# PHY 362K Homework 3

Xiaohui Chen
EID: xc2388

February 16, 2015

## 1

### (a)

From equation 1.25 in lecture note and the reduced mass correction, we get that $E_n = -\frac{1}{2}\left(\frac{m_e}{\hbar^2}\right)\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\left(\frac{m_p}{m_p+m_e}\right)\frac{Z^2}{n^2}$

We know that $m_p = 1.672621 * 10^{-27}kg$ and $m_e = 9.109 * 10^{-31}kg$

$\therefore \frac{m_p}{m_p+m_e} = 0.999456$

We also know that $Z = 2$

Plug in all the values of the constants, we get

$\boxed{E_1 = -54.393147eV}$

$\boxed{E_2 = -13.598287eV}$

$\boxed{E_3 = -6.043683eV}$

Equation 1.9 tells us $\frac{1}{\lambda_{nn'}} = \frac{E_n - E_{n'}}{hc}$, where $hc = 1240eV \cdot nm = 1.24 * 10^{-4}eV \cdot cm$

Therefore, in unit of $cm^{-1}$, we redefine energy $E_n' = \frac{E_n - E_1}{hc}$

$\therefore \boxed{E_1' = 0cm^{-1}}$

$\boxed{E_2' = 328991cm^{-1}}$

$\boxed{E'_3 = 389915 cm^{-1}}$

### (b)

The calculated energies and measured energies are shown in the table below:

| n | $E'_{n-calculated}$ $(cm^{-1})$ | $E'_{n-measured}$ $(cm^{-1})$ | fractional difference=$\frac{\lvert E'_{n-measured}-E'_{n-calculated}\rvert}{E'_{n-measured}}$ |
|---|---|---|---|
| 1 | 0 | 0 | N/A |
| 2 | 328991 | 329179.76197 | 0.000574019 |
| 3 | 389915 | 390140.964175 | 0.000579109 |

The fractional difference is also shown on the table above

### (c)

The Balmer-$\alpha$ transition is the transition between $n = 3$ and $n = 2$

$\frac{1}{\lambda_{32}} = E'_{3-measured} - E'_{2-measured} = 60961.2 cm^{-1}$

$\therefore \lambda_{32} \approx 164.039 nm$

According to the electromagnetic spectrum, the light emitted is within the ultraviolet region.

Therefore the light is not visible

## 2

### (a)

This part is omitted because we don't have to turn in any work for this part

## (b)

The Schrodinger equation for hydrogen eigenvalue problem is:

$\left[-\frac{\hbar^2}{2m_e}\frac{d^2}{dr^2} + V_{eff}(r)\right]u(r) = Eu(r)$ where $V_{eff} = -\frac{e^2}{4\pi\epsilon_0 r} + \frac{l(l+1)\hbar^2}{2m_e r^2}$

When $\rho = \frac{r}{a_0}$ and $\epsilon = \frac{E}{e^2/4\pi\epsilon_0 a_0}$, we get

$\rho^2 = \frac{r^2}{a_0^2}$, then $dr^2 = a_0^2 d\rho^2$

We also know that $a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}$, which means $\frac{e^2}{4\pi\epsilon_0 a_0} = \frac{\hbar^2}{m_e a_0^2}$

$\therefore \left[-\frac{\hbar^2}{2m_e a_0^2}\frac{d^2}{d\rho^2} - \frac{e^2}{4\pi\epsilon_0 a_0\rho} + \frac{l(l+1)\hbar^2}{2m_e a_0^2\rho^2}\right]u(\rho) = Eu(r)$

$\left[-\frac{1}{2}\frac{d^2}{d\rho^2} - \frac{1}{\rho} + \frac{l(l+1)}{2\rho^2}\right]u(\rho) = \frac{E}{e^2/4\pi\epsilon_0 a_0}u(r) = \epsilon u(\rho)$

$\therefore \left[-\frac{1}{2}\frac{d^2}{d\rho^2} + V_{eff}(\rho)\right]u(\rho) = \epsilon u(\rho)$ where $V_{eff}(\rho) = -\frac{1}{\rho} + \frac{l(l+1)}{2\rho^2}$

Therefore we have to solve the differential equation $-\frac{1}{2}u''(\rho) + (V_{eff}(\rho) - \epsilon)u(\rho) = 0$

The code for plotting $V_{eff}$ is:

```
Veff[\[Rho]_] := -1/\[Rho] + (l*(l + 1))/(2*\[Rho]^2)
Do[l := n;
 Plot[Veff[\[Rho]], {\[Rho], 0, 10},
   AxesLabel -> {"\[Rho]", "Veff(\[Rho])"},
   PlotLabel -> "Plot of Veff where l=" <> ToString[l]]
   // Print, {n, 0, 2}]


NDSolve[{-u''[\[Rho]]/2 +(Veff[\[Rho]]- \[Epsilon])*u[\[Rho]]==0,
  u[0] == 0, u'[0] == 5}, u, {\[Rho], 0, 5}]
Plot[u[\[Rho]] /. %, {\[Rho], 0, 3}]
```

The plot of $V_{eff}(\rho)$ when $l = 0$ is shown in 1

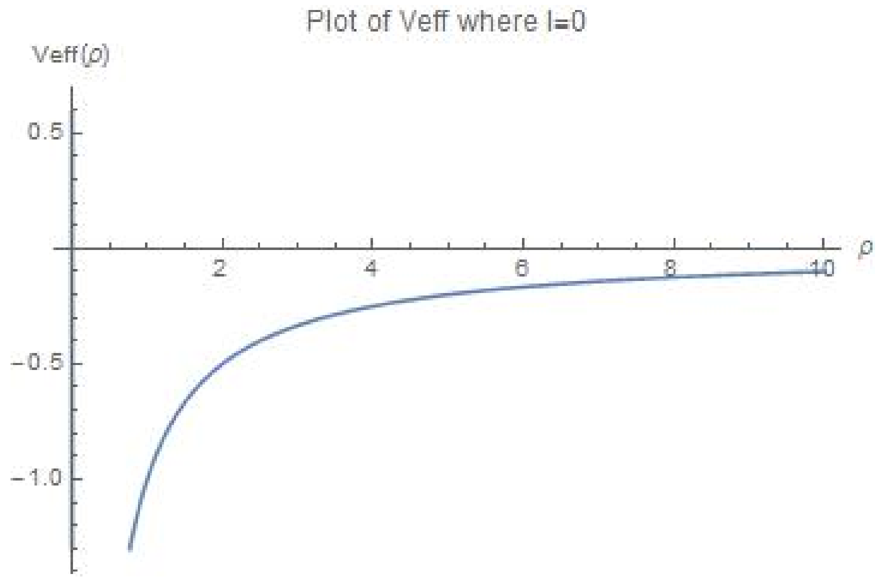


Figure 1: $V_{eff}(\rho)$ when $l = 0$

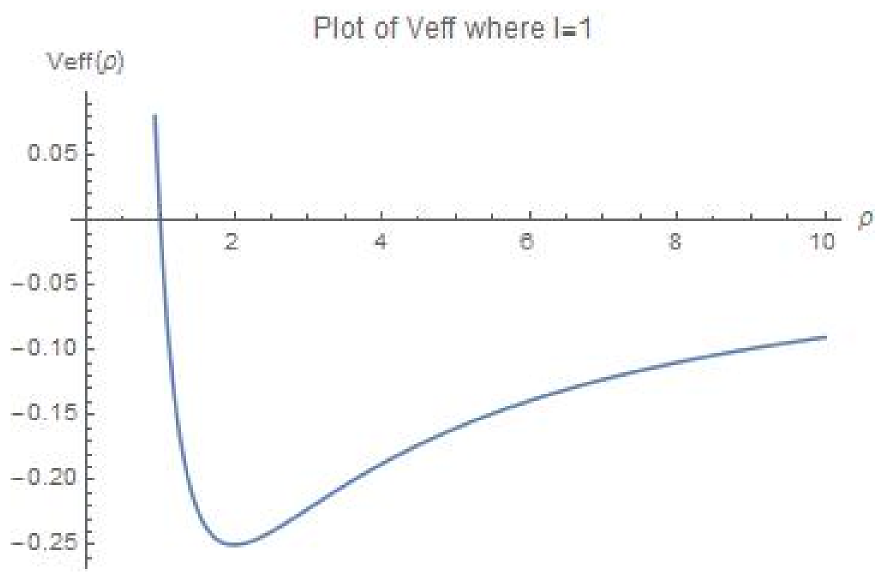


Figure 2: $V_{eff}(\rho)$ when $l = 1$

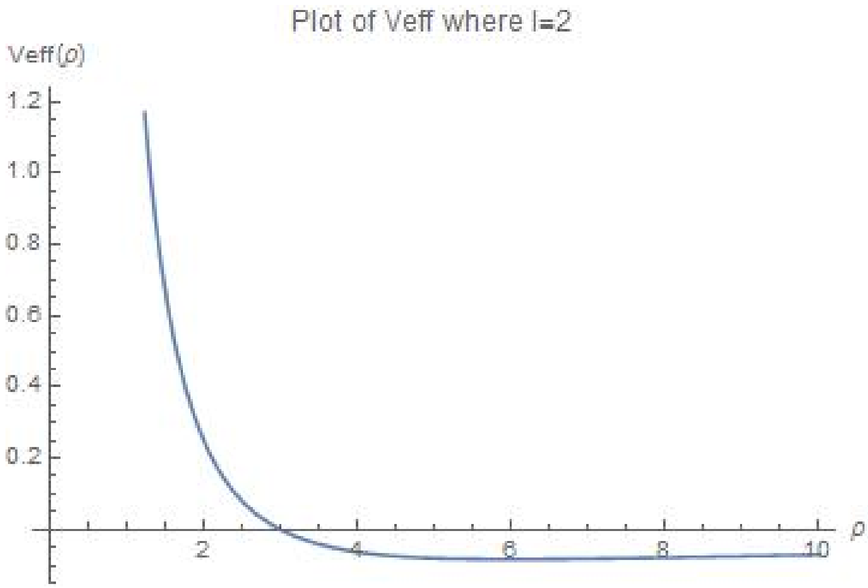


Figure 3: $V_{eff}(\rho)$ when $l = 2$

The plot of $V_{eff}(\rho)$ when $l = 1$ is shown in 2

The plot of $V_{eff}(\rho)$ when $l = 2$ is shown in 3

The code for finding and plotting $u(\rho)$ is:

```
l := 0

\[Epsilon] := -0.5

ep := $MachineEpsilon

NDSolve[{-u''[\[Rho]]/2+(Veff[\[Rho]]-

\[Epsilon])*u[\[Rho]] == 0,

  u[ep] == 0, u'[ep] == 2}, u, {\[Rho], ep, 10} ]

Plot[u[\[Rho]] /. %, {\[Rho], ep, 10},

 AxesLabel -> {"\[Rho]", "u[\[Rho]]"},

 PlotLabel ->
```

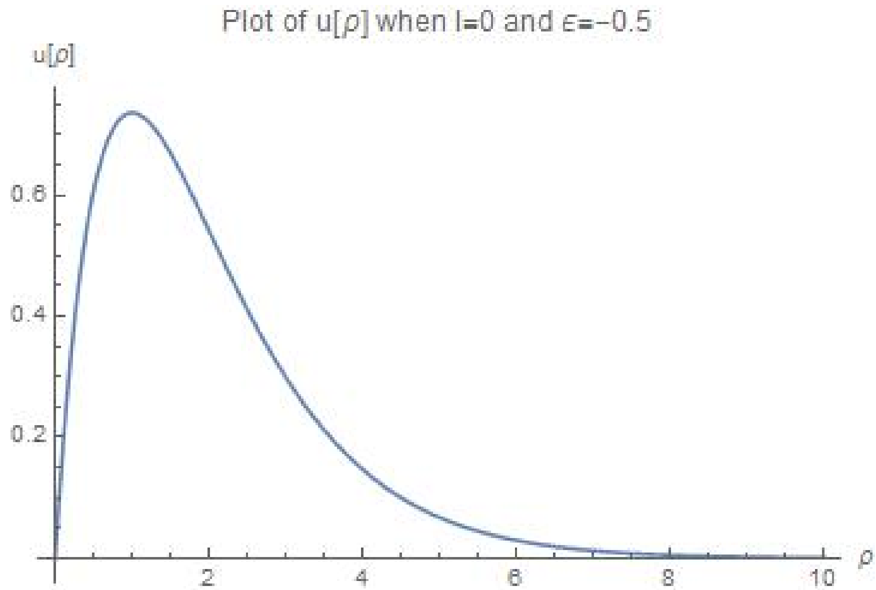


Figure 4: $u(\rho)$ when $l = 0$ and $n = 1$

```
"Plot␣of␣u[\[Rho]]␣when␣l=" <> ToString[l] <>
"␣and␣\[Epsilon]=" <> ToString[\[Epsilon]]]
```

Since $u(\rho)$ is singular, ep, which is a number slightly larger than 0, is used here

## (c)

From the property of wave functions, we know that $\lim_{\rho\to\infty} u(\rho) = 0$ must be true

In addition, when n=1, there are no node

When n=2, there is one node

When n=3, there are two nodes

From the differential equation shown in part (b), we know that the eigenvalue is $\epsilon$

When $l = 0$, the three eigenvalues occur at n=1,2,3 respectively

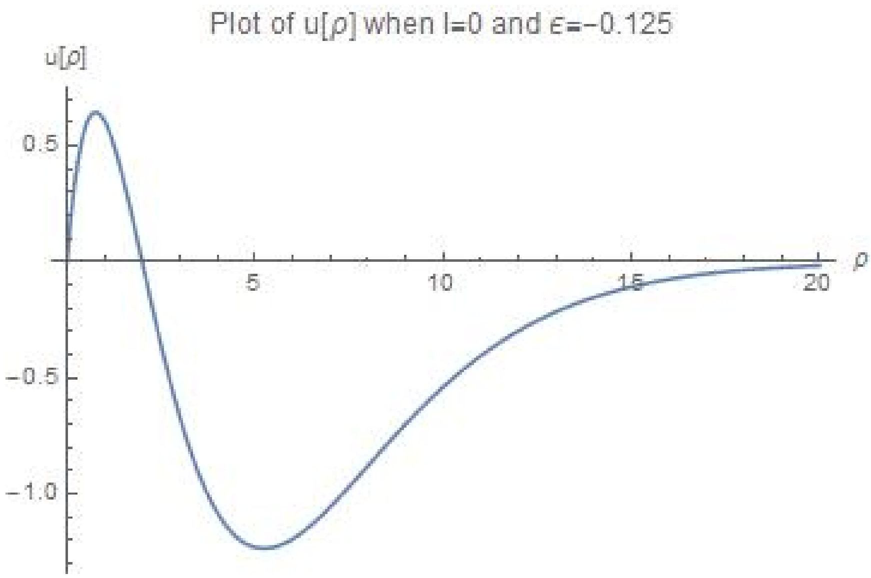


Figure 5: $u(\rho)$ when $l = 0$ and $n = 2$

Through experiments, I got the following approximated results:

When $l = 0$ and $n = 1$, the eigenvalue $\epsilon \approx -0.5$. The graph is shown in Figure 4

When $l = 0$ and $n = 2$, the eigenvalue $\epsilon \approx -0.125$. The graph is shown in Figure 5

When $l = 0$ and $n = 3$, the eigenvalue $\epsilon \approx -0.05556$. The graph is shown in Figure 6

When $l = 1$ and $n = 2$, the eigenvalue $\epsilon \approx -0.125$. The graph is shown in Figure 7

When $l = 1$ and $n = 3$, the eigenvalue $\epsilon \approx -0.05556$. The graph is shown in Figure 8

When $l = 2$ and $n = 3$, the eigenvalue $\epsilon \approx -0.05556$. The graph is shown in Figure 9

## (d)

$\because \epsilon = \frac{E}{e^2/4\pi\epsilon_0 a_0}$ and $\frac{e^2}{4\pi\epsilon_0 a_0} = \frac{\hbar^2}{m_e a_0^2}$

$\therefore E = \frac{\hbar\epsilon}{m_e a_0^2}$ where $m_e = 9.109 * 10^{-31} kg$ and $a_0 = 0.529 * 10^{-10} m$

When $\epsilon = -0.5$, $E \approx -2.18133 * 10^{-18} J = -13.61479 eV$

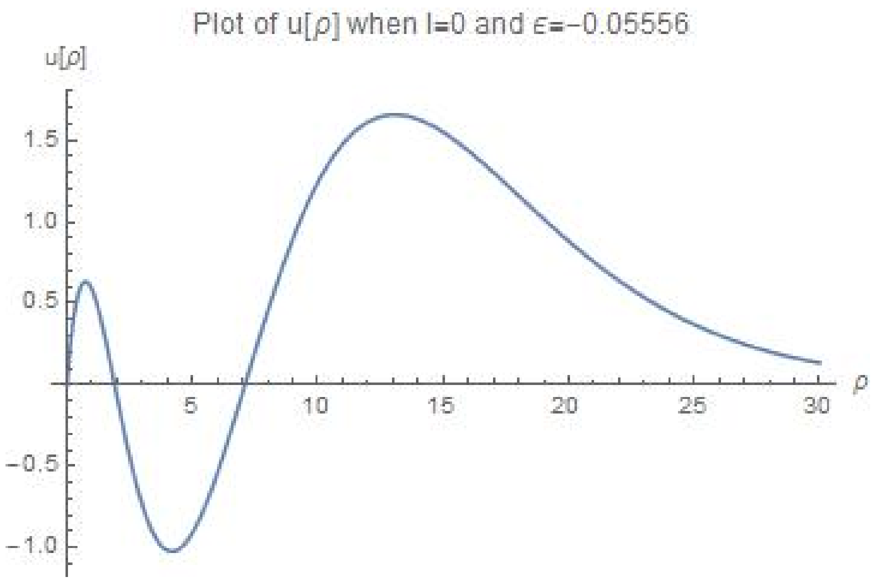


Figure 6: $u(\rho)$ when $l = 0$ and $n = 3$

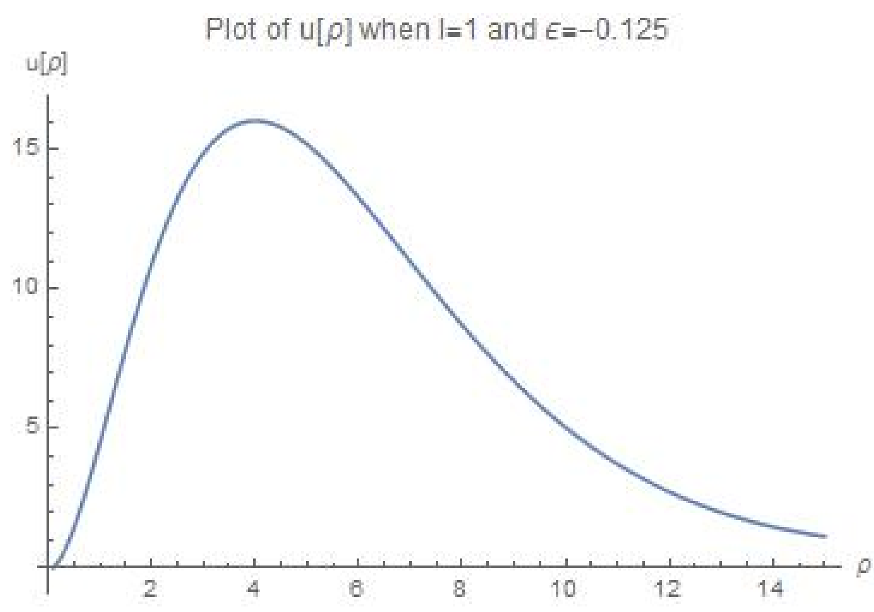


Figure 7: $u(\rho)$ when $l = 1$ and $n = 2$

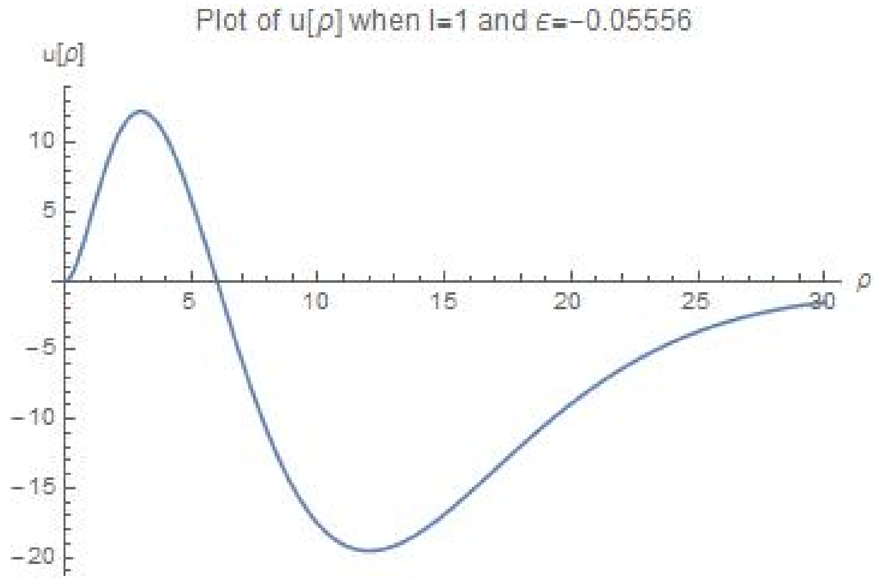


Figure 8: $u(\rho)$ when $l = 1$ and $n = 3$

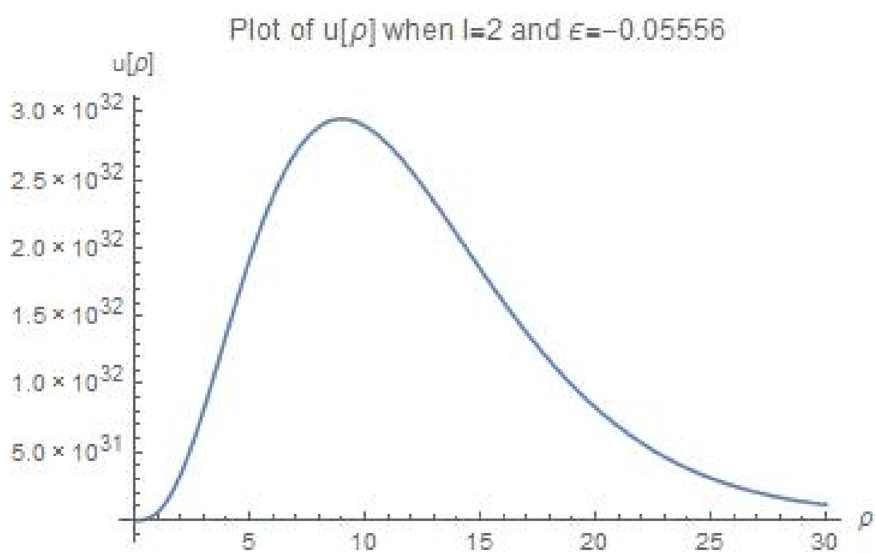


Figure 9: $u(\rho)$ when $l = 2$ and $n = 3$

When $\epsilon = -0.125$, $E \approx -5.45333 * 10^{-19}J = -3.403701eV$

When $\epsilon = -0.05556$, $E \approx -2.4239 * 10^{-19}J = -1.512879eV$

Therefore:

| Spectroscopic Label | Number of Nodes | $E_{n-calculated}(eV)$ | $E_{n-expected}(eV)$ |
|---|---|---|---|
| 1s | 0 | $-13.61479$ | $-13.6$ |
| 2s | 1 | $-3.403701$ | $-3.4$ |
| 2p | 0 | $-3.403701$ | $-3.4$ |
| 3s | 2 | $-1.512879$ | 1.511 |
| 3p | 1 | $-1.512879$ | 1.511 |
| 3d | 0 | $-1.512879$ | 1.511 |

From the table given above, we can know the calculated values of energies match the expected values

When $\rho$ approaches 0, $u(\rho)$ approaches to a number larger than 0 when $l = 0$. However, $u(\rho)$ approaches 0 when $\rho$ approaches when $l = 1$ and $l = 2$

However, since the question requires us to set $u[0] = 0$ in Mathematica, the graph shown in part (c) when $l = 0$ has a huge peak near $\rho = 0$. When $l = 1$ and $l = 2$, the wave function correctly approaches 0 as $\rho$ approaches 0. Therefore the wave functions plotted are considered having a correct dependence on r when r approaches 0.

# 3

## (a)

We know that $[L_z, z] = 0$, this means

$\langle\psi_{nlm}|[L_z, z]|\psi_{n'l'm'}\rangle = \langle\psi_{nlm}|(L_z z - z L_z)|\psi_{n'l'm'}\rangle = \hbar m\langle\psi_{nlm}|z|\psi_{n'l'm'}\rangle - \langle\psi_{nlm}|z|\psi_{n'l'm'}\rangle\hbar m' =$

$\hbar(m - m')\langle\psi_{nlm}|z|\psi_{n'l'm'}\rangle = 0$

Therefore this matrix element is zero unless $m = m'$

## (b)

From the equation of radial wave function, we get:

$R_{10} = 2a^{-3/2}\exp\left(-\frac{r}{a}\right)$

$R_{20} = \frac{a^{-3/2}\left(1-\frac{0.5r}{a}\right)\exp\left(-\frac{r}{2a}\right)}{\sqrt{2}}$

$R_{21} = \frac{a^{-3/2} r \exp\left(-\frac{r}{2a}\right)}{\sqrt{24}a}$

$R_{30} = \frac{2a^{-3/2}\left(\frac{2}{27}\left(\frac{r}{a}\right)^2 - \frac{2r}{3a} + 1\right)\exp\left(-\frac{r}{3a}\right)}{\sqrt{27}}$

$R_{31} = 8/(27 * \sqrt{6}) * a^{-3/2} * (1 - (1/6) * (r/a)) * (r/a) * \exp[-r/(3 * a)]$

$R_{32} = 4/(81 * \sqrt{30}) * a^{-3/2} * (r/a)^2 * \exp[-r/(3 * a)]$

Using mathematica, we get:

**(i)**

$\langle\psi_{200}|z|\psi_{100}\rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} R_{20}^* Y_{00}^* R_{10} Y_{00} r^2 \sin\theta r \cos\theta dr d\theta d\phi = 0$

**(ii)**

$\langle\psi_{210}|z|\psi_{100}\rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} R_{21}^* Y_{10}^* R_{10} Y_{00} r^2 \sin\theta r \cos\theta dr d\theta d\phi = \frac{128\sqrt{2}a}{243}$

**(iii)**

$\langle\psi_{300}|z|\psi_{100}\rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} R_{30}^* Y_{00}^* R_{10} Y_{00} r^2 \sin\theta r \cos\theta dr d\theta d\phi = 0$

**(iv)**

$\langle\psi_{310}|z|\psi_{100}\rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} R_{31}^* Y_{10}^* R_{10} Y_{00} r^2 \sin\theta r \cos\theta dr d\theta d\phi = \frac{27a}{64\sqrt{2}}$

**(v)**

$\langle\psi_{320}|z|\psi_{100}\rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} R_{32}^{*}Y_{20}^{*}R_{10}Y_{00}r^2\sin\theta r\cos\theta drd\theta d\phi = 0$

**(vi)**

$\langle\psi_{210}|z|\psi_{200}\rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} R_{21}^{*}Y_{10}^{*}R_{20}Y_{00}r^2\sin\theta r\cos\theta drd\theta d\phi = -3a$

According to equation 4.32 in textbook, we know that $Y_l^m\cos(\theta) = AY_{l+1}^m + B$ where A,B are constants

$\therefore \langle Y_l^m|z|Y_{l'}^{m'}\rangle = K\delta_{l+1,l'}\delta m, m'$ or $K'\delta_{l,l'+1}\delta m, m'$ where $K$ and $K'$ are constants

Therefore, as for the matrix elements, $m = m'$ should be true and $|l - l'| = 1$ should also be true

# 4

## (a)

We know that $\vec{B} = B\hat{z}$ and $\vec{r} = x\hat{x} + y\hat{y} + z\hat{z}$

$$\therefore \vec{A} = \frac{1}{2}\left(\vec{B}\times\vec{r}\right) = \frac{1}{2}\begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 0 & B \\ x & y & z \end{vmatrix} = \frac{1}{2}\left(-By\hat{x} + Bx\hat{y}\right) = \frac{B}{2}(-y\hat{x} + x\hat{y})$$

## (b)

The $\vec{p}$ operator can be written as $\vec{p} = -i\hbar\vec{\bigtriangledown}$

$\vec{A} = (-\frac{1}{2}By + \frac{\partial}{\partial x}(-\frac{1}{2}Bxy))\hat{x} + (\frac{1}{2}Bx + \frac{\partial}{\partial y}(-\frac{1}{2}Bxy))\hat{y} + \frac{\partial}{\partial z}(-\frac{1}{2}Bxy)\hat{z} = -By\hat{x}$

$\Phi = \frac{\partial}{\partial t} = 0$

$\therefore H = \frac{1}{2m}\left(\vec{p}^2 + e\vec{A}\cdot\vec{p} + e\vec{p}\cdot\vec{A} + e^2|\vec{A}|^2\right) = -\frac{\hbar^2}{2m}\vec{\bigtriangledown}^2 + \frac{i\hbar eBy}{2m}\frac{\partial}{\partial x} + \frac{i\hbar e}{2m}\frac{\partial By}{\partial} + \frac{e^2B^2y^2}{2m} = -\frac{\hbar^2}{2m}\vec{\bigtriangledown}^2 + \frac{i\hbar eBy}{2m}\frac{\partial}{\partial x} + \frac{e^2B^2y^2}{2m}$

## (c)

From the Hamiltonian in part (b), we get:

$H\psi(x,y) = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(x,y) + \frac{i\hbar eBy}{2m}\frac{\partial}{\partial x}\psi(x,y) + \frac{e^2B^2y^2}{2m}\psi(x,y) = -\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2}e^{ikx}f(y) + e^{ikx}\frac{\partial^2}{\partial y^2}f(y)) + \frac{i\hbar eBy}{2m}\frac{\partial}{\partial x}e^{ikx}f(y) + \frac{e^2B^2y^2}{2m}e^{ikx}f(y) = -\frac{\hbar^2}{2m}(-k^2e^{ikx}f(y) + e^{ikx}f''(y)) - \frac{k\hbar eBy}{2m}e^{ikx}f(y) + \frac{e^2B^2y^2}{2m}e^{ikx}f(y) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}\psi + \frac{1}{2}m\frac{e^2B^2}{m^2}y^2\psi + \frac{\hbar^2k^2 - k\hbar eBy}{2m}\psi$

The second term is indeed the potential $\frac{1}{2}m\omega_c^2x^2\psi$

$\therefore \boxed{\omega_c = \frac{eB}{m}}$

## 5

We know that $\hat{n} = \sin(\theta)\cos(\phi)\hat{x} + \sin(\theta)\sin(\phi)\hat{y} + \cos(\theta)\hat{z}$

$\therefore\ s_n = \vec{s}\cdot\hat{n} = s_x\sin(\theta)\cos(\phi) + s_y\sin(\theta)\sin(\phi) + s_z\cos(\theta) = \begin{pmatrix} 0 & \frac{\hbar}{2} \\ \frac{\hbar}{2} & 0 \end{pmatrix}\sin(\theta)\cos(\phi) + \begin{pmatrix} 0 & -\frac{1}{2}(i\hbar) \\ \frac{i\hbar}{2} & 0 \end{pmatrix}\sin(\theta)\sin(\phi) + \begin{pmatrix} \frac{\hbar}{2} & 0 \\ 0 & -\frac{\hbar}{2} \end{pmatrix}\cos(\theta) = \frac{\hbar}{2}\begin{pmatrix} \cos(\theta) & e^{-i\phi}\sin(\theta) \\ e^{i\phi}\sin(\theta) & \cos(\theta) \end{pmatrix}$

Let $\lambda$ denote eigenvalue and $c$ denote the eigenvector

Then $\frac{\hbar}{2}\begin{vmatrix} \cos(\theta) - \lambda I & e^{-i\phi}\sin(\theta) \\ e^{i\phi}\sin(\theta) & \cos(\theta) - \lambda I \end{vmatrix} = 0$

$\frac{\hbar^2}{4}(\cos(\theta) - \lambda I)(\cos(\theta) - \lambda I) - \frac{\hbar^2}{4}(e^{-i\phi}\sin(\theta))(e^{i\phi}\sin(\theta)) = 0$

The $s_n$ matrix is input to Mathematica. Using Eigensystem function in Mathematica, we therefore get

$\lambda_1 = -\frac{\hbar}{2}$ and $\lambda_2 = \frac{\hbar}{2}$

$\because \frac{\hbar}{2}\begin{pmatrix} \cos(\theta) & e^{-i\phi}\sin(\theta) \\ e^{i\phi}\sin(\theta) & \cos(\theta) \end{pmatrix} c_1 = -\frac{\hbar}{2}c_1$ and $\frac{\hbar}{2}\begin{pmatrix} \cos(\theta) & e^{-i\phi}\sin(\theta) \\ e^{i\phi}\sin(\theta) & \cos(\theta) \end{pmatrix} c_2 = \frac{\hbar}{2}c_2$

$$\therefore c_1 = \begin{pmatrix} -\frac{\sin(\theta)\cos(\phi) - i\sin(\theta)\sin(\phi)}{\cos(\theta)+1} \\ \\ 1 \end{pmatrix} = \begin{pmatrix} e^{-i\phi}\sin(\frac{\theta}{2}) \\ \\ -\cos(\frac{\theta}{2}) \end{pmatrix}$$

$$c_2 = \begin{pmatrix} -\frac{\sin(\theta)\cos(\phi) - i\sin(\theta)\sin(\phi)}{\cos(\theta)-1} \\ \\ 1 \end{pmatrix} = \begin{pmatrix} \cos(\frac{\theta}{2}) \\ \\ e^{i\phi}\sin(\frac{\theta}{2}) \end{pmatrix}$$

Therefore the eigenvalues are $-\frac{\hbar}{2}$ and $\frac{\hbar}{2}$, the corresponding eigenvectors are $\begin{pmatrix} e^{-i\phi}\sin(\frac{\theta}{2}) \\ \\ -\cos(\frac{\theta}{2}) \end{pmatrix}$ and $\begin{pmatrix} \cos(\frac{\theta}{2}) \\ \\ e^{i\phi}\sin(\frac{\theta}{2}) \end{pmatrix}$