Physics 560A Lecture 12

Jellium model of metals

$$H = \sum_{\vec{p},\sigma} \varepsilon_{\vec{p}}\, c^{\dagger}_{\vec{p}\sigma} c_{\vec{p}\sigma} + \sum_{\vec{q}} U(\vec{q})\, \hat{\rho}_{\vec{q}}$$

$$+ \frac{1}{2V} \sum_{\substack{\vec{q},\vec{k},\vec{k}' \\ \sigma,\sigma'}} V_{\vec{q}}\, c^{\dagger}_{\vec{k}+\vec{q}\sigma} c^{\dagger}_{\vec{k}'-\vec{q}\sigma'} c_{\vec{k}'\sigma'} c_{\vec{k}\sigma}$$

where $\rho(\vec{q}) = \sum_{\vec{k},\sigma} c^{\dagger}_{\vec{k}+\vec{q},\sigma} c_{\vec{k}\sigma}$

(density operator)

$$V_{\vec{q}} = \int d^3r\, e^{i\vec{q}\cdot\vec{r}}\, V(\vec{r}) \quad \text{(e-e int.)}$$

$$U(\vec{q}) = \int d^3r\, e^{i\vec{q}\cdot\vec{r}}\, U(\vec{r}) \quad \text{(e-ion int.)}$$

"pseudopotential"

$$V_{\vec{q}} = e^2 \int \frac{d^3r}{r} e^{i\vec{q}\cdot\vec{r}}$$

$$= 2\pi e^2 \int_0^\infty dr\, r \int_{-1}^{1} d(\cos\theta)\, e^{iqr\cos\theta}$$

$$= \frac{2\pi e^2}{iq} \int_0^\infty dr \left(e^{iqr} - e^{-iqr}\right)$$

$$= \frac{4\pi e^2}{q} \int_0^\infty dr \sin qr$$

$$= \frac{4\pi e^2}{q^2} \Big(1 - \cancel{\lim_{r\to\infty} \cos qr}\Big)$$

damps out

$$= \frac{4\pi e^2}{q^2}$$

Homogeneous electron gas

positive ions $\longrightarrow$ constant density

$$n_0 = \frac{N}{V}$$

Charge neutrality

$$n_0 = \frac{1}{V} \sum_{\vec{k},\sigma} \langle c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} \rangle$$

$\vec{q}=0$ term of e-e interaction:

$$\lim_{q\to 0} \frac{N(N-1)}{2V} V_{\vec{q}}$$

ion-ion interaction

$$\frac{1}{2} e^2 \int \frac{n_0^2 \, d^3r \, d^3r'}{|\vec{r}-\vec{r}'|} = \lim_{q\to 0} \frac{2\pi e^2}{q^2} \frac{N^2}{V}$$

e-ion interaction:

$$-e^2 \int \frac{n_0 \, \rho(\vec{r})}{|\vec{r}-\vec{r}'|} d^3r \, d^3r' = -\lim_{q\to 0} \frac{4\pi e^2}{q^2} \frac{N^2}{V}$$

$\Rightarrow$ cancels $\vec{q}=0$ term of e-e interaction.

Ground state energy

$$\sum_{\substack{\vec{k},\vec{k}' \\ \sigma,\sigma'}} c^{\dagger}_{\vec{k}+\vec{q}\,\sigma}\, c^{\dagger}_{\vec{k}'-\vec{q},\sigma'}\, c_{\vec{k}'\sigma'}\, c_{\vec{k}\sigma}$$

$$= \delta_{\vec{q}=0}\left(\sum_{\vec{k}\sigma} c^{\dagger}_{\vec{k},\sigma} c_{\vec{k},\sigma}\right)^2$$

$$\sum_{\substack{\vec{k},\vec{k}' \\ \sigma,\sigma'}} c^{\dagger}_{\vec{k}+\vec{q}\,\sigma}\, c^{\dagger}_{\vec{k}'-\vec{q},\sigma'}\, c_{\vec{k}'\sigma'}\, c_{\vec{k}\sigma}$$

$$= -\sum_{\substack{\vec{k},\sigma \\ \vec{k}',\sigma'}} n_{\vec{k}\sigma}\, n_{\vec{k}+\vec{q}\,\sigma}\, \delta_{\sigma\sigma'}\, \delta_{\vec{k};\vec{k}+\vec{q}} = -\sum_{\vec{k},\sigma} n_{\vec{k}\sigma}\, n_{\vec{k}+\vec{q}\,\sigma}$$

First-order perturbation theory:

$$H = H^{(1)} + \lambda H^{(2)}$$

$H^{(1)} =$ 1-body Hamiltonian

$H^{(2)} =$ 2-body Hamiltonian

Ground state of $H^{(1)}$:

$$|0_N\rangle = \prod_{\substack{|\vec{k}| \le k_F \\ \sigma = \uparrow, \downarrow}} c^{\dagger}_{\vec{k}\sigma} |0\rangle$$

$$\frac{1}{N} H^{(1)} |0_N\rangle = \frac{3}{5} \varepsilon_F |0_N\rangle$$

$$\frac{E_0}{N} = \frac{3}{5} \varepsilon_F + \frac{\lambda}{N} \langle 0_N | H^{(2)} | 0_N \rangle + \mathcal{O}(\lambda^2)$$

$$\frac{E_0^{(x)}}{N} \equiv \frac{1}{N} \langle 0_N | H^{(2)} | 0_N \rangle$$

$$= -\frac{1}{2NV} \sum_{\vec{k},\vec{q},\sigma} v_{\vec{q}}\, n_{\vec{k}\sigma}\, n_{\vec{k}+\vec{q}\,\sigma}$$

$$\sum_{\vec{k}} \rightarrow V \int \frac{d^3k}{(2\pi)^3}$$

$$v_{\vec{q}} = \frac{4\pi e^2}{q^2}$$

$$\frac{E_0^{(x)}}{N} = -\frac{4\pi e^2}{n_0} \int \frac{d^3k}{(2\pi)^3}\, n_{\vec{k}} \int \frac{d^3k'}{(2\pi)^3} \frac{n_{\vec{k}'}}{|\vec{k}-\vec{k}'|^2}$$

$$= -\frac{4\pi e^2}{n_0} \left(\frac{4\pi}{3} \frac{k_F^3}{8\pi^3} \right)^2 \left\langle \frac{1}{|\vec{k}-\vec{k}'|^2} \right\rangle$$

$$= -\pi n_0 e^2 \left\langle \frac{1}{|\vec{k}-\vec{k}'|^2} \right\rangle,$$

where we have used $n_0 = \frac{k_F^3}{3\pi^2}$

Here $\left\langle \frac{1}{|\vec{k}-\vec{k}'|^2} \right\rangle$ is the average over the Fermi sphere. Clearly

$$\left\langle \frac{1}{|\vec{k}-\vec{k}'|^2} \right\rangle = \frac{\text{Const.}}{k_F^2}$$

A detailed calculation gives

$$\left\langle \frac{1}{|\vec{k}-\vec{k}'|^2} \right\rangle = \frac{9}{4} \frac{1}{k_F^2}$$

$$\Rightarrow \quad \frac{E_0^{(x)}}{N} = -\frac{3e^2 k_F}{4\pi}$$

So

$$\frac{E_0}{N} = \frac{3}{5}\varepsilon_F - \lambda \frac{3}{4\pi} e^2 k_F + \mathcal{O}(\lambda^2)$$

<u>The parameter r_s</u>

$$\frac{4\pi}{3} r_s^3 = \frac{1}{n_0 a_0^3}$$

where $a_0 = \frac{\hbar^2}{me^2}$ = Bohr radius.

r_s is the radius, in atomic units, of a sphere containing, on average, one electron. The unit of energy is $Ry = \frac{me^4}{2\hbar^2}$.

$$\frac{E_F}{Ry} = \frac{3.6832}{r_s^2}$$

$$-\frac{3}{4\pi} e^2 k_F = -\frac{0.9163}{r_s} Ry$$

Thus, another way to write the series expansion for $\frac{E_0}{N}$ (setting $\lambda = 1$) is

$$\frac{E_0}{N} = \frac{2.2099}{r_s^2} - \frac{0.9163}{r_s} + \mathcal{O}(r_s^0)$$

We see that the perturbation series is really a high-density expansion. The next terms have been calculated (see e.g. Mahan, "Many-particle Physics") and are

$$\frac{E_0}{N} = \frac{2.2099}{r_s^2} - \frac{0.9163}{r_s} - 0.094 + 0.0622 \ln r_s + \cdots$$

The series converges rapidly for $r_s \ll 1$, and these terms give an accurate description for $r_s \leq 1$. However, real metals have

$$3 \lesssim r_s \lesssim 6 \quad !$$

Coulomb interactions not a small perturbation!