HOMEWORK VI

Problem 1

The one-dimensional momentum eigenstate

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

generalizes to

$$\psi_{\vec{k}}(x) = \left(\frac{1}{\sqrt{2\pi}}\right)^3 e^{i\vec{k}\cdot\vec{r}} = \left(\frac{1}{\sqrt{2\pi}}\right)^3 e^{i(k_x x + k_y y + k_z z)}$$

We want to show that this is the solution to the from part 1 TISE with the Laplacian used for the second derivative.

$$-\frac{\hbar^2}{2\mu}\nabla^2 \psi_{\vec{k}}(x) \overset{?}{=} E\psi_{\vec{k}}(x)$$

Calculate

$$\nabla^2 \psi_{\vec{k}}(x) = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\left(\frac{1}{\sqrt{2\pi}}\right)^3 e^{i(k_x x + k_y y + k_z z)}$$

$$= \left(\frac{1}{\sqrt{2\pi}}\right)^3 \left((ik_x)^2 + (ik_y)^2 + (ik_z)^2\right) e^{i(k_x x + k_y y + k_z z)}$$

$$= -(k_x^2 + k_y^2 + k_z^2)\psi_{\vec{k}}(x) = -k^2\psi_{\vec{k}}(x) \quad \text{where } k^2 = |\vec{k}|^2.$$

Thus,

$$\frac{-\hbar^2}{2\mu}\nabla^2\psi_{\vec{k}}(x) - \frac{\hbar^2 k^2}{2\mu}\psi_{\vec{k}}(x) = \frac{p^2}{2\mu}\psi_{\vec{k}}(x) = E\psi_{\vec{k}}(x) \checkmark$$

<u>Problem 2</u>

Write $\psi_\ell^\ell(r,\theta,\phi) = R_{E\ell}(r)Y_\ell^\ell(\theta,\phi)$. Let's further write that

$Y_\ell^\ell(\theta,\phi) = f_{\ell\ell}(\theta)g_\ell(\phi)$ and apply this to 12.5.28

$$\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)\psi_\ell^\ell(r,\theta,\phi) = 0$$

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

$$\Rightarrow g_\ell(\phi)f_{\ell\ell}'(\theta) + i\cot\theta\, f_{\ell\ell}(\theta)g_\ell'(\phi) = 0$$

$$\Rightarrow \frac{f_{\ell\ell}'(\theta)}{\cot\theta\, f_{\ell\ell}(\theta)} = -i\frac{g_\ell'(\phi)}{g_\ell(\phi)} = \ell$$

where ℓ is a chosen separation constant. This gives us for the ϕ-dependent part

$$-i\frac{dg_l(\phi)}{d\phi} = g_l(\phi)\cdot l \Rightarrow -i\hbar\frac{d}{d\phi}g(\phi) = l\hbar\, g(\phi)$$

Since $-i\hbar\, d/d\phi = L_z^{op}$, and $L_z = \hbar$ by the supposition of the problem, then we see that the separation constant $l = 1$ and

$$-i\frac{dg_1(\phi)}{d\phi} = g_1(\phi) \Rightarrow \frac{dg_1(\phi)}{d\phi} = i g_1(\phi)$$

$$\Rightarrow \boxed{g_1(\phi) = e^{i\phi}}$$ up to normalization.

The θ-dependent piece gives

$$\frac{df_{11}(\theta)}{d\theta} = \cot\theta\, f_{11}(\theta)$$ which has the solution

$$f_{11}(\theta) = \sin\theta$$ again up to normalization

whence

$$Y_1^1(\theta,\phi) = f_{11}(\theta)\, g_1(\phi) = C \sin\theta\, e^{i\phi}$$

Now, to normalize this, impose the requirement that

$$1 = \int C^2 \left(\sin\theta\, e^{-i\phi}\right)\left(\sin\theta\, e^{i\phi}\right) d\Omega$$

$$= C^2 \int_0^{\pi}\int_0^{2\pi} \sin^2\theta \sin\theta \, d\theta\, d\phi = 2\pi C^2 \int_{-1}^{1} \left(1-\cos^2\theta\right) d(\cos\theta) \quad \text{let } x = \cos\theta$$

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

$$= \frac{8\pi}{3} C^2 \Rightarrow C = \pm\sqrt{\frac{3}{8\pi}}$$

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_-

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

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

$$= \hbar e^{-i\phi}\sqrt{\frac{3}{8\pi}}\left[\cos\theta - i(i)\cos\theta\right] e^{i\phi} = \hbar\sqrt{\frac{3}{2\pi}}\cos\theta$$

But on the other hand

$$L_- |l, l\rangle = \hbar\sqrt{[(l+l)(1)]}\, |l, l-1\rangle \quad \text{so}$$

$$L_- |1,1\rangle = \sqrt{2}\,\hbar\, |1,0\rangle \Rightarrow \cancel{|1,0\rangle}$$

$$\Rightarrow |1,0\rangle = \frac{1}{\sqrt{2}\hbar} L_- |1,1\rangle = \frac{1}{\sqrt{2}\hbar}\,\hbar\sqrt{\frac{3}{2\pi}}\cos\theta = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta$$

$$\Rightarrow \boxed{Y_1^0 = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta}$$ again, as desired!

Problem 3

The $\ell=0$ radial solutions are of the form

$$j_0(\rho) = \frac{\sin\rho}{\rho} \qquad n_0(\rho) = \frac{-\cos\rho}{\rho}$$

where $\rho = kr$ and $k = \sqrt{2\mu E}/\hbar$

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

$$0 = j_0(kr_0) = \frac{\sin(kr_0)}{kr_0} \qquad 0 = n_0(kr_0) = -\frac{\cos(kr_0)}{kr_0}$$

There are satisfied for values of k for which $kr_0 = n\pi$, $n>0$ (j_0 case) or $kr_0 = (n-\frac{1}{2})\pi$ $n>0$ (n_0 case) so in general there is a solution whenever

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

This in turn implies

$$\frac{\sqrt{2\mu E_n}}{\hbar} = \frac{n\pi}{2r_0} \qquad \boxed{E_n = \frac{n^2\pi^2\hbar^2}{8\mu r_0}}$$

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 $V_{E\ell}$:

$$V'_{E\ell} = \frac{dV_{E\ell}}{d\rho} = (\ell+1)\rho^{\ell}\sum_{k=0}^{\infty} C_k\rho^k + \rho^{\ell+1}\sum_{1}^{\infty} kC_k\rho^{k-1}$$

$$V''_{E\ell} = (\ell)(\ell+1)\rho^{\ell-1}\sum_{0}^{\infty} C_k\rho^k + (\ell+1)\rho^{\ell}\sum_{0}^{\infty} kC_k\rho^{k-1} +$$

$$+ (\ell+1)\rho^{\ell}\sum_{0}^{\infty} kC_k\rho^{k-1} + \rho^{\ell+1}\sum_{0}^{\infty}(k)(k-1)\,C_k\rho^{k-2}$$

$$= (\ell)(\ell+1)\rho^{\ell-1}\sum_{0}^{\infty} C_k\rho^k + 2(\ell+1)\rho^{\ell}\sum_{0}^{\infty} kC_k\rho^{k-1} + \rho^{\ell+1}\sum_{0}^{\infty}(k)(k-1)C_k\rho^{k-2}$$

and so the differential constraint on $V_{E\ell}$ becomes

$$\cancel{(\ell)(\ell+1)\sum_{0}^{\infty} C_k\rho^{k+\ell-1}} + 2(\ell+1)\sum_{0}^{\infty} kC_k\rho^{k+\ell-1} + \sum_{0}^{\infty}(k)(k-1)C_k\rho^{k+\ell-1}$$

$$- 2(\ell+1)\sum_{0}^{\infty} C_k\rho^{k+\ell} - 2\sum_{0}^{\infty} kC_k\rho^{k+\ell} + e^2\lambda\sum_{0}^{\infty} C_k\rho^{k+\ell} -$$

$$- \cancel{\ell(\ell+1)\sum_{0}^{\infty} C_k\rho^{k+\ell-1}} = 0$$

We have ~~factors~~ terms that combine C_k w/ two different factors of ρ: $\rho^{k+\ell}$ and $\rho^{k+\ell-1}$. Collecting accordingly,

$$0 = \sum C_k \rho^{k+l} \left[-2(l+1) - 2k + e^2\lambda \right]$$

$$+ \sum C_k \rho^{k+l-1} \left[2(l+1)k + k(k-1) \right]$$

Now in the second of these let $k = m+1$, substitute, and then rename back $m \to k$ to get

$$0 = \sum C_k \rho^{k+l} \left[-2(l+1) - 2k + e^2\lambda \right] + \sum C_{k+1} \rho^{k+l} \left[2(l+1)(k+1) + (k+1)(k) \right]$$

whence we find that

$$\frac{C_{k+1}}{C_k} = -\frac{-2l-2-2k+e^2\lambda}{2lk+2l+2k+2+k^2+k} = \frac{-e^2\lambda + 2(l+k+1)}{k^2+3k+2lk+2l+2}$$

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

Now, we must truncate the recursion relation, which is to say that for some $k \geq 0$

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

$$\frac{2m}{\hbar^2 W} = \frac{4(k+l+1)^2}{e^4} \Rightarrow E = -W = -\frac{me^4}{2\hbar^2(k+l+1)^2} \quad \checkmark$$

Problem 5 We seek the $n=2$ $l=1$ state. From 13.1.15, which follows from 13.1.14 (which we just derived) ~~the~~

$$2 = n = k + l + 1 = k + 1 + 1 = k + 2 \quad \Rightarrow \quad k = 0$$

Then, from 13.1.10

$$V_{21} = \rho^{l+1} \sum_0^0 C_k \rho^k = \rho^2 \cdot C_0 \rho^0 = C_0 \rho^2 \quad \text{and}$$

$$U_{21} = \rho^{-\rho} V_{21} = C_0 \rho^2 e^{-\rho} \quad \text{and}$$

$$\psi_{210}(r,\theta,\phi) = R_{21}(r)\, Y_1^0(\theta,\phi) = U_{21}/\rho \cdot Y_1^0(\theta,\phi)$$

$$= C_0 \rho e^{-\rho} P_1(\theta) = C_0 \rho e^{-\rho} \cos\theta$$

Now $\rho = \dfrac{me^2}{\hbar^2 n} r = \dfrac{r}{2a_0}$ where $a_0 = \hbar^2/me^2$

Absorbing a constant or two into C_0, we thus write

$$\psi_{210}(r,\theta,\phi) = C r e^{-r/2a_0} \cos\theta$$

and all that is left is to determine the normalization constant C. To this end, we calculate

$$1 = C^2 \int r^2 e^{-r/a_0} \cos^2\theta \, r^2 dr \, d\Omega$$

$$= 2\pi C^2 \int_0^\infty r^4 e^{-r/a_0} dr \int_{-1}^{1} \cos^2\theta \, d\cos\theta$$

Let $x = \cos\theta$ $y = r/a_0 \Rightarrow dr = a_0 y$ $r^4 = a_0^4 y$ so

$$1 = 2\pi C^2 \left[\int_0^\infty a_0^5 y^4 e^{-y} dy \right] \left[\int_{-1}^{1} x^2 dx \right]$$

$$= 2\pi C^2 a_0^5 \left[\int_0^\infty y^4 e^{-y} dy \right] \left[\frac{x^3}{3} \right]_{-1}^{1} = 2\pi C^2 a_0^5 \left[4! \right] \left[\frac{2}{3} \right]$$

$$= 32\pi a_0^5 C^2 \Rightarrow C = \frac{1}{\sqrt{32\pi a_0^5}} = \frac{1}{\sqrt{32\pi a_0^3}} \frac{1}{a_0}$$

$$\boxed{\psi_{210}(r,\theta,\phi) = \frac{1}{\sqrt{32\pi a_0^3}} \frac{r}{a_0} e^{-r/2a_0} \cos\theta}$$

Problem 6

a) For the lowest value of n, the angular wavefunctions will be Y_{11} and Y_{21} for the two contributing eigenstates. Thus, we must allow values of l as large as 2, which means n must be at least 3.

$$\boxed{n = 3}$$

b) The angular part of the wavefunction is thus

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

The expectation value will be given by

$$\sqrt{\langle L^2 \rangle} = \left(\left\langle \tfrac{1}{\sqrt{2}}\left[Y_{11} + Y_{21}\right] \middle| L^2_{op} \middle| \tfrac{1}{\sqrt{2}}\left[Y_{11} + Y_{21}\right] \right\rangle\right)^{1/2}$$

$$= \left(\frac{1}{2}\left\langle Y_{11} + Y_{21} \middle| 2\hbar^2 Y_{11} + 6\hbar^2 Y_{21} \right\rangle\right)^{1/2}$$

$$= \left(\frac{1}{2}\left[2\hbar^2 + 6\hbar^2\right]\right)^{\frac{1}{2}} = \sqrt{4\hbar^2} = \boxed{2\hbar}$$

c) The full wave function is given by

$$\psi(r,\theta,\phi) = \frac{1}{\sqrt{2}}\left[R_{31}(r)\,Y_{11}(\theta,\phi) + R_{32}(r)\,Y_{21}(\theta,\phi)\right]$$

The result c) is given by

$$\int_0^\infty \int_0^{\pi/3} \int_0^{2\pi} \psi^*(r,\theta,\phi)\,\psi(r,\theta,\phi)\, r^2 dr \sin\theta\, d\theta\, d\phi$$

which, by the orthonormality of the R's reduces to

$$\int_0^{\pi/3} \int_0^{2\pi} \left(\frac{1}{\sqrt{2}}\right)^2 \left[Y_{11}^* Y_{11} + Y_{21}^* Y_{21}\right] d\Omega$$

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

$$\int_0^{\pi/3} \int_0^{2\pi} \left[Y_{11}^* Y_{11}\right] \sin\theta\, d\theta\, d\phi = \frac{3}{8\pi} \iint \sin^2\theta \sin\theta\, d\theta\, d\phi$$

$$= \frac{6}{8} \int_0^{\pi/3} (1-\cos^2\theta)(-d\cos\theta) = \frac{6}{8} \int_{1/2}^{1} (1-x^2)\, dx$$

$$= \frac{3}{4} \cdot \left[x - \frac{x^3}{3}\right]_{1/2}^{1} = \frac{3}{4}\left[1 - \frac{1}{2} - \frac{1}{3} + \frac{1}{24}\right] = \frac{15}{96}$$

and

$$\int_0^{\pi/3}\int_0^{2\pi}\left[Y_{21}^* Y_{21}\right]\sin\theta\, d\theta\, d\phi = \frac{15}{8\pi}\int_0^{\pi/3}\int_0^{2\pi}\sin^2\theta\cos^2\theta\sin\theta\, d\theta\, d\phi$$

$$= \frac{15}{4}\int_0^{\pi/3}(1-\cos^2\theta)\cos^2\theta\, d(-\cos\theta) = \frac{15}{4}\int_{1/2}^{1} x^2(1-x^2)\, dx$$

$$= \frac{15}{4}\int_{1/2}^{1}(x^2-x^4)\, dx = \frac{15}{4}\left[\frac{x^3}{3}-\frac{x^5}{5}\right]_{1/2}^{1}$$

$$= \frac{15}{4}\left[\frac{1}{3}-\frac{1}{24}-\frac{1}{5}+\frac{1}{160}\right] = \frac{15}{4}\left[\frac{47}{480}\right] = \frac{47}{128}$$

Thus, the probability is

$$\frac{1}{2}\left[\frac{15}{96}+\frac{47}{128}\right] \doteq .262 \text{ or about } \boxed{26.2\%}$$

d) The radial probability density is given by

$P(r) = r^2R^2(r)$, again, by the orthonormality of the Y_{lm}'s, we can ignore cross terms.

We want to take the ratio of $rR(r)$ for $r=a_0$ and $r=2a_0$ and then square and average.

Problem 7

The ground-state wavefunction for Hydrogen is

$$\psi(r,\theta,\phi) = \frac{1}{\sqrt{\pi}} a_0^{-3/2} e^{-r/a_0}$$

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

$$\phi(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int d^3r\, e^{-i\vec{k}\cdot\vec{r}} \psi(\vec{r})$$

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

$$1 = \int |\phi(k)|^2 d^3k = \int |\phi(k)|^2 \frac{d^3p}{\hbar^3} = \int \left|\frac{\phi(k)}{\hbar^{3/2}}\right|^2 d^3p$$

whence we conclude that $\phi(p) = \phi(k)/\hbar^{3/2}$, so

$$\phi(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \frac{1}{(\pi a_0)^{3/2}} \int r^2 dr \sin\theta d\theta d\phi\, e^{-ipr\cos\theta/\hbar} e^{-r/a_0}$$

where we have assume $\vec{p} = p\hat{z}$ w/out loss of generality. Following through,

$$\phi(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \frac{1}{(\pi a_0)^{3/2}} 2\pi \int_0^\infty r^2 dr\, e^{-r/a_0} \int_{-1}^{1} dx\, e^{-iprx/\hbar}$$

where we have substituted $x = \cos\theta$.

Now, $\int_{-1}^{1} dx\, e^{-ipr x/\hbar} = \frac{\hbar}{pr} i \left[e^{-ipr/\hbar} - e^{ipr/\hbar} \right] = \frac{\hbar}{pr} \cdot i \cdot 2i \sin\left(-\frac{pr}{\hbar}\right)$

$= \frac{2\hbar}{pr} \sin\left(\frac{pr}{\hbar}\right)$ and so

$$\phi(\vec{p}) = \frac{1}{(2\pi^2 \hbar^3 a_0^3)^{1/2}} \frac{2\hbar}{p} \int_0^\infty r e^{-r/a_0} \sin\left(\frac{pr}{\hbar}\right) dr$$

To evaluate this integral, consider the function

$F(a) = \int_0^\infty e^{-ay} \sin my\, dy$ which can be evaluated via

$$F(a) = \frac{1}{2i} \int_0^\infty e^{-ay} \left(e^{imy} - e^{-imy}\right) dy = \frac{1}{2i} \int_0^\infty \left[e^{-(a-im)y} - e^{-(a+im)y} \right] dy$$

$$= \frac{1}{2i} \left[\frac{1}{a-im} - \frac{1}{a+im} \right] = \frac{1}{2i} \left[\frac{a+im}{a^2+m^2} - \frac{a-im}{a^2+m^2} \right] = \frac{m}{a^2+m^2}$$

Our integral is closely related; it is of the form

$\int_0^\infty y e^{-ay} \sin my\, dy = -\frac{dF}{da} = \frac{2am}{(a^2+m^2)^2}$, yielding after application

$$\phi(\vec{p}) = 8\sqrt{\pi} \left(\frac{a_0}{2\pi\hbar}\right)^{3/2} \frac{1}{\left[1 + \left(\frac{a_0 p}{\hbar}\right)^2\right]^2}$$

Thus, the probability of finding the electron w/in d^3p of $\vec{p}$ is

$$P = |\phi(\vec{p})|^2 d^3p \qquad \text{where} \quad p = |\vec{p}|.$$

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

$$\left\langle \frac{p^2}{2\mu} \right\rangle = \int \frac{p^2}{2\mu} |\phi(\vec{p})|^2 d^3p$$

$$= \frac{1}{2\mu} 4\pi \int_0^\infty p^2 |\phi(\vec{p})|^2 p^2 dp = \frac{128\pi^2}{\mu} \left(\frac{a_0}{2\pi\hbar}\right)^3 \int_0^\infty \frac{p^4 dp}{[1+(a_0 p/\hbar)^2]^4}$$

$$= \frac{128\pi^2}{\mu} \left(\frac{a_0}{2\pi\hbar}\right)^3 \left(\frac{\hbar}{a_0}\right)^5 \int_0^\infty \frac{x^4}{[1+x^2]^2} dx$$

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

This integral can be looked up in the tables, yielding

$$\boxed{\left\langle \frac{p^2}{2\mu} \right\rangle = \frac{1}{2\mu} \left(\frac{\hbar}{a_0}\right)^2}$$

Finally, $V(r) = -e^2/r$, so $\langle V(r)\rangle = -e^2\left\langle \frac{1}{r}\right\rangle$. But

$$\left\langle \frac{1}{r}\right\rangle = \int |\psi(r)|^2 \frac{1}{r}\, d^3r = 4\pi \frac{1}{\pi a_0^3}\int_0^\infty r e^{-2r/a_0}\, dr$$

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

So, $\langle V(r)\rangle = -\frac{e^2}{a_0} = -\frac{\hbar^2}{\mu a_0^2}$ where we have used that $e^2 = \hbar^2/\mu a_0$.

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