Quantum Mechanics and Atomic Physics

Lecture 15:
Angular momentum and Central Potentials

http://www.physics.rutgers.edu/ugrad/361

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Last time

- S.E. in 3D and in spherical coordinates
- For a mass \( \mu \) moving in a central potential \( V(r) \)

\[ -\frac{\hbar^2}{2\mu} \left\{ \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r}) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \frac{\partial}{\partial \theta}) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right\} \psi(r, \theta, \phi) \]

\[ + V(r) \psi(r, \theta, \phi) = E \psi(r, \theta, \phi) \]

- Solutions separated into angular and radial parts

\[ \psi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi) \]
Rewrite this in terms of angular momentum of the system

\[-\frac{\hbar^2}{2\mu} \left\{ \frac{1}{r} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) \right\} + \left( V - E \right) r^2 = -\frac{1}{2\mu} L_{\phi}^2 \]

\[ L_{\phi}^2 = -\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \]
Angular Solutions

Solutions to $\Phi(\varphi)$:
$$\Phi(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im_\varphi}$$

$m_\varphi = 0, \pm 1, \pm 2, \ldots$

Solutions to $\Theta(\theta)$:
$$P_{lm}(\cos \theta)$$

$l = 0, 1, 2, \ldots$

$|m_\theta| \leq l$

Spherical harmonic functions

Associated Legendre functions

Magnetic quantum number

Orbital angular quantum number
Space Quantization

- The magnetic quantum number \( m_l \) expresses the quantization of direction of \( L \)

\[
L_z = m_l \hbar \\
L_z = L \cos \theta
\]

\[
\Rightarrow \cos \theta = \frac{L_z}{L} = \frac{m_l \hbar}{\sqrt{l(l+1)\hbar}} = \frac{m \hbar}{\sqrt{l(l+1)}}
\]

- So \( L \) can assume only certain angles, given above, with respect to the z-axis.
- This is called space quantization.

![Diagram showing space quantization with a cone and angles labeled.](image)
Example

For a particle with \( \ell = 2 \), what are the possible angels that \( \mathbf{L} \) can make with the z-axis?

\[
\ell = 2, \quad L = \sqrt{6} \hbar, \quad L_3 = m \hbar
\]

\[
\cos \theta = \frac{m_x}{\sqrt{\ell(\ell+1)}} = \frac{m_x}{\sqrt{6}}
\]

- \( m_x = 2 \Rightarrow \cos \theta = \frac{2}{\sqrt{6}} \Rightarrow \theta = 35.3^\circ \)
- \( m_x = 1 \Rightarrow \cos \theta = \frac{1}{\sqrt{6}} \Rightarrow \theta = 65.9^\circ \)
- \( m_x = 0 \Rightarrow \cos \theta = 0 \Rightarrow \theta = 90^\circ \)
- \( m_x = -1 \Rightarrow \cos \theta = -\frac{1}{\sqrt{6}} \Rightarrow \theta = 114^\circ \) or \(-66^\circ \)
- \( m_x = -2 \Rightarrow \cos \theta = \frac{1}{\sqrt{6}} \Rightarrow \theta = 145^\circ \) or \(-35^\circ \)

![Figure 6.5 Possible orientations of \( \mathbf{L} \) for \( \ell = 2, |L| = \sqrt{6}\hbar \).](image)
Plot of Spherical harmonics

- "3D" plots of:
  \[ r = |\mathcal{Y}_{\ell m}(\theta, \phi)|^2 \]

- \( \theta \) is measured from the +z axis
- Independent of \( \phi \)
  - So rotationally symmetric around z-axis
- These manifest themselves as the probability distributions

\( \text{distance}(r) \) from the origin represents the value \(|\mathcal{Y}_{\ell m}(\theta, \phi)|^2\)

\( \text{Figure 6.7} \) Poler diagrams of the absolute squares of spherical harmonics up to \( \ell = 3 \). Reproduced from Siegmund Brandt and Hans Gieter Dahmer, The Picture Book of Quantum Mechanics, John Wiley & Sons, Inc., New York, 1986, with the kind permission of the publisher.
Summary: Quantization of $L, L_z$ and space

\[ L^2 \mathcal{Y}_{\ell m \phi}(0, \Phi) = \left[ \hbar^2 \ell (\ell + 1) \right] \mathcal{Y}_{\ell, m \phi}(0, \Phi) \]

\[ \Rightarrow L = \sqrt{\ell (\ell + 1)} \hbar \]

\[ (L_\phi) \phi(\Phi) = m_\phi \hbar \phi(\Phi) \]

\[ \Rightarrow L_\phi = m_\phi \hbar \]

\[ \cos \theta = \frac{L_\phi}{L} = \frac{m_\phi}{\sqrt{\ell (\ell + 1)}} \]

Reed: Chapter 6
Radial Solutions

To find radial solutions:

\[-\frac{\hbar^2}{2\mu} \left\{ \frac{1}{r} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) \right\} + \left( V(r) - E \right) r^2 = -\frac{L^2}{2\mu r^2} \text{Y} \]

\[\Rightarrow -\frac{\hbar^2}{2\mu} \left\{ \frac{1}{r} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) - \ell (\ell + 1) \right\} + V(r) r^2 = Er^2 \]

This is called the radial equation
Solving the radial equation

- Note:

\[
\frac{1}{R} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \rho}{\partial r} \right) = \frac{\rho}{R} \frac{\partial^2}{\partial r^2} (r \rho)
\]

\[
\Rightarrow -\frac{\hbar^2}{2\mu} \left\{ \frac{\rho}{R} \frac{\partial^2}{\partial r^2} (r \rho) - l(l+1) \right\} + V(r) r^2 = \varepsilon r^2
\]

- Let’s introduce the auxiliary function:

\[
\mathcal{U}(r) = r \, R(r)
\]

- And plug it in above
\[ -\frac{\hbar^2}{2\mu} \left( \frac{\partial}{\partial r} \left( \frac{2}{r^2} (U) - \ell (l+1) \right) \right) + V(r) \frac{U}{R^2} - E \frac{U}{R^2} = 0 \]

Multiply by \( \frac{R^2}{U} \)

\[ -\hbar^2 \left( \frac{\partial^2 U}{\partial r^2} - \ell (l+1) \frac{R^2}{U} \right) + U(V - E) = 0 \]

Multiply by \( -\frac{2\mu}{\hbar^2} \) and \( \frac{\partial^2}{\partial r^2} \Rightarrow \frac{d^2}{dr^2} \)

\[ \Rightarrow \frac{d^2}{dr^2} U + \frac{2\mu}{\hbar^2} \left[ E - V(r) - \ell (l+1) \cdot \frac{\hbar^2}{2\mu} \right] U = 0 \]
The Total Wavefunction

- The total wavefunction

\[ \psi_{nlm,}(r, \theta, \phi) = R_n(r) Y_{l,m}(\theta, \phi) = \frac{U_{n}(r)}{r} Y_{\ell,m}(\theta, \phi) \]

- We will soon define \( n \) to be the quantum number that dictates the quantization of energy

- First let’s solve this for two simple cases
  - Infinite and finite spherical wells
  - Spherical analogs of particle in a box
  - Interest in nuclear physics: nuclei modeled as spherical potential wells 10’s of MeV deep and \( 10^{-14} \) m in radius

- Then we will obtain a detailed solution to the Coulomb potential for hydrogen (next time)
The Infinite Spherical Well

- A particle of mass $\mu$ is trapped in a spherical region of space with radius $a$ and an impenetrable barrier

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

- We will only deal with the simplest case of zero angular momentum

- (Otherwise: $l \neq 0 \Rightarrow$ Bessel $\&$ Neumann functions)
So, \( U(r) = U_0(r) \)

\[
\frac{d^2 U_0(r)}{dr^2} + \frac{2}{r} \frac{d U_0(r)}{dr} = 0 \quad \text{inside well.}
\]

\[
\lambda^2 = \left[ E - V(r) - \frac{\ell(\ell+1)}{r^2} \frac{\hbar^2}{2\mu} \right] \frac{2\mu}{\hbar^2} = \frac{2\mu E}{\hbar^2} \quad \text{since } V(r) = 0 \text{ inside.}
\]

Since \( \ell = 0 \) inside.

- Looks just like for 1D infinite potential well!
- So solutions are:

\[
U_{1D} = A \sin kr + B \cos kr
\]
Boundary Conditions

- Recall: 
  \[ R = \frac{u}{r} \]

- Boundary conditions should prevent divergence for \( R \) as \( r \to 0 \): Thus \( U = R^2 r = 0 \) as \( r \to 0 \):
  \[ \Rightarrow U(r=0) = 0 \Rightarrow B = 0 \]

- Boundary conditions also require that the barrier is impenetrable:
  \[ \Rightarrow U(r=a) = 0 \Rightarrow 0 = A \sin \kappa a \Rightarrow \kappa a = n\pi \]

- This gives us quantization of energy!
  \[ \Rightarrow E_n(l=0) = \frac{n^2 \alpha^2 \hbar^2}{2\mu a^2} \]
Total Wavefunction

\[ \Psi_{n\ell m}(r,\theta,\varphi) = R_n(r) Y_{\ell m}\theta(\theta,\varphi) \]

\[ = \frac{A}{\sqrt{4\pi r}} \sin\left(\frac{n\pi r}{a}\right) \]

Since: \[ Y_{0,0} = \frac{1}{\sqrt{4\pi}} \] and

\[ R_n(r) = \frac{U_n(r)}{r} = \frac{A}{r} \sin\left(\frac{n\pi r}{a}\right) \]

- To obtain A, we apply normalization ...
Normalization

\[
\int_0^a \int_\Phi^\pi \int_0^{2\pi} \Psi^* \Psi \frac{r^2 \sin \theta \, d\Phi \, d\theta \, dr}{d\text{Volume}} = 1
\]

\[
\int_0^a \int_\Phi^\pi \int_0^{2\pi} \frac{A^2}{4\pi \sigma^2} \sin^2 \left(\frac{n \pi r}{\sigma}\right) - r^2 \sin \theta \, d\Phi \, d\theta \, dr = 1
\]

\[
\int_0^{2\pi} \sin \theta \, d\Phi = 2\pi, \quad \int_0^\pi \sin \theta \, d\theta = 2, \quad \int_0^a \sin^2 \left(\frac{n \pi r}{\sigma}\right) \, dr = \frac{a}{2}
\]

\[
\Rightarrow \quad \frac{A^2}{4\pi} \cdot 2\pi \cdot 2 \cdot \frac{a}{2} = 1 \Rightarrow \quad A = \sqrt{\frac{2}{\sigma}}
\]

So,

\[
\Psi_{n,0,0} = \frac{1}{\sqrt{2\pi \sigma r}} \sin \left(\frac{n \pi r}{\sigma}\right)
\]
Normalization: simpler approach

\[ y_{n00}(r, \theta, \varphi) = R_n^0 Y_{00}(\theta, \varphi) \]

Because \( Y_{00} \) is already normalized, only \( R_n^0 \) needs 
\[ \left( \frac{1}{\sqrt{4\pi}} \right) \]
to be normalized. In other words
\[
1 = \int_0^a \int_0^\pi \int_0^{2\pi} \rho^2 r^2 \sin\theta \, d\rho \, d\varphi \, d\theta \\
= \int_0^a \left( \int_0^\pi \int_0^{2\pi} |Y_{00}|^2 \sin\theta \, d\varphi \, d\theta \right) r^2 \, dr \\
= \int_0^a \left( \frac{A}{r} \sin\left( \frac{n\pi}{a} r \right) \right)^2 r \, dr \\
= A^2 \int_0^a \sin^2\left( \frac{n\pi}{a} r \right) \, dr = A^2 \cdot \frac{a}{2} \Rightarrow A = \sqrt{\frac{2}{a}}
Example: what is $<r>$ for a particle in an infinite spherical well?

\[
<r> = \int_0^a \int_0^{2\pi} \int_0^{\pi} \left| \psi_{n\ell_0}^* \psi_{n\ell_0} \right|^2 r^2 \sin \theta \, d\phi \, d\theta \, dr
\]

\[
= \frac{1}{\pi a^3} \left[ \int_0^a r \sin^2 \left( \frac{n\pi r}{a} \right) \, dr \right] \left[ \int_0^{2\pi} \sin \theta \, d\theta \right] \left[ \int_0^\pi \, d\phi \right]
\]

\[
= \frac{2}{a} \int_0^a r \sin^2 \left( \frac{n\pi r}{a} \right) \, dr
\]

\[
= \frac{2}{n^2} \left[ \frac{r^2}{4} - \frac{r \sin \left( \frac{n\pi r}{a} \right)}{n \pi r/a} - \frac{\cos \left( \frac{n\pi r}{a} \right)}{8 \left( \frac{n\pi r}{a} \right)^2} \right]_0^a
\]

\[
= \frac{a^2}{4} \cdot \frac{2}{n^2} = \frac{a}{2}
\]

$<r>$ is independent of $n$!
Increasing the energy of the particle changes the probability distribution but not its average position.
This is not the case for non-zero angular momentum!
The Finite Spherical Well

- Analog of 1-D finite potential well.
- Could describe a particle trapped inside a nucleus

\[ V(r) = \begin{cases} V_0 & r > a \\ 0 & r < a \end{cases} \]

- Let’s find the bound state solutions, \( E < V_0 \)
- Again we consider only \( l = 0 \) case.
Inside and outside the well

- **Inside the well**

  \[ r < a \quad E \geq V(r) \Rightarrow E \geq 0 \]

  \[
  \frac{d^2 U_0}{dr^2} + \kappa_i^2 U_0 = 0
  \]

  \[
  \kappa_i = \frac{2\mu E}{\hbar^2}
  \]

  Just like infinite spherical well

  \[
  R_0 \text{\,\,\,inside} (r) = \frac{A \sin \kappa_i r}{r} \quad r < a
  \]

- **Outside the well**

  \[ r > a \quad E < V_0 \]

  \[
  \frac{d^2 U_0}{dr^2} = \kappa_2^2 U_0
  \]

  \[
  \kappa_2 = \frac{2\mu (V_0 - E)}{\hbar^2}
  \]

  \[
  U_0 \text{\,\,\,outside} (r) = Ce^{\kappa_2 r} + De^{-\kappa_2 r}
  \]

  \[
  \Rightarrow R_0 \text{\,\,\,outside} (r) = \frac{Ce^{\kappa_2 r}}{r} + \frac{De^{-\kappa_2 r}}{r}
  \]
Boundary conditions outside the well

- Boundary condition at \( r \to \infty \), \( u(r) \to 0 \)
  
  \[ \Rightarrow C = 0 \]

- Continuity @ \( r = a \) of \( R \) and \( \frac{dR}{dr} \)

  \[ A \sin k_a a = D e^{-k_a a} \]

  \[ -A \frac{\sin k_a a}{a^2} + A \frac{k_a \cos k_a a}{a} = -D \frac{k_a e^{-k_a a}}{a} - D e^{-k_a a} \]

  \[ \Rightarrow A \left[ k_a \cos k_a a - \sin k_a a \right] = -D e^{-k_a a} (a k_a + 1) \]
Divide the two equations:

\[
\lambda_2 \alpha \cot \lambda_2 \alpha - 1 = - (\alpha \lambda_2 + 1) \\
\lambda_1 \alpha \cot \lambda_1 \alpha = - \alpha \lambda_2 
\]

Define:

\[
\zeta = \lambda_1 \alpha \quad , \quad \eta = \lambda_2 \alpha \\
\zeta \cot \zeta = - \eta 
\]

This is a transcendental equation!

\[
\zeta^2 + \eta^2 = a^2 (k_1^2 + k_2^2) = a^2 \left[ \frac{2 \mu E}{\hbar^2} + \frac{2 \mu (V_0 - E)}{k^2} \right] \\
= a^2 \cdot \frac{2 \mu V_0}{k^2} = \text{const} \cdot \rho^2 
\]

\(\rho^2\) is the strength parameter
Sketch functions

\[ n = \begin{cases} \text{odd} & \text{odd} \\ \text{even} & \end{cases} \]

\[ \xi^2 + \eta^2 = \rho^2 \implies \]

\[ \lim_{\xi \to 0} \frac{\cos \xi}{\sin \xi} = 1 \]

\[ \cot \frac{\pi}{2} = \frac{\cos \frac{\pi}{2}}{\sin \frac{\pi}{2}} \]

\[ \xi \quad \eta \quad \rho \text{ radius} \]
Energy Eigenvalues

- This is an equation that describes a circle of radius $\rho$ in the $(\xi, \eta)$ plane.

$$\xi^2 + \eta^2 = \rho^2$$

- To find allowed bound state energies need to satisfy this equation and transcendental equation simultaneously

- Points of intersection of circles and the cotangent curves correspond to the quantized energy levels
Energy Eigenvalues

- Zeros of cotangent occur at:
  \[
  \cot \frac{\pi}{2} = 0,
  \]
  \[
  \frac{(2n-1)\pi}{2}, \quad n = 1, 2, 3, \ldots
  \]

- For a spherical well to possess n bound states it must have:
  \[
  \rho > \frac{(2n-1)\pi}{2}
  \]

- Or ...
  \[
  \rho^2 > \frac{(2n-1)^2\pi^2}{4} \Rightarrow \quad V_0a^2 \geq \frac{(2n-1)^2\pi^2h^2}{8\mu}
  \]

Note \(\rho=1\) has no bound states!
Example

- How many energy states are available to an alpha-particle trapped in a finite spherical well of depth 50 MeV and radius $10^{-14}$ m? Assume zero angular momentum.

\[
(2n-1)^2 \leq \frac{8 \mu a^2 V_0}{\hbar^2 \pi^2}
\]

\[
(2n-1)^2 \leq 8 \left( \frac{6.646 \times 10^{-27} \text{kg}}{10^{-14} \text{m}} \right)^2 \left( \frac{8 \times 10^{-12} \text{J}}{1.055 \times 10^{-34} \text{J} \cdot \text{s}} \right) \pi^2
\]

\[
(2n-1)^2 \leq 387
\]

\[
n \leq 10.3
\]
What is the energy of the lowest energy bound state for this system?

\[
\frac{3}{2} + n^2 = \frac{2m^2 e^2 V_0}{\hbar^2} = 955
\]

\[
3 \cot \psi = -n
\]

\[
3 \cot \psi + \sqrt{955 - 3^2} = 0
\]

Minimize \( \psi = 3.04305 \)

\[
\varepsilon = \frac{\hbar^2}{2m} \left( \frac{3}{2} \right) = \frac{3^2}{a^2} \frac{\hbar^2}{2m} = \frac{(3.04305)^2 (1.055 \times 10^{-31} \text{ J})^2}{(10^{14} \text{ m})^2 \cdot 2 \cdot (6.646 \times 10^{-19} \text{ kg})}
\]

\[
= 7.75 \times 10^{-14} \text{ J} \approx 0.48 \text{ MeV}
\]
Summary/Announcements

- Next time: The Coulomb Potential of the Hydrogen atom