Notes for Lectures on Quantum Mechanics *

Spherically Symmetric Potentials — Using Spherical Polar Coordinates

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Contents

We shall discuss energy eigenvalue problem in three dimensions for a spherically symmetric potential given. A spherically symmetric potential depends only on r and does not depend on θ and ϕ. The Hamiltonian for such a system is

$$H = \frac{p^2}{2m} + V(r) \tag{1}$$

For a spherically symmetric potential the Hamiltonian commutes with the angular momentum operators $\vec{L} = \vec{r} \times \vec{p}$ and the angular momentum components L_x, L_y, L_z are constants of motion and therefore $H, \vec{L}^2, L_z$ form a commuting set of operators. It is seen that the parity operators P commutes with all these operators and that the set of operators

$$H, "\vec{L}^2, L_z \text{and } P$$

is a complete set of commuting operators. This means that $\vec{L}^2, L_z, P$ are constants of motion and that the energy eigenfunctions can be selected to have definite values of $\vec{L}^2, L_z, P$ also. We shall see these features in the folowing specfic examples to be discussed later.

- Free Particle, $V(r) =$ constant.
- Hydrogen atom, $v(r) = -\dfrac{e^2}{r}$
- Square well and other similar potentials.

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1 Schrodinger Equation for Spherically Symmetric Potentials

The Schrodinger equation for a spherically symmetric potential is

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi = E\psi \tag{2}$$

The Laplacian ∇^2 in spherical polar coordinates is given by

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \tag{3}$$

Therefore, Eq,(2) takes the form

$$\left\{\frac{1}{r^2}\left(\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right\}\psi(r,\theta,\phi) \tag{4}$$

$$+ \frac{2m}{\hbar^2}(E - V(r))\psi(r,\theta,\phi) = 0. \tag{5}$$

2 Separation of Variables

Substitute

$$\psi(r,\theta,\phi) = R(r)Y(\theta,\phi) \tag{6}$$

in Eq,(4) and divide by $R(r)Y(\theta,\phi)$ to get

$$\frac{1}{R(r)}\frac{1}{r^2}\left(\frac{\partial}{\partial r}r^2\frac{\partial R}{\partial r}\right) + \frac{1}{Y}\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{Y}\frac{1}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2} + \frac{2m}{\hbar^2}(E - V(r)) = 0 \tag{7}$$

Multiply by r^2 and rearrange to get

$$\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{2m}{\hbar^2}(E - V(r))r^2 = -\frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\} = 0 \tag{8}$$

The left hand side of the above equation is a function of r alone and the right hand side is a function of θ and ϕ only. This is possible only when each side is a constant, say λ. Thus we get two ordinary differential equations

$$\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{2m}{\hbar^2}(E - V(r))r^2 = \lambda \tag{9}$$

and

$$\frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\} = -\lambda \tag{10}$$

On rearranging Eq,(9) we get the radial Schrodinger equation

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{2m}{\hbar^2}\left(E - V(r) - \frac{\lambda}{r^2}\right)R(r) = 0 \tag{11}$$

and Eq,(10) can be rewritten as

$$-\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\}=\lambda Y(\theta,\phi) \tag{12}$$

is seen to be just the eigenvalue problem for angular momentum operator $\vec{L}^2$. The variables θ and ϕ can be separated in Eq,(12) by writing

$$Y(\theta,\phi)=Q(\theta)E(\phi),$$

resulting partial differential equation

$$\left\{\frac{1}{P}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial P}{\partial\theta}\right)+\frac{1}{E}\frac{1}{\sin^2\theta}\frac{\partial^2 P}{\partial\phi^2}\right\}=\lambda \tag{13}$$

separates into two ordinary differential equations one of which is just the eigenvalue equation for L_z.

For these equations physically acceptable solutions are known to exist only when $\lambda=\ell(\ell+1), m=\ell,\ell-1,\cdots,-\ell-1,-\ell$. The solutions for Y are the spherical harmonics $Y_{\ell m}(\theta,\phi)$.

3 Summary of Results on Spherically Symmetric Potentials

The solutions of the Schrodinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2+V(r)\right]\psi=E\psi \tag{14}$$

for a spherically symmetric potential $V(r)$ are of the form

$$\psi(r,\theta,\phi)=R_\ell(r)Y_{\ell m}(\theta,\phi) \tag{15}$$

where $R_\ell(r)$ is called the radial wave function and satisfies the radial Schrodinger equation

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{2m}{\hbar^2}\left(E-V(r)-\frac{\lambda}{r^2}\right)R(r)=0 \tag{16}$$

The angular part of the wave function $Y_{\ell m}(\theta,\phi)$ is simultaneous eigenfunction of $\vec{L}^2$ and L_z with eigenvalues $\ell(\ell+1)\hbar^2$ and $m\hbar$, respectively. Note that only ℓ appears in the radial equation and that it does not contain m. Hence

1. The energy eigenvalues are independent of m; there are $2(\ell+1)$ linearly independent solutions for each fixed ℓ all having the same energy. Thus they are $(2\ell+1)$ fold degenerate.

2. The energy eigenvalues depend on ℓ and increase with increasing ℓ.

For a spherically symmetric potential we need to concentrate only on the radial equation. If we substitute $R(r)=\frac{1}{r}\chi(r)$, the radial equation takes the form of one dimensional Schrodinger equation. Using

$$\begin{aligned}
\frac{dR(r)}{dr} &= -\frac{1}{r^2}\chi(r) + \frac{1}{r}\chi(r) && (17)\\
r^2\frac{dR(r)}{dr} &= -\chi(r) + r\chi(r) && (18)\\
\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) &= \frac{1}{r^2}\left(-\frac{\partial\chi}{\partial r} + r\frac{\partial^2\chi}{\partial r^2} + \frac{\partial\chi}{\partial r}\right) && (19)\\
&= \frac{1}{r}\frac{\partial^2\chi}{\partial r^2} && (20)
\end{aligned}$$

Eq,(16) takes the form

$$-\frac{\hbar^2}{2m}\frac{d^2\chi}{dr^2} + \left(V(r) + \frac{\ell(\ell+1)\hbar^2}{2mr^2}\right)\chi = E\chi \tag{21}$$

This equation looks like one dimensional Schrodinger equation with potential $V(r)$ replaced with

$$V(r) + \frac{\ell(\ell+1)\hbar^2}{2mr^2} \equiv V_{\text{eff}}(r). \tag{22}$$

The second term in $V_{\text{eff}}(r)$ is just the centrifugal potential term which also appears in the classical equation for the radial motion. The radial Schrodinger equation Eq,(21) can be analyzed in the same manner as one dimensional problems. There is one difference however that we must demand

$$\chi(r) \to 0 \quad \text{as} \quad r \to 0, \tag{23}$$

so that the radial wave function $R(r) = \dfrac{\chi(r)}{r}$ does not become singular at $r = 0$. In addition to above boundary condition on the solutions, another difference between Eq,(21) and a one dimensional problem is that the variable r takes values in the interval $(0, \infty)$ instead of $(-\infty, \infty)$.