Problem 6: 3D Square Well (10 Points):

Consider a particle of mass m moving in a 3D spherical well given by the potential

$$V(\vec{r}) = -V_0 \quad 0 \le |\vec{r}| \le a_0, \qquad V(\vec{r}) = 0 \quad |\vec{r}| > a_0$$

where $V_0 > 0$ and $a_0 > 0$.

5?

In this problem, only consider bound states in this well, so $-V_0 < E < 0$.

? ✓ (a) (1 pt.) Show that the energy eigenstates for this potential can be written in the form:

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

r, θ, ϕ are the usual spherical coordinates. and Y_ℓ^m the spherical harmonics.

? ✓ (b) (1 pt.) Defining the function $u_{k,\ell}(r) = r f_{k,\ell}(r)$, write the radial Schrodinger equation for $u_{k,\ell}(r)$.

? ✓ (c) (2 pts.) Consider the zero angular momentum states, $\ell = 0$. Write down the functional form for the states $u_{k,0}(r)$ in the two regions, $0 \le r \le a_0$ and $r \ge a_0$. Define any constants that you use in these functions.

? ✓ (d) (1 pt.) What are the boundary conditions on the functions $u_{k,0}(r)$ as $r \to 0$, at $r = a_0$, and as $r \to \infty$? Hint: Consider the function $f_{k,\ell}(r)$ as $r \to 0$.

(e) (2 pts.) Using your boundary conditions, derive an equation that can be solved to give the bound state energies for the $\ell = 0$ states.

(f) (2 pt.) For a fixed value of the radius of the well, a_0, calculate the minimum depth, $V_0 = V_{min}$ for the potential well to have a bound state.

(g) (1 pt.) give a physical reason why there is always a bound state in a symmetric 1D quantum square well, but not in the 3D well studied in this problem.

In spherical coordinates, (L^2 is the usual angular momentum operator)

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\psi\right)$$

$$\nabla^2 \psi(\vec{r}) = \cancel{\frac{1}{r}\frac{\partial^2}{\partial r^2} r\psi(\vec{r})} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial \psi(\vec{r})}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \phi^2}\psi(\vec{r})$$

$$\nabla^2 \psi(\vec{r}) = \cancel{\frac{1}{r}\frac{\partial^2}{\partial r^2} r\psi(\vec{r})} - \frac{L^2}{\hbar^2 r^2}\psi(\vec{r})$$

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Quantum #6

a) $V(r) = \begin{cases} -V_0 & 0 \leq r \leq a_0 \\ 0 & r > a_0 \end{cases}$

* Note: We only consider the bound region

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

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

* Assuming a solution of the form $\psi = f_{k,\ell}(r)\, Y_\ell^m(\theta,\varphi)$

$$\frac{-\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right)\cdot Y + \frac{f}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{f}{r^2\sin^2\theta}\left(\frac{\partial^2 Y}{\partial\varphi^2}\right)\right] + VfY = EfY$$

* multiplying by $\frac{-2mr^2}{fY\hbar^2}$ yields

$$\frac{1}{f}\left(\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) - \frac{2mr^2 f(V-E)}{\hbar^2}\right) + \frac{1}{Y}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}\right) = 0$$

* Note: Our assumption of a seperable solution works where the angular equation can be solved to find that $Y_\ell^m(\theta,\varphi)$ is the solution we expect (ie spherical harmonics)

b) Defining $u_{k,\ell}(r) = r f_{k,\ell}(r) \Rightarrow f_{k,\ell} = \frac{u_{k,\ell}(r)}{r}$, the Schrödinger eqn becomes:

$$\frac{1}{f}\left(\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right)\right) - \frac{2mr^2 f(V-E)}{\hbar^2} = \ell(\ell+1)$$

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) - \frac{2mr^2 f(V-E)}{\hbar^2} = \ell(\ell+1)f$$

$$\frac{\partial}{\partial r}\left(r^2\frac{d}{dr}\left(\frac{u}{r}\right)\right) - \frac{2mr\,u_{k,\ell}(r)(V-E)}{\hbar^2} = \ell(\ell+1)\frac{u(r)}{r}$$

$$\frac{\partial}{\partial r}\left(\cancel{r^2}\left[\frac{r\,du/dr - u}{\cancel{r^2}}\right]\right) - \frac{2mr\,u(V-E)}{\hbar^2} = \frac{\ell(\ell+1)u}{r}$$

$$\frac{\partial}{\partial r}\left(r\frac{du}{dr} - u\right) - \frac{2mr\,u(V-E)}{\hbar^2} = \frac{\ell(\ell+1)u}{r}$$

$$\left[\frac{du}{dr} + r\frac{d^2u}{dr^2} - \frac{du}{dr}\right] - \frac{2mru(V-E)}{\hbar^2} = \frac{\ell(\ell+1)u}{r}$$

$$\frac{-\hbar^2}{2m}\frac{d^2u}{dr^2} + \left(V + \frac{\hbar^2\ell(\ell+1)}{2m}\right)u = Eu$$

#6 (cont)

c) If we only consider $l=0$, our equation becomes:

$$\frac{-\hbar^2}{2m}\frac{d^2u}{dr} + Vu = Eu$$

$$\hookrightarrow \frac{d^2u}{dr^2} = \frac{-2mE-V}{\hbar^2}u$$

let $k = \frac{\sqrt{2m(E+V_0)}}{\hbar}$ where $0 \le r \le a_0$

$$\frac{d^2u}{dr^2} = -k^2u \Rightarrow u = Ae^{ikr} + Be^{-ikr} = C\sin(kr) + D\cos(kr)$$

let $\kappa = \frac{\sqrt{+2mE}}{\hbar}$ where $r > a_0$

$$\frac{d^2u}{dr^2} = \kappa^2 u \Rightarrow u = Ae^{\kappa r} + Be^{-\kappa r}$$

d) Our function must go to 0 at $r=0$ and $r=\infty$

$$\hookrightarrow f = \frac{u}{r} = C\frac{\sin(kr)}{r} + D\frac{\cos(kr)}{r}$$ (Inside well)

$\sin(0) = 0$

$\cos(0) = 1 \Rightarrow D = 0$

$$f = \frac{u}{r} = A\frac{1}{r}e^{\kappa r} + B\frac{1}{r}e^{-\kappa r}$$

$e^{\kappa\infty} = \infty \Rightarrow A = 0$

$e^{-\kappa\infty} = 0$

e) Therefore, inside the well (bound states), it must be true that

$$\sin(kr) = 0 \Rightarrow kr = n\pi$$

$$\frac{\sqrt{2m(E+V_0)}\,r}{\hbar} = n\pi$$

$$2m(E+V_0) = \frac{n^2\pi^2\hbar^2}{r^2}$$

$$E = \frac{n^2\pi^2\hbar^2}{2mr^2} - V_0$$

#6 (cont.)

f) Assuming a_0 is fixed, we need to find the minimum depth for a bound state

↳ $E > 0 \Rightarrow \frac{n^2\pi^2\hbar^2}{2mr^2} > V_{min}$

* potential error in definitions of k an $\mathcal{K}$

$$\frac{n^2\pi^2\hbar^2}{2ma_0^2} = V_{min}$$