lecture 11 Interacting electron gas Screening

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§ Response-function approach (linear response)

Consider a many-body system with an external perturbation $H_e(t)$,

$t \to -\infty$ $H_e(t) = 0$. The Schrödinge Equation reads

$$i\hbar \frac{\partial}{\partial t} \psi = H\psi + H_e(t)\psi$$

in the interaction picture: $\psi(t) = \exp(-\frac{i}{\hbar} Ht)\, \varphi(t)$

$$i\hbar \frac{\partial \varphi(t)}{\partial t} = H_e'(t)\varphi = e^{\frac{i}{\hbar}Ht} H_e(t)\, e^{-\frac{i}{\hbar}Ht} \varphi(t)$$

the time evolution: $t \to +\infty$, $\varphi(t) = \Phi_0$ (ground state)

$$\varphi(t) = \Phi_0 + \frac{1}{i\hbar}\int_{-\infty}^{t} H_e'(t')\varphi(t')dt' \xrightarrow[\text{order}]{\text{linear}} \varphi(t) = \Phi_0 + \frac{1}{i\hbar}\int_{-\infty}^{t} H_e'(t')\Phi_0\, dt'$$

physical operator A's expectation value:

$$A(t) = e^{\frac{i}{\hbar}Ht} A\, e^{-\frac{i}{\hbar}Ht}$$

$$\bar{A} = \langle \varphi(t)|A(t)|\varphi(t)\rangle = \langle \Phi_0|A(t)|\Phi_0\rangle + \frac{1}{i\hbar}\int_{-\infty}^{t} \langle\Phi_0|[A(t), H_e'(t')]|\Phi_0\rangle\, dt'$$

$\because |\Phi_0\rangle$ is H's eigenstate $\Rightarrow \langle\Phi_0|A(t)|\Phi_0\rangle = \langle\Phi_0|A|\Phi_0\rangle$

$$\Rightarrow \boxed{\Delta A = \langle A\rangle_t - \langle A\rangle_{t=-\infty} = \frac{1}{i\hbar}\int_{-\infty}^{+\infty} dt'\, \theta(t-t')\langle\Phi_0|[A(t), H_e'(t')]|\Phi_0\rangle}$$

conside the example $H_e(t) = +\sum_q \frac{1}{V}\, \rho(-q,t)\, V_{ex}(q,t)$,

then

$$\delta\rho(q,t) = \frac{-i}{\hbar}\int_{-\infty}^{+\infty} dt'\, \theta(t-t')\, \frac{1}{V}\langle\Phi_0|\rho(q,t), \rho(-q,t')|\Phi_0\rangle V_{ex}(q,t')$$

$$= -\int_{-\infty}^{+\infty} dt'\, \chi_{ret}(q, t-t')\, V_{ex}(t')$$

thus $\boxed{\delta\rho(q\,\omega) = -\chi_{ret}(q,\omega)\; V_{ex}(q,\omega)}$

where $$\chi_{ret}(q,\omega) = \int_{-\infty}^{+\infty} dt\; e^{i(\omega + i\eta)t}\; \theta(t)\,(-)\left(\frac{-i}{\hbar}\right) \langle \Phi_0 | \rho(q\,t),\, \rho(-q,0) | \Phi_0 \rangle$$

this formula can be generalized to finite temperature, with thermal average $\langle \Phi_0 | \cdots | \Phi_0 \rangle \rightarrow \frac{1}{Z} \sum_m e^{-\beta E_m} \langle m | \cdots | m \rangle$.

The $\chi_{ret}(q,\omega)$ is the response function for interacting system. We can approximate it as follows:

$$\delta\rho(q,\omega) = -\chi_0(q,\omega)\; V_{tot}(q,\omega)$$, where χ_0 is the response of non-interacting system,

$$= -\chi_0(q,\omega)\,[\,V_{ext} + V_{ind}\,]$$

$$-\nabla^2 V_{ind} = 4\pi e^2\, \delta\rho(q,\omega) \Rightarrow V_{ind} = +\frac{4\pi e^2}{q^2}\,\delta\rho(q,\omega)$$

$$\Rightarrow \left(1 + \frac{4\pi e^2}{q^2}\chi_0(q,\omega)\right)\delta\rho(q,\omega) = -\chi_0(q,\omega)\; V_{ext}$$

$$\boxed{\chi(q,\omega) = \frac{\chi_0(q,\omega)}{1 + \frac{4\pi e^2}{q^2}\chi_0(q,\omega)}}$$ PRA response function

$$V_{tot} = V_{ext} + V_{ind} = V_{ext} - \frac{\chi_0(q\,\omega)}{1 + \frac{4\pi e^2}{q^2}\chi_0} \cdot \frac{4\pi e^2}{q^2}\, V_{ext} = \frac{V_{ext}}{1 + \frac{4\pi e^2}{q^2}\chi_0(q,\omega)}$$

$$\varepsilon(q,\omega) = 1 + \frac{4\pi e^2}{q^2}\chi_0(q,\omega)$$

Ex: prove χ_0 defined here is just the Lindhardt form!

Lecture 4: Interacting electron gas (II)

§: Static screening

$$\varepsilon(q,\omega) = 1 + \frac{2v(q)}{V}\sum_k n_k \left\{ \frac{1}{\hbar\omega_{kq} - (\hbar\omega + i\eta)} + \frac{1}{\hbar\omega_{kq} + (\hbar\omega + i\eta)} \right\}$$

$$\omega = 0 \Rightarrow \varepsilon(q,0) = 1 + \frac{2}{V} v(q) \sum_k n_k \frac{2}{E_{k+q} - E_k}$$

$$= 1 + \frac{4\pi e^2}{q^2} \sum_{k<k_F} \frac{4}{\frac{\hbar^2 k_f^2}{2m}\left[2\frac{\vec{k}}{k_f}\cdot\frac{\vec{q}}{k_f} + \left(\frac{q}{k_f}\right)^2\right]} = 1 + \frac{4\pi e^2}{q^2} \int \frac{k^2 dk}{(2\pi)^3} \int_{-1}^{1} d\cos\theta \, \frac{4\cdot 2\pi}{\varepsilon_f\left[\frac{2kq}{k_f^2}\cos\theta + \left(\frac{q}{k_f}\right)^2\right]}$$

$$= 1 + \frac{4\pi e^2}{q^2} \frac{k_f^3}{\varepsilon_f} \frac{1}{4\pi^2} \int_0^1 d\left(\frac{k}{k_f}\right)\left(\frac{k}{k_f}\right)^2 \int_{-1}^{1} d\cos\theta \, \frac{1}{\left[\frac{k}{k_f} x\cos\theta + x^2\right]} \qquad \left(x = \frac{q}{2k_f}\right)$$

$$= 1 + \frac{4\pi e^2}{q^2} N_0 \left[\frac{1}{2} + \frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right|\right]$$

① $q \to 0$, Thomas-Fermi Screening (N_0: density of states at FS)

$$\varepsilon(q) = 1 + \frac{4\pi e^2 N_0}{q^2}$$

$$V(q) = \frac{V_0(q)}{\varepsilon(q)} = \frac{4\pi e^2}{q^2} \Big/ 1 + \frac{4\pi e^2 N_0}{q^2} = \frac{4\pi e^2}{q^2 + (1/\lambda)^2}$$

$$\longrightarrow V(r) = \frac{e^{-\lambda r}}{r}$$

T-F $\quad -\nabla^2 V(r) = 4\pi(\rho_{ex} + \rho_{ind})e^2$

$$\rho_{ind} = -\left(\frac{\partial n}{\partial \mu}\right)\cdot V(r)$$

$$n(\mu = \mu_0 - V) - n(\mu) = -\frac{\partial n}{\partial \mu}\cdot V$$

the change of band bottom energy

$$\Rightarrow \left[-\nabla^2 + \left(\frac{\partial n}{\partial \mu}\right)4\pi e^2\right] V(r) = 4\pi e^2 \rho_{ex}$$

$$\Rightarrow V(r) = \frac{4\pi e^2}{q^2 + (1/\lambda)^2}$$

$$N_0 = 2\int \frac{d^3k}{(2\pi)^3}\,\delta\!\left(\varepsilon - \frac{\hbar^2 k^2}{2m}\right) = \frac{4\pi k_F^2}{\hbar^2 k_F/m}\;\frac{2}{8\pi^3} = \frac{m\,k_F}{\pi^2\hbar^2}$$

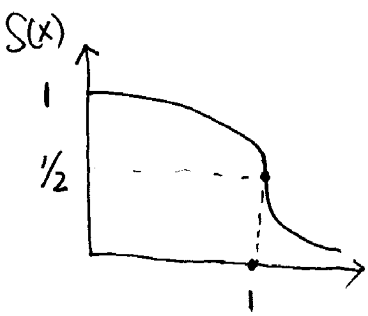
$$\lambda = \left(4\pi e^2 N_0\right)^{-1/2} \qquad \lambda\cdot k_F = \frac{1}{\left[4\pi e^2 \frac{m}{\pi^2\hbar^2 k_F}\right]^{1/2}}$$

$$\boxed{\lambda\cdot k_F = \frac{1}{\sqrt{4/\pi}}\;\frac{1}{\left[e^2\cdot k_F\Big/\frac{\hbar^2 k_F^2}{m}2\right]^{1/2}} \sim \sqrt{\frac{E_K}{E_{int}}}} \Rightarrow \boxed{\lambda \sim \sqrt{r_s}}$$

T-F screening length is at the order of $1/k_F$.

2 Friedel oscillation and Kohn's anomaly.

$$\varepsilon(q,0) = 1 + \frac{\lambda^2}{q^2}\,S\!\left(\frac{q}{2k_F}\right), \quad S(x) = \frac{1}{2}\left[1 + \frac{1-x^2}{2x}\ln\left|\frac{1-x}{1+x}\right|\right]$$



at $\boxed{x = \frac{q}{2k_F} \approx 1 \text{ S(x) has a sudden drop.}}$

(because $\omega_{in} = \frac{\hbar}{2m}\left[(\vec{k}-\vec{q})^2 - \vec{k}^2\right] > 0$ at $q > 2k_F$.

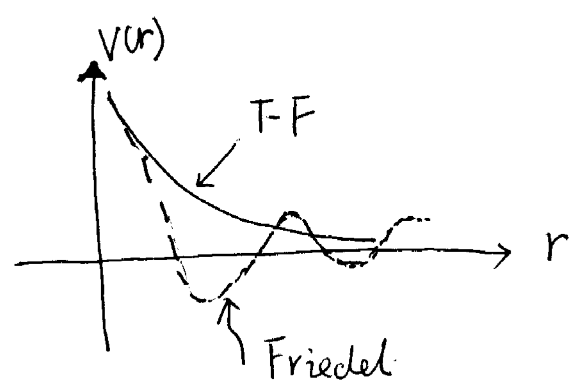
$$V(r) = \int d^3\vec{q}\; e^{i\vec{q}\cdot\vec{r}}\,\frac{4\pi Z e^2}{q^2 + \lambda^2 S\!\left(\frac{q}{2k_F}\right)}$$

screening potential by a charge impurity Ze

uncontinuity from the Fermi surface.

at $r \to +\infty$

$$V(r) \sim \text{const}\,\frac{\cos 2k_F r}{r^3}$$



b) at small wavevector $q/k_F \ll 1$

$$n(\vec{k}+\vec{q}/2) - n(\vec{k}-\vec{q}/2) = + \frac{\partial n}{\partial \mathcal{E}} \cdot v_F q\cos\theta = \delta(\mathcal{E})\, v_F q\cos\theta$$

$$S = \frac{\omega}{v_F q}$$

$$\chi_0(q,\mathcal{E}) = \frac{1}{(2\pi)^3}\, 2\int d\cos\theta \int d\varphi \int k_F^2\, dk\, \frac{(-)\, v_F q\cos\theta \;\; \delta(\mathcal{E}-\mathcal{E}(k))}{\omega - v_F q\cos\theta + i\eta}$$

$$= N_0 \int \frac{d\cos\theta\, d\varphi}{4\pi} \frac{v_F q\cos\theta}{\omega - v_F q\cos\theta + i\eta} = \frac{1}{2} N_0 \int_{-1}^{1} d\cos\theta \frac{-\cos\theta}{s - \cos\theta + i\eta}$$

$$\boxed{\begin{aligned} \mathrm{Re}\,\chi_0(q,\mathcal{E}) &= N_0\left[1 - \frac{S}{2}\ln\left|\frac{1+S}{1-S}\right|\right] \\ \mathrm{Im}\,\chi_0(q,\mathcal{E}) &= \begin{cases} \frac{\pi}{2} N_0 S & \text{for } 1 > S > -1 \\ 0 & \text{otherwise} \end{cases} \end{aligned}}$$

$$\chi_0(q,\mathcal{E}) = N_0 \cdot \begin{cases} 1 - s^2 + i\frac{\pi}{2} s\, \Theta(s<1) & (s \ll 1) \\ -\frac{1}{3}s^2 - \frac{1}{5}s^4 \cdot & (s \gg 1) \end{cases}$$

plasmon regime, $s \gg 1$

$$\mathcal{E}(q,\omega) = 1 + \frac{4\pi e^2}{q^2} N_0\left(-\frac{1}{3}s^2 - \frac{1}{5}s^4\right) = 1 - \underbrace{4\pi e^2}_{N_0}\left(\frac{v_F^2}{\omega^2} + \frac{3 v_F^4 q^2}{5\omega^4}\right)$$

$$= 1 - \left(\frac{\omega_p^2}{\omega^2} + \frac{3}{5}\frac{\omega_p^2 (v_F q)^2}{\omega^4}\right]$$

$$\Rightarrow \boxed{\frac{\omega^2}{\omega_p^2} = 1 + \frac{3}{10}\left(\frac{v_F q}{\omega_p}\right)^2}$$ no-damping!

$\boxed{\text{plasmon}}$

§: electron - electron interaction

Not only the external potential but also the interaction between electrons in renormalized into

$$V_{eff}(q,\omega) = \frac{4\pi e^2}{q^2 + 4\pi e^2 \chi_0(q,\omega)}, \quad \text{the HF difficulty}$$

$$\delta \varepsilon_{HF}(k) \to -\sum_q n_{k+q} \frac{4\pi e^2}{q^2 + 4\pi e^2 \chi_0(q,0)}$$

, then the exchange interaction is reduced!

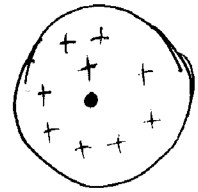
§: Wigner crystal:

$E_K \propto k_F^2$, $E_{int} \propto e^2/l \propto k_F$. define dimensionless parameter

$$r_s = \frac{E_{int}}{E_K} = \frac{\frac{e^2}{l}}{\frac{\hbar^2}{ml^2}} = \frac{l}{\frac{\hbar^2 e^2}{m}} \sim \frac{l}{a_0}$$

at low density region; $r_s \gg 1$, E_{int} is much stronger than E_K.

The above pertubative picture stop working. Electron starts to form regular crystal. In 3D, electrons form fcc lattice. In 2D electrons form triangular lattice.



vibration frequency.

$$E \cdot 4\pi \cdot r^2 = 4\pi \cdot \frac{4\pi}{3}\rho r^3$$

$$E = \frac{4\pi}{3}\rho r = \frac{4\pi}{3} \frac{e}{\frac{4\pi}{3} r_0^3} r = \frac{e}{r_0^3} r \Rightarrow \boxed{\omega^2 = \frac{e^2}{m(r_s a_0)^3} = \frac{1}{3}\omega_p^2}$$