EXCHANGE FORCE: INFINITE SQUARE WELL

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Section 5.1.2 & Problem 5.6.

We've seen that distinguishable particles and identical particles must be treated differently in quantum mechanics, resulting in different combinations of the single-particle wave functions in 2-particle systems. It's useful to work out what this means for some of the observables in a 2-particle system.

We can begin by looking at possibly the simplest case: the average positions of the two particles. If the particles are distinguishable, then the wave function is $\psi(x_a, x_b) = \psi_1(x_a) \psi_2(x_b)$ and

$$\langle x_a \rangle = \langle \psi \, | x_a | \, \psi \rangle \tag{1}$$

$$= \langle \psi_{1a} | x_a | \psi_{1a} \rangle \langle \psi_{2b} | \psi_{2b} \rangle \tag{2}$$

$$= \langle \psi_{1a} | x_a | \psi_{1a} \rangle \tag{3}$$

$$=\langle x\rangle_1\tag{4}$$

where the notation $|\psi_{1a}\rangle \equiv \psi_1(x_a)$ and so on.

That is, $\langle x \rangle$ is the mean value of x in state ψ_1 . We can drop the suffix a here, since x_a is just a dummy name for the integration variable in $\langle \psi_{1a} | x_a | \psi_{1a} \rangle$. For identical particles,

$$\psi_{\pm}(\mathbf{r}_{a},\mathbf{r}_{b}) = \frac{1}{\sqrt{2}} \left[\psi_{1}(\mathbf{r}_{a}) \psi_{2}(\mathbf{r}_{b}) \pm \psi_{2}(\mathbf{r}_{a}) \psi_{1}(\mathbf{r}_{b}) \right]$$
 (5)

This time, working out $\langle x_a \rangle$ is a bit messier but not too bad if we use the orthogonality of the two states.

$$2\langle x_a \rangle = \langle \psi_{1a} | x_a | \psi_{1a} \rangle \langle \psi_{2b} | \psi_{2b} \rangle + \langle \psi_{2a} | x_a | \psi_{2a} \rangle \langle \psi_{1b} | \psi_{1b} \rangle \tag{6}$$

$$\pm \langle \psi_{1a} | x_a | \psi_{2a} \rangle \langle \psi_{2b} | \psi_{1b} \rangle \pm \langle \psi_{2a} | x_a | \psi_{1a} \rangle \langle \psi_{1b} | \psi_{2b} \rangle \tag{7}$$

$$\langle x_a \rangle = \frac{1}{2} \left(\langle x \rangle_1 + \langle x \rangle_2 \right) \tag{8}$$

Thus the mean position of particle a is the average of its positions in the two states, which isn't all that surprising. We'd get the same result for

particle b of course, since the two particles are identical. This result is true for both bosons and fermions, since the plus/minus terms work out to zero due to the orthogonality of the states ψ_1 and ψ_2 .

What is a bit more interesting is the mean square separation of the two particles, that is $\left\langle (x_a-x_b)^2\right\rangle$. This can be worked out using the same procedure as above, and is done by Griffiths in his section 5.1.2, although his notation is a bit different from mine. (I've used a numerical suffix on the wave function, since this is the usual notation used for stationary states. Thus a letter suffix indicates which particle and a number suffix indicates which stationary state.) The results are, in my notation, first for distinguishable particles:

$$\left\langle \left(x_a - x_b\right)^2 \right\rangle = \left\langle x^2 \right\rangle_1 + \left\langle x^2 \right\rangle_2 - 2\left\langle x \right\rangle_1 \left\langle x \right\rangle_2 \tag{9}$$

For identical particles, we get

$$\left\langle (x_a - x_b)^2 \right\rangle_{\pm} = \left\langle x^2 \right\rangle_1 + \left\langle x^2 \right\rangle_2 - 2 \left\langle x \right\rangle_1 \left\langle x \right\rangle_2 \mp 2 \left| \left\langle x \right\rangle_{12} \right|^2 \tag{10}$$

where the plus (minus) sign on the left and minus (plus) on the right refer to bosons (fermions), and

$$\langle x \rangle_{12} \equiv \langle \psi_1 \, | x \, | \, \psi_2 \rangle \tag{11}$$

In general, then, since the term $2|\langle x\rangle_{12}|^2$ is always positive, bosons tend to be closer together than distinguishable particles while fermions are further apart. This is a sort of pseudo-force which is an entirely quantum mechanical effect of the symmetries of the wave functions. Although it's not really a force in the sense that electromagnetism and gravity are, it's known as the *exchange force*.

As an example, consider 2 particles in the infinite square well. The wave functions for a single particle are

$$\psi(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \tag{12}$$

where a is the width of the well. If the total wave function is a combination of states l and n, then if the particles are distinguishable

$$\langle (x_a - x_b)^2 \rangle = \langle x^2 \rangle_1 + \langle x^2 \rangle_2 - 2 \langle x \rangle_1 \langle x \rangle_2$$
(13)

$$= a^{2} \left(\frac{1}{3} - \frac{1}{2l^{2}\pi^{2}} \right) + a^{2} \left(\frac{1}{3} - \frac{1}{2n^{2}\pi^{2}} \right) - 2 \left(\frac{a}{2} \right) \left(\frac{a}{2} \right)$$
 (14)

$$=a^{2}\left(\frac{1}{6}-\frac{l^{2}+n^{2}}{2(\pi ln)^{2}}\right) \tag{15}$$

In line 2, we used the results of our earlier calculations for the infinite square well.

If the particles are identical, then

$$\langle x \rangle_{ln} = \langle \psi_l \, | \, x \, | \, \psi_n \rangle \tag{16}$$

$$= \frac{2}{a} \int_0^a \sin\left(\frac{l\pi x}{a}\right) \sin\left(\frac{n\pi x}{a}\right) x dx \tag{17}$$

$$= \left(-1 + (-1)^{n+l}\right) \frac{4anl}{\left[\pi \left(n^2 - l^2\right)\right]^2}$$
 (18)

This term is zero if n+l is even, so there is a difference in the separation only when n+l is odd. In general, we have

$$\left\langle (x_a - x_b)^2 \right\rangle_{\pm} = a^2 \left(\frac{1}{6} - \frac{l^2 + n^2}{2(\pi l n)^2} \right) \mp 2 \left[\left(-1 + (-1)^{n+l} \right) \frac{4anl}{\left[\pi \left(n^2 - l^2 \right) \right]^2} \right]^2$$
(19)

PINGBACKS

Pingback: Helium atom: parahelium and orthohelium

Pingback: Exchange force: harmonic oscillator