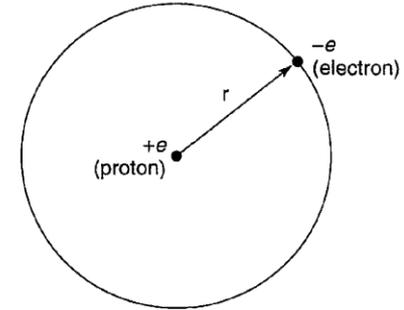


4.2: The Hydrogen Atom

Consider an electron orbiting a proton fixed at the origin of coordinates. The potential is (ϵ_0 = vacuum permittivity):

$$V(r) = -\frac{e^2}{4\pi\epsilon_0} \frac{1}{r}$$



The radial equation for "u(r)" (recall $R(r) = u(r)/r$) becomes:

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + \left[-\frac{e^2}{4\pi\epsilon_0} \frac{1}{r} + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} \right] u = E u$$

The **exact** solution of the Hydrogen atom potential is important because it influences on the understanding of **all atoms**.

We will focus on **bound states** i.e. $E < 0$ (there are also scattering states).

Thus, the combination used many times becomes:

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}$$

$$1/\kappa^2 = -\hbar^2/2mE$$

If you divide all by E , and move the effective potential to the right, you get:

$$\frac{1}{\kappa^2} \frac{d^2 u}{dr^2} = \left[1 - \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa} \frac{1}{(\kappa r)} + \frac{l(l+1)}{(\kappa r)^2} \right] u$$

This suggests $\rho \equiv \kappa r$ may be useful,
(dimensionless) and also

$$\rho_0 \equiv \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa}$$

The exact radial equation then becomes "simple":

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

As done for the "second" solution of the 1D harmonic oscillator (that led to the Hermite polynomials), we will study special cases expecting to simplify the problem:

Consider ρ large: $\frac{d^2 u}{d\rho^2} = u \quad \longrightarrow \quad u(\rho) \sim Ae^{-\rho}$

Unphysical diverging solutions discarded.

Consider ρ small: $\frac{d^2 u}{d\rho^2} = \frac{l(l+1)}{\rho^2} u \quad \longrightarrow \quad u(\rho) \sim C\rho^{l+1}$

Knowing the two asymptotic limits of ρ large and small, it makes sense to try a new definition:

$$u(\rho) = \rho^{l+1} e^{-\rho} v(\rho)$$

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

Exactly as done for the Hermite polynomials of 1D oscillator we try a series expansion:

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

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

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

* Check switch from j to $j+1$ by expanding the first few terms

Introducing this into the diff equation we arrive to a **recursive relation** for the coefficients:

$$c_{j+1} = \left\{ \frac{2(j+l+1) - \rho_0}{(j+1)(j+2l+2)} \right\} c_j$$

At very large j , then: $c_{j+1} \cong \frac{2}{j+1} c_j$

At large j , it can be shown (book) that the coefficients generate a growing exponential e^p . The **SAME** happened in Ch 2, 1D harmonic oscillator. Then, we must truncate the series (as with the Hermite polynomials). Long story short, **there is an upper limit** in j beyond which:

$$c_{(j_{\max}+1)} = 0$$

$c_0,$
 $c_0, c_1,$
 c_0, c_1, c_2, \dots

Thus, the series expansion with j running to ∞ becomes a polynomial.

You may recall that "magically" from that condition, the quantized levels of the 1D oscillator were deduced. Here is the **SAME** story.

Repeating the recursive relation:

$$c_{j+1} = \left\{ \frac{2(j+l+1) - \rho_0}{(j+1)(j+2l+2)} \right\} c_j$$

Then: $2(\underbrace{j_{\max} + l + 1}) - \rho_0 = 0$

Call this "n" (1,2,3,...).
Min l is 0. Min j_{\max} is 0.

By this procedure we arrive to a famous formula:

$$E_n = - \left[\frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \right] \frac{1}{n^2}$$

$n=1,2,3,\dots$

Remember

$$\rho_0 \equiv \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa}$$

and $\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}$

$$E_n = - \underbrace{\left[\frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \right]}_{E_1} \frac{1}{n^2}$$

$$E_1 = -13.6 \text{ eV} \quad \text{eV} = 1.6 \cdot 10^{-19} \text{ Joules}$$

Moreover, since $\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}$ then it can be shown:

$$\kappa = \left(\frac{me^2}{4\pi\epsilon_0\hbar^2} \right) \frac{1}{n} = \frac{1}{an} \quad \text{where } \underbrace{a = 0.529 \times 10^{-10} \text{ m}}_{\text{Bohr's radius.}}$$

$$u(\rho) = \rho^{l+1} e^{-\rho} v(\rho)$$

$$\rho \equiv \kappa r = (1/an) r$$

Bohr's radius.
The angstrom scale emerges.

Angstrom is the "natural" size of atoms. Remarkable!

How about the ground state wave function?

Remember:

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_l^m(\theta, \phi)$$

$$R_{nl}(r) = \frac{1}{r} \rho^{l+1} e^{-\rho} v(\rho) \quad u(\rho) = \rho^{l+1} e^{-\rho} v(\rho) \quad \rho \equiv \kappa r$$

$n=1$ is the lowest energy (the most negative).
Since $n = j_{\max} + l + 1$, then $l=0, j_{\max}=0$. Then

$$\psi_{100}(r, \theta, \phi) = R_{10}(r) Y_0^0(\theta, \phi)$$

with $R_{10}(r) = \frac{c_0}{a} e^{-r/a}$ because
the polynomial has only a
constant c_0 .

$$Y_0^0(\theta, \phi) = 1/\sqrt{4\pi}$$

We then **normalize**, which means we fix the value of c_0 :

$$\int_0^{\infty} |R_{10}|^2 r^2 dr = \frac{|c_0|^2}{a^2} \int_0^{\infty} e^{-2r/a} r^2 dr = |c_0|^2 \frac{a}{4} = 1$$

The very final result (harps, celestial music) is:

$$\psi_{100}(r, \theta, \phi) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$

which happened to be remarkably **simple**.