

Quantum Many Particle Theory

Despite of the enormous success of band theory in the single-electron approximation, one still needs to place these band theories within the more fundamental many-particle theory to seek justification or to show the limit.

For this purpose, one needs to include electron-electron interactions seriously.

We shall introduce several important approaches in this part.

Wave function approach

In this approach, one adopts the adiabatic approximation in which ions are assumed be fixed. In this approximation, one has

$$\hat{H} = \frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} + \sum_i V(\vec{r}_i)$$

$V(\vec{r}_i)$ is the potential due to ions.

Note that this approximation essentially decouples electrons & phonons and may break down in some cases such as Jahn-Teller effect.

In this case, one needs to solve the Schrödinger equation

$$\left[\underbrace{\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_i V(r_i)}_{H_0} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|r_i - r_j|} \right] \psi(r_1, r_2, \dots, r_N) = E \psi(r_1, r_2, \dots, r_N) \quad \text{--- (1)}$$

where $\psi(r_1, r_2, \dots, r_N)$ is many-electron wave function.

The Hartree Approximation

As a first step, neglecting the antisymmetric requirement,

$$\psi(r_1, r_2, \dots, r_N) = \prod_{i=1}^N \phi_i(r_i) \quad , \quad i \text{ includes } \delta = \uparrow \text{ \& \downarrow}$$

where ϕ_i is a one-particle wave function

Hartree suggested to use ψ to minimize

$$E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$$

This is a variational approach. One

requires $\frac{\delta E}{\delta \phi_i(r_i)} = 0$

This can be done by minimizing $\langle \psi | H | \psi \rangle$ under the constraint $\langle \phi_i | \phi_j \rangle = \delta_{ij}$

Now, $\langle \psi | H | \psi \rangle$

$$= \sum_i \int dr \phi_i^*(r) \left[\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \phi_i(r) \left[\prod_{j \neq i} \int dr_j \phi_j^*(r_j) \phi_j(r_j) \right] + \frac{e^2}{2} \int dr \int dr' \phi_i^*(r) \phi_i(r) \frac{1}{|r - r'|} \prod_{j \neq i} \phi_j^*(r_j) \phi_j(r_j)$$

Under the constraint $\int d\mathbf{r} \Phi_i^*(\mathbf{r}) \Phi_i(\mathbf{r}) = 1$, one introduces the Lagrangian multiplier ε_i and

$$\frac{\delta}{\delta \Phi_i^*(\mathbf{r})} \langle \Psi | H | \Psi \rangle - \varepsilon_i \frac{\delta}{\delta \Phi_i^*(\mathbf{r})} \left[\int d\mathbf{r} \Phi_i^*(\mathbf{r}) \Phi_i(\mathbf{r}) - 1 \right] = 0$$

we get

$$\left[\frac{-\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) + \sum_{j \neq i} e^2 \int \frac{|\Phi_j(\mathbf{r}')|^2}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \right] \Phi_i(\mathbf{r}) = \varepsilon_i \Phi_i(\mathbf{r}) \quad \text{--- (3)}$$

which looks like one-electron energy eigenvalue

problem with $V_{\text{eff}} = V(\mathbf{r}) + \sum_{j \neq i} e^2 \int \frac{|\Phi_j(\mathbf{r}')|^2}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'$

$\therefore$ In the Hartree approximation, the potential

seen by each electron is self-consistently

determined by the average distribution $\sum_{j \neq i} |\Phi_j(\mathbf{r}')|^2$ of other electrons.

Note that substituting eq (3) into eq. (2),

one finds

$$E = \langle \Psi | H | \Psi \rangle$$

$$= \sum_i \varepsilon_i - \frac{1}{2} \sum_{i \neq j} e^2 \iint \frac{|\Phi_i(\mathbf{r})|^2 |\Phi_j(\mathbf{r}')|^2}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}' \quad \text{--- (4)}$$

The Hartree equation (eq (3)) can be solved

by iteration: One first starts from a particular set of approximate $\phi_i^0(r)$ and then computes V_{eff}^0 . From V_{eff}^0 , one computes $\phi_i^1(r)$ from eq. (3) and then V_{eff}^1 . The iteration is repeated until it converges.

The Hartree - Fock Approximation

The Hartree approximation is obviously not realistic because the antisymmetric condition is not included.

If one replaces $\psi(r_1, r_2, \dots, r_N) = \prod_{i=1}^N \phi_i(r_i)$ by the Slater determinant

$$\psi(r_1, r_2, \dots, r_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(r_1) & \dots & \phi_1(r_N) \\ \phi_2(r_1) & \dots & \phi_2(r_N) \\ \vdots & & \vdots \\ \phi_N(r_1) & \dots & \phi_N(r_N) \end{vmatrix} \quad \dots (5)$$

and re-compute the minimization. It is known as the Hartree - Fock approximation.

For H_0 , one can easily see that eq. (5) doesn't change the result in eq. (2).

There are $N!$ equivalent contributions.

$$\therefore \langle \psi | H_0 | \psi \rangle = \sum_i \int dr \phi_i^*(r) \left[-\frac{\hbar^2}{2m} \nabla^2 + v(r) \right] \phi_i(r)$$

The crucial difference is the Coulomb term now containing the exchange term:

$$- \frac{e^2}{2} \sum_{i \neq j} \int dr \int dr' \phi_i^*(r) \phi_j(r) \frac{1}{|r-r'|} \phi_i(r') \phi_j^*(r')$$

For ϕ , one picks $\phi_j(r) \phi_i(r')$; while for ϕ^* , one picks $\phi_i^*(r) \phi_j^*(r')$. They are exchanged

in if j w.r.t. the term $\frac{e^2}{2} \sum_{i \neq j} \int dr \int dr'$

$$\phi_i^*(r) \phi_i(r) \frac{1}{|r-r'|} \phi_j(r') \phi_j^*(r')$$

In the determinant, permute (i, j) results in a minus sign.

$$\therefore \langle \psi | H | \psi \rangle$$

$$= \sum_i \int dr \phi_i^*(r) \left[-\frac{\hbar^2}{2m} \nabla^2 + v(r) \right] \phi_i(r)$$

$$+ \frac{e^2}{2} \sum_{i \neq j} \int dr \int dr' |\phi_i(r)|^2 \frac{1}{|r-r'|} |\phi_j(r')|^2$$

$$- \frac{e^2}{2} \sum_{i \neq j} \int dr \int dr' \phi_i^*(r) \phi_j(r) \frac{1}{|r-r'|} \phi_i(r') \phi_j^*(r') \quad \text{--- (6)}$$

Minimization leads to

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + v_{\text{eff}}(r) \right] \phi_i(r) = \underbrace{\sum_{j \neq i} \left[e^2 \int \frac{\phi_j^*(r') \phi_j(r')}{|r-r'|} dr' \right]}_{L = -\frac{e^2}{r}} \phi_j(r) = \sum_i \phi_i(r)$$

Just as the Hartree approximation, one also

needs to solve eq. (1) self-consistently to obtain the solution $\Phi_i(\vec{r})$ and thus the total energy $\sum_i \epsilon_i$.

However, the Hartree-Fock approximation can be also considered as an approximation to estimate

the energy without imposing self-consistent

condition. In the nearly-free electron approximation, one sets

$$\Phi_i(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}_i \cdot \vec{r}}$$

$$V(\vec{r}) = 0$$

$$\therefore V_{\text{eff}}(\vec{r}) = \sum_{j \neq i} e^2 \int \frac{|\Phi_j(\vec{r}')|^2}{|\vec{r} - \vec{r}'|} d\vec{r}' = \sum_j -e^2 \int \frac{|\Phi_j(\vec{r}')|^2}{|\vec{r} - \vec{r}'|}$$

$$= \frac{2e^2}{V} \underbrace{\sum_{\vec{k} \neq 0}^{\frac{k_F}{2}} \int \frac{d\vec{r}'}{|\vec{r} - \vec{r}'|}}_{\substack{\uparrow \\ |\Phi_j|^2 = \frac{1}{V}, \text{ spin} \Rightarrow \times 2}} - \frac{e^2}{V} \int \frac{d\vec{r}'}{|\vec{r} - \vec{r}'|}$$

Cancelled by
the background
charge of ions

$$\frac{e^2}{V} \int \frac{d\vec{r}'}{|\vec{r} - \vec{r}'|} = \frac{e^2}{V} \int \frac{d\vec{R}}{R} = \frac{e^2}{V} 4\pi \int_0^L R dR$$

$$\rightarrow \frac{1}{3} \times L^2 \rightarrow 0 \text{ as } L \rightarrow \infty$$

$$\therefore V_{\text{eff}} = 0 \quad \dots \textcircled{A}$$

$$\text{On the other hand, } V_{\text{exc}} = -\frac{e^2}{V} \sum_{\vec{k}_j \neq \vec{k}_i} \int d\vec{r}' \frac{e^{i(\vec{k}_j - \vec{k}_i) \cdot \vec{r}'}}{|\vec{r} - \vec{r}'|}$$

At 3D $\therefore \int \frac{e^{i\vec{k}\cdot\vec{r}}}{r} d^3r = \frac{4\pi}{k^2} \quad \left(\frac{1}{4\pi r} \rightarrow \frac{1}{k^2} \right)$

$$\therefore v_{exc} = \frac{-e^2}{V} \sum_{\vec{k}' \neq \vec{k}} \frac{4\pi}{(\vec{k}-\vec{k}')^2} \quad (\vec{k} \rightarrow \vec{k})$$

$$= -e^2 \int \frac{d^3k'}{(2\pi)^3} \frac{4\pi}{(\vec{k}-\vec{k}')^2}$$

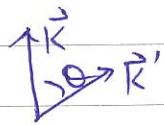
$$= -\frac{e^2}{2\pi^2} \int_0^{k_F} \frac{d^3k'}{(\vec{k}-\vec{k}')^2} \quad \dots (9)$$

Note that unlike the Hartree approximation, here we only consider one species of spin. Hence there is no factor of 2.

$$\therefore \epsilon_k = \frac{\hbar^2 k^2}{2m} - \frac{e^2}{2\pi^2} \int_0^{k_F} \frac{d^3k'}{(\vec{k}-\vec{k}')^2} \quad \dots (10)$$

If we align $\vec{k}$ along z-axis, we have

$$\int_0^{k_F} \frac{d^3k'}{(\vec{k}-\vec{k}')^2} = \int_0^{k_F} \int_0^\pi \frac{2\pi \sin\theta k'^2 dk' d\theta}{k'^2 - 2k'k \cos\theta + k^2}$$



$$= \int_0^{k_F} 2\pi \left(\int_{-1}^1 \frac{dx}{k^2 + k'^2 - 2k'kx} \right) k'^2 dk'$$

$$= \int_0^{k_F} 2\pi \frac{1}{2k'k} \ln \frac{k^2 + k'^2 + 2k'k}{k^2 + k'^2 - 2k'k} \times k'^2 dk'$$

$$= \frac{2\pi}{k} \int_0^{k_F} \ln \left| \frac{k+k'}{k-k'} \right| k' dk'$$

$$= \frac{2\pi}{k} k_F^2 \int_0^1 \ln \left| \frac{k_F + x}{k_F - x} \right| x dx$$

$$= 2\pi k_F \left[\int_0^1 \ln \left(\frac{y}{1-y} \right) x dx \right] \quad y = k/k_F$$

$$\frac{1}{y} \int_0^1 x \ln \left| \frac{y+x}{y-x} \right| dx$$

$$= \frac{1}{y} \int \ln \left| \frac{y+x}{y-x} \right| d\frac{x^2}{2}$$

$$= \frac{1}{y} \frac{x^2}{2} \ln \left| \frac{y+x}{y-x} \right|_0^1 - \frac{1}{2y} \int x^2 d \ln \left| \frac{y+x}{y-x} \right|$$

$$d \ln |y+x| = \frac{1}{2} d \ln (y+x)^2 = \frac{1}{2} \frac{1}{(y+x)^2} (2y+2x) dx$$

$$= \frac{1}{y+x} dx$$

$$- d \ln |y-x| = -\frac{1}{2} d \ln (y-x)^2 = -\frac{1}{2} \frac{2x-2y}{(y-x)^2} dx = \frac{1}{y-x} dx$$

$$\therefore d \ln \left| \frac{y+x}{y-x} \right| = \left(\frac{1}{y+x} + \frac{1}{y-x} \right) dx = \frac{2y}{y^2-x^2} dx$$

$$\therefore \frac{1}{y} \int_0^1 x \ln \left| \frac{y+x}{y-x} \right| dx$$

$$= \frac{1}{2y} \ln \left| \frac{1+y}{1-y} \right| - \int_0^1 \frac{x^2}{y^2-x^2} dx$$

$$= \frac{1}{2y} \ln \left| \frac{1+y}{1-y} \right| + 1 - y^2 \int_0^1 \frac{dx}{y^2-x^2}$$

$$\uparrow$$

$$x^2 = y^2 - y^2 + y^2$$

$$\frac{1}{2y} \ln \left| \frac{1+y}{1-y} \right|$$

$$= 1 + \frac{1-y^2}{2y} \ln \left| \frac{1+y}{1-y} \right|$$

$$\therefore \mathcal{E}_{1K} = \frac{\hbar^2 k_F^2}{2m} - \frac{e^2}{\pi} k_F \left[1 + \frac{k_F^2 k^2}{2k_F k} \ln \left| \frac{k_F+k}{k_F-k} \right| \right] \quad \text{--- (11)}$$

From eq. (6), the exchange energy is

$$\mathcal{E}_K = V \int \frac{d^3 k}{(2\pi)^3}$$

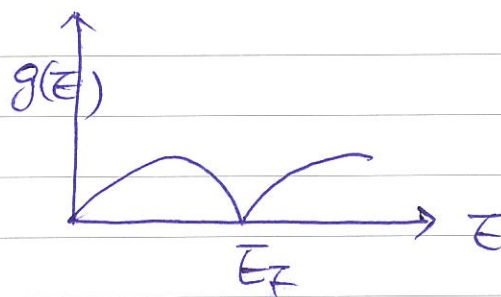
$$\downarrow$$

$$\frac{E_{exc}}{N} = \frac{V}{N} \int \frac{d^3 k}{(2\pi)^3} \times \underset{\text{spin}}{\frac{2}{1}} \times \frac{1}{2} \left(-\frac{e^2 k_F}{\pi} \right) \left[1 + \frac{1-y^2}{2y} \ln \left| \frac{1+y}{1-y} \right| \right]$$

$$1 \quad 4\pi k_F^3 / 3 \quad \uparrow \quad \left(\frac{1}{2} \times \frac{2}{1} \right) \quad \frac{1-y^2}{2y} \ln \left| \frac{1+y}{1-y} \right| = \frac{-3e^2 k_F}{4\pi} \quad \text{--- (11)-1}$$

$\therefore$ Exchange lowers down the energy.

However, if one looks at the density of state $g(E)$ by including the exchange energy, one finds $g(E_F) = 0$



Hence the Fermi surface is destroyed by the exchanged term. In fact, one can

combine exchange energy into $\Sigma(k)$ as shown

in eq. (1) and calculate the effective mass

m^*

$$\frac{m}{m^*} = \frac{\partial^2 \Sigma}{\partial k^2} \frac{1}{\Sigma^2} \left[\frac{1+y^2}{y} \ln \left| \frac{1+y}{1-y} \right| - 2 \right]$$

which diverges at $y \rightarrow 1$ (i.e. $k \rightarrow k_F$)

$\therefore m^* \rightarrow 0$ at $k = k_F$. This would indicate the electron gas is unstable, which is not consistent with the fact that alkali metals are stable. $\therefore$ This instability is an artifact

and should be removed by including higher orders as we shall see later. Alternatively, if one

uses screened potential, $\frac{1}{(k-k_F)^2} \rightarrow \frac{1}{(k-k_F)^2 + k_0^2}$

This singularity can be also removed.

Overall speaking, the HF approximation has been widely used by molecular orbital method of quantum chemistry as well as in the band calculation. But usually, itself is not sufficient, one must combine with other approaches to get more accurate results.

Density functional theory (DFT)

DFT represents one of the efforts in obtaining the ground wavefunctions of the condensed matter.

It is now among the most popular and

versatile methods in condensed matter physics and quantum chemistry.

To appreciate this method, one first realizes that even though the fundamental quantity that characterizes the ground state is the ground state wave function $\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$,

equivalently, one can replace it by density matrices.

Density Matrices

The single-particle density matrix of a state

ψ is defined as

$$\rho_i(\vec{r}, \vec{r}') = \int d\vec{r}_2 \dots \int d\vec{r}_N \psi(\vec{r}, \vec{r}_2, \dots, \vec{r}_N) \psi^*(\vec{r}', \vec{r}_2, \dots, \vec{r}_N)$$

where spin indices at $\vec{r}$ & $\vec{r}'$ are also summed over. (12)

When $\vec{r} \neq \vec{r}'$, ρ_i are off-diagonal terms.

$$\vec{r} = \vec{r}'$$

$\rho_i(\vec{r}, \vec{r}) \equiv n(\vec{r})$ is the density. Usually, $\rho_i(\vec{r}, \vec{r}') \rightarrow 0$ as $|\vec{r} - \vec{r}'| \rightarrow \infty$

However,

as we shall see later, for superfluidity,

$\lim_{|\vec{r} - \vec{r}'| \rightarrow \infty} \rho_i(\vec{r}, \vec{r}') \neq 0$ is termed as off-diagonal

long-range order by Onsager. (13)

Given $\rho_i(\vec{r}, \vec{r}')$, one obtains

$$n(\vec{r}) = \rho_i(\vec{r}, \vec{r}) \quad (\vec{r} = \vec{r}')$$

$$N = \text{Tr } \rho_i = \int d^3\vec{r} \rho_i(\vec{r}, \vec{r})$$

and $\hat{\rho}_i$ in other basis $\langle i | \hat{\rho}_i | j \rangle = \int d\vec{r} \int d\vec{r}'$
 $\times \phi_i^*(\vec{r}) \rho_i(\vec{r}, \vec{r}') \phi_j(\vec{r}')$

For ψ given by eq. (9), one finds

$$\rho_i(\vec{r}, \vec{r}') = \sum_{i=1}^N \phi_i(\vec{r}) \phi_i^*(\vec{r}')$$

Hence in k -space, $\langle \vec{r} | \rho_i | \vec{r}' \rangle = \int d\vec{k} d\vec{k}' \geq \theta(k - k')$
 $\uparrow \quad \uparrow$
 $\vec{r} \quad \vec{r}'$

$$\therefore \rho_1(\vec{r}, \vec{r}') = \frac{1}{V} \sum_{\vec{k}} e^{i\vec{k} \cdot \vec{r}} \langle \vec{r} | \rho_1 | \vec{r}' \rangle e^{-i\vec{k} \cdot \vec{r}'}$$

$$= \frac{2}{8\pi^3} \int_{|\vec{k}| < k_F} d^3\vec{k} e^{i\vec{k} \cdot (\vec{r} - \vec{r}')}$$

$$= \frac{k_F^3}{\pi^2} \frac{\sin k_F |\vec{r} - \vec{r}'| - k_F |\vec{r} - \vec{r}'| \cos k_F |\vec{r} - \vec{r}'|}{(k_F |\vec{r} - \vec{r}'|)^3}$$

L- (14)

$$\therefore \rho_1(\vec{r}, \vec{r}') = \frac{k_F^3}{3\pi^2} = n(\vec{r})$$

& $\rho_1(\vec{r}, \vec{r}')$ for free Fermions decays as $\frac{1}{|\vec{r} - \vec{r}'|^2}$.

Two-particle density matrix

Similarly, one defines the two-particle density matrix

$$\rho_2(\vec{r}_1, \vec{r}_2; \vec{r}_1', \vec{r}_2')$$

$$= C_N \int d\vec{r}_3 \dots d\vec{r}_N \psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots, \vec{r}_N) \psi^*(\vec{r}_1', \vec{r}_2', \vec{r}_3, \dots, \vec{r}_N)$$

$$\approx \frac{N(N-1)}{2!}$$

L- (15)

$$\text{Clearly, } \rho_1(\vec{r}, \vec{r}') = \frac{2}{N-1} \int d\vec{r}_2 \rho_2(\vec{r}, \vec{r}_2; \vec{r}', \vec{r}_2) \quad \text{--- (16)}$$

ρ_2 gives rise to the probability density

to find one particle at $\vec{r}_1$ and another at $\vec{r}_2$

$$n_2(\vec{r}_1, \vec{r}_2) = 2 \rho_2(\vec{r}_1, \vec{r}_2; \vec{r}_1, \vec{r}_2) \quad \text{--- (17)}$$

(... ..)

If Ψ is given by eq (5), we find

$$\rho_2(r_1, r_2; r_1', r_2')$$

$$= \frac{N(N-1)}{2} \int dr_3 \dots dr_N \left[\frac{1}{N!} \sum_P (r_1)^P \prod_i \phi_{P_i}(r_i) \right]$$

$$\times \left[\frac{1}{N} \sum_{P'} (r_1')^{P'} \prod_i \phi_{P'_i}^*(r_i') \right]$$

$$= \frac{N(N-1)}{2N!} \times (N-2)! \sum_{i,j=1}^N \left[\phi_i(\vec{r}_1) \phi_j(\vec{r}_2) \phi_i^*(\vec{r}_1') \phi_j^*(\vec{r}_2') \right] \begin{matrix} \text{exchange} \\ \downarrow \text{term} \end{matrix}$$

$$- \phi_i(\vec{r}_1) \phi_j(\vec{r}_2) \phi_j^*(\vec{r}_1') \phi_i^*(\vec{r}_2')$$

$$= \frac{1}{2} \sum_{i,j}^N \left[\underbrace{\phi_i(\vec{r}_1) \phi_j(\vec{r}_2) \phi_i^*(\vec{r}_1') \phi_j^*(\vec{r}_2')}_{\substack{\text{spins are the same} \\ \text{2x2}}} - \underbrace{\phi_i(\vec{r}_1) \phi_j(\vec{r}_2) \phi_j^*(\vec{r}_1') \phi_i^*(\vec{r}_2')}_{\substack{\text{spin same}}} \right]$$

Now, $N/2$ spatial orbitals are occupied for $\downarrow$ x_2 both spin directions. (18)

$$\therefore 2\rho_2(r_1, r_2, r_1', r_2') = \sum_{i,j}^{N/2} \left[4\phi_i(\vec{r}_1) \phi_j(\vec{r}_2) \phi_i^*(\vec{r}_1') \phi_j^*(\vec{r}_2') - 2\phi_i(\vec{r}_1) \phi_j(\vec{r}_2) \phi_j^*(\vec{r}_1') \phi_i^*(\vec{r}_2') \right]$$

Setting $r_1' = r_1, r_2' = r_2$, we get

$$n_2(\vec{r}_1, \vec{r}_2) = n(\vec{r}_1) n(\vec{r}_2) - \frac{1}{2} |\rho_1(\vec{r}_1, \vec{r}_2)|^2 \quad \text{--- (19)}$$

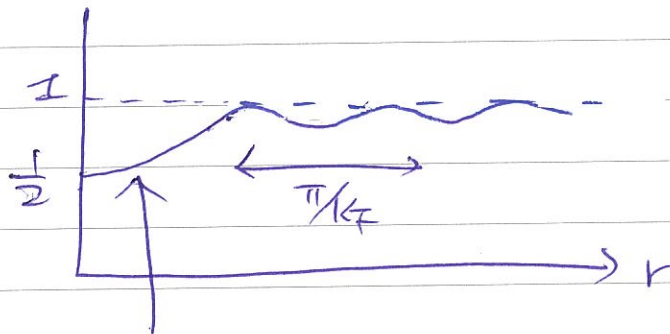
$$\uparrow$$

$$2 \sum_{i=1}^{N/2} \phi_i(\vec{r}) \phi_i^*(\vec{r}) = n(\vec{r})$$

From (19), we define the pair correlation function

$$g(r_1, r_2) = \frac{n_2(r_1, r_2)}{n(r_1) n(r_2)} = 1 - \frac{q}{2} \left[\frac{\sin kr - kr \cos kr}{(kr)^3} \right]^2$$

$$\therefore g(0) = 1/2$$



exchange hole

As one can see, the probability is suppressed once one electron is already at $r=0$.

The suppression can be traced back to the exchange of $\vec{r}_1$ & $\vec{r}_2$ in calculating ρ_2 , which has the same origin of exchange interaction in the Hartree - Fock term, is termed as exchange hole.

Expectation values

$$\hat{T} = \frac{\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2$$

$$\langle \hat{T} \rangle = \frac{\hbar^2}{2m} \int d^3r \sum_i \phi_i^*(\vec{r}) \nabla_i^2 \phi_i(\vec{r})$$

$$= \frac{\hbar^2}{2m} \int d^3r [\nabla^2 \rho_1(r, \vec{r}')] \Big|_{\vec{r}=\vec{r}'} \quad \dots (21)$$

Similarly, $\langle \sum_i v(\vec{r}_i) \rangle = \int d^3r v(\vec{r}) \rho_1(\vec{r}, \vec{r}') \Big|_{\vec{r}=\vec{r}'}$

For Coulomb interactions, one has

$$\hat{V}_C \equiv \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|}$$

We get

$$\begin{aligned} \langle \hat{V}_C \rangle &= \int d^3r \int d^3r' \frac{e^2}{|\vec{r} - \vec{r}'|} \rho_2(\vec{r}, \vec{r}', \vec{r}, \vec{r}') \quad \text{--- (23)} \\ &= \frac{1}{2} \int d^3r \int d^3r' \frac{e^2}{|\vec{r} - \vec{r}'|} n_2(\vec{r}, \vec{r}') \end{aligned}$$

Combining eqs. (1) & (23) (realizing $i=j$ gets

cancelled in (1)), one recovers the Hartree-Fock approximation in eq. (6).

Defining $h(\vec{r}_1, \vec{r}_2) = n_2(\vec{r}_1, \vec{r}_2) - n(\vec{r}_1)n(\vec{r}_2)$, we

get

$\rightarrow E_{\text{kin}}$

$\rightarrow E_{\text{ext.}}$

$$E = \langle \hat{H} \rangle = \frac{\hbar^2}{2m} \int d^3r [\nabla^2 \rho(\vec{r}, \vec{r}')]_{\vec{r}=\vec{r}'} + \int d^3r v(\vec{r}) n(\vec{r})$$

$$+ \frac{1}{2} \int d^3r \int d^3r' n(\vec{r}') w(|\vec{r} - \vec{r}'|) n(\vec{r}) \leftarrow E_H \text{ (Hartree)}$$

$$+ \frac{1}{2} \int d^3r \int d^3r' w(|\vec{r} - \vec{r}'|) h(\vec{r}', \vec{r}) \leftarrow E_{\text{xc}} \text{ (exchange and correlation energy)}$$

Where $w(|\vec{r} - \vec{r}'|)$ is two-body interaction & can be

$$\frac{e^2}{|\vec{r} - \vec{r}'|}$$

One sees that the exchange and correlation term has the hole effect reflecting the Pauli exclusion

From wavefunctions to density functional

The idea that the ground state can be expressed as a functional of density can be traced back to the Thomas - Fermi theory.

Is it possible to regard $n(r)$ as a basic variable in the calculation of electronic structure of solids & molecules?

This is not obvious. After all, ψ is complex and phases are also important in the phenomenon associated with interference.

The Thomas - Fermi theory provides the 1st attempt.

$$\therefore \frac{\frac{4\pi}{3} k_F^3}{\left(\frac{2\pi}{h}\right)^3} \times 2 = N$$

$$\therefore n = \frac{N}{L^3} = \frac{k_F^3}{3\pi^2} = \frac{1}{3\pi^2} \left(\frac{2m\mu}{\hbar^2} \right)^{3/2}$$

μ = chemical potential.

In the presence of external potential $V_{ex}(r)$, if it varies slowly in comparison to λ_F , one

approximates
$$n(r) = \frac{1}{3\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} (\mu - V_{ex}(r))^{3/2}$$

i.e. V_{ex} redefines the zero point of the energy so that μ is shifted.

Furthermore, $V_{\text{ex}}(\vec{r})$ should include electronic contribution.

$$\therefore V_{\text{ex}}(\vec{r}) = V(\vec{r}) + e^2 \int \frac{n(\vec{r}')}{|\vec{r} - \vec{r}'|} d\vec{r}'$$

However, Thomas-Fermi is only useful for describing some qualitative trends such as total energies. It's too crude to account for chemical binding, so its application to the electronic structure of solids is quite limited.

But the connection of $n(\vec{r})$ and $V(\vec{r})$ suggested by the Thomas-Fermi theory starts the development of density functional theory (DFT).

The key ideas of DFT are put forth by Hohenberg, Kohn & Sham.

It should be emphasized that it is not the density $n(\vec{r})$ that is unique to characterize the ground state. Instead, by coupling ^{interacting} electrons to external sources, can we uniquely

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This is quite similar to quantum field theories in which one introduces sources to couple the fundamental field ψ . In that case, if one needs to calculate correlation of

$\langle \psi^\dagger \psi \rangle$, one introduces $J^\dagger \psi + J \psi^\dagger$ by the term
coupling $J^\dagger$ & J to ψ & $\psi^\dagger$.

$\frac{d}{dJ^\dagger dJ}$ would lead to $\langle \psi^\dagger \psi \rangle$.

Similarly, if one needs to calculate $\langle \psi^\dagger(r) \psi^\dagger(r') \rangle$, one introduces $J_2^\dagger(r) \psi^2(r) + J_2(r) \psi^{2\dagger}(r)$.

Therefore, the key point is then how many sources (external potentials) can characterize the ground state?

The simplest source is the external potential $V(r)$ which couples to $n(r)$. In general, one can have $\Delta(r, r')$ that couples to superconducting order parameter $\Delta(r, r')$, and other sources that couple to order parameters due to symmetry broken.

We shall consider the simplest situation. v_{ex} and it is summarized in the following two theorems.

Hohenberg - Kohn theorem I

Given a Hamiltonian

$$\hat{H}[v] = \underbrace{\frac{\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2}_T + \underbrace{\sum_{i=1}^N v(\vec{r}_i) + \frac{1}{2} \sum_{i \neq j}^N \omega(|\vec{r}_i - \vec{r}_j|)}_U + \sum_{i=1}^N v_{ex}(\vec{r}_i) \quad \xrightarrow{U_{ee}}$$

the ground state energy

$$E = \min_{\psi} \langle \psi | \hat{H} | \psi \rangle$$

is obviously a functional of v_{ex}

$$\therefore E = E[v_{ex}]$$

It's clear $E[v_{ex} + \text{constant}] = E[v_{ex}] + \text{constant} \cdot N$
 $N = \# \text{ of particles}$

$\therefore$ Up to a constant, the theorem states

$$n[v_{ex}'] \neq n[v_{ex}^2] \Leftrightarrow v_{ex}' \neq v_{ex}^2$$

$\uparrow$
 density of the ground state
 is obviously a functional of v_{ex}

i.e. the ground-state density $n(\vec{r})$ determines
 $\rightarrow \dots \text{in } n!$

It's clear $E(V_{ex} + \text{constant}) = E(V_{ex}) + \text{const} \cdot N$

$N = \#$ of particles.

$\therefore$ Up to a constant, the theorem states

$$n[V_1] \neq n[V_2] \Leftrightarrow V_1 \neq V_2$$

↑
density as a functional of V .

i.e. the ground-state density $n(r)$ determines $V(r)$ uniquely.

p.f.: Let $n(r)$ be the non-degenerate ground-state density of N electrons in the potential $V(r)$ and the ground state wavefunction ψ_1 with the energy E_1 .

We have $E_1 = \langle \psi_1 | H_1 | \psi_1 \rangle$

$$= \langle \psi_1 | T + U | \psi_1 \rangle + \int V_{ex}(r) n(r) dr$$

$$H_1 \equiv T + U + \sum_i V_{ex}(r_i)$$

Suppose that there is another $V_2(r)$ with the ground state wavefunction $\psi_2 \neq \psi_1$ but gives the same $n(r)$, then

$$E_2 = \langle \psi_2 | H_2 | \psi_2 \rangle$$

$$E_2 = \int V_2(r) n(r) dr + \langle \psi_2 | T + U | \psi_2 \rangle$$

$\therefore E$ is non-degenerate, $\therefore E_1 < \langle \psi_2 | H_1 | \psi_2 \rangle$

$$= \int V_2(r) n(r) dr + \langle \psi_2 | T + U | \psi_2 \rangle$$

Pf: Let $n(\vec{r})$ be the non-degenerate ground-state density of N electrons in the potential $V(\vec{r})$ and the ground state wavefunction ψ_1 with the energy E_1

$$\begin{aligned} \text{We have } E_1 &= \langle \psi_1 | H_1 | \psi_1 \rangle \\ &= \langle \psi_1 | T + U | \psi_1 \rangle + \int V_{\text{ex}}(\vec{r}) n(\vec{r}) d^3\vec{r} \end{aligned}$$

$$H_1 \equiv T + U + \sum_i V_{\text{ex}}^i(\vec{r}_i)$$

Suppose that there is another $V_2(\vec{r})$ with the ground state wavefunction $\psi_2 \neq \psi_1$ but gives the same $n(\vec{r})$, then

$$\begin{aligned} E_2 &= \langle \psi_2 | H_2 | \psi_2 \rangle \\ &= \int V_{\text{ex}}^2(\vec{r}) n(\vec{r}) d\vec{r} + \langle \psi_2 | T + U | \psi_2 \rangle \end{aligned}$$

$$\begin{aligned} \because E \text{ is non-degenerate, } \therefore E_1 &< \langle \psi_2 | H_1 | \psi_2 \rangle \\ &= \int V_{\text{ex}}^1(\vec{r}) n(\vec{r}) d\vec{r} + \langle \psi_2 | T + U | \psi_2 \rangle \\ &= E_2 + \int [V_{\text{ex}}^1(\vec{r}) - V_{\text{ex}}^2(\vec{r})] n(\vec{r}) d\vec{r} \dots (24) \end{aligned}$$

$$\text{Similarly, } E_2 < \langle \psi_1 | H_2 | \psi_1 \rangle$$

$$= E_1 + \int [V_{\text{ex}}^2(\vec{r}) - V_{\text{ex}}^1(\vec{r})] n(\vec{r}) d\vec{r} \dots (25)$$

$$(24) + (25) \Rightarrow E_1 + E_2 < E_1 + E_2 \text{ which is incorrect.}$$

$\therefore$ For a given $n(r)$, $v(r)$ is given uniquely.

Theorem 2.

From the above theorem, since E is a functional of $v(r)$, one can perform a Legendre transformation to convert the functional dependence on $v(r)$ to the functional dependence on $n(r)$. This is possible because for a given $v(r)$, there is one $n(r)$. Collecting $\{n(r)\}$ for all possible $v(r)$ forms the functional space to define

$$F_{HK}[n] = E[v(r)] - \int dr v(r) n(r) \dots (26)$$

$$\therefore E = \min_{\psi} \langle \psi | \hat{H} | \psi \rangle$$

$$= \min_{\psi} \langle \psi | T + U | \psi \rangle + \int dr v(r) n(r)$$

$$\therefore F_{HK}[n] = \min_{\psi} \langle \psi | T + U | \psi \rangle \dots (27)$$

with $n(r) = \int \psi^*(r_1, \dots, r_N) \psi(r_1, \dots, r_N) dr_2 \dots dr_N$ fixed.

Now, clearly, the ground state energy

$E_0 = \min_{\psi} \langle \psi | T + U | \psi \rangle$ can be obtained by variation of $n(r)$.

Pf: Eq. (27) states $E_{HK}[n]$ is only a "local"

min when $n(r) = \int d^3r_2 \dots d^3r_N \psi^*(r, r_2, \dots, r_N) \psi(r, r_2, \dots, r_N)$

is fixed.

Let us indicate the wave function that minimize eq. (27) by $\psi_{\min}^n$.

$$\therefore \langle \psi_{\min}^n | T + U | \psi_{\min}^n \rangle \geq E_0$$

$$\therefore E_{HK}[n] \geq E_0$$

To obtain E_0 , one thus can vary n in $E_{HK}[n]$

so that $\underbrace{n = n_{GS}}_{\text{when}}, \quad E_{HK}[n_{GS}] = E_0$

In this case, $\psi_{\min}^{n_{GS}}$ becomes the Ground state $\psi_{\min}^{n_{GS}} = \psi_{GS}$ if the Ground state is non-degenerate.

If on the contrary, the ground state is degenerate, $\psi_{\min}^{n_{GS}} =$ one of the ground state.

Hence E_0 is determined by the density of ground state.

Example of DFT — the Thomas-Fermi theory
for the atom

$$E[n] = E_{\text{kinetic}} + \int v(r) n(r) dr + \frac{e^2}{2} \int dr' \int dr \frac{n(r) n(r')}{|r-r'|}$$

L - (20)

E_{kinetic} is given by free electrons:

$$\frac{k_F^3}{3\pi^2} = n$$

$$\begin{aligned} E_{\text{kinetic}} &= 2 \int_0^{k_F} \frac{4\pi k^2 dk}{(2\pi)^3} \cdot \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \times 4\pi \times \frac{1}{5} k_F^5 \times \frac{1}{(2\pi)^3} \\ &= \frac{2\hbar^2}{2m} \times \frac{4\pi}{5} \times (3\pi^2 n)^{\frac{5}{3}} \times \frac{1}{(2\pi)^3} \end{aligned}$$

$$\therefore E_{\text{kinetic}}[n] = \alpha n^{\frac{5}{3}} \quad \alpha = \frac{3}{10} (3\pi^2)^{\frac{2}{3}} \frac{\hbar^2}{m}$$

with $N = \int n(r) dr = \text{fixed}$.

$$\therefore \delta(E - \mu \int n dr) = 0$$

$$\frac{5}{3} \alpha n^{\frac{2}{3}} + v(r) - \mu + e^2 \int dr' \frac{n(r')}{|r-r'|} = 0$$

$$\therefore \text{One recovers } n = \frac{1}{3\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} (\mu - v_{\text{ex}}(\vec{r}))^{3/2}$$

Shortcomings: n diverges near nucleus. ($\sim 1/r$)
 does not decay exponentially $r \rightarrow \infty$
 for molecules, it does not produce binding and can't predict shell structures of atoms.

The Kohn - Sham formulation

The concrete Computation scheme after the Hohenberg - Kohn theorems is provided by the Kohn - Sham formulation.

The whole point is whether one can have faithful $E_{HK}[n]$.

The idea is to use non-interacting^{as} reference and to look for $\underline{v}$ such that the noninteracting system has the same ground state density as the real, interacting system.

The $v(r)$ turns out to depend on $n(r)$ and one has to solve it self-consistently.

$E_{HK}[n]$ is separated into the following terms:

$$E_{HK}[n] = E_{kin}[n] + \int dr v(r)n(r) + \frac{e^2}{2} \iint dr dr' \frac{n(r)n(r')}{|r-r'|} + E_{xc}[n]. \quad \dots (29)$$

where $E_{xc}[n]$ represents the exchange & correlation energies.

with $N = \int n(r) dr = \text{fixed}$, $\delta(F_{HK} - \mu N) = 0$

leads to

$$\int dr \delta n(r) \left[\frac{\delta E_{kin}}{\delta n(r)} + v(r) + e^2 \int \frac{n(r')}{|r-r'|} dr' + \frac{\delta E_{xc}[n]}{\delta n(r)} - \mu \right] = 0$$

$$\therefore \frac{\delta E_{kin}}{\delta n(r)} + v(r) + e^2 \int \frac{n(r')}{|r-r'|} dr' + \frac{\delta E_{xc}[n]}{\delta n(r)} = \mu$$

If we define $v_{xc}(r) = \frac{\delta E_{xc}[n]}{\delta n(r)}$, one

L - - (30)

$$\text{gets } v_{eff}(r) = v(r) + e^2 \int \frac{n(r')}{|r-r'|} dr' + v_{xc}(r) \quad (31)$$

The solution to eq. (30) can be found only when one knows $E_{kin}[n]$ & $E_{xc}[n]$.

Suppose $v_{xc}(r)$ is known, then eq. (30) is

solved by computing $E_{kin}[n]$ as follows:

One first solves $[E_{kin} \text{ is simply } \frac{\hbar^2}{2m} \sum_{i=1}^N \int |\phi_i(r)|^2 dr]$

$$\left[\frac{\hbar^2}{2m} \nabla^2 + v_{eff}(r) \right] \phi_i(r) = \epsilon_i \phi_i(r) \quad \dots (32)$$

to get $\phi_i(r)$ and then it yields

$$n(r) = \sum_{i=1}^N |\phi_i(r)|^2$$

Through eq. (31), one obtains $v_{eff}(r)$ and

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These self-consistent equations are called Kohn-Sham equations. 13-26

From the convergent ϕ_i & ϵ_i , one computes

$$\sum_i \epsilon_i = \sum_i \langle \phi_i | \frac{\nabla^2}{2m} + V_{\text{eff}}(r) | \phi_i \rangle$$

$$= E_{\text{kin}}[n] + \int dr n(r) V_{\text{eff}}(r)$$

$$= E_{\text{kin}}[n] + \int dr n(r) V(r) + e^2 \iint \frac{n(r)n(r')}{|r-r'|}$$

$$+ \int n(r) V_{\text{xc}}(r) dr$$

and hence $E_{\text{kin}}[n]$ is obtained.

Substituting $E_{\text{kin}}[n]$ into eq (29), one gets

$$E_0 = E_{\text{HK}}[n] = \sum_i \epsilon_i - \frac{e^2}{2} \iint \frac{n(r)n(r')}{|r-r'|} + E_{\text{xc}}[n]$$

$$- \int n(r) V_{\text{xc}}(r) dr.$$

As one can see, the whole scheme depends on the knowledge of $E_{\text{xc}}[n]$.

Note that, contrary to the HF theory, the single-particle wave functions $\phi_i(r)$ & ϵ_i have

no physical meaning, are only mathematical tools through which $n(r)$ & E_0 can be calculated. That

is, the occupied ϵ_i do not represent the physical

energies to excite molecules to the continuum

As we shall see later, the physical excitation energies $\hat{\epsilon}_i$ are solutions to the Dyson equation

$$-\frac{\nabla^2}{2m} \phi_i(r) + \int d\vec{r}' \Sigma(r, r'; \hat{\epsilon}_i) \phi_i(r') = \hat{\epsilon}_i \phi_i(r)$$

where Σ is the self energy and is non-local,

Σ is clearly different from $V_{eff}(r)$.

$\hat{\epsilon}_i$ is also complex. $\text{Re} \hat{\epsilon}_i$ is actually the pole of the Green's function.

The local density approximation (LDA)

As we indicated, the whole issue is to find E_{xc} or V_{xc} (the exchange-correlation potential). The first such approach is

to do the approximation: neglect the nonlocal aspect of V_{xc} .

The true $V_{xc}(r)$ will not only depend on the local density $n(r)$ but also on n at all other points $n(r')$.

For a system with slowly varying density,

One assumes nonlocality can be neglected.

$$E_{xc}[n] = \int E_{xc}[n(r)] n(r) d\vec{r} \quad \dots (33)$$

The justification of neglecting nonlocality was done in 1996 by Kohn (W. Kohn, PRL 76, 3168, 1996). He showed that the local static physical properties of a many-electron system at r are dependent on the particles in the neighbourhood of r and are insensitive to any change of potential outside this region. (for example, in metal, radius of the region $\sim \lambda_F(r)$, $\lambda_F(r) \equiv (3\pi^2 n(r))^{-1/3}$).

In the LDA calculation, E_{xc} is frequently separated into exchange and correlation parts.

$$E_{xc}[n] = E_x[n] + E_c[n] \quad \dots (34)$$

$$E_x[n] \approx -\frac{3e^2}{2\pi} (3\pi^2 n(r))^{\frac{1}{3}} \quad (3D)$$

$$E_F \approx 1 \times 2 \text{ eV}, \quad k_F = (3\pi^2 n)^{\frac{1}{3}}$$

A popular approximation for E_c (correlation) is

the Perdew-Wang 91 functional (Perdew and Wang, 1991)

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The Monte Carlo is done for several $n(r)$ and

then one tries to extract $E_c(n)$ by using

Padé approximants. For instance, in 2D

$$E_c[n] = a_0 \frac{1 + a_1 x}{1 + a_1 x + a_2 x^2 + a_3 x^3}$$

where $x = r_s^{1/2}$ with $r_s = (\pi n)^{-1/2}$ for 2D.

Here r_s is an important ^{length} parameter which we will use it quite often in below.

r_s is the average distance between electrons.

In 2D, $\frac{1}{\pi r_s^2} = n$. For 3D, $\frac{1}{n} = \frac{4\pi}{3} r_s^3$

For 1D, $\frac{1}{n} = 2r_s$.

For un polarized electrons (no magnetization, $n_\uparrow = n_\downarrow$),

$a_0 = -0.3568$, $a_1 = 1.1300$, $a_2 = 0.9052$, $a_3 = 0.4165$.

Many calculations by LDA produce good results even in the case when the density does not change slowly.

The LDA ^{also} produces good results for

the binding energy of atoms and diatomic molecules.

LSDA (local spin density approximation), CDF T (Current DFT)
and other generalization

As indicated in the above, one can not conclude that the ground state of a many-particle system is uniquely characterized by $n(r)$. Otherwise, how can one explain ferromagnetic states and other states. Instead, the ground state is characterized by sources (external potentials) that can couple to the system.

Several generalizations are taken.

For magnetic systems, the external magnetic field couples to $n_{\uparrow} - n_{\downarrow}$. Hence, in addition to $n(r) = n_{\uparrow} + n_{\downarrow}$, one needs to use $n_{\uparrow} - n_{\downarrow}$ to characterize the ground state.

This results in the local spin density approximation (LSDA).

In addition to magnetic systems, in the presence magnetic field, phases are explicitly important. For instance, LDA can't describe the Aharonov-Bohm effect. One needs to include current density.

This results in current density functional theory (CDFT) in which the parametric current

$$\text{density } \vec{j}_p(\vec{r}) = \frac{\hbar}{2m} [\psi^* \frac{1}{i} \nabla \psi - \psi \frac{1}{i} \nabla \psi^*]$$

Finally, to include superconductivity, one also need to include extra densities, This is done by including the anomalous density

$$\chi(r, r') = \langle \psi_{\uparrow}(r) \psi_{\downarrow}(r') \rangle$$

Whose corresponding potential is the non-local pairing potential $\Delta(r, r')$.

(L.N. Oliveira, Gross & Kohn, PRL 60, 2430, 1988).

Approach based on the 2nd quantization

The wavefunction approach, particular for fermions, is clumsy; especially, one needs to deal with a large determinant.

As we have seen, the method of the second quantization reduces computational effort a lot. Therefore, most methods

for many-electronic systems are based on the 2nd quantization. We shall start by 1st quantization.

2nd quantization for Fermions

Everything goes in the same way ^{as bosons} except that

(i) $n_i = 0$ or 1 (ii) antisymmetric.

the wave function has to be

To include the above properties, $a_\alpha, a_\beta^\dagger$ have to have different commuting properties:

$$* \quad a_\alpha^\dagger a_\beta^\dagger + a_\beta^\dagger a_\alpha^\dagger = 0$$

$$a_\alpha^\dagger a_\beta^\dagger |0\rangle = |\alpha \beta\rangle$$

$$a_\beta^\dagger a_\alpha^\dagger |0\rangle = |\beta \alpha\rangle$$

$$\therefore |\beta \alpha\rangle = -|\alpha \beta\rangle$$

$$\therefore a_\alpha^\dagger a_\beta^\dagger = -a_\beta^\dagger a_\alpha^\dagger, \quad a_\alpha^\dagger a_\beta^\dagger + a_\beta^\dagger a_\alpha^\dagger = 0$$

Taking the Hermitian conjugate, we get $a_\alpha a_\beta + a_\beta a_\alpha = 0$

$$* \quad \{a_\alpha, a_\beta^\dagger\} = \delta_{\alpha\beta}$$

The above commutation relation implies the Pauli principle:

$$\alpha = \beta, \quad (a_\alpha^\dagger)^2 = 0$$

i.e. one can not put two ^{identical} fermions to the

same state $|\alpha\rangle$.

$$\therefore n_\alpha = 0 \text{ or } 1.$$

This further implies that for fermions,

$$[a_\alpha, a_\beta^\dagger] = \delta_{\alpha\beta} \text{ is no longer correct}$$

because this commutation relation does constraint the number n_α to 0 or 1:

$$\begin{aligned} N_\alpha a_\alpha^\dagger |n\rangle &= a_\alpha^\dagger (a_\alpha^\dagger a_\alpha + 1) |n\rangle \\ &= (n+1) [a_\alpha^\dagger |n\rangle] \end{aligned}$$

$$\therefore a_\alpha^\dagger |1\rangle \neq 0$$

To remedy, one notices that we need

$$a_\alpha^\dagger |1\rangle = 0$$

$$a_\alpha^\dagger |0\rangle = |1\rangle$$

$$\therefore a_\alpha a_\alpha^\dagger |1\rangle = 0, \quad a_\alpha a_\alpha^\dagger |0\rangle = |0\rangle$$

$$\therefore a_\alpha a_\alpha^\dagger = 1 - n_\alpha$$

$$\therefore a_\alpha a_\alpha^\dagger + a_\alpha^\dagger a_\alpha = 1 \quad \text{i.e. } \{a_\alpha, a_\alpha^\dagger\} = 1$$

Can establish the requirement $n_\alpha = 0$ or 1.

The generalization of $\{a_\alpha, a_\beta^\dagger\} = \delta_{\alpha\beta}$

$$\{a_\alpha, a_\beta^\dagger\} = 0 \text{ for } \alpha \neq \beta, \text{ i.e., } a_\alpha a_\beta^\dagger + a_\beta^\dagger a_\alpha = 0.$$

To see it, we consider the following example:

$$\psi = \frac{1}{\sqrt{3!}} \begin{vmatrix} \phi_\alpha(x_1) & \phi_\alpha(x_2) & \phi_\alpha(x_3) \\ \phi_\beta(x_1) & \phi_\beta(x_2) & \phi_\beta(x_3) \\ \phi_\gamma(x_1) & \phi_\gamma(x_2) & \phi_\gamma(x_3) \end{vmatrix}$$

i.e. $|\psi\rangle \equiv a_\alpha^\dagger a_\beta^\dagger a_\gamma^\dagger |0\rangle$

$$\psi_1 = \frac{1}{\sqrt{3!}} \begin{vmatrix} \phi_\delta(x_1) & \phi_\delta(x_2) & \phi_\delta(x_3) \\ \phi_\beta(x_1) & \phi_\beta(x_2) & \phi_\beta(x_3) \\ \phi_\gamma(x_1) & \phi_\gamma(x_2) & \phi_\gamma(x_3) \end{vmatrix}$$

i.e. $|\psi_1\rangle = a_\delta^\dagger a_\beta^\dagger a_\gamma^\dagger |0\rangle$

$$\langle \psi_1 | = \langle 0 | a_\gamma a_\beta a_\delta$$

Now, $\langle \psi_1 | F | \psi \rangle = \langle \delta | f | \alpha \rangle$

i.e. $F = \sum_{m,n} \langle m | f | n \rangle a_m^\dagger a_n$

$$\begin{aligned} \langle \psi_1 | a_\delta^\dagger a_\alpha | \psi \rangle &= \langle 0 | a_\gamma a_\beta a_\delta a_\delta^\dagger a_\alpha a_\alpha^\dagger a_\beta^\dagger a_\gamma^\dagger | 0 \rangle \\ &= 1 \end{aligned}$$

On the other hand, $\langle \psi_1 | a_\alpha a_\delta^\dagger | \psi \rangle$

$$\begin{aligned} &= \langle 0 | a_\gamma a_\beta a_\delta a_\alpha a_\delta^\dagger a_\alpha^\dagger a_\beta^\dagger a_\gamma^\dagger | 0 \rangle \\ &\equiv \langle \tilde{\psi}_1 | \tilde{\psi} \rangle \end{aligned}$$

○ With $\hat{\psi} = \frac{1}{\sqrt{4}}$:

$\phi_8(x_1)$	$\phi_8(x_2)$	$\phi_8(x_3)$	$\phi_8(x_4)$
$\phi_2(x_1)$	$\phi_2(x_2)$	$\phi_2(x_3)$	$\phi_2(x_4)$
$\phi_3(x_1)$	$\phi_3(x_2)$	$\phi_3(x_3)$	$\phi_3(x_4)$
$\phi_7(x_1)$	$\phi_7(x_2)$	$\phi_7(x_3)$	$\phi_7(x_4)$

and $\tilde{\psi}_1 = \frac{1}{\sqrt{4}}$

$\phi_2(x_1)$	$\phi_2(x_2)$	$\phi_2(x_3)$	$\phi_2(x_4)$
$\phi_8(x_1)$	$\phi_8(x_2)$	$\phi_8(x_3)$	$\phi_8(x_4)$
$\phi_B(x_1)$	$\phi_B(x_2)$	$\phi_B(x_3)$	$\phi_B(x_4)$
$\phi_F(x_1)$	$\phi_F(x_2)$	$\phi_F(x_3)$	$\phi_F(x_4)$

Obviously, $\vec{v} = -\vec{v}_1$

i.e. $\langle \psi_1 | \psi_1 \rangle = -1$

$$\therefore \langle \psi_f | a a^\dagger | \psi \rangle = -1$$

$$\langle \psi | a_\alpha a_s^\dagger + a_s^\dagger a_\alpha | \psi \rangle = 0$$

In general, for $a \in \mathcal{O}_S^+$ & $a^* a \in \mathcal{O}_S^+$ to be non-vanishing, one must have:

$\mathcal{U}$ contains one row of Φ_α but no Φ_β

... ..

In the Fock space, we denote:

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The special case we considered in the above

corresponds to

$$\begin{array}{l}
 \begin{array}{c} f \quad \alpha \\ | \psi \rangle = | \dots 0 \dots \rangle \\ | \psi_1 \rangle = | \dots 1 \dots \rangle \end{array}
 \end{array}$$

$\Downarrow$ same $\Downarrow$ same

i.e., there are no rows between α & f . $\therefore \langle \psi_1 | \alpha \rangle = 1$

In the general case, one has

$$\begin{array}{c}
 \begin{array}{c} f \quad \alpha \qquad \qquad f \quad \alpha \\ | \dots 1 \dots 0 \dots | \dots 1 \dots 0 \dots \rangle \end{array} \\
 = \langle f | f | \alpha \rangle \cdot \underbrace{(-1)^{\# \text{ of rows between } \alpha \text{ \& } f}}_{11} \equiv R(\alpha, f)
 \end{array}$$

$(-1)^{\# \text{ of occupied states between } \alpha \text{ \& } \beta}$

The arising of the sign can be easily understood as follows: one first move

the row of ϕ_α to the row beside ϕ_f :

$$\begin{array}{l}
 | \psi \rangle = | \dots f \dots \alpha \dots \rangle \rightarrow (-1)^{R(f, \alpha)} | \dots f \alpha \dots \rangle \\
 | \psi_1 \rangle = | \dots 1 \dots 0 \dots \rangle = \begin{array}{c} \text{same} \quad \text{same} \\ | \dots 1 \dots 0 \dots \rangle \end{array}
 \end{array}$$

(there is no need to move ϕ_α in ψ_1 as it is vacant and be assigned in anywhere)

$\therefore$ for nearest neighbourly case of $f \neq \alpha$, one

$$\text{has } \langle \alpha | \psi_1 \rangle = 1$$

Now, to calculate $\langle \psi_1 | a_\alpha a_s^\dagger | \psi \rangle$, again,

We first move a to be the neighbour of s .

This introduces the sign $(-1)^{R(s, \alpha)}$.

However, there is an extra sign which we have in the example:

$$\begin{aligned} & \langle \dots \overset{s \alpha}{1 \ 0} \dots | a_\alpha a_s^\dagger | \dots \overset{s \alpha}{0 \ 1} \dots \rangle \\ &= (-1) \end{aligned}$$

$$\therefore \langle \psi_1 | a_\alpha a_s^\dagger | \psi \rangle = (-1) \cdot (-1)^{R(s, \alpha)} \quad (37)$$

$\therefore$ Combined with (F-2), we conclude

$$a_s^\dagger a_\alpha + a_\alpha a_s^\dagger = 0$$

$\therefore$ Generally, we must have $\{a_\alpha, a_s^\dagger\} = \delta_{\alpha s}$

Matix representation

The anti-commuting nature of fermionic operators

impose some difficulties in numerical work.

For ordinary operators, such as spins, spins at different sites commutes. Therefore, going from

one spin to many spins simply enlarges the Hilbert space (or the Fock space) by tensor product.

Example: $\sigma_z^1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $\sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

are one-body operators.

$\sigma_z^1 \sigma_z^2$ is a two-body operator that acts on two particles labelled by 1 & 2. $|\uparrow\rangle \otimes |\uparrow\rangle$

The basis for two particles are $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, hence $\sigma_z^1 \sigma_z^2$ is a 4×4 matrix,

written as $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ is the tensor product.

If one denotes $|\uparrow\uparrow\rangle = |\uparrow\rangle \otimes |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$

$|\uparrow\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$, $|\downarrow\uparrow\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$, $|\downarrow\downarrow\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$, one gets

$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}$ $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Similarly, $\delta z' \rightarrow \delta z \otimes \mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \mathbb{I}$

$$= \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\delta z^2 \rightarrow \mathbb{I} \otimes \delta z = \mathbb{I} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Clearly, $[\delta z', \delta z^2] = [\delta z \otimes \mathbb{I}, \mathbb{I} \otimes \delta z]$

$$= (\delta z \otimes \mathbb{I})(\mathbb{I} \otimes \delta z) - (\mathbb{I} \otimes \delta z)(\delta z \otimes \mathbb{I})$$

$$= (\delta z \mathbb{I}) \otimes (\mathbb{I} \delta z) - (\mathbb{I} \delta z) \otimes (\delta z \mathbb{I})$$

$$\because [\delta z, \mathbb{I}] = 0 \quad \therefore [\delta z', \delta z^2] = 0 \quad \dots (3f)$$

It is clearly, any operators by construction of tensor product would commute with each other!

Therefore, it would seem to be a problem

for realizing $\{\alpha, \alpha^\dagger\} = \delta_{\alpha\beta}$, $\{\alpha, \beta\} = 0$

$\{\alpha^\dagger, \beta^\dagger\} = 0$ in terms of

matrices.

It turns out that for Fermions, direct usage of tensor product does not work. One

needs to introduce a set of operators

and that would be source of difficulties.

in the numerical work of Fermions.

To construct any Fermions' related operators,

one first constructs $C_{\uparrow}^{\dagger}, C_{\downarrow}^{\dagger}$ on the same site.

If we set $|0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$, $|\uparrow\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$, $|\downarrow\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$

$|\uparrow\downarrow\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$, we find

$\langle 0 | C_{\uparrow}^{\dagger} | 0 \rangle = 1$, $\langle \uparrow | C_{\uparrow}^{\dagger} | \downarrow \rangle = 1$ other $\langle \alpha | C_{\uparrow}^{\dagger} | \beta \rangle = 0$

$\therefore C_{\uparrow}^{\dagger} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ Similarly $C_{\downarrow}^{\dagger} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$

L-3P

Note that $\langle \uparrow\downarrow | C_{\downarrow}^{\dagger} | \uparrow \rangle = \langle \uparrow\downarrow | \downarrow \uparrow \rangle = -1$

It's easy to check that on the same site,

$\{C_{\uparrow}^{\dagger}, C_{\uparrow}^{\dagger}\} = 0$, $\{C_{\downarrow}^{\dagger}, C_{\downarrow}^{\dagger}\} = 0$

$\{C_{\uparrow}, C_{\downarrow}^{\dagger}\} = 1$, $\{C_{\alpha}, C_{\beta}\} = 0$ are

Satisfied. From Eq. (3P), one can get $n_{\uparrow} = C_{\uparrow}^{\dagger} C_{\uparrow}$.

and $n_{\downarrow} = C_{\downarrow}^{\dagger} C_{\downarrow}$ and many other operators.

$$n_{\uparrow} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$n_{\downarrow} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \therefore n_{\uparrow} n_{\downarrow} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$n = n_{\uparrow} + n_{\downarrow} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}$$

So, for a single site, anti-commutations are constructed. What about many sites?

As indicated, direct usage of tensor product ^{considered at} as show in below does not work: (the following is ID)

$$\begin{matrix} 1 & 2 & 3 & & i & - & - & - & j \end{matrix}$$

$$\tilde{C}_{i\delta}^{\dagger} = I \otimes I \otimes I \otimes \dots \otimes C_{\delta}^{\dagger} \otimes I \otimes I \otimes \dots \otimes I \otimes I \otimes \dots$$

$$\tilde{C}_{j\delta}^{\dagger} = I \otimes I \otimes I \otimes \dots \otimes I \otimes \dots \otimes C_{\delta}^{\dagger} \otimes I \otimes \dots$$

$$[\tilde{C}_{i\delta}^{\dagger}, \tilde{C}_{j\delta}^{\dagger}] = 0 \text{ not anti commuting!}$$

To overcome it, it is often done by introducing a string operator from site 1 to the site (i) of the operator.

The idea is to notice that for any given

$$\text{state } |u\rangle = |n_1, n_2, n_3, \dots, n_i, \dots, n_j, \dots\rangle$$

with $n_k = 0$ or 1 but $n_i = n_j = 0$,

$$\tilde{C}_j^+ |\psi\rangle = |n_1, n_2, \dots, n_{i-1}, 0, n_{i+1}, \dots, n_{j-1}, 1, n_{j+1}, \dots\rangle$$

$$\tilde{C}_i^+ \tilde{C}_j^+ |\psi\rangle = |n_1, n_2, \dots, n_{i-1}, 1, n_{i+1}, \dots, n_{j-1}, 1, n_{j+1}, \dots\rangle$$

while $\tilde{C}_i^+ |\psi\rangle = |n_1, n_2, \dots, n_{i-1}, 1, n_{i+1}, \dots, n_{j-1}, 0, n_{j+1}, \dots\rangle$

$$\tilde{C}_j^+ \tilde{C}_i^+ |\psi\rangle = |n_1, n_2, \dots, n_{i-1}, 1, n_{i+1}, \dots, n_{j-1}, 1, n_{j+1}, \dots\rangle$$

If one introduces some kind of string from 1 to the site $\tilde{C}^+$ acts on, one can draw the pattern that

 associated with the string. The

combined operator is C^+ .

Clearly, if strings get cancelled by successive

C^+ operators, one sees  "plateau"

remains and there is a difference between in the configuration

$\tilde{C}_i^+ \tilde{C}_j^+$ & $\tilde{C}_j^+ \tilde{C}_i^+$:

$$\tilde{C}_i^+ \tilde{C}_j^+ \quad \begin{array}{c} \text{---} \boxed{0 \quad n_{i+1} \quad \dots \quad n_{j-1}} \text{---} \\ \text{---} \quad i \quad \quad \quad j \end{array}$$

$$\tilde{C}_j^+ \tilde{C}_i^+ \quad \begin{array}{c} \text{---} \boxed{1 \quad n_{i+1} \quad \dots \quad n_{j-1}} \text{---} \\ \text{---} \quad i-1 \quad i \quad \quad \quad j \end{array}$$

Obviously, the difference is 1 located at site i .

Therefore, if the string is designed to be

$$\hat{S} = (-1)^{\sum_{i=1}^{j-1} n_i} \quad \text{for } \tilde{C}_j^+, \text{ i.e., } \tilde{C}_j^+ = (-1)^{\sum_{i=1}^{j-1} n_i} \tilde{C}_j^+$$

then

$$C_{i8}^+ C_{j8}^+ + C_{j8}^+ C_{i8}$$

$$= (-1)^{0+n_1+1+\dots+n_{j-1}} \tilde{C}_{i8}^+ \tilde{C}_{j8}^+ +$$

$$+ (-1)^{1+n_1+1+\dots+n_{j-1}} \tilde{C}_{j8}^+ \tilde{C}_{i8}^+$$

$$= (-1)^{n_1+1+\dots+n_{j-1}} [\tilde{C}_{i8}^+, \tilde{C}_{j8}^+] = 0$$

$$\text{Now, } (-1)^n = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \equiv P \text{ (parity operator)}$$

$$\therefore C_{j8}^+ = P \otimes P \otimes \dots \otimes P \otimes C_{j8}^+ \otimes I \otimes \dots \otimes I \quad \dots (40)$$

1 2 j j+1

is the matrix representation for the electron creation operator.

Note that from the above construction, one sees that the string operator $\hat{S}$ can turn the bosonic operator into a fermionic operator. Viewed in the other way, $\hat{S}$ can also turn a fermion into a boson. The resulting transformation is essentially

the Jordan-Wigner transformation, which works well in 1D. Hence, there is no real difference in 1D for fermions & bosons

"Standard" models (Hamiltonians) in condensed

Matter Physics

In the adiabatic approximation (ions are fixed),

the Hamiltonian in the 1st quantized form is

$$\hat{H} = \sum_i \frac{\hbar^2}{2m} \nabla_i^2 + \sum_i V(r_i) + \frac{1}{2} \sum_{i \neq j} V(r_i - r_j) \quad \dots (41)$$

where $V(r_i)$ is the potential due to ions,

$V(r_i - r_j)$ is the electron-electron interaction.

In the 2nd quantized form, one has

$$\hat{H} = \sum_{ij\sigma} h_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \frac{1}{2} \sum_{ij\ell m} c_{j\sigma}^\dagger c_m^\dagger c_\ell c_i V_{ij\ell m}$$

$$\text{where } h_{ij} = \int d^3r \phi_i^*(r) \left[\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \phi_j(r)$$

$$V_{ij\ell m} = \int d^3r_1 \int d^3r_2 \phi_j^*(r_1) \phi_i(r_1) V(r_1 - r_2) \phi_m^*(r_2) \phi_\ell(r_2)$$

Note that the orders of indices in $V_{ij\ell m}$ has to be correct, otherwise, a minus sign may be induced.

In the plane wave representation (Valid for metals),

$$\text{one has } \phi_i \rightarrow \frac{1}{\sqrt{V}} e^{i\vec{k} \cdot \vec{r}}$$

$$\begin{aligned} \therefore \sum_{ij} h_{ij} c_{i\sigma}^\dagger c_{j\sigma} &\rightarrow \sum_{\vec{k}\sigma} \langle \vec{k} | \left[\frac{\hbar^2}{2m} p^2 + V(r) \right] | \vec{k} \rangle c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} \\ &= \sum_{\vec{k}} \epsilon_{\vec{k}} c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} + \sum_{\vec{q}} V_{\vec{q}} \rho_{\vec{q}} \end{aligned}$$

where $P(g) = \sum_{\mathbf{k}g} C_{\mathbf{k}+g}^\dagger C_{\mathbf{k}g}$:

$$\frac{1}{2} \sum_{ijlm} C_j^\dagger C_m^\dagger C_l C_i V_{ijlm}$$

$$\rightarrow \frac{1}{2} \sum_{\substack{\mathbf{k}_1, \mathbf{k}_2 \\ \mathbf{k}_3, \mathbf{k}_4}} \langle \mathbf{k}_1 \mathbf{k}_2 | V | \mathbf{k}_3 \mathbf{k}_4 \rangle C_{\mathbf{k}_1}^\dagger C_{\mathbf{k}_2}^\dagger C_{\mathbf{k}_4} C_{\mathbf{k}_3}$$

$$\langle \mathbf{k}_1 \mathbf{k}_2 | V | \mathbf{k}_3 \mathbf{k}_4 \rangle = \frac{1}{V^2} \int d\mathbf{r}_1 \int d\mathbf{r}_2 e^{i(\mathbf{k}_4 - \mathbf{k}_2) \cdot \mathbf{r}_1} e^{i(\mathbf{k}_3 - \mathbf{k}_1) \cdot \mathbf{r}_2} U(\mathbf{r}_1 + \mathbf{r}_2)$$

$$= \frac{1}{V^2} \int d\mathbf{r} e^{i(\mathbf{k}_4 - \mathbf{k}_2) \cdot \mathbf{r}} V(\mathbf{r}) \int d\mathbf{r}_2 e^{i(\mathbf{k}_4 + \mathbf{k}_3 - \mathbf{k}_2 - \mathbf{k}_1) \cdot \mathbf{r}_2}$$

$$= \frac{1}{V} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4} \int d\mathbf{r} V(\mathbf{r}) e^{i\mathbf{g} \cdot \mathbf{r}} \quad \mathbf{g} = \mathbf{k}_4 - \mathbf{k}_2$$

$$= \frac{V_g}{V} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4}, \text{ set } \mathbf{k}_3, \delta_3 = \mathbf{k}, \delta$$

$$\mathbf{k}_4, \delta_4 = \mathbf{k}', \delta'$$

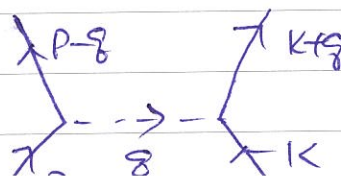
$$\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k} + \mathbf{k}', \quad \mathbf{k}_4 - \mathbf{k}_2 = \mathbf{g}, \quad \therefore \mathbf{k}_2 = \mathbf{k}' - \mathbf{g}$$

$$\therefore = \frac{1}{2V} \sum_{\substack{\mathbf{g}, \mathbf{k}, \mathbf{k}' \\ \delta, \delta'}} V_g C_{\mathbf{k}+g}^\dagger C_{\mathbf{k}-g}^\dagger C_{\mathbf{k}'} C_{\mathbf{k}} \delta_{\delta, \delta'}$$

$$\hat{H} = \sum_{\mathbf{k}g} \epsilon_{\mathbf{k}} C_{\mathbf{k}g}^\dagger C_{\mathbf{k}g} + \sum_{\mathbf{g}} V_g P_{\mathbf{g}} + \frac{1}{2V} \sum_{\substack{\mathbf{g}, \mathbf{k}, \mathbf{k}' \\ \delta, \delta'}} V_g C_{\mathbf{k}+g}^\dagger C_{\mathbf{k}-g}^\dagger C_{\mathbf{k}'} C_{\mathbf{k}} \delta_{\delta, \delta'}$$

--- (42)

the interaction can be represented graphically as



Eq. (42) is still too complicated to be solved.

Quite often, one makes a further approximation

by setting $V_g = 0$ & $\epsilon_g = \frac{\hbar^2 g^2}{2m} - \epsilon_F$. This describes

the homogeneous electron gas or electron liquid:

$$\hat{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \frac{1}{2V} \sum_{\substack{\mathbf{q} \\ \mathbf{k}, \mathbf{k}' \\ \sigma, \sigma'}} V_{\mathbf{q}} c_{\mathbf{k}+\mathbf{q}\sigma}^\dagger c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}'\sigma'} c_{\mathbf{k}'-\mathbf{q}\sigma'} \quad L - (43)$$

where $V_{\mathbf{q}} = \frac{4\pi e^2}{q^2}$ is the Coulomb interaction.

Even for eq. (43), there is no known exact solutions.

Electron - phonon interaction

The adiabatic approximation is by no means always

good. There are many important situations (such as

superconductivity & Peierls instability) in which

the phenomena are induced by phonons and can't be explained ^{without} phonons.

For a Bravais lattice, without electron-phonon interaction, the Hamiltonian is simply

$$\hat{H} = \hat{H}_n + \sum \hbar \omega_{\mathbf{q}} a_{\mathbf{q}}^\dagger a_{\mathbf{q}} \quad \dots (44)$$

Where $\hat{H}_e$ is given by eq (42), $a_{q\lambda}^+$ ($a_{q\lambda}$) are creation and annihilation operators for phonons, and $\omega_{q\lambda}$ is the phonon frequency with q & polarization λ .

The Fröhlich Hamiltonian.

If we assume that the potential due to a particular ion depends only on the distance of the electron to the center of the ion (rigid-ion approximation), we get

$$H_{e-p} = \sum_{K, K', n} \langle K | V(\vec{r} - \vec{r}_n - \vec{u}_n) | K' \rangle C_{K\alpha}^{\dagger} C_{K'\beta}$$

Where $V(r)$ is the potential due to a single ion at the origin, and $\vec{u}_n$ is the displacement of the ion whose equilibrium position is at $\vec{r}_n$.

$$\therefore \langle K | V(\vec{r} - \vec{r}_n - \vec{u}_n) | K' \rangle$$

$$= \int d\vec{r} \frac{1}{V} e^{i(\vec{K}' - \vec{K}) \cdot \vec{r}} V(\vec{r} - \vec{r}_n - \vec{u}_n) = \int d\vec{r} \frac{1}{V} e^{i(\vec{K}' - \vec{K}) \cdot \vec{r}}$$

$$\times \int d\vec{q} \frac{V_q}{N} e^{i\vec{q} \cdot (\vec{r} - \vec{r}_n - \vec{u}_n)}$$

$$= \frac{V}{N} \delta_{K-K'} e^{i(\vec{K}' - \vec{K}) \cdot (\vec{r}_n + \vec{u}_n)}$$

$$\therefore H_{e-p} = \sum_{K, K'} e^{i(\vec{K}' - \vec{K}) \cdot (\vec{r}_n + \vec{u}_n)} \frac{U_{K-K'}}{N} C_{K\alpha}^{\dagger} C_{K'\beta}$$

Assuming $(\vec{R}' - \vec{R}) \cdot \vec{u}_n \ll 1$, we find

$$e^{i(\vec{R}' - \vec{R}) \cdot \vec{u}_n} \approx 1 + i(\vec{R}' - \vec{R}) \cdot \vec{u}_n$$

$$= 1 + i \frac{1}{\sqrt{N}} (\vec{R}' - \vec{R}) \cdot \sum_{\vec{g}} e^{i\vec{g} \cdot \vec{r}_n} \vec{u}_{\vec{g}}$$

$$\therefore H_{e-p} = \frac{i}{N\sqrt{N}} \sum_{\substack{\vec{k}, \vec{k}' \\ n, \vec{g}}} e^{i(\vec{R}' - \vec{R} + \vec{g}) \cdot \vec{r}_n} (\vec{R}' - \vec{R}) \cdot \vec{u}_{\vec{g}} U_{\vec{k}-\vec{k}'} C_{\vec{k}\vec{g}}^{\dagger} C_{\vec{k}'\vec{g}}$$

$$\sum_n e^{i(\vec{k}' - \vec{k} + \vec{g}) \cdot \vec{r}_n} = N \sum_{\vec{g}} \delta(\vec{k}' - \vec{k} + \vec{g} - \vec{g})$$

$$\therefore H_{e-p} = \frac{i\sqrt{N}}{N} \sum_{\substack{\vec{k}, \vec{k}' \\ \vec{g}}} (\vec{R}' - \vec{R}) \cdot \vec{u}_{\vec{k}-\vec{k}'+\vec{g}} U_{\vec{k}-\vec{k}'} C_{\vec{k}\vec{g}}^{\dagger} C_{\vec{k}'\vec{g}}$$

Now the displacement operator can be written as (see page 4-45) (the convention for Fourier transform is different. $f(\vec{r}) = \sum e^{i\vec{r} \cdot \vec{r}_n} f(\vec{r}_n)$ is used here!)

$$\vec{u}_n = \frac{1}{\sqrt{N}} \sum_{\vec{k}} \sqrt{\frac{\hbar}{2M\omega_{\vec{k}}}} \left[\hat{a}_{\vec{k}} \vec{e}_{\vec{k}} e^{i\vec{k} \cdot \vec{r}_n} + \hat{a}_{\vec{k}+\vec{k}}^{\dagger} \vec{e}_{\vec{k}}^* e^{-i\vec{k} \cdot \vec{r}_n} \right]$$

$$= \frac{1}{\sqrt{N}} \sum_{\vec{k}} \sqrt{\frac{\hbar}{2M\omega_{\vec{k}}}} \left[\hat{a}_{\vec{k}} + \hat{a}_{-\vec{k}}^{\dagger} \right] \vec{e}_{\vec{k}} e^{i\vec{k} \cdot \vec{r}_n}$$

isotropic case
 $\vec{e}_{\vec{k}} = \text{real} \ \& \ \vec{e}_{\vec{k}} = \vec{e}_{-\vec{k}}$

$$\therefore \vec{u}_{\vec{g}} = \frac{1}{\sqrt{N}} \sqrt{\frac{\hbar}{2M\omega_{\vec{g}}}} (\hat{a}_{\vec{g}} + \hat{a}_{-\vec{g}}^{\dagger}) \vec{e}_{\vec{g}}$$

$$\therefore \hat{H}_{e-p} = \sum_{\substack{\vec{k}, \vec{g} \\ \lambda, \vec{g}}} M_{\vec{g}} (\hat{a}_{\vec{g}\lambda} + \hat{a}_{-\vec{g}\lambda}^{\dagger}) C_{\vec{k}-\vec{g}\vec{g}}^{\dagger} C_{\vec{k}\vec{g}} \quad \dots (45)$$

$$M_{\vec{g}} = i \sqrt{\frac{\hbar}{2M\omega_{\vec{g}}}} V_{\vec{g}} (\vec{g} \cdot \vec{e}_{\vec{g}\lambda})$$

Note that here summation over $\vec{q}$ includes all reciprocal lattice vectors $\vec{G}$!

More precisely, one can restrict $\vec{q}$ to the 1st B.Z. zone. In this case, only longitudinal mode $\vec{q} \parallel \vec{E}_{\vec{q}\lambda}$ contributes.

One has

$$H_{ep} = \sum_{\vec{q}, \vec{G}} M_{\vec{q}+\vec{G}} P_{\vec{q}+\vec{G}} (a_{\vec{q}} + a_{-\vec{q}}^{\dagger}) \quad \dots (46)$$

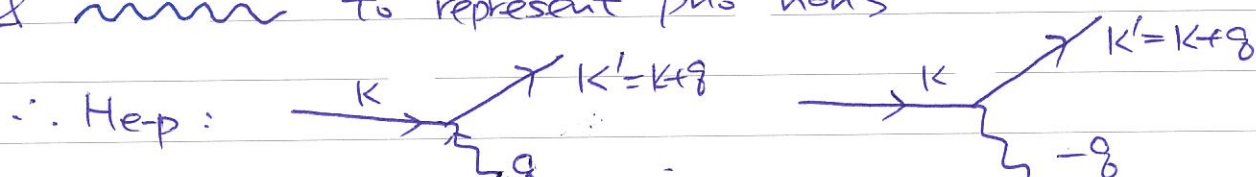
$$P_{\vec{q}+\vec{G}} = \sum_{\vec{k}} C_{\vec{k}+\vec{q}+\vec{G}}^{\dagger} C_{\vec{k}}$$

$$M_{\vec{q}+\vec{G}} = i \sqrt{\frac{\hbar}{2MN\omega_{\vec{q}\lambda}}} U_{\vec{q}} \underbrace{\vec{q} \cdot \vec{E}_{\vec{q}\lambda}}_{\parallel \vec{q} \parallel}$$

Combining H_{ep} with free electrons & phonons is the Fröhlich Hamiltonian

$$H_F = \sum_{\vec{k}} \epsilon_{\vec{k}} C_{\vec{k}}^{\dagger} C_{\vec{k}} + \sum_{\vec{q}} \hbar \omega_{\vec{q}} a_{\vec{q}}^{\dagger} a_{\vec{q}} + \sum_{\vec{q}} M_{\vec{q}+\vec{G}} P_{\vec{q}+\vec{G}} (a_{\vec{q}} + a_{-\vec{q}}^{\dagger}) \quad \dots (47)$$

Diagrammatically, one uses --- to represent electrons & ~~~~~ to represent phonons



Tight-binding Hamiltonian

As we discussed before, the plane-wave basis is only good for s, p orbitals. For transitional metals, with d-orbitals, the orbitals are more localized. It is therefore more convenient to use tight-binding approach.

In this approach, one has

$$\hat{H} = - \sum_{\langle i,j \rangle} t C_i^\dagger C_j - \sum_{\langle\langle i,j \rangle\rangle} t' C_i^\dagger C_j - t'' \dots + \text{h.c.}$$

(nearest neighbour)
(next nearest neighbour)
(next next nearest neighbour)

$$+ \sum_i \sum_{j \neq i} C_j^\dagger C_m^\dagger C_\ell C_i V_{ij\ell m}$$

Where i, j, ℓ, m are indices for sites of lattice points,

$C_j^\dagger C_m C_\ell C_i V_{ij\ell m} \Rightarrow n_i \frac{1}{|r_i - r_j|} n_j$ is usually long-ranged

In the extreme case when screening is maximal, one has the celebrated Hubbard model

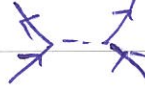
$$\hat{H} = - \sum_{\langle i,j \rangle} t (C_i^\dagger C_j + C_j^\dagger C_i) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

the Hubbard model represents the simplest model with hopping & interaction terms. As we shall see, it plays important role in understanding phenomena associated correlations.

Time-independent perturbation theory & Goldstone diagrams

Just as in the quantum mechanics, for a given 2nd quantized Hamiltonian,

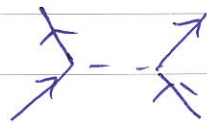
$$H = H_0 + H_I \quad (\text{for example.})$$

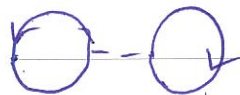
$H_I = e-e$ interaction , one

can develop perturbation theory in the energy space, in particular, for the ground state

$$E - E_0 = \underbrace{\langle \psi_0 | H_I | \psi_0 \rangle}_{\substack{\text{ground} \\ \text{state, energy} \\ |\psi_0\rangle}} + \sum_{n \neq 0} \frac{\langle \psi_0 | H_I | \psi_n \rangle \langle \psi_n | H_I | \psi_0 \rangle}{E_0 - E_n} + \dots \quad (48)$$

if $|\psi_0\rangle$ is non-degenerate,

If H_I is represented by , the 1st term can be represented by the diagram



For electron liquids (see eq. (43)), this corresponds

$$\text{to } \frac{1}{2V} U_{q=0} \sum_{\mathbf{k}, \mathbf{k}'} \langle C_{\mathbf{k}+\mathbf{q}}^\dagger C_{\mathbf{k}'} \rangle \langle C_{\mathbf{k}}^\dagger C_{\mathbf{k}'} \rangle$$

(direct term) or by the diagram.



$$\frac{-1}{2V} \sum_{\substack{q, k, k' \\ s, s'}} U_q \langle C_{k+q, s}^\dagger C_{k, s'} \rangle \langle C_{k, s}^\dagger C_{k+q, s} \rangle$$

$$= \frac{-1}{2V} \sum_{s, q, k} U_q \langle C_{k+q, s}^\dagger C_{k+q, s} \rangle \langle C_{k, s}^\dagger C_{k, s} \rangle$$

which is the exchange energy.

$$\therefore E - E_0 = \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \text{[diagram 4]} + \dots$$

These are known as Goldstone diagrams for the ground state energy.

In general, the Goldstone's theorem can be proved

$$E - E_0 = \langle \psi_0 | \hat{H}_I \sum_{n=0}^{\infty} \left(\frac{1}{E_0 - H_0} \hat{H}_I \right)^n | \psi_0 \rangle$$

Connected diagrams.

(We shall not prove it ^{now} but outline the prove later in the Green's function approach.)

Even though this is the standard perturbation theory, it usually provides useful approach / insights to difficult problems (such as deriving the t-J model from the Hubbard model..)

Kohn anomaly & Peierls transition

A typical usage of time-independent perturbation theory is to extract effective Hamiltonian to the lower orders.

We shall use the Fröhlich Hamiltonian (eq. (47)) as an example.

$$\text{Let } \hat{H}_0 \equiv \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} a_{\mathbf{q}}^\dagger a_{\mathbf{q}}$$

$$\hat{H}_{ep} = \sum_{\substack{\mathbf{k}, \mathbf{k}' \\ \mathbf{q} = \mathbf{k} - \mathbf{k}'}} M_{\mathbf{k}\mathbf{k}'} (a_{\mathbf{q}}^\dagger + a_{\mathbf{q}}) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}'\sigma}$$

$$\hat{H} = \hat{H}_0 + \hat{H}_{ep} \quad E_0 = \text{energy of } H_0 \text{ with } \underbrace{\text{of state } |\Phi\rangle}_{\text{ng phonons \& n}_{\mathbf{k}} \text{ electrons}}$$

To the 2nd order,

$$E = E_0 + \langle \Phi | \hat{H}_{ep} | \Phi \rangle + \underbrace{\langle \Phi | \hat{H}_{ep} \frac{1}{E_0 - H_0} \hat{H}_{ep} | \Phi \rangle}_{E_2}$$

Clearly, $\therefore$ # of phonons & electrons of $\hat{H}_{ep} |\Phi\rangle$ & $|\Phi\rangle$ are different. $\therefore \langle \Phi | \hat{H}_{ep} | \Phi \rangle = 0$

To conserve # of phonons & electrons (at $T=0$), 4

terms in E_2 is reduced to 2 terms (we shall suppress spin indices)

$$E_2 = \langle \Phi | \sum_{\mathbf{k}, \mathbf{k}'} M_{\mathbf{k}\mathbf{k}'} a_{\mathbf{q}}^\dagger c_{\mathbf{k}}^\dagger c_{\mathbf{k}'} (E_0 - H_0)^{-1} \sum_{\mathbf{k}'', \mathbf{k}'''} M_{\mathbf{k}''\mathbf{k}'''} a_{\mathbf{q}'} c_{\mathbf{k}''}^\dagger c_{\mathbf{k}'''} |\Phi\rangle \\ + \langle \Phi | \sum_{\mathbf{k}, \mathbf{k}'} M_{\mathbf{k}\mathbf{k}'} a_{\mathbf{q}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}'} (E_0 - H_0)^{-1} \sum_{\mathbf{k}'', \mathbf{k}'''} M_{\mathbf{k}''\mathbf{k}'''} a_{-\mathbf{q}'}^\dagger c_{\mathbf{k}''}^\dagger c_{\mathbf{k}'''} |\Phi\rangle$$

require $g' = -g$ $K'' = K'$, $K''' = K$ in the first term

$$\therefore E_2^1 = \langle \Phi | \sum_{K, K'} |M_{K, K'}|^2 (a_{-q}^\dagger c_{K'}^\dagger c_{K'} \frac{1}{E_0 - H_0} a_{-q} c_{K'}^\dagger c_K | \Phi \rangle$$

$\uparrow$
 $M_{K', K} = M_{K, K'}^*$

L -- (49)

$$(\vec{r} \cdot \vec{A}) \cdot \vec{E} \cdot \vec{V}_q = (\vec{r} \cdot \vec{E} \cdot \vec{V}_q)^*$$

A Feynman diagram illustrating the decay of a photon into an electron-positron pair. A horizontal line represents the photon, with a wavy line labeled γ entering from the left and a wavy line labeled γ exiting to the right. From the left end of the horizontal line, an electron line (solid line with an arrow pointing right) labeled e^- extends to the left. From the right end of the horizontal line, a positron line (solid line with an arrow pointing right) labeled e^+ extends to the right. The horizontal line is labeled k in the middle.

$$g' = -g, \quad k'' = k', \quad k''' = k$$
$$E_2^2 = \langle \Phi | \sum_{k, k'} |M_{k, k'}|^2 \left[a_g c_{k'}^\dagger c_{k'} - \frac{1}{E_0 - H_0} a_g^\dagger c_{k'}^\dagger c_k \right] | \Phi \rangle$$
$$iS = \Sigma_K - \hbar\omega_g + \Sigma_{K'} \quad \therefore E_0 - \hbar\omega_g \rightarrow \Sigma_K + \hbar\omega_g - \Sigma_{K'}$$

$$\therefore C_{Cl}^+ C_{Cl} \rightarrow n_{Cl} \quad , \quad C_{Cl'} C_{Cl'}^+ \rightarrow n_{Cl'} - 1$$

$$q_g^+ q_g \rightarrow n_g$$

Similarly, for the 2nd term

$$E_0 - H_0 \rightarrow \epsilon_K - \epsilon_{K'} - \hbar \omega_g, \quad a_g a_g^\dagger \rightarrow n_g + 1$$

$$\therefore E_2 = \sum_{K, K'} |M_{KK'}|^2 \langle n_K (1 - n_{K'}) \rangle \left[\frac{\langle n_g \rangle}{\epsilon_K - \epsilon_{K'} + \hbar \omega_g} + \frac{\langle n_g \rangle + 1}{\epsilon_K - \epsilon_{K'} - \hbar \omega_g} \right]$$

L - - (51)

We shall assume $\omega_g = \omega_g$, $\therefore \langle n_g \rangle = \langle n_g \rangle$

$$E = E_0 + \sum_{K, K'} |M_{KK'}|^2 \langle n_K \rangle \left[\frac{2(\epsilon_K - \epsilon_{K'}) \langle n_g \rangle}{(\epsilon_K - \epsilon_{K'})^2 - (\hbar \omega_g)^2} + \frac{1 - \langle n_{K'} \rangle}{\epsilon_K - \epsilon_{K'} - \hbar \omega_g} \right]$$

L - (52)

Where $\langle n_K \rangle \langle n_{K'} \rangle \langle n_g \rangle (\epsilon_K - \epsilon_{K'})$ is odd in $K \neq K'$
 $\therefore$ is cancelled.

From eq. (52), one can see the term $\propto \langle n_g \rangle$, the coefficient can be regarded as a correction to the phonon energy $\hbar \omega_g$

$$\therefore \hbar \omega_g^R = \hbar \omega_g + \sum_K |M_{KK'}|^2 \frac{2 \langle n_K \rangle (\epsilon_K - \epsilon_{K'})}{(\epsilon_K - \epsilon_{K'})^2 - (\hbar \omega_g)^2}$$

↑
(renormalized)

$$\approx \hbar \omega_g - \sum_K \frac{2 |M_{KK'}|^2 \langle n_K \rangle}{\epsilon_{K'} - \epsilon_K} + \dots$$

(neglect $(\hbar \omega_g)^2$)

$$= \hbar \omega_g - \sum_K |M_{KK'}|^2 \frac{\langle n_K \rangle - \langle n_{K'} \rangle}{\epsilon_{K'} - \epsilon_K} + \dots \quad (53)$$

$|M_{KK'}|^2 = |M_{K'K}|^2$

The 2nd term in

Eg. (53) has a simple graphical meaning:



electron bubble (electron-hole pair)
: excite electron from k
to k' $\therefore \epsilon_{k'} - \epsilon_k$

$$\therefore \text{wavy line} = \text{wavy line} + \text{wavy line} \circ \text{wavy line}$$

Just as impurity problem, $\circ$ acts as self energy
the

and correct twg!

Nesting & Kohn anomaly

in Eg. (53)

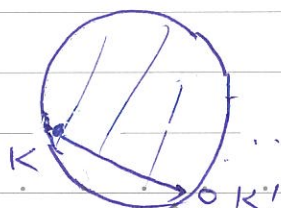
The 2nd term has the form $\frac{\langle n_k \rangle - \langle n_{k'} \rangle}{\epsilon_{k'} - \epsilon_k}$

which is interpreted as exciting an electron
at ϵ_k to $\epsilon_{k'}$: the denominator is
the energy difference, the numerator

$$= n_k (1 - n_{k'}) - (1 - n_k) n_{k'} = n_k - n_{k'}$$

$\uparrow$ $\uparrow$
 k occupied k'
 un-occupied

If the Fermi surface is spherical, the above
excitation can be represented graphically as



To evaluate the 2nd term in eq. (53), one

notices that $M_{KK'} \sim \frac{1}{\sqrt{\omega_g}} \underbrace{|k-k'|}_g \underbrace{V_{k-k'}}_{\sqrt{g}}$

$\rightarrow \text{const. as } g \rightarrow 0$

$\therefore$ One can roughly approximate $|M_{KK'}|^2$ by a constant in equation (53).

Hence the 2nd term is determined by (at $\omega=0$)

$$\chi(\vec{q}, \omega) = \int \frac{d^d K}{(2\pi)^d} \frac{\langle n_K \rangle - \langle n_{K+q} \rangle}{\epsilon_K - \epsilon_{K+q} + \omega + i0^+} \quad (K=K'+q, K \rightarrow K) \quad (54)$$

Which is known as the Lindhard response function.

The Lindhard function is often encountered when one investigates properties of electron gases.

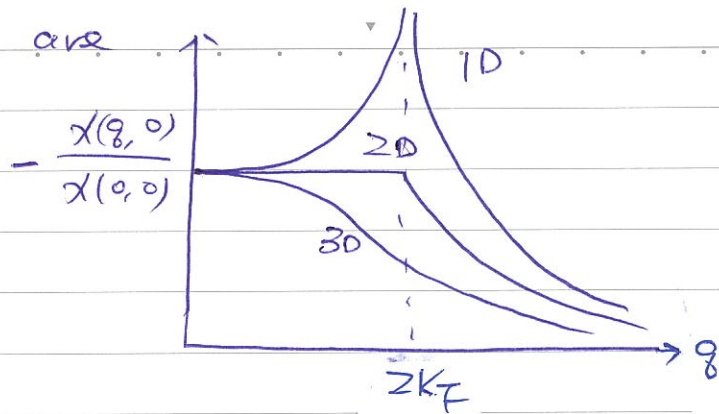
For 3D, $\epsilon_K = \frac{\hbar^2 K^2}{2m}$, one finds ($T=0$)

$$\begin{aligned} \chi(q, 0) &= \int \frac{d^3 K}{(2\pi)^3} \frac{\theta(K-K_F) - \theta(|K+q|-K_F)}{K^2 - (K+q)^2} \times \frac{2m}{\hbar^2} \\ &= -\frac{m K_F}{2\pi^2} \left[1 + \frac{1 - \left(\frac{q}{2K_F}\right)^2}{q/K_F} \ln \left| \frac{1 + q/2K_F}{1 - q/2K_F} \right| \right] \quad (\text{H.W.}) \end{aligned} \quad (55)$$

As one goes down to 1D, one finds

$$\chi(q, 0) = -\frac{m}{\pi K_F} \frac{1}{q/2K_F} \ln \left| \frac{1 - q/2K_F}{1 + q/2K_F} \right| \quad (56)$$

whose plots are



One sees that $\chi(z, 0)$ diverges at $z/k = 8$ for 1D.

The divergence of $\chi(q, 0)$ at $q = 2k_F$ is due to the particular topology of the Fermi surface, which is often termed nesting.

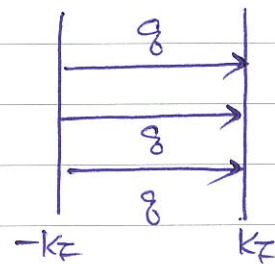
In eq. (54), when $\omega=0$, the dominant contribution comes from $\Sigma_K \simeq \Sigma_{K+g}$, which occurs at (with $K \equiv K_F$)

$$g = 2k_F$$

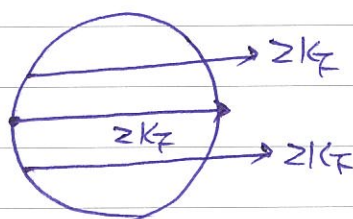
In ID, this is dominant

(one can view it as 2D

With no dependence on K_g)



However, in higher dimension, such paired states are reduced, hence there is no singularity.



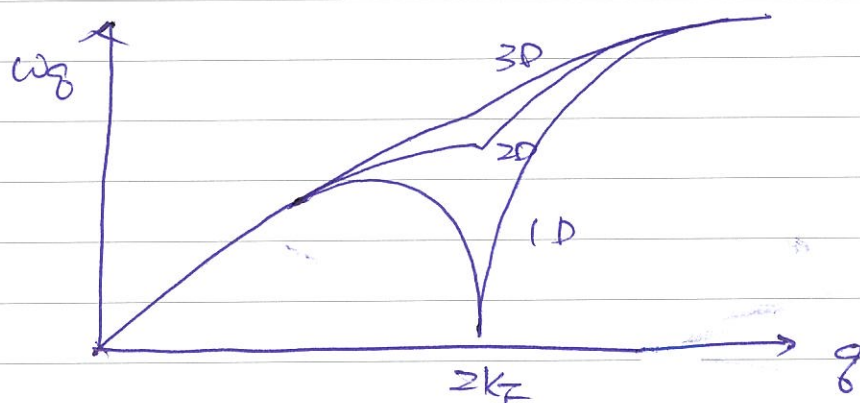
For general Fermi surfaces, as long as there are segments in the Fermi surfaces that differ by $2k_F$, it is termed that the

Fermi surface is nested. One expects that



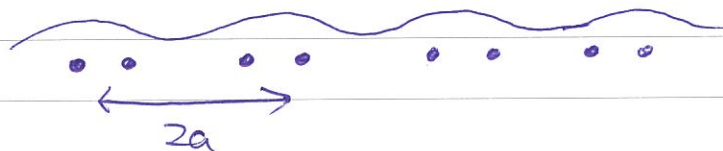
The divergence of $\chi(8,0)$ implies (from eq. (5))

That phonons get soft at $q = 2k_F$:



This is called the Kohn anomaly.

This would be pictured as

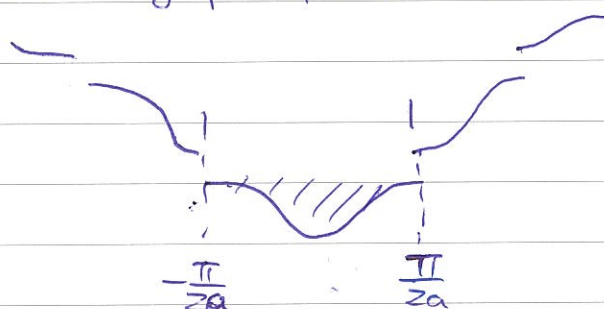


That is, it's dimerized with period $2a$.

Hence there is a charge modulation. Furthermore,

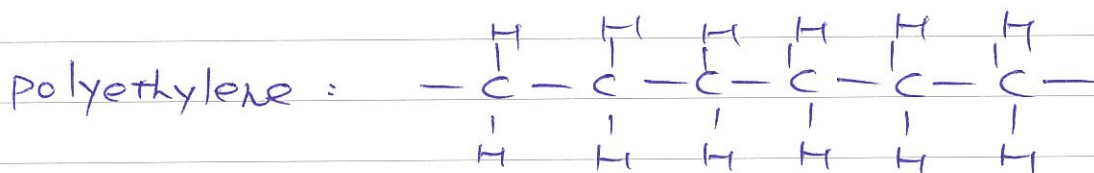
$\pm \frac{\pi}{2a}$ now become zone boundary of B.Z., it

must have band gap opened as follows



The system becomes an insulator. This is known as the Peierls transition.

Peierls transition happens in real 1D system. The most famous one is the polyacetylene:



(insulator, C's 4 bonds are used up.)



the extra electron per carbon can resonant through.

fluctuation of the double bonds but it is fixed with dimerized distances between Carbon atoms.

Mean-Field theory

The mean-field theory can be best adopted to describe the situation when an order happens.

Even if there is no ordering, by assuming appropriate averages, one can also help in

solving the problem. We shall start by

treating the Hartree-Fock approximation as a mean-field theory.

Hartree-Fock approximation

We start by Eq (41)-1 with $h_{ij} = \epsilon_i \delta_{ij}$ ($U=0$)

$$\hat{H} = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{i,j,k,l} \langle ij | U | kl \rangle c_i^\dagger c_j^\dagger c_l c_k$$

$$\begin{aligned} \langle ij | U | kl \rangle &= \int d\mathbf{r} \int d\mathbf{r}' \phi_i^*(\mathbf{r}) \phi_j^*(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \phi_k(\mathbf{r}) \phi_l(\mathbf{r}') \\ &= \langle ji | U | lk \rangle \quad (\text{exchange } \mathbf{r} \text{ \& } \mathbf{r}') \end{aligned}$$

where we have suppressed spin indices.

We now approximate the 4-Fermion term by

all possible average on $\langle c^\dagger c \rangle$:

$$c_i^\dagger c_j^\dagger c_\ell c_k \approx c_i^\dagger \langle c_j^\dagger c_\ell \rangle c_k + c_j^\dagger c_\ell \langle c_i^\dagger c_k \rangle - c_i^\dagger c_\ell \langle c_j^\dagger c_k \rangle - c_j^\dagger c_k \langle c_i^\dagger c_\ell \rangle \quad (17)$$

One further assumes that in the basis $\phi_i(\mathbf{r})$,

$$\langle c_i^\dagger c_\ell \rangle = \delta_{i\ell} \langle c_i^\dagger c_i \rangle = \bar{n}_i \delta_{i\ell}$$

Which in turns implies the other two indices

must be the same if $i, j, \ell \neq k$ are momentum

and momentum conservation implies $j = k$ too.

$$\therefore \sum_{ijkl} \langle ij | V | kl \rangle c_i^\dagger c_j^\dagger c_\ell c_k$$

$$\approx \sum_{ij} \langle ij | V | ij \rangle [\bar{n}_j c_i^\dagger c_i + \bar{n}_i c_j^\dagger c_j] - \langle ij | V | ji \rangle [\bar{n}_j c_i^\dagger c_i + \bar{n}_i c_j^\dagger c_j]$$

$$\therefore H = \sum_i E_i c_i^\dagger c_i$$

$\uparrow$ Hartree $\langle \phi_i(\mathbf{r}) |^2 V(\mathbf{r}-\mathbf{r}') | \phi_i(\mathbf{r}) |^2$
 $\uparrow$ Fock term $\langle \phi_i(\mathbf{r}) | V(\mathbf{r}-\mathbf{r}') | \phi_j(\mathbf{r}) \rangle$

$$E_i = \epsilon_i + \sum_j \bar{n}_j [\langle ij | V | ij \rangle - \langle ij | V | ji \rangle] \quad (18)$$

Clearly, one can think E_i as the energy eigenvalue to

$$\left\{ \frac{\hbar^2}{2m} \nabla^2 + \int d^3\mathbf{r}' V(\mathbf{r}, \mathbf{r}') \sum_j \bar{n}_j |\phi_j(\mathbf{r}')|^2 \right\} \phi_i = E_i \phi_i(\mathbf{r})$$

$$- \int d^3\mathbf{r}' V(\mathbf{r}, \mathbf{r}') \sum_j \bar{n}_j \phi_j^*(\mathbf{r}') \phi_i(\mathbf{r}') \phi_j(\mathbf{r}) = E_i \phi_i(\mathbf{r}) \quad (19)$$

One can easily verify that

$$\phi(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k} \cdot \vec{r}} \quad (s_m = \uparrow \& \downarrow)$$

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

$$\text{Eq. (50)} \Rightarrow E_k = \frac{\hbar^2 k^2}{2m} + \sum_{k'} n_{k'} [\langle k k' | V | k k' \rangle - \langle k k' | V | k' k \rangle]$$

$$\langle k k' | V | k k' \rangle = \int d\vec{r} \int d\vec{r}' \frac{1}{V^2} e^{i\vec{k} \cdot \vec{r}} e^{i\vec{k}' \cdot \vec{r}'} \frac{e^2}{|\vec{r} - \vec{r}'|} e^{i\vec{k}' \cdot \vec{r}} e^{i\vec{k} \cdot \vec{r}'}$$

$$= \frac{e^2}{V} \int d\vec{r} \frac{1}{R} = \frac{4\pi e^2}{V} \int_0^L R dR$$

$$\Rightarrow \frac{1}{3} \times L^2 \rightarrow 0 \text{ as } L \rightarrow \infty$$

$$\langle k k' | V | k' k \rangle = \int d\vec{r} \int d\vec{r}' \frac{1}{V^2} e^{i(\vec{k}' - \vec{k}) \cdot (\vec{r} - \vec{r}')} \frac{e^2}{|\vec{r} - \vec{r}'|}$$

$$= \frac{e^2}{V} \int d\vec{r} \frac{1}{R} e^{i(\vec{k}' - \vec{k}) \cdot \vec{r}}$$

$$= \frac{e^2}{V} \times \frac{4\pi}{|\vec{k}' - \vec{k}|^2}$$

$$\therefore E_k = \frac{\hbar^2 k^2}{2m} - \sum_{k'} n_{k'} \frac{e^2}{V} \frac{4\pi}{|\vec{k}' - \vec{k}|^2}$$

$$= \frac{\hbar^2 k^2}{2m} - \frac{e^2}{2\pi^2} \int_0^{k_F} \frac{d^3 k'}{(\vec{k}' - \vec{k})^2} \text{ which}$$

is the same as eq. (10)

$$\therefore E_k = \frac{\hbar^2 k^2}{2m} - \frac{e^2 k_F}{\pi} \left[1 + \frac{k_F^2 - k^2}{2k_F k} \ln \left| \frac{k_F + k}{k_F - k} \right| \right]$$

Consistent with eq. (11)

Stoner model of metallic ferromagnetism

There are magnets in which electrons both generate moments (magnetization) and also form the conduction band. This is known itinerant ferromagnetism.

Such metallic magnetism happens in transition metals (such as Fe, Co, Ni) where the conduction bands are formed by narrower d or f orbitals.

The simplest model to describe the Coulomb interaction in these orbitals is the

Hubbard model ($n \uparrow n \downarrow = \frac{1}{2}(n \uparrow + n \downarrow)^2 - (n \uparrow^2 + n \downarrow^2)/2 = \frac{1}{2}n^2 - n \uparrow^2$ ^{we shall neglect $n \uparrow^2$})

$$H = \sum_{\mathbf{k}\sigma} \sum_{\mathbf{k}'} C_{\mathbf{k}\sigma}^\dagger C_{\mathbf{k}\sigma} + \frac{U}{2U} \sum_{\mathbf{k}\mathbf{k}'} \underbrace{C_{\mathbf{k}+\mathbf{g}\sigma}^\dagger C_{\mathbf{k}\mathbf{g}\sigma'}^\dagger C_{\mathbf{k}'\sigma'} C_{\mathbf{k}\sigma}}_V$$

We can use the Hartree - Fock approximation to search for a ferromagnetic solution by getting

$$\begin{aligned} \langle C_{\mathbf{k}\uparrow}^\dagger C_{\mathbf{k}\uparrow} \rangle &= \delta_{\mathbf{k}\mathbf{k}'} \bar{n}_{\mathbf{k}\uparrow} \\ \langle C_{\mathbf{k}\downarrow}^\dagger C_{\mathbf{k}\downarrow} \rangle &= \delta_{\mathbf{k}\mathbf{k}'} \bar{n}_{\mathbf{k}\downarrow} \end{aligned} \quad \dots (60)$$

Here unlike the previous approach, one keeps

$\langle \rangle \langle \rangle$ terms. A more solid argument is to write

$$C_{\mathbf{k}\uparrow}^\dagger C_{\mathbf{k}\uparrow} = \langle C_{\mathbf{k}\uparrow}^\dagger C_{\mathbf{k}\uparrow} \rangle + \underbrace{(C_{\mathbf{k}\uparrow}^\dagger C_{\mathbf{k}\uparrow} - \langle C_{\mathbf{k}\uparrow}^\dagger C_{\mathbf{k}\uparrow} \rangle)}_{\delta C_{\mathbf{k}\uparrow}^\dagger C_{\mathbf{k}\uparrow}}$$

and assume the fluctuation $\delta(C_k^\dagger C_k) \ll \langle C_k^\dagger C_k \rangle$.

One gets

$$V = \frac{U}{2V} \left\{ \sum_{\substack{KK'g \\ \delta\delta'}} [\langle C_{k+g\delta}^\dagger C_{k\delta} \rangle + \delta C_{k+g\delta}^\dagger C_{k\delta}] [\langle C_{k'g\delta'}^\dagger C_{k'\delta'} \rangle + \delta C_{k'g\delta'}^\dagger C_{k'\delta'}] \right. \\ \left. - \sum_{\substack{KK'g \\ \delta\delta'}} [\langle C_{k+g\delta}^\dagger C_{k'\delta'} \rangle + \delta C_{k+g\delta}^\dagger C_{k'\delta'}] [\langle C_{k'g\delta'}^\dagger C_{k\delta} \rangle + \delta C_{k'g\delta'}^\dagger C_{k\delta}] \right\}$$

Now, the idea is to neglect $O(\delta^2)$ term. We obtain

$$V_{MF} = \frac{U}{2V} \sum_{\substack{KK'g \\ \delta\delta'}} [\langle C_{k+g\delta}^\dagger C_{k\delta} \rangle \delta C_{k'g\delta'}^\dagger C_{k'\delta'} + \langle C_{k'g\delta'}^\dagger C_{k'\delta'} \rangle \delta C_{k+g\delta}^\dagger C_{k\delta}] \\ - \frac{U}{2V} \sum_{\substack{KK'g \\ \delta\delta'}} [\langle C_{k+g\delta}^\dagger C_{k'\delta'} \rangle \delta C_{k'g\delta'}^\dagger C_{k\delta} + \langle C_{k'g\delta'}^\dagger C_{k\delta} \rangle \delta C_{k+g\delta}^\dagger C_{k'\delta'}] \\ + \frac{U}{2V} \sum_{\substack{KK'g \\ \delta\delta'}} \langle C_{k+g\delta}^\dagger C_{k\delta} \rangle \langle C_{k'g\delta'}^\dagger C_{k'\delta'} \rangle \\ - \frac{U}{2V} \sum_{\substack{KK'g \\ \delta\delta'}} \langle C_{k+g\delta}^\dagger C_{k'\delta'} \rangle \langle C_{k'g\delta'}^\dagger C_{k\delta} \rangle$$

Now, by changing $g \rightarrow -g$, $K' \leftrightarrow K$, $\delta \leftrightarrow \delta'$ for the 1st terms in the bracket $[\]$ of the 1st & 2nd terms, we get

$$V_{MF} = \frac{U}{V} \sum_{\substack{KK'g \\ \delta\delta'}} \langle C_{k'g\delta'}^\dagger C_{k'\delta'} \rangle C_{k+g\delta}^\dagger C_{k\delta} \\ - \frac{U}{V} \sum_{\substack{KK'g \\ \delta\delta'}} \langle C_{k+g\delta}^\dagger C_{k'\delta'} \rangle C_{k'g\delta'}^\dagger C_{k\delta} \\ - \frac{U}{2V} \sum_{\substack{KK'g \\ \delta\delta'}} \langle C_{k+g\delta}^\dagger C_{k\delta} \rangle \langle C_{k'g\delta'}^\dagger C_{k'\delta'} \rangle \quad \dots (61) \\ + \frac{U}{2V} \sum_{\substack{KK'g \\ \delta\delta'}} \langle C_{k+g\delta}^\dagger C_{k'\delta'} \rangle \langle C_{k'g\delta'}^\dagger C_{k\delta} \rangle$$

Using eq. (60), we find

$$U_{MF} = U \sum_{k\delta\delta'} C_{k\delta}^{\dagger} C_{k\delta} [\bar{n}_{\delta'} - \bar{n}_{\delta} f_{\delta\delta'}]$$

$$= \frac{UV}{2} \sum_{\delta\delta'} (\bar{n}_{\delta} \bar{n}_{\delta'} - f_{\delta\delta'} \bar{n}_{\delta}^2) \quad \dots (62)$$

where $\bar{n}_{\delta} \equiv \frac{1}{V} \sum_k \langle C_{k\delta}^{\dagger} C_{k\delta} \rangle = \frac{1}{V} \sum_k \langle C_{k\delta}^{\dagger} C_{k\delta} \rangle$

is the average particle density with spin δ .

Combining eq. (62) & ~~the~~ kinetic term, one gets

$$H_{MF} = \sum_{k\delta} \left[\underbrace{\frac{\epsilon_k}{2}}_{\substack{U_{MF} \\ \epsilon_k}} + U(\bar{n}_{\uparrow} + \bar{n}_{\downarrow} - \bar{n}_{\delta}) \right] C_{k\delta}^{\dagger} C_{k\delta} \\ - \frac{UV}{2} \sum_{\delta\delta'} \bar{n}_{\delta} \bar{n}_{\delta'} + \frac{UV}{2} \sum_{\delta} \bar{n}_{\delta}^2 \quad \dots (63)$$

From H_{MF} , one gets the self-consistent equation for $\bar{n}_{\uparrow}$ & $\bar{n}_{\downarrow}$ at $T=0$:

$$\bar{n}_{\delta} = \frac{1}{V} \sum_k \langle C_{k\delta}^{\dagger} C_{k\delta} \rangle = \frac{1}{V} \sum_k \theta(-\epsilon_k^{MF})$$

$$\therefore \bar{n}_{\uparrow} = \int \frac{d^3k}{(2\pi)^3} \theta\left(\epsilon_F - \frac{\hbar^2 k^2}{2m} - U\bar{n}_{\downarrow}\right) \quad \dots (64)$$

Define $\epsilon_F = \frac{\hbar^2 k_F^2}{2m} + U\bar{n}_{\downarrow}$ (65)

$$\therefore N_{\uparrow} = \frac{\frac{4}{3}\pi (k_F)^3}{\left(\frac{2\pi}{L}\right)^3} \Rightarrow \bar{n}_{\uparrow} = \frac{1}{6\pi^2} k_F^3, \quad k_F = (6\pi^2 \bar{n}_{\uparrow})^{\frac{1}{3}}$$

Similarly, $\bar{n}_\downarrow = \frac{1}{6\pi^2} k_{F\downarrow}^3$, $k_{F\downarrow} = (6\pi^2 \bar{n}_\downarrow)^{1/3}$

With $E_F = \frac{\hbar^2 k_F^2}{2m} + U \uparrow \uparrow$ -- (66)

$$\text{Eq. (65) - (66)} \Rightarrow \frac{\hbar^2}{2m} [k_{F\uparrow}^2 - k_{F\downarrow}^2] = U(\bar{n}_{\uparrow} - \bar{n}_{\downarrow})$$

$$\therefore \frac{\hbar^2}{2m} (6\pi^2)^{\frac{2}{3}} [\bar{n}_\uparrow^{\frac{2}{3}} - \bar{n}_\downarrow^{\frac{2}{3}}] = U(\bar{n}_\uparrow - \bar{n}_\downarrow) \quad \text{--- (6)}$$

Define $\xi \equiv \frac{n_T - \bar{n}}{\bar{n}}$ with $\bar{n} = \bar{n}_T + \bar{n}_D$, ξ = polarization fraction.

$$\frac{n_H}{n} = (1+\xi)/2, \quad \frac{n_J}{n} = (1-\xi)/2$$

$\therefore$ Eq. (67) becomes

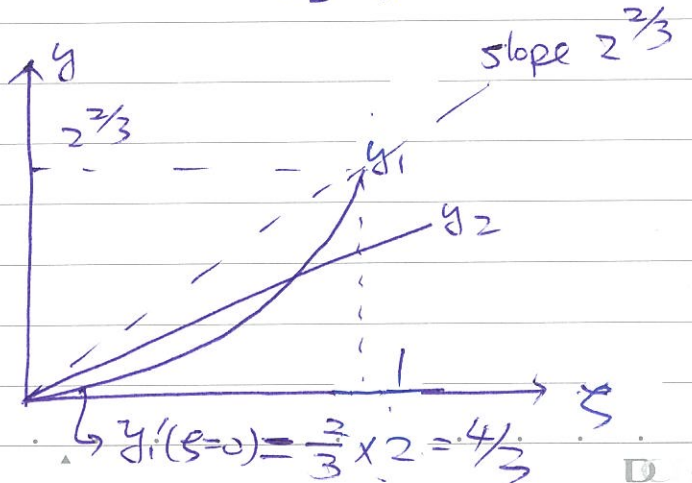
$$\delta \zeta = (1+\zeta)^{2/3} - (1-\zeta)^{2/3}, \quad \delta \equiv \frac{2mU \pi^{1/3}}{\hbar^2 (3\pi)^{2/3}}$$

Eg. (68) has to be solved to find ξ and hence the

magnetization $\mu_B \times N_T = M = \frac{\mu_B}{2} (1 + \xi)$.

To solve Eq. (6f), one plots $y_1 = (1+\xi)^{2/3} - (1-\xi)^{2/3}$
& $y_2 = 8\xi$

to find their intersection $\uparrow y$ slope $2^{2/3}$

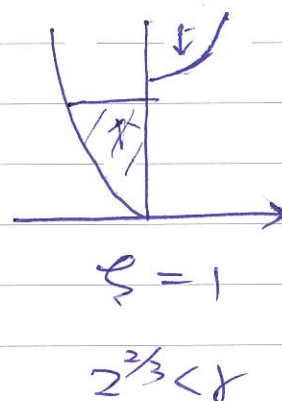
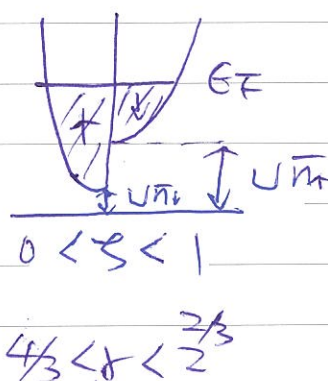
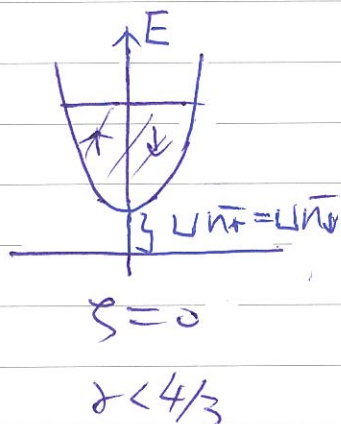


Clearly, there are three types of solutions:

$\delta < 4/3$, $\zeta = 0$ this is paramagnetic phase

$4/3 < \delta < 2^{2/3}$, $0 < \zeta < 1$, this is ferromagnetic phase

$\delta > 2^{2/3}$, $\zeta = 1$, fully polarization.



The emergent of ferromagnetism results from

the competition of loss of kinetic energy and gain of interaction energy (see the above figure, the zero point energy for different spin is shifted.)

When $\bar{n}_\uparrow \neq \bar{n}_\downarrow$, kinetic energy increases but it

is lowered down by shifting zero energy point.

One can also derive the self-consistent equation

(eq. (64)) by calculating $\langle H_{MF} \rangle \equiv E_{MF}$ and

minimizing E_{MF} : $\frac{dE_{MF}}{d\bar{n}_\uparrow} = 0$, $\frac{dE_{MF}}{d\bar{n}_\downarrow} = 0$ (For finite temperatures, one calculate F_{MF} instead).

The Stoner model gives a reasonable account of metallic magnets.

The Peierls transition we described before is a good example that one can use the mean-field approach to describe it quantitatively.

$$H = \sum_k \epsilon_k C_k^\dagger C_k + \sum_g \frac{1}{2} \hbar \omega_g a_g^\dagger a_g + \sum_{k, g} \lambda C_{k+g}^\dagger C_k (a_g^\dagger + a_g) \quad \text{--- (6f)}$$

To account for the static distortion, because

$$\lambda (\langle a_{2|k_F} \rangle + \langle a_{-2|k_F}^+ \rangle) = |\Delta| e^{i\phi} \quad \text{--- (7c)}$$

hence $\lambda (\langle a_{-1} \rangle + \langle a_{1F}^+ \rangle) = |\Delta| e^{i\phi}$

The displacement is then distorted into

$$\langle u(x) \rangle = \sqrt{\frac{\hbar}{2NM\omega_{2k_F}}} \left[\frac{1}{\lambda} |\Delta| e^{i\phi} e^{2ik_F x} + \frac{1}{\lambda} |\Delta| e^{-i\phi} e^{-2ik_F x} \right]$$

(both $q=2k_F$, $q=-2k_F$ had to be included in (10))

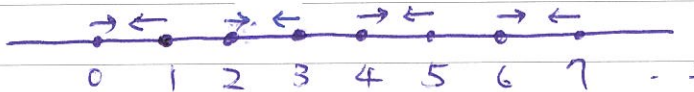
$$= \sqrt{\frac{\hbar}{2NM\omega_{2k_F}}} \cdot \frac{2|\Delta|}{\lambda} \cos(2k_F x + \phi)$$

$$\equiv \Delta u \cos(2k_F x + \phi) \quad \dots (11)$$

∴ One sees atoms have permanent displacement, i.e., the lattice is distorted.

$$\begin{aligned} X = na, \quad 2k_F &= 2 \cdot \frac{\pi}{2a} = \frac{\pi}{a} \quad \therefore \cos(2k_F x + \phi) \\ &= \cos(n\pi + \phi) \\ &= (-1)^n \cos \phi \end{aligned}$$

$\cos \phi > 0$



The system is dimerized.

In the mean-field assumption, ^{the electronic part} eg. (10), also changes the Hamiltonian into

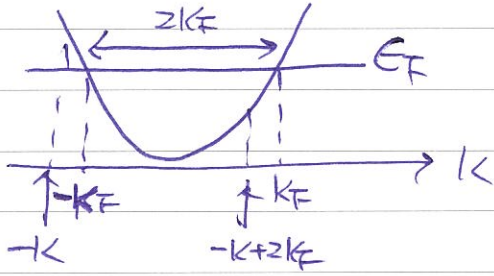
$$H_{MF}^e = \sum_k \epsilon_k c_k^\dagger c_k + \sum_k \left[\underbrace{|\Delta| e^{i\phi}}_{\Delta} c_{k+2k_F}^\dagger c_k + \underbrace{|\Delta| e^{-i\phi}}_{\Delta^*} c_k^\dagger c_{k+2k_F} \right] \quad (12)$$

It indicates that c_k & c_{k+2k_F} are coupled

(Note that $c_{k-2k_F} = c_{k+4k_F-2k_F} = c_{k+2k_F}$, $4k_F =$ reciprocal lattice vector $\frac{2\pi}{a}$)

How to solve the Hamiltonian of eq. (72)?

One needs to find the energy eigenvalues



$$\left. \begin{aligned} E_K &= -2t \cos K a - E_F = -\hbar v_F (-K - \frac{1}{2} K_F) \\ &= \hbar v_F (K + \frac{1}{2} K_F) \end{aligned} \right\} \text{for } K \sim -K_F$$

$$\left. \begin{aligned} E_{K+2K_F} &\simeq \hbar v_F (-K + \frac{1}{2} K_F, -K_F) \\ &= -\hbar v_F (K + \frac{1}{2} K_F) = -E_K \end{aligned} \right\} \rightarrow$$

using the same $K \sim -K_F$

$$\therefore \hat{H}_{MF}^e = \sum_K [G_K G_K^\dagger G_K - G_K G_{K+2K_F}^\dagger G_{K+2K_F}]$$

$$+ \sum_K [\Delta C_{K+2K_F}^+ C_K + \Delta^* C_K^+ C_{K+2K_F}] \dots (73)$$

With the understanding that $k \sim -k_z$.

Eq. (73) can be best solved by rewriting it as a matrix

$$\hat{H}_{MF}^e = \sum_{\mathbf{k}} (C_{\mathbf{k}}^\dagger \quad C_{\mathbf{k}+\mathbf{2}/\mathbf{k}}^\dagger) \underbrace{\begin{pmatrix} \epsilon_{\mathbf{k}} & \Delta^* \\ \Delta & -\epsilon_{\mathbf{k}} \end{pmatrix}}_{h_{\mathbf{k}}} \begin{pmatrix} C_{\mathbf{k}} \\ C_{\mathbf{k}+\mathbf{2}/\mathbf{k}} \end{pmatrix} \dots (74)$$

Clearly, to find excitation energies, one needs

to bring the matrix into a diagonal form.

We shall achieve it by a transformation

Let $\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} \equiv \begin{pmatrix} C_1 \\ C_2 \end{pmatrix}$, after transformation, it become

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \therefore \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \tilde{U} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \quad \tilde{U} = 2 \times 2 \text{ matrix}$$

$$\therefore \delta_i = \bigcup_j C_j$$

For Fermions, one requires $\{ \psi_i, \psi_j^\dagger \} = \delta_{ij}$ is still obeyed. Such transformation is called canonical.

$$\therefore \{ \hat{U}_{\alpha\alpha'} C_{\alpha'}, \hat{U}_{\beta\beta'}^* C_{\beta'}^\dagger \} = \delta_{\alpha\beta}$$

$$\therefore \hat{U}_{i,j} \hat{U}_{j,i}^* \underbrace{\{C_i, C_j^+\}}_{\delta_{i,j-1}} = \delta_{i,j}$$

$$\sum_i \hat{U}_{ij} \hat{U}_{ij}^* = \delta_{jj}, \text{ i.e., } UU^T = I \quad \text{--- (7)}$$

Hence the transformation is unitary and the excitation energy can be found by

Solving the secular equation:

$$\begin{vmatrix} G_K - E & \Delta^* \\ \Delta & -G_K - E \end{vmatrix} = 0 \quad \therefore E^2 = |\Delta|^2 + G_K^2$$

$$E_k = \pm \sqrt{\epsilon_k^2 + |\Delta|^2} \quad \dots \quad (76)$$

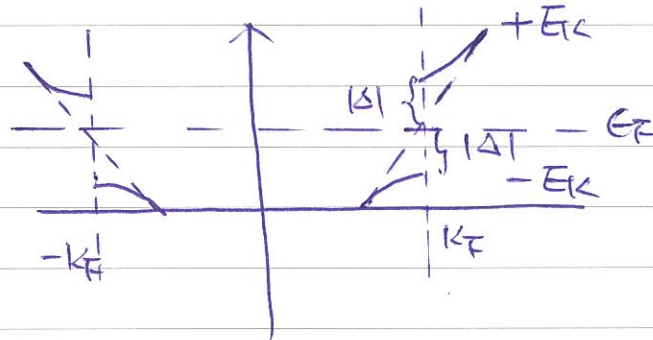
$$\therefore \hat{H}_{MF} = \sum_k (a_{1k}^\dagger \ a_{2k}^\dagger) U^\dagger h_{1k} U \begin{pmatrix} a_{1k} \\ a_{2k} \end{pmatrix}$$

$$= \sum_k (d_{1k}^+ d_{2k}^+) \begin{pmatrix} E_{1k} & 0 \\ 0 & -E_{1k} \end{pmatrix} \begin{pmatrix} d_{1k} \\ d_{2k} \end{pmatrix}$$

$$= \sum_{\mathbf{I}_K} E_{\mathbf{I}_K} (d_{\mathbf{I}_K}^+ d_{\mathbf{I}_K} - d_{\mathbf{I}_K}^- d_{\mathbf{I}_K}^-) \dots (77)$$

Clearly, the excitation energies are $\pm E_k = \sqrt{E_F^2 + |\Delta|^2}$

which show gaps opened near $\pm k_F$:

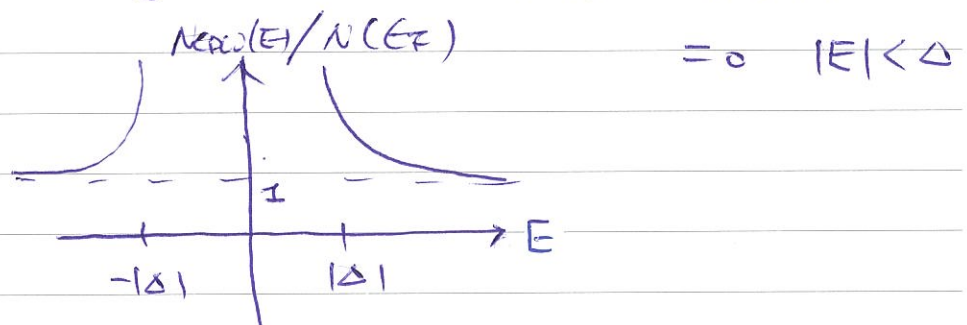


Since the transformation brings one k $\begin{pmatrix} C_k \\ C_{-k} \end{pmatrix}$ into one $\begin{pmatrix} \gamma_{1k} \\ \gamma_{2k} \end{pmatrix}$, the mapping is one to one. Hence # of states are conserved. One has

$$N_{CDW}(E) dE = N(E) dE = N(E_F) dE$$

$$\therefore \frac{N_{CDW}(E)}{N(E_F)} = \frac{dE}{dE}$$

$$\frac{dE}{dE} = \frac{E}{\sqrt{E^2 + |\Delta|^2}} = \frac{E}{\sqrt{E^2 + |\Delta|^2}} \quad \therefore \frac{N_{CDW}(E)}{N(E_F)} = \frac{E}{\sqrt{E^2 + |\Delta|^2}} \quad |E| > 0$$



Electronic charge density wave (CDW)

The distortion in ions must lead to uniform distribution of electronic charges. These are called charge density wave (CDW).

Note that in general,

The charge density wave needs not be induced

by ion distortion. It can be induced by

electron-electron interaction as long as perfect nesting happens. These are then called spontaneous CDW.

In the momentum space, $\therefore n(x) = \langle C^\dagger(x) C(x) \rangle$

$$= \frac{1}{N} \sum_{k, k'} \langle C_k^\dagger C_{k'} \rangle e^{i(k-k')x}$$

$$= \frac{1}{N} \sum_q \sum_k e^{-iqx} \langle C_k^\dagger C_{k+q} \rangle \quad \therefore n(q) = \sum_k \langle C_k^\dagger C_{k+q} \rangle$$

the charge density wave is characterized by $\sum_k \langle C_k^\dagger C_{k+q} \rangle$.
order parameter of

$\therefore$ The order parameter $n(q) = \sum_k \langle C_k^\dagger C_{k+q} \rangle$ -- (18)

In general, if $\frac{2\pi}{\theta} = \text{integer} \times \text{lattice constant}$, it is called Commensurate CDW. Otherwise, it's Incommensurate CDW.

For Peierls transition, $\theta = 2k_F = \frac{2\pi}{2a}$, $\therefore$ it's commensurate.

To evaluate $n(2k_F)$, we need to find the eigenvectors of $\hat{h}_k$.

Let eigenvector be $\begin{pmatrix} u_k e^{-i\phi/2} \\ v_k e^{i\phi/2} \end{pmatrix}$ with a appropriate

renormalization condition: $u_k^2 + v_k^2 = 1$ -- (19)

$$\therefore h_k \begin{pmatrix} u_k \\ v_k \end{pmatrix} = \begin{pmatrix} \epsilon_k & |d| e^{i\phi} \\ |d| e^{i\phi} & -\epsilon_k \end{pmatrix} \begin{pmatrix} u_k e^{-i\phi/2} \\ v_k e^{i\phi/2} \end{pmatrix} = E_k \begin{pmatrix} u_k e^{-i\phi/2} \\ v_k e^{i\phi/2} \end{pmatrix} \quad \text{--- (20)}$$

($e^{\pm i\phi/2}$ are to remove $e^{i\phi}$ so that u_k & v_k are real)

$$\therefore (E_k - E_k) u_k e^{-i\phi/2} + |\Delta| e^{-i\phi/2} v_k = 0$$

$$\therefore u_k = \frac{|\Delta|}{E_k - E_k} v_k \quad \dots (80)$$

Eq. (79) implies one can set $u_k = \sin \theta_k/2$, $v_k = \cos \theta_k/2$

$$\therefore \text{Eq. (80)} \quad \tan \frac{\theta_k}{2} = \frac{|\Delta|}{E_k - E_k}$$

$$\therefore \sqrt{(E_k - E_k)^2 + |\Delta|^2} = \sqrt{2E_k^2 - 2E_k E_k}$$

$$\therefore u_k = \sin \theta_k/2 = \frac{|\Delta|}{\sqrt{2E_k(E_k - E_k)}} = \frac{|\Delta| \sqrt{E_k + E_k}}{\sqrt{2E_k} |\Delta|}$$

$$\therefore u_k^2 = \frac{1}{2} \left(1 + \frac{E_k}{E_k} \right), \quad v_k^2 = \frac{1}{2} \left(1 - \frac{E_k}{E_k} \right) \quad \dots (81)$$

Now, the second eq. of (79) is

$$|\Delta| u_k - (E_k + E_k) v_k = 0$$

which suggest the eigenvector for $E = -E_k$ is

$$\begin{pmatrix} -v_k e^{-i\phi/2} \\ u_k e^{i\phi/2} \end{pmatrix} : \begin{pmatrix} E_k & |\Delta| e^{-i\phi} \\ |\Delta| e^{i\phi} & -E_k \end{pmatrix} \begin{pmatrix} -v_k e^{-i\phi/2} \\ u_k e^{i\phi/2} \end{pmatrix}$$

$$= \begin{pmatrix} (-E_k v_k + |\Delta| u_k) e^{-i\phi/2} \\ (-v_k |\Delta| - E_k u_k) e^{i\phi/2} \end{pmatrix} = -E_k \begin{pmatrix} -v_k e^{-i\phi/2} \\ u_k e^{i\phi/2} \end{pmatrix}$$

Hence the transformation matrix $U = \begin{pmatrix} u_k e^{-i\phi/2} & -v_k e^{-i\phi/2} \\ v_k e^{i\phi/2} & u_k e^{i\phi/2} \end{pmatrix}$

Now, $\begin{pmatrix} C_k \\ C_{k+2k_F} \end{pmatrix} = U \begin{pmatrix} \delta_{1k} \\ \delta_{2k} \end{pmatrix}$

$$= \begin{pmatrix} u_k e^{-i\phi/2} & -v_k e^{-i\phi/2} \\ v_k e^{i\phi/2} & u_k e^{i\phi/2} \end{pmatrix} \begin{pmatrix} \delta_{1k} \\ \delta_{2k} \end{pmatrix}$$

$$\therefore \left. \begin{aligned} C_k &= u_k e^{-i\phi/2} \delta_{1k} - v_k e^{-i\phi/2} \delta_{2k} \\ C_{k+2k_F} &= v_k e^{i\phi/2} \delta_{1k} + u_k e^{i\phi/2} \delta_{2k} \end{aligned} \right\} \dots (82)$$

$$\therefore C_x = \frac{1}{\sqrt{V}} \sum_k C_k e^{-ik_F x} + C_{k+2k_F} e^{ik_F x}$$

$$\therefore n(x) = \langle C_x^\dagger C_x \rangle$$

$$= \frac{1}{V} \sum_k \sum_{k'} [\langle C_k^\dagger C_{k'} \rangle + \langle C_{k+2k_F}^\dagger C_{k'+2k_F} \rangle + \langle C_k^\dagger C_{k'+2k_F} \rangle e^{2ik_F x} + \langle C_{k+2k_F}^\dagger C_{k'} \rangle e^{-2ik_F x}]$$

From eq. (1), at $T=0$, $\langle \delta_{2k}^\dagger \delta_{2k} \rangle = 1$

$$\langle \delta_{1k}^\dagger \delta_{1k} \rangle = 0, \quad \langle \delta_{1k}^\dagger \delta_{2k} \rangle = 0, \quad \langle \delta_{2k}^\dagger \delta_{1k} \rangle = 0$$

$$\therefore \langle C_k^\dagger C_{k'} \rangle = \delta_{kk'} v_k^2$$

$$\langle C_{k+2k_F}^\dagger C_{k'+2k_F} \rangle = \delta_{kk'} u_k^2$$

$$\langle C_k^\dagger C_{k'+2k_F} \rangle = -v_k u_k e^{i\phi} \times \delta_{kk'}$$

$$\langle C_{k+2k_F}^\dagger C_{k'} \rangle = -v_k u_k e^{-i\phi} \times \delta_{kk'}$$

$$\therefore n(x) = \frac{1}{V} \sum_k \underbrace{(u_k^2 + v_k^2)}_1 - 2 u_k v_k \cos(2k_F x + \phi)$$

$$= n_0 [1 + \alpha |\Delta| \cos(2k_F x + \phi)]$$

$$\alpha = \frac{-1}{V n_0} \int \frac{dk}{|E_k|} \sim \frac{-1}{n_0 v_F} \int^{\Lambda} \frac{dg}{\sqrt{g^2 + |\Delta|^2 / (\hbar v_F)^2}} \sim \frac{1}{n_0 v_F g_{k_F}}$$

$$(g = \frac{\lambda^2 n(\epsilon_F)}{\hbar \omega_{2k_F}} \text{ dimensionless e-p coupling})$$

The order parameter

$$n(\mathbf{r}) = -\sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} e^{i\phi}$$

$$= -\sum_{\mathbf{k}} \frac{|\Delta|}{2E_{\mathbf{k}}} e^{i\phi} \propto |\Delta| e^{i\phi} \propto \Delta$$

Therefore, electrons exhibit charge density waves.

Self-consistent equation for Δ

Eq. (17) is only the electronic part of eq. (6).

HMF actually contains $\sum_{\mathbf{g}} \hbar \omega_{\mathbf{g}} a_{\mathbf{g}}^{\dagger} a_{\mathbf{g}}$

$$\begin{aligned} \rightarrow \hbar \omega_{2\mathbf{k}} \langle a_{2\mathbf{k}}^{\dagger} a_{2\mathbf{k}} \rangle + f(2\mathbf{k}) \\ = 2 \hbar \omega_{2\mathbf{k}} \langle a_{2\mathbf{k}}^{\dagger} \rangle \langle a_{2\mathbf{k}} \rangle \end{aligned}$$

$$\therefore \lambda (\langle a_{2\mathbf{k}} \rangle + \langle a_{-2\mathbf{k}}^{\dagger} \rangle) = |\Delta| e^{i\phi}$$

$$\text{assume } \langle a_{2\mathbf{k}} \rangle = \langle a_{-2\mathbf{k}}^{\dagger} \rangle \quad \therefore \langle a_{2\mathbf{k}} \rangle = \frac{|\Delta|}{2\lambda} e^{i\phi}$$

$$\begin{aligned} \therefore 2 \hbar \omega_{2\mathbf{k}} \langle a_{2\mathbf{k}}^{\dagger} \rangle \langle a_{2\mathbf{k}} \rangle \\ = \frac{\hbar \omega_{2\mathbf{k}}}{2\lambda^2} |\Delta|^2 \end{aligned}$$

$$\text{At } T=0, \langle E_{\mathbf{g}} \rangle + \frac{\hbar \omega_{2\mathbf{k}}}{2\lambda^2} |\Delta|^2 \equiv E(|\Delta|)$$

$$\therefore E(|\Delta|) = \frac{\hbar \omega_{2\mathbf{k}}}{2\lambda^2} |\Delta|^2 - \sum_{\mathbf{k}} \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta|^2} \quad \dots (8) - 1$$

$$\frac{dE}{d|\Delta|} = 0 \Rightarrow \frac{\hbar \omega_{2\mathbf{k}}}{\lambda^2} |\Delta| - \sum_{\mathbf{k}} \frac{|\Delta|}{\sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta|^2}} = 0 \Rightarrow \frac{\hbar \omega_{2\mathbf{k}}}{\lambda^2} = \sum_{\mathbf{k}} \frac{1}{E_{\mathbf{k}}}$$

which determines $|\Delta|$!

density of states (not per volume)
at E_F

The energy E was chosen with zero point set at E_F .

$$\therefore \int dG = \int_{-E_F}^0 dE$$

$$\therefore \text{Eq. (3)} \Rightarrow \frac{\hbar \omega_{\text{KF}}}{n(E_F) \lambda^2} = \int_{-E_F}^0 d\epsilon \frac{1}{\sqrt{\epsilon^2 + |\Delta|^2}} = \int_0^{E_F} \frac{d\epsilon}{\sqrt{\epsilon^2 + |\Delta|^2}}$$

$$= \sinh^{-1} \frac{E_F}{|\Delta|}$$

$$\therefore \frac{f}{g} = \sinh^{-1} \frac{E_F}{T\Delta} \quad , \quad |\Delta| = \frac{E_F}{\sinh \frac{f}{g}}$$

For weak coupling, $g \ll 1$, $\sinh \frac{1}{g} \sim \frac{1}{2} e^{\frac{1}{g}}$

$$|\Delta| \simeq 2\epsilon_F e^{-\frac{1}{g}} \quad \dots \quad (84)$$

Which, as we shall see, is a typical form of the dependence of the order parameter on the coupling constant.

Mean field theory of Spin density waves (SDW)

Just as CDW, when the nesting happens, the system could also develop density waves in spins.

This was first discussed by Overhauser and the observations of SDW are now quite often.

For ^{example}, it's observed in $(\text{TM.TSE})_2\text{PF}_6$

(see Jerome & Schultz, Adv. Phys. 31, 299, 1982)

The order parameter of SDW in the most general form is given by

$$\vec{S}_Q = \sum_{\mathbf{k}} \langle C_{\mathbf{k}\alpha}^\dagger \frac{\vec{\sigma}_{\alpha\beta}}{2} C_{\mathbf{k}+\mathbf{Q}\beta} \rangle \quad \text{--- (85)}$$

When $\frac{2\pi}{Q} = \text{integer} \times \text{lattice constant}$, it is

commensurate, otherwise, it's incommensurate.

Here $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the Pauli matrix.

An additional feature of SDW is the vector nature of spin.

In principle, in real space, $\vec{S}(\mathbf{x})$ needs

not to point to the same direction and can

be spiral and behaves in ^{more} complicated ways.

These are also seen in experiments.

Here, to illustrate it, we shall examine

SDW in 1D Hubbard model

$$\hat{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} C_{\mathbf{k}\sigma}^\dagger C_{\mathbf{k}\sigma} + \frac{U}{V} \sum_{\mathbf{k}\mathbf{k}'\sigma} \overbrace{C_{\mathbf{k}\sigma}^\dagger C_{\mathbf{k}+\mathbf{Q}\sigma} C_{\mathbf{k}'\sigma}^\dagger C_{\mathbf{k}'+\mathbf{Q}\sigma}}^{UV \sum_{\sigma\delta} n_{\sigma\delta} n_{\delta-\sigma}} \quad \text{--- (86)}$$

Unlike the Stoner model, we shall not

assume eqs. (60). Instead, we assume

$$\frac{1}{V} \sum_{\mathbf{k}} \langle C_{\mathbf{k}\uparrow}^\dagger C_{\mathbf{k}+\mathbf{Q}\uparrow} \rangle = n_{\uparrow}(\mathbf{Q}) \neq 0, \quad \frac{1}{V} \sum_{\mathbf{k}} \langle C_{\mathbf{k}\downarrow}^\dagger C_{\mathbf{k}+\mathbf{Q}\downarrow} \rangle = n_{\downarrow}(\mathbf{Q}) \neq 0 \quad \text{--- (87)}$$

We first illustrate that perfect nesting implies

$$q = 2k_F$$

The difference of $n_{g\uparrow}$ and $n_{g\downarrow}$ is proportional to the magnetization $M_g = \mu_B (n_{g\uparrow} - n_{g\downarrow})$

Which couples to non-uniform magnetic field

$$H_I = \sum_g M_g H_g$$

H_g behaves similar to $(a_g^\dagger + a_g)$ (phonon, displacement) in the Fröhlich Hamiltonian.

Hence consider $H = H_0 + H_I$

$$\text{with } H_0 = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma}$$

To the 2nd order of H_I , we get

$$E = E_0 + \langle \Phi | H_I \frac{1}{E_0 - H_0} H_I | \Phi \rangle$$

To conserve # of electrons, we have exact the same situation as phonon's case. One finds

$$\sum_g H_g H_g \sum_k \left[\langle \Phi | c_{k+g\uparrow}^\dagger c_{k\uparrow} \frac{1}{E_0 - H_0} c_{k\uparrow}^\dagger c_{k+g\uparrow} | \Phi \rangle \right. \\ \left. (n_{g\uparrow}) \quad (n_{g\uparrow}) \right]$$

$$+ \langle \Phi | c_{k\downarrow}^\dagger c_{k+g\downarrow} \frac{1}{E_0 - H_0} c_{k+g\downarrow}^\dagger c_{k\downarrow} | \Phi \rangle \\ (n_{g\downarrow}) \quad (n_{g\downarrow})$$

$$= \sum_g H_g H_g \sum_k \left[\frac{\langle n_{k+g}^\uparrow (1 - n_k^\uparrow) \rangle}{\epsilon_{k+g} - \epsilon_k} + \frac{\langle n_k^\downarrow (1 - n_{k+g}^\downarrow) \rangle}{\epsilon_k - \epsilon_{k+g}} \right]$$

$$= \sum_{\vec{q}, k} |H_{\vec{q}}|^2 \frac{N_{k+\vec{q}}^0 - N_k^0}{\epsilon_{k+\vec{q}} - \epsilon_k} \quad \dots \textcircled{p8}$$

$$= \sum_{\vec{q}} |H_{\vec{q}}|^2 \chi(\vec{q})$$

One sees again that the Lindhard function determines the response of Fermi gas to the non-uniform magnetic field.

Since H - $\vec{q}$ couples to $M_{\vec{q}}$, $\therefore \underline{\langle M_{\vec{q}} \rangle = \chi(\vec{q}) H_{\vec{q}}}$. L -- (p9)

$\chi(\vec{q})$ has the meaning of spin susceptibility, representing the response of $\langle M_{\vec{q}} \rangle$ to the external magnetic field $H_{\vec{q}}$!

As we have seen, $\chi(\vec{q})$ is strongly peaked (divergent) at $q = 2k_F$. It implies that permanent $\langle M_{2F} \rangle$ may be developed spontaneously.

Hence we shall take $q = \pm 2k_F$ in eq. (p9).

$$\therefore C_{\delta}(x) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} e^{i\vec{k} \cdot \vec{x}} C_{\vec{k}\delta}$$

$$S(x) \equiv \frac{1}{2} [C_{\uparrow}^{\dagger}(x) C_{\uparrow}(x) - C_{\downarrow}^{\dagger}(x) C_{\downarrow}(x)] \quad \text{Spin density (z)}$$

$$= \frac{1}{2V} \sum_{\vec{k}, \vec{k}'} (C_{\vec{k}\uparrow}^{\dagger} C_{\vec{k}'\uparrow} - C_{\vec{k}\downarrow}^{\dagger} C_{\vec{k}'\downarrow}) e^{i(\vec{k}-\vec{k}') \cdot \vec{x}}$$

$$\therefore \langle S(x) \rangle = \frac{1}{2V} \sum_{\vec{k}} [\langle C_{\vec{k}\uparrow}^{\dagger} C_{\vec{k}+2\vec{k}\uparrow} \rangle - \langle C_{\vec{k}\downarrow}^{\dagger} C_{\vec{k}+2\vec{k}\downarrow} \rangle] e^{-i2\vec{k} \cdot \vec{x}} \\ + \frac{1}{2V} \sum_{\vec{k}} [\langle C_{\vec{k}\uparrow}^{\dagger} C_{\vec{k}-2\vec{k}\uparrow} \rangle - \langle C_{\vec{k}\downarrow}^{\dagger} C_{\vec{k}-2\vec{k}\downarrow} \rangle] e^{i2\vec{k} \cdot \vec{x}}$$

and redefine $k+2k_F = k$, the second term

Complex conjugate of the 1st term.

$$= \frac{1}{2} (\langle n_{2k_F \uparrow} \rangle - \langle n_{2k_F \downarrow} \rangle) = |s| e^{i\phi}$$

$$S(x) = 2|S| \cos(2kx + \phi) \quad \dots (90)$$

We shall assume the density modulations

(i.e. the same phase in $\uparrow$ & $\downarrow$ bands) so

as $\langle n_{\uparrow k \uparrow} \rangle + \langle n_{\uparrow k \downarrow} \rangle$ has no spatial variations.



and $N_{ZKF} = \langle N_{ZKF} \rangle + f N_{ZKF}$.

To *My Dear Cousin John*

$$UV \sum_{\mathbf{q}} n_{\mathbf{q}\uparrow} n_{\mathbf{q}\downarrow}$$

$$\approx UV \sum_{\mathbf{q}} \langle n_{\mathbf{q}\uparrow} \rangle n_{\mathbf{q}\downarrow} + n_{\mathbf{q}\downarrow} \langle n_{\mathbf{q}\uparrow} \rangle - \langle n_{\mathbf{q}\uparrow} \rangle \langle n_{\mathbf{q}\downarrow} \rangle$$

Setting $\mathbf{q} = \pm 2\mathbf{k}$ and realizing $n_{\pm 2\mathbf{k}\downarrow} = \frac{1}{V} \sum_{\mathbf{k}} \langle C_{\mathbf{k}\downarrow}^\dagger C_{\mathbf{k} \mp 2\mathbf{k}\downarrow} \rangle$

$$= \frac{1}{V} \sum_{\mathbf{k}} \langle C_{\mathbf{k}\downarrow}^\dagger C_{\mathbf{k}+2\mathbf{k}\downarrow} \rangle = n_{2\mathbf{k}\downarrow}$$

$$\therefore H_{MF} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} C_{\mathbf{k}\downarrow}^\dagger C_{\mathbf{k}\downarrow} + U \left[\sum_{\mathbf{k}} \langle n_{2\mathbf{k}\uparrow} \rangle C_{\mathbf{k}\downarrow}^\dagger C_{\mathbf{k}-2\mathbf{k}\downarrow} \right.$$

$$+ \sum_{\mathbf{k}} \langle n_{2\mathbf{k}\downarrow} \rangle C_{\mathbf{k}\uparrow}^\dagger C_{\mathbf{k}+2\mathbf{k}\uparrow} + \sum_{\mathbf{k}} \langle n_{2\mathbf{k}\uparrow} \rangle C_{\mathbf{k}\downarrow}^\dagger C_{\mathbf{k}+2\mathbf{k}\downarrow}$$

$$\left. + \sum_{\mathbf{k}} \langle n_{2\mathbf{k}\downarrow} \rangle C_{\mathbf{k}\uparrow}^\dagger C_{\mathbf{k}-2\mathbf{k}\uparrow} \right]$$

$$= UV \langle n_{2\mathbf{k}\uparrow} \rangle \langle n_{2\mathbf{k}\downarrow} \rangle - UV \langle n_{2\mathbf{k}\uparrow} \rangle \langle n_{2\mathbf{k}\downarrow} \rangle$$

Using eq (P1), setting $U|S| = \Delta$ and $\langle n_{2\mathbf{k}\downarrow} \rangle = \langle n_{2\mathbf{k}\uparrow} \rangle^*$,

We arrive at

$$H_{MF} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} C_{\mathbf{k}\downarrow}^\dagger C_{\mathbf{k}\downarrow} + \sum_{\mathbf{k}} K |e^{i\phi}| (C_{\mathbf{k}+2\mathbf{k}\downarrow}^\dagger C_{\mathbf{k}\downarrow} - C_{\mathbf{k}+2\mathbf{k}\uparrow}^\dagger C_{\mathbf{k}\uparrow})$$

$$+ \text{h.c.} + \frac{2V|\Delta|^2}{U} \quad \dots \quad (P2)$$

Eq. (P2) is similar to CDW in eq. (74) except that

now spin $\uparrow$ & $\downarrow$

there are two channels

$\therefore$ Eq. (92) - 1 is replaced by

$$E[|\Delta|] = \frac{2V}{U} |\Delta|^2 - \underbrace{2 \sum_{\substack{k \\ \text{spin } \uparrow \& \downarrow}} \sqrt{E_k^2 + |\Delta|^2}}_{\text{spin } \uparrow \& \downarrow} \dots \quad (93)$$

$$\frac{dE}{d|\Delta|} = 0 \Rightarrow \frac{2|\Delta|}{U} = \frac{1}{U} \sum_k \frac{|\Delta|}{\sqrt{E_k^2 + |\Delta|^2}}$$

$$\frac{2}{U} = \underbrace{N(E_F)}_{\text{DOS (per volume) at } E_F} \int dG \frac{1}{\sqrt{E^2 + |\Delta|^2}}$$

$$\therefore \frac{2}{UN(E_F)} = \sin^{-1} \frac{E_F}{|\Delta|}$$

$$|\Delta| \approx 2E_F e^{-\frac{1}{g_{SDW}}} \quad g_{SDW} = \frac{UN(E_F)}{2} \dots (94)$$

which, again, is singular in the coupling constant of U !