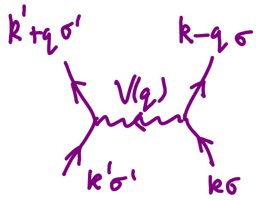
Ground State Energy of Interacting Electron Gas (AS 5.2)

$\boxed{PT1}$



$$\hat{H}_0 = \sum_k \frac{k^2}{2m} a^\dagger_{k\sigma} a_{k\sigma} \qquad (1)$$

$$\hat{V}_{ee} = \frac{1}{2L^d} \sum_{kk'} V_{ee}(q)\, a^\dagger_{k-q\sigma} a^\dagger_{k'+q\sigma'} a_{k'\sigma'} a_{k\sigma} \qquad (2)$$

How important is $\hat{V}_{ee}$? $\qquad V_{ee}(q) = \frac{e^2}{q^2} = \text{FT of } \frac{e^2}{|\vec{r}|}$

Suppose Volume per electron is r_0^3, then $\qquad \hbar = 1$

$$E_{\text{kinetic}} \text{ per electron} \sim \frac{1}{m r_0^2} \qquad \left(\text{since } r_0 \sim \frac{\hbar}{p_0}\right) \qquad (3)$$

$$E_{\text{pot}} \text{ per electron} \sim \frac{e^2}{r_0} \qquad (4)$$

$$\frac{E_{\text{pot}}}{E_{\text{kin}}} \sim e^2 m r_0 = \frac{r_0}{a_B} \equiv r_s = \text{dimensionless density parameter} \qquad (5)$$

↖ Bohr radius

$\boxed{PT2}$

$r_s \gg 1$: low density, interactions dominate, Wigner crystal

$r_s \ll 1$: high " , " don't dominate, Fermi liquid

real metals: $2 \lesssim r_s \lesssim 6$: (difficult for theory! but FL works surprisingly well in practice!)

We'll do pert. theory in r_s.

Free energy : $\qquad F = -T \ln Z, \qquad Z = \int \mathcal{D}(\bar{\psi},\psi)\, e^{-S} \qquad (1)$

$$S[\bar{\psi},\psi] = \sum_p \bar{\psi}_{p\sigma}\left(-i\omega_n + \frac{p^2}{2m} - \mu\right)\psi_{p\sigma} \qquad (2)$$

$$+ \frac{T}{2L^3} \sum_{\substack{pp' \\ q\neq 0}} \bar{\psi}_{p+q\,\sigma}\, \bar{\psi}_{p'-q\,\sigma'}\, V(q)\, \psi_{p'\sigma'}\, \psi_{p\sigma} \qquad (3)$$

$q \neq 0$ ← charge neutrality, ensured by background ions

where $\qquad p \equiv (\vec{p}, \omega_n) = $ four-momentum!

Free electron gas: $\boxed{PT3}$

after doing functional integral and $\sum_{\omega_n}$-summation.

$$F^{(0)} = -T \sum_{\vec{p}\sigma} \underset{(\partial_\varepsilon \varepsilon)}{\overset{1}{\shortparallel}} \ln\left(1 + e^{-\beta(\vec{p}^2/2m - \mu)}\right) \quad (1)$$

and int. by parts, $\partial_\varepsilon \ln = f(\varepsilon)$

$$= 2 \sum_{p^2/2m < \mu} \frac{p^2}{2m} \simeq \frac{L^3}{(2\pi)^3} 8\pi \, \frac{1}{5} \frac{p_F^5}{m} = \frac{3}{5} N\mu \quad (2)$$

where

chem. pot: $\mu = \frac{p_F^2}{2m}$,

$\#$ of part: $N = 2\sum_{|k|<k_F} = \frac{L^3}{(2\pi)^3} \frac{8\pi}{3} k_F^3 = \frac{L^3 p_F^3}{3\pi^2} = \frac{L^3 (2m\mu)^{3/2}}{3\pi^2}$ (3)

$\Rightarrow$ Energy per particle $= \frac{3}{5}\mu$.

In terms of $E_{Rydberg} = \frac{me^4}{2} = 13.6\,eV$ (ionization energy of Hydrogen)

$$\frac{F^{(0)}}{E_{Ryd}} \sim N \left(\frac{p_F^2}{m}\right)\left(\frac{1}{me^4}\right) \sim N \left(\frac{1}{me^2}\frac{1}{r_0}\right)^2 \sim \frac{N}{r_s^2} \quad (4)$$

Now add interactions: $\boxed{PT4}$

Expand

$$F = -T \ln Z = -T\left(\ln Z_0 + \frac{1}{Z}\int \mathcal{D}(\bar\psi,\psi)\, e^{-S_0}(-S_{int}) + \dots\right) \quad (1)$$

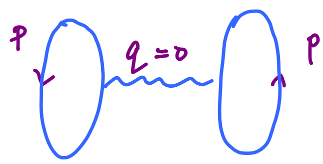
$$= F^{(0)} + \underbrace{T\langle S_{int}\rangle}_{F^{(1)}} + \dots \quad (2)$$

$$F^{(1)} = \frac{T^2}{2L^3} \left\langle \sum_{pp'q} \bar\psi_{p+q\sigma} \bar\psi_{p'-q\sigma'} V(\vec q)\, \psi_{p'\sigma'} \psi_{p\sigma} \right\rangle_0 \quad (3)$$

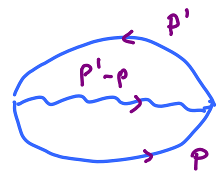
Wick: { Hartree

Fock

Hartree:



Fock:



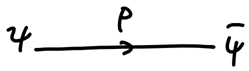
$F^{(1)}_{Hartree} \sim V(\vec q = 0) = 0$,

due to charge neutrality

$$F^{(1)}_{Fock} = -\frac{T^2}{2L^3} \sum_{pp'} \mathcal{G}_p \mathcal{G}_{p'} V(p-p') \quad (4)$$

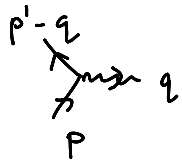
PT5

Feynman rules: (Detailed derivation: Negele & Orland, p. 74 – 100)



$$\langle \bar{\psi}_{p\sigma} \psi_{p\sigma} \rangle_0 \equiv \mathcal{G}_p \equiv \frac{1}{i\omega_n + \mu - \frac{p^2}{2m}} \qquad (1)$$

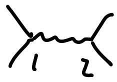
$$V(\vec{q}) \qquad (2)$$



: 4-momentum conservation (3)

Overall sign: $(-1)^{N_{loop}}$, N_{loop} = # of loops (4)

loop arises from:



$$\overbrace{(\bar{\psi}_1 \underbrace{\bar{\psi}_2 \psi_2 \psi_1}_{(+)})(\bar{\psi}_3 \underbrace{\bar{\psi}_4 \psi_4 \psi_3}_{(+)}) \cdots (\bar{\psi}_5 \underbrace{\bar{\psi}_6 \psi_6 \psi_5}_{(+)})}^{(-)} \qquad (5)$$

$$= (-)\, \psi_6 (\bar{\psi}_1 \psi_1 \, \bar{\psi}_2 \psi)(\bar{\psi}_3 \psi_3 \, \bar{\psi}_4 \psi_4) \cdots (\bar{\psi}_5 \psi_5 \bar{\psi}_6) \qquad (6)$$

$\Rightarrow$ (–) for every loop:

PT6

$$F^{(1)}_{Fock} \overset{(4.4)}{=} - \frac{T^2}{2L^3} \sum_{\vec{p}\vec{p}'} \sum_{\omega_n, \omega_n'} \mathcal{G}_p \mathcal{G}_{p'} V(p-p') \qquad (1)$$

Homework: do Matsubara sum !!

$$= -\frac{1}{L^3} \sum_{\vec{p}\vec{p}'} n_F(\varepsilon_p)\, n_F(\varepsilon_{p'}) \frac{e^2}{|\vec{p}-\vec{p}'|^2} \qquad (2)$$

$$\overset{T\to 0}{=} -\frac{1}{L^3} \underbrace{\sum_{\varepsilon_p, \varepsilon_{p'} < \mu}}_{L^3 \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3p'}{(2\pi)^3} \Big|_{|p|, |p'| < p_F}} \frac{e^2}{|\vec{p}-\vec{p}'|^2} \qquad (3)$$

(for sum, see Kittel, Quantum Theory of Solids, 1963)

$$= -e^2 \frac{L^3 p_F^4}{(2\pi)^4} \qquad (4)$$

(up to prefactors, result follows from dimensional analysis

$$\boxed{\frac{F^{(1)}_{Fock}}{E_{Ryd}} \sim \frac{N e^2 p_F}{m e^4} \sim \frac{N}{r_s} \sim F^{(0)} r_s} \qquad (5)$$

(so, pert. theory is valid if r_s is small)

But, closer analysis reveals problems. Rewrite $\boxed{PT7}$

$$\underset{(3.2)}{F^{(0)}} + \underset{(6.3)}{F^{(1)}} \overset{(T=0)}{=} \sum_{|p|<p_F} \underbrace{\left(\frac{|\vec{p}|^2}{2m} - \frac{1}{L^3} \sum_{|p'|<p_F} \frac{e^2}{|\vec{p}-\vec{p}'|} \right)}_{} \equiv \sum_{|p|<p_F} \tilde{\varepsilon}_p \quad (1)$$

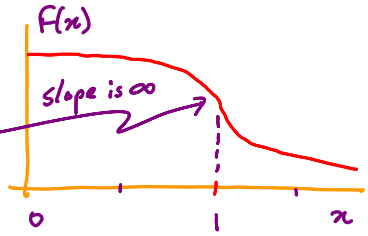
"renormalized" single-particle energies:

$$\frac{p^2}{2m} - \frac{e^2 p_F}{2\pi} \Gamma(|p|/p_F) = \tilde{\varepsilon}_p \quad (2)$$

[Exercise: check this!!]

where $\Gamma(x) = 2 + \frac{1-x^2}{x} \ln\left|\frac{1+x}{1-x}\right|$ (3)

$\Gamma'(x)$ diverges logarithmically at $x = 1$



Density of states:

$$\rho(\varepsilon) = \sum_{\vec{p}\sigma} \delta(\varepsilon - \varepsilon_p) = \frac{L^3}{(2\pi)^3} 4\pi \cdot 2 \int_0^\infty dp\, p^2\, \delta(\varepsilon - \varepsilon_p) \quad (4)$$

$\left[\int d\varepsilon\, \rho(\varepsilon) = \text{total number of states} \right]$

$$= \frac{L^3}{\pi^2} \int d\varepsilon_p \left(\frac{\partial p}{\partial \varepsilon_p}\right) p^2\, \delta(\varepsilon - \varepsilon_p) \quad (5)$$

$$= \frac{L^3}{\pi^2} p_\varepsilon^2 \left(\frac{\partial \varepsilon_p}{\partial p}\right)^{-1} \xrightarrow{\text{at } \varepsilon_F} \frac{1}{\infty} = 0 \quad (6)$$

$\Rightarrow$ prediction: $\rho(\varepsilon_F) = 0$, which is wrong (transport coeff. $\sim \rho(\varepsilon_F) \neq 0$)