Solutions to Problem Set 10
Physics 480 / Fall 1999
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Problem 1: Election In Spherical Box

(a) assume

$$\psi(\vec{r}) = u_{k,l}(r) Y_{lm}(\theta, \psi)$$

we have (7.20)

$$\left(-\frac{\hbar^2}{2m_e}\frac{1}{r}\partial_r^2 r + \frac{\hbar^2 l(l+1)}{2m_e r^2} + V(r) - E_{lm} \right) u_{E,l,m} = 0$$

Since this equation is independent of the quantum number m we drop the index m on the radial wave function $u_{E,l,m}$ and $E_{l,m}$.

$$V(r) = \begin{cases} \infty & for\, r \geq a \\ 0 & for\, r < a \end{cases}$$

we can rewrite the (7.20) as

$$\left(\frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r^2} + k^2 \right) r\, u_{k,l}(r) = 0$$

where $k^2 = \frac{2m_e E}{\hbar^2}$.
(b) see the mathematica notebook.
(c) k must satisfy the following equation since the wavefunction vanishes when $r \geq a$

$$j_l(k\,r)|_{r=a} = 0 \Longrightarrow \sqrt{\frac{\pi}{2ka}}\, J_{l+\frac{1}{2}}(ka) = 0$$

(d)(e)(f) see the notebook.
(g) the lowest energy of the system (ground state) is the lowest energy for l=0, the corresponding $x_0 = 3.14159$
the second lowest energy of the system is the lowest energy for l=1, the corrsponding $x_1 = 4.49341$(see the notebook).

$$\Longrightarrow \Delta E = \frac{\hbar^2}{2ma^2}(x_1^2 - x_0^2)$$

$\lambda \cong 5350\mathring{A}$ for green light

$$\Delta E = h\frac{c}{\lambda}$$

$$\Longrightarrow a = \sqrt{\frac{\hbar^2 \lambda (x_1^2 - x_0^2)}{2mhc}}$$

$$
\begin{aligned}
&= \sqrt{\frac{\hbar\lambda(x_1^2 - x_0^2)}{4\pi mc}} \\
&= 4.12 * 10^{-10}\ m \\
&= 4.12\AA
\end{aligned}
$$

Problem 2: Three Dimensional Harmonic Oscillator

(a) Since the equation is already seperate according to the variables x_1, x_2 and x_3 the solution will be of the form of the multiplication of the three independant one-dimensional harmonic oscillators

$$\Psi_E(\vec{r}) = \Psi_1(x_1)\Psi_1(x_2)\Psi_1(x_3) = constant * e^{-(\frac{1}{2}\alpha^2 r^2)} H_{n_1}(\alpha x_1) H_{n_2}(\alpha x_2) H_{n_3}(\alpha x_3) \quad (1)$$

where $\alpha = \sqrt{\frac{m\omega}{\hbar}}$ and the energy levels therefore will be

$$E_n = E_{n_1} + E_{n_2} + E_{n_3} = \hbar\omega(n_1 + n_2 + n_3 + \frac{3}{2}) \equiv \hbar\omega(n + \frac{3}{2}) \quad (2)$$

where n_1, n_2, n_3 and n are integers $0, 1, 2, \ldots.$ The degree of degeneracy of the nth level is equal to the number of ways in which n can be divided into the sum of three positive integral (or zero) numbers; this is

$$g_n = \frac{1}{2}(n+1)(n+2) \quad (3)$$

(b) By writing the Schrodinger‘s equation in spherical coordinates and using the fact that the angular part of the ∇^2 is just the $\widehat{L}^2$ operator in the coordinate basis up to a factor $(-\hbar^2 r^2)$ we get the radial equation

$$(-\frac{\hbar^2}{2\mu}[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}] + V(r))R(r) = ER(r) \quad (4)$$

To solve this equation we plug the form $R(r) = \frac{v_k l(r)}{r}$ into the equation and obtain

$$
\begin{aligned}
(-\frac{\hbar^2}{2\mu}[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}] + V(r))\frac{v_{kl}(r)}{r} &= E\frac{v_{kl}(r)}{r} \quad (5) \\
-\frac{\hbar^2}{2\mu}[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\dot{v}(r)r - v(r)}{r^2}] + (\frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2} + V(r))\frac{v_{kl}(r)}{r} &= E\frac{v_{kl}(r)}{r} \quad (6) \\
-\frac{\hbar^2}{2\mu}[\frac{1}{r^2}(\ddot{v_{kl}}(r)r + \dot{v_{kl}}(r) - \dot{v_{kl}}(r))] + (\frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2} + V(r))\frac{v_{kl}(r)}{r} &= E\frac{v_{kl}(r)}{r} \quad (7) \\
(-\frac{\hbar^2}{2\mu}[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}] + V(r))v_{kl}(r) &= Ev_{kl}(r) \quad (8)
\end{aligned}
$$

Writing $E = \frac{\hbar^2 k^2}{2m}$ and rearranging the terms, we obtain the desired result

$$(-\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{1}{2}m\omega^2 r^2 - k^2)v_{kl}(r) = 0 \tag{9}$$

(c) We should investigate the behaviour for large and small r in order to understand the general form of the wave function. For large r as $r \to \infty$ the dominant term in the equation will be the harmonic oscillator potential and the solution will look like

$$v_{kl}(r) \sim e^{-\frac{1}{2}\alpha^2 r^2} \tag{10}$$

and for small r as $r \to 0$ dominant term will be the angular momentum term which will behave like a centrifugal potential. Thus the solution to the equation

$$\ddot{v_{kl}}(r) \simeq \frac{l(l+1)}{r^2} v_{kl}(r) \tag{11}$$

will be $v_{kl}(r) \sim r^{l+1}$ or $v_{kl}(r) \sim r^{-l}$.Since the latter solution is irregular and so does not meet the boundary conditions, the correct form of the solution for small r should look like

$$v_{kl}(r) \sim r^{l+1} \tag{12}$$

Combining these two facts we can say that the general solution should be of the form

$$v_{kl}(r) = e^{-\frac{1}{2}\alpha^2 r^2} r^{l+1} \sum c_s r^s \tag{13}$$

For $v_{kl}(r)$ to have the right properties near $r = 0$ the sum should approach to a constant as $r \to 0$. Thus $c_0 \neq 0$ and since the second order differential equation will give us a two-term recursion relation, the only non-zero terms will be even coefficients.

(d) Plugging the series into the differential equation and with a little algebra we obtain the recursion relation

$$c_{s+2} = \frac{(s + l - \lambda) + 3/2}{(s + 2)(s + 2l + 3)/2} c_s \tag{14}$$

where $\lambda = E/(\hbar\omega)$. For the series to be finite, it should terminate at some c_s which is determined by the energy value that makes the numerator zero. From the equation

$$s + l - \lambda + 3/2 = 0 \tag{15}$$

$$\lambda = s + l + 3/2 = 2p + l + 3/2 \tag{16}$$

(e) If we define the principal quantum number

$$n = 2p + l \tag{17}$$

we get

$$E = (n + 3/2)\hbar\omega \tag{18}$$

And at each n, allowed l values turn out to be

$$l = n - 2p = n, n-2, n-4, ..., 1 \quad or \quad 0 \tag{19}$$

For the first three energy levels the quantum numbers will be

$$n = 0 \quad l = 0 \quad m = 0 \tag{20}$$
$$n = 1 \quad l = 1 \quad m = -1, 0, 1 \tag{21}$$
$$n = 2 \quad l = 0, 2 \quad m = -2, -1, 0, 1, 2 \tag{22}$$

(f) The l=0 states have radial symmetry, i.e. they don't have angular dependance. But the states obtained in (a) are functions of variables x_1, x_2, x_3 which possess directionality. To get rid of this directionality either we should construct a term like ${x_1}^2 + {x_2}^2 + {x_2}^3$ or get a constant using the six degenerate states having energies $7/2\hbar\omega$. If we look at the form of the Hermite polynomials for these states we immediately see that they look like

$$|\Psi>_{110} = const\ e^{-r^2} xy \tag{23}$$
$$|\Psi>_{101} = const\ e^{-r^2} xz \tag{24}$$
$$|\Psi>_{011} = const\ e^{-r^2} yz \tag{25}$$
$$|\Psi>_{200} = const\ e^{-r^2}(1 - 2x^2) \tag{26}$$
$$|\Psi>_{020} = const\ e^{-r^2}(1 - 2y^2) \tag{27}$$
$$|\Psi>_{002} = const\ e^{-r^2}(1 - 2z^2) \tag{28}$$

where $|\Psi>_{\{n_1,n_2,n_3\}}$ represents the states with quantum numbers n_1, n_2, n_3 obtained in (a). The only way to get rid of the directionality is to add the last three states and form a linear superposition which does not have angular dependance. So we can write the $l = 0$ state as

$$|\psi>_{200} = const \quad \{|\Psi>_{200} + |\Psi>_{020} + |\Psi>_{002}\} \tag{29}$$

Extra Problem: Hydrogen Atom in External Electric Field(Stark Effect in Hydrogen)

(a)

$$V = -e\,\vec{E} \cdot \vec{r} = -eEr\,\cos\theta$$

Whether the matrix element vanishes or not is determined by the angular momentum part.

$$Y_{00} = \frac{1}{\sqrt{4\pi}} \quad Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_{11} = -\sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi} \quad Y_{1-1} = \sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\phi}$$

$$< Y_{lm}|V|Y_{lm} >= \int_0^\pi \int_0^{2\pi} |Y_{lm}|^2 \cdot (-eEr\cos\theta) \cdot \sin\theta d\theta d\phi = 0$$

(note: $\sin\theta$ is symmetric with $\theta = \frac{\pi}{2}$.
$\cos\theta$ is anti-symmetric with $\theta = \frac{\pi}{2}$.
$|Y_{lm}|^2$ is symmetric with $\theta = \frac{\pi}{2}$)

$$\begin{aligned}
< Y_{00}|V|Y_{10} > &\propto \int_0^\pi \cos^2\theta \cdot \sin\theta d\theta \neq 0 \\
< Y_{00}|V|Y_{11} > &\propto \int_0^\pi \sin\theta\cos\theta \cdot \sin\theta d\theta = 0 \\
< Y_{00}|V|Y_{1-1} > &\propto \int_0^\pi \sin\theta\cos\theta \cdot \sin\theta d\theta = 0 \\
< Y_{10}|V|Y_{11} > &\propto \int_0^{2\pi} e^{i\phi} d\phi = 0 \\
< Y_{10}|V|Y_{1-1} > &\propto \int_0^{2\pi} e^{-i\phi} d\phi = 0 \\
< Y_{11}|V|Y_{1-1} > &\propto \int_0^\pi \sin^2\theta\cos\theta \cdot \sin\theta d\theta = 0
\end{aligned}$$

since$< Y_{l_1 m_1}|V|Y_{l_2 m_2} >=< Y_{l_2 m_2}|V|Y_{l_1 m_1} >$ for $V = -eE\,r\cos\theta$
we know that only

$$\epsilon =< 00|V|10 >=< 10|V|00 >\neq 0$$

(b) For $|nlm >= |200 >$ and $|nlm >= |210 >$

$$\psi_{200} = R_{20}Y_{00} = \frac{1}{\sqrt{2}a^{\frac{3}{2}}}(1 - \frac{r}{2a})e^{-\frac{r}{2a}} \cdot \frac{1}{\sqrt{4\pi}}$$

$$\psi_{210} = R_{21}Y_{10} = \frac{1}{2\sqrt{6}a^{\frac{3}{2}}} \frac{r}{a} e^{-\frac{r}{2a}} \cdot \sqrt{\frac{3}{4\pi}} \cos\theta$$

where $a = \frac{\hbar^2}{\mu e^2}$ (bohr radius), μ is the mass of an electron.

$$\begin{aligned}
\epsilon &= \int \psi_{200}\psi_{210} r^2 \sin\theta d\theta d\phi dr \\
&= \int_0^\infty \frac{1}{4\sqrt{3}a^3} \frac{r}{a}(1 - \frac{r}{2a})e^{-\frac{r}{a}}(-eEr) \cdot r^2 dr \\
&\quad \cdot \int_0^\pi \frac{\sqrt{3}}{4\pi} \cos^2\theta \cdot \sin\theta d\theta \cdot \int d\phi
\end{aligned}$$

$$= \quad -\frac{eEa}{4\sqrt{3}}\int_0^\infty (1-\frac{1}{2}\eta)\eta^4 e^{-\eta}d\eta \cdot \frac{\sqrt{3}}{4\pi}\int_0^\pi \cos^2\theta \sin\theta d\theta \cdot 2\pi$$

where $\eta = \frac{r}{a}$

$$\int_0^\infty (1-\frac{1}{2}\eta)\eta^4 e^{-\eta}d\eta = -36(you\ can\ use\ mathematica\ to\ evaluate\ this\ integral)$$

$$\int_0^\pi \cos^2\theta \sin\theta d\theta = -\int_0^\pi \cos^2\theta d\cos\theta = -\frac{1}{3}\cos^3\theta|_0^\pi = \frac{2}{3}$$

$$\Longrightarrow \epsilon = -\frac{eEa}{4\sqrt{3}} \cdot (-36) \cdot \frac{\sqrt{3}}{2} \cdot \frac{2}{3}$$

$$= 3eEa$$

(c)
assume $|200>$ $|211>$ $|210>$ $|21{-1}>$ are the base wavefunctions, then the Hamiltonian for perturbed $n = 2$ states is

$$H = H_0 + V = H_0 + \begin{pmatrix} 0 & 0 & \epsilon & 0 \\ 0 & 0 & 0 & 0 \\ \epsilon & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Since $E_0 = H_0\,|2lm>= -\frac{e^2}{2a} \cdot \frac{1}{n^2}|_{n=2} = -\frac{e^2}{8a}$ use *mathematica* command *Eigenvalues* and *Eigenvectors* to evaluate this matrix.

$$E_1 = E_2 = E_0$$

$$\phi_1 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad \phi_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$E_3 = E_0 - \epsilon = E_0 - 3eEa$$

$$\phi_3 = \begin{pmatrix} -1 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$E_4 = E_0 + \epsilon = E_0 + 3eEa$$

$$\phi_4 = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$