Problem Set 10
Physics 480 / Fall 1999
Professor Klaus Schulten

Problem 1: Electron in Spherical Box

An electron is trapped in a spherical box defined by the potential

$$V(r) \;==\; \begin{cases} \infty & \text{for } r \geq a \\ 0 & \text{for } r < a \end{cases} \;. \tag{1}$$

Determine the stationary states and corresponding energy eigenvalues proceeding as follows:

(a) Show that inside the spherical box the radial Schrödinger equation for a state at energy E can be written

$$\left(\frac{\partial^2}{\partial r^2} \;-\; \frac{\ell(\ell+1)}{r^2} \;+\; k^2 \right) r u_{k,\ell}(r) \;=\; 0 \;, \quad k^2 \;=\; \frac{2 m_e E}{\hbar^2} \tag{2}$$

for a wave function of the form

$$\psi(\vec{r}) \;=\; u_{k,\ell}(r)\, Y_{\ell m}(\theta, \phi) \;. \tag{3}$$

Equation (2) is the differential equation for the regular and irregular spherical Bessel functions $j_\ell(kr)$ and $n_\ell(kr)$, i.e.,

$$u_{k,\ell}(r) \;=\; A_\ell\, j_\ell(kr) \;+\; B_\ell\, n_\ell(kr) \;. \tag{4}$$

The coefficients B_ℓ must vanish since $n_\ell(kr)$ has a non-integrable singularity at $r = 0$. The regular spherical Bessel function $j_\ell(x)$ is given by

$$j_\ell(x) \;=\; \sqrt{\frac{\pi}{2x}}\, J_{\ell+\frac{1}{2}}(x) \tag{5}$$

where $J_n(x)$ is the so-called Bessel function of the first kind. You can evaluate $J_n(x)$ by the `Mathematica` command `BesselJ[n,x]` where n does not have to be integer.

(b) Using the `Mathematica` command `Plot3D[Sqrt[Pi/(2 x)] BesselJ[n+0.5,x], {x,0,10}, {n, 0,10}]` plot the functional behaviour of $j_\ell(kr)$.

(c) State the conditions which the values of k must satisfy for (3, 4) (for $B_\ell = 0$) to represent stationary states.

(d) Using `Mathematica` determine the allowed values of k for a chosen box radius a by using the `Mathematica` commands suggested above and either graphs of $j_\ell(kr)$, employing the `Mathematica` command `Plot[ ]`, or any method of your choice. Do this for the lowest five values of k for angular momentum states $\ell = 0, 2, 6$ and state the results in units $1/a$. What are the corresponding energies of the bound states.

(e) Using the `Mathematica` command `Plot[ ]` plot the radial parts of the wave function for the second lowest value of k and for $\ell = 2$.

(f) Do the same as in (e) for the angular part of the wave function for $m = -2, -1, 0, 1, 2$. Employ for this purpose the relationship for $m \geq 0$

$$Y_{\ell m}(\theta, \phi) = \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\, P_{\ell m}(\cos\theta)\, e^{im\phi} \,. \tag{6}$$

stated in the class notes. Employ the `Mathematica` commands `LegendreP[n, m, x]` for $P_{nm}(x)$ and a plot routine of your choice. Plot either the real or the imaginary part of the wave function.

(g) Determine the radius of the spherical box such that the energy to promote the system from the lowest to the second lowest stationary state corresponds approximately to the energy $\hbar\omega$ of green light.

Problem 2: Three-Dimensional Harmonic Oscillator

Consider the stationary states of a three-dimensional harmonic oscillator described by the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 r^2 \tag{7}$$

(a) Describe the stationary states first by solving the stationary Schrödinger equation through separation of variables, i.e., assume $\psi_E(\vec{r}) = \psi_1(x_1)\psi_2(x_2)\psi_3(x_3)$ and solve $(H - E)\psi_E(\vec{r}) = 0$ in the form

$$\Big(-\tfrac{\hbar^2}{2m}\tfrac{\partial^2}{\partial x_1^2} + \tfrac{1}{2}m\omega^2 x_1^2 - E_1 \Big)\, \psi_1(x_1)\psi_2(x_2)\psi_3(x_3) + \tag{8}$$

$$\Big(-\tfrac{\hbar^2}{2m}\tfrac{\partial^2}{\partial x_2^2} + \tfrac{1}{2}m\omega^2 x_2^2 - E_2 \Big)\, \psi_1(x_1)\psi_2(x_2)\psi_3(x_3) + \tag{9}$$

$$\Big(-\tfrac{\hbar^2}{2m}\tfrac{\partial^2}{\partial x_3^2} + \tfrac{1}{2}m\omega^2 x_3^2 - E_3 \Big)\, \psi_1(x_1)\psi_2(x_2)\psi_3(x_3) \quad = 0 \tag{10}$$

where $E = E_1 + E_2 + E_3$. Provide explicit expressions for the degeneracies of the energy levels, i.e., state your result in the form "there are n_o states of energy $E_o = \ldots$, there are ..."

(b) Employ then in a second approach separation of variables using spherical coordinates $\vec{r} = (r, \theta, \phi)$. Define for $k = \sqrt{2mE/\hbar^2}$

$$\psi_k(\vec{r}) = \frac{v_{k\ell}(r)}{r}\, Y_{\ell m}(\theta, \phi) \,. \tag{11}$$

Show that $v_{k\ell}(r)$ satisfies

$$\left(-\frac{d^2}{dr^2} \; + \; \frac{\ell(\ell+1)}{r^2} \; + \; \left(\frac{m\omega}{\hbar}\right)^2 r^2 \; - \; k^2 \right) v_{k\ell}(r) \; = \; 0 \; . \qquad (12)$$

(c) Argue why stationary state wave functions should be of the form

$$v_{k\ell}(r) \; = \; e^{-\beta r^2/2} \, g_{k\ell}(r) \; , \quad g_{k\ell}(r) \; = \; r^{\ell+1} \sum_{s=0}^{n} c_s r^s \qquad (13)$$

where $\beta \; = \; \sqrt{m\omega/\hbar}$ and n is a finite, non-negative number. Show that all coefficients c_s, for odd s, vanish.

(d) Derive a recursion equation for c_s and derive expressions for allowed k values (energy values) which ensure that $c_s = 0 \, , s > n$ holds.

(e) Show that the energies resulting from (d) agree with those derived in (a). State which angular momentum quantum numbers ℓ, m are realized for stationary states with energies (i) $E = \hbar\omega \cdot \frac{3}{2}$, (ii) $E = \hbar\omega \cdot (1 + \frac{3}{2})$, (iii) $E = \hbar\omega \cdot (2 + \frac{3}{2})$.

(f) Express the $\ell = 0$ state for $E = \hbar\omega \cdot (2 + \frac{3}{2})$ in terms of eigenstates derived in (a).

The problem set needs to be handed in by Tuesday, December 2. The web page of Physics 480 is at
`http://www.ks.uiuc.edu/Services/Class/PHYS480/`