

Lecture 10 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 $q \rightarrow 0$, and solve its frequency. We suppose every electron has a relative displacement respect to the background, this results in electric field $E = 4\pi\sigma = 4\pi enx$, where n is the electron density, and x is the displacement:

$$m\ddot{x} = -4\pi enx \Rightarrow \omega_p^2 = \frac{4\pi ne^2}{m}$$

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

$$\Rightarrow \hbar\omega_p/E_R = \sqrt{4\pi} (na_0^3)^{1/2}, \text{ where } a_0 = \frac{\hbar^2}{me^2} \text{ is the Bohr radius.}$$

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

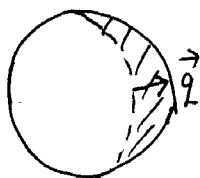
$\Rightarrow \hbar\omega_p$ is a very large energy scale $5 \sim 30 \text{ eV}$.

§2. particle-hole continuum: $C_{k+q} + C_k$

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

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

① For $q < 2k_f$,



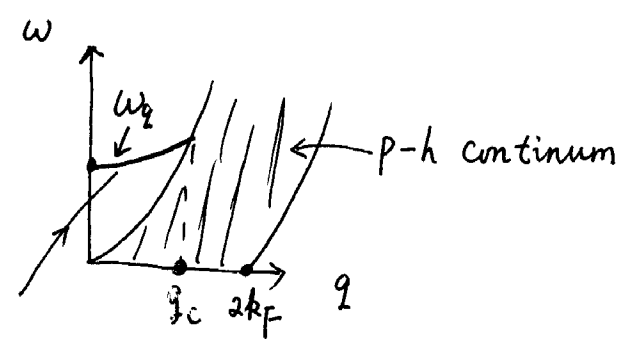
only particle inside the shaded area

can be excited, $\omega_{kq, \text{max}} = \frac{\hbar^2}{2m} (q^2 + 2kq)$

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

② For $q > 2k_F$, all the particles can be excited to create p-h

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



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:

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

Expand Coulomb interaction by using Fourier transform

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

where $P_q = \sum_j e^{-i\vec{q} \cdot \vec{r}_j}$, i.e. $\rho(r) = \sum_{i=1}^N \delta(r - r_i)$

the $q=0$ component $P_{q=0} = N$, $\Rightarrow \frac{V(0)}{2} [N^2 - N]$, this term

should just cancel the positive background charge. From now on,

we should get rid of the $q=0$ component.

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Change to ^{the} 2nd quantization

$$P_q = \sum_{k\sigma} C_{k-q,\sigma}^\dagger C_{k\sigma} \quad P_{-q} = \sum_{k,\sigma} C_{k\sigma}^\dagger C_{k+q,\sigma} \quad \rho(r) = \frac{1}{V} \sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}} \rho(\mathbf{q})$$

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

Equation of motion analysis

$$P_q^\dagger = \sum_{\mathbf{k}} P_{\mathbf{k}\mathbf{q},\sigma}^\dagger = \sum_{\mathbf{k}} C_{\mathbf{k}+\mathbf{q},\sigma}^\dagger C_{\mathbf{k}\sigma} \quad , \quad P_{\mathbf{k}\mathbf{q}} = \sum_{\mathbf{k}} C_{\mathbf{k}-\mathbf{q}}^\dagger C_{\mathbf{k}}$$

$$[H, P_q^\dagger] = \sum_{\mathbf{k}} [H, P_{\mathbf{k}\mathbf{q}}^\dagger] = \sum_{\mathbf{k}} [H_0, P_{\mathbf{k}\mathbf{q}}^\dagger] + \sum_{\mathbf{k}} [H_{\text{int}}, P_{\mathbf{k}\mathbf{q}}^\dagger]$$

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

$$[H_{\text{int}}, P_{\mathbf{k}+\mathbf{q}}^\dagger] = \sum_{\mathbf{q}'} \frac{1}{2} V(\mathbf{q}') \left\{ [P_{\mathbf{q}'}^\dagger, P_{\mathbf{k}\mathbf{q}}^\dagger] P_{\mathbf{q}'} + P_{\mathbf{q}'}^\dagger [P_{\mathbf{q}'}^\dagger, P_{\mathbf{k}+\mathbf{q}}^\dagger] \right\}$$

$$= \sum_{\mathbf{q}'} \frac{1}{2} V(\mathbf{q}') \left\{ [P_{\mathbf{q}'}^\dagger, P_{\mathbf{k}\mathbf{q}}^\dagger] P_{\mathbf{q}'}^\dagger + P_{\mathbf{q}'}^\dagger [P_{\mathbf{q}'}^\dagger, P_{\mathbf{k}+\mathbf{q}}^\dagger] \right\}$$

$$[P_{\mathbf{q}'}^\dagger, P_{\mathbf{k}\mathbf{q},\sigma}^\dagger] = \left[\sum_{\mathbf{k}'} C_{\mathbf{k}'-\mathbf{q}',\sigma}^\dagger C_{\mathbf{k}'\sigma}, \sum_{\mathbf{k}} C_{\mathbf{k}+\mathbf{q},\sigma}^\dagger C_{\mathbf{k}\sigma} \right] = C_{\mathbf{k}+\mathbf{q}-\mathbf{q}',\sigma}^\dagger C_{\mathbf{k}\sigma} - C_{\mathbf{k}+\mathbf{q},\sigma}^\dagger C_{\mathbf{k}+\mathbf{q}',\sigma}$$

$$\Rightarrow [H, P_{\mathbf{k}\mathbf{q},\sigma}^\dagger] = \hbar \omega_{\mathbf{k}\mathbf{q}} P_{\mathbf{k}\mathbf{q},\sigma}^\dagger + \frac{1}{2} V(\mathbf{q}) \left\{ (C_{\mathbf{k}\sigma}^\dagger C_{\mathbf{k}\sigma} - C_{\mathbf{k}+\mathbf{q},\sigma}^\dagger C_{\mathbf{k}+\mathbf{q},\sigma}) P_{\mathbf{q}}^\dagger + P_{\mathbf{q}}^\dagger (C_{\mathbf{k}\sigma}^\dagger C_{\mathbf{k}\sigma} - C_{\mathbf{k}+\mathbf{q},\sigma}^\dagger C_{\mathbf{k}+\mathbf{q},\sigma}) \right\}$$

$$+ \frac{1}{2} \sum_{\mathbf{q}' \neq \mathbf{q}} V(\mathbf{q}') \left\{ (C_{\mathbf{k}+\mathbf{q}-\mathbf{q}',\sigma}^\dagger C_{\mathbf{k}\sigma} - C_{\mathbf{k}+\mathbf{q},\sigma}^\dagger C_{\mathbf{k}+\mathbf{q}',\sigma}) P_{\mathbf{q}'}^\dagger + P_{\mathbf{q}'}^\dagger (C_{\mathbf{k}+\mathbf{q}-\mathbf{q}',\sigma}^\dagger C_{\mathbf{k}\sigma} - C_{\mathbf{k}+\mathbf{q},\sigma}^\dagger C_{\mathbf{k}+\mathbf{q}',\sigma}) \right\}$$

the second summation represents the coupling between electron-hole excitations with different momentum. This coupling will be neglected based

on the following argument:

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

thus $P_q \cdot P_{2-q}$ compared to $P_q P_{2-q} = P_q N$ is small. This approximation is called RPA.

We further replace $C_k^\dagger C_{k-\sigma} - C_{k+q}^\dagger C_{k+q-\sigma}$ with their expectation value

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

Let me assume the eigen operator is a linear superposition of P_{kq}^\dagger

$$\sum_{k\sigma} a_{k\sigma} P_{kq, \sigma}^\dagger, \text{ which satisfies } [H, \sum_{k\sigma} a_{k\sigma} P_{kq, \sigma}^\dagger] = \hbar \omega \sum_{k\sigma} a_{k\sigma} P_{kq, \sigma}^\dagger$$

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

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

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

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

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

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

§ dielectric function

Suppose we add an external potential

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

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

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

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

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

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

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

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

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

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

define $\chi_0(q, \omega) = \frac{2}{V} \sum_{\mathbf{k}} \frac{n_{\mathbf{k}+\mathbf{q}} - n_{\mathbf{k}}}{\hbar\omega - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) + i\eta}$ (vacuum polarization)

$$\langle P_{\mathbf{q}} \rangle_t = -\chi_0(q, \omega) V_{\text{tot}}(q, t)$$

$$\begin{aligned} V_{\text{tot}}(q, t) &= V_e(q, t) + V_{\text{induced}}(q, t) = V_e(q, t) + \frac{4\pi e^2}{q^2} \langle P_{\mathbf{q}} \rangle_t \\ &= V_e(q, t) - v(q) \chi_0(q, \omega) V_{\text{tot}}(q, t) \end{aligned}$$

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

Lindhard form of dielectric function (RPA approximation)

$$\epsilon(q, \omega) = 1 + v(q) \chi_0(q, \omega) = 1 + \frac{2}{V} v(q) \sum_{\mathbf{k}} \frac{n_{\mathbf{k}+\mathbf{q}} - n_{\mathbf{k}}}{(\hbar\omega + i\eta) - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})}$$

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

$$\epsilon = 1 + 4\pi \chi \leftarrow \text{polarizability}$$

$$\begin{aligned} \vec{j} &= \partial_t \vec{P}, \quad \text{i.e. } \vec{j}(\omega) = -i\omega \vec{P}(\omega) = -i \omega \chi(\omega) \vec{E}(\omega) \\ &= \frac{-i}{4\pi} (\epsilon - 1) \vec{E}(\omega) \end{aligned}$$

$$\text{or } \sigma(\omega) = \frac{-i}{4\pi} (\epsilon - 1) \omega, \quad \text{i.e. } \epsilon(\omega) = 1 + \frac{4\pi \sigma(\omega)}{\omega} i$$

$$\epsilon_1(q, \omega) = \text{Re } \epsilon(q, \omega) = 1 + \frac{2}{V} v(q) \sum_{\mathbf{k}} \mathcal{P} \left[\frac{n_{\mathbf{k}+\mathbf{q}} - n_{\mathbf{k}}}{\hbar\omega - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})} \right] \leftarrow \text{Principle value}$$

$$\epsilon_2(q, \omega) = \text{Im } \epsilon(q, \omega) = \frac{2\pi v(q)}{\hbar} \sum_{\mathbf{k}} n_{\mathbf{k}} \left\{ \delta(\omega - (\omega_{\mathbf{k}+\mathbf{q}} - \omega_{\mathbf{k}})) - \delta(\omega + (\omega_{\mathbf{k}+\mathbf{q}} - \omega_{\mathbf{k}})) \right\}$$