

Solutions to problems from Chapters 10 and 12.

1. The ground state wavefunction for hydrogen is

$$\psi(\vec{r}) = R_{10}(r)Y_{00}(\theta, \phi) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0},$$

where $r = |\vec{r}| = \sqrt{x^2 + y^2 + z^2}$ and a_0 is the Bohr radius. The state is spherically symmetric – there is no dependence on θ or ϕ .

$$\langle x \rangle = \int d^3\vec{r} \psi^*(\vec{r}) x \psi(\vec{r}) = \int d^3\vec{r} x \frac{1}{\pi a_0^3} e^{-2r/a_0} = 0,$$

because this is an odd function with respect to $x \rightarrow -x$ and we are integrating over the whole x axis (and indeed, the whole of three-space).

$$\begin{aligned} \langle x^2 \rangle &= \int d^3\vec{r} \psi^*(\vec{r}) x^2 \psi(\vec{r}) \\ &= \int r^2 dr \sin\theta d\theta d\phi (r \sin\theta \cos\phi)^2 \frac{1}{\pi a_0^3} e^{-2r/a_0} \\ &= \frac{1}{\pi a_0^3} \int_0^\infty dr r^4 e^{-2r/a_0} \int_0^\pi d\theta \sin^3\theta \int_0^{2\pi} d\phi \cos^2\phi \\ &= \frac{1}{\pi a_0^3} \left(\frac{3a_0^5}{4} \right) \left(\frac{4}{3} \right) (\pi) = a_0^2. \end{aligned}$$

Therefore,

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = a_0.$$

To compute $\langle p_x \rangle$ and $\langle p_x^2 \rangle$ we will need x derivatives of ψ . First note that since $r = \sqrt{x^2 + y^2 + z^2}$,

$$\frac{\partial r}{\partial x} = \frac{\frac{1}{2}(2x)}{\sqrt{x^2 + y^2 + z^2}} = \frac{x}{r}.$$

Using this repeatedly,

$$\begin{aligned}
\frac{\partial}{\partial x} \psi(\vec{r}) &= \frac{\partial}{\partial x} \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \\
&= \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \left(-\frac{1}{a_0} \right) \frac{\partial r}{\partial x} \\
&= \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \left(-\frac{x}{r a_0} \right); \\
\frac{\partial^2}{\partial x^2} \psi(\vec{r}) &= \frac{\partial}{\partial x} \left[\frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \left(-\frac{x}{r a_0} \right) \right] \\
&= \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \left(-\frac{x}{r a_0} \right)^2 + \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \frac{\partial}{\partial x} \left(-\frac{x}{r a_0} \right) \\
&= \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \left[\left(-\frac{x}{r a_0} \right)^2 - \frac{1}{a_0} \left(\frac{r - x \frac{x}{r}}{r^2} \right) \right] \\
&= \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \left[\left(\frac{x^2}{r^2 a_0^2} \right) - \frac{1}{a_0} \left(\frac{r^2 - x^2}{r^3} \right) \right] \\
&= \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \left[\left(\frac{x^2}{r^2 a_0^2} \right) - \left(\frac{y^2 + z^2}{a_0 r^3} \right) \right]
\end{aligned}$$

Therefore,

$$\begin{aligned}
\langle p_x \rangle &= \int d^3 \vec{r} \psi^*(\vec{r}) (-i\hbar) \frac{\partial}{\partial x} \psi(\vec{r}) \\
&= -i\hbar \int d^3 \vec{r} \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \left(-\frac{x}{r a_0} \right) = 0,
\end{aligned}$$

for the same reason $\langle x \rangle = 0$.

$$\begin{aligned}
\langle p_x^2 \rangle &= \int d^3 \vec{r} \psi^*(\vec{r}) \left(-i\hbar \frac{\partial}{\partial x} \right)^2 \psi(\vec{r}) \\
&= -\hbar^2 \int d^3 \vec{r} \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \left[\left(\frac{x^2}{r^2 a_0^2} \right) - \left(\frac{y^2 + z^2}{a_0 r^3} \right) \right] \\
&= -\hbar^2 \int r^2 dr \sin \theta d\theta d\phi \frac{1}{\pi a_0^3} e^{-2r/a_0} \left[\left(\frac{(r \sin \theta \cos \phi)^2}{r^2 a_0^2} \right) - \left(\frac{(r \sin \theta \sin \phi)^2 + (r \cos \theta)^2}{a_0 r^3} \right) \right] \\
&= \frac{\hbar^2}{3a_0^2}.
\end{aligned}$$

Finally,

$$\Delta p_x = \frac{\hbar}{a_0 \sqrt{3}}.$$

Note that $\Delta x \Delta p_x = \hbar/\sqrt{3} > \hbar/2$, so the uncertainty principle is satisfied. By spherical symmetry, we would find the same results for the y and z axes (or any other rectilinear coordinate axes we choose).

The ground state is an angular momentum eigenstate with eigenvalue zero, so the electron is not tracing any well-defined classical orbit. But it is moving with some non-zero (probability distribution of) linear momenta around the proton.

10.2 For the hydrogen atom in $|n, l, m\rangle$ basis, we are given

$$|\psi(t=0)\rangle = \frac{4}{5}|1, 0, 0\rangle + \frac{3i}{5}|2, 1, 1\rangle.$$

Applying the time evolution operator,

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle = \frac{4}{5}e^{-iE_1t/\hbar}|1, 0, 0\rangle + \frac{3i}{5}e^{-iE_2t/\hbar}|2, 1, 1\rangle.$$

$$\begin{aligned}\langle E \rangle &= \left| \frac{4}{5}e^{-iE_1t/\hbar} \right|^2 E_1 + \left| \frac{3i}{5}e^{-iE_2t/\hbar} \right|^2 E_2 \\ &= \frac{16}{25} \left(-\frac{\mu c^2 \alpha^2}{2} \right) + \frac{9}{25} \left(-\frac{\mu c^2 \alpha^2}{2(2)^2} \right) \\ &= -\frac{\mu c^2 \alpha^2}{2} \frac{73}{100}; \\ \langle \vec{L}^2 \rangle &= \left| \frac{4}{5}e^{-iE_1t/\hbar} \right|^2 (0) + \left| \frac{3i}{5}e^{-iE_2t/\hbar} \right|^2 \cdot 2\hbar^2 \\ &= \frac{18\hbar^2}{25}; \\ \langle \vec{L}_z \rangle &= \left| \frac{4}{5}e^{-iE_1t/\hbar} \right|^2 (0) + \left| \frac{3i}{5}e^{-iE_2t/\hbar} \right|^2 \cdot \hbar \\ &= \frac{9\hbar}{25}.\end{aligned}$$

Since all three operators commute with the Hamiltonian, their expectation values are independent of time.

10.5 For each problem, compute

$$\begin{aligned}a_0 &= \frac{\hbar}{\mu c \alpha} = \frac{\hbar^2}{\mu e^2}; & E_1 &= -\frac{\mu c^2 \alpha^2}{2}; \\ \frac{\hbar c}{\lambda_{21}} &= E_2 - E_1 = -\frac{\mu c^2 \alpha^2}{2(2)^2} + \frac{\mu c^2 \alpha^2}{2} = \frac{3}{4} \frac{\mu c^2 \alpha^2}{2}.\end{aligned}\tag{1}$$

The reduced mass is

$$\mu = \frac{m_1 m_2}{m_1 + m_2}.$$

For point of comparison, the values for hydrogen are

$$a_0 = .529 \text{ \AA}; \quad E_1 = -13.6 \text{ eV}; \quad \lambda_{21} = 1216 \text{ \AA (UV)},$$

and $\mu_H = \frac{m_e m_p}{m_e + m_p} = 9.104 \cdot 10^{-28}$ g, as compared to $m_e = 9.109 \cdot 10^{-28}$ g (to four sig figs).

- (a) 2H : A deuteron is a bound state of a neutron and proton, with mass $m_D \approx 2m_p$. Thus $\mu_{2H} = \frac{m_e \cdot 2m_p}{m_e + 2m_p} \approx 1.00027\mu_H$. The quantities in (1) differ from those for hydrogen by this small factor.
- (b) Positronium is a bound state of an electron and positron. $\mu_{pos} = m_e/2 \approx \mu_H/2$. The Bohr radius is doubled as compared to hydrogen and the ground state energy is halved. The wavelength is doubled, still in the UV.
- (c) The muon is 207 times more massive than the electron. $\mu = 186\mu_H$. The wavelength is $\lambda_{21} = 6.5 \text{ \AA}$, an x-ray.

10.7 The nuclear reaction changes $Z = 1$ to $Z = 2$ in the ground-state wavefunction

$$\psi(\vec{r}) = R_{10}(r)Y_{00}(\theta, \phi) = \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} e^{-Zr/a_0}.$$

The amplitude to remain in the ground state is

$$\begin{aligned} \langle He^3 \langle 1, 0, 0 | 1, 0, 0 \rangle_{tritium} &= \int d^3\vec{r} \left(\frac{2^3}{\pi a_0^3}\right)^{1/2} e^{-2r/a_0} \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0} \\ &= \frac{2\sqrt{2}}{\pi a_0^3} \int d^3\vec{r} e^{-3r/a_0} \\ &= \frac{2\sqrt{2}}{\pi a_0^3} (4\pi) \left(\frac{2a_0^3}{27}\right) = \frac{16\sqrt{2}}{27}. \end{aligned}$$

The probability is $512/729 \approx .70$.

12.2 The spin states symmetric under exchange of the particles are the triplet of states of total spin 1, i.e the three states

$$|s, m\rangle = |1, 1\rangle, |1, 0\rangle, \text{ or } |1, -1\rangle.$$

In class we used $|\chi\rangle_S$ to denote any of these three possible states. The state antisymmetric under particle exchange is the singlet of total spin 0,

$$|s, m\rangle = |0, 0\rangle,$$

which we denoted $|\chi\rangle_A$.

- (a) As we more or less worked out in class, the ground state and first excited states are:

$$\begin{aligned} \text{ground:} \quad & |0\rangle_1 |0\rangle_2 |\chi\rangle_A, \quad E_0 = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{2} = \hbar\omega; \\ \text{first excited:} \quad & \frac{1}{\sqrt{2}} \left(|0\rangle_1 |1\rangle_2 + |1\rangle_1 |0\rangle_2 \right) |\chi\rangle_A \\ & \text{or } \frac{1}{\sqrt{2}} \left(|0\rangle_1 |1\rangle_2 - |1\rangle_1 |0\rangle_2 \right) |\chi\rangle_S, \quad E_1 = \frac{\hbar\omega}{2} + \frac{3\hbar\omega}{2} = 2\hbar\omega. \end{aligned}$$

(b) The spin singlet has a symmetric spatial wavefunction; the spin triplet has an antisymmetric spatial wavefunction. The two particles are more likely to be found near each other when they have a symmetric spatial wavefunction. Since the potential is negative when $|x_1 - x_2| < a$, we expect the correction to the energy from their interaction to be more negative when they have a symmetric spatial wavefunction. For all of the states, the interaction will lower the total energy, but more so for the spin singlets than the spin triplet.