PHYS-505/551

Identical Particle in QM

Lecture-11

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Definitions

- Identical particles in QM are not distinguishable. But this has dramatic consequences in the quantum mechanical description of a system.
- Suppose we have a system of two electrons. The wave function of this system which contains information about position and spin is given by:

$$\Psi = \Psi\left(\mathbf{r}_1, s_1; \mathbf{r}_2, s_2\right) = \Psi\left(1,2\right)$$

$$1 \equiv \mathbf{r}_1, s_1 \text{ and } 2 \equiv \mathbf{r}_2, s_2$$

Definitions

- Since the particles are identical and not distinguishable then the mutual change 1<-> 2 must not have measurable consequences in the system's state. This means that:

$$\Psi(2,1) = e^{ia}\Psi(1,2)$$

and implies that $e^{i2a} = 1 \Rightarrow e^{ia} = \pm 1$ so the final form is

$$\Psi(2,1) = \pm\Psi(1,2)$$

Definitions

- This relation says to us that: **The wave-function of a system of two identical particles must be either symmetric or anti-symmetric with respect to the interchange of its variables.**
- Now the question is: which of the two signs, + and -, we must keep? The answer is given by Pauli's Principle:
- **All the particles with integer spin (bosons) are described by symmetrical wave-functions. All the particles with half-integer spin (fermions) are described by anti-symmetrical wave-functions**.

Implications

- Assume a system of two identical electrons interacting with electric only forces which they do not involve the spin.
- The total wave-function is the separable in a product of a spatial part and a spin part:

$$\Psi = \Psi\left(\mathbf{r}_1, s_1; \mathbf{r}_2, s_2\right) = \psi\left(\mathbf{r}_1, \mathbf{r}_2\right) X\left(s_1, s_2\right)$$

- We know that we have two different cases for the electron spins:

Implications

- A) The two electrons have parallel spins (total spin S=1). In this case

$$X_{\uparrow\uparrow}(s_1,s_2)=\begin{cases} X_{\uparrow}(s_1)X_{\uparrow}(s_2) \\ \frac{1}{\sqrt{2}}\left(X_{\uparrow}(s_1)X_{\downarrow}(s_2)+X_{\downarrow}(s_1)X_{\uparrow}(s_2)\right) \\ X_{\downarrow}(s_1)X_{\downarrow}(s_2) \end{cases}$$

- From where it is obvious that

$$X_{\uparrow\uparrow}(s_2,s_1)=X_{\uparrow\uparrow}(s_1,s_2)$$

Implications

- This has the following implication. Since the electrons are fermions the total wave-function must be symmetric, thus:

$$\Psi\left(\mathbf{r}_1, s_1; \mathbf{r}_2, s_2\right) = -\Psi\left(\mathbf{r}_2, s_2; \mathbf{r}_1, s_1\right) \Rightarrow$$

$$\psi\left(\mathbf{r}_1, \mathbf{r}_2\right) X\left(s_1, s_2\right) = -\psi\left(\mathbf{r}_2, \mathbf{r}_1\right) X\left(s_2, s_1\right) \Rightarrow$$

$$\psi\left(\mathbf{r}_1, \mathbf{r}_2\right) = -\psi\left(\mathbf{r}_2, \mathbf{r}_1\right)$$

Anti-symmetric spatial wave-function

Implications

- B) The two electrons have anti-parallel spins (total spin S=0). In this case

$$X_{\uparrow\downarrow}(s_1,s_2)=\frac{1}{\sqrt{2}}\left(X_{\uparrow}(s_1)X_{\downarrow}(s_2)-X_{\downarrow}(s_1)X_{\uparrow}(s_2)\right)$$

- From where it is obvious that

$$X_{\uparrow\downarrow}(s_2,s_1)=-X_{\uparrow\downarrow}(s_1,s_2)$$

Implications

- Since the electrons are fermions the total wave-function must be anti-symmetric, thus:

$$\Psi(\mathbf{r}_1, s_1; \mathbf{r}_2, s_2) = -\Psi(\mathbf{r}_2, s_2; \mathbf{r}_1, s_1) \Rightarrow$$

$$\psi(\mathbf{r}_1, \mathbf{r}_2) X(s_1, s_2) = -\psi(\mathbf{r}_2, \mathbf{r}_1)(-X(s_2, s_1)) \Rightarrow$$

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \psi(\mathbf{r}_2, \mathbf{r}_1)$$

Symmetric spatial wave-function

Implications

- If the wave-function is anti-symmetric then, as we said:

$$\psi\left(\mathbf{r}_1,\mathbf{r}_2\right) = -\psi\left(\mathbf{r}_2,\mathbf{r}_1\right)$$

- But if we put $\mathbf{r}_1 = \mathbf{r}_2 = \mathbf{r}$ we get

$$\psi\left(\mathbf{r},\mathbf{r}\right) = -\psi\left(\mathbf{r},\mathbf{r}\right) \Rightarrow \psi\left(\mathbf{r},\mathbf{r}\right) = 0$$

- This means that the probability to find two electrons **at the same** point of the space is **zero**! This is a special consequence of the Pauli exclusion principle.

Implications

- This has more interesting consequences. The zero value of the spatial wave-function means that as the two electrons approach each other the wave-function gets smaller values. Thus the probability becomes smaller or, in other words: **Electrons with parallel spins tend to "repel" each other.**
- On the contrary **when the spins are anti-parallel they tend to "attract" each other!**

Repulsion of parallel spins explains the ferromagnetism. The electrons, in order to minimize their electrostatic energy, develop parallel spins. Thus they create a large macroscopic magnet. The atomic magnets line up not because of their magnetic interaction but of the combination of electric repulsion and Pauli principle.

Pauli Exclusion Principle

- If we assume N particles that interact with a common external potential but **not** between each other then the total spatial wave-function is a product of N separate spatial wave-functions:

$$\psi\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right) = \psi\left(\mathbf{r}_1\right)\cdots\psi\left(\mathbf{r}_N\right)$$

- Assume now that we have the simplest multi-electron system which is the He atom and that one electron is placed at state α and the other at a state β such

$$\alpha \equiv n_1 l_1 m_1 \qquad \beta \equiv n_2 l_2 m_2$$

Pauli Exclusion Principle

- According to the what we said the spatial wave-function of the system has the form:

$$\psi_{\alpha\beta}(\mathbf{r}_1,\mathbf{r}_2)=\psi_\alpha(\mathbf{r}_1)\psi_\beta(\mathbf{r}_2)$$

electron 1 at state α,
electron 2 at state β

- But the electrons are identical particles so if we interchange the particles:

$$\psi_{\beta\alpha}(\mathbf{r}_1,\mathbf{r}_2)=\psi_\beta(\mathbf{r}_1)\psi_\alpha(\mathbf{r}_2)\equiv\psi_\alpha(\mathbf{r}_2)\psi_\beta(\mathbf{r}_1)$$

electron 1 at state β,
electron 2 at state α

Pauli Exclusion Principle

- Now what is the system spatial state? **Any linear combination is a solution of the Schrödinger equation.** To satisfy Pauli principle they must be either symmetric or anti-symmetric:

$$\psi_S = \frac{1}{\sqrt{2}}\left(\psi_{\alpha\beta} + \psi_{\beta\alpha}\right) = \frac{1}{\sqrt{2}}\left(\psi_\alpha\left(\mathbf{r}_1\right)\psi_\beta\left(\mathbf{r}_2\right) + \psi_\beta\left(\mathbf{r}_1\right)\psi_\alpha\left(\mathbf{r}_2\right)\right)$$

$$\psi_A = \frac{1}{\sqrt{2}}\left(\psi_{\alpha\beta} - \psi_{\beta\alpha}\right) = \frac{1}{\sqrt{2}}\left(\psi_\alpha\left(\mathbf{r}_1\right)\psi_\beta\left(\mathbf{r}_2\right) - \psi_\beta\left(\mathbf{r}_1\right)\psi_\alpha\left(\mathbf{r}_2\right)\right)$$

Pauli Exclusion Principle

- The total wave-functions for the cases of total spin (S=1, S=0) will be:

$$\psi_{\uparrow\uparrow} = \psi_A\left(\mathbf{r}_1,\mathbf{r}_2\right)X_{\uparrow\uparrow}\left(s_1,s_2\right) \qquad \psi_{\uparrow\downarrow} = \psi_S\left(\mathbf{r}_1,\mathbf{r}_2\right)X_{\uparrow\downarrow}\left(s_1,s_2\right)$$

- Note that if $\alpha=\beta$ then $\psi_A=0$ so the only spin state is this with opposite spins. This is the **Pauli exclusion principle**.

Exchange Degeneracy

- As we said in the transparency 14 "**Any linear combination is a solution of the Schrödinger equation".** This would bring a kind of degeneracy in the system. Even after a complete measurement there would be the so called **exchange degeneracy**. No further measurement would lift it because this would mean that there is a physical means to distinguish a particle from another. This would contradict the indistinguishability principle of identical particles.
- Pauli principle is not something arbitrary. It is the additional condition that lifts the exchange degeneracy!