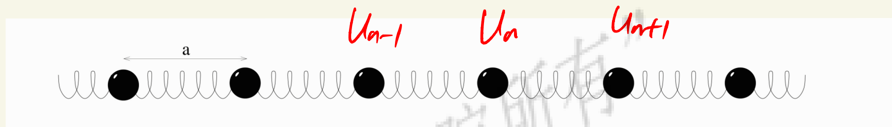
C phonons

Lesson 3

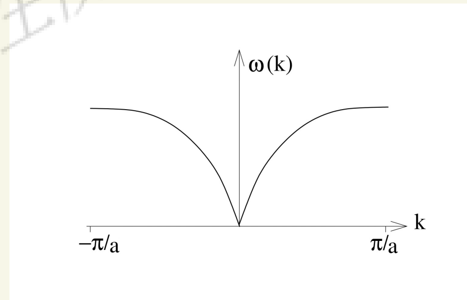
1 Lattice in 1D



$$m\ddot{u}_n = -\lambda\left(2u_n - u_{n-1} - u_{n+1}\right)$$

$$u_n = A\, e^{-i\omega t - ikna}$$

$$k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$$

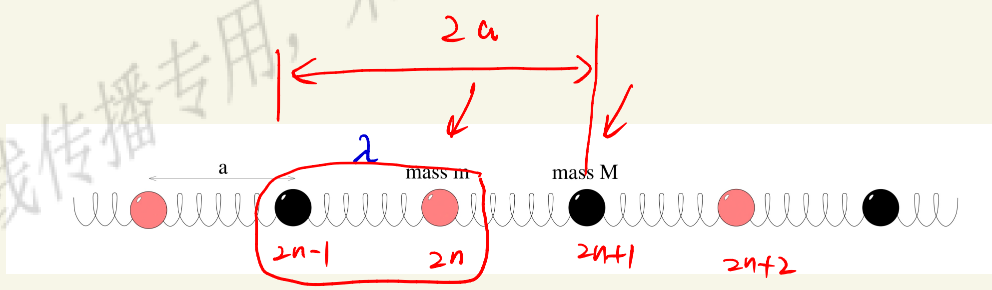


☆ $$m\omega^2 = \lambda\left(2 - e^{ika} - e^{-ika}\right) = 4\lambda \sin^2\left(\frac{ka}{2}\right)$$

$$\omega = 2\sqrt{\frac{\lambda}{m}}\left|\sin\left(\frac{ka}{2}\right)\right| \simeq \sqrt{\frac{\lambda}{m}}\, a\cdot k$$

speed of sound $\quad c_s = \sqrt{\frac{\lambda}{m}}$

* diatomic chain

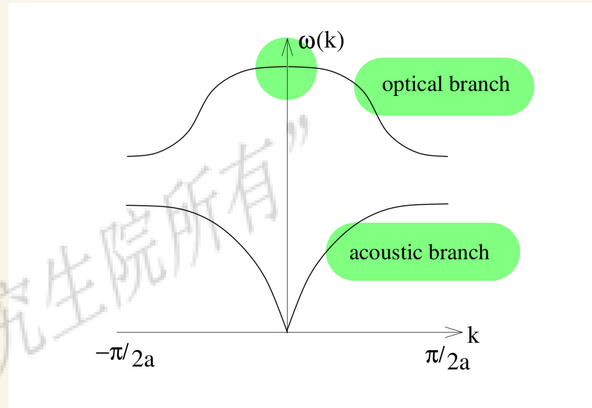


$$m\ddot{u}_{2n} = -\lambda\left[2u_{2n} - u_{2n-1} - u_{2n+1}\right]$$

$$M\ddot{u}_{2n+1} = -\lambda\left[2u_{2n+1} - u_{2n} - u_{2n+2}\right]$$

$$\omega^2\begin{pmatrix} m & \\ & M\end{pmatrix}\begin{pmatrix} A \\ B\end{pmatrix} = \lambda\begin{bmatrix} 2 & -1-e^{-2ika} \\ -(1+e^{2ika}) & 2\end{bmatrix}\begin{bmatrix} A \\ B\end{bmatrix}$$

$$\star \quad \omega_\pm^2 = \frac{\lambda}{mM}\left[m + M \pm \sqrt{(m-M)^2 + 4mM\cos^2 ka}\,\right]$$



$k \to 0 \quad \omega \propto k \qquad$ acoustic branch

$k \to 0 \quad \omega$ constant $\qquad$ optical branch

when $k = 0$; $\quad \omega_- = 0 \quad \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

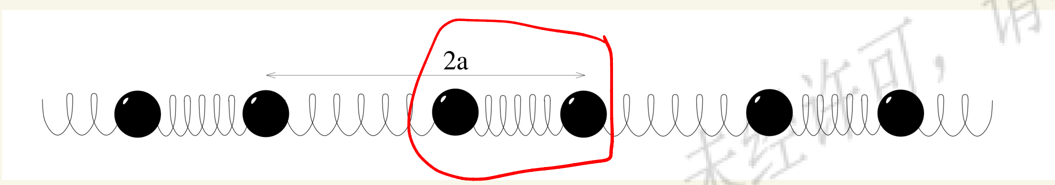
$$\omega_+^2 = 2\lambda\,(M^{-1} + m^{-1}) \Rightarrow \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} M \\ -m \end{pmatrix}$$

Peierls transitions ⟵ electron - phonon interaction.

charge density wave. ⟵ electron - electron interaction

spin

$a \longrightarrow 2a \qquad$ dimerized



(ω, k)

1D system $\qquad$ ① thermodynamic specific heat $\qquad \star$ ② transport resistance $\qquad$ ③ spectroscopy

Scattering of neutrons by Crystal.

$\qquad$ ⓪ scattering.
$\qquad$ ② tunelling. STM
$\qquad$ ⟶ local excitation

|A-M Book|

$$\Psi_i = \psi_p(r)\,\Phi_i \qquad \psi_p = \frac{1}{\sqrt{V}} e^{i\vec{p}\cdot\vec{r}/\hbar}$$

neutron $\qquad$ lattice

$$\varepsilon_i = E_i + \frac{p^2}{2M_n}$$

$$\Psi_f = \psi_{p'}(r)\,\Phi_f \qquad \psi_{p'} = \frac{1}{\sqrt{V}} e^{i\vec{p}'\cdot\vec{r}/\hbar}$$

$$\varepsilon_f = E_f + p'^2/2M_n$$

$$\hbar\omega = \frac{p'^2}{2M_n} - \frac{p^2}{2M_n} \qquad \text{neutron energy}$$

$$\hbar q = p' - p \qquad \text{and momentum transfer}$$

$$V(\vec{r}) = \sum_R V[r - r(R)] = \frac{1}{V}\sum_{k,R} V_k \, e^{ik[r - r(R_i)]}$$

$V_k \leftarrow V_0$ $\qquad V_0 \propto a$

$V \sim 10^{-15} m$ nuclear, subatomic scale.

$k \sim 10^{15} m^{-1}$; independent of wave vector $10^{10} m^{-1}$

scattering length a $\qquad$ Born approximation $\begin{cases} k \to 0 \\ V_k \to V_0 \end{cases}$

cross-section $4\pi a^2$

$$\boxed{V(r) = \frac{2\pi\hbar^2 a}{M_n \cdot V}\sum_{k,R} e^{ik[r - r(R)]}}$$

from "i" to "f" the probability is given by

"Fermi Golden Rule"

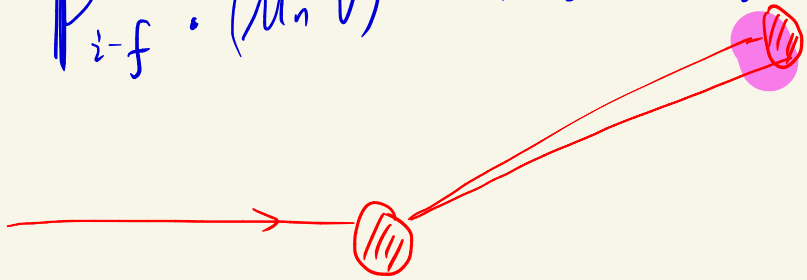
$$P_{i\to f} = \sum_f \frac{2\pi}{\hbar}\delta(\varepsilon_i - \varepsilon_f)\left|(\Psi_i, V\Psi_f)\right|^2$$

$$= \sum_f \frac{2\pi}{\hbar}\delta(E_f - E_i + \hbar\omega)\left|\frac{1}{V}\int dr\, e^{iqr}(\Phi_i, v(r)\Phi_f)\right|^2 \quad R$$

dynamical structure factor

$$= \frac{(2\pi\hbar)^3 a^2}{(M_n V)^2}\underbrace{\sum_f \delta(E_f - E_i + \hbar\omega)\left|\sum_R(\Phi_i, e^{iq\cdot r(R)}\Phi_f)\right|^2}_{S(q,\omega)}$$

$$\mathbb{P}_{i\to f}\cdot (M_n V)^2 \propto a^2\cdot S(q,\omega)$$



$j\cdot d\sigma$

$$dN = j\cdot d\sigma = \frac{\mathbb{P}\cdot V\, d^3p'}{(2\pi\hbar)^3} = \frac{\mathbb{P}\cdot V\, p'^2\, dp'\, d\Omega}{(2\pi\hbar)^3}$$

momentum

$$d\sigma\cdot j = d\sigma \frac{p}{M_n}|\psi_p|^2 = \frac{p}{V M_n}\cdot d\sigma = \frac{\mathbb{P}\cdot V\, M_n\, p'\, dE\, d\Omega}{(2\pi\hbar)^3}$$

$$\boxed{\frac{d\sigma}{d\Omega\cdot dE} = N\,\frac{p'}{p}\,a^2\, S(\vec{q},\omega)}$$

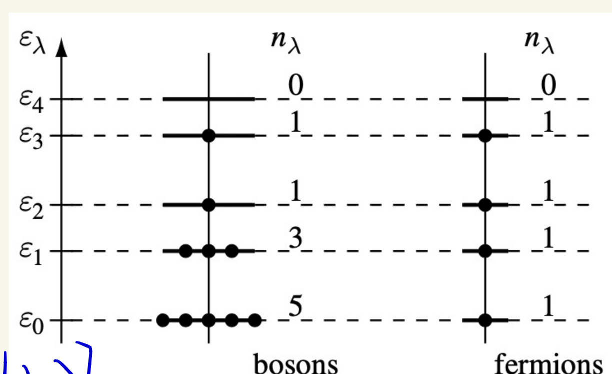
differential cross-section

$$S(\vec{q},\omega) = \sum_f \delta(E_f - E_i + \hbar\omega)\left|\sum_R \langle \Phi_i, e^{i\vec{q}\cdot r(R)}\Phi_f\rangle\right|^2$$

dynamical structure factor

2nd quantization

3rd lesson



* Notation

two particle

$$\psi_F(x_1,x_2) = \frac{1}{\sqrt{2}}\left[\langle x_1|\lambda_1\rangle\langle x_2|\lambda_2\rangle - \langle x_1|\lambda_2\rangle\langle x_2|\lambda_1\rangle\right]$$

$$\psi_B(x_1,x_2) = \frac{1}{\sqrt{2}}\left[\langle x_1|\lambda_1\rangle\langle x_2|\lambda_2\rangle + \langle x_1|\lambda_2\rangle\langle x_2|\lambda_1\rangle\right]$$

$$|\lambda_1,\lambda_2\rangle_{F(B)} = \frac{1}{\sqrt{2}}\left[\underset{x_1}{|\lambda_1\rangle} \otimes \underset{x_2}{|\lambda_2\rangle} + \xi\, \underset{x_1}{|\lambda_2\rangle} \otimes \underset{x_2}{|\lambda_1\rangle}\right]$$

$\xi = -1$; fermion ; $\xi = 1$ Boson.

$$|\lambda_1,\lambda_2,\cdots,\lambda_N\rangle = \frac{1}{\sqrt{N!\,\prod_{\lambda=0}^{\infty}(n_\lambda!)}}\sum_P \xi^{(1-\mathrm{sgn}P)/2}\,|\lambda_{P_1}\rangle\otimes|\lambda_{P_2}\rangle\otimes\cdots\otimes|\lambda_{P_N}\rangle$$

n_λ represents the particle number in state $|\lambda\rangle$

fermion $n_\lambda \le 1$

$$\boxed{\mathrm{sgn}\,P = \begin{cases} 1, & \text{even} \\ -1, & \text{odd} \end{cases}}$$

P : permutation Group.

$$(P_1, P_2, \cdots, P_N) \leftarrow (1, 2, \cdots, N)$$

$$(2, 3, 1, 4) \leftarrow (1, 2, 3, 4)$$

fermion case : slater determinant.

N - particle.

$$|\underbrace{1,1,1,1}_{4};\underbrace{2,2}_{2};\underbrace{3,3,3}_{3};\underbrace{4}_{1},\underbrace{\ }_{0}\underbrace{6,6}_{2};\cdots\rangle$$

$$|4, 2, 3, 1, 0, 2, \cdots\rangle$$ occupation number representation

$$\sum_i n_i = N \quad F^N \quad |\Psi\rangle = \sum_{\substack{n_1, n_2\cdots \\ \sum n_i = N}} C_{n_1,n_2\cdots}\,|n_1, n_2, \cdots\rangle$$

$$F = \bigoplus_{N=0}^{\infty} F^N \quad (2.2)$$ Fock space.

$a_i^\dagger : \mathcal{F} \to \mathcal{F}$

Boson 1

Fermion $(-1)^{S_i}$

(2.3)

$(*)$ $$a_i^\dagger |n_1, \cdots, n_i, \cdots\rangle \equiv \sqrt{n_i+1}\, \xi^{S_i} |n_1, \cdots, n_{i-1}, n_i+1, n_{i+1}, \cdots\rangle$$

$$S_i = \sum_{j=1}^{i-1} n_j \qquad \xi = \begin{cases} -1 & F \\ 1 & B \end{cases}$$

$$\boxed{|n_1, n_2, \cdots\rangle = \prod_i \frac{1}{\sqrt{n_i!}} (a_i^\dagger)^{n_i} |0\rangle} \qquad (2.4)$$

HW 1: $a^\dagger$: creation operator

$\forall i, j$

$\forall |n_1, n_2, \cdots\rangle$

easy to check

$$(a_i^\dagger a_j^\dagger - \xi a_j^\dagger a_i^\dagger) |n_1, n_2, \cdots\rangle = 0$$

$\forall i, j$ $\quad [a_i^\dagger, a_j^\dagger]_\xi = 0$; $\Rightarrow$ (2.5)

ETC

$$\langle n_1, \cdots, n_i, \cdots | a_i^\dagger | n_1', \cdots, n_i', \cdots\rangle = \sqrt{n_i'+1}\, \xi^{S_i'} \cdot \delta_{n_1 n_1'} \cdots \delta_{n_i, n_i'+1} \cdots$$

$\Updownarrow$

$$\langle n_1', \cdots, n_i', \cdots | a_i | n_1, \cdots n_i, \cdots\rangle^* = \sqrt{n_i}\, \xi^{S_i} \delta_{n_1' n_1} \cdots \delta_{n_i', n_i-1} \cdots$$

$$a_i |n_1, \cdots n_i, \cdots\rangle = \sqrt{n_i}\, \xi^{S_i} |n_1, \cdots, n_{i-1}, n_i - 1, n_{i+1}, \cdots\rangle$$

(2.6)

$a^\dagger : \mathcal{F}^N \to \mathcal{F}^{N+1}$

$a : \mathcal{F}^N \to \mathcal{F}^{N-1}$

ETC: $\forall i,j.$ $[a_i, a_j^\dagger]_\xi = \delta_{ij}$ $\quad [a_i, a_j]_\xi = 0; \quad [a_i^\dagger, a_j^\dagger]_\xi = 0;$

$$[A, B]_\xi = \begin{cases} AB + BA & F \\ AB - BA & B \end{cases}$$

$$\begin{cases} |\tilde{\lambda}\rangle = \sum_\lambda |\lambda\rangle\langle\lambda|\tilde{\lambda}\rangle \\ |\lambda\rangle \equiv a_\lambda^\dagger |0\rangle \\ |\tilde{\lambda}\rangle \equiv a_{\tilde{\lambda}}^\dagger |0\rangle \end{cases}$$

$$a_{\tilde{\lambda}}^\dagger = \sum_\lambda \langle\lambda|\tilde{\lambda}\rangle a_\lambda^\dagger \quad (2.8)$$

$$a_{\tilde{\lambda}} = \sum_\lambda \langle\tilde{\lambda}|\lambda\rangle a_\lambda$$

$$a_k = \int_0^L dx \, \langle k|x\rangle \, a(x) \qquad \langle k|x\rangle = \langle x|k\rangle^* = \frac{e^{-ikx}}{\sqrt{L}}$$

$$a(x) = \sum_k \langle x|k\rangle a_k \quad (2.9)$$

Representation of one body operator

$$\hat{T} = \sum_n p_n^2/2m \qquad \hat{V} = \sum_n V(\hat{x}_n) \qquad \sum_n \hat{S}_n$$

occupation number operator $\quad \hat{n}_\lambda = a_\lambda^\dagger a_\lambda \quad (2.10)$

ETC $\ast$ $\hat{n}_\lambda (a_\lambda^\dagger)^n |0\rangle = n (a_\lambda^\dagger)^n |0\rangle$

ETC $\ast$ $\hat{n}_{\lambda_j} |n_{\lambda_1}, n_{\lambda_2}, \cdots n_{\lambda_j}, \cdots\rangle = n_{\lambda_j} |n_{\lambda_1}, n_{\lambda_2}, \cdots\rangle$

$$\hat{O}_1 = \sum_i O_{\lambda_i} |\lambda_i\rangle\langle\lambda_i| \qquad O_{\lambda_i} = \langle\lambda_i|\hat{O}|\lambda_i\rangle$$

$$\langle n'_{\lambda_1}, n'_{\lambda_2} \cdots | \hat{O}_1 | n_{\lambda_1}, n_{\lambda_2}, \cdots\rangle = \sum_i O_{\lambda_i} \cdot n_{\lambda_i} \langle n'_{\lambda_1} n'_{\lambda_2} \cdots | n_{\lambda_1}, n_{\lambda_2}, \cdots\rangle$$

$$= \langle n'_{\lambda_1} n'_{\lambda_2} \cdots \Big| \sum_i O_{\lambda_i} \cdot \hat{n}_{\lambda_i} \Big| n_{\lambda_1}, n_{\lambda_2}, \cdots \rangle$$

$$\boxed{\hat{O}_1 = \sum_{\lambda=0}^{\infty} O_\lambda \hat{n}_\lambda = \sum_{\lambda=0}^{\infty} \langle \lambda | \hat{o} | \lambda \rangle a^\dagger_\lambda a_\lambda} \quad (2.11)$$

tranform to general basis: $\hat{O}_1 = \sum_{\mu\nu} \langle \mu | \hat{o} | \nu \rangle a^\dagger_\mu a_\nu$

$$\vec{S} = \frac{\hbar}{2} \vec{\sigma} \qquad (S_i)_{\alpha\alpha'} = \frac{\hbar}{2} (\sigma_i)_{\alpha\alpha'}$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad (2.12)$$

$$\hat{S} = \frac{\hbar}{2} \sum_{\lambda, \alpha\alpha'} a^\dagger_{\lambda\alpha'} \vec{\sigma}_{\alpha'\alpha} a_{\lambda\alpha} \quad (2.13)$$

One-body Hamiltonian in real space.

$$\hat{H} = \int d^d r \; a^\dagger(\vec{r}) \left[\frac{\hat{p}^2}{2m} + V(\vec{r}) \right] a(\vec{r}) \quad (2.14)$$

$$\hat{p} = -i\hbar\partial \quad (2.15)$$

Local density operator $\hat{\rho}(\vec{r}) = a^\dagger(\vec{r}) a(\vec{r})$

total density operator $\hat{N} = \int d^d\vec{r} \; a^\dagger(\vec{r}) a(\vec{r})$

$\hat{N} = \sum_i a^\dagger_i a_i$ discrete

Representation of two-body potential.

$$V(\vec{r}_m, \vec{r}_n) = V(\vec{r}_n, \vec{r}_m)$$

$$\hat{V} | r_1, r_2, \cdots, r_N \rangle = \sum_{n<m}^{N} V(r_n, r_m) | r_1, r_2, \cdots, r_N \rangle$$

$$= \frac{1}{2} \sum_{n \neq m}^{N} V(r_n, r_m) \, | r_1, r_2, \cdots, r_N \rangle$$

Guess

$$\hat{V} = \frac{1}{2} \int d^d r \int d^d r' \; a^{+}(r) \, a^{+}(r') \, \underbrace{V(r,r')}_{\text{c-number}} \, a(r') \, a(r)$$

$$a^{+}(r) \, a^{+}(r') \, a(r') \, a(r) \, | r_1, r_2, \cdots, r_N \rangle$$

$$= a^{+}(r) \, a^{+}(r') \, a(r') \, a(r) \, a^{+}(r_1) \, a^{+}(r_2) \cdots \underset{a^{+}(r_n)}{\cdot} \cdots a^{+}(r_N) | 0 \rangle$$

$$= \sum_{n=1}^{N} \xi^{n-1} \delta(r - r_n) \, a^{+}(r_n) \, \overbrace{a^{+}(r') \, a(r')}^{\rho(r')} \, a^{+}(r_1) \, a^{+}(r_2) \cdots a^{+}(r_{n-1}) \cdot a^{+}(r_{n+1}) \cdots a^{+}(r_N) | 0 \rangle$$

$$\to \sum_{m \neq n}^{N} \delta(r' - r_m)$$

$$= \sum_{n=1}^{N} \delta(r - r_n) \sum_{m \neq n} \delta(r' - r_m) \, \xi^{n-1} \, a^{+}(r_n) \, a^{+}(r_1) \, a^{+}(r_2) \cdots a^{+}(r_N) | 0 \rangle$$

$$= \sum_{n=1}^{N} \sum_{m \neq n}^{N} \delta(r - r_n) \, \delta(r' - r_m) \, | r_1, r_2, \cdots, r_N \rangle$$

$$[a(r), a^{+}(r_N)]_{\xi} = \delta(r - r_N)$$

$$\hat{V} = \frac{1}{2} \int d^d r \int d^d r' \; a^{+}(r) \, a^{+}(r') \, a(r') \, a(r) \, V(r, r')$$

$$\vec{S} = \frac{\hbar}{2} \vec{\sigma} \qquad \vec{S}_{\alpha\beta} = \frac{\hbar}{2} \vec{\sigma}_{\alpha\beta}$$

Spin-spin interaction.

$$\hat{V} = \frac{1}{2} \int d^d r \int d^d r' \sum_{\alpha\alpha'\beta\beta'} J(r, r') \, \vec{S}_{\alpha\beta} \cdot \vec{S}_{\alpha'\beta'} \, a^{+}_{\alpha}(r) \, a^{+}_{\alpha'}(r') \, a_{\beta'}(r') \, a_{\beta}(r)$$

$$\alpha = 1, 2 \qquad \beta = 1, 2$$

2.2 application of 2nd quantization.

$$\hat{H} = \hat{H}_0 + \hat{V}_{Le}$$

$$V_{ee} = \sum_{\sigma\sigma'} \frac{1}{2} \int d^d r \int d^d r' \, V(r-r') \qquad \sigma = \uparrow\downarrow$$

$$\times \; a_\sigma^+(r) \, a_{\sigma'}^+(r') \, a_{\sigma'}(r') \, a_\sigma(r)$$

$$H_0 = \int d^{\underset{\downarrow}{d=3}} r \quad a_\sigma^+(r) \left[\frac{\hat{p}^2}{2m} + V_{Le}(r) \right] a_\sigma(r)$$

$\hat{p} \Leftarrow -i\hbar\partial_x$

$$V_{Le} = \sum_i V_{Le}(r - R_i) \quad e\text{-}ph$$

$$a_k = \int_0^L dx \, \langle k|x\rangle \, a(x)$$

$$\psi_{k,n}(r) = e^{ikr} u_{k,n}(r) \qquad \langle k|x\rangle = e^{-ikx}/\sqrt{L} \quad (2.19)$$

ETC

$$\hat{H}_0 = \sum_k \frac{\hbar^2 k^2}{2m} a_{k\sigma}^+ a_{k\sigma} \quad \leftarrow \text{non-interacting electrons}$$

HW2

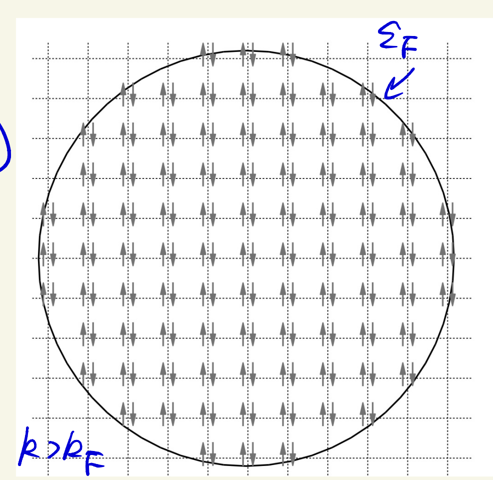
$$V_{ee} = \frac{1}{2V} \sum_{kk'q} V_{ee}(q) \, a^+_{k-q,\sigma} \, a^+_{k'+q,\sigma'} \, a_{k',\sigma'} \, a_{k,\sigma} \quad (2.19)$$

☆

$$V_{ee}(q) = \frac{e^2}{4\pi\varepsilon_0 q^2}$$

non-interacting e

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m} \qquad \varepsilon_F = \frac{\hbar^2 k_F^2}{2m}, \quad (2.20)$$



Ground state: $|\Omega\rangle = N_0 \prod_{|k|\le k_F, \sigma} a_{k\sigma}^+ |0\rangle$

⊛ $C_{k\sigma}|\Omega\rangle = 0$

$$C_{k\sigma} = \begin{cases} a_{k\sigma} & k > k_F \\ a_{k\sigma}^+ & k \le k_F \end{cases}, \quad C_{k\sigma}^+ = \begin{cases} a_{k\sigma}^+ & k > k_F \\ a_{k\sigma} & k \le k_F \end{cases} \quad (2.21)$$

Tight-binding systems:

$$\circledast \quad |\psi_{Rn}\rangle = \frac{1}{\sqrt{N}} \sum_{k}^{B.Z.} e^{-ikR} |\psi_{kn}\rangle \qquad (2.22) \Leftarrow$$

$$|\psi_{kn}\rangle = \frac{1}{\sqrt{N}} \sum_{R} e^{ikR} |\psi_{Rn}\rangle$$

$$\psi_{Rn}(r) \equiv \langle r|\psi_{Rn}\rangle \qquad R_n \sim r$$

converge when r is close to R_n

$\circledast$ $|\psi_{Rn}\rangle$ form an orthonormal basis

$$|r\rangle = \sum_{R} |\psi_R\rangle\langle\psi_R|r\rangle = \sum_{R} \psi^*_R(r)\, |\psi_R\rangle$$

$$a^+_\sigma(r) = \sum_{R} \psi^*_R(r)\, a^+_{R\sigma} = \sum_{i} \psi^*_{R_i}(r)\, a^+_{i\sigma} \qquad (2.23)$$

$$a^+_{k\sigma} = \frac{1}{\sqrt{N}} \sum_{i} e^{i\vec{k}\cdot\vec{R}_i} a^+_{i\sigma}$$

$$a^+_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{k}^{B.Z.} e^{-i\vec{k}\cdot\vec{R}_i} a^+_{k\sigma} \qquad (2.24)$$

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

$$\mathcal{H}_0 = \sum_{k} \varepsilon_k a^+_{k\sigma} a_{k\sigma} = \frac{1}{N} \sum_{i i'} \sum_{k} e^{ik(R_i - R_{i'})} \varepsilon_k\, a^+_{i\sigma} a_{i'\sigma}$$

$$t_{ij} = -t, \quad \langle i,j\rangle$$

$$= \sum_{i i'} a^+_{i\sigma}\, \underline{t_{ii'}}\, a_{i'\sigma} \simeq \sum_{\langle ij\rangle} a^+_{i\sigma}\, t_{ij}\, a_{j\sigma}$$

$$t_{ii'} = \frac{1}{N} \sum_{k} e^{i\underline{k(R_i - R_{i'})}} \varepsilon_k$$

$$|R_i - R_{i'}| = \begin{cases} 0 & \text{onsite} \checkmark \\ a & \text{N.N.} \checkmark \\ \vdots & \end{cases}$$

if ε_k is constant; $\quad \sum_{k} e^{i\underline{k(R_i - R_{i'})}} \propto \delta_{ii'}$

nearest neighbour N.N. $\quad \langle i, i'\rangle \quad t_{ii'} = -t$;

2D square lattice:

$$\varepsilon_k = -2t(\cos k_x a + \cos k_y a)$$

$k \to 0$; Taylor expansion: $m^* = \frac{\hbar^2}{2ta^2}$

* SSH model ← topological
  Su - Schrieffer - Heeger model

* tight-binding model interaction.
  → direct interaction
  → exchange interaction
  → Hubbard model

* FM / AFM spin wave.

Suggest reading:

Li Zhengzhong chapter 3, 4, 6

Taylor & Heinonen chapter 2, 3, 4, 6, 7, 10

Althand & Simons chapter 2

Khomskii chapter 5, 6, 7, 8, 9, 10, 11, 13

$$V = \frac{1}{2}\sum_{\sigma_1\sigma_2}\int dr_1\, dr_2\ \frac{e_0^2}{|r_2-r_1|}\ a^+_{\sigma_1}(r_1)\ a^+_{\sigma_2}(r_2)\ a_{\sigma_2}(r_2)\ a_{\sigma_1}(r_1)$$

$$e_0^2 = \frac{e^2}{4\pi\varepsilon_0}$$

$$V = \frac{1}{2}\sum_{\sigma_1\sigma_2}\ \sum_{\substack{k_1k_2\\k_3k_4}} \underbrace{\langle k_3\sigma_1\ k_4\sigma_2 |\, V\, | k_1\sigma_1\ k_2\sigma_2\rangle}\ a^+_{\underline{k_3}\sigma_1}\ a^+_{\underline{k_4}\sigma_2}\ a_{k_2\sigma_2}\ a_{k_1\sigma_1}$$

$$\frac{e_0^2}{V^2}\int \underset{dr_1}{\underline{d^3r_1}}\ \underset{d(r_2-r_1)}{\underline{d^3r_2}}\ \frac{e^{i(k_1r_1+k_2r_2-k_3r_1-k_4r_2)}}{|r_1-r_2|}$$

$$e^{i(k_1r_1+k_2r_2-k_3r_1-k_4r_2)} = e^{i[k_1-k_3+k_2-k_4]r_1}\, e^{i[k_2-k_4][r_2-r_1]}$$

$$\int e^{i[k_1-k_3+k_2-k_4]r_1} = V\cdot \underline{\delta_{k_3,k_1+q}} \qquad q\equiv k_2-k_4$$

$$V_q \equiv \int d^3r\ \frac{e_0^2}{r}\ e^{i\vec{q}\cdot\vec{r}} = \frac{4\pi e_0^2}{q^2}$$

ETC: $\int d^2r\ \frac{e_0^2}{r}\ e^{i\vec{q}\cdot\vec{r}} = \frac{2\pi e_0^2}{q}$

$$V = \frac{1}{2V}\sum_{\sigma_1\sigma_2}\ \sum_{k_1k_2q} V_q\cdot a^+_{k_1+q\,\sigma_1}\ a^+_{k_2-q,\sigma_2}\ a_{k_2\sigma_2}\ a_{k_1\sigma_1}$$

eg: SSH model

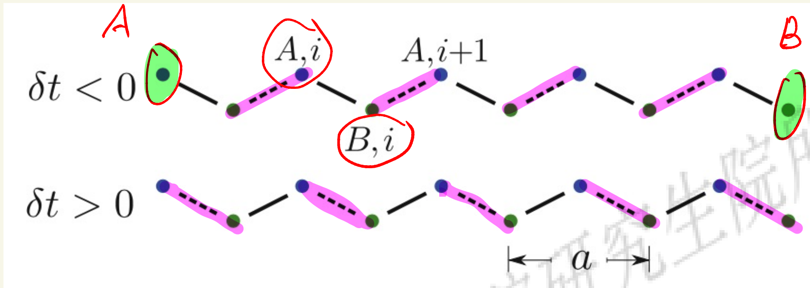
Su - Shrieffer - Heeger model

W.P. Su, J.R. Schrieffer, A.J. Heeger, Phys. Rev. Lett. **42**, 1698 (1979)

A.J. Heeger, S. Kivelson, J.R. Schrieffer, W.P. Su, Rev. Mod. Phys. **60**, 781 (1988)

$$\mathcal{H} = \sum_{n=1}^{N} (t+\delta t)\, \underline{C_{An}^{+} C_{Bn}} + \sum_{n=1}^{N-1} (t-\delta t)\, \underline{C_{A,n+1}^{+} C_{Bn}} + h.c.$$

Similar to 1D kitaev chain



Zero energy mode

Fourier transform: $a_k = \frac{1}{\sqrt{N}} \sum_n e^{-ik\cdot na} C_{A,n}$

$k \in [-\pi, \pi]$

$b_k = \frac{1}{\sqrt{N}} \sum_n e^{-ik\, na} C_{B,n}$.

$$\mathcal{H} = (t+\delta t) \sum_{k\in B.Z.} (a_k^+ b_k + b_k^+ a_k) + (t-\delta t) \sum_k \left(e^{ik} a_k^+ b_k + e^{-ik} b_k^+ a_k \right)$$

$$\psi_k = \begin{pmatrix} a_k \\ b_k \end{pmatrix}$$

$$\mathcal{H} = \sum_k \psi_k^+ \left\{ \begin{bmatrix} 0 & [(t+\delta t) + (t-\delta t)\cos k] - i \sin k\, (t-\delta t) \\ * & 0 \end{bmatrix} \right\} \psi_k$$

$$= \sum_k \psi_k^+ \left[[(t+\delta t) + (t-\delta t)\cos k]\, \sigma_x + (t-\delta t) \sin k \cdot \sigma_y \right] \psi_k .$$

$\sigma_x \to \sigma_z$, $\sigma_y \to \sigma_x$, $\sigma_z \to \sigma_y$; $k \to k+\pi$

massive Dirac equation

$$\mathcal{H} = \sum_k \psi_k^+ \left\{ \underbrace{\left[2\delta t + 2(t-\delta t) \sin^2 \tfrac{k}{2} \right]}_{\text{mass term}} \sigma_z - \underline{(t-\delta t) \sin k}\, \sigma_x \right\} .$$

$$\begin{cases} d_x = -(t-\delta t) \sin k \\ d_z = \underline{2\delta t} + \underline{2(t-\delta t) \sin^2 \frac{k}{2}} \end{cases}$$

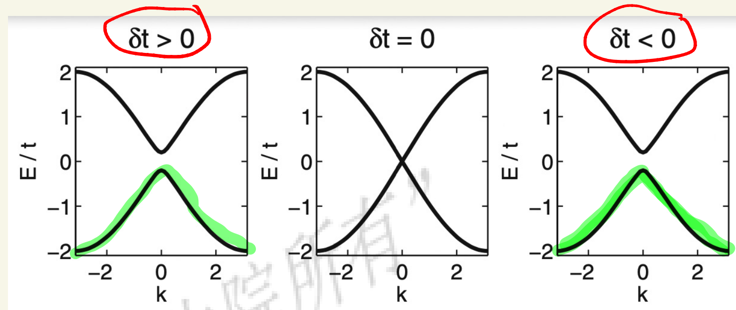
$E_\pm = \pm \sqrt{d_x^2 + d_z^2}$

$k = 0$; $d_x = 0$

$d_z = 2\cdot\delta t$

$\delta t < 0$; $\delta t \cdot t < 0$; mass change sign.

$\delta t = 0 \iff$ gap closing condition.



for negative energy band:

$$|\psi\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} \mathrm{sgn}(d_x)\sqrt{1 - \frac{d_z}{\sqrt{d_x^2 + d_z^2}}} \\ \sqrt{1 + \frac{d_z}{\sqrt{d_x^2+d_z^2}}} \end{bmatrix}$$

Zak phase

$$\gamma = \int_{-\pi}^{\pi} dk \, \langle \psi | i\partial_k | \psi \rangle = \frac{\pi}{2}\left[\mathrm{sgn}(t-\delta t) - \mathrm{sgn}(\delta t)\right]$$

$\delta t < 0 \; ; \; \gamma = \pi$

massive Dirac equation

$$H = \sum_k \psi_k^+ \left\{ \underbrace{\left[2\delta t + 2(t-\delta t)\sin^2\frac{k}{2}\right]}_{\text{mass term}} \sigma_z - (t-\delta t)\sin k \, \sigma_x \right\}.$$

Interaction effect in tight-binding system.

$$V = \frac{1}{2}\sum_{\sigma_1\sigma_2} \int dr dr' \frac{e_0^2}{|r-r'|} a_\sigma^+(r) \, a_{\sigma'}^+(r') \, a_{\sigma'}(r') \, a_\sigma(r)$$

$$a_\sigma^+(\vec{r}) = \sum_i \psi_{R_i}^*(\vec{r}) \cdot a_{i\sigma}^+ \qquad 2.2]$$

$$\boxed{\hat{V}_{ee} = \sum_{ii'jj'} U_{ii'jj'} \, a_{i\sigma}^+ \, a_{i'\sigma'}^+ \, a_{j'\sigma'} \, a_{j\sigma}}$$

$$U_{ii'jj'} = \frac{1}{2}\int d^d r \int d^d r' \, \psi_{R_i}^*(r) \, \psi_{R_j}(r) \, V(r-r') \, \psi_{R_{i'}}^*(r') \, \psi_{R_{j'}}(r')$$

(A) direct term $U_{ii'ii'} \equiv V_{ii'}$

When $i \neq i'$: $\sum_{\sigma\sigma'} \sum_{i \neq i'} V_{ii'} \, a^+_{i\sigma} a^+_{i'\sigma'} a_{i'\sigma'} a_{i\sigma}$

$= \sum_{\sigma\sigma'} \sum_{i \neq i'} V_{ii'} \, \hat{n}_{i\sigma} \hat{n}_{i'\sigma'}$ $\qquad \hat{n}_i = \sum_\sigma a^+_{i\sigma} a_{i\sigma}$

$= \sum_{i \neq i'} V_{ii'} \, \hat{n}_i \cdot \hat{n}_{i'}$ ← induce charge density wave

charge - charge

(B) exchange term $i \neq j$. $\qquad J^E_{ij} = U_{\underset{1\,2\,3\,4}{ijji}}$

Heisenberg model

$$\sum_{i\neq j} \underbrace{U_{ijji} \, a^+_{i\sigma} a^+_{j\sigma'} a_{i\sigma'} a_{j\sigma}} = \boxed{-2\sum_{i\neq j} J^E_{ij} \left(\hat{S}_i \cdot \hat{S}_j + \tfrac{1}{4} \hat{n}_i \cdot \hat{n}_j \right)}$$

spin - spin

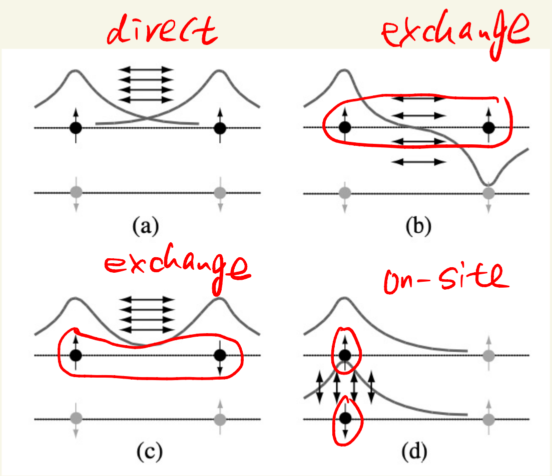
$\boxed{\hbar = 1}$ $\qquad \vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z) \quad \alpha, \beta = \{1, 2\}$, $\qquad \boxed{\text{Spin } 1/2}$ $\boxed{\text{High spin}}$ $2S+1$

Hint

$\hat{S}_i \equiv \frac{1}{2} \hat{a}^+_{i\alpha} \vec{\sigma}_{\alpha\beta} \hat{a}_{i\beta}$ $\qquad \vec{\sigma}_{\alpha\beta} \cdot \vec{\sigma}_{\gamma\delta} = 2 \delta_{\alpha\delta} \delta_{\beta\gamma} - \delta_{\alpha\beta} \delta_{\gamma\delta}$

$\hat{S}_j \equiv \frac{1}{2} \hat{a}^+_{j\gamma} \vec{\sigma}_{\gamma\delta} a_{j\delta}$

$$\boxed{\begin{aligned} \hat{S}_i \cdot \hat{S}_j &= \frac{1}{4} a^+_{i\alpha} a_{i\beta} a^+_{j\gamma} a_{j\delta} \left(\vec{\sigma}_{\alpha\beta} \cdot \vec{\sigma}_{\gamma\delta} \right) \\ &= -\tfrac{1}{2} a^+_{i\alpha} a^+_{j\beta} a_{i\beta} a_{j\alpha} - \frac{1}{4} \hat{n}_i \hat{n}_j \end{aligned}}$$



(a) (b) (c) (d)

(C) Atomic limit: 张礼 葛墨林 Chapter 3, 7, 10 ✓