Today

I. Last Time

II. Finish Power Series Method for Hydrogen

III. Saiqi's Guest Lecture on Spin

I. Last time

*Intro'd a power series solution to try and solve the Hydrogen atom radial wave function: part of that was $v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j$. (Recall v followed on from $u = rR(r)$.)

*The power series v came from stripping off the asymptotic behavior of $u = \rho^{\ell+1} e^{-\rho} v(\rho)$, where $\rho = kr$.

I. Our Result for the Radial Equation

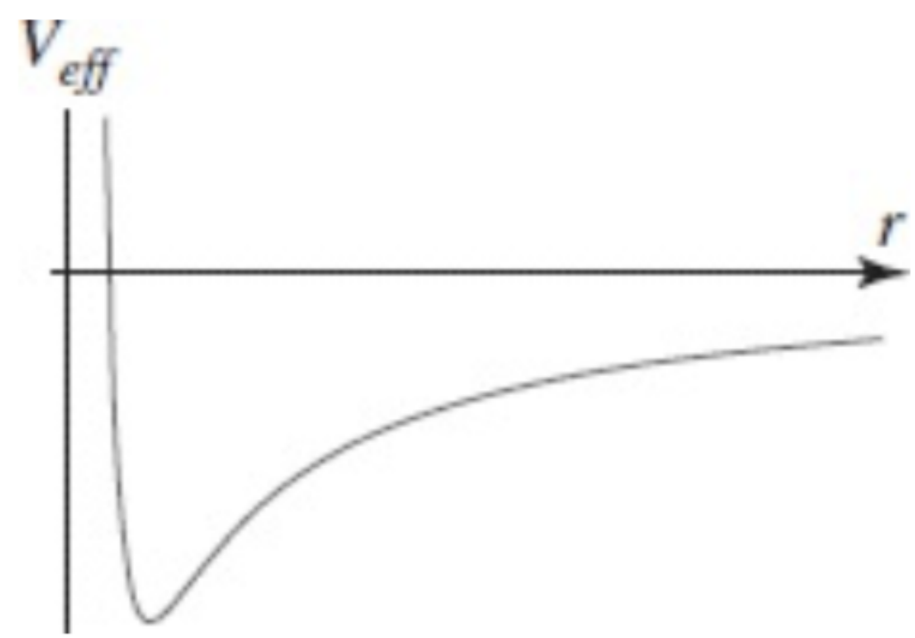
$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + V_{\text{eff}}u = Eu, \quad \text{where} \quad V_{\text{eff}}(r) = V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}$$

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,

$u(r) = rR(r)$.

I. Series Method for Hydrogen atom

Let's introduce a wave number for bound states

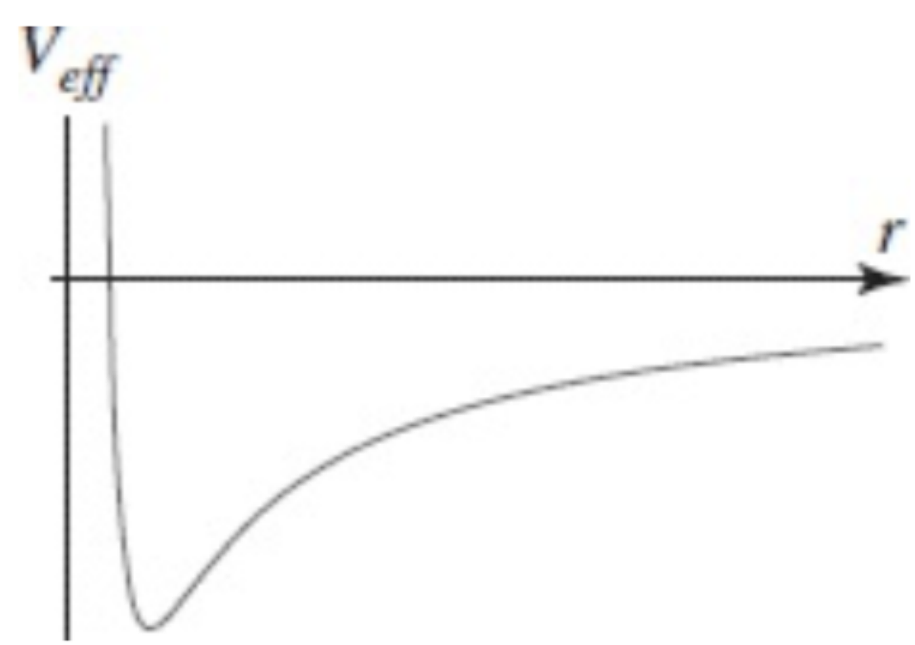
$$k = \frac{\sqrt{-2m_e E}}{\hbar}.$$

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

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

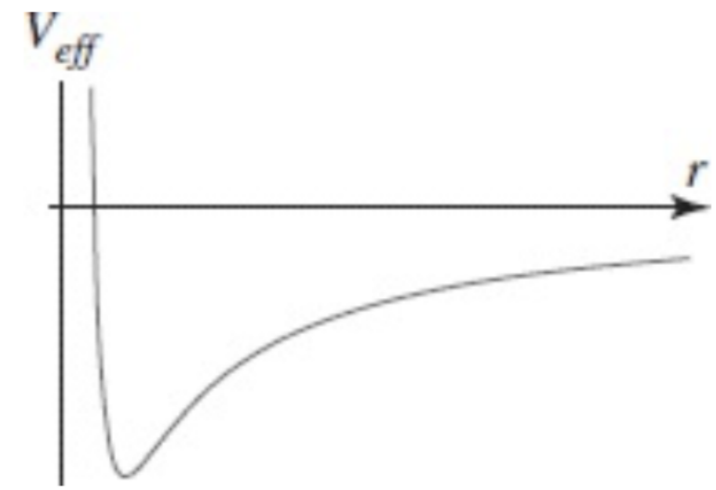


Then we have the clean form

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

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

I. 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, let's take up the case $\rho \to \infty$ where

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

and the solutions are just

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

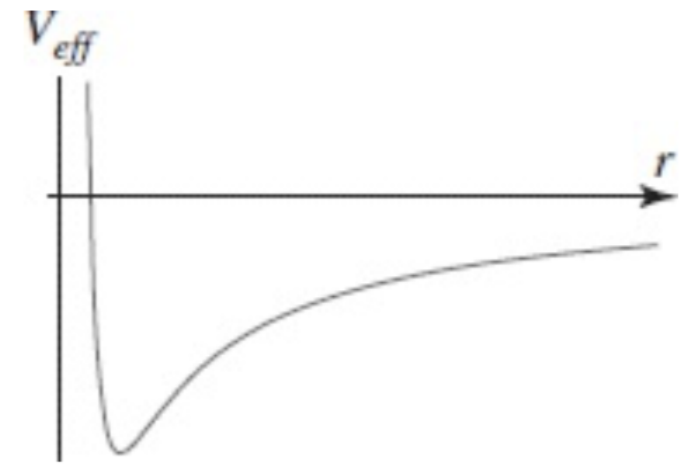
There's no way that the second term is normalizable, so we only keep

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

The other asymptotic regime is $\rho \to 0$, where

$$\frac{d^2u}{d\rho^2} = \frac{\ell(\ell+1)}{\rho^2}u,$$ with solution $u(\rho) = C\rho^{\ell+1} + D\rho^{-\ell}$ (check it).

I. Series Method for Hydrogen atom



Then we have the clean form

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

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

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

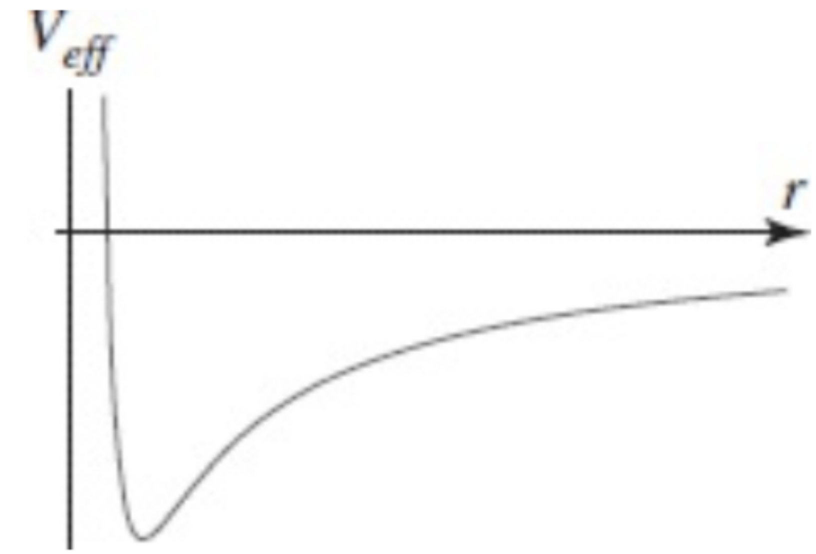
The other asymptotic regime is $\rho \to 0$, where

$\frac{d^2u}{d\rho^2} = \frac{\ell(\ell+1)}{\rho^2}u$, with solution $u(\rho) = C\rho^{\ell+1} + D\rho^{-\ell}$ (check it). 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

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

I. 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

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

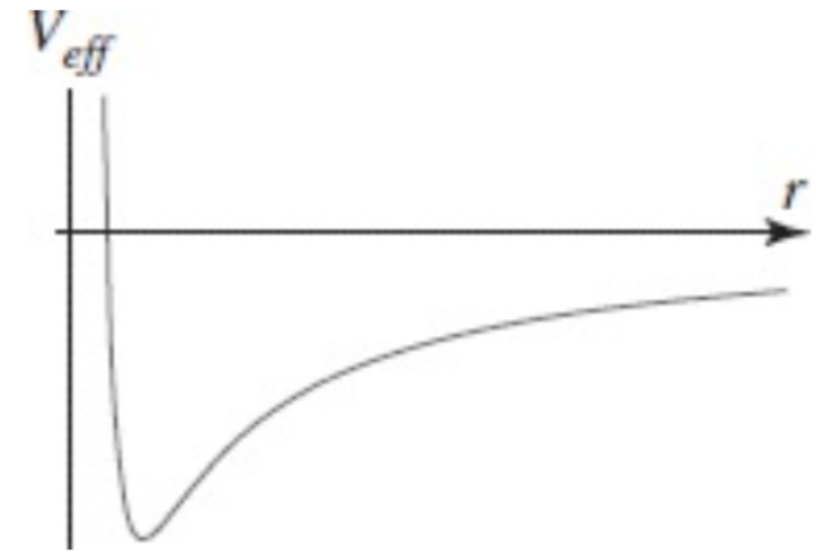
Now we grind

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

And for the second derivative

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

I. 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

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

And for the second derivative

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

$$\sum_{j=0}^{\infty} \left[j(j+1)c_{j+1}\rho^j + 2(\ell+1)j(j+1)c_{j+1}\rho^j - 2jc_j\rho^j + (\rho_0 - 2(\ell+1))c_j\rho^j \right] = 0$$

I. Series Method for Hydrogen atom

$$\sum_{j=0}^{\infty}\left[j(j+1)c_{j+1}\rho^j + 2(\ell+1)j(j+1)c_{j+1}\rho^j - 2jc_j\rho^j + (\rho_0 - 2(\ell+1))c_j\rho^j\right] = 0$$

Setting the coefficients of every term equal to zero we learn that

$$\left[j(j+1)c_{j+1} + 2(\ell+1)j(j+1)c_{j+1} - 2jc_j + (\rho_0 - 2(\ell+1))c_j\right] = 0.$$

This gives the recursion relation:

$$c_{j+1} = \frac{2(j+\ell+1)-\rho_0}{(j+1)(j+2\ell+2)}c_j.$$

Let's imagine for a moment that this recursion never ends, then for large j, we can approximate it in a simpler form:

$$c_{j+1} = \frac{2j}{j(j+1)}c_j = \frac{2}{j+1}c_j.$$

This new recursion and it has an approximate solution

$$c_j \approx \frac{2^j}{j!}c_0, \text{ which implies } v(\rho) \approx c_0\sum_{j=0}^{\infty}\frac{2^j}{j!}\rho^j = c_0e^{2\rho}; \text{ nota bene(!!!)...}$$

II. Series Method for Hydrogen atom

This new recursion and it has an approximate solution

$c_j \approx \frac{2^j}{j!} c_0$, which implies $v(\rho) \approx c_0 \sum_{j=0}^{\infty} \frac{2^j}{j!} \rho^j = c_0 e^{2\rho}$; nota bene(!!!)…

…this is a bad solution! It doesn't meet our boundary conditions, in particular, we can't normalize it. This means that we can't allow the recursion to continue to large j. So, instead we force it to end:

$c_{j+1} = \frac{2(j+\ell+1)-\rho_0}{(j+1)(j+2\ell+2)} c_j$ implies that the numerator should vanish for some value of j, which we will call N. Then

$2(N+\ell)-\rho_0 = 0$, then with $n \equiv N+\ell$, we get $\rho_0 = 2n$. We now have that

$$E = -\frac{\hbar^2 k^2}{2m} = -\frac{m_e e^4}{8\pi^2 \epsilon_0^2 \hbar^2 \rho_0^2} \implies E_n = -\left[\frac{m_e}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} = \frac{E_1}{n^2}$$

II. Series Method for Hydrogen atom

Then the total wave function is

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)Y_\ell^m(\theta,\phi),$$

Where

$$R_{n\ell}(r) = \frac{1}{r}\rho^{\ell+1}e^{-\rho}v(\rho),$$

Where $v(\rho)$ is determined by

$$c_{j+1} = \frac{2(j+\ell+1-n)}{(j+1)(j+2\ell+2)}c_j\,.$$

Also $\rho \equiv \dfrac{r}{an}$.