UNCERTAINTIES IN THE HARMONIC OSCILLATOR AND HYDROGEN ATOM

Link to: physicspages home page.

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

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 9, Exercises 9.4.1 - 9.4.2.

Here we'll look at a couple of calculations relevant to the application of the uncertainty principle to the hydrogen atom. When calculating uncertainties, we need to find the average values of various quantities. First, we'll look at an average in the case of the harmonic oscillator.

The harmonic oscillator eigenstates are

$$\psi_n(x)=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-m\omega x^2/2\hbar} \tag{1}$$

where H_n is the nth Hermite polynomial. For $n=1$, we have

$$H_1\left(\sqrt{\frac{m\omega}{\hbar}}x\right)=2\sqrt{\frac{m\omega}{\hbar}}x \tag{2}$$

so

$$\psi_1(x)=\frac{\sqrt{2}}{\pi^{1/4}}\left(\frac{m\omega}{\hbar}\right)^{3/4}x\,e^{-m\omega x^2/2\hbar} \tag{3}$$

For this state, we can calculate the average

$$\begin{aligned}\left\langle\frac{1}{X^2}\right\rangle &= \int_{-\infty}^{\infty}\psi_1^2(x)\frac{1}{x^2}dx &(4)\\ &= \frac{2}{\sqrt{\pi}}\left(\frac{m\omega}{\hbar}\right)^{3/2}\int_{-\infty}^{\infty}e^{-m\omega x^2/\hbar}dx &(5)\\ &= \frac{2}{\sqrt{\pi}}\left(\frac{m\omega}{\hbar}\right)^{3/2}\sqrt{\frac{\pi\hbar}{m\omega}} &(6)\\ &= \frac{2m\omega}{\hbar} &(7)\end{aligned}$$

where we evaluated the Gaussian integral in the second line.

We can compare this to $1/\left\langle X^2\right\rangle$ as follows:

$$\left\langle X^2 \right\rangle = \int_{-\infty}^{\infty} \psi_1^2(x) x^2 dx \tag{8}$$

$$= \frac{2}{\sqrt{\pi}} \left(\frac{m\omega}{\hbar}\right)^{3/2} \int_{-\infty}^{\infty} e^{-m\omega x^2/\hbar} x^4 dx \tag{9}$$

$$= \frac{2}{\sqrt{\pi}} \left(\frac{m\omega}{\hbar}\right)^{3/2} \frac{3\sqrt{\pi}}{4} \left(\frac{\hbar}{m\omega}\right)^{5/2} \tag{10}$$

$$= \frac{3}{2} \frac{\hbar}{m\omega} \tag{11}$$

$$\frac{1}{\langle X^2 \rangle} = \frac{2}{3} \frac{m\omega}{\hbar} \tag{12}$$

Thus $\left\langle \frac{1}{X^2} \right\rangle$ and $\frac{1}{\langle X^2 \rangle}$ have the same order of magnitude, although they are not equal.

In three dimensions, we consider the ground state of hydrogen

$$\psi_{100}(r) = \frac{1}{\sqrt{\pi} a_0^{3/2}} e^{-r/a_0} \tag{13}$$

where a_0 is the Bohr radius

$$a_0 \equiv \frac{\hbar^2}{me^2} \tag{14}$$

with m and e being the mass and charge of the electron. The wave function is normalized as we can see by doing the integral (in 3 dimensions):

$$\int \psi_{100}^2(r) d^3\mathbf{r} = \frac{4\pi}{\pi a_0^3} \int_0^{\infty} e^{-2r/a_0} r^2 dr \tag{15}$$

We can use the formula (given in Shankar's Appendix 2)

$$\int_0^{\infty} e^{-r/\alpha} r^n dr = \frac{n!}{\alpha^{n+1}} \tag{16}$$

We get

$$\int \psi_{100}^2(r) d^3\mathbf{r} = \frac{4\pi}{\pi a_0^3} \frac{2!}{2^3} a_0^3 = 1 \tag{17}$$

as required.

For a spherically symmetric wave function centred at $r = 0$,

$$(\Delta X)^2 = \left\langle X^2 \right\rangle - \langle X \rangle^2 = \left\langle X^2 \right\rangle \tag{18}$$

with identical relations for Y and Z. Since

$$r^2 = x^2 + y^2 + z^2 \tag{19}$$

$$\left\langle r^2 \right\rangle = \left\langle x^2 \right\rangle + \left\langle y^2 \right\rangle + \left\langle z^2 \right\rangle = 3\left\langle X^2 \right\rangle \tag{20}$$

$$\left\langle X^2 \right\rangle = \frac{1}{3}\left\langle r^2 \right\rangle \tag{21}$$

Thus

$$\left\langle X^2 \right\rangle = \frac{1}{3}\int \psi_{100}^2(r) r^2 d^3\mathbf{r} \tag{22}$$

$$= \frac{4\pi}{3\pi a_0^3}\int_0^\infty e^{-2r/a_0} r^4 dr \tag{23}$$

$$= \frac{4}{3a_0^3}\frac{4!}{2^5}a_0^5 \tag{24}$$

$$= a_0^2 \tag{25}$$

$$\Delta X = a_0 = \frac{\hbar^2}{me^2} \tag{26}$$

We can also find

$$\left\langle \frac{1}{r} \right\rangle = \int \psi_{100}^2(r)\frac{1}{r} d^3\mathbf{r} \tag{27}$$

$$= \frac{4\pi}{\pi a_0^3}\int_0^\infty e^{-2r/a_0} r\, dr \tag{28}$$

$$= \frac{4}{a_0^3}\frac{a_0^2}{4} \tag{29}$$

$$= \frac{1}{a_0} \tag{30}$$

$$\langle r \rangle = \int \psi_{100}^2(r) r\, d^3\mathbf{r} \tag{31}$$

$$= \frac{4\pi}{\pi a_0^3}\int_0^\infty e^{-2r/a_0} r^3 dr \tag{32}$$

$$= \frac{4}{a_0^3}\frac{6a_0^4}{16} \tag{33}$$

$$= \frac{3}{2}a_0 \tag{34}$$

Thus both $\left\langle\frac{1}{r}\right\rangle$ and $\frac{1}{\langle r\rangle}$ are of the same order of magnitude as $1/a_0 = me^2/\hbar^2$.

PINGBACKS

Pingback: Uncertainty principle and an estimate of the ground state energy of hydrogen