Problem Set 6, Physics 622 (Fall 2001)
Solutions

1 The potential of a 3-dimensional spherical box with perfectly rigid walls is given by

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

so $\psi(\vec{r}) = 0$ for $r \geq a$. For $r < a$, since V is spherically symmetric, we can write

$$\psi_{Elm}(\vec{r}) = R_{El}(r) Y_{lm}(\theta, \phi)$$

and $R_{El}(r)$ satisfies the radial Schrödinger equation,

$$\begin{aligned} \frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left[k^2 - \frac{l(l+1)}{r^2}\right] R &= 0 \qquad \left(k^2 = \frac{2mE}{\hbar^2}\right) \\ \rho^2 \frac{d^2R}{d\rho^2} + 2\rho\frac{dR}{d\rho} + \left[\rho^2 - l(l+1)\right] R &= 0 \qquad (\rho = kr) \\ \Rightarrow \qquad R_{El}(r) &= A j_l(kr) + B n_l(kr) \end{aligned}$$

where j_l and n_l are the spherical Bessel functions and spherical Neumann function. Boundary conditions:

$$\begin{aligned} R_{El}(0) \text{ is finite} \;&\Rightarrow\; B = 0 \quad (n_l(kr) \to -\infty \text{ as } r \to 0) \\ R_{el}(r = a) = 0 \;&\Rightarrow\; j_l(ka) = 0 \end{aligned}$$

$$\begin{aligned} E_{ln} &= \frac{\hbar^2}{2ma^2} z_{ln}^2 \qquad (z_{ln} = n^{th}\text{zero's of} j_l) \quad \blacksquare \\ \psi(\vec{r}) &= C j_l(kr) Y_{lm}(\theta, \phi) \quad \blacksquare \end{aligned}$$

The lowest three energy levels are $\frac{\hbar^2}{2ma^2} z_{10}^2$, $\frac{\hbar^2}{2ma^2} z_{11}^2$, $\frac{\hbar^2}{2ma^2} z_{12}^2$ where $z_{10} = \pi$, $z_{11} \approx 4.49$ and $z_{12} \approx 5.76$. $\blacksquare$

2 Start with the radial equation (for $\chi(r)$), with $l = 0$,

$$-\frac{\hbar^2}{2\mu}\frac{d^2\chi}{dr^2} + \left(-\frac{g}{d} e^{-\frac{r}{d}}\right) \chi = E\chi \qquad (E < 0)$$

let $x = ae^{-rb}$, $k^2 = \frac{2\mu|E|}{\hbar^2}$ and note that $\mu = \frac{M}{2}$

$$\begin{aligned} \frac{d^2\chi}{dr^2} + \left(\frac{Mg^2}{\hbar^2 d} e^{-\frac{r}{d}} - k^2\right) \chi &= 0 \\ x^2 \frac{d^2\chi}{dr^2} + x\frac{d\chi}{dx} + \left[\frac{Mg^2}{\hbar^2 d b^2} e^{-\frac{r}{d}} - \left(\frac{k}{b}\right)^2\right] \chi &= 0 \end{aligned}$$

Choose $b = \dfrac{1}{2d}$ and $a^2 = \dfrac{Mg^2}{\hbar^2 db^2}$ which implies $a = 2g\sqrt{\dfrac{M}{\hbar mc}}$ and $b = \dfrac{mc}{2\hbar}$, we obtain

$$x^2\frac{d^2\chi}{dr^2} + x\frac{d\chi}{dx} + [x^2 - (2dk)^2]\chi = 0$$

which is the Bessel's equation of order $2dk = \alpha$. Hence

$$\alpha = \frac{2\hbar}{mc}\frac{\sqrt{M|E|}}{\hbar} = \frac{2\sqrt{Mc^2|E|}}{mc^2} = 0.65$$

$$\therefore \qquad \chi \sim J_{0,65}(x)$$

Boundary condition: $\chi(r{=}0) = \chi(x{=}a) = 0 \quad \Rightarrow \quad J_{0.65}(x{=}a) = 0$

$$\begin{aligned} \therefore \qquad a &= 3.3 \\ 2g\sqrt{\frac{M}{\hbar mc}} &= 3.3 \\ g &\approx 0.64\sqrt{\hbar c} \quad \blacksquare \end{aligned}$$

3 Given the wavefunction

$$\begin{aligned} \psi_\pm(\vec{r}) &= \frac{e^{\pm ikr}}{r}Y_{lm}(\theta,\phi) \\ \vec{j} &= \frac{\hbar}{2mi}\left[\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right] \end{aligned}$$

In spherical coordinates,

$$\vec{\nabla} = \hat{r}\frac{\partial}{\partial r} + \frac{1}{r}\hat{\theta}\frac{\partial}{\partial\theta} + \frac{1}{r\sin\theta}\hat{\phi}\frac{\partial}{\partial\phi}$$

$$\hat{r}\cdot\vec{\nabla}\psi_\pm = \frac{\partial\psi_\pm}{\partial r} = \frac{e^{\pm ikr}}{r^2}(\pm ikr - 1)Y_{lm}$$

$$\begin{aligned} \psi_\pm^*\hat{r}\cdot n a \vec{b} l a \psi_\pm &= \frac{e^{\mp ikr}}{r}Y_{lm}^*\frac{e^{\pm ikr}}{r^2}(\pm ikr - 1)Y_{lm} \\ &= \frac{\pm ikr - 1}{r^3}|Y_{lm}|^2 \end{aligned}$$

$$\hat{r}\cdot\vec{j} = \frac{\hbar^2}{2mi}\frac{\pm 2ik}{r^2}|Y_{lm}|^2 = \frac{\pm\hbar k}{mr^2}|Y_{lm}|^2$$

$$\begin{aligned} \int_0^\pi\int_0^{2\pi}\sin\theta d\theta d\phi\hat{r}\cdot\vec{j} &= \pm\frac{\hbar k}{mr^2}\int_0^\pi\int_0^{2\pi}\sin\theta d\theta d\phi|Y_{lm}|^2 \\ &= \pm\frac{\hbar k}{mr^2} \quad \blacksquare \end{aligned}$$

4 Let $R(r)$ be the radial wavefunction, then $u(r) = rR(r)$ satisfies

$$\frac{d^2u}{dr^2} + \frac{2m}{\hbar^2}[E - V(r)]u = 0$$

Let $p = \sqrt{2m(E-V)}$ and $V(a) = E$, apply WKB analysis to the above 1-D equation,

$$\begin{aligned} u_I(r) &= \frac{A}{\sqrt{p}} \exp\left[\frac{i}{\hbar}\int_0^r p dr'\right] + \frac{B}{\sqrt{p}} \exp\left[-\frac{i}{\hbar}\int_0^r p dr'\right] \quad (r < a) \\ u_{II}(r) &= \frac{C}{\sqrt{|p|}} \exp\left[-\frac{1}{\hbar}\int_a^r |p| dr'\right] \qquad\qquad\qquad\qquad (r > a) \end{aligned}$$

$u_I(0) = 0 \ \Rightarrow \ A = -B,$ let $\varphi = \dfrac{1}{\hbar}\displaystyle\int_0^a p dr$

$$u_I(r) = \frac{A}{\sqrt{p}}\left\{e^{i\varphi}\exp\left[\frac{i}{\hbar}\int_a^r p dr'\right] - e^{-i\varphi}\exp\left[-\frac{i}{\hbar}\int_a^r p dr'\right]\right\}$$

Connecting u_I and u_{II},

$$\begin{pmatrix} Ae^{i\varphi} \\ \\ -Ae^{-i\varphi} \end{pmatrix} = \begin{pmatrix} e^{i\frac{\pi}{4}} & \frac{1}{2}e^{-i\frac{\pi}{4}} \\ \\ e^{-i\frac{\pi}{4}} & \frac{1}{2}e^{i\frac{\pi}{4}} \end{pmatrix} \begin{pmatrix} C \\ \\ 0 \end{pmatrix}$$

$$\begin{aligned} \Rightarrow \qquad Ae^{i\varphi} &= Ce^{i\frac{pi}{4}} \\ -Ae^{-i\varphi} &= Ce^{-i\frac{pi}{4}} \\ \therefore \qquad -e^{i2\varphi} &= e^{i\frac{\pi}{2}} \\ 2\varphi - \pi &= \frac{\pi}{2} + 2n\pi \qquad (-1 = e^{-i\pi}) \\ \varphi &= n\pi + \frac{3\pi}{4} \\ \text{therefore,} \qquad 2\int_0^a dr\sqrt{2m(E-V)} &= (n + \frac{3}{4})\hbar \quad \blacksquare \end{aligned}$$

5 Without loss of generality, assume $A > 0$, hence $E > 0$.

(a) Let $\alpha = \dfrac{2mA}{\hbar^2}$, $\beta = \dfrac{2mB}{\hbar^2}$ and $k^2 = \dfrac{2mE}{\hbar^2}$,

$$\begin{aligned} \left[\frac{-\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) + \frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right]R(r) &= ER(r) \\ \frac{d^2R}{dr^2} + \frac{2}{r}\frac{d}{dr} + \left[k^2 - (\alpha + \beta r) - \frac{l(l+1)}{r^2}\right]R &= 0 \end{aligned}$$

$\underline{r \to 0}$ Since $r = 0$ is a regular singular point, we can expand $R(r)$ in the vicinity of the origin as

$$R(r) = r^s \sum_{n-0}^{\infty} c_n r^n$$

Substituting the expansion in the radial equation, we obtain the indicial equation for s,

$$\begin{aligned} & s^2 + s - l(l+1) = 0 \\ \Rightarrow \quad & s = l, -(l+1) \\ \Rightarrow \quad & R(r) \sim r^l \text{ as } r \to 0 \end{aligned}$$

$\underline{r \to \infty}$ let $u = rR$

$$\begin{aligned} \frac{d^2u}{dr^2} - r\beta u &= 0 \\ \frac{d^2u}{dz^2} - zu &= 0 \qquad (z = \beta^{\frac{1}{2}} r) \end{aligned}$$

$$\therefore \quad u(z) \sim Ai(z) \to \frac{e^{-\frac{2}{3}z^{\frac{3}{2}}}}{z^{\frac{1}{4}}} \quad \text{as} \quad z \to \infty$$

$$R(r) \sim r^{-\frac{5}{4}} e^{-\frac{2}{3}\beta^{\frac{1}{2}} r^{\frac{3}{2}}} \quad \text{as} \quad r \to \infty$$

Therefore,

$$\psi(\vec{r}) \sim Y_{lm}(\theta, \phi)\, r^l \, \frac{e^{-\frac{2}{3}\beta^{\frac{1}{2}} r^{\frac{3}{2}}}}{r^{\frac{5}{4}}} w(r) \quad \blacksquare$$

(b) From (a), $R(r) = r^l \, \frac{e^{-\frac{2}{3}\beta^{\frac{1}{2}} r^{\frac{3}{2}}}}{r^{\frac{5}{4}}} w(r) = G(r)v(r)$ where $G(r) = r^l e^{-\frac{2}{3}\beta^{\frac{1}{2}} r^{\frac{3}{2}}}$ and $v(r) = r^{-\frac{5}{4}} w(r)$.

$$\begin{aligned} G'(r) &= \left(\frac{l}{r} - \beta^{\frac{1}{2}} r^{\frac{1}{2}}\right) G(r) \\ G''(r) &= \left[\beta r - 2\left(l + \frac{1}{4}\right)\beta^{\frac{1}{2}} r^{-\frac{1}{2}} + \frac{l(l-1)}{r^2}\right] G(r) \\ R' &= G'V + GV' \\ R'' &= G''V + 2G'V' + GV'' \end{aligned}$$

By substitution, the equation for $v(r)$ is :

$$v'' + 2\left(\frac{l+1}{r} - \beta^{\frac{1}{2}} r^{\frac{1}{2}}\right) v' + \left[k^2 - \alpha - 2\left(l + \frac{5}{4}\right)\frac{\beta^{\frac{1}{2}}}{r^{\frac{1}{2}}}\right] v = 0 \quad \blacksquare$$

(c) Let E_0 be the ground state energy and $A + Ba = E_0$,

$$\begin{aligned}
2\int_0^a [2m(E-A-Br)]^{\frac{1}{2}}\,dr &= \frac{3}{4}h \\
\int_0^{\frac{E_0-A}{B}} \sqrt{E_0-A-Br}\,dr &= \frac{3h}{8\sqrt{2m}} \\
E_0 &= A + \left(\frac{9Bh}{16\sqrt{2m}}\right)^{\frac{2}{3}}
\end{aligned}$$ ■

6 Let $\omega^2 = k/m$,

$$V(r) = \frac{1}{2}kr^2 = \frac{1}{2}m\omega^2 r^2$$

$$\psi_{Elm}(\vec{r}) = R_{El}(r)Y_{lm}(\theta,\phi)$$

The radial equation for $u(r) = rR_{El}(r)$ is

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2mE}{\hbar^2} - \frac{m^2\omega^2 r^2}{\hbar^2}\right]u(r) = 0$$

Let $\rho = \alpha r$ where $\alpha = \left(\frac{mk}{\hbar^2}\right)^{\frac{1}{4}} = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}$ and $\lambda = \frac{2E}{\hbar\omega}$,

$$\left[\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + \lambda - \rho^2\right]u(\rho) = 0$$

Analysis of $u(\rho)$ as $\rho \to 0$ and $\rho \to \infty$ suggests looking for solutions in the form

$$u(\rho) = \rho^{l+1}e^{-\frac{\rho^2}{2}}w(\rho)$$

Upon substitution, we find $w(\rho)$ satisfies

$$\frac{d^2w}{d\rho^2} + 2\left(\frac{l+1}{\rho} - \rho\right)\frac{dw}{d\rho} + \left[\lambda - 2\left(l+\frac{3}{2}\right)\right]w(\rho) = 0$$

$$\text{or}\qquad \zeta\frac{d^2w}{d\zeta^2} + \left[\left(l+\frac{3}{2}\right) - \zeta\right]\frac{dw}{d\zeta} - \left[\frac{1}{2}\left(l+\frac{3}{2}\right) - \frac{\lambda}{4}\right]w(\zeta) = 0 \qquad (\zeta = \rho^2)$$

which is the Kummer-Laplace equation whose solution, regular at the origin is given by the confluent hypergeometric function,

$$w(\zeta) = C\;{}_1F_1\left[\frac{1}{2}\left(l+\frac{3}{2}\right) - \frac{\lambda}{4}\,,\; l+\frac{3}{2}\,,\; \zeta\right] \qquad (C = \text{constant})$$

$$\text{as } \zeta \to \infty, {}_1F_1\left[\frac{1}{2}\left(l+\frac{3}{2}\right) - \frac{\lambda}{4}\,,\; l+\frac{3}{2}\,,\; \zeta\right] \sim \zeta^{-\frac{1}{2}(l+\frac{3}{2}+\frac{\lambda}{2})}e^{\zeta}$$

Therefore, if the series ${}_1F_1$ does not terminate,

$$u(\rho) \sim \rho^{-\frac{\lambda+1}{2}} e^{\frac{\rho^2}{2}} \qquad (\rho \to \infty)$$

which is inadmissible. The only way to avoid this divergence is to transform the confluent hypergeometric series into a polynomial of degree n_r, by requiring that

$$\begin{aligned}
\frac{1}{2}(l+\frac{3}{2}) - \frac{\lambda}{4} &= -n_r & \qquad n_r &= 0,1,2,\ldots \\
\lambda &= 2(n+\frac{3}{2}) & n &= 2n_r + l = 0,1,2,\ldots \\
\Rightarrow \qquad E_n &= (n+\frac{3}{2})\hbar\omega \quad \blacksquare
\end{aligned}$$

The wavefunction is given by

$$\psi_{Elm}(\vec{r}) = N e^{-\frac{\alpha^2 r^2}{2}} r^l \, {}_1F_1(-n_r, l+\frac{3}{2}, \alpha^2 r^2) Y_{lm}(\theta,\phi) \quad \blacksquare$$

– END –