UNCERTAINTY PRINCIPLE AND AN ESTIMATE OF THE GROUND STATE ENERGY OF HYDROGEN

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 9, Exercise 9.4.3.

The uncertainty principle can be used to get an estimate of the ground state energy in some systems. In his section 9.4, Shankar shows how this is done for the hydrogen atom, treating the system as a proper 3-d system.

A somewhat simpler analysis can be done by treating the hydrogen atom as a one-dimensional system. The Hamiltonian is

$$H=\frac{P^{2}}{2m}-\frac{e^{2}}{\left(R^{2}\right)^{1/2}} \tag{1}$$

where m and e are the mass and charge of the electron. The operators P and R stand for the 3-d momentum and position:

$$P^{2} = P_{x}^{2}+P_{y}^{2}+P_{z}^{2} \tag{2}$$

$$R^{2} = X^{2}+Y^{2}+Z^{2} \tag{3}$$

If we ignore the expansions of P^2 and R^2 and treat the Hamiltonian as a function of the operators P and R on their own, we can use the uncertainty principle to get a bound on the ground state energy. By analogy with one-dimensional position and momentum, we assume that the uncertainties are related by

$$\Delta P\cdot\Delta R\geq\frac{\hbar}{2} \tag{4}$$

By using coordinates such that the hydrogen atom is centred at the origin, and from the spherical symmetry of the ground state, we have

$$(\Delta P)^{2}=\left\langle P^{2}\right\rangle-\langle P\rangle^{2}=\left\langle P^{2}\right\rangle \tag{5}$$

$$(\Delta R)^{2}=\left\langle R^{2}\right\rangle-\langle R\rangle^{2}=\left\langle R^{2}\right\rangle \tag{6}$$

We can then write 1 as

$$\langle H\rangle = \frac{\langle P^2\rangle}{2m} - e^2\left\langle\frac{1}{(R^2)^{1/2}}\right\rangle \tag{7}$$

$$\simeq \frac{\langle P^2\rangle}{2m} - \frac{e^2}{\left\langle\sqrt{\langle R^2\rangle}\right\rangle} \tag{8}$$

where in the last line we used an argument similar to that considered earlier, in which we showed that, for a one-dimensional system,

$$\left\langle\frac{1}{X^2}\right\rangle \simeq \frac{1}{\langle X^2\rangle} \tag{9}$$

where the $\simeq$ sign means 'same order of magnitude'. We can now write the mean of the Hamiltonian in terms of the uncertainties:

$$\langle H\rangle \simeq \frac{(\Delta P)^2}{2m} - \frac{e^2}{\Delta R} \tag{10}$$

$$\gtrsim \frac{\hbar^2}{8m(\Delta R)^2} - \frac{e^2}{\Delta R} \tag{11}$$

We can now minimize $\langle H\rangle$:

$$\frac{\partial\langle H\rangle}{\partial(\Delta R)} = -\frac{\hbar^2}{4m(\Delta R)^3} + \frac{e^2}{(\Delta R)^2} = 0 \tag{12}$$

$$\Delta R = \frac{\hbar^2}{4me^2} \tag{13}$$

This gives an estimate for the ground state energy of

$$\langle H\rangle_{g.s.} \simeq -\frac{2me^4}{\hbar^2} \tag{14}$$

The actual value is

$$E_0 = -\frac{me^4}{2\hbar^2} \tag{15}$$

so our estimate is too large (in magnitude) by a factor of 4. For comparison, the estimate worked out by Shankar for the 3-d case is

$$\langle H\rangle \gtrsim -\frac{2me^4}{9\hbar^2} \tag{16}$$

This estimate is too small by around a factor of 2.