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Chapter 1

Density functional theory

1.1 Kohn-Heisenberg theorem

We consider a system with Halmiltonian

$$H = T + V + U \quad \begin{cases} T = \int d^3r \psi_\sigma^\dagger \left(-\frac{\hbar^2}{2m} \right) \nabla^2 \psi_\sigma \\ V = \int d^3r \psi_\sigma^\dagger V(r) \psi_\sigma \\ u = \frac{e^2}{2} \int d^3r d^3r' \frac{\psi_\sigma^\dagger(r) \psi_\sigma^\dagger(r') \psi_\sigma(r') \psi_\sigma(r)}{|r - r'|} \end{cases} \quad (1.1)$$

The hamiltonian is determined by potential $V(r)$. In the language of field theory, H is the functional of $V(r)$. Furthermore, the ground state $|\psi_a\rangle$ and the ground density $\rho(r)$ are also functionals of $V(r)$.

$$V(r) \rightarrow |\psi_a\rangle \rightarrow \rho(r) \quad (1.2)$$

The variables $\rho(r)$ and $V(r)$ are conjugate variables. We could also describe system in terms of $\rho(r)$.

First, we denote ground state for $H = T + U + V$ as $\psi(r_1, \dots, r_n)$ and ground state for $H' = T + U + V'$ as $\psi'(r_1, \dots, r_n)$. It's obvious that the state $\psi'(r_1, \dots, r_n)$ isn't ground state of H . Otherwise, we will deduce that $V(r)$ and $V(r')$ are same potential.

$$\begin{cases} (T + U + V)\psi(r_1, \dots, r_n) = E\psi(r_1, \dots, r_n) \\ (T + U + V')\psi(r_1, \dots, r_n) = E\psi(r_1, \dots, r_n) \end{cases} \implies (V - V')\psi(r_1, \dots, r_n) = (E - E')\psi(r_1, \dots, r_n) \quad (1.3)$$

Hence, the state $\psi'(r_1, \dots, r_n)$ isn't ground state for H if $\psi(r_1, \dots, r_n)$ is ground state for H . We could have

$$\langle \psi' | H | \psi' \rangle > \langle \psi | H | \psi \rangle \iff \langle \psi' | H + V' - V | \psi' \rangle < \langle \psi | H | \psi \rangle \quad (1.4)$$

By the same way,

$$\langle \psi | H + V - V' | \psi \rangle > \langle \psi' | H | \psi' \rangle \quad (1.5)$$

Adding Eq(1.4,1.5),

$$\int d^3r (\rho'(r) - \rho(r)) (V(r) - V'(r)) > 0 \quad (1.6)$$

The Eq(1.6) tells that different $V(r)$ gives different $\rho(r)$. This is just Khon -Heisenberg theorem , where the ground state of any interacting many particle systems with a given fixed interparticle interaction is a unique functional of the electron.

Now we discuss the benefits of theory in terms of $\rho(r)$. We defined the ground state energy functional

$$\begin{cases} E_G[\rho(r)] = F[\rho(r)] + \int d^3r V(r)\rho(r) \\ F[\rho(r)] = \langle \psi_G | T + U | \psi_G \rangle \end{cases} \quad (1.7)$$

The ground state energy is separated into two parts , where F only depends on density $\rho(r)$ and the other term depends on lattice potential $V(r)$.

1.2 LDA

We can use local approximation such that we use the results from uniform electron gas at different values of ρ to approximate $F[\rho(r)]$. We express the ground state energy into

$$E_G[\rho(r)] = T_o[\rho(r)] + V_H[\rho(r)] + E_{xc}[\rho(r)] + \int d^3r V(r)\rho(r) \quad (1.8)$$

The ground state could be approximated with Slater determinant $\phi_{i\sigma}(r)$,which is also determined by $\rho(r)$.

•

$$T_o[\rho(r)] = \int d^3r \sum_{i,\sigma} \phi_{i\sigma}^*(r) \left(-\frac{\hbar^2}{2m} \nabla^2 \right) \phi_{i\sigma}(r) \quad (1.9)$$

This is not real ground state of system. The slater determinant will distorted by interaction.

•

$$V_H(\rho) = \frac{1}{2} \int d^3r d^3r' \rho(r) \frac{e^2}{|r - r'|} \rho(r') \quad (1.10)$$

•

$$E_{xc}[\rho(r)] = F[\rho(r)] - T_o[\rho(r)] - V_H[\rho(r)] \quad (1.11)$$

We spproximate $E_{xc}[\rho(r)]$ with function of density $\rho[\rho(r)]$ in a local way . The energy $E_{xc}[\rho(r)]$ doesn;t depend on $\nabla\rho$, which implies that it doesn't depend on fluctuations of density $\rho(r)$. We minimize energy functional under constraint of $\int d^3r \phi_{i\sigma}^* \phi_{i\sigma} = 1$.

We write down the energy functional explicitly

$$E_G\rho(r) = \sum_{i\sigma} \int d^3r \psi_{i\sigma}^* \left(-\frac{\hbar^2}{2m} \nabla^2 + V(r) + \right) \psi_{i\sigma} + V_H + \int d^3r E_{xc}[\rho(r)] - \sum_{i\sigma} \int d^3r \lambda_{i\sigma} (\phi_{i\sigma}^* \phi_{i\sigma} - 1) \quad (1.12)$$

We take variation with respect to $\phi_{i\sigma}^*(r)$ to obtain motion equation

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V(r) \right) \psi_{i\sigma} + \int d^3r' \frac{e^2}{|r - r'|} \rho(r') + \frac{\delta E_{xc}(\rho)}{\delta \rho(r)} \psi_{i\sigma} = \lambda_{i\sigma} \psi_{i\sigma} \quad (1.13)$$

The Eq(1.13) is analogous to single particle Schrodinger equation. We define effective potential as

$$V_{\text{eff}}(r) = V(r) + V'(r) + \frac{\delta E_{xc}(r)}{\delta \rho(r)} \quad (1.14)$$

We need to assume an initial density contribution $\rho(r)$, then we have V_{eff} . We can solve the band structure and obtain revisited $\rho(r)$. This process is iterated continually untill convergence. The unknown $\frac{\delta E_{xc}(\rho)}{\delta \rho(r)} \psi_{i\sigma}$ can be obtained through homogeneous electron gas at density ρ .

1.2.1 Exchange energy E_{xc}

We solve the exchange energy for electron with $k < k_F$ with Hatree-Fock theory.

$$\varepsilon_{Fock}(k) = -\frac{2e^2}{\pi} k_F F(x) \quad \text{where} \quad F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \log \left| \frac{1+x}{1-x} \right| \quad (1.15)$$

The total energy could be founded as

$$\sum_k \varepsilon_{Fock}(k) = \frac{V}{(2\pi)^3} \int -\frac{2e^2}{\pi} k_F F(x) = -N \left(\frac{3e^2}{4\pi} \right) k_F \quad (1.16)$$

Note:-

$$\begin{aligned} \int_0^1 x^2 F(x) dx &= \int_0^1 x^2 \left(\frac{1}{2} + \frac{1-x^2}{4x} \log \left| \frac{1+x}{1-x} \right| \right) dx \\ &= \frac{1}{6} + \frac{1}{4} \int_0^1 (1-x^2) x \log \left| \frac{1+x}{1-x} \right| dx \\ &= \frac{1}{6} + \frac{1}{2} \int_0^1 x(1-x^2) \sum_{n=0}^{+\infty} \frac{1}{2n+1} x^{2n+1} dx \\ &= \frac{1}{6} + \frac{1}{2} \sum_{n=0}^{+\infty} \frac{1}{(2n+1)(2n+3)} - \frac{1}{(2n+1)(2n+5)} \\ &= \frac{1}{6} + \sum_{n=0}^{+\infty} \frac{1}{(2n+1)(2n+3)(2n+5)} \\ &= \frac{1}{6} + \frac{1}{2} \sum_{n=0}^{\infty} B\left(n + \frac{1}{2}, 3\right) \\ &= \frac{1}{6} + \frac{1}{2} \int_0^1 \sum_{n=0}^{\infty} x^{n-\frac{1}{2}} (1-x)^2 \\ &= \frac{1}{4} \end{aligned}$$

Hence, the Eq(1.16) reads

$$\sum_k \varepsilon_{Fock}(k) = -\frac{V}{(2\pi)^3} \cdot \frac{2e^2 k_F^4}{\pi} \int d\Omega \int_0^{+\infty} x^2 F(x) dx = -\frac{V e^2 k_F^4}{4\pi^3} = -\frac{3e^2}{4\pi} k_F N \quad k_F^3 = \frac{3\pi^2 N}{V} \quad (1.17)$$

With the definition of density ρ

$$\rho \frac{4\pi}{3} (r_s a_0)^3 = 1 \quad r_s = \left(\frac{3\rho}{4\pi} \right)^{\frac{1}{3}} \frac{1}{a_0} \quad (1.18)$$

The correlation energy could be written as

$$\varepsilon_x = -\frac{e^2}{2a_0} \frac{3^{\frac{4}{3}}}{2\pi^{\frac{1}{3}}} \rho^{\frac{4}{3}} a_0 \quad (1.19)$$

1.3 Thomas-Fermi approximation

The energy functional could be written as

$$E[\rho(r)] = \int d^3r T[\rho(r)] + \frac{e^2}{2} \int \frac{\rho(r)\rho(r')}{|r-r'|} d^3r d^3r' + \int d^3r E_{xc}[\rho(r)] + \int d^3r V(r)\rho(r) - \mu \int d^3r (\rho(r) - N) \quad (1.20)$$

We make variation with respect to $\rho(r)$.

$$\int d^3r \delta\rho(r) \left[\frac{\delta T(\rho)}{\delta\rho} + V(r) + e^2 \int d^3r' \frac{\rho(r')}{|r-r'|} + \frac{\delta E_{xc}(\rho)}{\delta\rho(r)} - \mu \right] = 0 \quad (1.21)$$

The kinetic energy could be expressed into density

$$\int d^3r T[\rho(r)] = \int d^3r \rho(r) \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} = \frac{3}{10} \frac{\hbar^2}{m} (3\pi^2)^{\frac{2}{3}} \int \rho^{\frac{5}{3}}(r) d^3r \implies \frac{\delta T[\rho(r)]}{\delta\rho(r)} = \frac{\hbar^2}{2m} (3\pi^2 \rho)^{\frac{2}{3}} \quad (1.22)$$

We can derive motion equation

$$\frac{\hbar^2}{2m} (3\pi^2 \rho)^{\frac{2}{3}} + V(r) + V_i(r) = \mu \quad (1.23)$$

Chapter 2

Heisenberg model

2.1 Exchange interaction

Heisenberg proposed the nearest exchange interaction to explain the spontaneous magnetization . The hydrogen molecular model provide key clue to this problem. As shown in Fig1.1, two electrons labeled by 1,2 located on the 1s orbit. The spatial wavefunction can be written as

$$\begin{cases} \phi_S = \frac{1}{\sqrt{2}} (\phi_a(r_1)\phi_b(r_2) + \phi_a(r_2)\phi_b(r_1)) \\ \phi_A = \frac{1}{\sqrt{2}} (\phi_a(r_1)\phi_b(r_2) - \phi_a(r_2)\phi_b(r_1)) \end{cases}$$

which corresponds to the energy

$$\begin{cases} E_S = 2\varepsilon_0 + K + J_e \\ E_A = 2\varepsilon_0 + K - J_e \end{cases}$$

The ε_0 is the on-site energy for 1s orbit electron . K is the Coulomb interaction

$$K = \int V_{ab} |\psi_a(r_1)|^2 |\psi_b(r_2)|^2$$

The V_{ab} is the Coulomb interaction

$$V_{ab} = e^2 \int \left(\frac{1}{r_{12}} + \frac{1}{r_{ab}} - \frac{1}{r_{a2}} - \frac{1}{r_{b1}} \right)$$

The J is the exchange energy

$$J = \int V(ab) \psi_a(r_1) \psi_a(r_2)^* \psi_b(r_1) \psi_b(r_2)^*$$

Pauli principle restrict that the product of the spatial wavefunction and spin wavefunction must be anti-symmetry. In the other words, the coherent energy of hydrogen atom depend on the spin orientation. Hence, Heisenberg written out the hamiltonian based on the exchange interaction.

$$H = - \sum_{\langle i,j \rangle} J_{ij} S_i \cdot S_j$$

The exchange integral originates from Pauli principle.

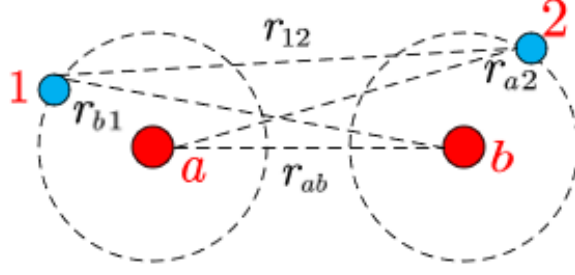


Fig 2.1: Hydrogen molecule exchange interaction

2.2 Heisenberg ferromagnetism

The Holstein-Primakoff transformation swap the angular momentum operator into bosonic operator.

$$\begin{cases} \hat{S}^z = S - \hat{b}^\dagger \hat{b} \\ \hat{S}^\dagger = \sqrt{2S} \left(1 - \frac{\hat{b}^\dagger \hat{b}}{2S}\right) \hat{b} \\ \hat{S}^- = \sqrt{2S} \hat{b}^\dagger \left(1 - \frac{\hat{b}^\dagger \hat{b}}{2S}\right) \end{cases}$$

In the limit that expectations of \hat{S}_z on each site are near to S , there are very few excitations in the bosonic representation, this mapping may be mapped into

$$\begin{cases} S^z = S - \hat{b}^\dagger \hat{b} \\ S^\dagger = \sqrt{2S} \hat{b} \\ \hat{S}^- = \sqrt{2S} \hat{b}^\dagger \end{cases}$$

Consider the exchange energy J is larger than zero, where the spins on the sites tend to align in the same direction. The ground state of ferromagnetism can be written as

$$| \text{Ground} \rangle = \bigotimes_i | S, S \rangle$$

Using the Holstein-Primakoff transformation to reduce the heisenberg hamiltonian into

$$H = -J \sum_{\langle i,j \rangle} S^2 - JS \sum_{\langle i,j \rangle} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i - \hat{b}_i^\dagger \hat{b}_i - \hat{b}_j^\dagger \hat{b}_j)$$

This system is translationally invariant, which can be taken Fourier transformation . The result is

$$H = -\frac{1}{2}JS^2NZ + \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} \quad \varepsilon_{\mathbf{k}} = 2J \sum_i (1 - \cos k_i)$$

The decription of the excitations can be reduce into harmonic oscillator like modes .Because the ferromagnet is an eigenstate of Hamiltonian, there no zero-point fluctuations. At the lower energy sector, the dispersion is propotional to the k^2

$$\varepsilon_{\mathbf{k}} \sim |k^2|$$

These excitation modes are Goldstone mode which arise from the spin rotational symmetry broken. According to the Ginzburg -Landau theory, the symmetry broken can be described by an parameter -magnetization .We will study the magnetization

$$M = \frac{1}{N} \sum_i \langle S - \hat{b}_i^\dagger \hat{b}_i \rangle = S - \frac{1}{N} \sum_{\mathbf{k}} \langle \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} \rangle$$

The fluctuation of magnetization is just the occupation number for the bosonic modes .

$$\begin{aligned} \Delta M &= \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{e^{\beta \varepsilon_{\mathbf{k}}} - 1} = \frac{1}{V} \int_{\text{BZ}} d^d \mathbf{k} \frac{1}{e^{\beta \varepsilon_{\mathbf{k}}} - 1} \\ &= T \int_0^{\sqrt{T/SJ}} \frac{k^{d-1} dk}{SJk^2} \\ &\sim T^{1.5} (d=3) \end{aligned}$$

The magnetization fluctuation is divergent in the $d \leq 2$, where the Mermin-Wagner theorem tells us that there is no continue symmetry broken at finite temperature. The three dimension is just the Bloch $T^{1.5}$ law ,that the magnetization fluctuation is propotional to $T^{1.5}$.

2.3 Heisenberg anti-ferromagnet

The Hamiltonian minimized the energy when the spin on the nearset site is opposite. This is also know as the Neel state shown in Fig 1.2

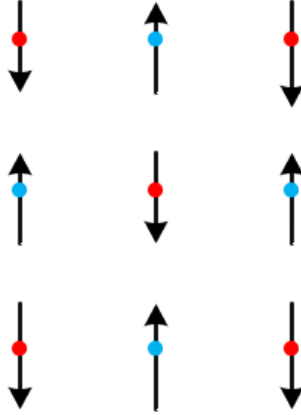


Fig 2.2: Neel state

We decompose the lattice into two sublattice A, B . For A sublattice, all spins on the site are oriented up . The Holstein-Primakoff for the A sublattice is the same as the ferromagnet .

However, We should change the forms of Holstein-Primakoff for the A sublattice.

Now we use this to rewrite the Heiseberg hamiltonian into such forms

$$H = -J \sum_{i,j} S^2 + JS \sum_{\langle i,j \rangle} \left[\hat{a}_i^\dagger \hat{a}_i + \hat{a}_j^\dagger \hat{a}_j + \hat{a}_i^\dagger \hat{a}_j^\dagger + \hat{a}_i \hat{a}_j \right]$$

We introduce the new coordinate x, d , where x is the coordinate for the all sites and the d is the nearest vector running over all nearest sites.

$$\begin{cases} S^z = S - \hat{b}^\dagger \hat{b} & |S, S\rangle & \text{---} & |0\rangle \\ \hat{S}^\dagger = \sqrt{2S} \hat{b} & |S, S-1\rangle & \text{---} & |1\rangle \\ \hat{S}^- = \sqrt{2S} \hat{b}^\dagger & |S, S-2\rangle & \text{---} & |2\rangle \\ & \vdots & & \end{cases}$$

Fig 2.3: Holstein-Primakoff for A sublattice

$$\begin{cases} & \vdots \\ S^z = -S + \hat{b}^\dagger \hat{b} & |S, -S+2\rangle & \text{---} & |2\rangle \\ \hat{S}^\dagger = \sqrt{2S} \hat{b}^\dagger & |S, -S+1\rangle & \text{---} & |1\rangle \\ \hat{S}^- = \sqrt{2S} \hat{b} & |S, -S\rangle & \text{---} & |0\rangle \end{cases}$$

Fig 2.4: Holstein-Primakoff for B sublattice

$$H = -\frac{JS^2 Nz}{2} + \frac{JSz}{2} \sum_{x,d} \left[2\hat{a}_x^\dagger \hat{a}_x + \hat{a}_z^\dagger \hat{a}_{x+d}^\dagger + \hat{a}_z \hat{a}_{x+d} \right]$$

which transforms into momentum representation

$$H = -\frac{JS(S+1)Nz}{2} + \frac{JSz}{2} \sum_{\mathbf{k}} \begin{bmatrix} \hat{a}_{\mathbf{k}}^\dagger & \hat{a}_{-\mathbf{k}} \end{bmatrix} \begin{bmatrix} 1 & \gamma_{\mathbf{k}} \\ \gamma_{\mathbf{k}} & 1 \end{bmatrix} \begin{bmatrix} \hat{a}_{\mathbf{k}} \\ \hat{a}_{-\mathbf{k}}^\dagger \end{bmatrix} \quad \gamma_{\mathbf{k}} = \sum_i \cos k_i$$

This Hamiltonian is the same as the BCS superconductor hamiltonian which can be diagonalized by Bogoliubov transformation.

$$\begin{bmatrix} \hat{a}_{\mathbf{k}} \\ \hat{a}_{-\mathbf{k}}^\dagger \end{bmatrix} = \begin{bmatrix} \cosh \theta_{\mathbf{k}} & -\sinh \theta_{\mathbf{k}} \\ -\sinh \theta_{\mathbf{k}} & \cosh \theta_{\mathbf{k}} \end{bmatrix} \begin{bmatrix} \hat{\alpha}_{\mathbf{k}} \\ \hat{\alpha}_{-\mathbf{k}}^\dagger \end{bmatrix}$$

The result is given by

$$H = -\frac{JS(S+1)Nz}{2} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \left(\hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} + \frac{1}{2} \right)$$

where

$$\epsilon_{\mathbf{k}} = JSz \sqrt{1 - \gamma_{\mathbf{k}}} \sim JSz |k|$$

The energy spectrum exists the zero point energy, which leads to the fluctuation even at the zero temperature. The magnetization fluctuation is given by

$$\begin{aligned} \Delta M &= \frac{1}{N} \sum_{\mathbf{k}} \langle (u_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^\dagger + v_{\mathbf{k}} \hat{\alpha}_{-\mathbf{k}}) (u_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}} + v_{\mathbf{k}} \hat{\alpha}_{-\mathbf{k}}^\dagger) \rangle \\ &= \frac{1}{N} \sum_{\mathbf{k}} \left(u_{\mathbf{k}}^2 \langle \hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} \rangle + v_{\mathbf{k}}^2 \langle \hat{\alpha}_{-\mathbf{k}} \hat{\alpha}_{-\mathbf{k}}^\dagger \rangle \right) \\ &= \frac{1}{N} \sum_{\mathbf{k}} \left(u_{\mathbf{k}}^2 \langle \hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} \rangle + v_{\mathbf{k}}^2 \langle \hat{\alpha}_{-\mathbf{k}}^\dagger \hat{\alpha}_{-\mathbf{k}} \rangle + v_{\mathbf{k}}^2 \right) \end{aligned}$$

At the zero temperature , the bosonic occupation number vanishes . We only consider zero point term

$$\begin{aligned}\Delta M &= \frac{1}{N} \sum_{\mathbf{k}} v_{\mathbf{k}}^2 \\ &= \frac{1}{2V} \int_{\text{BZ}} \left[\frac{1}{\sqrt{1 - \gamma_{\mathbf{k}}}} - 1 \right] \\ &= \frac{1}{4zV} \int dk k^{d-2}\end{aligned}$$

This integral is divergent in the 1d and convergent in $d \geq 2$.

2.4 Bethe ansatz

The Heisenberg model has the $SU(2)$ symmetry , but we only consider the spin rotational symmetry around the z axis. The total spin $S_z = \sum_n s_n^z$ is a conserved quantity , which leads to a good quantum number $S_z = \frac{N}{2} - M$.

The state is the ferromagnetic ground state with eigenvalue $E_0 = -\frac{JN}{4}$ when $M = 0$.

$$|\psi_0\rangle = |\uparrow, \uparrow, \dots, \uparrow\rangle$$

We consider the sector $M = 1$ where the eigenstate is the superposition of the n basis. The basis label by n which can be constructed by the lower operator

$$|n\rangle = S_n^- |\uparrow, \uparrow, \dots, \uparrow\rangle$$

We write the eigenstate $|\psi_1\rangle$ in the sector $M = 1$ as

$$|\psi_1\rangle = \sum_{n=1}^N f(n) |n\rangle$$

Define the translational operator T as

$$T |n\rangle = |(n+1) \pmod{N}\rangle$$

Consider the translational invariance on the Heisenberg model

$$T |\psi_i\rangle = \sum_{n=1}^N f(n) |n+1\rangle$$

which implies that

$$f(n+1) = \mu f(n)$$

We use the periodic condition to find out μ

$$T^N |\psi_0\rangle = \mu^N \sum_{n=1}^N f(n) |n\rangle \implies \mu^N = 1$$

Now the eigenstate can be written as

$$|\psi_1\rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^N e^{ikn} |n\rangle$$

The eigenvalue for the $|\psi_1\rangle$ is the

$$E = E_0 + 2J(1 - \cos k) \quad k = \frac{2\pi}{N}$$

Let's write down the generic eigenstate for the sector $M = 2$

$$|\psi_2\rangle = \sum_{1 \leq n_1 \leq n_2 \leq N} f(n_1, n_2) |n_1, n_2\rangle$$

where

$$|n_1, n_2\rangle = S_{n_1}^- S_{n_2}^- |\uparrow, \uparrow, \dots, \uparrow\rangle$$

Bethe made an ansatz that the coefficient is determined by

$$f(n_1, n_2) = A e^{i(k_1 n_1 + k_2 + n_2)} + A' e^{i(k_1 n_2 + k_2 n_1)}$$

We substitute this state into eigenequation

$$2(E - E_0)f(n_1, n_2) = J(4f(n_1, n_2) - f(n_1 \pm 1, n_2) - f(n_1, n_2 \pm 1))$$

which implies the eigenvalue

$$E = E_0 + 2 \sum_{i=1,2} (1 - \cos k_i)$$

On the other hand, the we can derive another equation if $n_2 = n_2 + 1$

$$2(E - E_0)f(n_1, n_2) = J(2f(n_1, n_2) - f(n_1 - 1, n_2) - f(n_1, n_2 + 1))$$

This equation leads to the relation of coefficient A, A'

$$\frac{A}{A'} = e^{i\theta} = -\frac{e^{i(k_1+k_2)} + 1 - 2e^{ik_1}}{e^{i(k_1+k_2)} + 1 - 2e^{ik_2}} \implies 2 \cot \frac{\theta}{2} = \cot \frac{k_1}{2} - \cot \frac{k_2}{2}$$

The phase shift θ reflect the interaction between the magnons. And we use the periodic condition to determine the quasi momentum k_1, k_2

$$f(n_1, n_2) = f(n_2, n_1 + N) \implies Nk_1 = 2\pi n_1 + \theta \quad Nk_2 = 2\pi n_2 - \theta$$

Bethe generalize this idea to construct generic wavefunction

$$|\psi\rangle = \sum_{1 \leq n_1 \leq n_2 \leq \dots \leq n_M} f(n_1, n_2, \dots, n_M) |n_1, n_2, \dots, n_M\rangle$$

where

$$f(n_1, n_2, \dots, n_M) = \sum_{P \in S_M} \exp \left(i \sum_{j=1}^M k_{P(j)} n_j + \frac{1}{2} \sum_{l, l < j} \theta_{P(l)P(j)} \right)$$

The phase angle is given by

$$e^{i\theta_{lj}} = -\frac{e^{i(k_l+k_j)} + 1 - 2e^{ik_l}}{e^{i(k_l+k_j)} + 1 - 2e^{ik_j}}$$

In virtue of translational symmetry , which means that $f(n_1, n_2, \cdots n_M) = f(n_2, \cdots n_M, n_1 + N)$

$$\sum_{j=1}^M k_{P(j)} n_j + \frac{1}{2} \sum_{l, l < j} \theta_{P(l)P(j)} = \sum_{j=2}^M k_{P'(j-1)} n_j + P'(j)$$

Chapter 3

Plasmon and Lindhard function

3.1 Random phase approximation

Electrons on the positive charge background could be described by hamiltonian

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^N \frac{\nabla_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|r_i - r_j|} + H_{\text{positive charge background}} \quad (3.1)$$

The Columb interaction could be expanded into momentum space by Fourier transformation

$$\begin{aligned} \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|r_i - r_j|} &= \frac{1}{2} \sum_q v(q) e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} = \frac{1}{2} \sum_q v(q) \left(\sum_{i=1}^N \sum_{j=1}^N v(q) e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} - N \right) \\ &= \sum_q v(q) (\rho_q^\dagger \rho_q - N) \end{aligned} \quad (3.2)$$

where $\rho_q = \sum_j e^{-i\vec{q} \cdot \vec{r}_j}$, $\rho(r) = \sum_{i=1}^N \delta(r - r_i)$. The background charge corresponds to $q = 0$ components, namely $\frac{V(0)}{2}(N^2 - N)$. We should remove it .

The hamiltonian (3.1) written into second quantization form

$$H = \sum_{k\sigma} (\varepsilon_{k\sigma} - \mu) c_{k\sigma}^\dagger c_{k\sigma} + \frac{1}{2V} \sum_{k, k' \text{ prime}} \sum_{q \neq 0} \frac{4\pi e^2}{q^2} c_{k+q, \sigma}^\dagger c_{k'-q, \sigma'}^\dagger c_{k'-q, \sigma'} c_{k+q, \sigma} \quad (3.3)$$

We remove the background charge contribution. We define the density operator ρ_q as

$$\rho_q = \sum_k c_{k+q}^\dagger c_k \quad \sum_k \rho_q^\dagger = \sum_k c_{k+q}^\dagger c_{k+q} = \rho_{-q} \quad (3.4)$$

Note:-

$$\begin{aligned} [H_0, \rho_q] &= \sum_{k\sigma} \varepsilon_k [c_{k\sigma}^\dagger c_{k\sigma}, c_{k+q\sigma}^\dagger c_{k\sigma}] = \sum_{k\sigma} \varepsilon'_k c_{k'\sigma}^\dagger [c_{k'\sigma}, c_{k+q\sigma}^\dagger c_{k\sigma}] + \varepsilon'_k [c_{k'\sigma}^\dagger, c_{k+q\sigma}^\dagger c_{k\sigma}] c_{k'\sigma} \\ &= \sum_k (\varepsilon_{k+q} - \varepsilon_k) c_{k+q\sigma}^\dagger c_{k\sigma} \\ &= \sum_k \hbar \omega_{kq} \rho_{kq} \end{aligned} \quad (3.5)$$

$$\begin{aligned}
[\rho_{q_1}, \rho_{q_2}] &= \sum_{k_1, k_2} [c_{k_1+q_1}^\dagger c_{k_1}, c_{k_2+q_2}^\dagger c_{k_2}] = \sum_{k_1, k_2} c_{k_1+q_1}^\dagger [c_{k_1}, c_{k_2+q_2}^\dagger c_{k_2}] + [c_{k_1+q_1}^\dagger, c_{k_2+q_2}^\dagger c_{k_2}] c_{k_1} \\
&= \sum_{k_1, k_2} c_{k_1+q_1}^\dagger \{c_{k_1}, c_{k_2+q_2}^\dagger\} c_{k_2} - c_{k_2+q_2}^\dagger \{c_{k_1+q_1}^\dagger, c_{k_2}\} c_{k_1} \\
&= \sum_k c_{k+q_1+q_2}^\dagger c_k - c_{k+q_2}^\dagger c_{k-q_1}
\end{aligned} \tag{3.6}$$

$$\begin{aligned}
\frac{1}{2} \sum_{q \neq 0} v(q') [\rho_{p'} \rho_{-q'}, \rho_q] &= \frac{1}{2} \sum_{q \neq 0} v(q') [\rho_{q'}, \rho_q] \rho_{-q'} + v(q') \rho_{q'} [\rho_{-q'}, \rho_q] \\
&= \frac{1}{2} \sum_{k, q \neq 0} v(q') (c_{k+q'+q\sigma}^\dagger c_{k\sigma} - c_{k+q\sigma}^\dagger c_{k-q'\sigma}) \rho_{-q'} + (c_{k-q'+q\sigma}^\dagger c_{k\sigma} - c_{k+q\sigma}^\dagger c_{k+q'\sigma}) \rho_{q'}
\end{aligned} \tag{3.7}$$

$$\tag{3.8}$$

The $\rho_q = \sum_i e^{-i\vec{q} \cdot \vec{r}_i}$ is a summation of phase, which is random at high densities. Hence, the RPA could be applied.

$$\rho_{q_1} \rho_{q_2 - q_1} = \sum_{k_1, k_2} e^{-i\vec{q}_1 \cdot \vec{r}_i} \cdot e^{-i(\vec{q}_2 - \vec{q}_1) \cdot \vec{r}_i} \approx N \rho_{q_2} \tag{3.9}$$

Hence, the commutator becomes

$$[H, \rho_{k\sigma}] = \hbar \omega_{kq} \rho_{kq\sigma} + v(q)(n_k - n_{k+q}) \rho_q \tag{3.10}$$

Let's consider the eigenequation, which reads

$$[H, \sum_k a_k \rho_k] = \hbar \omega \sum_k a_k \rho_k \tag{3.11}$$

which is equivalent to

$$[H, \sum_k a_k \rho_k] = \sum_k a_k (\hbar \omega_{kq} \rho_{kq\sigma} + v(q)(n_k - n_{k+q}) \rho_q) = \hbar \omega \sum_k a_k \rho_{kq} \tag{3.12}$$

Note:-

Let's derive consistent equation. We can derive from Eq(3.12)

$$\begin{aligned}
\hbar \omega_{kq} a_k + \sum_{k', \sigma'} v(q)(n_{k'} - n_{k'+q}) a_{k'\sigma'} &= \hbar \omega a_k \\
\Rightarrow a_k &= \frac{v(q)}{\hbar(\omega - \omega_{kq})} \sum_{k', \sigma'} (n_{k'} - n_{k'+q}) a_{k'} \\
\Rightarrow \sum_k (n_k - n_{k+q}) a_k &= \sum_{k', \sigma} \frac{v(q)(n_{k'} - n_{k'+q})}{\hbar(\omega - \omega_{kq})} \sum_k (n_k - n_{k+q}) a_k \\
\Rightarrow \sum_{k', \sigma} \frac{v(q)(n_{k'} - n_{k'+q})}{\hbar(\omega - \omega_{kq})} &= 1
\end{aligned}$$

3.2 Dielectric function

Suppose we add an external potential ,

$$H_e(t) = \sum_i V_e(r_i) e^{-i\omega t + \eta t} = \frac{1}{V} \sum_q V_e(q) e^{-i\omega t + \eta t} \rho_q \quad (3.13)$$

The motion equation reads as

$$-i\hbar \dot{\rho}_k = [H, \rho_k] + [H_e(t), \rho_k] \quad (3.14)$$

Note:-

With RPA approximation,

$$[H_e(t), \rho_{kq}] = \sum_{q'} V_e(q) e^{-i\omega t + \eta t} [\rho_{q'}, \rho_{kq}] = \frac{2}{V} V_e(q) (n_{k+q} - n_k) e^{-i\omega t + \eta t}$$

Hence, we can derive

$$\begin{aligned} -\omega \langle \rho_{kq} \rangle &= \omega_{kq} \langle \rho_{kq} \rangle + \frac{2}{V} V_e(q) (n_k - n_{k-q}) + \frac{2}{V} (n_{k+q} - n_k) \langle \rho_q \rangle \\ \implies \langle \rho_{kq} \rangle &= - \sum_k \frac{2}{V} \frac{n_{k+q} - n_k}{\hbar\omega - \omega_{kq}} \underbrace{(V_e(q) + V(q) \langle \rho_q \rangle)}_{V_{tot}} \end{aligned} \quad (3.15)$$

We define the vacuum polarization as

$$\chi(q, \omega) = \frac{2}{V} \sum_k \frac{n_{k+q} - n_k}{\hbar\omega - \omega_{kq}} \quad (3.16)$$

The total potential V_{tot} can be expressed as

$$V_{tot} = V_e(q, t) + \frac{4\pi e^2}{q^2} \langle \rho_q \rangle = V_e - V(q) \chi(q, \omega) V_{tot} \implies V_{tot} = \frac{V_e}{(1 + v(q) \chi(q, \omega))} \quad (3.17)$$

Note:-

From the classical Laplace equation

$$-\nabla^2 V = 4\pi(-e)^2 \langle \rho \rangle \implies V_{tot} = \frac{4\pi e^2}{q^2} \langle \rho_q \rangle \quad (3.18)$$

We define dielectric function with Lindhard function

$$\varepsilon(q, \omega) = 1 + v(q) \chi(q, \omega) = 1 + \frac{2v(q)}{V} \sum_k \frac{n_{k+q} - n_k}{\hbar\omega - \omega_{kq}} \quad (3.19)$$

Let's consider the real part and imaginary part of dielectric function.

$$\begin{cases} \varepsilon_1(q, \omega) = 1 + v(q) \chi(q, \omega) = 1 + \frac{2v(q)}{V} \sum_k \mathcal{P} \left(\frac{n_{k+q} - n_k}{\hbar\omega - \omega_{kq}} \right) \\ \varepsilon_2(q, \omega) = \frac{2\pi v(q)}{\hbar V} \sum_k n_k [\delta(\omega - (\omega_{k+q} - \omega_k)) + \delta(\omega + (\omega_{k+q} - \omega_k))] \end{cases} \quad (3.20)$$

3.3 Lindhard function

Let's discuss some typical behaviour of Lindhard function.

- $\frac{q}{k_F} \rightarrow 0$, $n_{k+q} - n_k = \frac{\partial n}{\partial \varepsilon} \nabla_q \varepsilon = -\delta(\varepsilon - \varepsilon_F) q v_F \cos \theta$

$$\begin{aligned}
 \chi_0(q, \omega) &= \frac{2}{V} \sum_k \frac{n_{k+q} - n_k}{\hbar\omega - \omega_{kq}} = 2 \int \frac{d^3k}{(2\pi)^3} \frac{-\delta(\varepsilon - \varepsilon_F) v_F q \cos \theta}{\omega - q v_F \cos \theta + i\eta} \\
 &= 2N(0) \int \frac{d \cos \theta d\varphi}{4\pi} \frac{-q v_F \cos \theta}{\omega - q v_F \cos \theta + i\eta} \\
 &= N(0) \int_{-1}^1 dx \frac{-x}{s - x + i\eta} \\
 &= N(0) \int_{-1}^1 dx \left[\mathcal{P} \left(\frac{x}{x-s} \right) + i\pi \delta(x-s) \right] \\
 &= 2N(0) \left(1 - \frac{s}{2} \log \left| \frac{1+s}{1-x} \right| \right) + iN(0)\pi s \Theta(|s^2 - 1|) \quad (3.21)
 \end{aligned}$$

Note:-

$$\begin{aligned}
 N &= \left(\frac{4\pi k^3}{3} \right) \cdot \left(\frac{L}{2\pi} \right)^3 \implies \log N = \frac{3}{2} \log \varepsilon \implies D(\varepsilon) = \frac{dN}{d\varepsilon} = \frac{3N}{2\varepsilon} \\
 \frac{1}{(2\pi)^3} k^2 dk &= \frac{1}{(2\pi)^3} \cdot \frac{1}{4\pi} \frac{d\frac{4\pi}{3} k^3}{d\varepsilon} \cdot d\varepsilon = \frac{N(\varepsilon)}{4\pi} d\varepsilon
 \end{aligned}$$

We consider two different limits

$$\chi_0(q, \omega) = \begin{cases} 2N(0) \left(1 - s^2 + i\frac{\pi}{2} \right) & (s \ll 1) \\ 2N(0) \left(-\frac{1}{3s^2} - \frac{1}{5s^4} \right) & (s \gg 1) \end{cases} \quad (3.22)$$

In the plasmon region, the imaginary part of Lindhard vanishes.

$$\varepsilon(q, \omega) = 1 + \frac{4\pi e^2}{q^2} \cdot 2N(0) \left(-\frac{1}{3s^2} - \frac{1}{5s^4} \right) \quad (3.23)$$

Chapter 4

Fermi Liquid

4.1 Quasi-particles and Landau interaction parameters

4.2 Renormalization to physical properties

Let's consider a simple classical example. The object is connected by string . The other end of string is fixed on wall.

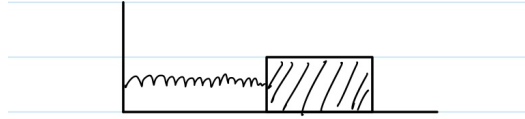


Fig 4.1

The input of system is force F and response is displacement s . The susceptibility is defined as

$$x = -\frac{x}{F} = \frac{1}{k} \quad (4.1)$$

The energy of sytem is described as

$$E = E_{\text{Ela}} - kx = \frac{1}{2}kx^2 - Fx \rightarrow E = -\frac{1}{2}\chi F^2 \quad (4.2)$$

The susceptibility also can be defined from energy

$$\chi = -\frac{\partial^2 E}{\partial F^2} \quad (4.3)$$

Example 4.2.1 (.)

We consider magnetism system . where the external field H will response to magnetization M . The energy increment is gien by

$$dE = HdM \quad (4.4)$$

Hence , the total energy is given by

$$E = E_M - HM \rightarrow \chi = -\frac{\partial^2 E}{\partial H^2} \quad (4.5)$$

Now we consider a more complex system, where object is connected with two springs . By the same way , the susceptibility is given by

$$\chi = \frac{1}{k_0 + k'} = \frac{\chi_0}{1 + \frac{k'}{k_0}} \quad (4.6)$$

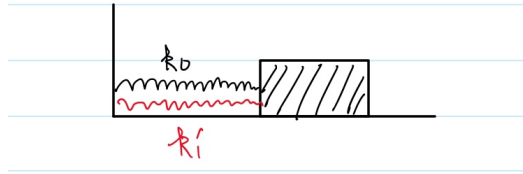


Fig 4.2

We understood this process with close loop process as shown on ().

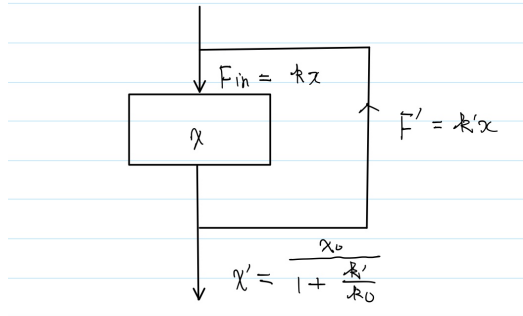


Fig 4.3

The feedback process will change the susceptibility. We expand the renormalized susceptibility into Taylor series

$$\chi' = \chi_0 + \chi_1 + \chi_2 \dots \text{where } \chi_n = \chi_0 \left(-\frac{k'}{k} \right)^n \quad (4.7)$$

Question 1: .

If the k' is negative, what interesting things will be happen?

4.2.1 Magnetic susceptibility

We consider energy fnctional with second order . The spin index is polarized at z axis. Hnece, the desnity variation are diagonal.

$$f^a(p, p') \vec{\sigma}_{\alpha\beta} \cdot \vec{\sigma}_{\gamma\delta} \delta n_{\beta\alpha}(p) \cdot \delta n_{\delta\gamma}(p') \rightarrow f^a(p, p') \vec{\sigma} \cdot \vec{\sigma} \delta n_{p\sigma} \delta n_{p'\sigma'} \quad (4.8)$$

Hence, we can derive that

$$\delta\varepsilon^{(2)} = \frac{1}{2N_0V} F_0^a \sum \sigma \cdot \sigma' \delta n_{p\sigma} \delta n_{p'\sigma'} = \frac{V}{2N_0} F_0^a (S_z)^2 \quad (4.9)$$

We introduce molecular field h_{mol} , which induces energy increment ΔV

$$\Delta V = -V \int h_{\text{mol}} \cdot dS_z \implies h_{\text{mol}} = -\frac{1}{V} \frac{\partial E}{\partial S} = -\frac{1}{N_0} F_0^a S_z \quad (4.10)$$

The total magnetic field is given by

$$h_{\text{tot}} = h_{\text{ex}} + h_{\text{mol}} \quad (4.11)$$

The total magnetization S_z and total field can be related with susceptibility χ_0

$$S_z = \chi_0 h_{\text{tot}} = \chi(0) (h_{\text{ex}} - N_0^{-1} F_0^a S_z) \implies \chi = \frac{\chi_0}{1 + \chi_0 N_0^{-1} F_0^a} \quad (4.12)$$

4.2.2 Compressibility

In this subsection, we will discuss another quantity, namely compressibility.

Note:-

The definition of compressibility is

$$\chi_{\text{comp}} = -\frac{1}{V} \frac{\partial V}{\partial p} \quad (4.13)$$

We can use observable quantity n and μ to express the compressibility.

$$V = \frac{N}{n} \quad PV = N\mu \quad (4.14)$$

The compressibility can be written as

$$\chi = -\frac{1}{N} \frac{d}{d\mu} \left(\frac{N}{n} \right) = \frac{1}{n^2} \frac{dn}{d\mu} \quad (4.15)$$

The density variation functional could be written as

$$\delta\varepsilon^{(2)} = \frac{1}{2N_0V} F_0^s \sum_{p,p'} \delta n_p \delta n_{p'} = \frac{V}{2N_0} F_0^s \sum (\delta n)^2 \quad (4.16)$$

By the same way, we can define molecular field

$$h_{\text{mol}} = -\frac{F_0^s \delta n}{N_0} \quad (4.17)$$

which means that

$$\chi = \frac{\chi_0}{1 + F_0^s} \quad (4.18)$$

4.2.3 Effective mass

The effective mass is renormalized with p wave channel . We will derive the explicit form below. The density on the real space could be written as

$$n(r, t) = \sum_{\sigma} \int \frac{d^3 p}{(2\pi)^3} n_p(r, t) \quad (4.19)$$

The current is given by

$$\vec{j}(r, t) = \sum_{\sigma} \int \frac{d^3 p}{(2\pi)^3} \nabla_p \varepsilon(p, \sigma) n_{p\sigma}(r, t) \quad (4.20)$$

We take linear order approximation

$$\begin{cases} \varepsilon_{p\sigma}(r, t) = \varepsilon_p^0 + \int \frac{d^3 p'}{(2\pi)^3} f_{\sigma\sigma'}(p, p') \delta n_{p'\sigma'} \\ n_{p\sigma} = n_{p,\sigma}^0 + \delta n_{p\sigma}(r, t) \end{cases} \quad (4.21)$$

We substitute the EQ(4.21) into (4.22)

$$\vec{j}(r, t) = \sum_{\sigma} \int \frac{d^3 p}{(2\pi)^3} \nabla_p \left(\varepsilon_p^0 + \int \frac{d^3 p'}{(2\pi)^3} f_{\sigma\sigma'}(p, p') \delta n_{p'\sigma'} \right) (n_{p,\sigma}^0 + \delta n_{p\sigma}(r, t)) \quad (4.22)$$

We remove the background current, then we have

$$\begin{aligned} \vec{j}(r, t) &= \sum_{\sigma} \int \frac{d^3 p}{(2\pi)^3} \left[\nabla_p \varepsilon_p^0 \delta n_{p\sigma}(r, t) + \nabla_p \int \frac{d^3 p'}{(2\pi)^3} f_{\sigma\sigma'}(p, p') \delta n_{p'\sigma'} n_{p,\sigma}^0 \right] \\ &= \int \frac{d^3 p}{(2\pi)^3} \left[\nabla_p \varepsilon_p^0 \delta n_{p\sigma}(r, t) - \int \frac{d^3 p'}{(2\pi)^3} f_{\sigma\sigma'}(p, p') \delta n_{p'\sigma'} \nabla_p n_{p,\sigma}^0 \right] \\ &= \int \frac{d^3 p}{(2\pi)^3} \nabla_p \varepsilon_p^0 \delta n_{p\sigma}(r, t) - \int \frac{d^3 p}{(2\pi)^3} \frac{\partial n_{p,\sigma}^0}{\partial \varepsilon} \vec{v}_F \int \frac{d^3 p'}{(2\pi)^3} f_{\sigma\sigma'}(p, p') \delta n_{p'\sigma'} \\ &= \int \frac{d^3 p}{(2\pi)^3} \nabla_p \varepsilon_p^0 \delta n_{p\sigma}(r, t) - \int \frac{d^3 p}{(2\pi)^3} \frac{\partial n_{p,\sigma}^0}{\partial \varepsilon} v_F \frac{4\pi}{2l+1} \sum_l P_l(\cos \theta) P_l(\cos \theta') \int \frac{d^3 p'}{(2\pi)^3} \delta n_{p'\sigma'} \\ &= \int \frac{d^3 p}{(2\pi)^3} \vec{v}_F \left(1 + \frac{F_0^s}{3} \right) \Rightarrow \frac{1}{m^*} = \frac{1}{m} \int \frac{d^3 p}{(2\pi)^3} \end{aligned} \quad (4.23)$$

4.2.4 Arbitrary channel contribution

We define the radial density by integrate out momentum p

$$\delta n = V \int \frac{d^3 p}{(2\pi)^3} \delta n(p) = V \int \frac{p^2 dp}{(2\pi)^3} \delta n(p) \int d\Omega = V \int d\Omega \delta n(\Omega) \quad (4.24)$$

The angular density distribution could be expand into normal modes

$$\delta n(\Omega) = \sum_{l,m} n_{l,m} Y_{l,m}(\Omega) \quad (4.25)$$

The kinetic increment could be decomposed into normal modes

$$\begin{aligned}
\Delta E^2 &= \frac{1}{2V} \int \frac{dp^3}{(2\pi)^3} f_{\sigma,\sigma'}(p,p') \delta n_{p\sigma} \delta n_{p'\sigma'} \\
&= \frac{V}{2} \int d\Omega_p d\Omega_{p'} f_{\sigma,\sigma'}(p,p') \delta n(\Omega_p) \delta n(\Omega'_p) \\
&= \frac{V}{2} N^{-1}(0) \int d\Omega_p d\Omega_{p'} \left(\sum_{l_1} \sum_{m_1=-l_1}^{l_1} F_{l_1}^s Y_{l_1 m_1}(\Omega_p) \bar{Y}_{l_1 m_1}(\Omega'_p) \right) \left(\sum_{l_2} \sum_{m_2=-l_2}^{l_2} n_{l_2 m_2} Y_{l_2 m_2}(\Omega_p) \right) \\
&\quad \left(\sum_{l_3} \sum_{m_3=-l_3}^{l_3} n_{l_3 m_3} Y_{l_3 m_3}(\Omega'_p) \right) + (s \leftrightarrow a) \\
&= \frac{V}{2} N^{-1}(0) \sum_l \frac{4\pi}{2l+1} \sum_{m=-l}^l F_l^s |\delta n_{lm}|^2 + (s \leftrightarrow a)
\end{aligned} \tag{4.26}$$

We consider the first order increment

$$\delta E^{(0)} = \sum_p \varepsilon_p \delta n_p = \int \frac{d^3 p}{(2\pi)^3} \varepsilon_p \delta n \tag{4.27}$$

4.2.5 Pomeranchuk instability

4.3 The Boltzmann equation and zero sound

4.3.1 Boltzmann equation

We start from Boltzmann equation. The particle density on the phase space is described by distribution function $f(\mathbf{r}, \mathbf{p}, t)$. In the other words ,

$$f(\mathbf{r}, \mathbf{p}, t) d\mathbf{r}^3 d\mathbf{p}^3 \tag{4.28}$$

Due to occurence of collisions, the particle number lying on the phase space will change . We consider the particle variation on the phase space. The Liouville theorem tells us phase space volumme conservation.

$$\Delta N_{\text{Collision}} = (f(\mathbf{r} + \Delta \mathbf{r}, \mathbf{p} + \Delta \mathbf{p}, t) - f(\mathbf{r}, \mathbf{p}, t)) d\mathbf{r}^3 d\mathbf{p}^3 \tag{4.29}$$

The total differential of f is

$$df = \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial x} \frac{\partial p}{\partial t} dt + \frac{\partial f}{\partial p} \frac{\partial p}{\partial t} dt = \left(\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla_{\mathbf{r}} f + \vec{F} \cdot \nabla_{\mathbf{p}} f \right) dt \tag{4.30}$$

We can see that the particle number flow comprise real space flow and momentum space flow. The total flow is equal to collision section. The collision section consists of forward process and reverse process.

$$I = \int d^3 \mathbf{r} d^3 \mathbf{p} I(\Omega) (f(\mathbf{r}'_1, \mathbf{p}'_1, t) f(\mathbf{r}'_1, \mathbf{p}'_1, t) - f(\mathbf{r}_1, \mathbf{p}_1, t) f(\mathbf{r}_1, \mathbf{p}_1, t)) \tag{4.31}$$

The $I(g, \Omega)$ is scattering section , which can be determined by Fermin golden rule. We consider the fermion system, the density distribution has very strong limit in virtue of Pauli principle.

$$I = \frac{1}{V^2} \sum |\langle 3, 4 | V | 1, 2 \rangle|^2 \delta_{p_1+p_2=p_3+p_4} \delta_{\sigma_1+\sigma_2=\sigma_3+\sigma_4} \delta_{\varepsilon_1+\varepsilon_2=\varepsilon_3+\varepsilon_4} (n_1 n_2 (1-n_3)(n_4) - (1-n_2)(1-n_2) n_3 n_4) \tag{4.32}$$

Note:-

If we consider random approximation , then the collision section will turns into

$$\langle I \rangle = -\frac{\delta N}{\tau} \quad (4.33)$$

Hence, the solution will recover into equilibrium distrition gradually.

$$N(T) = N_0(1 - e^{-\frac{T}{\tau}}) \quad (4.34)$$

4.4 Zero sound

We consider collisonless cases . Hence, the Boltzman equation could be written as

$$\frac{\partial n(\mathbf{r}, \mathbf{p}, t)}{\partial t} + \nabla_{\mathbf{p}} \varepsilon(\mathbf{p}, t) \nabla_{\mathbf{r}} n(\mathbf{r}, \mathbf{p}, t) - \nabla_{\mathbf{r}} \varepsilon(\mathbf{p}, t) \nabla_{\mathbf{p}} n(\mathbf{r}, \mathbf{p}, t) = 0 \quad (4.35)$$

It's self-evident that Eq(4.35) is a nonlinear equation . We expand the density distribution and energy functional.

$$\begin{cases} \varepsilon(\mathbf{r}, \mathbf{p}, t) = \varepsilon_0(p) + \frac{1}{V} \sum_{p'} f^s(\mathbf{p}, \mathbf{p}') \delta n_{\mathbf{p}'}(\mathbf{r}, t) \\ n(\mathbf{r}, \mathbf{p}) = n_0(\mathbf{r}, \mathbf{p}) + \delta n(\mathbf{r}, \mathbf{p}, t) \end{cases} \quad (4.36)$$

At the equibrillium state, the density distribution and energy functional don't rely on space position \mathbf{r} . The Boltzmann equation can be expanded into first order in relative with $\delta(\mathbf{r}, \mathbf{p}, t)$.

$$\frac{\partial \delta n(\mathbf{r}, \mathbf{p}, t)}{\partial t} + \vec{v}_{\mathbf{p}} \cdot \nabla_{\mathbf{r}} \delta n(\mathbf{r}, \mathbf{p}, t) - \nabla_{\mathbf{p}} \varepsilon \cdot \frac{1}{V} \sum_{p'} f^s(p, p') \nabla_{\mathbf{r}} \delta n(\mathbf{r}, \mathbf{p}', t) = 0 \quad (4.37)$$

We insert relation $\nabla_{\mathbf{p}} \varepsilon = \frac{\partial \varepsilon}{\partial \varepsilon} \nabla_{\mathbf{p}} \varepsilon$ into Eq(??). The Boltzmann equation will reduce into

$$\frac{\partial \delta n(\mathbf{r}, \mathbf{p}, t)}{\partial t} + \vec{v}_{\mathbf{p}} \cdot \left(\nabla_{\mathbf{r}} \delta n(\mathbf{r}, \mathbf{p}, t) - \frac{\partial n}{\partial \varepsilon} \cdot \frac{1}{V} \sum_{p'} f^s(p, p') \nabla_{\mathbf{r}} \delta n(\mathbf{r}, \mathbf{p}', t) \right) = 0 \quad (4.38)$$

We expand the density fluactuation into Fourier modes, namely

$$\delta n(\mathbf{r}, \mathbf{p}, t) = \sum_{\mathbf{q}} \delta n(\mathbf{p}) e^{i(\vec{q} \cdot \vec{r} - \omega t)} \quad (4.39)$$

where wavevector \vec{q} is small . We insert Fourier mode into Eq(4.39)

$$(\omega - \vec{q} \cdot \vec{v}_F) \delta n(\mathbf{p}) + (\vec{v}_F \cdot \vec{q}) \frac{\partial n}{\partial \varepsilon} \frac{1}{V} \sum_{p'} f^s(\mathbf{p}, \mathbf{p}') \delta n(\mathbf{p}) = 0 \quad (4.40)$$

We define the dimensionless quantty $s = \frac{\omega}{qv_F}$ and choose direction of \vec{v}_F as z axis. Now we integrate out the radial part by $\int \frac{p^2 dp}{2\pi}$

$$(s - \cos \theta) \delta \hat{n}(\Omega) - \cos \theta \underbrace{\int \frac{p^2 dp}{2\pi} \frac{\partial n}{\partial \varepsilon}}_{\frac{N(0)}{4\pi}} \frac{1}{V} \sum_{p'} f^s(\mathbf{p}, \mathbf{p}') \delta n(\mathbf{p}) = 0 \quad (4.41)$$

The oscillation on the Fermi surface is tensor wave. The Fermi surface oscillation is transferred by Landau interaction. Hence, we consider decomposing the density $\hat{n}(\Omega)$ into $SO(3)$ irreducible tensors.

$$\frac{1}{V} \sum_{p'} f^s(\mathbf{p}, \mathbf{p}') \delta n(\mathbf{p}) = \int d\Omega' \left(F_l^s \sum_l \sum_{m=-l}^l \frac{4\pi}{2l+1} Y_{lm}(\Omega) \bar{Y}_{lm}(\Omega') \right) \left(\sum_{l'} \sum_{m=-l'}^{l'} u_l' Y_{l'm'}(\Omega') \right) \quad (4.42)$$

$$= \sum_{l'} \frac{4\pi}{2l'+1} u_{l'} F_{l'}^s Y_{l'm}(\Omega) \quad (4.43)$$

where Ω is the solid angle expanded by momentum p and Ω' expanded by Ω' . We insert Eq(4.43) into Eq(4.41) to derive such identity

$$\sum_{l'} \sum_{m=-l'}^{l'} n_{l'} Y_{l'm} - \sum_{l'} \sum_{m=-l'}^{l'} \frac{1}{2l'+1} \frac{\cos \theta}{s - \cos \theta} u_{l'} F_{l'}^s Y_{l'm}(\Omega) = 0 \quad (4.44)$$

We can see from Eq(4.44) that the angular momentum m can be viewed as internal gauge. Hence, We fix m to zero. Now, we can derive from Eq(4.44)

$$\frac{u_l}{\sqrt{(2l+1)}} - \sum_{l'} \frac{1}{\sqrt{(2l'+1)(2l+1)}} \int d\Omega \frac{\cos \theta}{s - \cos \theta} Y_{l0}(\Omega) Y_{l'0}(\Omega) F_{l'}^s \frac{u_{l'}}{\sqrt{2l'+1}} = 0 \quad (4.45)$$

We define the integral $\Omega_{ll'}$ as below.

$$\Omega_{ll'} = - \frac{1}{\sqrt{(2l'+1)(2l+1)}} \int d\Omega \frac{\cos \theta}{s - \cos \theta} Y_{l0}(\Omega) Y_{l'0}(\Omega) F_{l'}^s \quad (4.46)$$

We consider the zero order of Eq(4.45).

$$u_0 + \Omega_{00} F_0^s = 0 \implies \frac{1}{F_0^s} = -\Omega_{00} \quad (4.47)$$

Note:-

We give some details about calculation of Ω_{00}

$$\begin{aligned} \Omega_{00} &= - \int \frac{d\Omega}{4\pi} \frac{\cos \theta}{s - \cos \theta} = - \frac{1}{2} \int_{-1}^1 \frac{x dx}{s - x} = - \frac{1}{2} \int_{-1}^1 \left[x \mathcal{P}\left(\frac{1}{s-x}\right) + i\pi \delta(s-x) \right] dx \\ &= - \frac{1}{2} \int_{-1}^1 \left[\frac{s}{s-x} - 1 + i\pi \delta(s-x) \right] dx \\ &= - \frac{s}{2} \log \frac{s+1}{s-1} + 1 - i \frac{\pi}{2} \Theta(|s^2 - 1|) \end{aligned} \quad (4.48)$$

The solution of the Eq(4.47) could be depicted in Fig (4.4)

Note:-

We consider two limits

- $s \rightarrow 1^+$

$$-\frac{s}{2} \log \left| \frac{s+1}{s-1} \right| + 1 \approx 1 + \log \left| \frac{s-1}{2} \right| = \frac{!}{F_o^s} \Rightarrow s \approx 1 + e^{-\frac{2}{F_o^s}} \quad (4.49)$$

- $s \rightarrow \infty$

$$\frac{s}{2} \log \left| \frac{s-1}{s+1} \right| = \frac{s}{2} \left(-\frac{1}{s} - \frac{1}{2s^2} - \frac{1}{3s^3} - \frac{1}{s} + \frac{s^2}{2} - \frac{1}{3s^3} \right) + 1 = -\frac{1}{3s^2} \Rightarrow s = \sqrt{\frac{F_o^s}{3}} \quad (4.50)$$

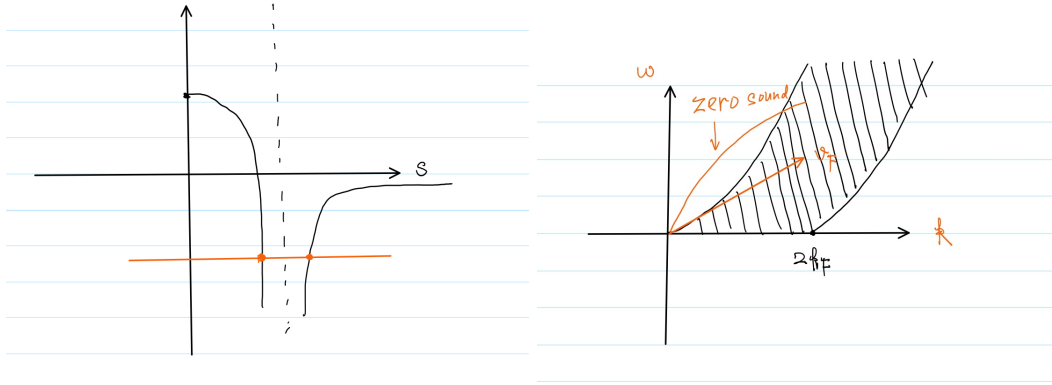


Fig 4.4

The real physical solution lies on region $s > 1$. Otherwise, it will collapse into particle-hole continuum.

Chapter 5

Superconductor

5.1 Phenomenology of superconductor

5.2 BCS theory

5.3 BCS theory

5.4 Unconventional superconductor

5.5 Josephson diode

Chapter 6

Many body methods

6.1 Green function and Feymann diagram

6.2 Luttinger theorem

Chapter 7

Bosonization

Chapter 8

Spin model

8.1 One-dimensional tranverse Ising model

In this section, we will introduce the most simple quantum spin model, namely one dimensional tranverse Ising model. This model is constructed from classical Ising model . We also need to add tranverse term to generate quantum fluctuations.

$$H = J \sum_n \sigma_n^x \sigma_n^x + h \sum_n \sigma_n^z \quad (8.1)$$

In order to deal with spin operator, we use Jordon-Wigner transformation to translate into fermions language. The fermion occupied state $|1\rangle$ represents spin up \uparrow and fermion vacuum state represents spin down $|\downarrow\rangle$. Hence, we can write down Jordon-Wigner transformation.

$$\begin{cases} \sigma_n^+ = e^{i\pi \sum_{m<n} c_m^\dagger c_m} c_n^\dagger \\ \sigma_n^- = e^{i\pi \sum_{m<n} c_m^\dagger c_m} c_n \\ \sigma_z = 2c_n^\dagger c_n - 1 = [c_n^\dagger, c_n] \end{cases} \quad (8.2)$$

Note:-

The reverse transformation is

$$\begin{cases} c_n^\dagger = \prod_{m<n} \sigma_m^x \sigma_n^+ \\ c_n = \prod_{m<n} \sigma_m^x \sigma_n^- \\ [c_n^\dagger, c_n] = \sigma_n^z \end{cases} \quad (8.3)$$

Under the Jordon-Wigner transformation, the spin model could be transformed into fermion model , which reads as

$$H = J \sum_n (c_n^\dagger + c_n)(c_{n+1}^\dagger - c_{n+1}) + h \sum_n [c_n^\dagger, c_n] \quad (8.4)$$

The Hamiltonian(8.4) has Majorana representation. The fermionic operator is splitted into two real Majorana operator

$$\begin{cases} \beta_n = (c_n^\dagger + c_n) \\ \gamma_n = -i(c_n^\dagger - c_n) \end{cases} \quad (8.5)$$

Note:-

The Majorana operator satisfies to relation

$$\begin{cases} \{\beta_n, \beta_m\} = \{\gamma_n, \gamma_n\} = 2\delta_{nm} \\ \{\beta_n, \gamma_m\} = 0 \\ i\beta_n\gamma_n = [c_n^\dagger, c_n] \end{cases}$$

The Majorana Hamiltonian reads

$$H = -iJ \sum_n \beta_n \gamma_{n+1} + ih \sum_n \beta_n \gamma_n \quad (8.6)$$

The spectrum could be solved by Fourier transformation

$$\begin{aligned} H &= -\frac{i}{2} \sum_k \beta_k \gamma_{-k} e^{ik} + \frac{i}{2} \sum_{-k} \gamma_{-k} \beta_k e^{-ik} + \frac{h}{2} \sum_k \beta_k \gamma_{-k} - \gamma_{-k} \beta_k \\ &= \frac{i}{2} \begin{pmatrix} \beta_k & \gamma_{-k} \end{pmatrix} \begin{pmatrix} 0 & -Je^{ik} + h \\ Je^{-ik} - h & 0 \end{pmatrix} \begin{pmatrix} \beta_k \\ \gamma_{-k} \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} \beta_k & \gamma_{-k} \end{pmatrix} \begin{pmatrix} 0 & J \sin k + i(h - J \cos k) \\ J \sin k - i(h - J \cos k) & 0 \end{pmatrix} \begin{pmatrix} \beta_k \\ \gamma_{-k} \end{pmatrix} \end{aligned} \quad (8.7)$$

From the Eq(8.7), we solve the eigenvalue and eigenvector

$$\varepsilon_k^\pm = \pm \sqrt{(J-h)^2 + 4Jh \sin^2 \frac{k}{2}} \quad \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-\frac{i}{2}\phi_k} \\ \pm e^{\frac{i}{2}\phi_k} \end{pmatrix} \quad (8.8)$$

The Hamiltonian in the real space could be dealt with fermions

$$\begin{aligned} H &= J \sum_n c_n c_{n+1}^\dagger - c_n^\dagger c_{n+1} + c_n^\dagger c_{n+1}^\dagger - c_n^\dagger c_{n+1} + h \sum_n c_n^\dagger c_n - c_n c_n^\dagger \\ &= J \sum_k c_k c_k^\dagger e^{-ik} - c_k^\dagger c_k e^{ik} + c_k^\dagger c_{-k}^\dagger e^{-ik} - c_k^\dagger c_{-k} e^{ik} + h \sum_k c_k^\dagger c_k - c_k c_k^\dagger \\ &= \sum_k (h - J \cos k) c_k^\dagger c_k - c_k c_k^\dagger - i \sin k \sum_k c_k^\dagger c_{-k}^\dagger + c_{-k} c_k \\ &= \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \begin{pmatrix} h - J \cos k & -iJ \sin k \\ -iJ \sin k & h - J \cos k \end{pmatrix} \begin{pmatrix} c_k^\dagger \\ c_{-k} \end{pmatrix} \end{aligned} \quad (8.9)$$

The hamiltonian could be diagonalized with fermionic Bogliubov transformation

$$\begin{pmatrix} \eta_k \\ \eta_{-k}^\dagger \end{pmatrix} = \begin{pmatrix} \cos \theta_k & i \sin \theta_k \\ -i \sin \theta_k & \cos \theta_k \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} \quad (8.10)$$

where $\tan 2\theta_k = \frac{J \sin k}{h - J \cos k}$. The hamiltonian transforms into

$$H = \sum_k \varepsilon_k [\eta_k^\dagger, \eta_k] \quad (8.11)$$

The ground state is annihilated by operator η_k

$$c_k^\dagger c_k = \left(\cos \theta_k \eta_k^\dagger - i \sin \theta_k \eta_{-k} \right) \left(\cos \theta_k \eta_k + i \sin \theta_k \eta_{-k}^\dagger \right) = \sin^2 \theta_k = \frac{1 - \cos 2\theta_k}{2} = \frac{1}{2} \left(1 - \frac{h - J \cos k}{\varepsilon_k} \right) \quad (8.12)$$

The order parameter is

$$M_z = \langle c_k^\dagger c_k \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{J \cos k - h}{\varepsilon_k} dk \quad (8.13)$$

Chapter 9

Semiconductor