Phys 726 - Lecture 2

Recap:

* Last class, we introduced field operators

$$\hat{\psi}(\vec{r}), \ \hat{\psi}(\vec{r})^{\dagger}$$

that destroy and create a quantum particle at position $\vec{r}$.

* "Second-quantization" framework handles all the bookkeeping associated with enforcing particle statistics (symmetrization and antisymmetrization

* It does so via commutation / anticommutation rules

bosons $\quad [\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}\,')^{\dagger}] = [\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}\,')^{\dagger}]_{-}$

$$= \hat{\psi}(\vec{r})\hat{\psi}(\vec{r}\,')^{\dagger} - \hat{\psi}(\vec{r}\,')^{\dagger}\hat{\psi}(\vec{r}) = \delta(\vec{r}-\vec{r}\,')$$

$$[\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}\,')] = [\hat{\psi}(\vec{r})^{\dagger}, \hat{\psi}(\vec{r}\,')^{\dagger}] = 0$$

fermions $\{\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}')^\dagger\} = [\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}')^\dagger]_+$

$$= \hat{\psi}(\vec{r})\hat{\psi}(\vec{r}')^\dagger + \hat{\psi}(\vec{r}')^\dagger \psi(\vec{r}) = \delta(\vec{r}-\vec{r}')$$

$$\{\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}')\} = \{\hat{\psi}(\vec{r})^\dagger, \hat{\psi}(\vec{r})^\dagger\} = 0$$

Exercise: show that the anticommutation relation *implies* Pauli exclusion

* In terms of the field operators, we can write down a many-body Hamiltonian

$$\hat{H} = \int d^3r\, \hat{\psi}(\vec{r})^\dagger T(\vec{r})\, \hat{\psi}(\vec{r})$$

$$+ \frac{1}{2}\iint d^3r\, d^3r'\, \hat{\psi}(\vec{r})^\dagger \hat{\psi}(\vec{r}')^\dagger V(\vec{r},\vec{r}')\, \hat{\psi}(\vec{r}')\hat{\psi}(\vec{r})$$

$$= \hat{H}_0 + \hat{V}$$

two-body term, biquadratic in the fields

one-body term, bilinear in the fields

* Sometimes convenient to use a basis of single-particle states

→ take the conventional T.I.S.E. for the one-body kernel

differential operator

$$T\phi_k = E_k \phi_k$$

mode label

$\phi_k(\vec{r})$ is a real-space wavefunction

→ $\{\phi_k(\vec{r}), E_k\}$ is a complete set of eigenfunction, energy-eigenvalue pairs

→ assume orthonormality

$$\int d^3r\, \phi_k(\vec{r})^* \phi_{k'}(\vec{r}) = \delta_{k,k'}$$

$$\& \sum_k \phi_k(\vec{r})^* \phi_k(\vec{r}\,') = \delta(\vec{r}-\vec{r}\,')$$

→ express the field operators in this language, expanding them as a series in the creation and annihilator ops for each mode:

fermions

$$\hat{\psi}(\vec{r}) = \sum_k \phi_k(\vec{r})\, c_k$$

$$\hat{\psi}(\vec{r})^\dagger = \sum_k \phi_k(\vec{r})^* c_k^\dagger$$

check:

$$\{\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}\,')^\dagger\} = \sum_{k,k'} \Big(\phi_k(\vec{r})\, c_k\, \phi_{k'}(\vec{r}\,')^* c_{k'}^\dagger + \phi_{k'}(\vec{r}\,')^* c_{k'}^\dagger\, \phi_k(\vec{r})\, c_k \Big)$$

$$= \sum_{k,k'} \phi_k(\vec{r})\, \phi_{k'}(\vec{r}\,')^* \underbrace{\{c_k, c_{k'}^\dagger\}}_{\equiv\, \delta_{kk'} \text{ for fermions}}$$

$$= \sum_k \phi_k(\vec{r})\, \phi_k(\vec{r}\,')^* = \delta(\vec{r} - \vec{r}\,')$$

bosons

$$\hat{\psi}(\vec{r}) = \sum_k \phi_k(\vec{r})\, a_k$$

$$\hat{\psi}(\vec{r})^\dagger = \sum_k \phi_k(\vec{r})^* a_k^\dagger$$

check:

$$[\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}\,')^\dagger] = \sum_{k,k'} \Big(\phi_k(\vec{r}) a_k \phi_{k'}(\vec{r}\,')^* a_{k'}^\dagger$$

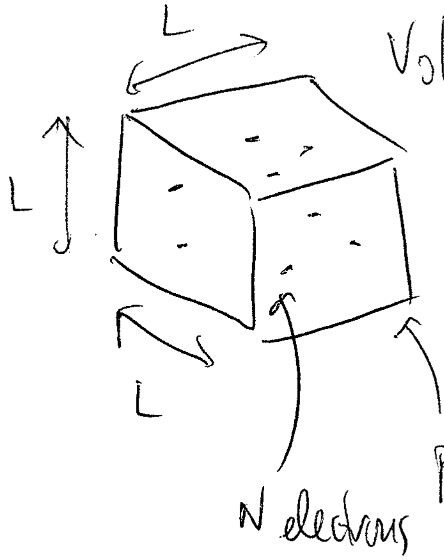
$$- \phi_{k'}(\vec{r}\,')^* a_{k'}^\dagger \phi_k(\vec{r})\, a_k \Big)$$

$$= \sum_{k,k'} \phi_k(\vec{r}) \phi_{k'}(\vec{r}\,')^* \underbrace{[a_k, a_k^\dagger]}_{\equiv\, \delta_{kk'} \text{ for bosons}}$$

$$= \sum_k \phi_k(\vec{r}) \phi_k(\vec{r}\,')^* = \delta(\vec{r} - \vec{r}\,')$$

Let's return to the Degenerate Electron gas

EXAMPLE



Volume $V = L^3$ (assume periodic boundary conditions; irrelevant in the $L \to \infty$ limit)

positive, uniform charge density

$$\rho(\vec{r}) = \text{const} = +\frac{eN}{V}$$

Interacting via the Yukawa potential $\sim \dfrac{e^{-\mu r}}{r}$

μ acts as a regularization parameter. We can choose a length scale $\frac{1}{\mu} \sim L$ so that $\mu \to 0$ as $L \to \infty$ in the end

* Single-particle wavefunctions for free, $s = 1/2$ particles

$$\phi_{\vec{k},\alpha}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} \chi_\alpha$$

* Hamiltonian

$$H = H_{el} + H_b + H_{el-b}$$

electrons only

background charge self-interaction

interaction between electrons and the background

(via transl. invariance)

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

boring constant

all the physics is here

→ in the old notation

$$H_{el} = -\frac{\hbar^2}{2m} \sum_{j=1}^{N} \nabla_j^2 + \sum_{j<j'} \frac{e^2 e^{-\mu|\vec{r}_j - \vec{r}_{j'}|}}{|\vec{r}_j - \vec{r}_{j'}|}$$

→ in second-quantized notation

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

$$= \int d^3r \sum_{k,\alpha} \frac{1}{\sqrt{V}} e^{-i\vec{k}\cdot\vec{r}} \chi_\alpha^\dagger c_{k,\alpha}^\dagger \left(-\frac{\hbar^2\nabla^2}{2m}\right) \sum_{k',\alpha'} \frac{1}{\sqrt{V}} e^{i\vec{k}'\cdot\vec{r}} \chi_{\alpha'} c_{k'\alpha'}$$

$$= \sum_{\substack{kk' \\ \alpha\alpha'}} \frac{1}{2m} \underbrace{\left(\frac{1}{V}\int d^3r\, e^{i(\vec{k}'-\vec{k})\cdot\vec{r}}\right)}_{\delta_{k,k'}} \hbar^2 \vec{k}'\cdot\vec{k}'\, \underbrace{\chi_\alpha^\dagger \chi_{\alpha'}}_{\delta_{\alpha\alpha'}}\, c_{k,\alpha}^\dagger c_{k',\alpha'}$$

$$= \sum_{k,\alpha} \frac{\hbar^2 k^2}{2m} c_{k\alpha}^\dagger c_{k\alpha} = \sum_{k,\alpha} \frac{\hbar^2 k^2}{2m} \hat{n}_{k,\alpha}$$

interaction term...

$$\frac{1}{2}\iint d^3r\, d^3r' \sum_{k_1\alpha_1} \frac{1}{\sqrt{V}} e^{-i\vec{k}_1\cdot\vec{r}} \chi_{\alpha_1}^{+} c_{k_1\alpha_1}^{+} \cdot \sum_{k_2\alpha_2} \frac{1}{\sqrt{V}} e^{-i\vec{k}_2\cdot\vec{r}'} \chi_{\alpha_2}^{+} c_{k_2\alpha_2}^{+}$$

$$\cdot \frac{e^2 \cdot e^{-\mu|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \cdot \sum_{k_3\alpha_3} \frac{1}{\sqrt{V}} e^{+i\vec{k}_3\cdot\vec{r}'} \chi_{\alpha_3} c_{k_3\alpha_3} \sum_{k_4\alpha_4} \frac{1}{\sqrt{V}} e^{+i\vec{k}_4\cdot\vec{r}} \chi_{\alpha_4} c_{k_4\alpha_4}$$

with the understanding that $\cdots\chi_{\alpha_1}^{+}\cdots\chi_{\alpha_2}^{+}\cdots\chi_{\alpha_3}\cdots\chi_{\alpha_4}\cdots$ pairs as $(\chi_{\alpha_1}^{+}\chi_{\alpha_4})(\chi_{\alpha_2}^{+}\chi_{\alpha_3}) = \delta_{\alpha_1\alpha_4}\delta_{\alpha_2\alpha_3}$

$$= \frac{e^2}{2V^2}\iint d^3r\, d^3r' \sum_{\substack{k_1k_2k_3k_4 \\ \alpha_1\alpha_2\alpha_3\alpha_4}} e^{i(k_4-k_1)\cdot\vec{r}} e^{i(\vec{k}_3-\vec{k}_2)\cdot\vec{r}'} \cdot \delta_{\alpha_1\alpha_4}\delta_{\alpha_2\alpha_3}$$

$$\cdot \frac{e^{-\mu|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} c_{k_1\alpha_1}^{+} c_{k_2\alpha_2}^{+} c_{k_3\alpha_3} c_{k_4\alpha_4}$$

change of variables: let $\vec{r} \to \vec{r}+\vec{r}'$

$$= \frac{e^2}{2V^2} \iint d^3r \, d^3r' \sum_{\substack{\{k\} \\ \{\alpha\}}} e^{i(\vec{k}_4 - \vec{k}_1)\cdot \vec{r}} \, e^{i(\vec{k}_4 + \vec{k}_3 - \vec{k}_1 - \vec{k}_2)\cdot \vec{r}\,'}$$

$$\delta_{\alpha_1 \alpha_4} \delta_{\alpha_2 \alpha_3} \quad \frac{e^{-\mu r}}{r} c^{+}_{k_1\alpha_1} c^{+}_{k_2\alpha_2} c_{k_3\alpha_3} c_{k_4\alpha_4}$$

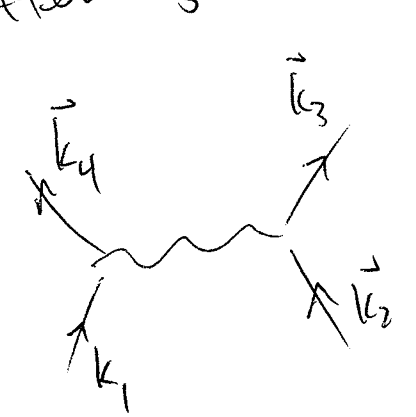
$$= \frac{e^2}{2V} \int d^3r' \sum_{\substack{\{k\} \\ \{\alpha\}}} \left(\frac{1}{V} \int d^3r \, e^{i(\vec{k}_4 - \vec{k}_1)\cdot \vec{r}} \frac{e^{-\mu r}}{r} \right) e^{i(\vec{k}_4 + \vec{k}_3 - \vec{k}_1 - \vec{k}_2)\cdot \vec{r}\,'}$$

$$\delta_{\alpha_1 \alpha_4} \delta_{\alpha_2 \alpha_3} \quad c^{+}_{k_1\alpha_1} c^{+}_{k_2\alpha_2} c_{k_3\alpha_3} c_{k_4\alpha_4}$$

$$\text{F.T.} \left[\frac{e^{-\mu r}}{r} \right] = \frac{4\pi}{k^2 + \mu^2}$$

"after" $\vec{k}_3 + \vec{k}_4$

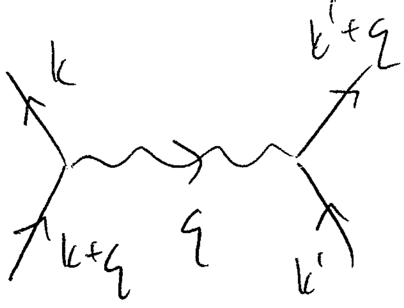
momentum conservation



$$\frac{1}{V} \int d^3r' \, e^{i(k_4 + k_3 - \vec{k}_1 + \vec{k}_2)\cdot \vec{r}\,'} = \delta(k_4 + k_3 - k_1 - k_2)$$

or $\delta_{k_1+k_2,\, k_3+k_4}$

"before" $k_1 + k_2$



process that transfers moment q between a pair of particles

$k_1 = k+q$

$k_2 = k'$

$k_3 = k'+q$

$k_4 = k$

→ momentum "before" and "after" is $k+k'+q$.

→ collapses one momentum sum

$$= \frac{e^2}{2V} \sum_{\{\alpha\}} \sum_{\substack{\vec{k}\vec{k}' \\ \vec{q}}} \frac{4\pi}{q^2+\mu^2} c^{\dagger}_{k+q,\alpha_1} c^{\dagger}_{k',\alpha_2} c_{k'+q,\alpha_3} c_{k,\alpha_4} \cdot \delta_{\alpha_1\alpha_4} \delta_{\alpha_2\alpha_3}$$

$$= \frac{e^2}{2V} \sum_{\alpha\beta} \sum_{\substack{kk' \\ q}} \frac{4\pi}{q^2+\mu^2} c^{\dagger}_{k+q,\alpha} c^{\dagger}_{k',\beta} c_{k'+q,\beta} c_{k,\alpha}$$

Separate out the uniform (i.e. $\vec{q}=0$) component

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

$$+ \underbrace{\frac{e^2}{2V}\sum_{\alpha\beta}\sum_{kk'} \frac{4\pi}{\mu^2}\, c^\dagger_{k,\alpha}\, c^\dagger_{k',\beta}\, c_{k',\beta}\, c_{k,\alpha}}$$

EXERCISE: Show that this is equal to $\frac{e^2}{2V}\cdot\frac{4\pi}{\mu^2}\left(\hat{N}^2-\hat{N}\right)$