# Phys 726 – Lecture 3

Recap:

* Last class, we continued to work through the example of N electrons in a uniform background of compensating charge

→ N electrons of charge $-e$ have charge density
$$\rho_e(\vec{r}) = \sum_{i=1}^{N} (-e)\,\delta(\vec{r}-\vec{r}_i)$$

and total charge

$$Q_e = \int d^3r \, \rho_e(\vec{r}) = -eN$$

→ positive background charge $\rho(\vec{r}) = \text{const} = +\frac{eN}{L^3}$

$$= \frac{eN}{V}$$

$$Q = \int d^3r \, \rho(\vec{r}) = +eN$$

→ charge neutrality $Q_e + Q = 0$

* Neutrality is a delicate balance and requires exact cancellation of terms that diverge in the thermodynamic limit ($L \to \infty$ with $\frac{N}{V}$ fixed)

→ mathematical regularization via the Yukawa potential $\frac{e^{-\mu r}}{r}$ with a length scale $\mu^{-1} \sim L$ such that $\mu \to 0$ as $L \to \infty$ at the end of the calculation

→ $\mu$ cuts off divergent integrals. For the Hamiltonian, we found

self-interaction of the background charge

interactions between electrons and the background

$$H = \underbrace{H_b}_{-\frac{1}{2} e^2 \frac{N^2}{V} \cdot \frac{4\pi}{\mu^2}} + H_{el-b} + H_{el}$$

kinetic energy and mutual interactions of the electrons only

evaluates to a constant, and we expect it to exactly cancel a term in $H_{el}$

* Second-quantized Hamiltonian

$$\hat{H}_{el} = \int d^3r\, \hat{\psi}(\vec{r})^\dagger\, T\, \psi(\vec{r}) + \frac{1}{2}\iint d^3r\, d^3r'\, \hat{\psi}(\vec{r})^\dagger\, \hat{\psi}(\vec{r}')^\dagger$$

anti-commuting fermion field operators

$$\times\, V(\vec{r},\vec{r}')\, \hat{\psi}(\vec{r}')\, \hat{\psi}(\vec{r})$$

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

→ we evaluated the single-particle term with the substitutions $T = -\frac{\hbar^2}{2m}\nabla^2$

and $\hat{\psi}_\alpha(\vec{r}) = \sum_{\vec{k}} \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}\, \chi_\alpha\, c_{k\alpha}$ ← annihilation op for electron with momentum $\hbar\vec{k}$ and spin proj. $\alpha$

unrestricted sum over all wavevectors (momenta $\vec{p} = \hbar\vec{k}$)

eigenfunctions of the single-particle ~~[illegible]~~ contribution

$$T \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} = \frac{\hbar^2 k^2}{2m} \cdot \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$$

→ we showed that

$$\hat{H}_{el}^{(1)} = \sum_{\vec{k},\alpha} \frac{\hbar^2 k^2}{2m} c_{k\alpha}^{\dagger} c_{k\alpha} = \sum_{\vec{k},\alpha} \frac{\hbar^2 k^2}{2m} \hat{n}_{k\alpha}$$

occupation number operator on each mode

Ignoring the interaction term, the ground state would be the Fermi sea

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

with the Fermi wave vector $k_F$ chosen such that

$$\hat{N}|F\rangle = \sum_{k,\alpha} \hat{n}_{k,\alpha} |F\rangle = N|F\rangle$$

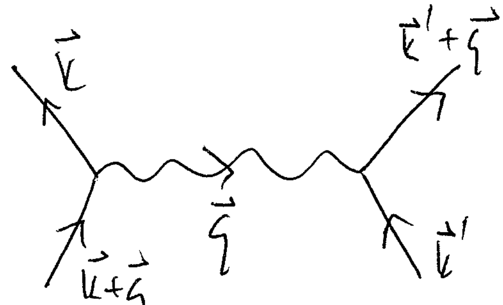
$|F\rangle$ is a state of definite number, which is possible since

$$[\hat{H}_{el}^{(1)}, \hat{N}] = 0$$

EXERCISE: Prove this.

→ We also showed that

$$\hat{H}_{el}^{(2)} = \frac{e^2}{2V} \sum_{\alpha\beta} \sum_{\substack{kk' \\ q}} \frac{4\pi}{q^2+\mu^2} c^\dagger_{k+q,\alpha} c^\dagger_{k',\beta} c_{k'+q,\beta} c_{k,\alpha}$$




all $\vec{q} \neq 0$ contributions cut off this divergence, and only the $\vec{q}=0$ term blows up as $\mu \to 0$.

momentum-conserving interaction mediated by a "photon" of infinite velocity that carries momentum $\vec{q}$

→ Separated out, the uniform term looks like

$$\frac{e^2}{2V} \sum_{\alpha\beta} \sum_{kk'} \frac{4\pi}{\mu^2} \underbrace{c^\dagger_{k\alpha} c^\dagger_{k'\beta} c_{k'\beta} c_{k\alpha}}_{\text{normal ordered}}$$

instead, try to pair up $c^\dagger_{k\alpha}$ and $c_{k\alpha}$, $c^\dagger_{k'\beta}$ and $c_{k'\beta}$

Recall that $\{c_{k\alpha}, c^{\dagger}_{k'\beta}\} = \delta_{kk'}\delta_{\alpha\beta}$

and $\{c_{k\alpha}, c_{k'\beta}\} = \{c^{\dagger}_{k\alpha}, c^{\dagger}_{k'\beta}\} = 0,$

So $c^{\dagger}_{k,\alpha} c^{\dagger}_{k'\beta} c_{k'\beta} c_{k\alpha}$

$$= - c^{\dagger}_{k\alpha}\left(c^{\dagger}_{k'\beta} c_{k\alpha}\right) c_{k'\beta}$$

$$= - c^{\dagger}_{k\alpha}\left(\delta_{kk'}\delta_{\alpha\beta} - c_{k\alpha} c^{\dagger}_{k'\beta}\right) c_{k'\beta}$$

$$= c^{\dagger}_{k\alpha} c_{k\alpha} c^{\dagger}_{k'\beta} c_{k'\beta} - \delta_{\alpha\beta}\delta_{kk'} c^{\dagger}_{k\alpha} c_{k\alpha}$$

$$= \hat{n}_{k\alpha}\hat{n}_{k'\beta} - \delta_{\alpha\beta}\delta_{kk'}\hat{n}_{k\alpha}$$

Hence, $\frac{e^2}{2V}\sum_{\alpha\beta}\sum_{kk'}\frac{4\pi}{\mu^2}\left(\hat{n}_{k\alpha}\hat{n}_{k'\beta} - \delta_{\alpha\beta}\delta_{kk'}\hat{n}_{k\alpha}\right)$

$$= \frac{e^2}{2V}\cdot\frac{4\pi}{\mu^2}\left[\left(\sum_k\sum_\alpha \hat{n}_{k\alpha}\right)\left(\sum_{k'}\sum_\beta \hat{n}_{k'\beta}\right) - \sum_k\sum_\alpha \hat{n}_{k\alpha}\right]$$

$$= \frac{e^2}{2V}\cdot\frac{4\pi}{\mu^2}\left(\hat{N}^2 - \hat{N}\right)$$

* Already argued that $[\hat{H}_{el}^{(1)}, \hat{N}]=0$

→ also true that $[\hat{H}_{el}^{(2)}, \hat{N}]=0$, so we can use states of definite particle number

→ Select a ground state $|\psi_0^{(N)}\rangle$ with exactly ~~[illegible]~~ $N$ particles: i.e.,

$$\hat{N}|\psi_0^{(N)}\rangle = N|\psi_0^{(N)}\rangle$$

and

$$\frac{e^2}{2V}\cdot\frac{4\pi}{\mu^2}(\hat{N}^2-\hat{N})|\psi_0^{(N)}\rangle$$

$$= \frac{e^2}{2V}\cdot\frac{4\pi}{\mu^2}(N^2-N)|\psi_0^{(N)}\rangle$$

$$= \frac{1}{2}e^2\frac{N^2}{V}\cdot\frac{4\pi}{\mu^2}\left(1-\frac{1}{N}\right)|\psi_0^{(N)}\rangle$$

vanishingly small contribution as $L\to\infty$, $N\to\infty$

* Exact cancellation of divergent terms from the uniform ($\vec{q}=0$) contribution

$$\hat{H} = -\frac{1}{2} e^2 \frac{N^2}{V} \cdot \frac{4\pi}{\mu^2} + \hat{H}_{el}$$

$$= -\frac{1}{2} e^2 \frac{N^2}{V} \cdot \frac{4\pi}{\mu^2} + \frac{1}{2} e^2 \frac{N^2}{V} \cdot \frac{4\pi}{\mu^2}\left(1-\frac{1}{N}\right)$$

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

restricted sum

now safe to take the limit

$$\xrightarrow[\mu\to 0]{L\to\infty,\ N\to\infty} \frac{e^2}{2V} \sum_{\alpha\beta} \sum_{\substack{\vec{k}\vec{k}' \\ \vec{q}\neq 0}} \frac{4\pi}{q^2} c^\dagger_{k+q,\alpha} c^\dagger_{k'\beta} c_{k'+q,\beta} c_{k\alpha}$$

* Now have $\hat{H}_{el} = \hat{H}_{el}^{(1)} + \hat{H}_{el}^{(2)}$

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

straightforward to solve: Fermi Sea ground state

complicated scattering terms: perturbation weak or strong?

→ convenient to scale to dimensionless variables:

① length scale $r_0$ defined in terms of the volume per particle, $V = \frac{4}{3}\pi r_0^3 N$ (interparticle spacing)

② second length scale, the Bohr radius $a_0 = \frac{\hbar^2}{me^2}$, which is associated with the strength of the Coulomb interaction

The relevant dimensionless quantities are

$$r_s \equiv \frac{r_0}{a_0} \qquad \bar{k} = r_0 k$$

$$\bar{k}' = r_0 k'$$

$$\bar{V} = r_0^{-3} V \qquad \bar{q} = r_0 q$$

Then

$$\hat{H}_{el} = \frac{e^2}{a_0 r_s}\left(\sum_{\bar{k}\alpha} \frac{1}{2}\bar{k}^2 c^{\dagger}_{\bar{k}\alpha} c_{\bar{k}\alpha} + \frac{r_s}{2\bar{V}} \sum_{\substack{\bar{k}\bar{k}' \\ \bar{q}\neq 0}} \frac{4\pi}{\bar{q}^2} c^{\dagger}_{\bar{k}+\bar{q}\alpha} c^{\dagger}_{\bar{k}'\beta} c_{\bar{k}+q,\beta} c_{\bar{k}\alpha}\right)$$

overall energy scale

controls the relative strength of the perturbation

Counterintuitive: perturbation is small in the high-density limit ($r_s \to 0$), even though the Coulomb potential is strong

* Attempt first-order perturbation theory

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

solvable base Hamiltonian

perturbation, small in the high-density limit

→ Use the ground state of $\hat{H}_{el}^{(1)}$, which is the N-electron Fermi Sea, $|F\rangle$

→ Evaluate the energy as

$$E = \langle F | \hat{H}_{el} | F \rangle$$

$$= \langle F | \hat{H}_{el}^{(1)} | F \rangle + \langle F | \hat{H}_{el}^{(2)} | F \rangle$$

→ Remember that $|F\rangle$ describes a state with single-particle levels in momentum space filled up to $k_F$

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

Heaviside

$$= V \int \frac{d^3k}{(2\pi)^3} \sum_{\alpha} \theta(k_F - k) = 2V \cdot \frac{1}{8\pi^3} \int_0^{k_F} 4\pi k^2 dk$$

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

$$= \frac{V}{\pi^2} \int_0^{k_F} k^2 = \frac{V}{3\pi^2} k_F^3 \equiv N$$

$$\text{or} \quad k_F = \left(3\pi^2 \frac{N}{V}\right)^{1/3}$$

$$= \left(\frac{3\pi^2 N}{\frac{4}{3}\pi r_0^3 N}\right)^{1/3}$$

$$= \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{r_0} \doteq 1.92 \frac{1}{a_0 r_s}$$

→ can use the same tricks to evaluate $\langle F | \hat{H}^{(1)}_{el} | F \rangle$

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

EXERCISE: Show all the steps

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

→ Somewhat harder to evaluate the first-order energy shift

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

What conditions on $k, k', \alpha, \beta$ must apply so that the matrix element doesn't vanish?