

VARIATIONAL PRINCIPLE AND THE HYDROGEN ATOM

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 7.13.

Another example of the variational principle this time to estimate the ground state of the hydrogen atom. This is the first example we've done in three dimensions, although since it's spherically symmetric, the integral isn't much more complicated.

The trial function here is

$$(0.1) \quad \psi = Ae^{-br^2}$$

First, we normalize it:

$$(0.2) \quad A^2 \int e^{-2br^2} r^2 \sin\theta d\phi d\theta dr = 1$$

$$(0.3) \quad A = \left(\frac{2b}{\pi}\right)^{3/4}$$

We now find $H\psi$:

$$(0.4) \quad H\psi = -\frac{\hbar^2}{2m}\nabla^2\psi - \frac{e^2}{4\pi\epsilon_0 r}\psi$$

$$(0.5) \quad = -\left(\frac{2b}{\pi}\right)^{3/4} e^{-br^2} \left[\frac{\hbar^2(2b^2r^2 - 3b)}{m} + \frac{e^2}{4\pi\epsilon_0 r} \right]$$

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

$$(0.6) \quad \langle H \rangle = -\left(\frac{2b}{\pi}\right)^{3/2} \int e^{-2br^2} \left[\frac{\hbar^2(2b^2r^2 - 3b)}{m} + \frac{e^2}{4\pi\epsilon_0 r} \right] r^2 \sin\theta d\phi d\theta dr$$

$$(0.7) \quad = \frac{3\hbar^2}{2m}b - \frac{e^2}{\sqrt{2}\pi^{3/2}\epsilon_0}\sqrt{b}$$

Taking the derivative w.r.t. b and setting to zero gives

$$(0.8) \quad b_{min} = \frac{m^2 e^4}{18 \hbar^4 \pi^3 \epsilon_0^2}$$

Substituting back into 0.7 gives

$$(0.9) \quad \langle H \rangle_{min} = -\frac{me^4}{12 \hbar^2 \pi^3 \epsilon_0^2}$$

$$(0.10) \quad = -11.6 \text{ eV}$$

This is significantly above the correct value of -13.6 eV .