Problem Set 11

1. (a) The probability of finding the particle somewhere between r_1 and r_2 is $\int_{r_1}^{r_2} R^2(r)\, r^2\, dr$.

(b) $R_{10}(r) = \frac{2}{a_0^{3/2}} e^{-\frac{r}{a_0}}$.

For small r, Taylor expand the radial wavefunction to first order

$$R_{10}(r) \approx \frac{2}{a_0^{3/2}} \left(1 + \left(-\frac{r}{a_0}\right) + O\left(r^2\right)\right).$$

The probability of finding the electron inside the proton is therefore

$$P = \int_0^{r_p} R_{10}^2(r)\, r^2\, dr$$

In[1]:= $a_0 = 5.29 \times 10^{-11}$; (* in unit of m *)
$r_p = 10^{-15}$; (* in unit of m *)

$$\int_0^{r_p} \left(\frac{2}{a_0^{3/2}}\right)^2 \left(1 + \left(-\frac{r}{a_0}\right)\right)^2 r^2\, dr$$

Out[3]= 9.00657×10^{-15}

The probability of finding the electron inside the proton is very small, hence we can treat the proton as a positive point charge.

(c) $R_{21}(r) = \frac{1}{(2 a_0)^{3/2}} \frac{r}{\sqrt{3}\, a_0} e^{-\frac{r}{2 a_0}}$.

For small r, Taylor expand the radial wavefunction to first order

$$R_{21}(r) \approx \frac{1}{(2 a_0)^{3/2}} \frac{r}{\sqrt{3}\, a_0} \left(1 + \left(-\frac{r}{2 a_0}\right) + O\left(r^2\right)\right).$$

The probability of finding the electron inside the proton is therefore

$$P = \int_0^{r_p} R_{21}^2(r)\, r^2\, dr$$

In[4]:= $$\int_0^{r_p} \left(\frac{1}{(2 a_0)^{3/2}} \frac{r}{\sqrt{3}\, a_0}\right)^2 \left(1 + \left(-\frac{r}{2 a_0}\right)\right)^2 r^2\, dr$$

Out[4]= 2.01156×10^{-26}

The probability of finding the excited electron inside the proton is even smaller than the ground state electron.

2. We already know that the probability density does not depend on the azimuthal angle ϕ. In the absence of information about the z - component of angular momentum, it is likely that the electron would have any of the allowed values. Adding the angular probability densities with equal weights, we have

$$\Theta_{1,0}(\theta) + \Theta_{1,+1}(\theta) + \Theta_{1,-1}(\theta) = \left(\sqrt{\frac{3}{4\pi}}\cos\theta\right)^2 + \left(\sqrt{\frac{3}{8\pi}}\sin\theta\right)^2 + \left(\sqrt{\frac{3}{8\pi}}\sin\theta\right)^2$$

$$= \frac{3}{4\pi}\cos^2\theta + 2\,\frac{3}{8\pi}\sin^2\theta = \frac{3}{4\pi}.$$

This has no dependence on either ϕ or θ.

3. (a) The expectation value of the potential energy is

$$\overline{U} = \int_0^\infty U(r)\,P(r)\,dr = \int_0^\infty \left(\frac{1}{4\pi\epsilon_0}\frac{-e^2}{r}\right)\left(\frac{2}{a_0^{3/2}}e^{-\frac{r}{a_0}}\right)^2 r^2\,dr$$

$$= \frac{-e^2}{\pi\epsilon_0 a_0^3}\int_0^\infty r e^{-\frac{2r}{a_0}}\,dr = \frac{-e^2}{\pi\epsilon_0 a_0^3}\frac{1}{-\frac{2}{a_0}}\int_0^\infty r\,d\left(e^{-\frac{2r}{a_0}}\right)$$

$$= \frac{-e^2}{\pi\epsilon_0 a_0^3}\frac{1}{-\frac{2}{a_0}}\left(r e^{-\frac{2r}{a_0}}\Big|_0^\infty - \int_0^\infty e^{-\frac{2r}{a_0}}\,dr\right) = \frac{-e^2}{\pi\epsilon_0 a_0^3}\frac{1}{\left(-\frac{2}{a_0}\right)^2}\left(e^{-\frac{2r}{a_0}}\Big|_0^\infty\right)$$

$$= \frac{-e^2}{\pi\epsilon_0 a_0^3}\frac{1}{\left(-\frac{2}{a_0}\right)^2} = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{a_0}$$

$$= -\left(8.99\times10^9\,\text{N}\cdot\text{m}^2/\text{C}^2\right)\frac{(1.6\times10^{-19}\,\text{C})^2}{0.0529\times10^{-9}\,\text{m}} = 4.35\times10^{-18}\,\text{J} = -27.2\,\text{eV}.$$

In[20]:=
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ϵ0 = 8.854 × 10^-12;      (* in units of C^2/N·m^2 *)
e = 1.6 × 10^-19; (* in units of C *)
∫_0^∞ ((1/(4 π ϵ0) (-e^2/r)) (2/a0^(3/2) E^(-r/a0))^2 r^2) dr      (* in units of J *)
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$$\int_0^\infty\left(\left(\frac{1}{4\pi\epsilon_0}\frac{-e^2}{r}\right)\left(\frac{2}{a_0^{3/2}}E^{-\frac{r}{a_0}}\right)^2 r^2\right)dr$$

Out[22]= -4.34946×10^{-18}

(b) The expectation value of the total energy is a well defined - 13.6 eV. Hence the expectation value of the kinetic energy must be -13.6 eV - (-27.2 eV) = +13.6 eV.

4. (a) We search between $\theta = 0$ and $\theta = \frac{\pi}{3}$, and between $\theta = \frac{2\pi}{3}$ and $\theta = \pi$.

By symmetry we would double the integral from 0 to $\frac{\pi}{3}$. Hence the probabiliry is

$$2\int_0^{\frac{\pi}{3}}\left(\sqrt{\frac{3}{4\pi}}\cos\theta\right)^2 2\pi\sin\theta\, d\theta = 3\int_0^{\frac{\pi}{3}}\cos^2\theta\sin\theta\, d\theta$$

$$= -\cos^3\theta \,\Big|_0^{\frac{\pi}{3}} = 0.875.$$

(b) The radial part of the wave function is all that is involved, and $R_{11}(r)$ is the same for an $(n, l, m_l) = (2, 1, 0)$ state as for a $(2, 1, +1)$ state. Therefore, the probability is the same as in Example 7.9 : 0.662.

(c) $0.875 \times 0.662 = 0.58$.