions of the degree of anisotropy in the XY model.

tion of the relevant determinants. Because $G_r = 0$ for even r, these determinants simplify somewhat. Thus

$$\rho^x_{2n-1} = \tfrac{1}{4}R_{n-1}R_n \tag{2.45a}$$

and

$$\rho^x_{2n} = \tfrac{1}{4}R_n^2 \tag{2.45b}$$

where

$$R_n = \begin{vmatrix} G_{-1} & G_{-3} & \cdots & & G_{-(2n-1)} \\ G_1 & G_{-1} & G_{-3} & & \\ \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \\ \cdot & & \cdot & \cdot\ \cdot & \\ & & & G_1\ G_{-1} & G_{-3} \\ G_{2n-3} & & & G_1 & G_{-1} \end{vmatrix} \tag{2.46a}$$

and

$$R_0 = 1. \tag{2.46b}$$

Similar expressions can be derived for ρ^y_{2n-1} and ρ^z_{2n}. One has only to let $G_r \to G_{-r}$. Numerical evaluation of this determinant for several values of n leads to a very slowly converging sequence for ρ_n, even for $\gamma = 0$, the case expected to be most rapidly converging. Results for $\gamma = 0$ and $\gamma = 0.10102$ are summarized as shown in the tabulation.

n	1	2	3	4	5	6
$\rho_n(\gamma = 0)$	−0.1592	0.1013	−0.0860	0.0730	−0.0661	0.0597
$\rho_n(\gamma = 0.10102)$	−0.2007	0.1611	−0.1555	0.1500	−0.1483	0.1467

Now let us investigate the long-range order. The cases $\gamma = 0$ and $\gamma \neq 0$ exhibit entirely different long-range order characteristics because of the difference in asymptotic behavior of G_r for these two cases. We first consider the isotropic case, which is simpler and, as we now show, has no long-range order.

We seek the limits of ρ_n^x, ρ_n^y, and ρ_n^z as $n \to \infty$ for $\gamma = 0$. The fact that we have first taken the limit $N \to \infty$ in passing from sums to integrals ensures that we never come round the circle when $n \to \infty$.

$$\rho_n{}^x = \rho_n{}^y = \frac{1}{4}\begin{vmatrix} G_{-1} & G_{-2} & \cdots & G_{-n} \\ G_0 & G_{-1} & G_{-2} & \\ \cdot & & \cdot & \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & & \cdot & \\ & & \cdot & \cdot \ G_{-2} \\ G_{n-2} & & G_0 & G_{-1} \end{vmatrix} \equiv \frac{1}{4} D_n , \tag{2.47a}$$

$$\rho_n{}^z = \tfrac{1}{2}\delta_{n0} - \tfrac{1}{4} G_n G_{-n} \xrightarrow[n \to \infty]{} -(\pi n)^{-2} \to 0. \tag{2.47b}$$

An upper bound to $| D_n |$ may be obtained with Hadamard's Theorem (*15*), which states that

$$| \det_n \mathbf{C} |^2 \leqq \prod_{i=1}^{n} \left(\sum_{j=1}^{n} C_{ij}^2 \right) \equiv \prod_{i=1}^{n} d_{i,n}^2 , \tag{2.48}$$

if $d_{i,n}$ is the norm of the ith row of $\mathbf{C}$. The equality holds only when the rows are all mutually orthogonal. We divide the rows of D_n into three groups, those near the top (the first n_0 rows, where n_0 is independent of n and $\ll n$), those near the bottom (the last n_0 rows) and those in the middle. Because $d_{i,n}^2 \leqq 1$ for all i from the unitarity of $\mathbf{G}$, we may replace $d_{i,n}$ by 1 for the first and third groups in (2.48):

$$D_n{}^2 \leqq \prod_{i=n_0+1}^{n-n_0} d_{i,n}^2 . \tag{2.49}$$

In the middle group

$$\begin{aligned} d_{i,n}^2 = \sum_{j=1}^{n} G_{i-1-j}^2 = 1 - 2 \sum_{M(i,n)}^{\infty} G_r^2 - \sum_{m(i,n)}^{M(i,n)-1} \\ G_r{}^2 \leqq \exp\left[-2 \sum_{M}^{\infty} G_r{}^2 - \sum_{m}^{M-1} G_r{}^2 \right], \end{aligned} \tag{2.50}$$

where

$$M(i,n) = \max\,(i - 1, n + 2 - i) \tag{2.51a}$$

and

$$m(i,n) = \min\,(i - 1, n + 2 - i). \tag{2.51b}$$

But

$$\sum_{0}^{b} G_r{}^2 \geqq (2/\pi)^2 \frac{1}{2} \int_{a+1}^{b} k^{-2}\, dk = (2/\pi)^2 \frac{1}{2} \left(\frac{1}{a+1} - \frac{1}{b} \right), \tag{2.52}$$

so that

$$\prod_{i=n_0+1}^{n-n_0} d_{i,n}^2 \leqq \exp\left\{-(2/\pi)^2\frac{1}{2}\left[\sum_{n_0+1\leqq i\leqq \frac{1}{2}(n+3)}\left(\frac{1}{n+2-i}+\frac{1}{i}\right)\right.\right.$$
$$\left.\left.+\sum_{\frac{1}{2}(n+3)<i\leqq n-n_0}\left(\frac{1}{i-1}+\frac{1}{n+3-i}\right)\right]\right\}. \tag{2.53}$$

Furthermore

$$\sum_a^b (1/k) \geqq \int_a^b (dk/k) = \ln(b/a),$$

so that each sum in the exponent of (2.53) can be replaced by a lower bound:

$$D_n^2 \leqq \exp\left\{-(2/\pi)^2\frac{1}{2}\left[\ln 2\left(\frac{n-n_0+1}{n+1}\right)+\ln 2\left(\frac{n-n_0-1}{n+1}\right)\right.\right.$$
$$\left.\left.+\ln\frac{1}{2}\left(\frac{n+3}{n_0+1}\right)+\ln\frac{1}{2}\left(\frac{n+3}{n_0+3}\right)\right]\right\}. \tag{2.54}$$

As $n \to \infty$

$$D_n^2 \leqq (n+3)^{-(2/\pi)^2} \times \text{constant}, \tag{2.55}$$

and so

$$\rho_n^x = \rho_n^y \to 0 \quad \text{as} \quad n \to \infty. \tag{2.56}$$

When $\gamma \neq 0, |G_r| < Ar^{-4}$ for $r > r_0$ and the preceding development gives only the very weak result

$$D_n^2 \leqq \text{constant} \quad \text{as} \quad n \to \infty,$$

which does not exclude the possibility that either ρ_n^x, ρ_n^y, or both approach finite limits as $n \to \infty$ (n even). Not only the norms of the rows but the overlap between rows must now be considered to improve the estimate. Conceivably a more powerful theorem would show that either or both the order parameters tend to zero as $n \to \infty$, although no such theorem has been found. Instead, when we consider the spins at the ends of a long chain with free ends, we find for $\gamma > 0$ that $\rho_{iN}^x \neq 0$ although $\rho_{iN}^y = O(1/N)$ (and the reverse for $\gamma < 0$), as we now show.

D. End-to-End Order in the Ground State

It is easy to calculate the order between the first and last spins of a chain of N spins, even if evaluation of the intermediate-range order is difficult. This is

because what is involved is an $(N-1) \times (N-1)$ minor of the $N \times N$ determinant $\det \mathbf{G}$, where $\mathbf{G}$ is unitary. Thus

$$\rho^x_{1N} = \tfrac{1}{4} \begin{vmatrix} G_{12} & \cdots & G_{1N} \\ \vdots & & \vdots \\ G_{N-1,2} & \cdots & G_{N-1,N} \end{vmatrix} = (-1)^{N-1} \tfrac{1}{4} (\mathbf{G}^{-1})_{1N} \det \mathbf{G}. \quad (2.57)$$

Because $\mathbf{G}$ is unitary

$$(\mathbf{G}^{-1})_{1N} = G_{N1}. \quad (2.58)$$

Therefore, using (2.36), we have

$$\rho^x_{1N} = (-1)^{N-1} \tfrac{1}{4} G_{N1} \det \mathbf{G} = -\tfrac{1}{4} G_{N1} \det(\mathbf{A} - \mathbf{B})/|\det(\mathbf{A} - \mathbf{B})|. \quad (2.59a)$$

We have assumed only that $\Lambda_k \neq 0$ for all k. In a similar way

$$\rho^y_{1N} = -\tfrac{1}{4} G_{1N} \det(\mathbf{A} - \mathbf{B})/|\det(\mathbf{A} - \mathbf{B})|. \quad (2.59b)$$

As before

$$\rho^z_{1N} = \tfrac{1}{4} (G_{11} G_{NN} - G_{1N} G_{N1}). \quad (2.59c)$$

An alternative way to derive (2.59a,b) which bypasses the general problem of calculating ρ_{lm}, is as follows:

$$\rho^x_{1N} = \tfrac{1}{4} \langle \Psi_0 | (c_1^\dagger + c_1)(c_N^\dagger - c_N) \exp(i\pi \mathfrak{I}) | \Psi_0 \rangle. \quad (2.60)$$

Because $[\exp(i\pi \mathfrak{I}), H_\gamma] = 0$, the nondegeneracy of Ψ_0 (assured by $\Lambda_k \neq 0$) implies that Ψ_0 is an eigenstate of $\exp(\pi i \mathfrak{I})$ belonging to one of the eigenvalues ± 1. Thus $\rho^x_{1N} = \mp \tfrac{1}{4} G_{N1}$. To determine which sign is in fact correct, we use the fact that the sign is independent of the continuous variable γ, and evaluate it for $\gamma = 0$. We find finally

$$\rho^x_{1N} = -\tfrac{1}{4} G_{N1} \det \mathbf{A} / |\det \mathbf{A}|, \quad (2.61)$$

which agrees with (2.59a) providing $\Lambda_k \neq 0$ for all k (and thus $\det(\mathbf{A} - \mathbf{B}) \neq 0$ and $\det \mathbf{A} \neq 0$). For the cyclic chain the simplicity of the end-to-end order is of no interest because the sites 1 and N are nearest neighbors, and we obtain only the short-range order. For the chain with free ends, however, this is indeed a measure of the long-range order as $N \to \infty$. Certainly, if there is a finite end-to-end order, then there is finite long-range order as defined in the previous section, although the two calculations may give slightly different numerical results because of end effects. We investigate these end effects at the end of this section.

Consider then a chain of N spins with free ends. To ensure that Ψ_0 be non-

degenerate, or equivalently that $\Lambda_k \neq 0$ for all k, we assume N to be even.[5] We are then calculating the order between two spins that have a tendency, however small, to be antiparallel.

The relevant matrices are

$$\mathbf{A}-\mathbf{B}=\tfrac{1}{2}\begin{pmatrix} 0 & 1-\gamma & & & & & & \\ 1+\gamma & 0 & 1-\gamma & & & & \mathbf{0} & \\ & \cdot & \cdot & \cdot & & & & \\ & & \cdot & \cdot & \cdot & & & \\ & & & \cdot & \cdot & \cdot & & \\ & & & & 1+\gamma & 0 & 1-\gamma & \\ & \mathbf{0} & & & & 1+\gamma & 0 & \end{pmatrix} = (\mathbf{A}+\mathbf{B})^T, \quad (2.62)$$

$$(\mathbf{A}-\mathbf{B})(\mathbf{A}+\mathbf{B})$$

$$=\tfrac{1}{4}\begin{pmatrix} (1-\gamma)^2 & 0 & 1-\gamma^2 & & & & & \\ 0 & 2(1+\gamma^2) & 0 & 1-\gamma^2 & & & \mathbf{0} & \\ 1-\gamma^2 & 0 & 2(1+\gamma^2) & 0 & 1-\gamma^2 & & & \\ & \cdot & \cdot & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \cdot & \\ & \mathbf{0} & & & 1-\gamma^2 & 0 & 2(1+\gamma^2) & 0 \\ & & & & & 1-\gamma^2 & 0 & (1+\gamma)^2 \end{pmatrix}. \quad (2.63)$$

Because the problem is no longer cyclic, the first, second, $(N-1)$st and Nth rows of $(\mathbf{A}-\mathbf{B})(\mathbf{A}+\mathbf{B})$ are different from all the rest.

The vectors ϕ_k and ψ_k are readily found and are of two kinds.

Modes of the first kind:

[5] It is readily seen that for N odd, $\det(\mathbf{A}-\mathbf{B})=0$, so there exists a zero eigenvalue of $(\mathbf{A}-\mathbf{B})(\mathbf{A}+\mathbf{B})$. The existence of this excitation corresponds to the fact that because both $R_x \equiv \exp[\pi i \sum_1^N S^x_i]$ and $R_z \equiv \exp[\pi i \sum_1^N S^z_i]$ commute with H and because there are an odd number of sites, every eigenstate is degenerate. Suppose Ψ is an eigenstate of H and R_z so that $R_z\Psi = \pm i\Psi$ (the eigenvalues of R_z are $\pm i$ for an odd number of spins). Then $\Psi' \equiv R_x\Psi$ is distinct from Ψ because $R_z\Psi' = \mp i\Psi'$ and yet it is an energy eigenstate degenerate with Ψ.

$$\phi_k^{\mathrm{I}} = A_k \begin{pmatrix} 0 \\ \sin 2k \\ 0 \\ \sin 4k \\ \vdots \\ 0 \\ \sin Nk \end{pmatrix} \quad \text{and} \quad \psi_k^{\mathrm{I}} = -A_k \delta_k \begin{pmatrix} \sin Nk \\ 0 \\ \sin(N-2)k \\ 0 \\ \vdots \\ \sin 2k \\ 0 \end{pmatrix}, \tag{2.64a}$$

where

$$\delta_k = \text{sign of } \cos(N+1)k, \tag{2.64b}$$

$$\Lambda_k = [1 - (1-\gamma^2)\sin^2 k]^{\frac{1}{2}}, \tag{2.64c}$$

and A_k is the normalization constant,

$$A_k \equiv \left[\sum_{n=1}^{N/2} \sin^2 2nk\right]^{-\frac{1}{2}} = 2\left[N + 1 - \frac{\sin 2(N+1)k}{\sin 2k}\right]^{-\frac{1}{2}}. \tag{2.64d}$$

The k's are the roots of the equation

$$\sin(N+2)k/\sin Nk = (1-\gamma)/(1+\gamma) = -\lambda, \tag{2.64e}$$

which we discuss below. It can then be shown that

$$\Lambda_k = \cos k / |\cos(N+1)k|\,. \tag{2.64f}$$

The parameter λ, previously introduced in (2.43b), is a convenient alternate characterization of the anisotropy, the isotropic case corresponding to $\lambda = 1$ and the Ising limits being $\lambda = 0, \infty$.

Modes of the second kind:

$$\phi_k^{\mathrm{II}} = A_k \begin{pmatrix} \sin Nk \\ 0 \\ \sin(N-2)k \\ 0 \\ \vdots \\ \sin 2k \\ 0 \end{pmatrix} \quad \text{and} \quad \psi_k^{\mathrm{II}} = -A_k \delta_k \begin{pmatrix} 0 \\ \sin 2k \\ 0 \\ \sin 4k \\ \vdots \\ 0 \\ \sin Nk \end{pmatrix}, \tag{2.65a}$$

where δ_k, Λ_k, and A_k are as before, and the k's are the roots of the equation

$$\sin(N+2)k/\sin Nk = -1/\lambda. \tag{2.65b}$$

Assuming $\gamma > 0$, we represent the functions $\sin(N+2)k/\sin Nk$, λ, and $1/\lambda$ diagrammatically in Fig. 3. The roots of (2.64e) are of the form

$$k_m^{\mathrm{I}} = (\pi/N)(m - \nu_m^{\mathrm{I}}) + O(1/N^2), \qquad m = 1, \cdots, \tfrac{1}{2}N, \tag{2.66}$$

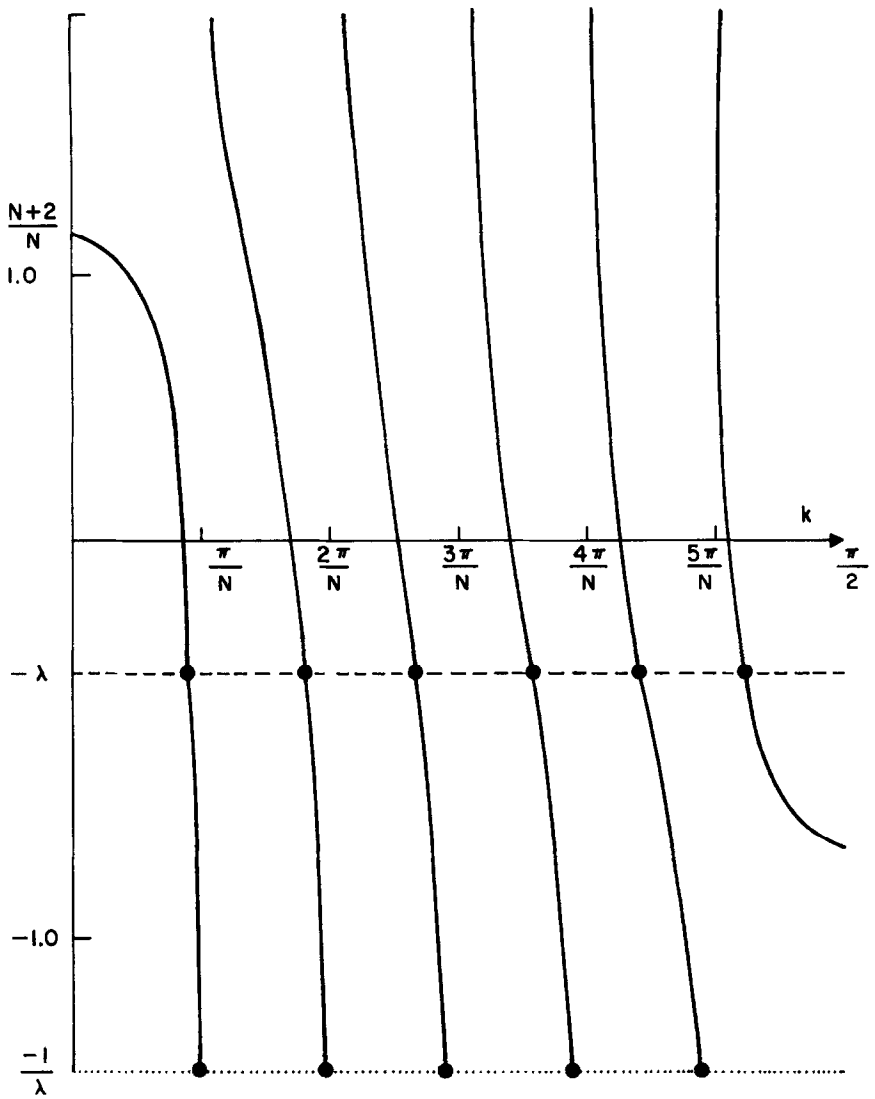

FIG. 3. Sin $(N+2)k/\sin Nk$ (continuous curve), $-\lambda$ (dashed line) and $-1/\lambda$ (dotted line) versus k for $N = 12$ and a typical value of λ. The intersections of these curves define the k^{I}'s and k^{II}'s in the XY model with free ends.

where $\nu_m{}^{\mathrm{I}}$, defined by

$$\cot \nu_m{}^{\mathrm{I}}\pi = [\lambda + \cos(2m\pi/N)]/\sin(2m\pi/N), \tag{2.67}$$

is found to be

$$\nu_m{}^{\mathrm{I}} = (m/N) + (1/\pi) \tan^{-1} [\gamma \tan(m\pi/N)]. \tag{2.67'}$$

Similarly, the *real* roots of (2.65b) are of the form

$$k_m^{\mathrm{II}} = (\pi/N)(m - \nu_m^{\mathrm{II}}) + O(1/N^2), \qquad m = 1, \cdots, \tfrac{1}{2}N - 1, \quad (2.68)$$

where

$$\nu_m^{\mathrm{II}} = (m/N) - (1/\pi)\tan^{-1}[\gamma \tan(m\pi/N)]. \quad (2.69)$$

There is also one complex root of (2.65b) which is very important:

$$k_0 = (\pi/2) + iv, \quad (2.70)$$

where v is the solution of

$$\cosh 2v + \coth Nv \sinh 2v = 1/\lambda. \quad (2.71)$$

In the zeroth approximation, we may set $\coth NV = 1$, so that

$$e^{2v} = 1/\lambda = (1 + \gamma)/(1 - \gamma). \quad (2.72)$$

In the next approximation

$$e^{2v} = 1/\lambda - (1 - \lambda^2)\lambda^{N-1} = \left(\frac{1+\gamma}{1-\gamma}\right) - \frac{4\gamma}{(1+\gamma)^2}\left(\frac{1-\gamma}{1+\gamma}\right)^{N-1}. \quad (2.72')$$

The ϕ and ψ vectors for this special mode are

$$\phi_{k_0} = A_{k_0}\begin{pmatrix} \sinh Nv \\ 0 \\ \vdots \\ (-1)^{\frac{1}{2}N-2}\sinh 4v \\ 0 \\ (-1)^{\frac{1}{2}N-1}\sinh 2v \\ 0 \end{pmatrix}$$

$$\text{and } \psi_{k_0} = (-1)^{\frac{1}{2}N+1}\begin{pmatrix} 0 \\ (-1)^{\frac{1}{2}N-1}\sinh 2v \\ 0 \\ (-1)^{\frac{1}{2}N-2}\sinh 4v \\ 0 \\ \vdots \\ 0 \\ \sinh Nv \end{pmatrix}, \quad (2.73a)$$

where

$$A_{k_0}^2 = 4\left[\frac{\sinh 2(N+1)v}{\sinh 2v} - N - 1\right]^{-1}$$
$$\simeq 4(1 - \lambda^2)\lambda^N = 16(\gamma/(1+\gamma)^2)\left(\frac{1-\gamma}{1+\gamma}\right)^N. \quad (2.73b)$$

This exhausts the normal modes because, for any mode with k' in $(\frac{1}{2}\pi, \pi)$, there is a mode with $k = \pi - k'$ that differs from the first only by a sign.

It is obvious from (2.64c) that $\Lambda_k > 0$ for all real k's. It is also readily seen that for the special mode k_0

$$\Lambda_{k_0} \simeq (1 + \lambda)\lambda^{N/2} = [2/(1 + \gamma)]\,[(1 - \gamma)/(1 + \gamma)]^{\frac{1}{2}N}. \tag{2.73c}$$

Thus, although the ground state is, strictly speaking, nondegenerate for any finite N, it becomes degenerate with the state carrying the k_0 excitation in the limit $N \to \infty$. It is observed in the next section that these two states have the same end-to-end order to $O(1/N)$. In terms of the customary definition of long-range order, the preponderance of spins up on one sublattice to spins up on the other, neither of these states shows any long-range order, if by "spins up" we mean spins in the x-direction. However, a linear combination of these two states in equal proportions will show a long-range order according to the customary definition.

We can now compute the various relevant G functions, recalling that $G_{ij} = -\sum_k \psi_{ki}\phi_{kj}$:

$$G_{1N} = \sum_{k^{\mathrm{I}}} A_k^{\,2}\,\delta_k \sin^2 Nk, \tag{2.74a}$$

$$G_{N1} = \sum_{k^{\mathrm{II}}\ \mathrm{real}} A_k^{\,2}\,\delta_k \sin^2 Nk + A_{k_0}^2\,(-1)^{\frac{1}{2}N} \sinh^2 Nv. \tag{2.74b}$$

Except for the factor δ_k, the summands in (2.74) are slowly varying functions of k, as shown in Appendix D, and each term is $O(1/N)$. The factor δ_k alternates in sign, the first δ_k being -1, etc. Thus a pair of consecutive terms in the summand is approximately

$$(d/dm)\,(A_{k_m}^2 \sin^2 Nk_m)$$

and the sums go over to Riemann integrals:

$$\tfrac{1}{2}\int_0^{\frac{1}{2}N} (d/dm)(A_{k_m}^2 \sin^2 Nk_m)\,dm = O(1/N). \tag{2.75}$$

Finally we have

$$G_{1N} = O(1/N), \tag{2.76a}$$

$$\begin{aligned} G_{N1} = A_{k_0}^2\,(-1)^{\frac{1}{2}N} \sinh^2 Nv + O(1/N) \\ = (-1)^{\frac{1}{2}N}\,(1 - \lambda^2) + O(1/N). \end{aligned} \tag{2.76b}$$

To calculate the end-to-end order in the ground state using (2.59), we note that

$$\det(\mathbf{A} - \mathbf{B}) = (-1)^{\frac{1}{2}N}\,(1 - \gamma^2)^{\frac{1}{2}N}. \tag{2.77}$$

so that

$$\rho_{1N}^{x} = -\tfrac{1}{4}(-1)^{\frac{1}{2}N} G_{N1} \tag{2.78a}$$

and

$$\rho_{1N}^{y} = -\tfrac{1}{4}(-1)^{\frac{1}{2}N} G_{1N} . \tag{2.78b}$$

Because $G_{1N} = O(1/N)$, only ρ_{1N}^{x} of the order parameters is finite for $\gamma > 0$ as $N \to \infty$.

$$\rho_{1N}^{x} = -\tfrac{1}{4}(1 - \lambda^2) + O(1/N) = -[\gamma/(1 + \gamma)^2] + O(1/N). \tag{2.79}$$

The ground state of the one-dimensional XY model thus shows no end-to-end order in the isotropic case, but a finite end-to-end order for any finite amount of anisotropy.

As anticipated, we see explicitly that the various contributions to the order parameter are nonanalytic functions of γ at $\gamma = 0$. The limiting contribution $\rho_{1\infty}^{x}$, for example, is finite for $\gamma > 0$ but zero for $\gamma < 0$.

As we have already remarked, the order ρ_{1N}^{x} may differ from $\lim_{n\to\infty} \rho_n{}^{x}$ obtained for the cyclic chain because of end effects. To see how important these effects are, it is useful to compute the order between two spins situated near but not at the two ends of the chain. Somewhat simpler is the "end-to-almost-end" order calculated between the qth spin and the Nth spin, where q is small. Just as ρ_{1N}^{x} can be expressed with a 1×1 determinant, ρ_{qN}^{x} can be expressed with a $q \times q$ determinant as we now show.

$$\begin{aligned}
\rho_{qN}^{x} &= \tfrac{1}{4} \langle \Psi_0 \mid (a_q^{\dagger} + a_q)(a_N^{\dagger} + a_N) \mid \Psi_0 \rangle, \\
&= \tfrac{1}{4} \left\langle \Psi_0 \middle| \exp\left(i\pi \sum_{1}^{q-1} c_j^{\dagger} c_j \right)(c_q^{\dagger} + c_q)(c_N^{\dagger} + c_N) \exp\left(i\pi \sum_{1}^{N-1} c_j^{\dagger} c_j \right) \middle| \Psi_0 \right\rangle, \\
&= \tfrac{1}{4} \langle \Psi_0 \mid A_1 B_1 A_2 B_2 \cdots A_{q-1} B_{q-1} A_q B_N e^{i\pi \mathfrak{N}} \mid \Psi_0 \rangle.
\end{aligned} \tag{2.80}$$

But according to (2.61),

$$\exp(i\pi \mathfrak{N}) \mid \Psi_0 \rangle = (\det \mathbf{A} / \mid \det \mathbf{A} \mid) \mid \Psi_0 \rangle = (-1)^{\frac{1}{2}N} \mid \Psi_0 \rangle. \tag{2.81}$$

The evaluation of ρ_{qN}^{x} now gives, using Wick's theorem,

$$\rho_{qN}^{x} = \frac{(-1)^q (-1)^{\frac{1}{2}N}}{4} \begin{vmatrix} G_{11} & G_{12} & \cdots & G_{1q} \\ G_{21} & G_{22} & \cdots & G_{2q} \\ \vdots & \vdots & & \vdots \\ G_{q-1,1} & G_{q-1,2} & & G_{q-1,q} \\ G_{N1} & G_{N2} & & G_{Nq} \end{vmatrix} . \tag{2.82}$$

ρ_{qN}^{y} is obtained by letting $G_{ij} \to G_{ji}$. It should be borne in mind that the G_{ij}'s are now calculated for the chain with free ends; they are not the G_{ij}'s discussed

in the last section. We introduce the notation G^f_{ij} and G^c_{ij} for the free chain and cyclic chain, respectively. Then there are simple relations, proved in Appendix E, between the two kinds of G's provided $|i-j| = o(N)$.

$$G^f_{ij} = G^c_{i-j} - G^c_{i+j} \qquad \text{for } i \text{ odd}, j \text{ even}; \tag{2.83a}$$

$$G^f_{ij} = G^c_{i-j} - G^c_{-(i+j)} \qquad \text{for } i \text{ even}, j \text{ odd}; \tag{2.83b}$$

$$G^f_{ij} = 0 \qquad \text{for } i-j \text{ even}. \tag{2.83c}$$

The determinant in (2.82) can be simplified in two ways. First recall that

$$\rho^x_{1N} = -\tfrac{1}{4}(-1)^{\frac{1}{2}N} G^f_{N1} \tag{2.78a}$$

and observe that if j is odd and $j = o(N)$,

$$G^f_{Nj} = (-1)^{\frac{1}{2}(j-1)} \lambda^{j-1}, \tag{2.84}$$

so that (2.82) simplifies to

$$\rho^x_{qN} = (-1)^{q-1} \rho^x_{1N} \begin{vmatrix} G^f_{11} & \cdots & G^f_{1q} \\ \vdots & & \\ G^f_{q-1,1} & \cdots & G^f_{q-1,q} \\ 1 \;\; 0 & -\lambda^2 \;\; 0 \;\; \lambda^4 & \cdots \end{vmatrix}. \tag{2.85}$$

Second, because of (2.83), the determinant can be simplified in analogy with (2.45a, b) giving

$$\rho^x_{2q,N} = (-1)^{q+1} S_q T_q \rho^x_{1N}, \tag{2.86a}$$

$$\rho^x_{2q-1,N} = (-1)^{q+1} S_q T_{q-1} \rho^x_{1N}, \tag{2.86b}$$

where

$$T_q = \begin{vmatrix} G^f_{12} & G^f_{14} & \cdots & G^f_{1,2q} \\ G^f_{32} & G^f_{34} & \cdots & G^f_{3,2q} \\ \vdots & \vdots & & \vdots \\ G^f_{2q-1,2} & G^f_{2q-1,4} & \cdots & G^f_{2q-1,2q} \end{vmatrix} \tag{2.87a}$$

and

$$S_q = \begin{vmatrix} G^f_{21} & G^f_{23} & \cdots & G^f_{2,2q-1} \\ G^f_{41} & G^f_{43} & \cdots & G^f_{4,2q-1} \\ \vdots & & & \vdots \\ G^f_{2q-2,1} & & \cdots & G^f_{2q-2,2q-1} \\ 1 & (i\lambda)^2 & \cdots & (i\lambda)^{2q-2} \end{vmatrix}. \tag{2.87b}$$

Numerical evaluation of ρ^x_{qN}/ρ^x_{1N} for $\gamma = 0.10102$ and $q = 2, 3, \cdots, 7$ shows a rapid convergence to a value differing by only a few percent from unity; but surprisingly, the order does not increase in absolute value monotonically as q increases.

E. Order in Excited States and at Finite Temperatures

The order parameters in excited states are given by simple modifications of (2.33). For example, the state with the elementary excitations $k_1, \cdots, k_s$ excited can be regarded as the vacuum state of a new set of η_k operators, where η_k and $\eta_k^\dagger$ are interchanged for $k_1, \cdots, k_s$. For these k's, this is equivalent to letting $\psi_{ki} \to -\psi_{ki}$ and $\Lambda_k \to -\Lambda_k$. Instead of (2.32c) we have

$$G_{ij}(k_1 \cdots k_s) = -\sum_{k \text{ unexc.}} \psi_{ki}\phi_{kj} + \sum_{k \text{ exc.}} \psi_{ki}\phi_{kj}. \tag{2.88}$$

Because s of the Λ_k's now are negative,

$$\det \mathbf{G}(k_1 \cdots k_s) = (-1)^s \det \mathbf{G}. \tag{2.89}$$

For the cyclic chain, the change of sign of a few of the terms contributing to G_{ij}, as given in (2.88) has a negligible effect on G_{ij}, because each term is $O(1/N)$. Thus in very low-lying excited states, the order between spins a fixed distance apart, (as $N \to \infty$) is the same as in the ground state, although this in itself does not imply long-range order at finite temperatures. For the end-to-end order in the chain with free ends, the sign of the order is changed with each additional excitation (except for k_0) because det $\mathbf{G}$ changes sign, so that at finite temperatures the end-to-end order vanishes. It is interesting to note, however, that for the one extremely low-lying excitation k_0, *both* det $\mathbf{G}$ *and* G_{N1} change sign so that this very low-lying excited state has the same end-to-end order as the ground state, to order $O(1/N)$.

The systematic generalization to finite temperatures of the treatment of order using Wick's theorem is simply achieved by introducing temperature-dependent contractions (*16*):

$$\langle B_i A_j \rangle = \operatorname{tr}[B_i A_j \exp(-\beta H_\gamma)]/\operatorname{tr} \exp(-\beta H_\gamma) \equiv G_{ij}(\beta). \tag{2.90}$$

The explicit evaluation of G_{ij} at finite temperatures is given in Appendix C. In matrix notation

$$\mathbf{G}(\beta) = -\boldsymbol{\psi}^T \tanh(\tfrac{1}{2}\beta\boldsymbol{\Lambda})\boldsymbol{\phi}. \tag{2.91}$$

$G(\beta)$ is no longer a unitary matrix. In fact, the norm of the entire ith row is

$$d_{i,N}(\beta) = \left[\sum_{j=1}^{N} (G_{ij}(\beta))^2\right]^{\frac{1}{2}} \leqq \tanh(\tfrac{1}{2}\beta\Lambda_{\max}) < 1. \tag{2.92}$$

Thus, even though $G_{i-j}(\beta) \sim A(\beta)/(i-j)^4$ for *all*[6] γ, the long-range order is zero at any finite temperature by Hadamard's theorem. In fact

$$\rho_n{}^x \leqq \tfrac{1}{4} \tanh^n \tfrac{1}{2}\beta \underset{n\to\infty}{\to} 0 \tag{2.93}$$

because

$$\Lambda_{\max} = 1,$$

and similarly for $\rho_n{}^y$.

F. Relationship between Heisenberg and XY Models

It is unfortunately not obvious that the Heisenberg model shows either a stronger or weaker tendency to order than the XY model. On the one hand, one might argue that the Heisenberg model, in which all three components of the spin want to align antiparallel, should show more order than the XY model, in which only two components have this tendency. Equivalently, because the ordering effect of the transverse terms alone in the Heisenberg model is less than that of the transverse terms alone in the XY model, one might conclude that the disordering effect is also correspondingly less in the Heisenberg model. On the other hand, one might argue with perhaps equal justification that the disordering tendency of the transverse terms in the Heisenberg model is greater, there being twice as many such terms. We have so far been unable to show rigorously that either model has a stronger tendency to long-range order than the other.

Lacking a general theorem, it is most interesting for heuristic reasons to consider a simple soluble but nontrivial special case: a chain of six spin $\frac{1}{2}$'s in both the isotropic Heisenberg and isotropic XY models.[7]

For the Heisenberg model a direct diagonalization of the Hamiltonian matrix among the sixty-four possible states is greatly simplified by the knowledge that the ground state is a singlet. It can be further simplified because under reversal of the ordering of the six sites, one of the five singlets of such a chain is even and four (including the ground state) are odd. Diagonalizing the resulting 4×4 matrix, one finds for the ground state

$$\begin{aligned}\Psi_0 = {} & 0.635\,\Phi_{135} - 0.436(\Phi_{136} + \Phi_{235}) - 0.336\,\Phi_{145} \\ & - 0.186(\Phi_{125} + \Phi_{134}) + 0.114(\Phi_{126} + \Phi_{234}) + 0.086\,\Phi_{124} - 0.014\,\Phi_{123}\,,\end{aligned} \tag{2.94}$$

where

$$\Phi_{ijk} = 2^{-\frac{1}{2}}(a_i{}^\dagger a_j{}^\dagger a_k{}^\dagger - a_{6-i}^\dagger a_{6-j}^\dagger a_{6-k}^\dagger)\Phi_0 \tag{2.95}$$

[6] The asymptotic behavior is given by (2.41) with $f(k) \to f(k;\beta) \equiv f(k) \times \tanh \frac{1}{2}\beta\Lambda_k$. It is observed that $f'(0;\beta) = f'(\pi/2;\beta) = 0$ even for $\gamma = 0$, when $\beta \neq 0$ (see footnote 4).

[7] The four-spin problem, though nontrivial, shows too large end effects to be interesting.

and Φ_0 is the state with all spins down.

For the XY model one can specialize the general formalism developed in Section II D to the case $N = 6$. One finds

$$k_m^{\mathrm{I}} = k_m^{\mathrm{II}} = m\pi/7, \tag{2.96}$$

which gives the following G matrix:

$$\mathsf{G} = \begin{pmatrix} 0 & -0.875 & 0 & 0.388 & 0 & -0.300 \\ -0.875 & 0 & -0.485 & 0 & 0.087 & 0 \\ 0 & -0.485 & 0 & -0.774 & 0 & 0.388 \\ 0.388 & 0 & -0.774 & 0 & -0.485 & 0 \\ 0 & 0.087 & 0 & -0.485 & 0 & -0.875 \\ -0.300 & 0 & 0.388 & 0 & -0.875 & 0 \end{pmatrix}. \tag{2.97}$$

The various order parameters may be computed for the Heisenberg model directly from the ground state. ρ_{ij}^z is the simplest to compute; ρ_{ij}^x and ρ_{ij}^y have the same value because Ψ_0 is a singlet. For the XY model the various order parameters may be computed from the appropriate subdeterminants of G. In Table II we exhibit the order parameter ρ_{1j}^x between the first spin and each of the other five. It is immediately clear that the XY model has a stronger tendency to order except for neighboring spins.

The parameter ρ_{1j}^x for the six-spin problem differs from its value when spin $\aleph 1$ is in the middle of an infinite chain because of end effects from both ends. To see the effects of each end for the XY model, we have also tabulated ρ_{1j}^x for a semi-infinite chain (i.e., spin $\aleph 1$ is at one end but the chain is infinitely long) and for an infinite chain (i.e., both the first and jth spins are far from either end). The results for the semi-infinite chain show that the end at the sixth site has a very small effect on the order ρ_{1j}^x; while the results for the infinite chain show that the fact that spin $\aleph 1$ is at an end position has a noticeable but not dominating effect for the six-spin and semi-infinite cases. The results strongly suggest that as $j \to \infty$, ρ_{1j}^x for the semi-infinite and infinite Heisenberg models is dominated by the corresponding parameter for the XY models, which we know

TABLE II

ρ_{1j}^x FOR $j = 2, \ldots, 6$ IN VARIOUS ONE-DIMENSIONAL MODELS

j	2	3	4	5	6
Heis.: 6 spins	−0.222	0.064	−0.077	0.032	−0.047
XY: 6 spins	−0.219	0.106	−0.105	0.065	−0.075
XY: Semi-infinite	−0.212	0.108	−0.102	0.075	−0.077
XY: Infinite	−0.159	0.101	−0.086	0.073	−0.066

TABLE III

$\rho^x_{j,j+1}$ FOR SEVERAL j IN VARIOUS ONE-DIMENSIONAL MODELS

j	1	2	3	∞	$\frac{1}{4}(\rho^x_{12} + 2\rho^x_{23} + \rho^x_{34})$
Heis.:					
6 spins	−0.222	−0.092	−0.202		−0.152
Semi-infinite				−0.148	
XY:					
6 spins	−0.219	−0.121	−0.193		−0.163
Semi-infinite	−0.212	−0.127	−0.182	−0.159	−0.162

tends to zero; i.e., *the isotropic Heisenberg model appears to have vanishing long-range order.*

The end effects on the nearest neighbor order $\rho^x_{j,j+1}$ can also be examined on the basis of values given in Table III. We have exhibited only the cases $j = 1, 2, 3$ because j and $6 - j$ are equivalent for this parameter. We see that for both models the nearest neighbor order oscillates strongly because j is near a free end. However, the effects of the farther end are seen to be small. Furthermore, if the simplest imaginable extrapolation from the six-spin problem is made, a good estimate of the true short-range order in an infinite chain is obtained for both models. Calculations of $\rho^x_{j,j+2}$ and $\rho^x_{j,j+3}$, as well as analogous calculations for the total order parameter, ρ_{ij}, all agree with these conclusions, so they are not exhibited.

III. THE HEISENBERG-ISING MODEL

A. FORMULATION OF GROUND-STATE PROBLEM

The second model consists of $2N$ spin $\frac{1}{2}$'s also arranged in a row and having only nearest neighbor interactions. The interactions are alternately Ising and isotropic Heisenberg interactions, so that the Hamiltonian for a chain with free ends is

$$\begin{aligned} H_\lambda &= \sum_1^N \mathbf{S}_{2i-1}\cdot\mathbf{S}_{2i} + 2\lambda \sum_1^{N-1} S^z{}_{2i}\mathbf{S}^z{}_{2i+1} \\ &= H_0 + H_1 . \end{aligned} \tag{3.1}$$

The parameter λ is to be considered variable but positive and characterizes the relative strength of the two types of interaction.[8]

The particular simplicity of this Hamiltonian is noticed if the representation diagonalizing H_0 is introduced. For the ith pair of spins we introduce the four eigenfunctions of $\mathbf{S}_{2i-1}\cdot\mathbf{S}_{2i}$:

[8] The symbol λ is chosen because this parameter appears in many expressions in exactly the same way as does λ for the XY model. In both models, λ ranges from 0 to ∞.

$$\Phi^i_{11} = \uparrow\uparrow, \qquad \Phi^i_{1-1} = \downarrow\downarrow,$$
$$\Phi^i_{10} = \frac{1}{\sqrt{2}}(\downarrow\uparrow + \uparrow\downarrow), \quad \text{and} \quad \Phi^i_{00} = \frac{1}{\sqrt{2}}(\downarrow\uparrow - \uparrow\downarrow); \tag{3.2}$$

where the first and second arrows refer to the $(2i-1)$st and $2i$th spins, respectively, and represent states of a single spin in the positive and negative z-direction. The first subscript of Φ^i refers to the quantum number J_i and the second to M_i for the ith pair. Application of either $S^z_{2i-2}\,S^z_{2i-1}$ or $S^z_{2i}\,S^z_{2i+1}$ to any of these four states leaves the values of M_i unchanged. Thus the assignment of one of the three possible values $(\pm 1, 0)$ to each of the N M_i's defines a subspace of the 2^{2N} dimensional space of all states. The Hamiltonian, having no matrix components between states in different subspaces, can be diagonalized separately in each. It will be shown in Section III E that the ground state is in the subspace for which $M_i = 0$ for all i, a subspace we now consider.

We are faced with a situation that is formally similar to that encountered in the XY model: a set of dynamical systems (in this case a pair of spins) each having two possible states (in this case Φ_{10} and Φ_{00}) and interacting only with the nearest neighbor systems. If we call the states Φ^i_{10} the "up" states and Φ^i_{00} the "down" states, we can formally introduce raising and lowering operators for the ith pair having the usual properties:

$$a_i^\dagger \Phi^i_{00} = \Phi^i_{10}, \qquad a_i^\dagger \Phi^i_{10} = 0, \tag{3.3a}$$

and

$$a_i \Phi^i_{00} = 0, \qquad a_i \Phi^i_{10} = \Phi^i_{00}, \tag{3.3b}$$

so that

$$\{a_i, a_i^\dagger\} = 1 \quad \text{and} \quad a_i^2 = a_i^{\dagger 2} = 0. \tag{3.4}$$

It is to be emphasized that a_i and $a_i^\dagger$ do not lower and raise a particular spin as they did for the XY model. It is only a *formal* analogy between the states Φ^i_{10} and Φ^i_{00} on the one hand, and the up and down orientations of a single spin $\frac{1}{2}$ that we are exploiting.

Because of the fundamental relations

$$S^z_{2i-1}\Phi^i_{10} = -\Phi^i_{00}, \qquad S^z_{2i-1}\Phi^i_{00} = -\Phi^i_{10} \tag{3.5a}$$

and

$$S^z_{2i}\Phi^i_{10} = \Phi^i_{00}, \qquad S^z_{2i}\Phi^i_{00} = \Phi^i_{10}, \tag{3.5b}$$

we may represent S^z_{2i-1} and S^z_{2i} in the $M_i \equiv 0$ subspace by means of a_i and $a_i^\dagger$:

$$S^z_{2i-1} \to -\tfrac{1}{2}(a_i^\dagger + a_i); \qquad S^z_{2i} \to \tfrac{1}{2}(a_i^\dagger + a_i). \tag{3.6}$$

Because the diagonal energies of the states Φ_{10}^i and Φ_{00}^i are, respectively, $\frac{1}{4}$ and $-\frac{3}{4}$, the ith term in H_0 can also be expressed in terms of a_i and $a_i^\dagger$:

$$\mathbf{S}_{2i-1}\cdot\mathbf{S}_{2i} \rightarrow a_i^\dagger a_i - \tfrac{3}{4}. \tag{3.7}$$

In the subspace defined by $M_i \equiv 0$, the total Hamiltonian is then

$$H_\lambda = -\tfrac{3}{4}N + \sum_1^N a_i^\dagger a_i - \tfrac{1}{2}\lambda\sum_1^{N-1}(a_i^\dagger + a_i)(a_{i+1}^\dagger + a_{i+1}), \tag{3.8}$$

where, in addition to (3. 4), we have

$$[a_i,a_j] = [a_i^\dagger,a_j^\dagger] = [a_i,a_j^\dagger] = 0. \tag{3.9}$$

The eigenstates and associated energies of H_λ can be found exactly as for the XY model by introducing a complete set of Fermi operators, through (2.5), in terms of which H_λ is given by

$$H_\lambda = -\tfrac{3}{4}N + \sum_1^N c_i^\dagger c_i - \tfrac{1}{2}\lambda\sum_1^{N-1}(c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1}). \tag{3.10}$$

B. Ground State of the Cyclic Chain

It is convenient in this section to consider the "c-cyclic" case obtained by letting $\sum_1^{N-1} \rightarrow \sum_1^N$ in H_1 and defining

$$c_{N+1} \equiv c_1 \quad \text{and} \quad c_{N+1}^\dagger \equiv c_1\,. \tag{3.11}$$

The matrices relevant to the diagonalization of H_λ are then

$$\mathbf{A} - \mathbf{B} = \begin{pmatrix} 1 & & & -\lambda \\ -\lambda & 1 & \mathbf{0} & \\ & \cdot & \cdot & \\ & & \cdot & \cdot \\ & & & \cdot \\ \mathbf{0} & & -\lambda & 1 \end{pmatrix} = (\mathbf{A} + \mathbf{B})^T \tag{3.12}$$

and

$$(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B}) = \begin{pmatrix} 1+\lambda^2 & -\lambda & & & -\lambda \\ -\lambda & 1+\lambda^2 & -\lambda & \mathbf{0} & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & \mathbf{0} & & \cdot & \cdot \\ -\lambda & & & -\lambda & 1+\lambda^2 \end{pmatrix}. \tag{3.13}$$

For $\lambda \neq 1$ the normal modes are characterized by the functions

$$\phi_{kj} = \begin{cases} (2/N)^{\frac{1}{2}} \sin kj \\ (2/N)^{\frac{1}{2}} \cos kj \end{cases} \tag{3.14a}$$

and

$$\psi_{kj} = \Lambda_k^{-1}[(1 - \lambda \cos k)\phi_{kj} - \lambda \sin k\, \phi_{-kj}], \tag{3.14b}$$

belong to the eigenvalues

$$\Lambda_k = [(1 + \lambda)^2 - 4\lambda \cos^2 \tfrac{1}{2}k]^{\frac{1}{2}}, \tag{3.14c}$$

where

$$k = 2\pi m/N \tag{3.14d}$$

and

$$\begin{aligned} m &= -\tfrac{1}{2}N, \cdots, 0, \cdots, \tfrac{1}{2}N - 1 \quad \text{for } N \text{ even}, \\ m &= -\tfrac{1}{2}(N-1), \cdots, 0, \cdots \tfrac{1}{2}(N-1) \quad \text{for } N \text{ odd}. \end{aligned} \tag{3.14e}$$

We take the upper solution for ϕ_{kj} if $k > 0$, the lower solution if $k \leqq 0$. For $\lambda = 1$ and $m = 0$, we have $\Lambda_k = 0$. For this particular k,

$$\phi_{kj} = N^{-\frac{1}{2}}, \qquad \psi_{kj} = \pm N^{-\frac{1}{2}}. \tag{3.14'}$$

The sign, which is arbitrary, will be taken positive.

It is convenient to introduce the parameter γ, ranging from $+1$ to -1, by

$$\gamma = (1 - \lambda)/(1 + \lambda); \tag{3.15}$$

then

$$\Lambda_k = (1 + \lambda)\,[1 - (1 - \gamma^2)\cos^2 \tfrac{1}{2}\, k]^{\frac{1}{2}}, \tag{3.16}$$

which resembles the spectrum of the XY model.

We see that except for $\lambda = 1$ or $\gamma = 0$ the spectrum of elementary excitations has an energy gap. It should be emphasized, however, that the ground state together with states of all possible combinations of these elementary excitations are but a small subset of the complete set of stationary states, all the rest having one or more $M_i = \pm 1$. Thus, the behavior of the system for finite temperatures is not immediately apparent from the knowledge of the excitation spectrum (3.14c).

The ground-state energy, according to (A-12) is

$$E_0 = -\tfrac{3}{4}N + \tfrac{1}{2}\left(\sum_1^N 1 - \sum_k \Lambda_k\right). \tag{3.17}$$

As $N \to \infty$,

$$E_0/N = -\tfrac{1}{4} - (2/\pi)[1/(1 + \gamma)]\, \mathcal{E}(1 - \gamma^2). \tag{3.18}$$

We notice that E_0/N is not analytic at $\lambda = 1$ ($\gamma = 0$) although it has power

series expansions in λ and $1/\lambda$. This nonanalytic behavior at $\lambda = 1$ is associated with the appearance of long-range order for $\lambda > 1$ as we now show.

C. Short- and Long-Range Order in the Ground State

Define the order parameter in the ground state between pair sites l and m to be

$$\rho_{lm} = \langle \Psi_0 \mid \mathbf{S}_{2l} \cdot \mathbf{S}_{2m} \mid \Psi_0 \rangle; \tag{3.19}$$

i.e., it is the order between the second spin of each pair. The order between other pairs of spins can be calculated from ρ_{lm} because

$$\langle \Psi_0 \mid \mathbf{S}_{2l} \cdot \mathbf{S}_{2m-1} \mid \Psi_0 \rangle = - \langle \Psi_0 \mid \mathbf{S}_{2l} \cdot \mathbf{S}_{2m} \mid \Psi_0 \rangle, \quad \text{etc.} \tag{3.20}$$

Furthermore, the only nonzero contribution to ρ_{lm} is

$$\rho^z_{lm} = \langle \Psi_0 \mid S^z_{2l} S^z_{2m} \mid \Psi_0 \rangle = \tfrac{1}{4} \langle \Psi_0 \mid (a_l^\dagger + a_l)(a_m^\dagger + a_m) \mid \Psi_0 \rangle, \tag{3.21}$$

because S^x_{2l} and S^y_{2l} both change M_l and S^x_{2m} and S^y_{2m} both change M_m. The structure of ρ^z_{lm} is identical with the structure of ρ^x_{lm} for the XY model, so that ρ^z_{lm} is given by the determinant (2.33a) with G_{ij} defined by (2.32c).

For the cyclic chain, $G_{ij} = G_{i-j}$ and in the limit $N \to \infty$ with $r = i - j$ fixed, G_r is found to be given by

$$G_r = (-1)^{r+1} [\tfrac{1}{2}(1 + \gamma) L_{2r}(\gamma) + \tfrac{1}{2}(1 - \gamma) L_{2r+2}(\gamma)], \tag{3.22}$$

where $L_r(\gamma)$ is defined in (2.83b). For the special case of vanishing energy gap, $\lambda = 1$ or $\gamma = 0$,

$$G_r = (2/\pi) [(-1)^{r+1}/(2r + 1)]. \tag{3.23a}$$

For the limiting case of noninteracting Heisenberg pairs,

$$G_r = -\delta_{r0}. \tag{3.23b}$$

In the limit $\lambda \to \infty$ or $\gamma = -1$, which we shall later show to be the Ising limit,

$$G_r = \delta_{r,-1}. \tag{3.23c}$$

In general, for $\lambda \neq 1$,

$$| G_r | < A r^{-4} \quad \text{for} \quad | r | > r_0, \tag{3.24}$$

just as in the XY model.

Hadamard's theorem is sufficient to show that there is no long-range order for $\lambda = 1$, because of the r^{-1} behavior of G_r. For $\lambda \neq 1$, Hadamard's theorem is again too weak, because of the r^{-4} dependence. In the limiting cases $\lambda = 0$ and $\lambda \to \infty$, however, there is no order and perfect order, respectively. This suggests that for $\lambda \leqq 1$ there is no long-range order and for $\lambda > 1$ there is finite long-range

order, a conjecture that is confirmed for the end-to-end order of a free chain, which we now investigate.

D. End-to-End Order in the Ground State

For a chain of N pairs, the order between the first and last pairs, as in (2.59a) is

$$\rho^z_{1N} = -\tfrac{1}{4} G_{N1} \det (\mathbf{A} - \mathbf{B}) / |\det (\mathbf{A} - \mathbf{B})| \tag{3.25}$$

providing $\lambda \neq 1$ (to ensure $\Lambda_k \neq 0$). If the chain has free ends,

$$\mathbf{A} - \mathbf{B} = \begin{pmatrix} 1 & & & \\ -\lambda & 1 & & \mathbf{0} \\ & \cdot & \cdot & \\ & & \cdot & \cdot \\ & \mathbf{0} & -\lambda & 1 \end{pmatrix} = (\mathbf{A} + \mathbf{B})^T, \tag{3.26}$$

so that

$$\det (\mathbf{A} - \mathbf{B}) = 1 \quad \text{and} \quad \rho^z_{1N} = -\tfrac{1}{4} G_{N1}\,. \tag{3.27}$$

The functions ϕ_{kj} and ψ_{kj} needed to compute G_{N1} are found to be

$$\phi_{kj} = A_k \sin k(N + 1 - j) \quad \text{and} \quad \psi_{kj} = A_k \delta_k \sin kj, \tag{3.28a}$$

where

$$\delta_k = \text{sign of } \sin k/\sin kN. \tag{3.28b}$$

The corresponding eigenvalue is

$$\Lambda_k = [(1 + \lambda)^2 - 4\lambda \cos^2 \tfrac{1}{2}k]^{\frac{1}{2}}, \tag{3.28c}$$

and the normalization constant is

$$A_k = 2\{2N + 1 - [\sin (2N + 1)k]/\sin k\}^{-\frac{1}{2}}. \tag{3.28d}$$

The k's are the roots of

$$\sin k(N + 1)/\sin kn = \lambda. \tag{3.28e}$$

For these k's Λ_k reduces to

$$\Lambda_k = |\sin k/\sin Nk|. \tag{3.28f}$$

For $\lambda \leqq 1$, there are N real roots, exhausting the normal modes. For $\lambda > 1$, there are $N - 1$ real roots and one imaginary root,

$$k_0 = iv, \tag{3.29}$$

with v defined by

$$\sinh (N + 1)v/\sinh Nv = \lambda. \tag{3.30}$$

For $NV \gg 1$ [i.e., $\lambda - 1 \neq O(1/N)$],

$$e^{r} = \lambda - [(\lambda^2 - 1)/\lambda](1/\lambda)^{2N}. \tag{3.31}$$

For this particular mode

$$\phi_{k_0 j} = A_{k_0} \sinh (N + 1 - \mathrm{j})v \quad \text{and} \quad \psi_{k_0 j} = A_{k_0} \sinh jv, \tag{3.32a}$$

$$A_{k_0} = 2e^{-Nv}(1 - e^{-2v})^{\frac{1}{2}}, \tag{3.32b}$$

and

$$\Lambda_{k_0} = (\lambda^2 - 1)/\lambda^{N+1}. \tag{3.32c}$$

In evaluating $G_{N1} = -\sum \psi_{kN}\phi_{k1}$, we use the fact (proved in analogy with the XY model, Appendix D) that, except for the mode k_0 and the factor δ_k, the factors in the summand are slowly varying functions of k, and δ_k alternates in sign. Thus

$$G_{N1} = -\psi_{k_0 N}\,\phi_{k_0 1} + O(1/N) = -(1 - \lambda^{-2}) + O(1/N), \tag{3.33}$$

and

$$\begin{aligned} \rho_{1N} &= \tfrac{1}{4}(1 - \lambda^{-2}) + O(1/N), \qquad \lambda \geqq 1, \\ &= O(1/N), \qquad \lambda < 1. \end{aligned} \tag{3.34}$$

The order in the extremely low-lying excited state with the k_0 excitation present is the same as in the ground state to $O(1/N)$.

E. Excited States

In addition to the excited states produced with the creation operators $\eta_k^{\dagger}$, there are also all the states lying in subspaces characterized by one or more $M_i \neq 0$. Although it is possible to find states in these subspaces for which each of these M_i is definitely $+1$ or -1, it is much more convenient to work with certain linear combinations of these states. To see why this is, consider the subspace defined by

$$M_1 = 1 \quad \text{and} \quad M_i = 0, \qquad i \neq 1. \tag{3.35}$$

The Hamiltonian in this subspace corresponding to (3.10) is

$$\begin{aligned} H_\lambda = &-\tfrac{3}{4}(N - 1) + \sum_{2}^{N} c_i^{\dagger}c_i \\ &- \tfrac{1}{2}\lambda \sum_{2}^{N-1} (c_i^{\dagger} - c_i)(c_{i+1}^{\dagger} + c_{i+1}) - \tfrac{1}{2}\lambda(c_1^{\dagger} + c_1). \end{aligned} \tag{3.36}$$

Because this Hamiltonian is no longer purely quadratic in the c's and $c^\dagger$'s, it fails to conserve the number of fermions and cannot be diagonalized by a simple principal axis transformation. The difficulty is even greater if the $M = 1$ site is not at the left end, but at $i = p$; for then H_λ is

$$H_\lambda = -\frac{3}{4}(N-1) + \sum_{i\neq p} c_i^\dagger c_i - \frac{1}{2}\lambda \sum_{i\neq p-1,p} (c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1}) - \frac{1}{2}\lambda \Big[(c_{p-1}^\dagger - c_{p-1}) \exp\Big(i\pi \sum_1^{p-1} c_j^\dagger c_j\Big) + (c_{p+1}^\dagger + c_{p+1}) \exp\Big(i\pi \sum_1^{p} c_j^\dagger c_j\Big)\Big], \tag{3.36'}$$

which is obviously not directly diagonalizable.

The way around these difficulties is to consider the states with $M_p = \pm 1$ simultaneously, introducing raising and lowering operators $a_p^\dagger$ and a_p which take Φ_{1-1}^p into Φ_{11}^p and vice versa. The Hamiltonian is then a quadratic form in the a's and $a^\dagger$'s (including a_p and $a_p^\dagger$) which remains quadratic, and so is readily diagonalizable, when expressed in the c's and $c^\dagger$'s. The ground state (and all excited states) in this subspace must be doubly degenerate, corresponding to the two linearly independent combinations of Φ_{1-1}^p and Φ_{11}^p, and this must manifest itself in the fact that $\Lambda_k = 0$ for some k. Stationary states with $M_p = \pm 1$ can then be projected from any state if one is so inclined.

Let us consider this procedure more explicitly as generalized to the case of an arbitrary number of sites with $M = \pm 1$. In fact, let

$$|M_i| = 1 \quad \text{for} \quad i = p_1, p_2, \cdots, p_s$$

and (3.37)

$$M_i = 0 \quad \text{for} \quad i \neq p_1, p_2, \cdots, p_s.$$

The pairs at pair sites $p_1, \cdots, p_s$ can be considered as "impurity pairs" embedded in a perfect chain of $M = 0$ pairs. Each set of p's identifies a different subspace and now, because each impurity can also be in two states, all subspaces are still of dimension 2^N.

For an impurity pair at p, we introduce the "up" and "down" states

$$\Phi_+^p = \frac{1}{\sqrt{2}}(\Phi_{11}^p + \Phi_{1-1}^p) = \frac{1}{\sqrt{2}}(\uparrow\uparrow + \downarrow\downarrow), \tag{3.38a}$$

$$\Phi_-^p = \frac{1}{\sqrt{2}}(\Phi_{11}^p - \Phi_{1-1}^p) = \frac{1}{\sqrt{2}}(\uparrow\uparrow - \downarrow\downarrow), \tag{3.38b}$$

and the raising and lowering operators $a_p^\dagger$ and a_p :

$$a_p^\dagger \Phi_-^{\,p} = \Phi_+^{\,p}, \qquad a_p^\dagger \Phi_+^{\,p} = 0; \tag{3.39a}$$

$$a_p \Phi_-^{\,p} = 0, \qquad a_p \Phi_+^{\,p} = \Phi_-^{\,p}. \tag{3.39b}$$

Because

$$S^z_{2p-1}\Phi_+^{\,p} = S^z_{2p}\Phi_+^{\,p} = \tfrac{1}{2}\Phi_-^{\,p} \tag{3.40a}$$

and

$$S^z_{2p-1}\Phi_-^{\,p} = S^z_{2p}\Phi_-^{\,p} = \tfrac{1}{2}\Phi_+^{\,p}, \tag{3.40b}$$

we may represent S^z_{2p-1} and S^z_{2p} in this subspace by

$$S^z_{2p-1} = S^z_{2p} = \tfrac{1}{2}(a_p^\dagger + a_p). \tag{3.41}$$

The pth term in H_0 will be simply $\frac{1}{4}$. The interaction of the impurity at p with the $(p-1)$st pair is

$$\tfrac{1}{2}\lambda(a_{p-1}^\dagger + a_{p-1})(a_p^\dagger + a_p), \tag{3.42a}$$

whether the $(p-1)$st pair is an impurity or not. The interaction of the impurity at p with the $(p+1)$st pair is

$$\tfrac{1}{2}\lambda(a_p^\dagger + a_p)(a_{p+1}^\dagger + a_{p+1}) \tag{3.42b}$$

provided $p+1$ is an impurity, and it is

$$-\tfrac{1}{2}\lambda(a_p^\dagger + a_p)(a_{p+1}^\dagger + a_{p+1}) \tag{3.42c}$$

if $p+1$ is not an impurity.

To make all interactions look alike and the same as between two $M = 0$ pairs, it is convenient to introduce new canonical variables in the following way. We make the canonical transformation

$$a_i \to -a_i \quad \text{and} \quad a_i^\dagger \to -a_i^\dagger \tag{3.43}$$

for $p_1 \leqq i < p_2$, $p_3 \leqq i < p_4$, $p_5 \leqq i < p_6$, etc., but leave the other a's and $a^\dagger$'s unchanged. The Hamiltonian in this subspace is then

$$H_\lambda(p_1 \cdots p_s) = -\tfrac{3}{4}N + \varepsilon + \sum_{i \neq p_1, \cdots, p_s} a_i^\dagger a_i - \tfrac{1}{2}\lambda \sum_1^{N-1} (a_i^\dagger + a_i)(a_{i+1}^\dagger + a_{i+1}) \tag{3.44}$$

or simply

$$H_\lambda(p_1 \cdots p_s) = H_\lambda + \sum_{r=1}^{s} (1 - a_{p_i}^\dagger a_{p_i}), \tag{3.44'}$$

where H_λ is the Hamiltonian (3.8) for the case all $M_i = 0$. Although the a's and $a^\dagger$'s on impurity pair sites have a different meaning from the other a's and $a^\dagger$'s, they all have the same formal properties and so (3.44′) is a meaningful statement. It is now clear that the ground state lies in the subspace with no impurities, because if Ψ_0', with energy E_0', is the lowest energy state corresponding to a given set of s impurities, then

$$\left\langle \Psi_0' \middle| \sum_{i=1}^{s} (1 - a^\dagger_{p_i} a_{p_i}) \middle| \Psi_0' \right\rangle = s/2. \tag{3.45}$$[9]

Thus

$$E_0' = \langle \Psi_0' \mid H_\lambda \mid \Psi_0' \rangle + \tfrac{1}{2}s \geqq E_0 + \tfrac{1}{2}s, \tag{3.46}$$

showing that the ground state has all $M_i = 0$, as previously asserted.

We might mention at this point that, contrary to appearances, we have really included as much anisotropy as is possible, through the variability of λ. An apparent generalization that is still soluble would be to replace H_0 by

$$H_0' = \sum_{1}^{N} [\alpha_1(S^x_{2i-1}S^x_{2i} + S^y_{2i-1}S^y_{2i}) + \alpha_2 S^z_{2i-1}S^z_{2i}]. \tag{3.47}$$

The corresponding generalization of $H_\lambda(p_1 \cdots p_s)$ is

$$H_\lambda'(p_1 \cdots p_s) = \alpha_1 H_{\lambda/\alpha_1} - \tfrac{1}{4} N(\alpha_2 - \alpha_1) + \tfrac{1}{2}\alpha_2 s + \alpha_1 \sum_{i=1}^{s} (\tfrac{1}{2} - a^\dagger_{p_i} a_{p_i}). \tag{3.48}$$

We see that α_2 has no effect on the stationary states, its only effect being on the energy needed to create impurities. For any $\alpha_2 \geqq 0$, the ground state has no impurities. Only the ratio λ/α_1 has any effect on the wave functions. Thus, without loss of generality, we have chosen $\alpha_1 = \alpha_2 = 1$. Now, provided $\lambda > 0$, this choice of α_2 is exactly equivalent (for the ground-state wave function) to

[9] To prove this, note that the unitary transformation

$$U^{-1}a_{pi}U = a^\dagger_{pi} \quad \text{and} \quad U^{-1}a^\dagger_{pi}U = a_{pi} \quad \text{for all } i$$

leaves $H_\lambda(p_1 \cdots p_s)$ unchanged, i.e., $[H_\lambda(p_1 \cdots p_s), U] = 0$. It is thus possible to choose Ψ_0' to be an eigenstate of U as well as of $H_\lambda(p_1 \cdots p_s)$. Then

$$\langle \Psi_0' \mid a^\dagger_{pi}a_{pi} \mid \Psi_0' \rangle = \langle U\Psi_0' \mid a_{pi}a^\dagger_{pi} \mid U\Psi_0' \rangle = \langle \Psi_0' \mid (1 - a^\dagger_{pi}a_{pi}) \mid \Psi_0' \rangle$$

or

$$\langle \Psi_0' \mid a^\dagger_{pi}a_{pi} \mid \Psi_0' \rangle = \tfrac{1}{2} \quad \text{for} \quad i = 1, \cdots, s.$$

the choice $\alpha_2 = 2\lambda$. But with the second choice, $H_\lambda/2\lambda$ becomes the Ising Hamiltonian in the limit $\lambda \to \infty$. Thus the limit $\lambda \to \infty$ is also the Ising limit for the choice $\alpha_2 = \alpha_1 = 1$.

The introduction of impurities at pair sites $p_1, \cdots, p_s$ reduces the matrix $(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B})$ into a set of square blocks along the main diagonal of order $p_1, p_2 - p_1, \cdots, N - p_s$, corresponding to the dynamical independence of the different $M = 0$ segments of the chain. Any distribution of impurities can be solved, in principle, because of this independence. The particularly simple distributions of impurities are those in which the first impurity is at the extreme left and the last is at the extreme right, because for such distributions all the nontrivial square blocks have the same structure. It is then convenient to assume the chain has $N + 1$ pair sites and $s + 1$ impurities, the first being at $p_0 = 0$. Then

$$(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B}) = \begin{pmatrix} 0 & & & \\ & \mathbf{L}_{q_1} & & \mathbf{0} \\ & & \mathbf{L}_{q_2} & \\ \mathbf{0} & & & \ddots \\ & & & & \mathbf{L}_{q_s} \end{pmatrix}, \tag{3.49}$$

where

$$\mathbf{L}_q = \begin{pmatrix} 1+\lambda^2 & -\lambda & & \mathbf{0} \\ -\lambda & 1+\lambda^2 & -\lambda & \\ & \ddots & \ddots & \ddots \\ & & -\lambda & 1+\lambda^2 & \lambda \\ \mathbf{0} & & & -\lambda & \lambda^2 \end{pmatrix} \begin{matrix} \\ \\ \\ \\ q \text{ rows and columns} \end{matrix}, \tag{3.50}$$

and $q_i = p_i - p_{i-1}$, the "length" of the ith subchain (including the impurity at the right end, but not the one at the left when the ordering is from left to right).

Let us consider first the case with impurities only at the ends ($p_0 = 0$ and $q_1 = p_1 = N$). One normal mode is

$$\phi_0 = \begin{pmatrix} 1 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{pmatrix} \quad \text{and} \quad \psi_0 = \begin{pmatrix} 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ 1 \end{pmatrix} \tag{3.51a}$$

belonging to

$$\Lambda_0 = 0. \tag{3.51b}$$

The other normal modes are

$$\phi_k^{q_1} = A_k^{q_1} \begin{pmatrix} 0 \\ \sin k \\ \cdot \\ \cdot \\ \cdot \\ \sin q_1 k \end{pmatrix} \quad \text{and} \quad \psi_k^{q_1} = -A_k^{q_1}\, \delta_k^{q_1} \begin{pmatrix} \sin q_1 k \\ \cdot \\ \cdot \\ \cdot \\ \sin k \\ 0 \end{pmatrix} \tag{3.52a}$$

with Λ_k given by (3.14c) and

$$\delta_k^{q_1} = \text{sign of } \sin k / \sin\,(q_1 + 1)k. \tag{3.52b}$$

The k's are the roots of

$$\sin\,(q_1 + 1)k / \sin\, q_1 k = 1/\lambda, \tag{3.52c}$$

and so they, and the corresponding Λ_k's, depend on q_1. The excitation of the $\Lambda = 0$ mode corresponds to a reversal of the spins of both impurity pairs and hence of all intervening $M = 0$ pairs, which is why it costs no energy. The two degenerate "ground states" for the chain terminated by two impurity pairs are Ψ_{0-} and Ψ_{0+} defined by

$$\eta_k \Psi_{0-} = 0, \quad \text{all} \quad k, \tag{3.52d}$$

and

$$\eta_k \Psi_{0+} = 0, \qquad k \neq 0 \quad \text{and} \quad \eta_0^{\dagger} \Psi_{0+} = 0. \tag{3.52e}$$

For $\lambda < 1$, there is an imaginary root k_0 of (3.52c) which for $q_1 \to \infty$, has a vanishingly small excitation energy, $\Lambda_{k0} = (\lambda^{-2} - 1)\lambda^{q_1+1}$; but for $\lambda > 1$, there is an energy gap. The creation of the k_0 excitation reverses the relative orientation of the two impurity pairs, as shown in Appendix F. Thus, for $\lambda < 1$ and $q_1 \to \infty$, states with parallel and antiparallel impurity pair alignments have the same energy, a reflection of the absence of long-range order in the intervening $M = 0$ chain. For $\lambda > 1$, on the other hand, the state with antiparallel alignment lies lower in energy by a finite amount, a reflection of the presence of long-range order.

Consider now the same chain but extended to an impurity pair at p_2. In addition to the $\Lambda = 0$ mode, the normal modes are now of two kinds:

$$\phi_k^{q_1} = A_k^{q_1} \begin{pmatrix} 0 \\ \sin k \\ \sin 2k \\ \cdot \\ \cdot \\ \cdot \\ \sin q_1 k \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{pmatrix} \quad \text{and} \quad \psi_k^{q_1} = A_k^{q_1}\, \delta_k^{q_1} \begin{pmatrix} 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ \sin q_1 k \\ \cdot \\ \cdot \\ \cdot \\ \sin 2k \\ \sin k \\ 0 \end{pmatrix}, \tag{3.53}$$

with $\delta_k^{q_1}$ and k defined by (3.52b) and 3.52c); and

$$\phi_k^{q_2} = A_k^{q_2} \begin{pmatrix} 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ \sin k \\ \sin 2k \\ \cdot \\ \cdot \\ \cdot \\ \sin q_2 k \end{pmatrix} \quad \text{and} \quad \psi_k^{q_2} = A_k^{q_2}\, \delta_k^{q_2} \begin{pmatrix} \sin q_2 k \\ \cdot \\ \cdot \\ \cdot \\ \sin 2k \\ \sin k \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{pmatrix}, \tag{3.54}$$

with $\delta_k^{q_2}$ and k defined by the analogs of (3.52b) and (3.52c). Arguments similar to those in Appendix F can be used to show that in the lowest state, successive impurity pairs are aligned antiparallel. Any odd number of excitations of the left segment results in a parallel alignment of impurity pairs at p_0 and p_1; and similarly odd numbers of excitations of the right segment result in parallel alignment of pair sites p_1 and p_2. If $\lambda < 1$, and p_1 is far from one end, the k_0 excitation of this long segment gives the corresponding parallel alignment at a negligible cost of energy. But if $\lambda > 1$, these parallel alignments cost finite amounts of energy, a consequence of the long-range order.

The above discussion is obviously generalizable immediately to any number of impurities. For a chain of length $N + 1$, the lowest energy in a subspace characterized by the impurity pairs at $p_0 = 0, p_1, \cdots, p_{s-1}, p_s = N$, or by the chain segments $q_1, \cdots, q_s, \sum_1^s q_r = N$ is

$$E_0(q_1, \cdots, q_s) = -\frac{1}{4}(N-1) + \frac{1}{2}\sum_{r=1}^{s}\left[1 - \sum_{k(q_r)} \Lambda_k\right]. \tag{3.55}$$

The quantity $\frac{1}{2}[1 - \sum_{k(q)} \Lambda_k] \equiv \mathcal{U}(q)$ can be simply interpreted as the sum of the self-energy of an impurity embedded in an $M = 0$ chain and the interaction energy of this impurity with another one, q pair sites away. It can be more simply regarded, however, just as the energy of a chain segment (with an impurity at the right end) of length q; the entire chain is then a collection of noninteracting segments, arbitrary in number, obeying only the constraint $\sum_1^s q_r = N$.

F. Statistical Mechanics

To evaluate the partition sum of the Heisenberg–Ising model, we first evaluate it for all the internal degrees of freedom in each segment, which leads to a temperature dependent $\mathcal{U}(q)$:

$$\exp\left[-\beta\mathcal{U}(q;\beta)\right] \equiv \prod_{k(q)} (1 + \exp(-\beta\Lambda_k)). \tag{3.56}$$

We then sum over all configurations of $s - 1$ internal impurities and then sum over s:

$$Z_N(\beta) = \sum_s \sum_{\substack{q_1,\cdots q_r \\ \Sigma q_r = N}} \exp\left[-\beta \sum_{r=1}^{s} \mathcal{U}(q_r;\beta)\right] \tag{3.57}$$

It is appealing to handle the constraint $\sum q_r = N$ in analogy with the grand canonical ensemble, but because the exact free energy increases linearly with N for large N, such a method fails. Rather the constraint can be introduced explicitly using the integral representation for the Kronecker delta:

$$\delta_{\Sigma q,N} = (1/2\pi) \int_{-\pi}^{\pi} \exp[i\theta(\textstyle\sum q - N)]d\theta. \tag{3.58}$$

Then

$$Z_N(\beta) = \sum_s \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \exp(-i\theta N)[z(\theta;\beta)]^s = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \frac{\exp(-i\theta N)}{1 - z(\theta;\beta)}, \tag{3.59}$$

where

$$z(\theta;\beta) = \sum_{q=1}^{\infty} \exp[-\beta\mathcal{U}(q;\beta) + i\theta q]. \tag{3.60}$$

This reduces the problem to quadratures, which we shall not carry out.

G. The Approximation of Ruijgrok and Rodriguez

It is interesting to consider the most successful of the approximate procedures for the Heisenberg model, that of Ruijgrok and Rodriguez (*10*), (henceforth, RR), to see how accurately it gives the various properties of the Heisenberg–

Ising (HI) model that are known exactly. The procedure of RR is to introduce operators ξ_k and $\xi_k^\dagger$ similar to η_k and $\eta_k^\dagger$ of the XY model, operators that annihilate or create particles (i.e., spins up) in Bloch wave single particle states with two sites per unit cell rather than in plane wave single particle states as we did for the cyclic isotropic XY model. The best form for the Bloch waves is determined variationally. Thus their method gives the isotropic XY model exactly (the Bloch waves reduce to plane waves), but it is not really suited to the anisotropic XY model because the latter fails to conserve the number of particles, whereas the RR method is particle conserving. The Heisenberg–Ising model, on the other hand, is also particle conserving, if by particles we mean single up-spins, not to be confused with up and down pair states. Furthermore, the HI Hamiltonian is invariant under translations by an even number of spin sites, providing it is made suitably cyclic. It is thus appropriate for a test of the RR procedure.

The cyclic HI-Hamiltonian in terns of the c's and $c^\dagger$'s introduced in (2.5a, b) is

$$H_\lambda = \sum_{j=1.3\cdots}^{2N-1} [(c_j^\dagger c_j - \tfrac{1}{2})(c_{j+1}^\dagger c_{j+1} - \tfrac{1}{2}) + \tfrac{1}{2}(c_j^\dagger c_{j+1} - c_j c_{j+1}^\dagger)] + 2\lambda \sum_{j=2,4\cdots}^{2N} (c_j^\dagger c_j - \tfrac{1}{2})(c_{j+1}^\dagger c_{j+1} - \tfrac{1}{2}). \tag{3.61}$$

Following RR, operators ξ_k and $\xi_k^\dagger$ are introduced to diagonalize H approximately:

$$\xi_k = \sum_j e^{ikj} u_k(j) c_j = (\xi_k^\dagger)^\dagger \tag{3.62}$$

with

$$u_k(j) = (2N)^{-\frac{1}{2}} [\cos \alpha(k) + (-1)^j \sin \alpha(k)]. \tag{3.63}$$

TABLE IV

COMPARISON OF THE RUIJGROK–RODRIGUEZ APPROXIMATE LONG-RANGE ORDER IN THE GROUND STATE OF THE HI MODEL WITH THE CORRESPONDING EXACT VALUES FOR VARIOUS VALUES OF λ

λ	0	½	1	2.5	5
E_{RR}/N	−0.485	−0.615	−0.829	−1.541	−2.771
E_0/N	−0.750	−0.782	−0.887	−1.550	−2.775
$\rho_{xz,RR}$	0.057	0.162	0.202	.234	.245
$\rho_{xz\ exact}$	0.000	0.000	0.000	.210	.240

The function $\alpha(k)$ is chosen to minimize the expectation value of H_λ in the Fermi sea of ξ-particles. The energy per spin is found to be

$$E_{\mathrm{RR}}/N = [1/4(1 + 2\lambda)] - [(1 + 2\lambda)/\pi^2]\mathfrak{K}^2(\mu^2), \tag{3.64}$$

where μ is the solution of the transcendental equation

$$\mu\mathfrak{D}(\mu^2) = \pi/2(1 + 2\lambda). \tag{3.65}$$

$\mathfrak{K}$ and $\mathfrak{D}$ are again complete elliptical integrals. In Table IV we compare the energy per spin and long-range order calculated for the RR approximate ground state with the exact energy per spin and end-to-end order, for several values of λ. We see that although the RR procedure gives the asymptotically correct energy as $\lambda \to \infty$, and a good approximation to the energy for $\lambda > 1$, it may give the order quite incorrectly. This emphasizes the danger of relying on a variational approach for the long-range order, a result which is not surprising in view of the fact that states with no long-range order can be constructed with energy/spin above the ground state by only $O(N^{-2})$.

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APPENDIX A. TO DIAGONALIZE A GENERAL QUADRATIC FORM IN FERMI OPERATORS

We wish to diagonalize the quadratic form

$$H = \sum_{i,j} [c_i^\dagger A_{ij} c_j + \tfrac{1}{2}(c_i^\dagger B_{ij} c_j^\dagger + \text{h.c.})], \tag{A-1}$$

where the c_i's and $c_i^\dagger$'s are Fermi annihilation and creation operators and H is Hermitian. The Hermiticity of H requires that $\mathbf{A}$ be a Hermitian matrix, while the anticommutation rules among the c_i's require that $\mathbf{B}$ be an antisymmetric matrix. In the situations of interest *here*, one can always arrange that $\mathbf{A}$ and $\mathbf{B}$ are real.

We try to find a linear transformation of the form

$$\eta_k = \sum_i (g_{ki} c_i + h_{ki} c_i^\dagger), \tag{A-2a}$$

$$\eta_k^\dagger = \sum_i (g_{ki} c_i^\dagger + h_{ki} c_i), \tag{A-2b}$$

with the g_{ki} and h_{ki} real, which is canonical (i.e., the η_k's and $\eta_k^\dagger$'s should also be Fermi operators) and which gives for H the form

$$H = \sum \Lambda_k \eta_k^\dagger \eta_k + \text{constant}. \tag{A-3}$$

If this is possible, then

$$[\eta_k , H] - \Lambda_k \eta_k = 0. \tag{A-4}$$

Substituting (A-2) in (A-4) and setting the coefficients of each operator equal to zero, we obtain a set of equations for the g_{ki} and h_{ki} :

$$\Lambda_k g_{ki} = \sum_j (g_{kj} A_{ji} - h_{kj} B_{ji}), \tag{A-5a}$$

$$\Lambda_k h_{ki} = \sum_j (g_{kj} B_{ji} - h_{kj} A_{ji}). \tag{A-5b}$$

These are simplified by introducing the linear combinations

$$\phi_{ki} = g_{ki} + h_{ki} \tag{A-6a}$$

and

$$\psi_{ki} = g_{ki} - h_{ki} \tag{A-6b}$$

in terms of which the coupled equations are

$$\phi_k(\mathbf{A} - \mathbf{B}) = \Lambda_k \psi_k \tag{A-7a}$$

and

$$\psi_k(\mathbf{A} + \mathbf{B}) = \Lambda_k \phi_k \tag{A-7b}$$

in an obvious matrix notation. Either ψ_k or ϕ_k can be eliminated from (A-7) giving either

$$\phi_k(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B}) = \Lambda_k^2 \phi_k \tag{A-8a}$$

or

$$\psi_k(\mathbf{A} + \mathbf{B})(\mathbf{A} - \mathbf{B}) = \Lambda_k^2 \psi_k . \tag{A-8b}$$

For $\Lambda_k \neq 0$, either (A-8a) or (A-8b) is solved for ϕ_k or ψ_k and the other vector is then obtained from (A-7a) or (A-7b).

For $\Lambda_k = 0$, both ϕ_k and ψ_k are determined by (A-8), or more simply by (A-7), their relative sign being arbitrary. Changing the sign of ψ_k , but not of ϕ_k , interchanges g_{kj} and h_{kj} , hence η_k and $\eta_k^\dagger$, and thus interchanges the definitions of occupied and unoccupied for this zero-energy mode. That the choice of definition is arbitrary is not surprising, because it has no effect on the energy.

Because $\mathbf{A}$ is symmetric and $\mathbf{B}$ is antisymmetric, $(\mathbf{A} + \mathbf{B})^T = \mathbf{A} - \mathbf{B}$, so that both $(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B})$ and $(\mathbf{A} + \mathbf{B})(\mathbf{A} - \mathbf{B})$ are symmetric and at least positive semi-definite. Thus all the Λ_k's are real and it is possible to choose all the ϕ_k's and ψ_k's to be real as well as orthogonal. If the ϕ_k's are normalized

vectors ($\sum_i \phi_{ki}^2 = 1$), then the ψ_k's are also automatically normalized when $\Lambda_k \neq 0$ or can be so chosen when $\Lambda_k = 0$. This ensures that

$$\sum_i (g_{ki}g_{k'i} + h_{ki}h_{k'i}) = \delta_{kk'} \tag{A-9a}$$

and

$$\sum_i (g_{ki}h_{k'i} - g_{k'i}h_{ki}) = 0, \tag{A-9b}$$

the necessary and sufficient conditions that the η_k's and $\eta_k^\dagger$'s be canonical Fermi operators.

The constant in H can be determined by substituting (A-3) in (A-1) or, less tediously, from the invariance of tr H under the canonical transformation (A-2). From (A-1)

$$\text{tr } H = 2^{N-1} \sum_i A_{ii} \tag{A-10}$$

while from (A-3)

$$\text{tr } H = 2^{N-1} \sum_k \Lambda_k + 2^N \times \text{constant}. \tag{A-11}$$

The constant is thus $\frac{1}{2}(\sum_i A_{ii} - \sum_k \Lambda_k)$ and

$$H = \sum_k \Lambda_k \eta_k^\dagger \eta_k + \frac{1}{2}(\sum_i A_{ii} - \sum_k \Lambda_k). \tag{A-12}$$

APPENDIX B. NONDEGENERACY OF THE GROUND STATE AND ABSENCE OF AN ENERGY GAP IN THE HEISENBERG MODEL

We prove two exact theorems about the ground state and excitation spectrum for a Heisenberg model with nearest neighbor interactions in one dimension. The generalization to longer range interactions and higher-dimensional lattices is indicated. A further generalization to particles of spin $\neq \frac{1}{2}$ and a discussion of the ordering of excited state energy levels has been submitted for publication in the *Journal of Mathematical Physics* by Lieb and Mattis.

THEOREM 1. For a linear chain of spin $\frac{1}{2}$'s with nearest neighbor antiferromagnetic Heisenberg interactions, the ground state is nondegenerate (hence $S = 0$).

Proof. We first remark that this is a stronger theorem than that due to Marshall (7), who proved that there is a singlet ground state, but who did not exclude the possibility of there being several degenerate ground states, some of which may not be singlets. We consider the Hamiltonian

$$H = \sum S^z{}_i S^z{}_j + \tfrac{1}{2} \sum S^+{}_i S^-{}_j + S^-{}_i S^+{}_j, \tag{B-1}$$

where i and j are on the A and B sublattices respectively and the sums run over all interacting pairs. It is convenient to make the canonical transformation rotating all spins on the B sublattice ($S^x{}_j \to -S^x{}_j$, $S^y{}_j \to -S^y{}_j$, $S^z{}_j \to S^z{}_j$), so that instead of (B-1) we consider

$$H' = \sum S^z{}_i S^z{}_j - \tfrac{1}{2}\sum S^+{}_i S^-{}_j + S^-{}_i S^+{}_j . \tag{B-2}$$

Because $[S_z, H] = 0$, let us consider only states having $S_z = 0$ and show that only one such state has the ground-state energy. A complete set of states in the $S_z = 0$ subspace is the set of configurations in which $N/2$ spins are up and $N/2$ spins are down. We denote these states by Φ_μ where $1 \leqq \mu \leqq \binom{N}{\frac{1}{2}N}$. Any eigenfunction Ψ of H' can be expanded as

$$\Psi = \sum C_\mu \Phi_\mu , \tag{B-3}$$

and Schrödinger's equation in this representation reduces to a set of coupled linear equations

$$(E - \epsilon_\mu) C_\mu = \tfrac{1}{2} \sum_{\mu'(\mu)} C_{\mu'} , \tag{B-4}$$

where

$$\epsilon_\mu \Phi_\mu = (\sum S^z{}_i S^z{}_j)\Phi_\mu ,$$

and the $\Phi_{\mu'(\mu)}$ are the set of configurations which connect to Φ_μ via the interaction. Because the Hamiltonian is real, we may assume without loss of generality that all C's are real. Essential to the proof is the following lemma:

LEMMA 1. For any ground state with $S_z = 0$, all $C_\mu \neq 0$.

Proof. Suppose the contrary, i.e., for some ground state Ψ_0 having the ground-state energy E_0,

$$C_\mu = 0 \quad \text{for} \quad \mu = \mu_1 , \cdots , \mu_r . \tag{B-5a}$$

For these C's (B-2) reduces to

$$0 = \tfrac{1}{2} \sum_{\mu'(\mu)} C_{\mu'}, \qquad \mu = \mu_1 , \cdots , \mu_r . \tag{B-5b}$$

Now in at least one of these equations, say the μ_pth, some of the $C_{\mu'}$'s $\neq 0$ (otherwise H would break into blocks with no matrix elements connecting $\Phi_{\mu_1} , \cdots , \Phi_{\mu_r}$ with the other configurations, which is readily seen to be impossible); therefore (B-5b) implies that there are nonzero C's of *both* signs. Consider then the trial function Ψ_0':

$$\Psi_0' = \sum | C_\mu | \Phi_\mu . \tag{B-6}$$

On the one hand, Ψ_0' is not an eigenstate because

$$| C_{\mu_p} | = 0 \quad \text{but} \quad \sum_{\mu\ (\mu_p)} | C_{\mu'} | \neq 0, \tag{B-7}$$

so that, from the variational principle, we have for its energy

$$E_0' > E_0 . \tag{B-8}$$

On the other hand, explicit evaluation gives

$$E_0' = \sum \epsilon_\mu C_\mu^2 - \tfrac{1}{2} \sum_{\mu} \sum_{\mu'(\mu)} | C_\mu | \, | C_{\mu'} | \tag{B-9a}$$

and

$$E_0 = \sum \epsilon_\mu C_\mu^2 - \tfrac{1}{2} \sum_{\mu} \sum_{\mu'(\mu)} C_\mu C_{\mu'} , \tag{B-9b}$$

from which it follows that

$$E_0' \leqq E_0 . \tag{B-10}$$

The contradiction between (B-8) and (B-10) proves the lemma.

We now prove a lemma which is a stronger version of the lemma due to Peierls and used by Marshall.

LEMMA 2. For every ground state with $S_z = 0$, all C_μ's have the same sign.

Proof. For Ψ_0 to be a ground state, the equality must hold in (B-10). This occurs if, and only if, all the terms $C_\mu C_{\mu'}$ occuring in (B-9b) are positive, (they are all nonzero by lemma 1), i.e., the coefficients of all configurations connected through the interaction with each other should have the same sign. But as we have remarked, each configuration is ultimately connected with every other through repeated applications of the interaction, proving the lemma.

It is now obvious that there can be only one ground state with $S_z = 0$; otherwise, the several states would all have all positive coefficients and so could not be orthogonal to one another. Now Marshall has shown that *at least* one ground state has $S = 0$. The existence of another ground state, whatever its multiplicity, would imply that there is a second ground state with $S_z = 0$, which we have shown to be impossible. The entire proof is immediately generalizable to any number of dimensions and any lattice which is decomposable into two equivalent sublattices with antiferromagnetic Heisenberg interactions between spins on different sublattices and ferromagnetic Heisenberg interactions between spins on the same sublattice. Also, although Marshall's proof, used above, requires periodic boundary conditions to ensure translational invariance, this restriction may also be dropped if the lattice has reflection symmetry about some plane (so that there is a transformation mapping the A and B sublattices into each other but leaving the Hamiltonian unchanged).

Next we investigate the nature of the excitation spectrum and prove

THEOREM 2. There is an excited state for the cyclic linear chain with nearest neighbor Heisenberg interactions having vanishingly small excitation energy in the limit that the length of the chain becomes infinite.

Proof. Consider the state

$$\Psi_k = \exp\,(ik\sum nS^z{}_n)\Psi_0 \equiv \mathcal{O}^k\Psi_0\,. \tag{B-11}$$

We first show that if $k = (2\pi/N) \times$ odd integer, Ψ_k is orthogonal to the ground state. Consider the unitary operator U_x that displaces all the spins by one site cyclically:

$$U_x\mathbf{S}_iU_x^{-1} = \mathbf{S}_{i+1}\,, \qquad \mathbf{S}_{N+1} = \mathbf{S}_1\,. \tag{B-12}$$

Because

$$[H,U_x] = 0,$$

if Ψ_0 is an eigenstate of H, so is $U_x\Psi_0$. By the nondegeneracy of Ψ_0

$$U_x\Psi_0 = e^{i\alpha}\Psi_0\,. \tag{B-13}$$

Thus

$$\begin{aligned}\langle\Psi_0 \mid \Psi_k\rangle &= \langle\Psi_0 \mid \mathcal{O}^k \mid \Psi_0\rangle \\ &= \langle\Psi_0 \mid U_x\mathcal{O}^kU_x^{-1} \mid \Psi_0\rangle.\end{aligned} \tag{B-14}$$

But

$$U_x\mathcal{O}^kU_x^{-1} = \mathcal{O}^k \exp\,(ikNS^z{}_1) \exp\,(-ik\sum_1^N S^z{}_n). \tag{B-15}$$

Because Ψ_0 is a singlet

$$\exp\,(-ik\sum_1^N S^z{}_n)\Psi_0 = 0. \tag{B-16}$$

Furthermore, in the most convenient representation

$$S^z{}_1 = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} \tag{B-17a}$$

so that

$$\exp(ikNS^z{}_1) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \tag{B-17b}$$

in this or any other representation, providing

$$k = 2\pi m/N, \quad m \text{ an odd integer.} \tag{B-18}$$

Thus

$$\langle \Psi_0 \mid \Psi_k \rangle = -\langle \Psi_0 \mid \Psi_k \rangle = 0. \tag{B-19}$$

Note that we have not proved the Ψ_k's to be orthogonal among themselves. The energy of Ψ_k is also readily calculated.

$$\langle \Psi_k \mid H \mid \Psi_k \rangle = \langle \Psi_0 \mid \mathcal{O}_x^{k-1} H \mathcal{O}^k \mid \Psi_0 \rangle. \tag{B-20}$$

Using,

$$\mathcal{O}^{k-1} S^x{}_n \mathcal{O}^k = S^x{}_n \cos kn + S^y{}_n \sin kn, \tag{B-21a}$$

$$\mathcal{O}^{k-1} S^y{}_n \mathcal{O}^k = -S^x{}_n \sin kn + S^y{}_n \cos kn, \tag{B-21b}$$

and

$$\mathcal{O}^{k-1} S^z{}_n \mathcal{O}^k = S^z{}_n , \tag{B-21c}$$

we find

$$\langle \Psi_0 \mid \mathcal{O}^{k-1} H \mathcal{O}^k \mid \Psi_0 \rangle = \Big\langle \Psi_0 \Big| H + (\cos k - 1) \sum_1^N (S^x{}_n S^x{}_{n+1} + S^y{}_n S^y{}_{n+1}) + \sin k \sum_1^N (S^x{}_n S^y{}_{n+1} - S^y{}_n S^x{}_{n+1}) \Big| \Psi_0 \Big\rangle. \tag{B-22}$$

Use has been made of (B-18) in the term arising from $\mathbf{S}_N \cdot \mathbf{S}_1$. Consider the terms on the right in (B-22), one by one, for $k = 2\pi/N$.

(i) $$\langle \Psi_0 \mid H \mid \Psi_0 \rangle = E_0 . \tag{B-23a}$$

(ii) $$(\cos k - 1) \Big\langle \Psi_0 \Big| \sum_1^N (S^x{}_n S^x{}_{n+1} + S^y{}_n S^y{}_{n+1}) \Big| \Psi_0 \Big\rangle$$

$$= \Big[-\tfrac{1}{2} \Big(\frac{2\pi}{N} \Big)^2 - O(N^{-4}) \Big] \sum_1^N \langle \Psi_0 \mid S^x{}_n S^x{}_{n+1} + S^y{}_n S^y{}_{n+1} \mid \Psi_0 \rangle \tag{B-23b}$$

$$\leq \Big(\frac{2\pi}{N} \Big)^2 \frac{N}{2} + O(N^{-3}).$$

(iii) $$\sin k \Big\langle \Psi_0 \Big| \sum_1^N (S^x{}_n S^y{}_{n+1} - S^y{}_n S^x{}_{n+1}) \Big| \Psi_0 \Big\rangle = -i \sin k \, \langle \Psi_0 \mid [\textstyle\sum n S^z{}_n , H] \mid \Psi_0 \rangle = 0. \tag{B-23c}$$

Thus for $k = 2\pi/N$,

$$\langle \Psi_k \mid H \mid \Psi_k \rangle \leqq E_0 + (2\pi^2/N), \tag{B-24}$$

and there is no energy gap.

In two dimensions we consider a square lattice of N sites in the x-direction and of $M = O(N^\nu)$ sites in the y-direction, where $0 < \nu < 1$. The Hamiltonian is assumed cyclic in the sense that

$$\mathbf{S}_{n,\,M+1} = \mathbf{S}_{n,\,1} \tag{B-25a}$$

and

$$\mathbf{S}_{N+1,\,m} = \mathbf{S}_{1,\,m}\,, \tag{B-26}$$

i.e., the lattice is wrapped on a torus. We take for the operator $\mathcal{O}^k$,

$$\mathcal{O}^k = \exp\left(ik \sum_{n=1}^{N} \sum_{m=1}^{M} n S^z{}_{n,m}\right). \tag{B-27}$$

This operator twists the direction of all spins with the same x-coordinate by the same amount. Ψ_k is constructed and its orthogonality to the ground state is proved precisely as in one dimension. Instead of (B-24), one now has

$$\langle \Psi_k \mid H \mid \Psi_k \rangle \leqq E_0 + (2\pi^2/N^{1-\nu}); \tag{B-28}$$

so again there is no energy gap. Because the excitation energy of exact low-lying states should not depend on the shape of the entire lattice, there should be no energy gap for a lattice of $N \times N$ sites either. The particular state Ψ_k is unfortunately not sufficiently like an exact low-lying excited state to give this result.

A similar extension to three dimensions is obvious.

APPENDIX C. CALCULATING $G_{ij}(\beta)$ FOR THE XY MODEL

By definition

$$G_{ij} = \langle B_i A_j \rangle. \tag{C-1}$$

In the ground state

$$G_{ij} = \langle \Psi_0 \mid B_i A_j \mid \Psi_0 \rangle \tag{C-2a}$$

while at finite temperature

$$G_{ij} = \langle B_i A_j \rangle_\beta\,,$$

where $\langle \ldots \rangle_\beta$ denotes an average over the canonical ensemble at temperature $T = 1/k$. Thus

$$\begin{aligned} G_{ij}(\beta) &= \sum_{kk'} \psi_{ki} \phi_{k'j} \langle (\eta_k{}^\dagger - \eta_k)(\eta_{k'}{}^\dagger + \eta_{k'}) \rangle_\beta \\ &= \sum_k \psi_{ki} \phi_{kj} (\langle \eta_k{}^\dagger \eta_k \rangle_\beta - \langle \eta_k \eta_k{}^\dagger \rangle_\beta). \end{aligned} \tag{C-3}$$

But

$$\langle \eta_k^\dagger \eta_k \rangle = [\exp(\beta\Lambda_k) + 1]^{-1}, \text{ etc.},$$

so that

$$G_{ij}(\beta) = -\sum_k \psi_{ki}\phi_{kj} \tanh(\tfrac{1}{2}\beta\Lambda_k) = -(\psi^T \tanh(\tfrac{1}{2}\beta\mathbf{\Lambda})\phi)_{ij}. \quad \text{(C-4)}$$

For the cyclic chain, the sum in (C-4) can be considerably simplified. First, combining the summands for k and $-k$,

$$G_{ij}(\beta) = -(2/N) \sum_{k>0} \Lambda_k^{-1} \tanh(\tfrac{1}{2}\beta\Lambda_k) \cdot [\cos k \cos k(i-j) - \gamma \sin k \sin k(i-j)]. \quad \text{(C-5)}$$

Second, combining the summands for k and $\pi - k$,

$$G_{ij}(\beta) = -(4/N) \frac{1-(-1)^{i-j}}{2} \sum_{0<k<\pi/2} \Lambda_k^{-1} \tanh(\tfrac{1}{2}\beta\Lambda_k) \cdot [\cos k \cos k(i-j) - \gamma \sin k \sin k(i-j)]. \quad \text{(C-6)}$$

For $N \to \infty$ with $i - j = r$ fixed,

$$G_r = -\left[\frac{1+\gamma}{2} L_{r+1} + \frac{1-\gamma}{2} L_{r-1}\right], \qquad r \text{ odd}$$

$$G_r = 0, \qquad r \text{ even}, \quad \text{(C-7)}$$

where

$$L_r = (2/\pi) \int_0^{\pi/2} dk \Lambda_k^{-1} \tanh(\tfrac{1}{2}\beta\Lambda_k) \cos kr. \quad \text{(C-8)}$$

G_r for the ground state is obtained by setting $\tanh(\tfrac{1}{2}\beta\Lambda_k) \equiv 1$.

APPENDIX D. DEPENDENCE OF $\sin^2 Nk$ AND A_k^2 ON k FOR A CHAIN WITH FREE ENDS, XY MODEL

In this appendix we wish to show that for a chain with free ends, A_k^2 and $\sin^2 Nk$ are smoothly varying functions of k in the sense that the change in either of them when k_m is replaced by k_{m+1} is $O(1/N)$ (except when k_{m+1} is k_0, the bound state).

First consider $\sin^2 Nk$.

$$\Delta \sin^2 Nk_m = \tfrac{1}{2}(\cos 2Nk_m - \cos 2Nk_{m+1}) = \tfrac{1}{2}(\cos 2\nu_m\pi - \cos 2\nu_{m+1}\pi). \quad \text{(D-1)}$$

But because ν_m is obviously a slowly varying function of m, from (2.67′) or (2.69), we have

$$\Delta \sin^2 Nk_m = \pi \sin 2\nu_m \pi \, \Delta\nu_m = O(1/N). \tag{D-2}$$

Second, consider A_k. Letting

$$\chi_m = \sin 2(N+1)k_m / \sin 2k_m ,$$

we have

$$\Delta A_{k_m}^2 \equiv A_{k_{m+1}}^2 - A_{k_m}^2 = 4(N+1-\chi_m)^{-2} \Delta\chi_m \tag{D-3}$$

providing

$$\Delta\chi_m/(N+1-\chi_m) \ll 1. \tag{D-4}$$

Now, as $N \to \infty$,

$$\chi_m = \frac{\sin[(2m/N) - \nu_m]\pi}{\sin(2m\pi/N)} = \cos \nu_m \pi - \cot \frac{2m\pi}{N} \sin \nu_m \pi \tag{D-5}$$

and

$$\Delta\chi_m = -[\sin \nu_m\pi + \cot(2m\pi/N) \cos \nu_m\pi]\pi\Delta\nu_m - \sin \nu_m\pi \, \Delta\cot(2m\pi/N). \tag{D-6}$$

For $\frac{1}{2}N - m = O(N)$, these relations give

$$\chi_m = O(1) \quad \text{and} \quad \Delta\chi_m = O(1/N), \tag{D-7}$$

so that (D-4) is satisfied and (D-3) gives

$$\Delta A_{k_m}^2 = O(1/N^3). \tag{D-8}$$

For $\frac{1}{2}N - m \equiv m' = o(N) \neq 0$, one must be more careful. Then

$$\Delta A_{k_m}^2 = 4\Delta\chi_m/(N+1-\chi_{m+1})(N+1-\chi_m). \tag{D-9}$$

In this limit

$$\chi_m = \cos \nu_m\pi + (N/2m'\pi) \sin \nu_m\pi = (N/2m'\pi) \sin \nu_m\pi + o(N). \tag{D-10}$$

Thus

$$\Delta\chi_m = (N/2\pi) \, [\sin \nu_m\pi/m'(m'-1)] + o(N), \tag{D-11}$$

so that

$$\Delta A_{k_m}^2 = O(1/N). \tag{D-12}$$

APPENDIX E. G_{ij} FOR THE XY MODEL WITH FREE ENDS

In this appendix we derive simple relations between G^f_{ij} for the XY model with free ends and G^c_{i-j} for the cyclic XY model, valid except when i and j are near opposite ends.

In general

$$G_{ij} = -\sum_k \psi_{ki}\phi_{kj}\,. \tag{E-1}$$

For free ends, the sum on k is over modes of Type I and Type II. If i is odd $\psi^{\mathrm{II}}_{ki} = 0$ so that only Type I modes contribute; but for Type I modes, $\phi^{\mathrm{I}}_{kj} = 0$ unless j is even. Thus

$$G^f_{ij} = -\sum_{k^{\mathrm{I}}} \psi^{\mathrm{I}}_{ki}\phi^{\mathrm{I}}_{kj} = \sum_{k^{\mathrm{I}}} A_k{}^2\delta_k \sin[(N-i+1)k]\sin jk \quad \text{for } i \text{ odd}, j \text{ even}; \tag{E-2a}$$

similarly,

$$G^f_{ij} = \sum_{k^{\mathrm{II}}} A_k{}^2\delta_k \sin ik \sin[(N+1-j)k] \quad \text{for } i \text{ even}, j \text{ odd}; \tag{E-2b}$$

and finally,

$$G^f_{ij} = 0 \quad \text{for } i \text{ and } j \text{ both even or both odd.} \tag{E-2c}$$

Furthermore, $k_{\mathrm{I}} \leftrightarrow k_{\mathrm{II}}$ is equivalent to $\gamma \to -\gamma$, so that

$$G^f_{ij}(\gamma) = G^f_{ji}(-\gamma), \tag{E-3a}$$

and for the cyclic chain we have a similar relation

$$G^c_{i-j}(\gamma) = G^c_{j-i}(-\gamma). \tag{E-3b}$$

Therefore we need consider only the case i odd and j even.

Defining

$$r = i - j, \tag{E-4a}$$

$$s = i + j, \tag{E-4b}$$

we obtain

$$G^f_{ij} = \tfrac{1}{2}\sum_{k^{\mathrm{I}}} A_k{}^2\delta_k[\cos(N+1-s)k - \cos(N+1-r)k], \tag{E-5}$$

and we have two sums on the right of identical structure. Suppose first that $s = o(N)$. Then using (2.66) and neglecting terms of $O(1/N)$ we find

$$\cos(N+1-s)k_m{}^{\mathrm{I}} = (-1)\cos\{\nu_m{}^{\mathrm{I}} - [(1-s)m/N]\}\pi. \tag{E-6}$$

From (2.67′) it follows immediately that

$$\tfrac{1}{2}\sum_{k\mathrm{I}} A_k^2\delta_k \cos\,(N+1-s)k = -G_s^c \tag{E-7}$$

so that

$$G_{ij}^f = G_{i-j}^c - G_{i+j}^c \quad \text{for} \quad i \text{ odd}, j \text{ even}, \mid i-j \mid = o(N), \quad \text{and} \quad i+j = o(N). \tag{E-8a}$$

From (E-3a, b) we have also

$$G_{ij}^f = G_{i-j}^c - G_{-(i+j)}^c \quad \text{for} \quad i \text{ even}, j \text{ odd}, \mid i-j \mid = o(N) \quad \text{and} \quad i+j = o(N). \tag{E-8b}$$

If both i and j are far from the ends but not far from each other, we suppose $r = o(N)$ but $s = \sigma N$ where $\sigma = O(1)$. Then, using (2.66) and neglecting terms of $O(1/N)$, we find

$$\begin{aligned}\frac{1}{2}\sum_{k\mathrm{I}} A_k^2\delta_k \cos(N+1-s)k \\ = \frac{1}{4}\sum_m [\cos(2-\sigma)m\pi + \cos\sigma m\pi]A_{k_m}^2 \cos\left((1-\sigma)\nu_m - \frac{m}{N}\right)\pi \\ + \frac{1}{4}\sum_m [\sin(2-\sigma)m\pi - \sin\sigma m\pi]A_{k_m}^2 \sin\left((1-\sigma)\nu_m - \frac{m}{N}\right)\pi.\end{aligned} \tag{E-9}$$

The terms in brackets in each sum are rapidly oscillating functions of m while their coefficients are slowly changing functions of m, as $N \to \infty$. The sums are therefore $O(1/N)$ and can be neglected. Thus

$$G_{ij}^f = G_{i-j}^e, i \text{ odd} \quad \text{and} \quad j \text{ even}, \mid i-j \mid = o(N), i+j = O(N) \tag{E-10}$$

The same result holds for i even and j odd.

APPENDIX F. ALIGNMENT OF SPINS IN SUCCESSIVE IMPURITY PAIRS, HI MODEL

In this appendix we show that the spins of successive impurity pairs in the HI model are aligned parallel or antiparallel, depending on whether the number of elementary excitations (excluding the trivial $k = 0$ "excitation") is respectively odd or even. We shall consider only the special case that the impurity pairs are at opposite ends of a finite chain, but the generalization to any number of impurity pairs in any positions is obvious.

Although neither of the states Ψ_{0+} and Ψ_{0-} defined by (3.52d, e), are eigenstates of $S^z{}_0$ or $S^z{}_N$, we wish to show that these two states involve only configurations

in which the first two spins are antiparallel to the last two. Because the first two spins (and also the last two) are themselves parallel, it is sufficient to show that

$$S^z{}_0 S^z{}_N \Psi_{0\pm} = -\tfrac{1}{4}\Psi_{0\pm} . \tag{F-1}$$

More generally, we shall show that

$$S^z{}_0 S^z{}_N \eta^\dagger_{k_1} \ldots \eta^\dagger_{k_n} \Psi_{0\pm} = -(-1)^n \tfrac{1}{4} \eta^\dagger_{k_1} \ldots \eta^\dagger_{k_n} \Psi_{0\pm} , \tag{F-2}$$

where $k_i \neq 0$ for all i.

Taking into account (3.41) and (3.43), we have

$$\begin{aligned} S^z{}_0 S^z{}_N \eta^\dagger_{k_1} \cdots \eta^\dagger_{k_n} \Psi_{0\pm} &= -\tfrac{1}{4}(a_0{}^\dagger + a_0)(a_N{}^\dagger + a_N)\, \eta^\dagger_{k_1} \ldots \eta^\dagger_{k_n} \Psi_{0\pm} , \\ &= -\tfrac{1}{4} \exp(i\pi\mathfrak{N})(c_0{}^\dagger + c_0)(c_N{}^\dagger + c_N) \eta^\dagger_{k_1} \ldots \eta^\dagger_{k_n} \Psi_{0\pm} , \\ &= -\tfrac{1}{4} \exp(i\pi\mathfrak{N})(\eta_0 \eta_0{}^\dagger - \eta_0{}^\dagger \eta_0) \eta^\dagger_{k_1} \ldots \eta^\dagger_{k_n} \Psi_{0\pm} , \\ &= \pm\tfrac{1}{4} \exp(i\pi\mathfrak{N}) \eta^\dagger_{k_1} \ldots \eta^\dagger_{k_n} \Psi_{0\pm} , \end{aligned} \tag{F-3}$$

where $\mathfrak{N} = \sum_0^N c_j{}^\dagger c_j$. Now it is easily seen that

$$\exp(i\pi\mathfrak{N}) \eta_k{}^\dagger \exp(-i\pi\mathfrak{N}) = -\eta_k{}^\dagger . \tag{F-4}$$

Therefore

$$S^z{}_0 S^z{}_N \eta^\dagger_{k_1} \ldots \eta^\dagger_{k_n} \Psi_{0\pm} = \pm\, (-1)^n \tfrac{1}{4} \eta^\dagger_{k_1} \ldots \eta^\dagger_{k_n} \exp(i\pi\mathfrak{N})\, \Psi_{0\pm} . \tag{F-5}$$

The result that the spin alignment of successive impurities goes from parallel to antiparallel or vice versa with each additional excitation is now obvious from the factor $(-1)^n$.

To determine the alignment in the states $\Psi_{0\pm}$ we must evaluate $\exp(i\pi\mathfrak{N})\Psi_{0\pm}$. First observe from (F-4) that

$$\eta_k \exp(i\pi\mathfrak{N})\Psi_{0-} = -\exp(i\pi\mathfrak{N})\eta_k \Psi_{0-} = 0, \quad \text{for all } k, \tag{F-6}$$

so that

$$\exp(i\pi\mathfrak{N})\Psi_{0-} = \exp(i\alpha)\Psi_{0-} , \tag{F-7}$$

where α is a phase angle to be determined. But

$$\exp(2i\pi\mathfrak{N}) = 1 \tag{F-8}$$

so that

$$\exp(i\alpha) = \pm 1. \tag{F-9}$$

Thus Ψ_{0-} involves states either with only even numbers of "c-particles" or only odd numbers of c-particles. To find out which is the case, consider the expansion of Ψ_{0-} in states with definite sets of c-particles:

$$\Psi_{0-} = [f_0^- + \sum_i f_1^-(i)c_i^\dagger + \sum_{ij} f_2^-(ij)c_i^\dagger c_j^\dagger + \cdots]\Phi_0 , \qquad \text{(F-10)}$$

where Φ_0 is the c-particle vacuum. Then, using the transformation (A-2), the defining equations for Ψ_{0-} reduce to

$$\{[\sum_l g_{kl} f_1^-(l)] + [f_0^- + \sum_l g_{kl}(f_2^-(li) - f_2^-(il))]c_i^\dagger + \cdots\}\Phi_0 = 0, \qquad \text{(F-11)}$$

from which we have a set of coupled equations for f_0^-, f_1^-, f_2^-, etc.:

$$\sum_l g_{kl} f_1^-(l) = 0, \qquad \text{(F-11a)}$$

$$f_0^- + \sum_l g_{kl}(f_2^-(li) - f_2^-(il)) = 0, \quad \text{all } i, \text{ etc. } \cdots , \qquad \text{(F-11b)}$$

where

$$g_{ki} = \phi_{ki} + \psi_{ki} . \qquad \text{(F-12)}$$

Similarly, from the defining equations for Ψ_{0+}, we obtain a set of coupled equations for the expansion coefficients f_0^+, f_1^+, f_2^+, etc.:

$$\sum_l m_{kl} f_1^+(l) = 0, \qquad \text{(F-13a)}$$

$$f_0^+ + \sum_l m_{kl}[f_2^+(li) - f_2^+(il)] = 0, \quad \text{all } i, \text{ etc. } \cdots , \qquad \text{(F-13b)}$$

where

$$\begin{aligned} m_{ki} = g_{ki} &= \phi_{ki} + \psi_{ki} \quad \text{for} \quad k \neq 0, \\ &= \phi_{ki} - \psi_{ki} \quad \text{for} \quad k = 0. \end{aligned} \qquad \text{(F-14)}$$

A study of det $\mathbf{g}$ and det $\mathbf{m}$ reveals that, in general, $\mathbf{m}$ is singular and $\mathbf{g}$ is not. Thus

$$f_1^- = f_3^- = f_5^- = \cdots = 0 \qquad \text{(F-15)}$$

and

$$f_0^+ = f_2^+ = f_4^+ = \cdots = 0, \qquad \text{(F-16)}$$

from which we conclude that

$$\exp(i\pi\mathfrak{N})\Psi_{0\pm} = \pm\,\Psi_{0\pm} \tag{F-17}$$

and

$$S^z{}_0 S^z{}_N \eta^\dagger_{k_1} \cdots \eta^\dagger_{k_n}\Psi_{0\pm} = -(-1)^n \tfrac{1}{4}\eta^\dagger_{k_1} \cdots \eta^\dagger_{k_n}\Psi_{0\pm}\,. \tag{F-18}$$

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