The many-body problem in quantum mechanics

So far we have dealt with a single particle only. The wave function for a single particle is a function of time, spatial coordinates, and, possibly spin:

$$\Psi = \Psi(\vec{r}, s, t) = \begin{pmatrix} \varphi_\uparrow(\vec{r},t) \\ \varphi_\downarrow(\vec{r},t) \end{pmatrix} \quad \text{(assuming spin } 1/2\text{)}$$

For a system of N particles things become more complicated. If we ignore spin for the moment, the wave function depends on $\vec{r}_i$ $i = 1 \dots N$ and t:

$$\Psi = \Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots \vec{r}_N, t)$$

For a general case of interacting particles the dependence on $\vec{r}_i$'s is very nontrivial. The time evolution is still governed by the Schrödinger equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi$$

Here the Hamiltonian for the whole system is:

$$\hat{H} = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m_i} + V(\vec{r}_1, \vec{r}_2, \dots \vec{r}_N, t) = \sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \vec{\nabla}_i^2 + V(\vec{r}_1, \dots \vec{r}_N, t)$$

The statistical interpretation carries over in the obvious way:

$$|\Psi(\vec{r}_1, \vec{r}_2, \dots \vec{r}_N, t)|^2 \, d\vec{r}_1 \, d\vec{r}_2 \dots d\vec{r}_N$$

is the probability of finding particle 1 in the element of volume $d\vec{r}_1$ and at the same time particle 2 in the element of volume $d\vec{r}_2$, particle 3 in $d\vec{r}_3$ and so on. This probability is a function of the

Since the probability of finding any particle anywhere must be equal to unity, the normalization condition for the wave function is

$$\int |\Psi(\vec{r}_1, \ldots, \vec{r}_N, t)|^2 \, d\vec{r}_1 \ldots d\vec{r}_N = 1$$

If the potential V is time independent (e.g. there is no explicit dependence on t) we can, again, as before, use the separation of variables approach to represent the general solution as

$$\Psi(\vec{r}_1, \ldots \vec{r}_N, t) = \sum_k' c_k \psi_k(\vec{r}_1, \ldots \vec{r}_N) \, e^{-\frac{iE_k t}{\hbar}}$$

where ψ_k's are stationary (or partial) solutions that satisfy the time-independent Schrödinger equation

$$\left[-\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \nabla_i^2 + V(\vec{r}_1, \ldots \vec{r}_N) \right] \psi_k(\vec{r}_1, \ldots \vec{r}_N) = E_k \psi_k(\vec{r}_1, \ldots \vec{r}_N)$$

In most practical application potential V is a sum of single-particle and pairwise interparticle interactions:

$$V = \underbrace{\sum_{\substack{i,j=1 \\ i>j}}^{N}{}' V_{ij}(\vec{r}_i, \vec{r}_j)}_{\text{two-body potential}} + \underbrace{\sum_{i=1}^{N} U_i^{ext}(\vec{r}_i)}_{\text{external potential}}$$

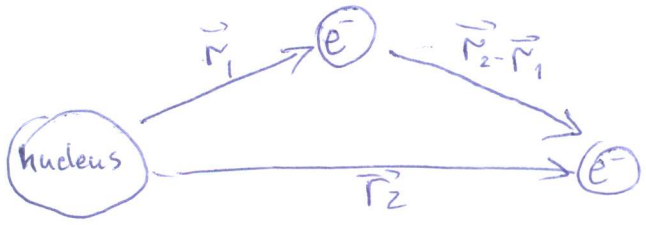
Moreover, oftentimes, V_{ij} is central and depends only on the distance between particles:

$$V_{ij}(\vec{r}_i, \vec{r}_j) = V_{ij}(|\vec{r}_i - \vec{r}_j|) = V_{ij}(r_{ij})$$

The solution of the N-particle Schrödinger equation is, generally, a very difficult task, even in the stationary case. Various numerical approaches have been developed to tackle this problem.

A simple example of a many-body problem in quantum mechanics is the He atom (or He-like ion):

$$\hat{H} = -\frac{\hbar^2}{2m_n}\vec{\nabla}_n^2 - \frac{\hbar^2}{2m_e}\vec{\nabla}_1^2 - \frac{\hbar^2}{2m_e}\vec{\nabla}_2^2 - \frac{Ze^2}{|\vec{r}_1-\vec{r}_n|} - \frac{Ze^2}{|\vec{r}_2-\vec{r}_n|} + \frac{e^2}{|\vec{r}_1-\vec{r}_2|}$$



Here m_n is the mass of the nucleus and m_e is the mass of the electron

Identical particles

Suppose we have a system of two particles that have the same mass, charge, etc. In other words, suppose the two particles are of exactly the same nature. Now if we suppose particle 1 is in the one-particle state (assume no interaction) $\psi_a(\vec{r})$, and particle 2 is in the state $\psi_b(\vec{r})$. If we ignore spin for the moment then the total wave function is a simple product:

$$\psi(\vec{r}_1, \vec{r}_2) = \psi_a(\vec{r}_1)\,\psi_b(\vec{r}_2)$$

This assumes that we can tell particles apart.

In classical mechanics we can always tell particles apart. In quantum mechanics the situation is fundamentally different. We cannot paint or label particles. We cannot track them as tracking must involve some sort of a measurement that inevitably and unpredictably alter its state. Because of that we cannot be sure that particles switch places. The fact is, all particles of the same nature (e.g. electrons) are utterly identical.

Quantum mechanics neatly accomodates the existence of particles that are indistinguishable in principle. We simply construct a wave function that does not discriminate between particles and is non-committal as to which particle is in which state

$$\psi_{\pm}(\vec{r}_1, \vec{r}_2) = A\left[\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) \pm \psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\right]$$

The theory admits two kinds of particles; bosons (the plus sign) and fermions (the minus sign). Relativistic theory establishes a connection between spin of particles and statistics. It turns out that all fermions have half integer spin and vice versa. All particles with integer spin are bosons.

It follows that two identical fermions cannot occupy the same (single-particle) state. This is because

$$\psi_-(\vec{r}_1, \vec{r}_2) = A\left[\psi_a(\vec{r}_1)\psi_a(\vec{r}_2) - \psi_a(\vec{r}_2)\psi_a(\vec{r}_1)\right] = 0$$

This constitutes the well-known Pauli exclusion principle.

To consider things in a more formal way let us