Phys. 528 Lecture 13

Quantum Many-particle systems

$$\hat{H} = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i=1}^{N} U(\vec{r}_i, t) + \sum_{i<j} V(\vec{r}_i, \vec{r}_j),$$

where e.g., $V(\vec{r}_i, \vec{r}_j) = \dfrac{e^2}{|\vec{r}_i - \vec{r}_j|}$.

Because all of the particles have exactly the same mass, charge, spin, etc., $\hat{H}$ has a symmetry under particle interchange. Define the particle exchange operator

$$\hat{P}_{ij} f(\vec{r}_1, \ldots, \vec{r}_i, \ldots, \vec{r}_j, \ldots, \vec{r}_N)$$
$$= f(\vec{r}_1, \ldots, \vec{r}_j, \ldots, \vec{r}_i, \ldots, \vec{r}_N)$$

Clearly, $[\hat{P}_{ij}, \hat{H}] = 0$.

The eigenstates of $\hat{H}$ may thus be chosen as eigenstates of $\hat{P}_{ij}$.
This is a fundamental symmetry of nature.

1) Noninteracting particles

For simplicity, let's drop the 2-body interaction $V(\vec{r}_i, \vec{r}_j)$ for the moment.

Then $$\hat{H} = \sum_{i=1}^{N} \hat{H}_i ,$$

$$\hat{H}_i = \frac{\vec{p}_i^{\,2}}{2m} + U(\vec{r}_i)$$

The eigenstates and eigenvalues of $\hat{H}_i$ are

$$\hat{H}_i \psi_n(\vec{r}_i) = \varepsilon_n \psi_n(\vec{r}_i) .$$

It is easy to construct an eigenstate of the total Hamiltonian:

$$\Psi_D(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N) = \prod_{i=1}^{N} \psi_{n_i}(\vec{r}_i)$$

with eigenvalue

$$E = \sum_{i=1}^{N} \varepsilon_{n_i} .$$

However, Ψ_D is not an eigenstate of $\hat{P}_{ij}$ (unless $n_i = n_j$). The only such product wavefunction that is an eigenstate of all the $\hat{P}_{ij}$ is the one with $n_i = n \ \forall i$, which is clearly not the most general quantum state of the system.

In quantum mechanics, it is not possible to tell the difference between two identical particles, because we cannot follow their individual trajectories (due to the uncertainty principle) to tell which is which. Thus, all physical observables should be invariant under particle exchange.

For example

$$|\hat{P}_{ij}\psi|^2 = |\psi|^2.$$

2) Eigenstates of $\hat{P}_{ij}$

suppose $\hat{P}_{ij}\psi = \lambda\psi$

$$\hat{P}_{ij}^2\psi = \lambda^2\psi.$$

But $\hat{P}_{ij}^2\psi(\ldots,\vec{r}_i,\ldots,\vec{r}_j,\ldots) = \psi(\ldots,\vec{r}_i,\ldots\vec{r}_j\ldots)$

so $\lambda^2 = 1 \qquad \lambda = \pm 1$

i) N = 2

Given two 1-body wavefunctions $\psi_1(\vec{r})$ and $\psi_2(\vec{r})$, we can construct symmetric and antisymmetric 2-body states as follows

$$\Psi_\pm(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}\left[\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) \pm \psi_2(\vec{r}_1)\psi_1(\vec{r}_2)\right]$$

$$\hat{P}_{12}\Psi_\pm = \pm\Psi_\pm$$

Fermions and bosons

Depending on their (intrinsic) spin, systems of identical particles are either symmetric under particle exchange (bosons) or antisymmetric (fermions):

particle type	spin	symmetry under $\hat{P}_{12}$
boson	integer	$+$
fermion	half-odd integer	$-$

(spin-statistics theorem)

Examples of fermions:

electron, proton, neutron, quark, neutrino, atom with half-odd integer total angular monetum

Examples of bosons:

photon, gluon, $W^{\pm}$, Z, phonon, atom with integer total angular momentum

Pauli principle

Two fermions of the same species cannot have the same wavefunction — they cannot occupy the same quantum state.

Proof Suppose each occupied some state $\psi(\vec{r})$. Then

$$\Psi_-(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}\left[\psi(\vec{r}_1)\psi(\vec{r}_2) - \psi(\vec{r}_2)\psi(\vec{r}_1)\right]$$
$$= 0$$

$\Rightarrow$ not allowed state (un-normalizable)

ii) General N

Let $P \in S_N$ be a permutation of the N particles.

$$\Psi_\pm(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \frac{1}{\sqrt{N!}} \sum_P (\pm 1)^P \prod_{i=1}^{N} \psi_{n_i}(\vec{r}_{P_i})$$

Factor is -1 if P is an odd permutation, $+1$ if P is an even permutation (for fermions).

Slater determinant

$$\psi_-(\vec{r}_1, \ldots, \vec{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_{n_1}(\vec{r}_1) & \psi_{n_1}(\vec{r}_2) & \cdots & \psi_{n_1}(\vec{r}_N) \\ \psi_{n_2}(\vec{r}_1) & \cdots & & \vdots \\ \vdots & & & \\ \psi_{n_N}(\vec{r}_1) & \cdots & & \psi_{n_N}(\vec{r}_N) \end{vmatrix}$$