S 2013

Problem 6: Spherical Square Well

Consider a spin 0 particle of mass m moving in a 3D square well, given by the potential

$$V(\vec{r}) = -V_0 \quad 0 \leq |\vec{r}| \leq a_0\ , \qquad V(\vec{r}) = 0 \quad |\vec{r}| > a_0 \quad (V_0 > 0). \tag{1}$$

In this problem we will only consider the bound states of this well, so that $-V_0 < E < 0$.

(a) [1 pt] Explain why we can write the eigenstates of this potential as

$$\Psi_{k,l,m} = f_{k,l}(r) Y_l^m(\theta, \phi). \tag{2}$$

(b) [2 pts] Defining the function $u_{k,l}(r) = r f_{k,l}(r)$, write the radial Schrödinger equation for $u_{k,l}(r)$.

(c) [2 pts] For $l = 0$, write the form for the function $u_{k,0}(r)$ in the regions $0 \leq r \leq a_0$ and $r \geq a_0$. Define any constants that you use.

(d) [3 pts] Using the boundary conditions on the function $u_{k,0}(r)$, derive an equation that gives the bound state energies for the $l = 0$ states. Hint: Considering that $f(r) = u(r)/r$, what is the boundary condition on u as $r \to 0$?

(e) [2 pts] For a fixed radius for the potential, a_0, calculate the minimum depth, $V_0 = V_{min}$, for the potential to have a bound state.

(a)

We can write the eigenstates of the spherical well as a product of the radial and angular portions due to the separability of the Schrödinger equation and the symmetry of our system.

(b)

In spherical coordinates, the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\nabla^2\psi + U\psi = E\psi.$$

In this case,

$$U = -V_0$$

for $0 \le |\vec{r}| \le a_0$. So we have

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial^2}{\partial r^2}r\psi + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right] - V_0\psi = E\psi.$$

Let

$$\psi_{k\ell m} = f_{k\ell}(r)\,Y_\ell^m(\theta,\phi).$$

Then

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r}Y_\ell^m\frac{d^2}{dr^2}rf_{k\ell} + \frac{1}{r^2\sin\theta}f_{k\ell}\frac{d}{d\theta}\left(\sin\theta\frac{dY_\ell^m}{d\theta}\right) + \frac{1}{r^2\sin^2\theta}f_{k\ell}\frac{d^2Y_\ell^m}{d\phi^2}\right] - V_0 f_{k\ell}Y_\ell^m = Ef_{k\ell}Y_\ell^m$$

$$-\frac{\hbar^2}{2m}\left[\frac{r}{f_{k\ell}}\frac{d^2}{dr^2}rf_{k\ell} + \frac{1}{\sin\theta}\frac{1}{Y_\ell^m}\frac{d}{d\theta}\left(\sin\theta\frac{dY_\ell^m}{d\theta}\right) + \frac{1}{\sin^2\theta}\frac{1}{Y_\ell^m}\frac{d^2Y_\ell^m}{d\phi^2}\right] - V_0 r^2 = Er^2$$

Then we must have

$$-\frac{\hbar^2}{2m}\frac{r}{f_{k\ell}}\frac{d^2}{dr^2}rf_{k\ell} - V_0r^2 - Er^2 = \frac{\hbar^2\ell(\ell+1)}{2m},$$

where ℓ is an integer $(\ell = 0,1,2,\dots)$.

(b), cont'd...

Define $u_{k\ell}(r) = r f_{k\ell}(r)$. Then $f_{k\ell}(r) = \frac{1}{r} u_{k\ell}(r)$ and

$$-\frac{\hbar^2}{2m} \frac{r}{\frac{1}{r}u_{k\ell}} \frac{d^2}{dr^2} u_{k\ell} - r^2 (V_0 + E) = \frac{\hbar^2 \ell(\ell+1)}{2m}$$

$$-\frac{\hbar^2}{2m} \frac{r^2}{u_{k\ell}} \frac{d^2 u_{k\ell}}{dr^2} - r^2 (V_0 + E) = \frac{\hbar^2 \ell(\ell+1)}{2m}$$

$$\frac{r^2}{u_{k\ell}} \frac{d^2 u_{k\ell}}{dr^2} + \frac{2m}{\hbar^2} r^2 (V_0 + E) = -\ell(\ell+1)$$

$$\frac{d^2 u_{k\ell}}{dr^2} + \frac{2m}{\hbar^2} (V_0 + E) u_{k\ell} = -\frac{\ell(\ell+1)}{r^2} u_{k\ell}$$

Let

$$k^2 = \frac{2m(V_0 + E)}{\hbar^2}.$$

Then our radial Schrödinger equation is

$$\frac{d^2 u_{k\ell}}{dr^2} + k^2 u_{k\ell} = -\frac{\ell(\ell+1)}{r^2} u_{k\ell}$$

$$\boxed{\frac{d^2 u_{k\ell}}{dr^2} + \left[k^2 - \frac{\ell(\ell+1)}{r^2}\right] u_{k\ell} = 0}$$

(c)

If $l=0$, we have

$$\frac{d^2 u_{k,0}}{dr^2} + k^2 u_{k,0} = 0$$

$$\frac{d^2 u_{k,0}}{dr^2} = -k^2 u_{k,0}$$

In the region $0 \le r \le a_0$, our solution is

$$u_{k,0}(r) = A \sin(k_1 r), \quad (1)$$

where

$$k_1^2 = \frac{2m(V_0 + E)}{\hbar^2}.$$

We know $V=0$ in the regions $|\vec{r}| > a_0$, so

$$\frac{-\hbar^2}{2m} \frac{d^2 u_{k,0}}{dr^2} = +E u_{k,0}.$$

Let

$$k_2 = \frac{\sqrt{-2mE}}{\hbar^2}.$$

Then

$$\frac{d^2 u_{k,0}}{dr^2} = k_2^2 u_{k,0}.$$

The general solution is

$$u_{k,0}(r) = Be^{-k_2 r} + Ce^{k_2 r}. \quad (2)$$

(c), cont'd...

For $|\vec{r}| > a_0$, we must have $C = 0$ to keep ② from blowing up. So ② becomes

$$u_{k,0}(r) = Be^{-k_2 r}.$$

We must have ① = ② at $|\vec{r}| = a_0$ and $\frac{d①}{dr} = \frac{d②}{dr}$ at $|\vec{r}| = a_0$. So

$$A\sin(k_1 r)\Big|_{a_0} = Be^{-k_2 r}\Big|_{a_0}$$

$$A\sin(k_1 a_0) = Be^{-k_2 a_0}$$

and

$$Ak_1\cos(k_1 a_0) = -Bk_2 e^{-k_2 a_0}.$$

Normalizing ①, we know

$$A = \sqrt{\frac{2}{a_0}}.$$

So

$$\sqrt{\frac{2}{a_0}}\sin(k_1 a_0) = Be^{-k_2 a_0}$$

$$B = \sqrt{\frac{2}{a_0}}\sin(k_1 a_0)\, e^{k_2 a_0}$$

and our function is

$$\boxed{u_{k,0}(r) = \begin{cases} \sqrt{\frac{2}{a_0}}\sin(k_1 r), & 0 < r < a_0 \\ \sqrt{\frac{2}{a_0}}\sin(k_1 a_0)\, e^{k_2(a_0 - r)}, & r > a_0 \end{cases}}$$

(d)

From the boundary conditions, we know

$$A k_1 \cos(k_1 a_0) = -B k_2 e^{-k_2 a_0}$$

$$\sqrt{\frac{2}{a_0}} \left(\frac{\sqrt{2m(V_0+E)}}{\hbar}\right) \cos\left(\frac{\sqrt{2m(V_0+E)}}{\hbar} a_0\right)$$

$$= -\sqrt{\frac{2}{a_0}} \sin\left(\frac{\sqrt{2m(V_0+E)}}{\hbar} a_0\right) e^{\frac{\sqrt{-2mE}}{\hbar} a_0} \sqrt{-\frac{2mE}{\hbar^2}}\, e^{-\frac{\sqrt{-2mE}}{\hbar} a_0}$$

$$\frac{\sqrt{2m(V_0+E)}}{\hbar} \cot\left(\frac{\sqrt{2m(V_0+E)}}{\hbar} a_0\right) = -\frac{\sqrt{-2mE}}{\hbar} \qquad (3)$$

$$\boxed{\cot\left(\frac{\sqrt{2m(V_0+E)}}{\hbar} a_0\right) = \sqrt{-\frac{E}{V_0+E}}}$$

This transcendental equation gives the bound state energies for the $l=0$ states.

(e) From (3), we can leave this in the form

$$k_1 \cot(k_1 a_0) = -k_2 .$$

Let $z = k_1 a_0$. Then

$$-\frac{k_1}{k_2} = \tan(k_1 a_0)$$

$$-\frac{k_1}{k_2} = \tan(z)$$