Problem 4.54

What is the probability that an electron in the ground state of hydrogen will be found *inside the nucleus*?

(a) First calculate the *exact* answer, assuming the wave function (Equation 4.80) is correct all the way down to $r = 0$. Let b be the radius of the nucleus.

(b) Expand your result as a power series in the small number $\epsilon \equiv 2b/a$, and show that the lowest-order term is the cubic: $P \approx (4/3)(b/a)^3$. This should be a suitable approximation, provided that $b \ll a$ (which it *is*).

(c) Alternatively, we might assume that $\psi(r)$ is essentially constant over the (tiny) volume of the nucleus, so that $P \approx (4/3)\pi b^3|\psi(0)|^2$. Check that you get the same answer this way.

(d) Use $b \approx 10^{-15}$ m and $a \approx 0.5 \times 10^{-10}$ m to get a numerical estimate for P. Roughly speaking, this represents the "fraction of its time that the electron spends inside the nucleus."

Solution

Part (a)

According to Born's statistical interpretation, the probability that an electron in the ground state of hydrogen will be found inside the nucleus is the volume integral over the nucleus of the modulus squared of the ground state wave function. Note that $\psi_{100}(r, \theta, \phi)$ is given in Equation 4.80 on page 148, and the nucleus is a ball with radius b.

$$P = \iiint\limits_{\text{nucleus}} |\Psi_{100}|^2 \, d\mathcal{V}$$

$$= \int_0^\pi \int_0^{2\pi} \int_0^b \left|\psi_{100}(r, \theta, \phi)e^{-iE_nt/\hbar}\right|^2 (r^2 \sin\theta \, dr \, d\phi \, d\theta)$$

$$= \int_0^\pi \int_0^{2\pi} \int_0^b \left[\frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} e^{-iE_nt/\hbar}\right]^* \left[\frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} e^{-iE_nt/\hbar}\right] (r^2 \sin\theta \, dr \, d\phi \, d\theta)$$

$$= \int_0^\pi \int_0^{2\pi} \int_0^b \left[\frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} e^{iE_nt/\hbar}\right] \left[\frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} e^{-iE_nt/\hbar}\right] (r^2 \sin\theta \, dr \, d\phi \, d\theta)$$

$$= \frac{1}{\pi a_0^3} \left(\int_0^\pi \sin\theta \, d\theta\right) \left(\int_0^{2\pi} d\phi\right) \left(\int_0^b r^2 e^{-2r/a_0} \, dr\right)$$

$$= \frac{1}{\pi a_0^3}(2)(2\pi) \int_0^b r^2 e^{-2r/a_0} \, dr$$

$$= \frac{4}{a_0^3} \int_0^b \frac{\partial^2}{\partial k^2} \left(a_0^2 e^{kr/a_0}\right)\bigg|_{k=-2} dr$$

Evaluate the integral, take two derivatives with respect to k, and plug in $k = -2$.

$$\begin{aligned}
P &= \frac{4}{a_0}\frac{d^2}{dk^2}\left(\int_0^b e^{kr/a_0}\,dr\right)\bigg|_{k=-2} \\
&= \frac{4}{a_0}\frac{d^2}{dk^2}\left[\left(\frac{a_0}{k}e^{kr/a_0}\right)\bigg|_0^b\right]\bigg|_{k=-2} \\
&= 4\frac{d^2}{dk^2}\left(\frac{e^{kb/a_0}-1}{k}\right)\bigg|_{k=-2} \\
&= 4\frac{d}{dk}\left[\frac{e^{kb/a_0}(kb-a_0)+a_0}{a_0k^2}\right]\bigg|_{k=-2} \\
&= 4\left[\frac{e^{kb/a_0}(b^2k^2-2a_0bk+2a_0^2)-2a_0^2}{a_0^2k^3}\right]\bigg|_{k=-2} \\
&= 4\left[\frac{e^{-2b/a_0}(4b^2+4a_0b+2a_0^2)-2a_0^2}{-8a_0^2}\right] \\
&= -\frac{e^{-2b/a_0}}{a_0^2}(2b^2+2a_0b+a_0^2)+1
\end{aligned}$$

Therefore,

$$\boxed{P = 1-\left(\frac{2b^2+2a_0b+a_0^2}{a_0^2}\right)e^{-2b/a_0}.}$$

Part (b)

Write this probability in terms of $\epsilon = 2b/a_0$.

$$\begin{aligned}
P &= 1-\left(\frac{2b^2}{a_0^2}+\frac{2b}{a_0}+1\right)e^{-2b/a_0} \\
&= 1-\left[\frac{1}{2}\left(\frac{2b}{a_0}\right)^2+\left(\frac{2b}{a_0}\right)+1\right]e^{-(2b/a_0)} \\
&= 1-\left(\frac{1}{2}\epsilon^2+\epsilon+1\right)e^{-\epsilon}
\end{aligned}$$

Since b is orders of magnitude smaller than the Bohr radius ($b \ll a_0$), ϵ is extremely close to zero; the closer ϵ is to zero, the better the first few terms of the Taylor series expansion of $e^{-\epsilon}$ about $\epsilon = 0$ will approximate the function.

$$P = 1-\left(\frac{1}{2}\epsilon^2+\epsilon+1\right)\left(1-\epsilon+\frac{\epsilon^2}{2}-\frac{\epsilon^3}{6}+\cdots\right)$$

Multiply the terms together and simplify the result.

$$P = 1 - \left[1\left(\frac{1}{2}\epsilon^2 + \epsilon + 1\right) - \epsilon\left(\frac{1}{2}\epsilon^2 + \epsilon + 1\right) + \frac{\epsilon^2}{2}\left(\frac{1}{2}\epsilon^2 + \epsilon + 1\right) - \frac{\epsilon^3}{6}\left(\frac{1}{2}\epsilon^2 + \epsilon + 1\right) + \cdots\right]$$

$$= \cancel{1} - \left[\left(\cancel{\frac{1}{2}\epsilon^2} + \cancel{\epsilon} + \cancel{1}\right) - \left(\frac{1}{2}\epsilon^3 + \cancel{\epsilon^2} + \cancel{\epsilon}\right) + \left(\frac{1}{4}\epsilon^4 + \frac{\epsilon^3}{2} + \cancel{\frac{\epsilon^2}{2}}\right) - \left(\frac{1}{12}\epsilon^5 + \frac{\epsilon^4}{6} + \frac{\epsilon^3}{6}\right) + \cdots\right]$$

$$= \frac{\epsilon^3}{6} + \text{terms on the order of } \epsilon^4,\ \epsilon^5, \text{ and higher}$$

Because of how small ϵ is, the higher-order terms are negligible compared to $\epsilon^3/6$.

$$P \approx \frac{\epsilon^3}{6}$$

$$\approx \frac{1}{6}\left(\frac{2b}{a_0}\right)^3$$

$$\approx \frac{8}{6}\left(\frac{b}{a_0}\right)^3$$

A good approximation for P is therefore

$$\boxed{P \approx \frac{4}{3}\left(\frac{b}{a_0}\right)^3.}$$

Part (c)

Because of how small the volume of the nucleus is, another way to approximate P is to treat $\psi_{100}(r, \theta, \phi)$ as a constant in the triple integral.

$$P = \iiint_{\text{nucleus}} |\Psi_{100}|^2 \, d\mathcal{V}$$

$$\approx \int_0^\pi \int_0^{2\pi} \int_0^b \left|\psi_{100}(0, \theta, \phi) e^{-iE_n t/\hbar}\right|^2 (r^2 \sin\theta \, dr \, d\phi \, d\theta)$$

$$\approx \int_0^\pi \int_0^{2\pi} \int_0^b \left[\frac{1}{\sqrt{\pi a_0^3}} e^0 e^{-iE_n t/\hbar}\right]^* \left[\frac{1}{\sqrt{\pi a_0^3}} e^0 e^{-iE_n t/\hbar}\right] (r^2 \sin\theta \, dr \, d\phi \, d\theta)$$

$$\approx \int_0^\pi \int_0^{2\pi} \int_0^b \left[\frac{1}{\sqrt{\pi a_0^3}} e^{iE_n t/\hbar}\right] \left[\frac{1}{\sqrt{\pi a_0^3}} e^{-iE_n t/\hbar}\right] (r^2 \sin\theta \, dr \, d\phi \, d\theta)$$

$$\approx \frac{1}{\pi a_0^3} \left(\int_0^\pi \sin\theta \, d\theta\right) \left(\int_0^{2\pi} d\phi\right) \left(\int_0^b r^2 \, dr\right)$$

$$\approx \frac{1}{\pi a_0^3} (2)(2\pi) \left(\frac{b^3}{3}\right) = \frac{4}{3}\left(\frac{b}{a_0}\right)^3$$

Part (d)

If $b \approx 10^{-15}$ m and $a_0 \approx 0.5 \times 10^{-10}$ m, then

$$P = 1 - \left(\frac{2b^2 + 2a_0 b + a_0^2}{a_0^2}\right) e^{-2b/a_0} \approx 1.076916333886402 \times 10^{-14}$$

$$P \approx \frac{4}{3}\left(\frac{b}{a_0}\right)^3 \approx 1.0666666666666667 \times 10^{-14}.$$

The percent difference between the exact and approximate values is less than 1%.

$$\begin{aligned} \text{Percent Difference} &= \frac{\text{Exact} - \text{Approximate}}{\text{Approximate}} \times 100\% \\ &\approx \frac{1.076916333886402 \times 10^{-14} - 1.0666666666666667 \times 10^{-14}}{1.0666666666666667 \times 10^{-14}} \times 100\% \\ &\approx 0.960906\% \end{aligned}$$