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 μ moving in a central potential V(r)

$$-\frac{\hbar^2}{2\mu}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2}\frac{1}{\sin^2\theta}\left(\frac{\partial^2}{\partial\varphi^2}\right)\right\}\Psi(r,\theta,\varphi)$$

$$+V(r)\,\Psi(r,\theta,\varphi)=E\,\Psi(r,\theta,\varphi)$$

- Solutions separated into angular and radial parts

$$\Psi(r,\theta,\varphi)=R(r)\underbrace{Y(\theta,\varphi)}_{\Theta(\theta)\Phi(\varphi)}=R(r)\,\Theta(\theta)\,\Phi(\varphi)$$

Rewrite this in terms of angular momentum of the system

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

$$L_{op}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\left(\frac{\partial^2}{\partial\varphi^2}\right)\right]$$

Angular Solutions

Solutions to $\Phi(\varphi)$:

$$\Phi(\varphi) = \sqrt{\frac{1}{2\pi}}\, e^{i m_\ell \varphi}$$

Magnetic quantum number

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

Solutions to $\Theta(\theta)$:

Associated Legendre functions

$P_{\ell m_\ell}(\cos\theta)$

$\ell = 0, 1, 2, 3, \ldots$

Orbital angular quantum number

Solutions to $Y(\theta, \varphi)$: Spherical harmonic functions

$$Y_{\ell, m_\ell}(\theta, \varphi) = \Theta_{\ell m_\ell}(\theta) \cdot \Phi_{m_\ell}(\varphi)$$

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

$|m_\ell| \leq \ell$.

Space Quantization

- The magnetic quantum number m_ℓ expresses the quantization of direction of **L**

$$L_z = m_\ell \hbar \qquad L_z = L\cos\theta$$

$$\Rightarrow \cos\theta = \frac{L_z}{L} = \frac{m_\ell \hbar}{\sqrt{\ell(\ell+1)}\,\hbar} = \frac{m_\ell}{\sqrt{\ell(\ell+1)}}$$

Space quantization.

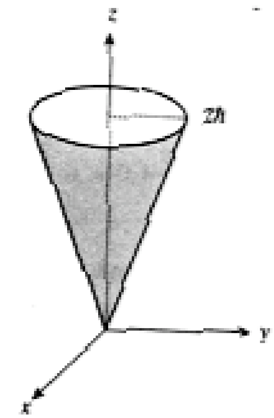

FIGURE 6.6 For $\ell = 2$, $m = 2$, L lies anywhere on the cone.

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

Example

- For a particle with ℓ=2, what are the possible angels that **L** can make with the z-axis?

$\ell = 2, \quad L = \sqrt{6}\,\hbar \qquad L_z = m_\ell \hbar$

$m_\ell = -2, -1, 0, 1, 2$

$\cos\theta = \frac{m_\ell}{\sqrt{\ell(\ell+1)}} = \frac{m_\ell}{\sqrt{6}}$

- $m_\ell = 2 \Rightarrow \cos\theta = \frac{2}{\sqrt{6}} \Rightarrow \theta = 35.3^\circ$
- $m_\ell = 1 \Rightarrow \cos\theta = \frac{1}{\sqrt{6}} \Rightarrow \theta = 65.9^\circ$
- $m_\ell = 0 \Rightarrow \cos\theta = 0 \Rightarrow \theta = 90^\circ$
- $m_\ell = -1 \Rightarrow \cos\theta = -\frac{1}{\sqrt{6}} \Rightarrow \theta = 114^\circ$ or -66°
- $m_\ell = -2 \Rightarrow \cos\theta = -\frac{2}{\sqrt{6}} \Rightarrow \theta = 145^\circ$ or -35

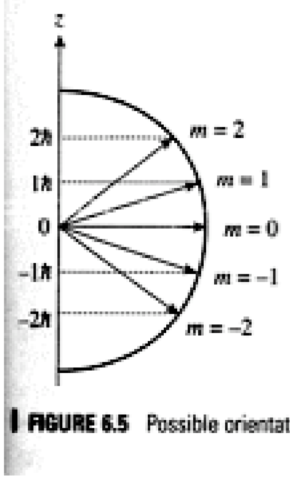

FIGURE 6.5 Possible orientations of **L** for $\ell = 2$, $|L| = \sqrt{6}\hbar$.

Plot of Spherical harmonics

- "3D" plots of:

$$r = \left| Y_{\ell m_\ell}(\theta, \varphi) \right|^2$$

- θ is measured from the +z axis
- Independent of ϕ
  - So rotationally symmetric around z-axis
- These manifest themselves as the probability distributions

distance (r) from the origin represents the value $|Y_{\ell m_\ell}(\theta,\varphi)|^2$

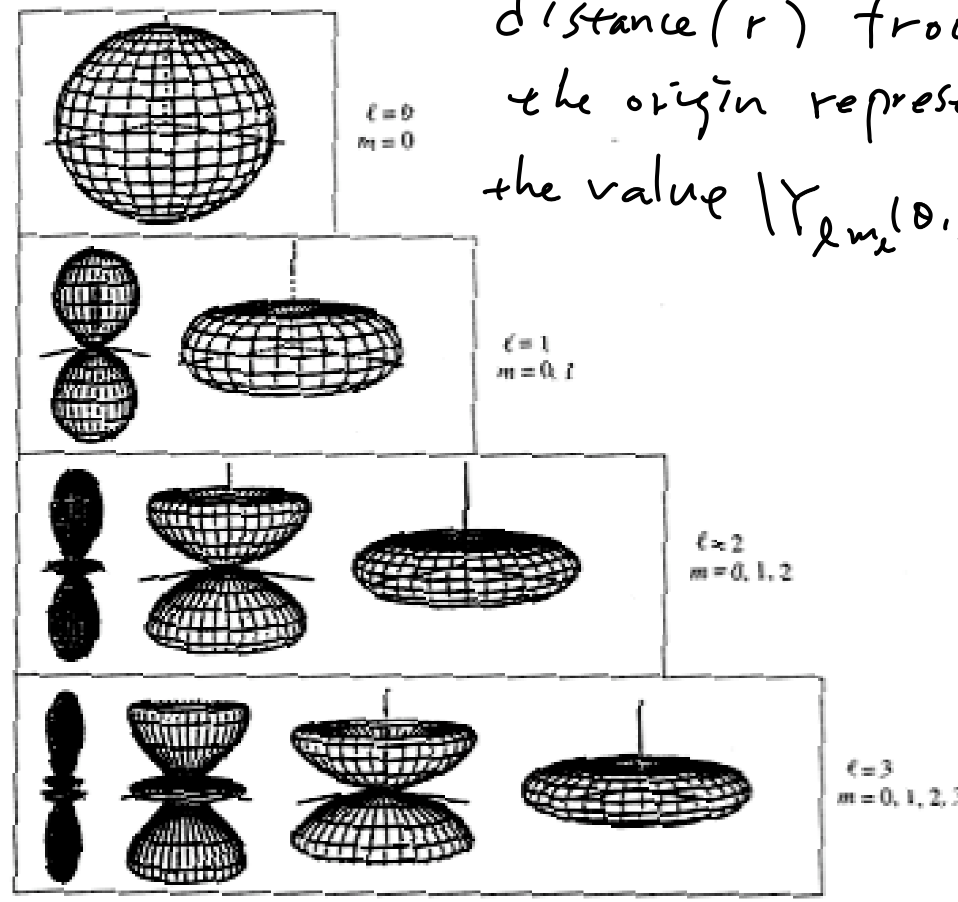

FIGURE 6.7 Polar diagrams of the absolute squares of spherical harmonics up to $\ell = 3$. Reproduced from Siegmund Brandt and Hans Dieter Dahmen, *The Picture Book of Quantum Mechanics*, John Wiley & Sons, Inc., New York, 1985, with the kind permission of the publisher.

Summary: Quantization of L, L_z and space

$$L_{op}^2 Y_{\ell,m_\ell}(\theta,\varphi) = \left[\hbar^2 \cdot \ell(\ell+1)\right] Y_{\ell,m_\ell}(\theta,\varphi)$$

$$\Rightarrow \; L = \sqrt{\ell(\ell+1)}\,\hbar$$

$$(L_z)_{op}\,\Phi(\varphi) = m_\ell \hbar\, \Phi(\varphi)$$

$$\Rightarrow \; L_z = m_\ell \hbar$$

$$\cos\theta = \frac{L_z}{L} = \frac{m_\ell}{\sqrt{\ell(\ell+1)}}$$

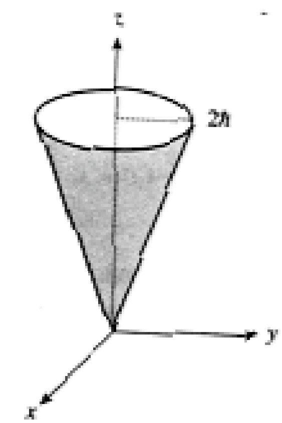

FIGURE 6.6 For $\ell = 2$, $m = 2$, L lies anywhere on the cone.

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Radial Solutions

- To find radial solutions:

$$-\frac{\hbar^2}{2\mu}\left\{\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)\right\} + [V(r)-E]r^2 = -\frac{1}{2\mu Y}\overbrace{[\hbar^2 l(l+1)]Y}^{L_{op}^2 Y}$$

$$\Rightarrow -\frac{\hbar^2}{2\mu}\left\{\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) - l(l+1)\right\} + V(r)r^2 = Er^2$$

  - This is called the ***radial equation***

Solving the radial equation

- Note:

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)=\frac{r}{R}\frac{\partial^2}{\partial r^2}(rR)$$

$$\Rightarrow -\frac{\hbar^2}{2\mu}\left\{\frac{r}{R}\frac{\partial^2}{\partial r^2}(rR)-\ell(\ell+1)\right\}+V(r)\,r^2=Er^2$$

- Let's introduce the auxiliary function:

$$u(r)=r\,R(r)$$

  - And plug it in above

$$\Rightarrow \quad -\frac{\hbar^2}{2\mu}\left(\frac{u}{R^2}\frac{\partial^2}{\partial r^2}(u) - \ell(\ell+1)\right) + V(r)\frac{u^2}{R^2} - E\frac{u^2}{R^2} = 0$$

Multiply by $\frac{R^2}{u}$

$$-\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial r^2}u - \ell(\ell+1)\underbrace{\frac{R^2}{u}}_{\frac{u}{r^2}}\right] + u(V-E) = 0$$

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

$$\Rightarrow \quad \frac{d^2}{dr^2}u + \frac{2\mu}{\hbar^2}\left[E - V(r) - \frac{\ell(\ell+1)}{r^2}\cdot\frac{\hbar^2}{2\mu}\right]u = 0$$

The Total Wavefunction

- The total wavefunction

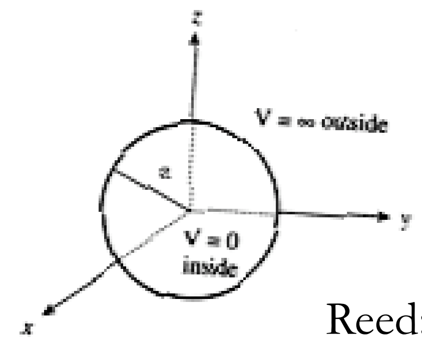
$$\psi_{n\ell m_\ell}(r,\theta,\varphi) = R_{n\ell}(r)\, Y_{\ell,m_\ell}(\theta,\varphi) = \frac{u_{n\ell}(r)}{r} Y_{\ell,m_\ell}(\theta,\varphi)$$

- 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 μ is trapped in a spherical region of space with radius a and an impenetrable barrier

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



Reed: Chapter 7

FIGURE 7.1 Infinite Spherical Well.

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

$$\ell = 0$$

- (Otherwise: $\ell \neq 0 \Rightarrow$ Bessel & Neumann functions)

So . $u(r) \Rightarrow u_0(r)$

$$\frac{d^2 u_0(r)}{dr^2} + k^2 u_0(r) = 0 \qquad \text{inside well.}$$

$$k^2 = \left[E - V(r) - \frac{\ell(\ell+1)}{r^2}\frac{\hbar^2}{2\mu}\right]\frac{2\mu}{\hbar^2}$$

$$= \frac{2\mu E}{\hbar^2} \qquad \text{since } V(r) = 0 \text{ inside and } \ell = 0$$

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

$$u_0(r) = A \sin kr + B \cos kr$$

Boundary Conditions

- Recall: $R = u/r$
- Boundary conditions should prevent divergence for R as r→0: Thus U=R*r =0 as r→0:

$$\Rightarrow u(r=0) = 0 \Rightarrow B = 0$$

- Boundary conditions also require that the barrier is impenetrable:

$$\Rightarrow u(r=a) = 0 \Rightarrow 0 = A\sin ka \Rightarrow ka = n\pi$$

- This gives us quantization of energy!

$$\Rightarrow E_n(\ell=0) = \frac{n^2\pi^2\hbar^2}{2\mu a^2}$$

Total Wavefunction

$$\psi_{n00}(r,\theta,\varphi) = R_n(r)\, Y_{0,0}(\theta,\varphi)$$
$$= \frac{A}{\sqrt{4\pi}\, r} \sin\left(\frac{n\pi r}{a}\right)$$

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

$$\int_0^a \int_0^\pi \int_0^{2\pi} \psi^* \psi \underbrace{r^2 \sin\theta \, d\varphi \, d\theta \, dr}_{d\,\text{Volume}} = 1$$

$$\int_0^a \int_0^\pi \int_0^{2\pi} \frac{A^2}{4\pi r^2} \sin^2\left(\frac{n\pi r}{a}\right) \cdot r^2 \sin\theta \, d\varphi \, d\theta \, dr = 1$$

$$\int_0^{2\pi} d\varphi = 2\pi, \quad \int_0^\pi \sin\theta \, d\theta = 2 \qquad \int_0^a \sin^2\left(\frac{n\pi r}{a}\right) dr = \frac{a}{2}$$

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

So,

$$\boxed{\psi_{n,0,0} = \frac{1}{\sqrt{2\pi a}\, r} \sin\left(\frac{n\pi r}{a}\right)}$$

Normalization: simpler approach

$\psi_{n00}(r,\theta,\varphi) = R_n(r) Y_{00}(\theta,\varphi)$

Because Y_{00} is already normalized, only $R_n(r)$ needs $\left(" \frac{1}{\sqrt{4\pi}} \right)$

to be normalized. In other words

$$1 = \int_0^a \int_0^\pi \int_0^{2\pi} |\psi_n|^2 r^2 \sin\theta \, d\varphi \, d\theta \, dr$$

$$= \int_0^a |R_n|^2 r^2 dr \underbrace{\int_0^\pi \int_0^{2\pi} |Y_{00}|^2 \sin\theta \, d\theta \, d\varphi}_{\underset{1}{\shortparallel}}$$

$$= \int_0^a \left(\frac{A}{r} \sin\left(\frac{n\pi}{a} r \right) \right)^2 r^2 dr$$

$$= A^2 \int_0^a \sin^2\left(\frac{n\pi}{a} r \right) dr = A^2 \cdot \frac{a}{2} \Rightarrow A = \sqrt{\frac{2}{a}}$$

Example: what is <r> for a particle in an infinite spherical well?

$$\langle r\rangle = \int_0^a\int_0^\pi\int_0^{2\pi}\left[\psi^*_{n00}\, r\, \psi_{n00}\right] r^2\sin\theta\, d\varphi\, d\theta\, dr$$

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

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

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

$$= \frac{2}{a}\cdot\frac{a^2}{4} = \frac{a}{2}$$

$$\langle r\rangle = \frac{a}{2}$$

<r> is independent of n!

Increasing the energy of the particle changes the probability distribution but not it's 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

$$V(r) = \begin{cases} V_0 & r \geq a \\ 0 & r < a \end{cases}$$

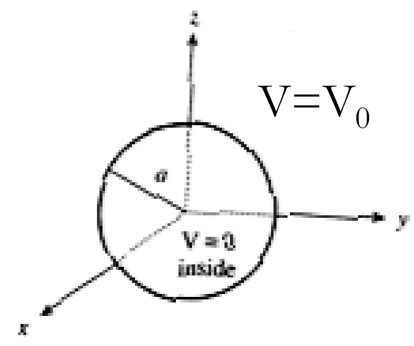


FIGURE 7.1 Infinite Spherical Well.

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- 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 $r < a$ $E > V(r) \Rightarrow E > 0$

$$\frac{d^2 u_0^{in}}{dr^2} + k_1^2 u_0^{in} = 0 \qquad k_1^2 = \frac{2\mu E}{\hbar^2}$$

Just like infinite spherical well

$$R_0^{inside}(r) = \frac{A}{r}\sin k_1 r \qquad r<a$$

- Outside the well $r \geq a$ $E < V_0$

$$\frac{d^2 u_0^{out}}{dr^2} = k_2^2 u_0^{out} \qquad k_2^2 = \frac{2\mu}{\hbar^2}(V_0 - E)$$

$$u_0^{out}(r) = C e^{k_2 r} + D e^{-k_2 r}$$

$$\Rightarrow R_0^{out}(r) = \frac{Ce^{k_2 r}}{r} + \frac{De^{-k_2 r}}{r}$$

Boundary conditions outside the well

- Boundary condition at $r \to \infty$, $U(r) \to 0$

$\Rightarrow C = 0$

$$R_0^{out}(r) = \frac{De^{-k_2 r}}{r}$$

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

$$A \sin k_1 a = De^{-k_2 a}$$

$$-\frac{A \sin k_1 a}{a^2} + \frac{A k_1 \cos k_1 a}{a} = \frac{-Dk_2 e^{-k_2 a}}{a} - \frac{De^{-k_2 a}}{a^2}$$

$$\Rightarrow A\left[k_1 a \cos k_1 a - \sin k_1 a\right] = -De^{-k_2 a}(ak_2 + 1)$$

- Divide the two equations:

$$k_1 a \cot k_1 a - 1 = -(a\kappa_2 + 1)$$

$$k_1 a \cot k_1 a = -a\kappa_2$$

- Define:

$$\xi = k_1 a \quad , \quad \eta = \kappa_2 a \qquad\qquad \xi \cot \xi = -\eta$$

This is a transcendental equation!

$$\xi^2 + \eta^2 = a^2 (k_1^2 + \kappa_2^2) = a^2 \left[\frac{2\mu E}{\hbar^2} + \frac{2\mu}{\hbar^2}(V_0 - E) \right]$$

$$= a^2 \cdot \frac{2\mu V_0}{\hbar^2} = \text{const} = \rho^2$$

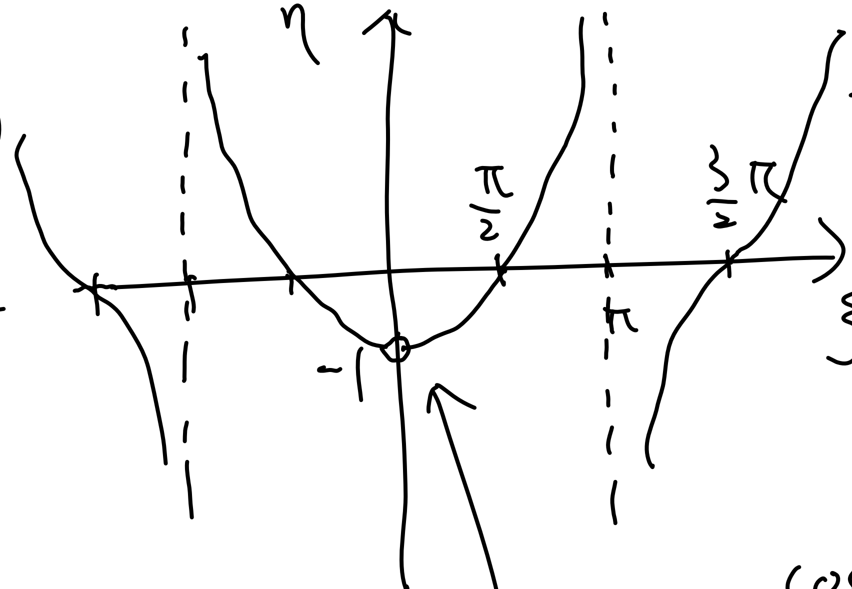
ρ^2 is the strength parameter

Sketch functions

$$\eta = \underbrace{-\xi \; \cot\xi}_{\text{even}}$$

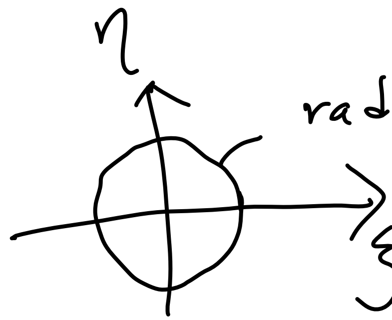
odd odd

$$\cot\frac{\pi}{2} = \frac{\cos\frac{\pi}{2}}{\sin\frac{\pi}{2}} = \frac{0}{1} = 0$$



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

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



radius ρ

Energy Eigenvalues

- This is an equation that describes a circle of radius ρ in the (ξ,η) plane.

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

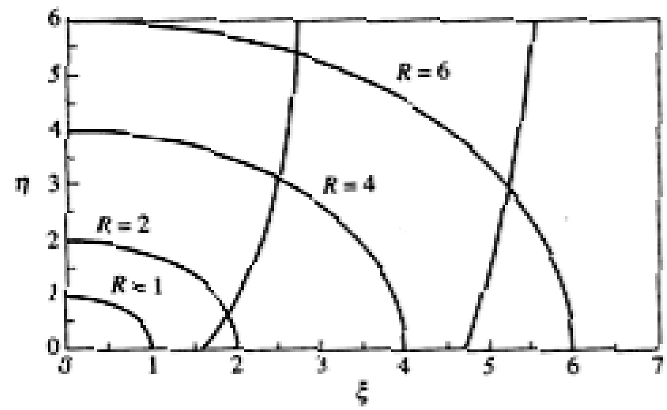


FIGURE 7.2 Illustration of the Solution for Energy Eigenvalues for a Finite Spherical Well.

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- 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:

$$\cot \xi = 0$$

$$(2n-1)\frac{\pi}{2}, \quad n = 1, 2, 3, \ldots$$

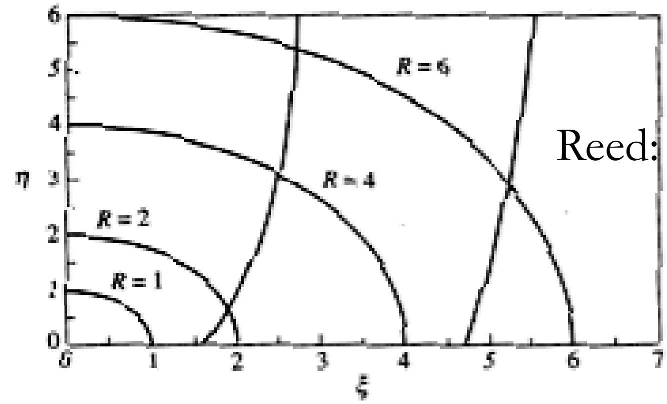

FIGURE 7.2 Illustration of the Solution for Energy Eigenvalues for a Finite Spherical Well.

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Note ρ=1 has no bound states!

- For a spherical well to possess n bound states it must have:

$$\rho \geq (2n-1)\frac{\pi}{2}$$

$$\xi^2 + \eta^2 = a^2(k_1^2 + \kappa_2^2) = a^2\left[\frac{2\mu E}{\hbar^2} + \frac{2\mu}{\hbar^2}(V_0 - E)\right]$$

$$= a^2 \cdot \frac{2\mu V_0}{\hbar^2} = \text{const} \equiv \rho^2$$

- Or …

$$\rho^2 \geq (2n-1)^2\frac{\pi^2}{4} \Rightarrow V_0 a^2 \geq \frac{(2n-1)^2\pi^2\hbar^2}{8\mu}$$

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.

$$(2n-1)^2 \le \frac{8\mu a^2 V_0}{\hbar^2 \pi^2}$$

$$(2n-1)^2 \le \frac{8(6.646\times10^{-27}\,\text{kg})(10^{-14}\,\text{m})^2 \overbrace{(8.0\times10^{-12}\,\text{J})}^{50\,\text{MeV}\times\frac{1.6\times10^{-19}\,\text{J}}{\text{eV}}}}{(1.055\times10^{-34}\,\text{J}\cdot\text{s})^2\,\pi^2}$$

$$(2n-1)^2 \le 387$$

$$n \le 10.3$$

- What is the energy of the lowest energy bound state for this system?

$$\xi^2 + \eta^2 = \frac{2\mu a_0^2 V_0}{\hbar^2} = 955$$

$$\xi \cot \xi = -\eta$$

$$\xi \cot \xi + \sqrt{955 - \xi^2} = 0$$

Minimize $\quad \xi = 3.04305$

$$E = \frac{k_1^2 \hbar^2}{2\mu} = \frac{\xi^2}{a^2} \frac{\hbar^2}{2\mu} = \frac{(3.04305)^2 (1.055 \times 10^{-34}\ J)^2}{(10^{-14} m)^2 \cdot 2 \cdot (6.646 \times 10^{-27} kg)}$$

$$= 7.75 \times 10^{-14}\ J \approx \underline{0.48 MeV}$$

Summary/Announcements

- Next time: The Coulomb Potential of the Hydrogen atom