## <u>Today</u>

- I. Last Time
- II. Harmonic Oscillator Wave Functions
- III. Power Series Method for Hydrogen
- I. Last time

\*Analytical method for solving Sch. Equation in the harmonic oscillator. Based on using an infinite power series to solve the differential equation. Steps: 0. Try to adopt variables that make the equation as simple as possible. Key is to look for dimensionless combinations of the parameters in the problem.

- 1. Find limiting (asymptotic) behavior of solutions (e.g. as  $x \to \pm \infty$ ).
- 2. Peel off this limit behavior and look for a power series that solves the remaining differential equation:  $u(\rho) = \sum c_j \rho^j$ .
- 3. Find a recursion relationship on the  $c_j$  and require that it truncates at some point if the sum wouldn't otherwise converge.

I. The 'Old' Quantum Theory of Hydrogen (The Bohr Model)

The classical mechanics gave us:  

$$E = \left(-\frac{L^2}{2mr^2}\right) = -\frac{1}{2}\frac{k_e e^2}{r}.$$
Bohr quantization:  $L_n = n\hbar$ ,  $E_n = -\left[\frac{m_e}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2}$ 

$$\frac{k_e e^2}{r_n} = \frac{(n\hbar)^2}{mr_n^2}.$$

Solve this for the radius to find  $r_n = \left(\frac{\hbar^2}{k_e e^2 m}\right) n^2 = an^2$ ,

where *a* is the Bohr radius and has the value  $0.529*10^{(-10)}$  m. This also leads to

$$E_n = \left(-\frac{1}{2}\frac{k_e e^2}{r_n}\right) = -E_g \frac{1}{n^2}$$
, where  $E_g = \frac{1}{2}\frac{k_e e^2}{a} = 13.6$ eV.

I. The 'Old' Quantum Theory of Hydrogen (The Bohr Model)

In quantum theory the energy eigenstates are stationary states and the Hydrogen atom is not accelerated in the classical sense. This is what allows the atom to be stable and not radiate.

On the other hand, if we add energy into the system we can excite the electron to a higher energy state and it can radiatively decay to lower energy states.

$$E_{\gamma} = h\nu = |E_{n_i} - E_{n_f}|$$





I. Intuition for making sketches and the power series method



When we find the asymptotic form for the solution to a differential equation, we're doing the same thing of filling in the boundaries that we need to interpolate between. This

## I. Our Result for the Radial Equation

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + V_{\text{eff}}u = Eu, \text{ where } V_{\text{eff}}(r) = V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}$$

Let's consider a particular potential, just to get a feel for what this looks like. The hydrogen atom potential is

$$V(r) = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{r} = -\frac{k_e e^2}{r},$$
  
then the effective potential is  
$$V_{\text{eff}} = -\frac{k_e e^2}{r} + \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2}.$$



Here little *u*,

u(r) = rR(r).

II. Series Method for Hydrogen atom Let's introduce a wave number for bound states

$$k = \frac{\sqrt{-2m_eE}}{\hbar}.$$

Plugging this in we find

$$\frac{1}{k^2}\frac{d^2u}{dr^2} = \left[1 - \frac{m_e e^2}{2\pi\epsilon_0 \hbar^2 k}\frac{1}{(kr)} + \frac{\ell(\ell+1)}{(kr)^2}\right]u,$$

Let's introduce nice variables

$$\rho = kr \quad \text{and} \quad \rho_0 = \frac{m_e e^2}{2\pi\epsilon_0 \hbar^2 k}.$$

Then we have the clean form  $\frac{d^2u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{\ell(\ell+1)}{\rho^2}\right]u.$ 



Let's look for the asymptotic behavior of this equation, let's take up the case  $\rho \rightarrow \infty$ ...

II. Series Method for Hydrogen atom

Then we have the clean form

$$\frac{d^2u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{\ell(\ell+1)}{\rho^2}\right]u.$$



Let's look for the asymptotic behavior of this equation, i.e.  $\sigma$  the case  $\rho \to \infty$  where

 $\frac{d^2u}{do^2} = u,$ 

and the solutions are just

 $u(\rho) = Ae^{-\rho} + Be^{\rho}.$ 

There's no way that the second term is normalizable, so we only keep

 $u(\rho) \sim A e^{-\rho}.$ 

The other asymptotic regime is  $\rho \to 0$ , where  $\frac{d^2 u}{d\rho^2} = \frac{\ell(\ell+1)}{\rho^2} u, \text{ with solution } u(\rho) = C\rho^{\ell+1} + D\rho^{-\ell} \text{ (check it)}.$ 

II. Series Method for Hydrogen atom

Then we have the clean form

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 $u(\rho) \sim A e^{-\rho}.$ 

The other asymptotic regime is  $\rho \to 0$ , where  $\frac{d^2u}{d\rho^2} = \frac{\ell(\ell+1)}{\rho^2}u, \text{ with solution } u(\rho) = C\rho^{\ell+1} + D\rho^{-\ell} \text{ (check it)}. \text{ The}$ normalizable one is  $u \sim C\rho^{\ell+1}$ . Then our full ansatz for the power series method is going to be  $u(\rho) = \rho^{\ell+1}e^{-\rho}v(\rho).$  Putting this in the resulting differential equation is

$$\rho \frac{d^2 v}{d\rho^2} + 2(\ell + 1 - \rho) \frac{dv}{d\rho} + [\rho_0 - 2(\ell + 1)]v = 0$$

II. Series Method for Hydrogen atom

Starting with

$$\rho \frac{d^2 v}{d\rho^2} + 2(\ell + 1 - \rho) \frac{dv}{d\rho} + [\rho_0 - 2(\ell + 1)]v = 0,$$

we now guess a solution of the form

$$v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j.$$

Now we grind

$$\frac{dv}{d\rho} = \sum_{j=0}^{\infty} jc_j \rho^{j-1} = \sum_{j=0}^{\infty} (j+1)c_{j+1}\rho^j$$

And for the second derivative

$$\frac{d^2 v}{d\rho^2} = \sum_{j=0}^{\infty} j(j+1)c_{j+1}\rho^{j-1}$$

