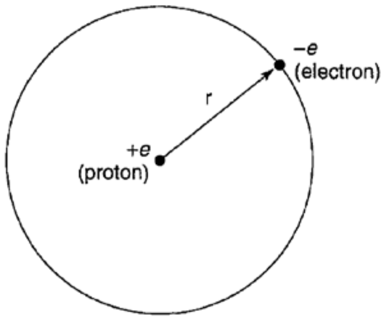
4.2: The Hydrogen Atom

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:

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

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:

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

This suggests $\rho \equiv \kappa r$ may be useful, and also $\rho_0 \equiv \dfrac{me^2}{2\pi\epsilon_0\hbar^2\kappa}$

(dimensionless)

The exact radial equation then becomes "simpler":

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

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

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

Unphysical diverging solutions discarded.

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

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

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

$\rho = \kappa r$ so we know all solutions will decay exponentially

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

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 Eq.4.63:

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

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^{ρ}. 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 only then $j_{max}=0$
c_0, c_1 only then $j_{max}=1$
c_0, c_1, c_2, …

Thus, the series expansion with *j* running in principle to ∞, becomes in practice 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 from 2 pages back:

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

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

Call this "*n*" (1,2,3,...). I.e. ρ_0=2n.

Min angular momentum *l* is 0. Min j_{max} is 0. You can achieve the same "*n*" with various j_{max} and *l*.

Remember

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

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

By this procedure we arrive to the very famous **Bohr's 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,...

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

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

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

$$\kappa = \left(\frac{me^2}{4\pi\epsilon_0\hbar^2}\right)\frac{1}{n} = \frac{1}{an}$$ where $a = 0.529 \times 10^{-10}$ m

Bohr's radius.

The angstrom scale, and thus the typical atomic size, emerges.

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

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

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