VARIATIONAL PRINCIPLE AND THE YUKAWA POTENTIAL

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 7.14.

A result from quantum field theory is the Yukawa potential which, when applied to the Coulomb potential, gives

$$V=-\frac{e^{2}}{4\pi\varepsilon_{0}}\frac{e^{-\mu r}}{r} \tag{1}$$

where $\mu=m_{\gamma}c/\hbar$ and m_{γ} is the mass of the particle mediating the force, which in the case of electromagnetism is the photon. Thus if the photon did have a non-zero mass, this exponential factor would appear in the potential.

We can use the variational principle to estimate the effect of this potential on the ground state of the hydrogen atom. We can try as a trial function

$$\psi=Ae^{-br/a} \tag{2}$$

where a is the Bohr radius and b is the parameter we can vary to find the minimum upper bound on the energy. Most of the calculations from here onwards were done using Maple, as they get a bit messy in places.

First, we normalize it:

$$A^{2}\int e^{-2br/a}r^{2}\sin\theta d\phi d\theta dr=1 \tag{3}$$

$$A=\frac{1}{\sqrt{\pi}}\left(\frac{b}{a}\right)^{3/2} \tag{4}$$

We now find $H\psi=(T+V)\psi$:

$$T\psi = -\frac{\hbar^2}{2m}\nabla^2\psi \tag{5}$$

$$= \frac{\hbar^2\,(2a-br)\,b^{5/2}e^{-br/a}}{2m\sqrt{\pi}a^{7/2}r} \tag{6}$$

$$V\psi = -\frac{e^2}{4\pi^{3/2}\varepsilon_0}\frac{e^{-\mu r}}{r}\left(\frac{b}{a}\right)^{3/2}e^{-br/a} \tag{7}$$

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

$$\langle T\rangle = \frac{\hbar^2 b^4}{2\pi m a^5}\int (2a-br)\,e^{-2br/a}r\sin\theta\,d\phi\,d\theta\,dr \tag{8}$$

$$= \frac{\hbar^2 b^2}{2a^2 m} \tag{9}$$

$$\langle V\rangle = -\frac{e^2 b^3}{4\pi^2 a^3\varepsilon_0}\int e^{-\mu r}e^{-2br/a}r\sin\theta\,d\phi\,d\theta\,dr \tag{10}$$

$$= -\frac{e^2 b^3}{\pi\varepsilon_0 a\,(4b^2+4b\mu a+\mu^2a^2)} \tag{11}$$

$$\langle H\rangle = \frac{\hbar^2 b^2}{2a^2 m} - \frac{e^2 b^3}{\pi\varepsilon_0 a\,(4b^2+4b\mu a+\mu^2a^2)} \tag{12}$$

At this stage, we'd take the derivative w.r.t. b and set to zero to find $\langle H\rangle_{min}$. As you can see, the derivative is quite complicated, so we'll do this by software. After substituting $x\equiv\mu a$ we get

$$\frac{d\langle H\rangle}{db} = \frac{b\hbar^2}{ma^2} - \frac{3b^2e^2}{\pi\varepsilon_0 a\,(4bx+x^2+4b^2)} + \frac{b^3e^2\,(8b+4x)}{\pi\varepsilon_0 a\,(4bx+x^2+4b^2)^2} \tag{13}$$

For $\mu=0, b=1$ since that just gives us the exact hydrogen wave function for the normal Coulomb potential. Since $x=\mu a\ll 1$, we'd expect b to be very close to 1, so we can write $b=1+y$ where $y\ll 1$. Therefore we can try expanding the expression in a Taylor series, first in x about $x=0$ and then in y about $y=0$, and saving only terms that are second order in products of x and y. First, we expand around $x=0$:

$$\frac{d\langle H\rangle}{db} = \frac{b\hbar^2}{ma^2} - \frac{e^2}{4\pi\varepsilon_0 a} + \frac{3e^2}{16\pi\varepsilon_0 ab^2}x^2 + \mathcal{O}\left(x^3\right) \tag{14}$$

Now we substitute $b=1+y$ and expand about $y=0$, saving only terms where the combined powers of x and y are ≤ 2:

$$\frac{d\langle H\rangle}{db} \approx \frac{\hbar^2}{ma^2} - \frac{e^2}{4\pi\varepsilon_0 a} + \frac{\hbar^2}{ma^2}y + \frac{3e^2}{16\pi\varepsilon_0 a}x^2 \tag{15}$$

Now we can set this to zero and solve for y (since we're trying to find b_{min}):

$$b_{min} = 1 + y_{min} = 1 + \frac{4me^2a - 16\pi\hbar^2\varepsilon_0 - 3e^2max^2}{16\pi\varepsilon_0\hbar^2} \tag{16}$$

We can substitute this back into 12 and then take the Taylor expansion of the result around $x = 0$. The result is:

$$\langle H\rangle_{min} = -\frac{me^4}{32\pi^2\hbar^2\varepsilon_0^2} + \frac{e^2}{4\pi\varepsilon_0 a}x - \frac{3\hbar^2}{4ma^2}x^2 + \mathcal{O}\left(x^3\right) \tag{17}$$

Substituting in for the Bohr radius:

$$a = \frac{4\pi\varepsilon_0\hbar^2}{me^2} \tag{18}$$

we get

$$\langle H\rangle_{min} = -\frac{me^4}{32\pi^2\hbar^2\varepsilon_0^2}\left(1 - 2x + \frac{3}{2}x^2 + \mathcal{O}\left(x^3\right)\right) \tag{19}$$

$$= E_1\left(1 - 2x + \frac{3}{2}x^2 + \mathcal{O}\left(x^3\right)\right) \tag{20}$$

where E_1 is the exact ground state energy for hydrogen.

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