Bohr Radius

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PHYS 4352 - Concepts of Modern Physics
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August 20, 2020

In today's lecture we proposed a simple way to find the Bohr radius a_0. The main idea is to consider the energy of the electron in the frame of the inertial frame of the proton

$$E = T + V = \frac{p^2}{2m} - \frac{kq^2}{a_0}$$

and then set $\frac{\partial E}{\partial a_0} = 0$ and solve for a_0. An intermediate consideration was the position–momentum uncertainty principle, which helped us write $\frac{p^2}{2m} \sim \frac{\hbar^2}{2ma_0^2}$. But I think the application of the uncertainty principle is tenuous, since the uncertainty principle is really saying $\Delta a_0 \Delta p \sim \hbar$, not $a_0 p \sim \hbar$.

The variational principle offers a more rigorous calculation of the Bohr radius:

Using some trial wave function $\psi(r) = Ae^{-\alpha r}$, where $\alpha \equiv \frac{1}{a}$, we can normalize to find A:

$$\begin{aligned}
1 = \int\int\int |\psi|^2 \, \mathrm{d}\vec{r} &= 4\pi \int_0^\infty r^2 |\psi|^2 \, \mathrm{d}r \\
&= 4\pi A^2 \int_0^\infty r^2 e^{-2\alpha r} \, \mathrm{d}r \\
&= \frac{A^2 \pi}{\alpha^3} = 1 \\
\text{so we find } A &= \sqrt{\frac{\alpha^3}{\pi}}
\end{aligned}$$

Now we seek to find some α_{optimal} such that $\langle H \rangle(\alpha_{\text{optimal}})$ is a minimum. Note

$$\langle H \rangle(\alpha) = \langle V \rangle(\alpha) + \langle T \rangle(\alpha)$$

Let's find the expectation values of the potential and kinetic energies:

$$\begin{aligned}
\langle V \rangle &= \int\int\int V(r) |\psi|^2 \, \mathrm{d}\vec{r} \\
&= -4\pi \int r^2 \frac{kq^2}{r} e^{-2\alpha r} \\
\text{integration}\ldots &= -kq^2 \alpha
\end{aligned}$$

Meanwhile,

$$
\begin{aligned}
\langle T \rangle &= \int\int\int \psi^* \left(\frac{\hbar}{2m} \tfrac{\partial^2}{\partial r^2} \right) \psi \, \mathrm{d}\vec{r} \\
\text{by parts: } &= \frac{4\pi\hbar^2}{2m} \int r^2 |\tfrac{\partial \psi}{\partial r}|^2 \, \mathrm{d}r \\
&= \frac{4\pi\hbar^2}{2m} A^2 \int r^2 \tfrac{\partial e^{-2\alpha r}}{\partial r} \, \mathrm{d}r \\
\text{integration\dots } &= \frac{\hbar\alpha^2}{2m}
\end{aligned}
$$

So

$$\langle H \rangle(\alpha) = \langle V \rangle(\alpha) + \langle T \rangle(\alpha) = -kq^2\alpha + \frac{\hbar\alpha^2}{2m}$$

We want α_{optimal} such that $\langle H \rangle(\alpha_{\text{optimal}})$ is a minimum:

$$\frac{\partial \langle H \rangle}{\partial \alpha} = -kq^2 + \frac{k^2\alpha}{m} = 0$$

Solving, we find that $\alpha_{\text{optimal}} = \frac{kq^2m}{\hbar^2}$. But $\alpha \equiv \frac{1}{a}$, so the Bohr radius is

$$\boxed{a_0 = \frac{\hbar}{kq^2m}}$$

Incidentally,

$$\langle H \rangle(\alpha_{\text{optimal}}) = \langle V \rangle(\alpha_{\text{optimal}}) + \langle T \rangle(\alpha_{\text{optimal}}) = \frac{k^2q^4m}{2\hbar^2} - \frac{k^2q^4m}{\hbar^2} = -\frac{k^2q^4m}{2\hbar^2} = -R_y$$

where R_y is the Rydberg energy. It is nice that $\frac{1}{2}\langle V \rangle = \langle T \rangle$. This is what we expect from the virial theorem.