HYDROGEN ATOM - MIXED INITIAL STATE AND MEAN POTENTIAL ENERGY

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.15.

We've looked at the stationary states of the hydrogen atom, but suppose an atom starts off in a mixture of two states, as in

$$\Psi(\mathbf{r},0)=\frac{1}{\sqrt{2}}\left(\psi_{211}+\psi_{21-1}\right) \tag{1}$$

We've already worked out the two stationary states:

$$\begin{aligned}
\psi_{211} &= -\frac{1}{8\sqrt{\pi}}\frac{r}{a^{5/2}}e^{-r/2a}\sin\theta e^{i\phi} && (2)\\
\psi_{21-1} &= \frac{1}{8\sqrt{\pi}}\frac{r}{a^{5/2}}e^{-r/2a}\sin\theta e^{-i\phi} && (3)
\end{aligned}$$

Since both states have the same value of n, they both have the same energy, so the time-dependent wave function is

$$\begin{aligned}
\Psi(\mathbf{r},t) &= \frac{1}{\sqrt{2}}e^{-iE_2t/\hbar}\left(\psi_{211}+\psi_{21-1}\right) && (4)\\
&= \frac{1}{\sqrt{2}}e^{-iE_2t/\hbar}\frac{1}{8\sqrt{\pi}}\frac{re^{-r/2a}}{a^{5/2}}\sin\theta\left(-2i\sin\phi\right) && (5)\\
&= -\frac{ri}{4\sqrt{2\pi a^5}}e^{-r/2a}e^{-iE_2t/\hbar}\sin\theta\sin\phi && (6)
\end{aligned}$$

where we have used $e^{i\phi}-e^{-i\phi}=2i\sin\phi$.

We can now calculate $\langle V\rangle$, the average of the potential. The potential function is (from Coulomb's law)

$$V(r)=-\frac{e^2}{4\pi\varepsilon_0 r} \tag{7}$$

We do the integral

$$
\begin{aligned}
\langle V\rangle &= \int \Psi^* V \Psi d^3\mathbf{r} &(8)\\
&= \frac{-e^2}{128\pi^2 a^5\varepsilon_0}\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} r^3 e^{-r/a}\sin^3\theta\sin^2\phi\, dr d\theta d\phi &(9)\\
&= -\frac{e^2}{16\pi a\varepsilon_0} &(10)\\
&= -1.09\times 10^{-18}\, Joules &(11)\\
&= -6.81\, eV &(12)
\end{aligned}
$$

using the values (in MKS units):

$$
\begin{aligned}
e &= 1.6\times 10^{-19}\,\text{Coulombs} &(13)\\
\frac{1}{4\pi\varepsilon_0} &= 8.99\times 10^{9}\, Nm^2/C^2 &(14)\\
a &= 0.529\times 10^{-10}\, m &(15)
\end{aligned}
$$

The value in eV is given by the conversion 1 eV = 1.6×10^{-19} Joules. The average potential is independent of time, since the time appears only in the complex exponential which cancels out when we take the square modulus of Ψ.