Phys 726 - Lecture 1

* Quantum mechanics of a collection of mutually interacting, nonrelativistic particles

→ wave function $\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, t)$

probability amplitude

coordinate positions of the N particles

global time clock

→ governed by the Schrödinger equation

$$\left\{ -\frac{\hbar^2}{2m} \sum_{j=1}^{N} \nabla_j^2 + \sum_{j<j'} V(\vec{r}_j - \vec{r}_{j'}) + \sum_j U(\vec{r}_j) \right\} \Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

Hamiltonian
= operator expression of the total system energy

two-body interaction term

external potential

"Theory of Everything"

→ phase of Ψ is ambiguous with respect to the classical probability $|\Psi|^2$

$$\Psi(\text{particle at } A, \text{particle at } B)$$

$$= e^{i\theta}\, \Psi(\text{particle at } B, \text{particle at } A)$$

↗ phase arising from exchange

Indistinguishability implies that

$$e^{2i\theta} = 1 \quad \text{or} \quad e^{i\theta} = \begin{cases} +1 & \text{bosons} \\ -1 & \text{fermions} \end{cases}$$

* Second quantization is the key technical innovation

→ connection between $\underset{\substack{\text{ket in the}\\ \text{abstract state}\\ \text{space}}}{|\Psi(t)\rangle}$ and $\underset{\substack{\text{many body}\\ \text{wavefunction}}}{\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, t)}$

is overlap with a ket $|\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N\rangle$ in the position representation

→ Suppose the existence of single-body creation operator $\hat{\psi}(\vec{r})^\dagger$ such that

$$|\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N\rangle = \hat{\psi}(\vec{r}_1)^\dagger \hat{\psi}(\vec{r}_2)^\dagger \cdots \hat{\psi}(\vec{r}_N)^\dagger \underset{\text{vacuum state}}{|vac\rangle}$$

then

$$\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, t) = \underbrace{\langle vac|\hat{\psi}(\vec{r}_N) \cdots \hat{\psi}(\vec{r}_1)}_{\text{dual bra}}|\Psi(t)\rangle$$

* exchange statistics impose the operator algebra

$$\Psi(\vec{r}_1, \vec{r}_2) = \langle vac | \hat{\psi}(r_2) \hat{\psi}(r_1) | \Psi \rangle$$

$$\Psi(\vec{r}_2, \vec{r}_1) = \pm \Psi(\vec{r}_1, \vec{r}_2) \qquad \vec{r}_1 \neq \vec{r}_2$$

$$= \pm \langle vac | \hat{\psi}(\vec{r}_1) \hat{\psi}(\vec{r}_2) | \Psi \rangle$$

$$\Rightarrow \hat{\psi}(\vec{r}_1) \hat{\psi}(\vec{r}_2) = \pm \hat{\psi}(\vec{r}_2) \hat{\psi}(\vec{r}_1)$$

bosons commute

fermions anticommute

* Pauli exclusion

$$\Psi(\vec{r}_2, \vec{r}_1) = - \Psi(\vec{r}_1, \vec{r}_2)$$

$$\xrightarrow{\vec{r}_2 \to \vec{r}_1} \Psi(\vec{r}_1, \vec{r}_1) = - \Psi(\vec{r}_1, \vec{r}_1) \equiv 0 \quad \text{no weight}$$

→ in the fermion case

$$\hat{\psi}(\vec{r})^2 = \hat{\psi}(\vec{r})\,\hat{\psi}(\vec{r}) = 0$$

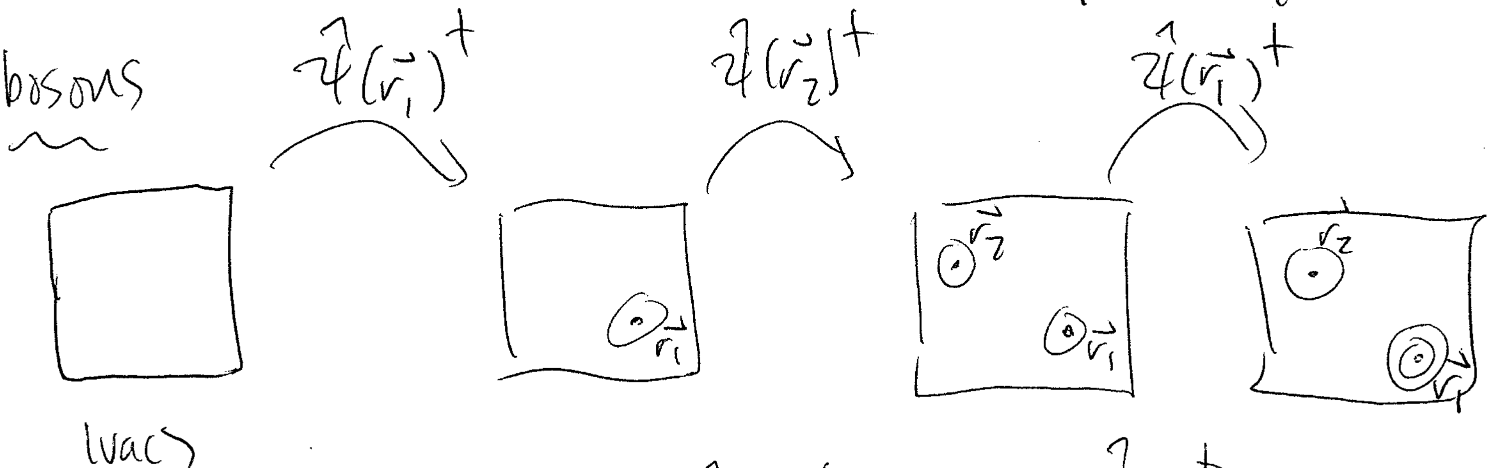
Schematically

$|vac\rangle$

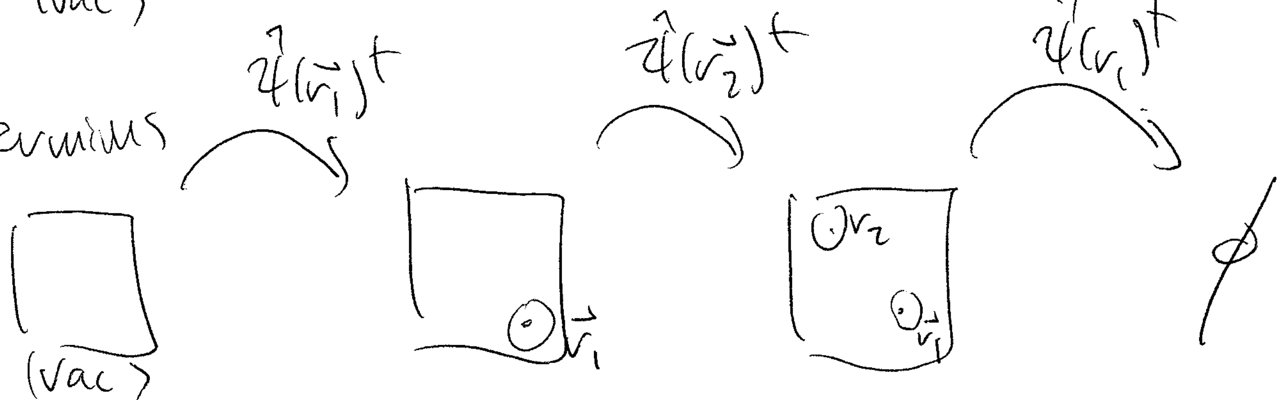
1-particle state
$\hat{\psi}(\vec{r}_1)^\dagger|vac\rangle$

3-particle state
$\hat{\psi}(\vec{r}_3)^\dagger\hat{\psi}(\vec{r}_2)^\dagger\hat{\psi}(\vec{r}_1)^\dagger|vac\rangle$

bosons



fermions



bosons $\hat{\psi}(\vec{r}_1)^\dagger \hat{\psi}(\vec{r}_2)^\dagger \hat{\psi}(\vec{r}_1)^\dagger |vac\rangle$

free to swap

$= (\hat{\psi}(\vec{r}_1)^\dagger)^2 \hat{\psi}(\vec{r}_2)^\dagger |vac\rangle$ canonical ordering

fermions $\hat{\psi}(\vec{r}_1)^\dagger \hat{\psi}(\vec{r}_3)^\dagger \psi(\vec{r}_2)^\dagger |vac\rangle$

$= - \hat{\psi}(r_1)^\dagger \hat{\psi}(r_2)^\dagger \hat{\psi}(r_3)^\dagger |vac\rangle$

$\xrightarrow{\vec{r}_3 \to \vec{r}_2} - \hat{\psi}(r_1)^\dagger \cancel{(\hat{\psi}(r_2)^\dagger)^2}^{\,0} |vac\rangle \equiv 0$

* Commutation / anticommutation relations

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

$-$ bosons, $+$ fermions

$$= \delta(\vec{r}-\vec{r}')$$

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

* Hamiltonian expressed in terms of field operators

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

$$\times \, V(\vec{r}, \vec{r}') \, \underbrace{\hat{\psi}(\vec{r}') \, \hat{\psi}(\vec{r})}_{\text{note the ordering}}$$

1-body kinetic energy e.g. $-\frac{\hbar^2 \nabla^2}{2m}$

2-body interaction potential

note the ordering (encompasses fermi and bose cases)

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

→ customary to express the field operators in terms of creation / annihilation ops for the 1-body modes that ~~sat~~ satisfy the eigenequation $T \phi_k = E_k \phi_k$

mode label (often momentum or crystal mom.)

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

← usually written c for fermions and a for bosons

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

→ the $\phi_k(\vec{r})$ states ~~are~~ form an orthonormal set, so

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

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

→ generic, local, 1-body operator (<u>bilinear</u> in the fields) looks like

$$\hat{J} = \int d^3r \; \hat{\psi}(\vec{r})^\dagger J(\vec{r}) \hat{\psi}(\vec{r})$$

$$= \int d^3r \; \sum_k \phi_k(\vec{r})^* c_k^\dagger \; J(\vec{r}) \sum_{k'} \phi_{k'}(\vec{r}) c_{k'}$$

$$= \sum_{kk'} \underbrace{\left\{ \int d^3r \; \phi_k^*(\vec{r}) J(\vec{r}) \phi_{k'}(\vec{r}) \right\}}_{\text{matrix element}} c_k^\dagger c_{k'}$$

$$= \sum_{kk'} \langle k | J | k' \rangle c_k^\dagger c_k$$

e.g. number-density operator

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

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

and the total particle number

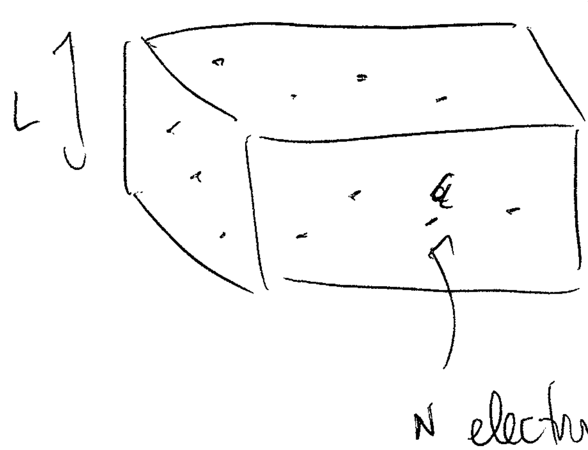
$$\hat{N} = \int d^3r\, \hat{n}(\vec{r}) = \sum_{kk'} \underbrace{\int d^3r\, \phi_k(\vec{r})^* \phi_{k'}(\vec{r})}_{\delta_{kk'}}\, c_k^\dagger c_{k'}$$

$$= \sum_k c_k^\dagger c_k \equiv \sum_k \hat{n}_k$$

$\hat{n}_k = c_k^\dagger c_k$ is the occupation number operator on each mode k

EXAMPLE: Degenerate electron gas

→ interacting gas of negative charges in a uniformly distributed background of compensating positive charge



Volume $V = L^3$

← charge density $+eN/V$

Single-particle wave functions

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

↑ spinor $\chi_\uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$\chi_\downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

necessary for $S=1/2$ particles

$\vec{k} = \frac{2\pi}{L}(\mathbb{Z}, \mathbb{Z}, \mathbb{Z})$ because of periodic

boundary conditions

Hamiltonian is sum of three terms

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

$$H_{el} = \sum_{j=1}^{N} \frac{p_j^2}{2m} + \frac{1}{2} \sum_{i \neq j} \frac{e^{-\mu |\vec{r}_i - \vec{r}_j|}}{|r_i - r_j|}$$

(we'll take $\mu \to 0$ at the end)

Yukawa potential for regularization

charge ~~number~~ density of background +ve

$$H_b = \frac{1}{2} \iint d^3r \, d^3r' \, \frac{\rho(\vec{r}) \rho(\vec{r}\,') e^{-\mu |\vec{r} - \vec{r}\,'|}}{|\vec{r} - \vec{r}\,'|}$$

$$H_{el-b} = - e \sum_{i=1}^{N} \int d^3r \, \frac{\rho(\vec{r}) e^{-\mu |\vec{r} - \vec{r}_i|}}{|\vec{r} - \vec{r}_i|}$$

Background is inert (no dynamical quantum degrees of freedom)

$$\rho = e\frac{N}{V} = \text{const}$$

$$H_b = \frac{1}{2}e^2\left(\frac{N}{V}\right)^2 \iint d^3r\, d^3r' \, \frac{e^{-\mu|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}$$

$$= \frac{1}{2}e^2\left(\frac{N}{V}\right)^2 \cdot V \cdot \int d^3r \, \frac{e^{-\mu r}}{r} \quad \text{(transl. invariance)}$$

$$\boxed{= \frac{1}{2}e^2 \frac{N^2}{V} \cdot \frac{4\pi}{\mu^2}} \quad \text{(divergent as } \mu \to 0\text{)}$$

$$H_{el-b} = -e^2 \sum_{i=1}^{N} \frac{N}{V} \int d^3r \, \frac{e^{-\mu|\vec{r}-\vec{r}_i|}}{|\vec{r}-\vec{r}_i|}$$

$$= -e^2 \sum_{i=1}^{N} \frac{N}{V} \int d^3r \, \frac{e^{-\mu r}}{r}$$

$$\boxed{= -e^2 \frac{N^2}{V} \frac{4\pi}{\mu^2}}$$

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

All the interesting physical effects are contained in H_{el}

Kinetic energy part...

$$\langle \vec{k}_1 \alpha_1 | T | \vec{k}_2 \alpha_2 \rangle = \frac{1}{V} \int d^3r \, e^{-i\vec{k}_1 \cdot \vec{r}} \chi_{\alpha_1} \left(-\frac{\hbar^2}{2m} \nabla^2 \right) \times e^{+i\vec{k}_2 \cdot \vec{r}} \chi_{\alpha_2}$$

$$= \frac{\hbar^2 k_2^2}{2mV} \delta_{\alpha_1 \alpha_2} \underbrace{\int d^3r \, e^{i(\vec{k}_2 - \vec{k}_1) \cdot \vec{r}}}_{V \delta_{k_1 k_2}}$$

$$= \frac{\hbar^2 k_2^2}{2m} \delta_{\alpha_1 \alpha_2} \delta_{k_1 k_2}$$

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

potential energy part

$$\langle \vec{k}_1\, \alpha_1\, \vec{k}_2\, \alpha_2 \,|\, V \,|\, \vec{k}_3\, \alpha_3\, \vec{k}_4\, \alpha_4 \rangle$$