VI Identical particles

In principle QM formalism easy to generalize to N particles. E.g. coordinates $\bar{r}_i$ and spins $(\bar{S}_i^2, S_{iz})$ form a complete commuting set of observables, and wave function would be

$$\psi(\bar{r}_1, \underbrace{s_1, s_{1z}}_{\text{shorthand } s_1}; \bar{r}_2, s_2, s_{2z}; \dots; \bar{r}_N, s_N, s_{Nz}) = \langle \bar{r}_1 s_1 \bar{r}_2 s_2 \dots \bar{r}_N s_N | \psi \rangle$$

If particles are independent, i.e. mutually noninteracting
⇒ separate variables
⇒ wave function product of <u>individual</u> wave functions

$$\psi = \varphi_1(\bar{r}_1, s_1)\, \varphi_2(\bar{r}_2, s_2) \cdots \varphi_N(\bar{r}_N, s_N)$$

(same structure for momentum representation)

Hamiltonian depends on $\{\bar{r}_i, \bar{p}_i, s_i\}$

$$\hat{H} = \hat{H}(\bar{p}_1, \bar{r}_1, s_1; \dots; \bar{p}_N, \bar{r}_N, s_N)$$

If particles are distinguishable (eg. different mass, charge, spin, ...) nothing new.

For <u>identical</u> particles new interesting features

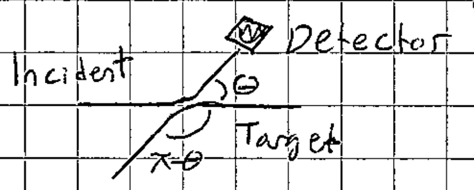
$\hat{H}$ (and other observables → operators) must be <u>symmetric in particle exchange</u>

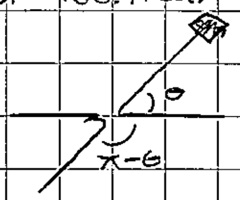
$$H(\dots; \bar{p}_i \bar{r}_i s_i; \dots; \bar{p}_j \bar{r}_j s_j; \dots) = H(\dots; \bar{p}_j, \bar{r}_j, s_j; \dots; \bar{p}_i, \bar{r}_i, s_i; \dots)$$

since physical properties of system must not change.

Similar argument holds in classical mechanics, but there particles retain their identity in following well-defined trajectories.

Think of scattering of identical particles:





In classical mechanics, detector rate is the sum of incident and target particles (identical) flying to detector:

$$\frac{d\sigma_I}{d\Omega} = \frac{d\sigma(\Theta)}{d\Omega} + \frac{d\sigma(\pi-\Theta)}{d\Omega}$$

incident — target to det., incident at angle $\pi-\Theta$

In QM, cannot distinguish beam and target particles after collision ⇒ scattering amplitude a superposition

$$\frac{d\sigma_I}{d\Omega} = |f(\Theta) + f(\pi-\Theta)|^2 = \frac{d\sigma(\Theta)}{d\Omega} + \frac{d\sigma(\pi-\Theta)}{d\Omega} + 2\,\mathrm{Re}\, f^*(\Theta) f(\pi-\Theta)$$

↑ $\sigma \sim |f|^2$ — ↑ extra term, interference

Define exchange operator $\hat{P}_{ij}$, which exchanges two particles i, j

$$\hat{P}_{ij}\,\psi(\ldots; \bar{r}_i, s_i; \ldots; \bar{r}_j, s_j; \ldots) = \psi(\ldots; \bar{r}_j, s_j; \ldots; \bar{r}_i, s_i; \ldots)$$

Hamiltonian is invariant in this transformation

$$\hat{P}_{ij}\,\hat{H}\,\hat{P}_{ij}^{-1} = \hat{H} \quad \Rightarrow \quad [\hat{P}_{ij}, \hat{H}] = 0$$

Clearly $\hat{P}_{ij}^2 = 1 \Rightarrow \hat{P}_{ij}^{-1} = \hat{P}_{ij}$

Easy to see by integrating

$$\langle \varphi | P_{ij} \psi \rangle = \langle \psi | P_{ij} \varphi \rangle^* \Rightarrow \text{Hermitian},$$

eigenvalues $\pi_{ij} = \pm 1$

π_{ij} constant of motion, eigenstates of $\hat{H}$ can be chosen as eigenstates of $\hat{P}_{ij}$, i.e. symmetric or antisymmetric.

$$\hat{P}_{ij}\,\psi^S(\ldots,i,\ldots,j,\ldots) = \psi^S(\ldots,j,\ldots,i,\ldots) = +\psi^S(\ldots,i,\ldots,j,\ldots)$$

$$\hat{P}_{ij}\,\psi^A(\ldots,i,\ldots,j,\ldots) = \psi^A(\ldots,j,\ldots,i,\ldots) = -\psi^A(\ldots,i,\ldots,j,\ldots)$$

Example: two identical particles, $\psi(1,2)$ any function

$$\psi^S(1,2) = N_S\left[\psi(1,2)+\psi(2,1)\right]$$
$$\psi^A(1,2) = N_A\left[\psi(1,2)-\psi(2,1)\right]$$

$$N_{S/A} = \left[2 \pm 2\,\mathrm{Re}\,\langle\psi(1,2)|\psi(2,1)\rangle\right]^{-1/2}$$

Example: three particles
completely (anti) symmetric states

$$\psi^S(1,2,3) = N_{3S}\left[\psi(1,2,3)+\psi(2,3,1)+\psi(3,1,2)+\psi(2,1,3)+\psi(3,2,1)+\psi(1,3,2)\right]$$

$$\psi^A(1,2,3) = N_{3A}\left[\psi(1,2,3)+\psi(2,3,1)+\psi(3,1,2)-\psi(2,1,3)-\psi(3,2,1)-\psi(1,3,2)\right]$$

In addition, there are 4 other linearly independent combinations, with different eigenvalues π_{ij} for different pairs (e.g. $\pi_{12}=+1$, $\pi_{23}=-1$).
These mixed symmetries do not appear in nature!

States of identical particles either fully symmetric or antisymmetric in any pair exchange.

symmetric: bosons — integer spin
$\gamma, \pi, W^\pm, Z, g,$ "α" — Bose-Einstein statistics

antisymmetric: fermions — half-integer spin
$q, e^\pm, p, \bar{p}, \nu,$ "^{3}He" — Fermi-Dirac statistics

Spin-statistics theorem

VI.2 Fermion system

System of N noninteracting identical fermions:
- electrons in atom
- nucleons in nucleus
- electrons in solids

(interelectron forces approximated by a mean field)

Common potential $V(\bar{r})$,

$$\hat{H} = \sum_{i=1}^{N} \hat{H}_1(\bar{p}_i, \bar{r}_i, s_i) \quad , \quad \hat{H}_1(\bar{p}, \bar{r}, s) = \frac{\bar{p}^2}{2m} + V(\bar{r}, s)$$

one-particle Hamiltonian

Assume eigenstates of $\hat{H}_1$ known,

$$\hat{H}_1 u_k(\bar{r}, s) = E_k u_k(\bar{r}, s)$$

A solution of N-particle Schrödinger equation would be

$$H\Psi = E\Psi \quad \text{with} \quad \Psi(1, \dots, N) = u_{k_1}(1)\, u_{k_2}(2) \cdots u_{k_N}(N)$$

$$E = E_{k_1} + E_{k_2} + \dots + E_{k_N}$$

but this is not antisymmetric!
Any permutation also solution with same energy

$\Rightarrow$ totally antisymmetric linear combination of permutations

Slater's determinant

$$\Psi(1, \dots, N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} u_{k_1}(1) & u_{k_1}(2) & \dots & u_{k_1}(N) \\ u_{k_2}(1) & u_{k_2}(2) & \dots & u_{k_2}(N) \\ u_{k_3}(1) & & & \vdots \\ \vdots & & & \\ u_{k_N}(N) & & & u_{k_N}(N) \end{vmatrix}$$

2-particle exchange = exchange two columns, change of sign

Every particle in every state with same probability as others

State known, when we know which one-particle states appear, or are <u>occupied</u>.

If two one-body states are same, det = 0

⇒ <u>Pauli's exclusion principle</u>: two identical fermions cannot be in same state

Note: determinant normalized correctly, as all 1-body states are orthogonal → permutation terms orthogonal ($N!$ of them)

Also if two coordinates are same, w.f. → 0
⇒ statistical repulsion (even without interaction)

<u>Example</u>: two spin-$\frac{1}{2}$ fermions

same spin: $\frac{1}{\sqrt{2}}\begin{vmatrix} u_1(\bar{r}_1)\uparrow_1 & u_1(\bar{r}_2)\uparrow_2 \\ u_2(\bar{r}_1)\uparrow_1 & u_2(\bar{r}_2)\uparrow_2 \end{vmatrix} = \frac{1}{\sqrt{2}}\left(u_1(\bar{r}_1)u_2(\bar{r}_2) - u_1(\bar{r}_2)u_2(\bar{r}_1)\right)\uparrow_1\uparrow_2$ ← $|11\rangle$

different spin $\frac{1}{\sqrt{2}}\begin{vmatrix} u(\bar{r}_1)\uparrow_1 & u(\bar{r}_2)\uparrow_2 \\ u(\bar{r}_1)\downarrow_1 & u(\bar{r}_2)\downarrow_2 \end{vmatrix} = u(\bar{r}_1)u(\bar{r}_2)\underbrace{\frac{1}{\sqrt{2}}\left(\uparrow_1\downarrow_2 - \downarrow_1\uparrow_2\right)}_{|00\rangle}$

symmetric spin ⇔ antisymmetric space
(triplet)
antisymmetric spin ⇔ symmetric space
(singlet)

Eg. helium ground state symmetric in space
~ 2 hydrogens ⇒ spins in singlet state $s=0$

<u>Example 2</u>: expectation value of separation

Distinguishable: $\psi(1,2) = \psi_a(1)\psi_b(2) \Rightarrow \langle (x_1-x_2)^2\rangle_d = \langle x^2\rangle_a + \langle x^2\rangle_b - 2\langle x\rangle_a\langle x\rangle_b$

Identical $\begin{cases}\text{bosons} \\ \text{fermion}\end{cases}$ $\psi = \frac{1}{\sqrt{2}}\left[\psi_a(1)\psi_b(2) \pm \psi_a(2)\psi_b(1)\right] \Rightarrow \langle (x_1-x_2)^2\rangle_{B/F} = \langle (x_1-x_2)^2\rangle_d \mp 2|\langle x\rangle_{ab}|^2$

where $\langle x\rangle_{ab} = \int x\,\psi_a^*(x)\,\psi_b(x)\,dx$

If no overlap, no interference

Inter-particle interactions

$$\hat{H} = \sum_{i=1}^{N} \hat{H}_1(i) + \sum_{i<j} \hat{V}_2(i,j)$$

$\hat{V}_2$ ~ 2-body operator

In principle Ψ can be expanded in terms of Slater determinants, but difficult without approximations

Common & useful: mean field approximation

$$\sum_{i<j} \hat{V}_2(i,j) \approx \sum_i \hat{W}(i) \; ; \quad \hat{H}_1 \to \frac{\hat{p}^2}{2m} + \hat{V}_1(\bar{r},s) + \hat{W}(\bar{r},s)$$

⇒ 1-body solutions form Slater determinants, deviations from $\hat{W}$ residual interactions best treated in perturbation theory

Shell models:

lowest energy states occupied, each state has one fermion ⇒ each spatial state 2, if spin-½

atoms:

each shell $(n\ell)$ can take $2\times(2\ell+1)$ electrons

ns	2	8 = period in periodic tables
np	6	

- heavier atoms also d, f states, energies close to other shells: e.g. $3d \sim 4s$, $4f \sim 5d \sim 6s$

(- approximate spherically symmetric mean field)

nudei:

$|n\ell s m_\ell m_s\rangle \to |n\ell s j m_j\rangle$

strong spin-orbit coupling $\bar{L}\cdot\bar{S} = \frac{1}{2}(J^2 - L^2 - S^2)$

⇒ m_ℓ, m_s not good quantum numbers, need $\bar{J} = \bar{L} + \bar{S}$ & m_j

energy independent of m_j ⇒ shells of $2j+1$ protons + $2j+1$ neutrons

- classification of shells by nj, full shell has $2(2j+1)$ nucleons

Example: degeneracy pressure

Assume a Fermi gas with all lowest energy states occupied

remember, that in a box of side length L $\quad \bar{p} = \frac{2\pi\hbar}{L}(n_x, n_y, n_z)$

$\Rightarrow$ number of states with $|\bar{p}| \leq p_{max} \equiv p_F$

$$N = \frac{4}{3}\pi p_F^3 \cdot \left(\frac{L}{2\pi\hbar}\right)^3 \cdot 2$$

(2: spin-½)

density $\rho_0 = \frac{N}{V} = \frac{N}{L^3} = \frac{p_F^3}{3\pi^2\hbar^3} \equiv \frac{k_F^3}{3\pi^2}$

$\rightarrow k_F = (3\pi^2\rho_0)^{1/3}$ Fermi-momentum

$$E_F = \frac{\hbar^2 k_F^2}{2m}$$

Density of states of energy E:

$$\rho(E) = \frac{dN}{dE} = \frac{d}{dE}\left(\frac{L^3}{3\pi^2}\left(\frac{2mE}{\hbar^2}\right)^{3/2}\right) = \frac{L^3}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}$$

$\Rightarrow$ total energy $E_{tot} = \int_0^{E_F} dE\, \rho(E)\, E = \frac{L^3}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^{E_F} dE\, E^{3/2}$

$$= \frac{L^3}{5\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_F^{5/2} = \frac{L^3}{5\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left[\frac{\hbar^2}{2m}\left(3\pi^2\frac{N}{L^3}\right)^{2/3}\right]^{5/2}$$

$$= \frac{\hbar^2}{10m\pi^2}(3\pi^2 N)^{5/3} V^{-2/3} \qquad V = L^3$$

Pressure: $dE = -p\,dV$

$$\Rightarrow p = -\frac{dE}{dV} = \frac{\hbar^2}{15m\pi^2}\left(3\pi^2\frac{N}{V}\right)^{5/3} = \frac{\hbar^2}{5m}(3\pi^2)^{2/3}\rho_0^{5/3}$$

No heat, no interactions, just electrons in ground state

$\Rightarrow$ pressure

This prevents neutron stars and white dwarves from collapsing.