Lecture 5 Interacting electron gas: random phase approximation

Lindhardt response -- beyond single electron

§1 Plasmons:

Let us consider the fluctuation of electron density in the background of positive charge background. We use the Fourier component ρ_q as collective coordinate. We first consider the long wave length limit $q \to 0$, and solve its frequency. We suppose every electron has a relative displacement respect to the background, this results in electric field $E = 4\pi\sigma = 4\pi e n x$, where n is the electron density, and x is the displacement:

$$m\ddot{x} = -4\pi e n x \quad \Rightarrow \quad \omega_p^2 = \frac{4\pi n e^2}{m}$$

Let us compare $\hbar\omega_p$ with Rydberg energy $E_R = \frac{me^4}{\hbar^2}$

$$\Rightarrow \hbar\omega_p / E_R = \sqrt{4\pi}\,(n a_0^3)^{1/2}, \quad \text{where } a_0 = \frac{\hbar^2}{me^2} \text{ is the Bohr radius.}$$

in metal $n^{1/3} a_0 \approx 0.1 \sim 1$

$\Rightarrow \hbar\omega_p$ is a very large energy scale $5 \sim 30\,eV$.

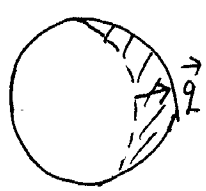
§2. particle-hole continuum:

$$C^\dagger_{k+q\,\sigma} C_{k\sigma}$$

Let's consider an excitation of moving an electron at $\vec{k}$ (inside the FS) to $\vec{k}+\vec{q}$ (outside the FS)

the excitation energy is $\hbar\omega_{kq} = \frac{\hbar^2}{2m}(q^2 + 2\vec{k}\cdot\vec{q})$

① For $q < 2k_F$,

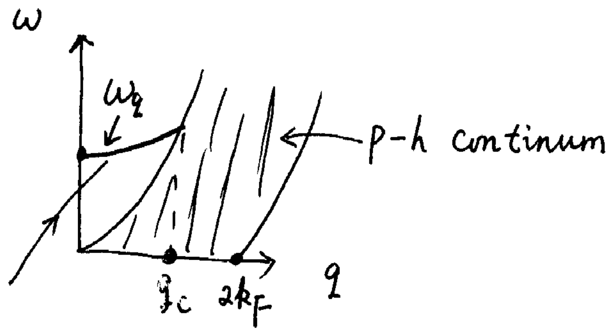


only particle inside the shaded area can be excited, $\omega_{kq,\max} = \frac{\hbar^2}{2m}(q^2 + 2kq)$

$\omega_{kq\,\min} = 0$

② For $q > 2k_F$, all the particle can be excited to creat p-h excitation.

$$\hbar\omega_{kq,\max} = \frac{\hbar^2}{2m}(q^2+2kq) \qquad \hbar\omega_{k,q\,\min} = \frac{\hbar^2}{2m}(q^2-2kq)$$



dispersion of plasmons.

At $q < q_c$, plasmon excitation lies outside the p-h continuum. it is not damped.

At $q > q_c$, plasmon can decay into p-h continuum.

§3: Random phase approximation:

$$H = -\sum_{i=1}^{N}\frac{\hbar^2\nabla_i^2}{2m} + \frac{1}{2}\sum_{ij}{}'\frac{e^2}{|r_i-r_j|} + H_{\text{positive charge background}}$$

Expand Coulomb interaction by using Fourier transform

$$\frac{1}{2}\sum_{i\neq j}\frac{e^2}{|r_i-r_j|} = \frac{1}{2}\sum_q\sum_{i\neq j} v(q)\, e^{i\vec{q}\cdot(\vec{r}_i-\vec{r}_j)} = \frac{1}{2}\sum_q v(q)\Big[\sum_i e^{i\vec{q}\cdot\vec{r}_i}\sum_j e^{-i\vec{q}\cdot\vec{r}_j} - N\Big]$$

$$= \frac{1}{2}\sum_q v(q)\left[\rho_q^{+}\rho_q - N\right]$$

where $\rho_q = \sum_j e^{-iq\cdot r_j}$, i.e $\rho(r) = \sum_{i=1}^{N}\delta(r-r_i)$

the $q=0$ component $\rho_{q=0} = N$, $\Rightarrow \frac{V(0)}{2}[N^2-N]$, this term should just cancel the positive background charge. From now on, we should get rid of the $q=0$ component.

Change to the 2nd quantization

$$\rho_q = \sum_{k\sigma} C^{\dagger}_{k-q,\sigma} C_{k\sigma} \qquad \rho_{-q} = \sum_{k,\sigma} C^{\dagger}_{k\sigma} C_{k\pm q,\sigma}\,, \quad \rho(r) = \frac{1}{V}\sum_q e^{-iqr}\rho(q)$$

$$\boxed{H = \sum_{k\sigma}(\varepsilon_{k\sigma}-\mu)\, C^{\dagger}_{k\sigma} C_{k\sigma} + \frac{1}{2V}\sum_{kk'}\sum_{q\neq 0}\frac{4\pi e^2}{q^2}\, C^{\dagger}_{k+q,\sigma} C^{\dagger}_{k'-q,\sigma'} C_{k',\sigma'} C_{k,\sigma}}$$

Equation of motion analysis

$$\rho^{\dagger}_q = \sum_k \rho^{\dagger}_{kq,\sigma} = \sum_k C^{\dagger}_{k+q_\sigma} C_{k\sigma}\,, \qquad \rho_{kq} = \sum_k C^{\dagger}_{k-q} C_k$$

$$[H, \rho^{\dagger}_q] = \sum_k [H, \rho_{kq}] = \sum_k [H_0, \rho^{\dagger}_{kq}] + \sum_k [H_{int}, \rho^{\dagger}_{kq}]$$

$$[H_0, \rho^{\dagger}_{kq,\sigma}] = \left\{\frac{\hbar^2}{2m}(k+q)^2 - \frac{\hbar^2}{2m}k^2\right\}\rho_{kq,\sigma} = \hbar\omega_{k+q}\, \rho^{\dagger}_{kq,\sigma}$$

$$[H_{int}, \rho^{\dagger}_{k+q_\sigma}] = \sum_{q'} \frac{1}{2} V(q')\left\{[\rho^{\dagger}_{q'}, \rho^{\dagger}_{kq_\sigma}]\rho_{q'} + \rho^{\dagger}_{q'}[\rho_{q'}, \rho^{\dagger}_{k+q_\sigma}]\right\}$$

$$= \sum_{q'} \frac{1}{2} V(q')\left\{[\rho_{q'}, \rho^{\dagger}_{kq_\sigma}]\rho^{\dagger}_{q'} + \rho^{\dagger}_{q'}[\rho_{q'}, \rho_{k+q_\sigma}]\right\}$$

$$[\rho_{q'}, \rho^{\dagger}_{kq,\sigma}] = [\sum_{k'} C^{\dagger}_{k'-q',\sigma} C_{k'_\sigma}, C^{\dagger}_{k+q_\sigma} C_{k_\sigma}] = C^{\dagger}_{k+q-q'_\sigma} C_{k_\sigma} - C^{\dagger}_{k+q_\sigma} C_{k+q'_\sigma}$$

$$\Rightarrow [H, \rho^{\dagger}_{kq,\sigma}] = \hbar\omega_{kq}\,\rho^{\dagger}_{kq} + \frac{1}{2}V(q)\{(C^{\dagger}_{k_\sigma}C_{k_\sigma} - C^{\dagger}_{k+q_\sigma}C_{k+q_\sigma})\,\rho^{\dagger}_q + \rho^{\dagger}_q(C^{\dagger}_{k_\sigma}C_{k\sigma} - C^{\dagger}_{k+q_\sigma}C_{k+q_\sigma})\}$$

$$+ \frac{1}{2}\sum_{q'\neq q} V(q')\left\{(C^{\dagger}_{k+q-q'_\sigma}C_{k_\sigma} - C^{\dagger}_{k+q_\sigma}C_{k+q'_\sigma})\,\rho^{\dagger}_{q'} + \rho^{\dagger}_{q'}(C^{\dagger}_{k+q-q'_\sigma}C_{k_\sigma} - C^{\dagger}_{k+q_\sigma}C_{k+q'_\sigma})\right\}$$

the second summation represents the coupling between electron-hole excitations with different momentum. This coupling will be neglected basing on the following argument:

$\rho_q = \sum_j e^{-iq\cdot r_j}$ is a summation of phases, which are "random" at high densities.

thus $\rho_{q'}\rho_{q-q'}$ compared to $\rho_q \rho_{q-q} = \rho_q N$ is small. This approximation

is called RPA.

We futher replace $C^\dagger_{k\sigma} C_{k\sigma} - C^\dagger_{k+q\sigma} C_{k+q\sigma}$ with their expectation value

$$\Rightarrow [H, \rho^\dagger_{kq,\sigma}] = \hbar\omega_{kq}\rho^\dagger_{kq,\sigma} + V(q)(n_k - n_{k+q})\,\rho^\dagger{}_q$$

Let me assume the eigen operator is a linear superposition of $\rho^\dagger_{kq}$

$\sum a_{k\sigma}\rho^\dagger_{kq,\sigma}$, which satisfies $[H, \sum_{k\sigma} a_{k\sigma}\rho^\dagger_{kq,\sigma}] = \hbar\omega \sum_{k\sigma} a_{k\sigma}\rho^\dagger_{kq,\sigma}$

$$\Rightarrow \sum_{k\sigma} \hbar\omega_{kq}\underset{a_{k\sigma}}{\rho^\dagger_{kq,\sigma}} + \sum_{k\sigma} V(q)(n_k - n_{k+q})\,a_{k\sigma}\,\rho^\dagger_q = \hbar\omega\sum_{k\sigma} a_{k\sigma}\rho^\dagger_{kq,\sigma}$$

$$\Rightarrow \sum_{k\sigma}\left\{\hbar\omega_{kq}a_{k\sigma} + \sum_{k'\sigma'} V(q)(n_{k'} - n_{k'+q})a_{k'\sigma'}\right\}\rho^\dagger_{kq,\sigma} = \hbar\omega\sum_{k\sigma} a_{k\sigma}\rho^\dagger_{kq,\sigma}$$

i.e. $\hbar\omega_{kq}a_{k,\sigma} + \sum_{k'\sigma'} V(q)(n_{k'} - n_{k'+q})a_{k'\sigma'} = \hbar\omega a_{k\sigma}$

$$\frac{V(q)}{\hbar(\omega-\omega_{kq})}\sum_{k'\sigma'}(n_{k'} - n_{k'+q})a_{k'\sigma'} = a_{k\sigma}$$

$$2V(q)\sum_k \frac{(n_k - n_{k+q})}{\hbar(\omega-\omega_{kq})}\cdot\sum_{k'\sigma'}(n_{k'} - n_{k'+q})a_{k'\sigma'} = \sum_{k\sigma}(n_{k'} - n_{k'+q})a_{k\sigma}$$

$$\Rightarrow \boxed{1 + 2V(q)\sum_k \frac{n_{k+q} - n_k}{\hbar(\omega-\omega_{kq})} = 0}$$

§ dielectric function

Suppose we add an external potential

$$H_e(t) = \sum_i V_e(r_i)\, e^{-i\omega t + \eta t} = \frac{1}{V} \sum_q \left[V_e(q) e^{-i\omega t + \eta t} \right] \rho_q^{+}$$

$\Rightarrow$ ρ_q and ρ_{kq} should have the same $e^{-i\omega t + \eta t}$ dependence

$$\rho_{kq} = \sum_\sigma \rho_{kq,\sigma} \Rightarrow -i\hbar \dot{\rho}_{kq} = [H, \rho_{kq}] + [H_e(t)\, \rho_{kq}]$$

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

$$-\omega \langle \rho_{kq} \rangle_t = \frac{1}{V} V(q)\, 2(n_k - n_{k-q}) \langle \rho_q \rangle_t + \frac{2}{V} V_e(q)(n_k - n_{k-q})\, e^{-i\omega t + \eta t}$$
$$+ \hbar\omega_{k,-q} \langle \rho_{kq} \rangle_t$$

$$\Rightarrow (\hbar\omega + E_{k-q} - E_k) \langle \rho_{kq} \rangle_t + \frac{2}{V}(n_k - n_{k-q}) \left[V_e(q) e^{-i\omega t + \eta t} + V(q) \langle \rho_q \rangle_t \right) = 0$$

$$\Rightarrow \langle \rho_q \rangle_t = \sum_k \langle \rho_{kq} \rangle_t = -\sum_k \frac{2}{V} \frac{(n_k - n_{k-q})}{[\hbar\omega - (E_k - E_{k-q})]} \left\{ V_e(q) e^{-i\omega t + \eta t} + V(q) \langle \rho_q \rangle_t \right\}.$$

$$-\nabla^2 V_i(r,t) = 4\pi(-e)^2 \rho_i(r) = 4\pi(-e)^2 \sum_{q \neq 0} \langle \rho_q \rangle e^{iqr - i\omega t + \eta t}$$

$$V_i(q,t) = \frac{4\pi e^2}{q^2} \langle \rho_q \rangle_t$$

$$\Rightarrow \quad \langle \rho_q \rangle_t = -\sum_k \frac{2}{V} \frac{(n_k - n_{k-q})}{[\hbar\omega - (\varepsilon_k - \varepsilon_{k-q})]} \underbrace{\left[V_e(q,t) + V_i(q,t) \right]}_{V_{tot}(q,t)}$$

define $\chi_0(q,\omega) = \frac{2}{V}\sum_k \frac{n_{k+q} - n_k}{\hbar\omega - (\mathcal{E}_{k+q} - \mathcal{E}_k) + i\eta}$, (vaccum polarization)

$$\boxed{\langle \rho_q \rangle_t = -\chi_0(q,\omega)\, V_{tot}(q,t)}$$

$$V_{tot}(q,t) = V_e(q,t) + V_{induced}(q,t) = V_e(q,t) + \frac{4\pi e^2}{q^2}\langle \rho_q \rangle_t$$

$$= V_e(q,t) - v(q)\chi_0(q,\omega)\, V_{tot}(q,t)$$

$$V_{tot}(q,t) = V_e(q,t) \big/ [1 + v(q)\chi_0(q,\omega)]$$

Lindhard form of dielectric function (RPA approximation)

$$\boxed{\mathcal{E}(q,\omega) = 1 + v(q)\chi_0(q,\omega) = 1 + \frac{2}{V} v(q) \sum \frac{n_{k+q} - n_k}{(\hbar\omega + i\eta) - (\mathcal{E}_{k+q} - \mathcal{E}_k)}}$$

$$\nabla\cdot\vec{D} = 4\pi\rho_e, \quad \vec{D} = \vec{E} + 4\pi\vec{P} = \vec{E} + 4\pi\chi\vec{E} = \mathcal{E}\vec{E}$$

$\mathcal{E} = 1 + 4\pi\chi$ ← polarizibility

$$\vec{j} = \partial_t \vec{P}, \quad \text{i.e} \quad \vec{j}(\omega) = -i\omega P(\omega) = -i\,\omega\chi(\omega)\vec{E}(\omega)$$

$$= \frac{-i}{4\pi}[\mathcal{E} - 1]\,\omega\,\vec{E}(\omega)$$

or $\sigma(\omega) = \frac{-i}{4\pi}(\mathcal{E} - 1)\,\omega$, i.e $\boxed{\mathcal{E}(\omega) = 1 + \frac{4\pi\sigma(\omega)}{\omega} i}$

$$\mathcal{E}_1(q,\omega) = \mathrm{Re}\,\mathcal{E}(q,\omega) = 1 + \frac{2}{V} v(q) \sum_k P\left(\frac{n_{k+q} - n_k}{\hbar\omega - (\mathcal{E}_{k+q} - \mathcal{E}_k)}\right) \leftarrow \text{Principle value}$$

$$\mathcal{E}_2(q,\omega) = \mathrm{Im}\,\mathcal{E}(q,\omega) = \frac{2\pi v(q)}{\hbar} \sum_k n_k \left\{ \delta[\omega - (\omega_{k+q} - \omega_k)] - \delta(\omega + [\omega_{k+q} - \omega_k]) \right\}$$