Lecture 29:
Motion in a Central Potential

Phy851 Fall 2009

Side Remarks

- Counting quantum numbers:
  - 3N quantum numbers to specify a basis state for N particles in 3-dimensions
      - It will go up to 5N when we include spin
  - When does it work:
    - All of the standard basis choices
      - Position eigenstates, Momentum eigenstates, angular momentum eigenstates, …
    - Any basis formed from energy eigenstates of an analytically solvable system:
      - Harmonic oscillator states, hydrogen orbitals, ...
      - These problems are solvable due to a high degree of symmetry
    - Any basis formed from eigenstates of an exactly solvable system plus a weak symmetry breaking perturbation
      - We can watch the levels evolve as we increase the perturbation strength, and therefore keep track of the quantum numbers
  - When it does not work
    - Strongly interacting systems with minimal symmetry
      - These are problems that you could only solve numerically, they won't be encountered in class or in textbooks

` And’ versus ‘or’ paradigm

$$I = I^{(C)} \otimes I^{(R)}$$

$$I^{(R)} = I^{(R)}_{bound} + I^{(R)}_{continuum}$$

- Hilbert subspace Hierarchy:

$$\mathcal{H}$$

$$\mathcal{H}^{(C)}, \mathcal{H}^{(R)}$$

$$\mathcal{H}^{(R)}_{bound}, \mathcal{H}^{(R)}_{continuum}$$

  - To specify the state of the full system, we **must** specify a state in $\mathcal{H}^{(R)}$ **AND** a state in $\mathcal{H}^{(C)}$

  - To specify the state of the relative motion we **may** specify a state entirely in $\mathcal{H}^{(R)}_{bound}$ **OR** a state entirely in $\mathcal{H}^{(R)}_{continuum}$ **OR** a state partially in both

Review of Separation of Variables and Angular Momentum

$$H = H_{CM} + H_r$$

$$\left|E\right\rangle = \left|E_{CM}\right\rangle^{(C)} \otimes \left|E_r\right\rangle^{(R)}$$

$$E = E_{CM} + E_r$$

- The center-of-mass motion is that of a free particle
- We thus only need to determine to state of relative motion:

$$H_r = \frac{P_r^2}{2\mu} + \frac{L^2}{2\mu R^2} + V(R)$$

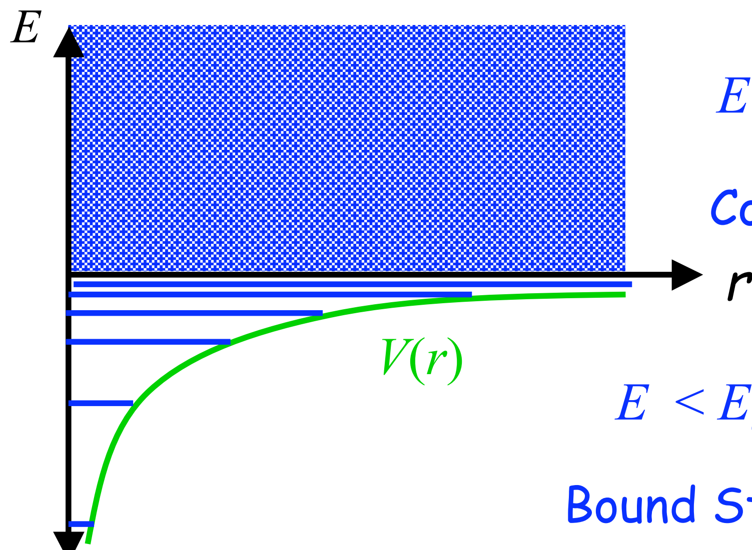
- As long as V depends only r and not on θ, ϕ then simultaneous eigenstates of H_r , L^2 and L_z exist:

$$[L^2, R] = 0 \qquad [L^2, P_r] = 0$$

$$[L_z, R] = 0 \qquad [L_z, P_r] = 0$$

Simultaneous Eigenstates of Energy and Angular Momentum

The spectrum of H_r typically has bound-states and continuum states



$E > E_c$:

Continuum

$E < E_c$:

Bound States

- Bound state basis:

$$\{|n,\ell,m\rangle\}: \qquad |n,\ell,m\rangle = |n,\ell\rangle^{(r)} \otimes |\ell,m\rangle^{(\Omega)}$$

$$H|n,\ell,m\rangle = E_n|n,\ell,m\rangle$$

$$L^2|n,\ell,m\rangle = \hbar^2\ell(\ell+1)|n,\ell,m\rangle$$

$$L_z|n,\ell,m\rangle = \hbar m|n,\ell,m\rangle$$

The energy levels and radial wavefunctions can be found via the series solution method

- Continuum basis:

$$\{|k,\ell,m\rangle\}: \qquad |k,\ell,m\rangle = |k,\ell\rangle^{(r)} \otimes |\ell,m\rangle^{(\Omega)}$$

$$H|k,\ell,m\rangle = E(k)|k,\ell,m\rangle$$

$$L^2|k,\ell,m\rangle = \hbar^2\ell(\ell+1)|k,\ell,m\rangle$$

$$L_z|k,\ell,m\rangle = \hbar m|k,\ell,m\rangle$$

Derivation of Radial Wave Equation

- We start from the energy eigenvalue equation:

$$E_n \left| n, \ell, m \right\rangle = H_r \left| n, \ell, m \right\rangle$$

- Hit with $\{ |r\ell m\rangle \}$ basis state from left:

$$R \left| r, \ell, m \right\rangle = r \left| r, \ell, m \right\rangle$$

$$E_n \left\langle r, \ell, m \middle| n, \ell, m \right\rangle = \left\langle r, \ell, m \middle| H_r \middle| n, \ell, m \right\rangle$$

- Define the radial wavefunction:

$$\psi_{n,\ell}(r) = \left\langle r, \ell, m \middle| n, \ell, m \right\rangle$$

$$\left\langle r, \theta, \phi \middle| n, \ell, m \right\rangle = \psi_{n,\ell}(r) Y_\ell^m(\theta, \phi)$$

$$E_n \psi_{n,\ell}(r) = \left\langle r, \ell, m \right| \frac{P_r^2}{2\mu} \left| n, \ell, m \right\rangle + \frac{1}{2\mu} \left\langle r, \ell, m \right| \frac{L^2}{R^2} \left| n, \ell, m \right\rangle + \left\langle r, \ell, m \middle| V(R) \middle| n, \ell, m \right\rangle$$

$$E_n \psi_{n,\ell}(r) = \left(-\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} + V(r) \right) \psi_{n,\ell}(r)$$

Solving the Radial Wave eq.

$$E_{n,\ell}\psi_{n,\ell}(r)=\left(-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)+\frac{\hbar^2\ell(\ell+1)}{2\mu r^2}+V(r)\right)\psi_{n,\ell}(r)$$

- Let: $\psi_{n,\ell}(r)=\frac{1}{r}R_{n,\ell}(r)$

$$\psi'_{n,\ell}(r)=\frac{1}{r}R'_{n,\ell}(r)-\frac{1}{r^2}R_{n,\ell}(r)$$

$$\psi''_{n,\ell}(r)=\frac{1}{r}R''_{n,\ell}(r)-\frac{2}{r^2}R'_{n,\ell}(r)+\frac{2}{r^3}R_{n,\ell}(r)$$

$$\begin{aligned}\psi''_{n,\ell}(r)+\frac{2}{r}\psi'_{n,\ell}(r)&=\frac{1}{r}R''_{n,\ell}(r)-\frac{2}{r^2}R'_{n,\ell}(r)+\frac{2}{r^3}R_{n,\ell}(r)\\&\quad+\frac{2}{r^2}R'_{n,\ell}(r)-\frac{2}{r^3}R_{n,\ell}(r)\\&=\frac{1}{r}R''_{n,\ell}(r)\end{aligned}$$

$$E_{n,\ell}R_{n,\ell}(r)=\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2}+\frac{\hbar^2\ell(\ell+1)}{2\mu\, r^2}+V(r)\right)R_{n,\ell}(r)$$

Effective 1-D motion

$$E_{n,\ell}R_{n,\ell}(r) = -\left(\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2} + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} + V(r)\right)R_{n,\ell}(r)$$

- The wavefunction, $R_{n,\ell}(r)$, is that of a particle of mass μ in one dimension, subject to the effective potential:

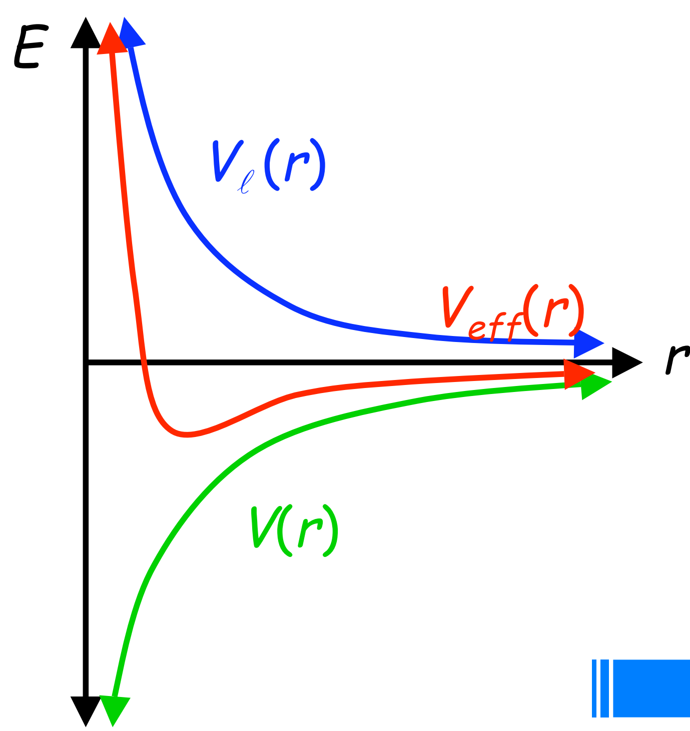
$$V_{eff}(r) = \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} + V(r)$$

- For $\ell \neq 0$, angular momentum creates as a repulsive effective potential

- Example:

$$V(r) = -\frac{a}{r}$$

$$V_{eff}(r) = \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} - \frac{a}{r}$$



Example 1 : Spherically symmetric Harmonic Oscillator

- Let:

$$V(r) = \frac{1}{2}\mu\omega^2 r^2$$

$$E_{n,\ell} R_{n,\ell}(r) = \left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2} + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} + \frac{1}{2}\mu\omega^2 r^2 \right) R_{n,\ell}(r)$$

- Switch to dimensionless variables:

$$r = \lambda\rho$$

$$R_{n,\ell}(\lambda\rho) = u(\rho) \qquad \lambda = \sqrt{\frac{\hbar}{\mu\omega}}$$

$$E_n = \hbar\omega\varepsilon_n$$

$$\hbar\omega\varepsilon_n u(\rho) = \left(-\frac{\hbar^2}{2\mu\lambda^2}\frac{\partial^2}{\partial\rho^2} + \frac{\hbar^2 \ell(\ell+1)}{2\mu\lambda^2\rho^2} + \frac{1}{2}\mu\omega^2\lambda^2\rho^2 \right) u(\rho)$$

- Dropping common factors gives:

$$0 = -\frac{1}{2}u'' + \left(\frac{\ell(\ell+1)}{2\rho^2} + \frac{1}{2}\rho^2 - \varepsilon_n \right) u$$

How to solve the differential equation

$$u'' + \left(-\frac{\ell(\ell+1)}{\rho^2} - \rho^2 + 2\varepsilon_n \right) u = 0$$

- From 'Handbook of Mathematical Functions', p. 781:
    - Authors: Abramowitz and Stegun
    - No copyright, full text free online
  - If: $$y'' + \left(4n_r + 2\alpha + 2 - x^2 + \frac{1 - 4\alpha^2}{4x^2} \right) y = 0$$
  - Then solution is:

$$y(x) = Ne^{-\frac{x^2}{2}} x^{\alpha + \frac{1}{2}} L_{n_r}^{(\alpha)}(x^2)$$

Generalized Laguerre Polynomial

- Physicists never solve differential equations by hand

- Let:

$$\frac{1 - 4\alpha^2}{4} = -\ell(\ell+1)$$

$$\alpha^2 = \ell^2 + \ell + \frac{1}{4}$$

$$\alpha = \ell + \frac{1}{2}$$

$$4n_r + 2\alpha + 2 = 2\varepsilon_n$$

$$\varepsilon_n = 2n_r + \alpha + 1$$

$$\varepsilon_n = 2n_r + \ell + \frac{3}{2}$$

Full Solution to spherical harmonic oscillator

$$\varepsilon_n = 2n_r + \ell + \frac{3}{2} \qquad n_r = 0,1,2,3,\ldots$$

- n_r is the number of nodes in the radial wavefunction
  - Note that $2n_r + \ell$ is always an integer
- We can define the *principle quantum number:*

$$n = 2n_r + \ell \qquad n = 0,1,2,\ldots$$

$$\varepsilon_n = n + \frac{3}{2}$$

  - Solution is then: $u(\rho) = Ne^{-\frac{\rho^2}{2}}\rho^{\ell+1}L_{\frac{n-\ell}{2}}^{(\ell+\frac{1}{2})}(\rho^2)$

- In original Units we have:

$$E_n = \hbar\omega\left(n + \frac{3}{2}\right)$$

$$\psi_{n,\ell,m}(r,\theta,\phi) = \sqrt{\frac{n!}{\Gamma(n+\ell+3/2)}}\, e^{-\frac{r^2}{2\lambda^2}}\frac{r^\ell}{\lambda^{\ell+1}}L_{\frac{n-\ell}{2}}^{(\ell+1/2)}\left(\frac{r^2}{\lambda^2}\right)Y_\ell^m(\theta,\phi)$$

Degeneracy of n[th] level

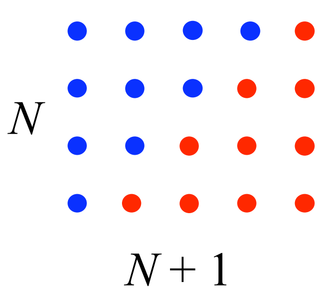
$$n = 2n_r + \ell \qquad \begin{cases} n_r = 0,1,2,3,\ldots \\ \ell = 0,1,2,3,\ldots \end{cases}$$

- Case I: n is even:
  - ℓ must then be even also: $\ell = 2k$
  - $\ell_{\max} = n$: $k_{\max} = \frac{n}{2}$
  - Degeneracy factor:

$$d_\ell = \sum_{m=-\ell}^{\ell} 1 = 2\ell + 1$$

$$d_n = \sum_{k=0}^{n/2} d_k = \sum_{k=0}^{n/2} (4k+1) = 4\sum_{k=1}^{n/2} k + \left(\frac{n}{2}+1\right)$$

$$\sum_{k=1}^{N} k = \frac{1}{2} N(N+1)$$



$$d_n = 4\frac{1}{2}\frac{n}{2}\left(\frac{n}{2}+1\right) + \left(\frac{n}{2}+1\right)$$

$$= (n+1)\left(\frac{n}{2}+1\right)$$

$$d_n = \frac{1}{2}\left(n^2 + 3n + 2\right)$$

Degeneracy Continued…

- Case II: n is odd:
  - ℓ is odd: $\ell = 2k+1$
  - $\ell \le n$: $k_{\max} = \dfrac{n-1}{2}$

$$d_k = (2\ell+1) = 2(2k+1)+1 = 4k+3$$

$$d_n = \sum_{k=0}^{(n-1)/2} d_k = \sum_{k=0}^{(n-1)/2}(4k+3) = 4\sum_{k=1}^{(n-1)/2} k + 3\left(\frac{n-1}{2}+1\right)$$

$$= 4\,\frac{1}{2}\,\frac{n-1}{2}\left(\frac{n-1}{2}+1\right) + 3\left(\frac{n-1}{2}+1\right)$$

$$= (n+2)\left(n+\frac{1}{2}\right)$$

$$d_n = \frac{1}{2}\left(n^2+3n+2\right)$$

- Result is same for odd or even n*!*

Summary

- For Spherically Symmetric Harmonic Oscillator, we have:

$$V(r) = \frac{1}{2} m\omega^2 r^2$$

$$E_n = \hbar\omega\left(n + \frac{3}{2}\right) \qquad n = 0,1,2,\ldots$$

$$d_n = \frac{1}{2}\left(n^2 + 3n + 2\right)$$

$$\psi_{n,\ell,m}(r,\theta,\phi) = \sqrt{\frac{n!}{\Gamma(n+\ell+3/2)}}\, e^{-\frac{r^2}{2\lambda^2}} \frac{r^\ell}{\lambda^{\ell+1}} L_{\frac{n-\ell}{2}}^{(\ell+1/2)}\left(\frac{r^2}{\lambda^2}\right) Y_\ell^m(\theta,\phi)$$

$$\lambda = \sqrt{\frac{\hbar}{m\omega}} \qquad \begin{array}{l} n = 2n_r + \ell \\ n_r, \ell = 0,1,2,\ldots,\infty \end{array} \qquad n \text{ fixed} \rightarrow \begin{cases} n_r = 0,1,2,\ldots,\frac{n}{2} \\ \ell = 0,1,2,\ldots,n \end{cases}$$

n	d_n	
0	1	$n_r=0,\ \ell=0,\ m=0$
1	3	$n_r=0,\ \ell=1,\ m=-1,0,1$
2	6	$n_r=1,\ \ell=0,\ m=0$; $n_r=0,\ \ell=2,\ m=-2,-1,0,1,2$
3	10	$n_r=1,\ \ell=1,\ m=-1,0,1$; $n_r=0,\ \ell=3,\ m=-3,-2,-1,0,1,2,3$
…	…	…