Phys 726 – Lecture 4

Recap:

* Last class, we reduced the charge-compensated electron gas to the form

$$\hat{H}_{el} = \hat{H}^{(1)}_{ee} + \hat{H}^{(2)}_{ee}$$

$$= \sum_{\vec{k},\alpha} \frac{\hbar^2 k^2}{2m} c^\dagger_{\vec{k}\alpha} c_{\vec{k}\alpha} + \frac{e^2}{2V} \sum_{\alpha\beta} \sum_{\substack{\vec{k}\vec{k}' \\ \vec{q}\neq 0}} \frac{4\pi}{q^2} c^\dagger_{\vec{k}+\vec{q},\alpha} c^\dagger_{\vec{k}',\beta} c_{\vec{k}'+\vec{q},\beta} c_{\vec{k},\alpha}$$

one-body term bilinear in $c^\dagger, c$ and diagonal w.r.t. the representation in wavevector $\vec{k}$ and spin projection α

two-body term biquadratic in $c^\dagger, c$ and off-diagonal; functions as a scattering term

* Argued that equal numbers of c and $c^\dagger$ operators in each term of the Hamiltonian

$$\Rightarrow [\hat{H}_{el}, \hat{N}] = 0$$

$\Rightarrow$ Eigenstates are states of definite particle number

* Ground state of $\hat{H}_{el}^{(1)}$ is the N-particle Fermi Sea

$$|F\rangle = \left(\prod_{|\vec{k}| < k_F} c^\dagger_{\vec{k}\uparrow} c^\dagger_{\vec{k}\downarrow} \right) |vac\rangle$$

* Scaling argument suggests that at <u>high</u> electronic density, $\hat{H}_{el}^{(2)}$ is a small perturbation

$\rightarrow$ try to use $|F\rangle$ as a starting point for first-order perturbation theory

→ Unperturbed ground state energy

$$\langle F | H_{el}^{(1)} | F \rangle = \frac{\hbar^2}{2m} \sum_{\vec{k}\alpha} k^2 \langle F | \hat{n}_{k\alpha} | F \rangle$$

$$= \frac{e^2}{2a_0} \cdot \frac{N}{r_s^2} \cdot \frac{3}{5} \left(\frac{9\pi}{4} \right)^{2/3} \doteq \frac{e^2}{2a_0} \cdot N \cdot \frac{2.21}{r_s^2}$$

Here, $a_0 = \frac{\hbar^2}{me^2}$ is the Bohr radius

and r_s is the dimensionless interparticle spacing defined by $V = \frac{4}{3}\pi r_0^3 = \frac{4}{3}\pi a_0^3 r_s^3$.

→ First order energy shift due to interactions is

$$\langle F | \hat{H}_{el}^{(2)} | F \rangle = \frac{e^2}{2V} \sum_{\substack{kk'\\ q\neq 0}} \frac{4\pi}{q^2} \langle F | c^+_{k+q,\alpha} c^+_{k'\beta} c_{k'+q,\beta} c_{k\alpha} | F \rangle$$

Evaluating expectation values of operators in the Fermi Sea

$$|F\rangle = \left(\prod_{|\vec{k}|<k_F} c^{+}_{k\uparrow} c^{+}_{k\downarrow} \right) |vac\rangle$$

= tensor product of all filled states inside the fermi surface and all empty states outside it

$$= \underbrace{\underset{k=0,\uparrow}{|1\rangle} \otimes \underset{k=0,\downarrow}{|1\rangle} \otimes \cdots \otimes |1\rangle}_{\text{corresponding to } |\vec{k}|<k_F} \otimes \underbrace{|0\rangle \otimes |0\rangle \otimes |0\rangle \otimes \cdots}_{|\vec{k}|>k_F}$$

$$\hat{n}_{k,\alpha} |F\rangle = \begin{cases} |F\rangle & \text{if } |\vec{k}|<k_F \\ 0 & \text{if } |\vec{k}|>k_F \end{cases}$$

Heavyside function

$$= \theta(k_F - k) \, |F\rangle$$

and $\langle F | \hat{n}_{k,\alpha} | F \rangle = \theta(k_F - k)$

Consider the expectation value of a more general bilinear operator

$$\langle F | c^\dagger_{k\alpha} c_{k'\beta} | F \rangle = \left(\langle F | c^\dagger_{k\alpha} \right) \cdot \left(c_{k'\beta} | F \rangle \right)$$

$$\equiv \langle \Psi_{k,\alpha} | \Psi_{k'\beta} \rangle$$

where $|\Psi_{k\alpha}\rangle = c_{k\alpha} |F\rangle$

$$= c_{k\alpha} c^\dagger_{\lambda_N} c^\dagger_{\lambda_{N-1}} \cdots c^\dagger_{\lambda_2} c^\dagger_{\lambda_1} |vac\rangle$$

where $\{\lambda_1, \lambda_2 \dots, \lambda_N\} = \{k_1\uparrow, k_1\downarrow, \dots, k_{\frac{N}{2}}\uparrow, k_{\frac{N}{2}}\downarrow\}$

label the N states in the Fermi Sea.

→ want to manipulate the position of $c_{k\alpha}$ in the operator string to bring it into normal order

→ Two possibilities

① $k\alpha$ is not occupied in $|F\rangle$

i.e. $\vec{k},\alpha$ does not correspond to any of $\lambda_1,\dots,\lambda_N$

so that

$$c_{k\alpha}c^\dagger_{\lambda_N}\cdots c^\dagger_{\lambda_1}|vac\rangle = (-1)^N c^\dagger_{\lambda_N}\cdots c^\dagger_{\lambda_1}\cancelto{0}{c_{k\alpha}|vac\rangle}$$

$$\Rightarrow \quad \langle F|c^\dagger_{k\alpha}c_{k'\beta}|F\rangle \sim \theta(k_F-|\vec{k}|)\,\theta(k_F-|\vec{k}'|)$$

(2) $k\alpha$ corresponds to a particular λ_n

$$c_{k\alpha}c^\dagger_{\lambda_N}\cdots c^\dagger_{\lambda_1}|vac\rangle = (-1)^{N-n}c^\dagger_{\lambda_N}\cdots c^\dagger_{\lambda_{n+1}}c_{\vec{k},\alpha}c^\dagger_{\lambda_n} \times c^\dagger_{\lambda_{n-1}}\cdots c^\dagger_{\lambda_1}|vac\rangle$$

$$= (-1)^{N-n}c^\dagger_{\lambda_N}\cdots c^\dagger_{\lambda_{n+1}}\left(1-c^\dagger_{\lambda_n}c_{\vec{k}\alpha}\right)c^\dagger_{\lambda_{n-1}}\cdots c^\dagger_{\lambda_1}|vac\rangle$$

$$= (-1)^{N-n}\Big[c^\dagger_{\lambda_N}\cdots c^\dagger_{\lambda_{n+1}}c^\dagger_{\lambda_{n-1}}\cdots c^\dagger_{\lambda_1}|vac\rangle$$

Fermi sea with $\vec{k},\alpha$ removed

Here even or odd depending on α

$$-(-1)^{n-1}c^\dagger_{\lambda_N}\cdots c^\dagger_{\lambda_1}\cancelto{0}{c_{k\alpha}|vac\rangle}\Big]$$

annihilates the vacuum

Finally, we get

$$|\Psi_{k\alpha}\rangle = c_{k\alpha}|F\rangle$$

$$= \begin{cases} 0 & \text{if } k > k_F \\ \pm\,|F \text{ with } k\alpha \text{ removed}\rangle & \text{if } k < k_F \end{cases}$$

$+$ for spin $\alpha = \uparrow$
$-$ for spin $\alpha = \downarrow$ in our convention

and so $\langle F | c^{\dagger}_{k\alpha} c_{k'\beta} | F\rangle = \langle \Psi_{k\alpha} | \Psi_{k'\beta}\rangle$

$$= (\pm)_{\alpha} (\pm)_{\beta}\, \theta(k_F - k)\, \theta(k_F - k')$$

$$\times \underbrace{\langle F \text{ with } k\alpha \text{ removed} \,|\, F \text{ with } k'\beta \text{ removed}\rangle}_{\text{only has overlap if these are the identical state}}$$

$$= (\pm)_{\alpha} (\pm)_{\beta}\, \delta_{kk'}\, \delta_{\alpha\alpha'}\, \theta(k_F - k)\, \theta(k_F - k')$$

$$= \delta_{kk'}\, \delta_{\alpha\beta}\, \theta(k_F - k) = \delta_{kk'}\, \delta_{\alpha\beta} \langle F | \hat{n}_{k\alpha} | F\rangle$$

We can make a similar argument for

$$\langle F | c^\dagger_{k\alpha} c^\dagger_{k'\beta} c_{k''\mu} c_{k'''\nu} | F \rangle$$

$$\equiv \langle \Psi_{k\alpha;k'\beta} | \Psi_{k''\mu,k'''\nu} \rangle$$

where $|\Psi_{k\alpha;k'\beta}\rangle = c_{k'\beta} c_{k\alpha} |F\rangle$

$$= - c_{k\alpha} c_{k\beta} |F\rangle$$

$$= - |\Psi_{k'\beta;k\alpha}\rangle$$

exchange of fermions

Expect

$$\langle \Psi_{k\alpha;k'\beta'} | \Psi_{k''\mu;k'''\nu} \rangle$$

$$= \left[\delta_{kk'''} \delta_{k'k''} \delta_{\alpha\nu} \delta_{\beta\mu} \right.$$

$$\left. - \delta_{kk''} \delta_{k'k'''} \delta_{\alpha\mu} \delta_{\beta\nu} \right] \theta(k_F - k)\, \theta(k_F - k')$$

Let's apply this result to our expression for the first-order energy shift in the interacting electron gas

$$\langle F | \hat{H}_{el}^{(2)} | F \rangle = \frac{e^2}{2V} \sum_{\alpha\beta k k'} \sum_{q \neq 0} \frac{4\pi}{q^2} \langle F | c^{\dagger}_{k+q,\alpha} c^{\dagger}_{k'\beta} c_{k'+q,\beta} c_{k\alpha} | F \rangle$$

$$= \frac{e^2}{2V} \sum_{\alpha\beta k k'} \sum_{q \neq 0} \frac{4\pi}{q^2} \Big(\overbrace{\delta_{k+q,k}\, \delta_{\alpha\alpha}\, \delta_{k',k'+q}}^{\delta_{q,0}}\, \delta_{\beta\beta}\, \theta(k_F - k)\, \theta(k_F - k')$$

$$- \underbrace{\delta_{k'+q,k+q}\, \delta_{\alpha\beta}}_{\delta_{k,k'}\, \delta_{\alpha\beta}}\, \delta_{k',k}\, \delta_{\alpha\beta}\, \theta(k_F - |\vec{k}+\vec{q}|)\, \theta(k_F - k) \Big)$$

$$= -\frac{e^2}{2V} \sum_{\alpha} \sum_{k, q \neq 0} \frac{4\pi}{q^2} \theta(k_F - |\vec{k}+\vec{q}|)\, \theta(k_F - k)$$

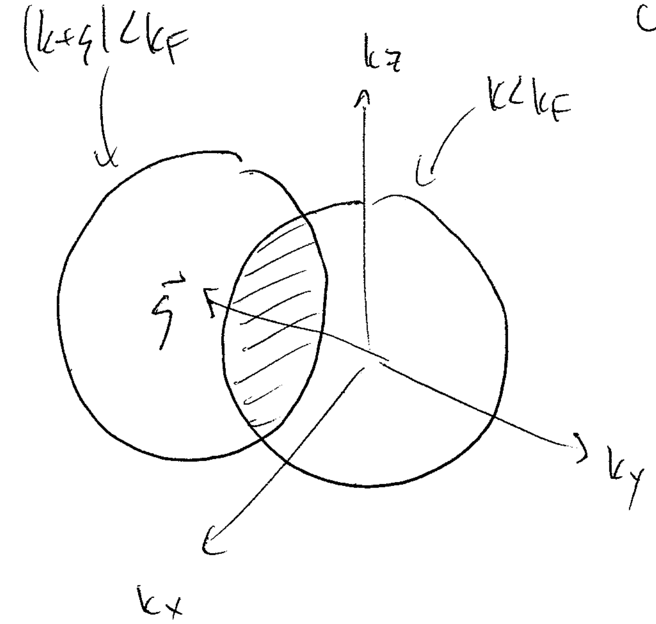
two copies for $\alpha = \uparrow, \downarrow$

let sums pass over to integrals in the thermodynamic limit $\sum_k \to V \int \frac{d^3k}{(2\pi)^3}$

$$= -e^2 4\pi V \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3q}{(2\pi)^3} \frac{1}{q^2} \theta(k_F - |\vec{k}+\vec{q}|)\, \theta(k_F - k)$$

all points in a Fermi Sea centered at $\vec{q}$

all points in a Fermi Sea centred at zero momentum



→ integration over the Fermi Sea when $q = 0$

→ as q increases the region of overlap shrinks

→ no overlap when $q > 2k_F$

Overlap volume

$$\Rightarrow \int d^3k\, \theta(k_F - |\vec{k}+\vec{q}|)\, \theta(k_F - k)$$

$$= \frac{4\pi}{3} k_F^3 \left(1 - \frac{3}{2}x + \frac{1}{2}x^3\right) \theta(1-x)$$

with $x = \dfrac{q}{2k_F}$

Energy shift

$$-e^2 4\pi V \cdot \frac{1}{(2\pi)^6} \underbrace{\int d^3q \cdot \frac{1}{q^2}}_{} \frac{4\pi}{3} k_F^3 \left(1 - \frac{3}{2}x + \frac{1}{2}x^3\right) \theta(1-x)$$

$$4\pi q^2 dq \cdot \frac{1}{q^2} = 4\pi \, dq = 8\pi k_F \, dx$$

$$= -4\pi e^2 V (2\pi)^{-6} \frac{4}{3}\pi k_F^3 \cdot 8\pi k_F \int_0^1 dx \left(1 - \frac{3}{2}x + \frac{1}{2}x^3\right)$$

$$= -\frac{e^2}{2a_0} \frac{N}{r_s} \left(\frac{9\pi}{4}\right)^{1/3} \frac{3}{2\pi} = -\frac{e^2}{2a_0} N \frac{0.916}{r_s}$$

Ground-state energy per particle in the high-density limit

$$\frac{E}{N} \xrightarrow{r_s \to 0} \frac{e^2}{2a_0} \left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + \cdots \right)$$