Problem 2

The one-dimensional momentum eigenstate

\[ \psi_k(x) = \frac{1}{\sqrt{2\pi}} \ e^{ikx} \]

generates to

\[ \psi_{k'}(x) = \left( \frac{1}{\sqrt{2\pi}} \right)^3 e^{i(k'x + k'y + k'z)} \]

We want to show that this is the solution to the TISE with the Laplacian used for the second derivative:

\[ -\frac{\hbar^2}{2\mu} \nabla^2 \psi_{k'}(x) = E \psi_{k'}(x) \]

Calculate

\[ \nabla^2 \psi_{k'}(x) = \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial t^2} \right) \left( \frac{1}{\sqrt{2\pi}} \right)^3 e^{i(k'x + k'y + k'z)} \]

\[ = \left( \frac{1}{\sqrt{2\pi}} \right)^3 \left( (ik_x)^2 + (ik_y)^2 + (ik_z)^2 \right) e^{i(k'x + k'y + k'z)} \]

\[ = -\left( k_x^2 + k_y^2 + k_z^2 \right) \psi_{k'}(x) = -k^2 \psi_{k'}(x) \text{ where } k^2 = (k')^2. \]
Thus,\[
\frac{\hbar^2}{2\mu} \nabla^2 \psi_k(x) - \frac{\hbar^2 k^2}{2\mu} \psi_k(x) = \frac{p^2}{2\mu} \psi_k(x) = E \psi_k(x).
\]

**Problem 2**

Write \( \Psi^d(r, \theta, \phi) = R_{\ell \ell}(r) Y^d_{\ell \ell}(\theta, \phi) \). Let us further write that \( Y^d_{\ell \ell}(\theta, \phi) = f_{\ell \ell}(\theta) g_{\ell \ell}(\phi) \) and apply this to 12.5.28

\[
\left( \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right) \psi^d_{\ell \ell}(r, \theta, \phi) = 0
\]

\[
\Rightarrow \quad R_{\ell \ell}(r) \left( \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right) f_{\ell \ell}(\theta) g_{\ell \ell}(\phi) = 0
\]

\[
\Rightarrow \quad f_{\ell \ell}(\theta) f'_{\ell \ell}(\theta) + i \cot \theta f_{\ell \ell}(\theta) g_{\ell \ell}(\phi) = 0
\]

\[
\Rightarrow \quad \frac{f'_{\ell \ell}(\theta)}{f_{\ell \ell}(\theta)} = -i \frac{g_{\ell \ell}(\phi)}{g_{\ell \ell}(\phi)} = \ell
\]

when \( \ell \) is a chosen separation constant. This gives us for the \( \phi \)-dependence for...
\[-i \frac{d}{d\phi} \phi = \phi \frac{\partial}{\partial \phi} \phi, \lambda \Rightarrow -i \hbar \frac{d}{d\phi} \phi = \hbar \frac{\partial}{\partial \phi} \phi\]

Since \(-i \hbar \frac{d}{d\phi} \phi = \phi \frac{\partial}{\partial \phi} \phi = 0\) due to the properties of the function, then we see that the separation constant \(\lambda = 0\) and

\[-i \frac{d}{d\phi} \phi = \phi \Rightarrow \frac{d}{d\phi} \phi = i \phi\]

\[
\Rightarrow \phi \phi = e^{i\phi} \quad \text{up to normalization.}
\]

The \(\Theta\)-dependent piece gives

\[
\frac{d}{d\Theta} f_n(\Theta) = \cot \Theta f_n(\Theta) \quad \text{which has the solution}
\]

\[f_n(\Theta) = \sin \Theta \quad \text{again up to normalization, when}
\]

\[Y_n(\theta, \phi) \cdot f_n(\Theta) \phi = C \sin \Theta e^{i\phi}
\]

Now, to normalize this, impose the requirement that
\[ 1 = \int \cos^2 \left( \sin \theta e^{i \phi} \right) \left( \sin \theta e^{i \phi} \right) d\Omega \]

\[ = C^2 \int_0^\pi \left[ \frac{\sin^2 \theta}{2} \right] d\theta \int_0^{2\pi} \cos \theta d\phi = \pi C^2 \int_0^\pi \left( 1 - \cos^2 \theta \right) d(\cos \theta) \int_0^{2\pi} d\phi \]

\[ = 2\pi C^2 \left[ \frac{x - \frac{x^3}{3}}{3} \right]_{-1}^1 = 2\pi C^2 \left[ 1 - \frac{1}{3} \left( -\frac{1}{3} \right) \right] \]

\[ = \frac{8\pi}{3} C^2 \quad \Rightarrow \quad C = \sqrt{\frac{3}{8\pi}} \]

By convention we choose the negative square root ($l = 1$) so

\[ Y_1^1(\theta, \phi) = -\sqrt{\frac{3}{8\pi}} \sin \theta e^{i\phi} \quad \text{as desired} \]

Now, let's operate on this with \( L \)

\[ L \cdot Y_1^1(\theta, \phi) = -\hbar e^{-i\phi} \left[ \frac{2}{\theta} - i \cot \theta \frac{\partial}{\partial \phi} \right] \left[ \sqrt{\frac{3}{8\pi}} \sin \theta e^{i\phi} \right] \]

\[ = \hbar e^{-i\phi} \sqrt{\frac{3}{8\pi}} \left[ \cos \theta e^{i\phi} - i \cot \theta \sin \theta e^{i\phi} \right] \]

\[ = \hbar e^{-i\phi} \sqrt{\frac{3}{8\pi}} \left[ \cos \theta - i (i \cos \theta) \right] e^{i\phi} = \hbar \sqrt{\frac{3}{2\pi}} \cot \theta \]
But in the other hand

\[ L(l, l) = \sqrt{l(l+1)} | l, l \rangle \]

\[ L(-l, l) = \sqrt{2l+1} | l, 0 \rangle \]

\[ L(l, -l) = \sqrt{2l+1} \]

\[ L(-l, -l) = \sqrt{l(l+1)} \]

\[ \langle 1, 0 | L | 1, 1 \rangle = \frac{1}{\sqrt{2l}} \]

\[ \langle 1, 0 | \frac{1}{\sqrt{2l}} \sqrt{2l+1} \rangle = \frac{1}{\sqrt{2l}} \sqrt{2l+1} \]

\[ \cos \theta = \frac{1}{2} \sqrt{\frac{3}{2l}} \cos \theta \]

\[ Y_{l}^{0} = \frac{1}{2} \sqrt{\frac{3}{2l}} \cos \theta \]

Again, as desired.
Problem 3

The $l=0$ radial solutions are of the form

$$j_0(r) = \frac{\sin l}{r}, \quad n_0(r) = -\frac{\cos l}{r}$$

where $l = kr$ and $k = \sqrt{\frac{2\mu E}{\hbar^2}}$.

To satisfy the boundary conditions for the proverbial "spherical box", we must have $j=0$ at $r=r_0$, or

$$0 = j_0(kr_0) = \frac{\sin (kr_0)}{kr_0}, \quad 0 = n_0(kr_0) = \frac{\cos (kr_0)}{kr_0}$$

These are satisfied for values of $k$ for which $kr_0 = n\pi$, $n > 0$ (j-case) or $kr_0 = (n-\frac{1}{2})\pi$, $n > 0$ (n-case).

In general, thus, in a solution whenever

$$kr_0 = \frac{n\pi}{2}, \quad n > 0$$

This in turn implies

$$\frac{2\mu E}{\hbar} = \frac{n\pi}{2r_0} \quad \frac{E_0}{8\mu kr_0} = \frac{n^2\pi^2\hbar^2}{8\mu r_0^2}$$

for any strictly positive integer $n$. 


Problem 4

It's good to work through one of these recursion relation solutions at some point, so here we go. We need derivatives of $V_{ee}$:

$$ V_{ee}' = \frac{d}{dg} V_{ee} = (l+1) g^l \sum_{k=0}^{\infty} C_k g^k + g^{l+1} \sum_{k=0}^{\infty} k C_k g^{k-1} $$

$$ V_{ee}'' = (l)(l+1) g^{l-1} \sum_{k=0}^{\infty} C_k g^k + (l+1) g^l \sum_{k=0}^{\infty} \frac{kC_k g^{k-1}}{k} + $$

$$ + (l+1) g^l \sum_{k=0}^{\infty} \frac{kC_k g^{k-1}}{k} + g^{l+1} \sum_{k=0}^{\infty} \frac{(k)(k-1)}{k} C_k g^{k-2} $$

$$ = (l)(l+1) g^{l-1} \sum_{k=0}^{\infty} \frac{C_k g^k}{k} + 2(l+1) g^l \sum_{k=0}^{\infty} \frac{kC_k g^{k-1}}{k} + g^{l+1} \sum_{k=0}^{\infty} \frac{(k)(k-1)}{k} C_k g^{k-2} $$

and so the differential constraint on $V_{ee}$ becomes

$$ (l)(l+1) \sum_{k=0}^{\infty} \frac{C_k g^{k+l-1}}{k} + 2(l+1) \sum_{k=0}^{\infty} \frac{kC_k g^{k+l-1}}{k} + g^{l+1} \sum_{k=0}^{\infty} \frac{(k)(k-1)}{k} C_k g^{k+l-1} $$

$$ - z(l+1) \sum_{k=0}^{\infty} C_k g^{k+1} - 2 \sum_{k=0}^{\infty} kC_k g^{k+2} + e^2 \chi \sum_{k=0}^{\infty} C_k g^{k+2} $$

$$ - \frac{\ell}{(l+1)} \sum_{k=0}^{\infty} C_k g^{k+l-1} = 0 $$

We have terms that combine $C_k$ with two different powers of $g$: $g^{k-1}$ and $g^{k+2}$. Collecting accordingly,
\[ O = \sum_c g^{k+l} \left[ -2(l+1) - 2k + e^2 \lambda \right] + \sum_c g^{k+l} \left[ \lambda (l+1) k + k(l-1) \right] \]

Now in the second at these, let \( k = m+1 \), substitute, and then rename back \( m \rightarrow k \) to get

\[ O = \sum_c g^{k+l} \left[ 2(l+1) - 2k + e^2 \lambda \right] + \sum_c g^{k+l} \left[ 2(l+1)(k+1) + (k+1)(l) \right] \]

Whence we find that

\[ \frac{C_{k+1}}{C_k} = \frac{-2l - 2 - 2k + e^2 \lambda}{2kl + 2l + 2k + 2 + e^2 \lambda} = \frac{-e^2 \lambda + 2(l+k+1)}{k^2 + 3k + 2kl + 2l + 2} \]

\[ = \frac{-e^2 \lambda + 2(k+1)}{(k+1)^2} \quad \text{as desired} \]

Now we must truncate the recursion relation, which is to say that for \( \sum k \geq 0 \)

\[ 0 = -e^2 \lambda + 2(k+l+1) \quad \Rightarrow \quad 2(k+l+1) = e^2 \sqrt{\frac{2m}{k^2}} \quad \text{so} \]

\[ \frac{2m}{k^2} \frac{1}{e^4} \quad \Rightarrow \quad E^2 - W = \frac{Me^4}{2e^4(k+1)^2} \quad \checkmark \]
Problem 5: We seek the \( n = 2 \) \( l = 1 \) state. From 13.1.15, which follows from 13.1.14 (which we just derived), we have

\[
2 = n = k + l + 1 = k + 1 + 1 = k + 2 \quad \Rightarrow \quad k = 0
\]

Thus, from 12.1.10,

\[
\psi_{21} = \sum_{k} C_k g^k = g^2 \cdot C_0 g^0 = C_0 g^2 \quad \text{and}
\]

\[
\psi_{21} = g^2 \psi_{21} = C_0 g^2 e^{-\frac{r}{\alpha}} \quad \text{and}
\]

\[
\psi_{21} (r, \theta, \phi) = R_{21} (r) Y^0 (\theta, \phi) = \frac{U_{21} V}{g} \cdot Y^0 (\theta, \phi)
\]

\[
= C_0 g e^{-\frac{r}{\alpha}} \theta \cos \theta = C_0 g e^{-\frac{r}{\alpha}} \cos \theta
\]

Now \( g = \frac{m e^2}{\hbar^2 \alpha^2} r = \frac{r}{2\alpha} \) when \( \alpha = \frac{\hbar^2}{m e^2} \).

Absorbing a constant or two into \( C_0 \), we thus write

\[
\psi_{21} (r, \theta, \phi) = C e^{-\frac{r}{2\alpha}} \cos \theta
\]

and all that is left is to determine the normalization constant \( C \). To this end, we calculate.
\[ 1 = \frac{C^2}{\pi} \int_{r_0}^{\infty} \frac{e^{-r/a_0}}{r^2 \cos^2 \Theta} \, r \, dr \, d\Omega \]

\[ = 2\pi C^2 \int_0^1 r^2 e^{-r/a_0} \, dr \int_{-\pi}^{\pi} \cos \Theta \, d\cos \Theta \]

Let \( \chi = \cos \Theta \) and \( y = \frac{r}{a_0} \), then \( r = a_0 \chi y \) and \( \nu = a_0 \chi y \), so

\[ 1 = 2\pi C^2 \left[ \int_0^\infty y^4 e^{-y} \, dy \right] \left[ \int_0^1 \chi^2 \, d\chi \right] \]

\[ = 2\pi C^2 a_0^5 \left[ \int_0^\infty y^4 e^{-y} \, dy \right] \left[ \frac{\chi^2}{3} \right] \cdot 2\pi C^2 a_0^5 \left[ y^3 \right] \left[ \frac{2}{3} \right] \]

\[ = 32 \pi a_0^5 C^2 \Rightarrow C^2 = \frac{1}{132 \pi a_0^5} \Rightarrow \frac{1}{132 \pi a_0^5} \frac{1}{B2 \pi a_0} \frac{1}{a_0} \]

\[ y_{2,10}(r, \Theta, \phi) = \frac{1}{132 \pi a_0^5} \frac{r}{a_0} e^{-r/2a_0} \cos \Theta \]

\[ \frac{1}{2\pi a_0} \frac{e^{-r/2a_0} \cos \Theta}{\frac{r}{a_0}} \]
Problem 6

a) For the lowest value of \( n \), the angular wavefunctions will be \( \chi_n \) and \( \chi_{21} \) for the two contributing eigenstates. Thus, we must allow values of \( \ell \) as large as \( 2 \), which means \( n \) must be at least 3.

\[ \boxed{\ell = 3} \]

b) The angular part of the wavefunction is thus

\[ Y_{\ell \ell}(\theta, \phi) = \frac{1}{\sqrt{2}} \left[ Y_{11}(\theta, \phi) + Y_{21}(\theta, \phi) \right] \]

The expectation value will be given by

\[ \sqrt{\langle U^2 \rangle} = \left( \langle \frac{1}{2} \left[ Y_{11} + Y_{21} \right] | L_{x}^{2} \left| \frac{1}{2} \left[ Y_{11} + Y_{21} \right] \right. \rangle \right)^{\frac{1}{2}} \]

\[ = \left( \frac{1}{2} \left[ Y_{11} + Y_{21} \right] | 2 \hat{x}^{2} Y_{11} + 6 \hat{x}^{2} Y_{21} \rangle \right)^{\frac{1}{2}} \]

\[ = \left( \frac{1}{2} \left[ 2 \hat{x}^{2} + 6 \hat{x}^{2} \right] \right)^{\frac{1}{2}} = \sqrt{4 \hbar^2} = 2 \hbar \]
2) The full wave function is given by

\[ \psi(r, \theta, \phi) = \frac{1}{L} \left[ R_{31}(r) Y_{11}(\theta, \phi) + R_{32}(r) Y_{21}(\theta, \phi) \right] \]

The result (c) is given by

\[ \iint_{0}^{2\pi} \int_{0}^{\pi} Y_{n_{1}}^{*}(r, \theta, \phi) \psi(r, \theta, \phi) r^2 \sin \theta \, d\theta \, d\phi \]

which, by the orthonormality of the \( R_{l} \)'s reduces to

\[ \sum_{l} \int_{0}^{2\pi} \int_{0}^{\pi} \left[ Y_{l}^{*} + Y_{l}^* \right] d\Omega \]

So take it one term at a time and then average the results.

\[ \int_{0}^{2\pi} \int_{0}^{\pi} \left[ Y_{l_{1}}^{*} Y_{l_{1}} \right] \sin \theta \, d\theta \, d\phi = \frac{3\pi}{8\pi} \int_{0}^{\pi} \sin^2 \theta \, d\theta \, d\phi \]

\[ = \frac{6}{8} \int_{0}^{\pi} (1 - \cos^2 \theta) \, d\cos \theta = \frac{6}{8} \int_{1/2}^{1} (1 - x^2) \, dx \]

\[ = \frac{3\pi}{8} \left[ 1 - \frac{x^2}{3} \right]_{1/2}^{1} = \frac{3\pi}{8} \left[ 1 - \frac{1}{3} - \frac{1}{2} + \frac{1}{2} \right] = \frac{15}{96} \]

and
\[ \int_0^{\frac{\pi}{2}} \int_0^{2\pi} [Y_{21}^* Y_{21}] \sin \theta \, d\theta \, d\phi = \frac{15}{8\pi} \int_0^{\frac{\pi}{2}} \sin^2 \theta \cos^2 \theta \sin \theta \, d\theta \]

\[ = \frac{15}{4} \int_0^{\frac{\pi}{2}} (1 - \cos^2 \theta) \cos^2 \theta \, d\theta \]

\[ = \frac{15}{4} \int_0^{\frac{\pi}{2}} \cos^2 \theta (1 - \sin^2 \theta) \, d\theta \]

\[ = \frac{15}{4} \int_0^{\frac{\pi}{2}} (\cos^2 \theta - \sin^2 \theta) \, d\theta \]

\[ = \frac{15}{4} \left[ \frac{\sin^2 \theta}{2} - \frac{\cos^2 \theta}{2} \right]_0^{\frac{\pi}{2}} \]

\[ = \frac{15}{4} \left[ \frac{1}{2} - \frac{1}{2} \right] = \frac{15}{4} \cdot \frac{1}{2} = \frac{15}{8} \]

Thus, the probability is

\[ \frac{1}{2} \left[ \frac{15}{96} + \frac{47}{128} \right] \approx 0.262 \text{ or about 26.2%} \]

(d) The radial probability density is given by

\[ p(r) = r^2 R^2(r) \]

again, by the orthogonality of the Yms. We can ignore cross terms.

We want to take the ratios of \( R_2(r) \) for \( r = 0, \pi, \) and \( 2\pi \), and then square each ratio.
Problem 7

The ground-state wavefunction for Hydrogen is

\[ \psi(r, \theta, \phi) = \frac{1}{4\pi} \frac{a}{a_0}^{-2\frac{3}{2}} e^{-r/a_0} \]

To compute the requested probability, we need to transform \( \psi(r) \) to \( \phi(p) \). We know

\[ \phi(p) = \frac{1}{(2\pi)^{3/2}} \int d^3r \ e^{-i\vec{p} \cdot \vec{r}} \psi(r) \]

To write this instead in terms of \( \phi(p) \) we note that

\[ 1 = \int |\psi(k)|^2 d^3k = \int |\phi(p)|^2 \frac{d^3p}{2\pi^2} = \int \left| \frac{\phi(k)}{k\frac{\hbar}{2\pi}} \right|^2 d^3p \]

where we conclude that \( \phi(p) = \phi(k)/k\frac{\hbar}{2} \), so

\[ \phi(p) = \frac{1}{(2\pi)^{3/2}} \frac{1}{(\pi a_0^2)^{3/2}} \int r^2 dr \sin \theta \sin \phi \ e^{-i\vec{p} \cdot \vec{r} / \hbar} \ e^{-r/a_0} \]

where we have assumed \( \vec{p} = p\hat{z} \) without loss of generality. Follow through

\[ \phi(p) = \frac{1}{(2\pi)^{3/2}} \frac{1}{(\pi a_0^2)^{3/2}} 2\pi \int_0^\infty \! r^2 dr \ e^{-r/a_0} \int_0^{2\pi} \sin \phi \ e^{-ipr/a_0} \]

where we have substituted \( \chi = \cos \Theta \).
Now, \[ \int_{-\infty}^{\infty} \frac{dx}{x} e^{-i \pi x / \hbar} = \frac{i}{\pi} \left[ e^{i \pi / \hbar} - e^{-i \pi / \hbar} \right] = \frac{2}{\pi} \sin \left( \frac{\pi \hbar}{\hbar} \right) \]

= \frac{2 i}{\pi} \sin \left( \frac{\pi \hbar}{\hbar} \right) \quad \text{and so}

\[ \phi(\beta) = \frac{1}{(2\pi \hbar^2 \alpha^3)^{1/2}} \frac{2 i}{\pi} \int_{0}^{\infty} e^{-r/\alpha} \sin \left( \frac{\pi \hbar}{\hbar} \right) \, dr \]

To evaluate this integral, consider the function

\[ F(a) = \int_{0}^{\infty} e^{-ay} \sin \beta y \, dy \quad \text{which can be evaluated via} \]

\[ F(a) = \frac{1}{2i} \int_{0}^{\infty} e^{-ay} (e^{i \beta y} - e^{-i \beta y}) \, dy = \frac{1}{2i} \left[ \left( e^{-a + i \beta} \right) - \left( e^{-a - i \beta} \right) \right] \\
= \frac{1}{2i} \left[ \frac{1}{a - i \beta} + \frac{1}{a + i \beta} \right] = \frac{1}{2i} \left[ \frac{a + i \beta}{(a - i \beta)(a + i \beta)} + \frac{a - i \beta}{(a + i \beta)(a - i \beta)} \right] = \frac{a}{a^2 + \beta^2} \]

An integral is closely related to this of the form

\[ \int_{0}^{\infty} ye^{-a y} \sin \beta y \, dy = -\frac{dF}{da} = \frac{2 \alpha m}{(a^2 + \beta^2)^2}, \quad \text{yielding after application} \]

\[ \phi(\beta) = 8 \frac{\alpha \hbar}{(2\pi \hbar)^{3/2}} \frac{1}{\left[ 1 + \left( \frac{q \beta}{\alpha \hbar} \right)^2 \right]^2} \]

15
Thus, the probability of finding the electron w/ \( \varphi(\vec{r}) \) at \( \vec{r} \) is

\[
P = |\varphi(\vec{r})|^2 d^3\vec{r}
\]

where \( r = |\vec{r}| \).

Now, we can use this to find the mean kinetic energy.

\[
\left< \frac{p^2}{2\mu} \right> = \int \frac{1}{2\mu} |\varphi(\vec{r})|^2 d^3\vec{r}
\]

\[
= \frac{1}{2\mu} \frac{1}{4\pi} \int_0^\infty r^2 |\varphi(r)|^2 r^2 dr = \frac{128\pi^2}{\mu} \left( \frac{a_0}{2\pi\hbar} \right)^2 \int_0^\infty \frac{p^2 dp}{[1 + (\kappa a_0)^2]^4}
\]

\[
= \frac{128\pi^2}{M} \left( \frac{a_0}{2\pi\hbar} \right)^2 \left( \frac{\hbar}{a_0} \right)^5 \int_0^\infty \frac{x^4}{[1 + x^2]^2} dx
\]

\[
= \frac{16}{\mu \pi} \left( \frac{\hbar}{a_0} \right)^2 \int_0^\infty \frac{x^4}{[1 + x^2]^2} dx
\]

This integral can be looked up in the tables, yielding

\[
\left< \frac{p^2}{2\mu} \right> = \frac{1}{2\mu} \left( \frac{k}{a_0} \right)^2
\]
Finally, \( V(r) = -\frac{\Theta}{r} \), so \( \langle V(r) \rangle = -e^2 \langle \frac{1}{r} \rangle \). But

\[
\langle \frac{1}{r} \rangle = \int |y(r)|^2 \frac{1}{r} \, d^3 r = 4\pi \frac{1}{a_0^3} \int_0^\infty re^{-2r/a_0} \, dr,
\]

\[
= \frac{4}{a_0^3} \left( \frac{a_0}{2} \right)^2 \int_0^\infty y^2 e^{-y} \, dy = \frac{1}{a_0},
\]

So, \( \langle V(r) \rangle = -\frac{\Theta}{a_0} = -\frac{4\pi}{\mu a_0^3} \) when we have used that \( e^2 = \frac{1}{\mu a_0} \).

Thus, we confirm the Fermi result \( \langle KE \rangle = -\frac{1}{2} \langle V \rangle \).