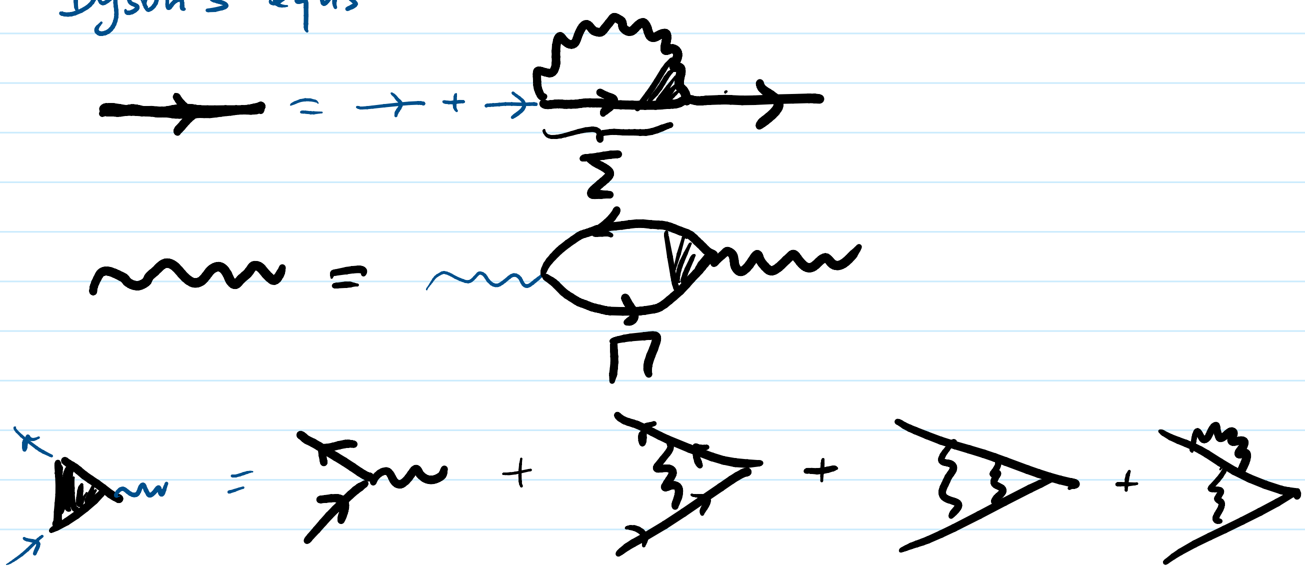
Lecture 4 - Polarisation operator. Plasmons. RKKY interaction.

22 February 2023 14:00

Last time:

Dyson's eqns



In case of Coulomb,

$$V = \frac{\tilde{e}^2}{\varepsilon r},$$

$$r_s = \frac{V}{T} \sim \frac{\lambda_F}{a_B}$$ is the parameter that allows to choose leading diagrams when it's small.

Today: <u>Coulomb</u>:

1. Diagrams for GS energy
2. Polarisation operator
3. Effective excitations (quasiparticles).
4. RKKY

① $E = \langle 0|\hat{H}|0\rangle = \langle 0|H_0 + H_{int}|0\rangle$

We had $S = S_0 + S_{int}$

We again expand $e^{iS_{int}} = \sum_{n=0}^{\infty} \frac{(iS_{int})^n}{n!}$

$S_{int} = \frac{1}{2}\int_{xx'} \bar{\psi}\bar{\psi} V \psi\psi$

Averaging $\equiv$ connecting $\bar{\psi}$-ψ pairs in all possible ways.

This gives the partition f-n, Z.

$\ln Z$ contains all connected diagrams

In stat. phys., we had

$$E = -\frac{d\ln Z}{d\beta}, \quad \beta = \frac{1}{kT}.$$

To have the analogue of β, we change

$$\hat{H}_{int} \to \lambda H_{int}, \text{ where } \lambda \in [0,1].$$

$\ln Z$ diagrams by themselves are not graphically summable:

when we consider all closed connected diagrams like

 etc,

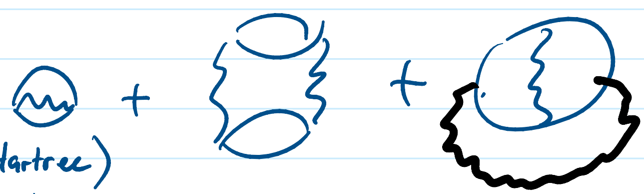
we have only $(n-1)!$ relevant permutation of S_{int} in the n^{th} order.

Consider $\left\langle \int_0^1 \frac{d\lambda}{\lambda} (\lambda S_{int})^n \right\rangle = \int_0^1 \lambda^{n-1} S_{int}^n \, d\lambda = \frac{1}{n}\langle S_{int}^n \rangle$

Then, the energy is obtained by

$$E = -\frac{d\ln Z}{d\lambda}.$$

This is called the adiabatic switching on the interaction.

$\langle H_{int} \rangle =$  $+ \dots$

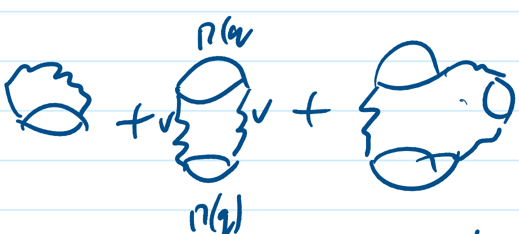
(Hartree)
Fock
approximation

Hartree:  $\rightarrow 0$

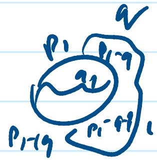
For Coulomb, $V(\underline{q}) = \frac{4\pi e^2}{q^2}$

It's divergent in the longwave limit, $q \to 0$

The most divergent in a given perturbative order, diagrams a those with simple bubbles:

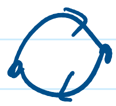
 $+ \dots$ most divergent diagrams.

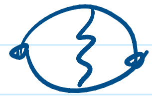
$\sim \frac{1}{q^4}$ $\qquad \sim \frac{1}{q^6}$

while 

$\rightarrow$ two q integrals divergent when $q \to 0$ and $q_1 \to 0$, but two q-integrations.

Alternatively,

$\Pi =$ 

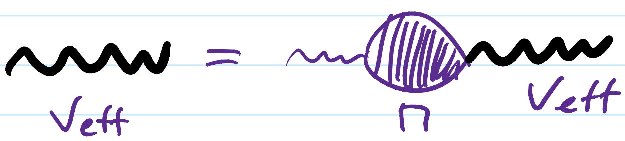
$+$ 

$+ \; + \; \cdots$

$\downarrow$

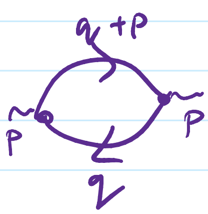
power-law estimate gives that $\frac{\Pi_1}{\Pi_0} \sim r_s$

In $r_s \ll 1$ limit, we can reduce Π to Π_0.



$$\Rightarrow \quad V_{eff}(q) = \frac{V_0}{1 - V_0 \Pi} \rightarrow \frac{V_0}{1 - V_0 \Pi_0}$$

Calculating even Π_0 gives a lot information.

$\Pi_0(p) =$ 

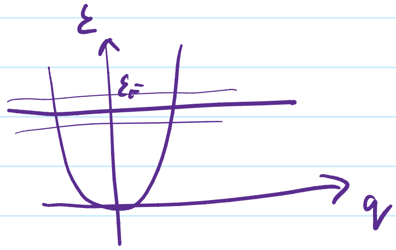
$= -2 \int G_0(q) G_0(p+q)\, dq$

$\uparrow$ Fermionic loop $\quad \uparrow$ spin

For electrons in metals (semiconductors)

$$G(q) = \frac{1}{\varepsilon - \xi_q + i\delta\,\mathrm{sgn}\,\varepsilon}\,; \qquad \xi_q = \varepsilon_q - \varepsilon_F = \frac{q^2}{2m} - \frac{p_F^2}{2m}$$

$$\mathrm{sgn}\,\varepsilon = \mathrm{sgn}\,\xi_q$$

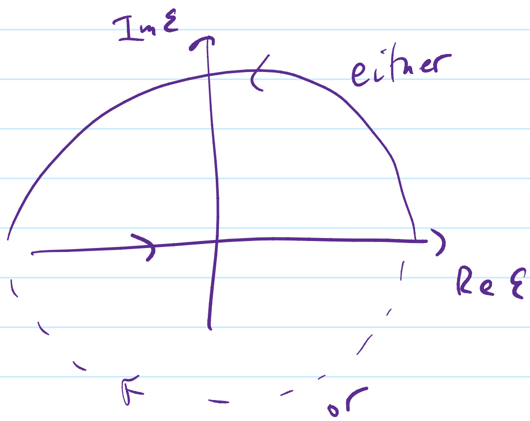


$$p \equiv \underline{p}, \omega$$

$$q \equiv \underline{q}, \varepsilon \quad \| \quad d\vec{q} = \frac{d^d q}{(2\pi)^d}$$

$$-i\Pi(p) = 2\int d\vec{q}\,\frac{d\varepsilon}{2\pi}\,\frac{1}{\varepsilon - \xi_{\underline{q}} + i\delta\,\mathrm{sgn}\,\xi_{\underline{q}}}\;\frac{1}{\omega + \varepsilon - \xi_{\underline{q}+\underline{p}} + i\delta\,\mathrm{sgn}\,\xi_{\underline{q}+\underline{p}}}$$

We should always integrate over ε first.



If both $\xi_{\underline{q}}$ & $\xi_{\underline{q}+\underline{p}}$ have the same sign, then both poles are in the same half-plane — close in the opposite half-plane to get $\int = 0$.

Hence, the signs are opposite, e.g.

$$\frac{q^2}{2m} - \varepsilon_F < 0 \quad \text{but} \quad \frac{(\underline{q}+\underline{p})^2}{2m} - \varepsilon_F > 0$$

or other way around.

This means that $\int$ is proportional to $n_{\underline{p}+\underline{q}} - n_{\underline{q}}$

where n is the Fermi distribution $= \Theta$-f-n at $T=0$.

Hence, we make the pole integration over ε to get

$$\Pi = -2 \int d\underline{q} \, \frac{n_{\underline{p}+\underline{q}} - n_{\underline{q}}}{\omega + \xi_{\underline{q}} - \xi_{\underline{q}+\underline{p}} + i\delta \, \mathrm{sgn}\, \omega}$$

(the "i" factor should be in the original expression for Π).

Let's see how small ω, p work:

$\omega \ll \varepsilon_F$, $|\underline{p}| \ll p_F$

Then, $n_{\underline{p}+\underline{q}}$ can be Taylor-expanded in small $|\underline{p}|$:

$$n_{\underline{p}+\underline{q}} = n_{\underline{q}} + \underline{p} \cdot \frac{\partial n_{\underline{q}}}{\partial \underline{q}}\Big|_{p=0} + \dots$$

$$= n_{\underline{q}} + \underline{p} \cdot \underbrace{\frac{\partial n_q}{\partial \varepsilon_q}}_{= \frac{1}{v_F}\delta(|\underline{q}| - p_F)} \cdot \frac{\partial \varepsilon_{q+p}}{\partial \underline{q}}\Big|_{p=0};$$

$\varepsilon_{q+p} = \dfrac{q^2 + 2\underline{p}\cdot\underline{q} + p^2}{2m}$

$\dfrac{\partial \varepsilon}{\partial \underline{q}} \approx \varepsilon_{q+p} - \varepsilon_p \approx$

$\approx \dfrac{\underline{p}\cdot\underline{q}}{m}$, neglecting small $\dfrac{p^2}{2m}$.

$$\left(\frac{q^2}{2m} - \frac{p_F^2}{2m} = \frac{(q - p_F)(q + p_F)}{2m} \approx \frac{p_F}{m}(q - p_F) = v_F (q - p_F) \right)$$

$$\therefore \quad n_{\underline{p}+\underline{q}} - n_{\underline{q}} = \frac{\underline{q}\cdot\underline{p}}{m v_F} \delta(q - p_F) \underset{\text{in 3D}}{=}$$

$$= \frac{q p \cos\theta}{p_F}\,\delta(q-p_F) = p\cos\theta\,\delta(q-p_F).$$

Hence, $$\Pi_0 = -2\int_0^\infty \frac{q^2\,dq}{(2\pi)^3}\int_0^{2\pi} d\varphi \int_0^\pi \sin\theta\,d\theta\;\frac{p\cos\theta\,\delta(q-p_F)}{\omega + (\varepsilon_q - \varepsilon_{p+q}) + i\delta\,\mathrm{sgn}\,\omega}$$

$$\eta \equiv \cos\theta$$

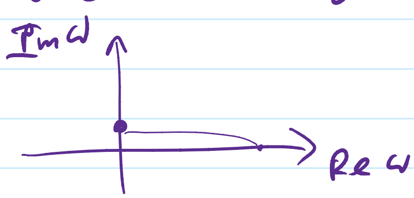
$$= -2\,\frac{p_F^2}{(2\pi)^2}\int_{-1}^{1} d\eta\,\frac{1}{v_F}\,\frac{\omega - p\eta v_F - \omega}{\omega - v_F p\eta + i\delta\,\mathrm{sgn}\,\omega}$$

$$= -2\,\underbrace{\frac{2 m v_F}{2\pi^2}}_{\equiv \nu_0}\left[1 + \frac{\omega}{2 v_F p}\ln\frac{\omega - p v_F + i\delta\,\mathrm{sgn}\,\omega}{\omega + p v_F + i\delta\,\mathrm{sgn}\,\omega}\right]$$

DoS for spinless el

We have $\ln z = \ln|z|e^{i\arg z}$ where $z = |z|e^{i\arg z}$

$$\arg(\omega + p_F + i\delta\,\mathrm{sgn}\,\omega) = \frac{\pi}{2}\,\mathrm{sgn}\,\omega$$



Similar for $\arg(\omega - p_F + i\delta\,\mathrm{sgn}\,\omega)$ but

when $0 < \omega < p_F$, the argument is $\frac{3\pi}{2}$.

The result is

$$\Pi = -\nu_0\left\{1 + \frac{\omega}{v_F p}\left[\ln\left|\frac{\omega - v_F p}{\omega + v_F p}\right| + i\pi\,\Theta(v_F p - \omega)\right]\right\}$$

When $\omega < v_F p$, there's imaginary part in Π.

$$V_{eff}(\omega,p) = \frac{V_0}{1 - V_0 \Pi} = \frac{1}{V_0^{-1} - \Pi} = \frac{1}{\frac{p^2}{4\pi} - e^2 \Pi(p,\omega)}$$

When $\mathrm{Im}\,\Pi = 0$, we have the pole at

$$p^2 = 4\pi e^2 \, \Pi(p,\omega).$$

Although both ω and $v_F p$ are small, there are opposite limits for $\left|\frac{\omega}{v_F p}\right|$.

For $\omega \gg v_F p$, we have

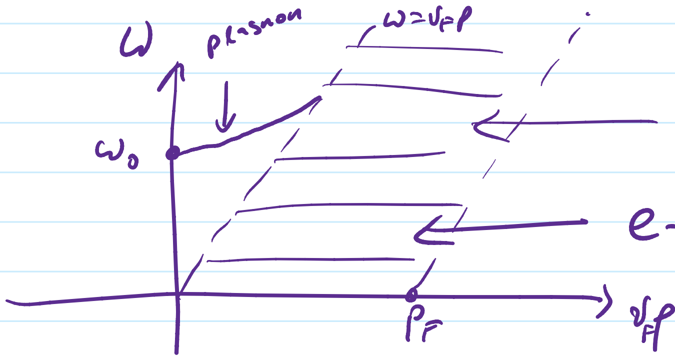
$$\ln\left|\frac{\omega - v_F p}{\omega + v_F p}\right| = \ln\left|\frac{1 - \frac{v_F p}{\omega}}{1 + \frac{v_F p}{\omega}}\right| \simeq -\frac{2 v_F p}{\omega}$$

Substituting into V_{eff}, we find that it diverges at $\omega_0 = \frac{4\pi n e^2}{m}$, n is density

$\left(\frac{v_F^2 \nu_0}{3} = \frac{p_F^2}{3\pi^2 m} = \frac{n}{m} \right)$ $\uparrow$ plasmon frequency.

Expanding to the next order gives

$$\omega(p) = \omega_0 \left(1 + \frac{3}{10} \left(\frac{v_F p}{n} \right)^2 \right)$$



V_{eff} has the denominator with imaginary part $\equiv$ damping the effective excitations.

The ultimate (opposite to $\frac{\omega}{v_F p} >> 1$) limit is the static one, $\omega \to 0$; where $\Pi_0 = -\nu_0$.

$$\therefore \quad V_{eff}(\omega=0, p) = \frac{1}{\frac{p^2}{4\pi} - e^2 \Pi_0} = \frac{1}{\frac{q^2}{4\pi} + \nu_0 e^2}$$

$$= \frac{4\pi}{q^2 + \underbrace{4\pi\nu_0 e^2}_{\varkappa^2 = \frac{1}{r_0^2}}}$$

where r_0 is the Debye screening

$$\mathrm{IFT}\left(\frac{4\pi}{q^2+q_0^2}\right) = \frac{e^2}{r} e^{-r/r_0}$$

Actually, $\Pi_0(\underline{p}, \omega)$ can be calculated exactly (Lindhardt formula).

$$-\Pi_0(\underline{p},\omega) = I(\underline{p},\omega) + I(-\underline{p},-\omega)$$

where

$$I(\underline{p},\omega) = 2\int \frac{n_{\underline{q}}\, d\vec{q}}{\omega - \xi_{\underline{q}+\underline{p}} + \xi_{\underline{q}} + i\delta\,\mathrm{sgn}\,\omega}$$

since

$$I(-\underline{p},-\underline{\omega}) = 2\int \frac{d\vec{q}\; n_{\vec{q}}}{-\omega - \xi_{\underline{q}-\underline{p}} + \xi_{\underline{q}} - i\delta\,\mathrm{sgn}\,\omega}$$

shift $\vec{q} \to \vec{q} + \vec{p}$, $\underline{q}-\underline{p} \to \underline{q}$

$$= -2\int \frac{n_{q+p}\; d\vec{q}}{\omega + \xi_{\underline{q}} - \xi_{\underline{q}+\underline{p}} + i\delta\,\mathrm{sgn}\,\omega} = -I(\underline{p},\underline{\omega}).$$

$$I(\underline{p},\omega) = -2\,\frac{2\pi}{(2\pi)^3}\int_0^{p_F} q^2\,dq \int_{-1}^{1} d\eta\; \frac{1}{\omega + \xi_p - \xi_{\underline{p}+\underline{q}} + i\delta\,\mathrm{sgn}\,\omega}$$

$$= -\frac{1}{2\pi^2}\int_0^{p_F} q^2\,dq \int_{-1}^{1} d\eta\; \frac{1}{\xi_+ - \frac{pq\eta}{m}}.$$

where $\xi_+ = \omega - \frac{q^2}{2m} + i\delta\,\mathrm{sgn}\,\omega$

$$= -\frac{m}{2\pi^2 p}\int_0^{p_F} q\,dq\; \ln \frac{\xi_+ - \frac{qp}{m}}{\xi_+ + \frac{qp}{m}}$$

The log-integration is cumbersome but straightforward

The result - Lindhardt formula.