SQ4

In previous course, we have learned that (from Schrödinger) the energy levels of hydrogen is $-\frac{13.6}{n^2}$ eV.

However, when we tried to look for the experimental data in SQ2, we saw that the numbers are slightly off

(e.g. for $n=2$, there are in fact 3 values regarding the angular configuration $2p\,(J=\frac{1}{2})$, $2p\,(J=\frac{3}{2})$, $2S$, not simply depend only on n)

One correction we can think of is the relativistic effect. Instead of $T=\frac{p^2}{2m}$, we use $T=\frac{p^2}{2m}+(\text{correction})$

a. Take Bohr's Model,

$E_n = -\frac{13.6}{n^2}$ eV, remember that E_n is the total energy of the atom.

By virial theorem, the kinetic energy $T = +\frac{13.6}{n^2}$ eV.

For ground state ($n=1$), assume that $T_1 = \frac{1}{2}mv_1^2 = 13.6$ eV,

where $m = 0.51 \times 10^6$ eV$/c^2$ is the mass of an electron.

$$\therefore \quad \frac{1}{2}(0.51\times10^6)\,v_1^2 = 13.6\,c^2$$

$$\Rightarrow \quad \frac{v_1}{c} = 0.00729 \approx \frac{1}{137}$$

This ratio ($<1\%$) is called the fine structure constant α and it is famous in high energy physics.

b. Remember $E_n = -\frac{13.6}{n^2}$ eV is coming from ~~the~~ a combination of constants s.t. $E_n = -\frac{1}{2}\left(\frac{e^2}{4\pi\epsilon_0\hbar}\right)^2\frac{m}{n^2}$.

ie, $E_1 = -\frac{1}{2}\left(\frac{e^2}{4\pi\epsilon_0\hbar}\right)^2 m$, $T_1 = +\frac{1}{2}\left(\frac{e^2}{4\pi\epsilon_0\hbar}\right)^2 m$

This impl $v_1 = \frac{e^2}{4\pi\epsilon_0\hbar}$

The electron rest energy E_{rest}, is of course mc^2.

$$\therefore \quad \frac{E_1}{E_{rest}} = -\frac{1}{2}\left(\frac{e^2}{4\pi\epsilon_0\hbar}\right)^2 m \;\frac{1}{mc^2}$$

b. (cont.)

$$\frac{E_1}{E_{rest}} = -\frac{1}{2}\left(\frac{e^2}{4\pi\epsilon_0\hbar}\right)^2 \frac{1}{c^2}.$$

$\because$ $v_1 = \frac{e^2}{4\pi\epsilon_0\hbar}$,

$$\therefore \quad \frac{E_1}{E_{rest}} = -\frac{1}{2}\left(\frac{v_1}{c}\right)^2 = -\frac{1}{2}\alpha^2.$$

$$\Rightarrow \quad \alpha = \sqrt{\frac{2E_1}{E_{rest}}}$$ //

c. In relativistic expression, the kinetic energy

$$T = \sqrt{p^2c^2 + m^2c^4} - mc^2$$

$$\Rightarrow \quad T = mc^2\sqrt{1+\left(\frac{p}{mc}\right)^2} - mc^2$$

For small relativistic correction, $\frac{p}{mc}$ is small

(reference $\frac{v}{c} \approx \frac{1}{137} <$ 1%.)

We can expand the 1st term in the powers of $\left(\frac{p}{mc}\right)^2$,

$\because$ for $f(x) = \sqrt{1+x}$, $\quad f'(x) = \frac{1}{2}(1+x)^{-\frac{1}{2}}$, $\quad f''(x) = -\frac{1}{4}(1+x)^{-\frac{3}{2}}$

$$f(x) = 1 + f'(0)x + \frac{1}{2}f''(0)x^2 + O(x^3) \quad \text{for } |x|<1$$

$$= 1 + \frac{1}{2}x - \frac{1}{8}x^2 + O(x^3)$$

Plug $x = \left(\frac{p}{mc}\right)^2$,

$$T \approx mc^2\left(1+\frac{1}{2}\left(\frac{p}{mc}\right)^2 - \frac{1}{8}\left(\frac{p}{mc}\right)^4\right) - mc^2$$

$$\approx \frac{p^2}{2m} - \frac{p^4}{8m^3c^2}$$ //

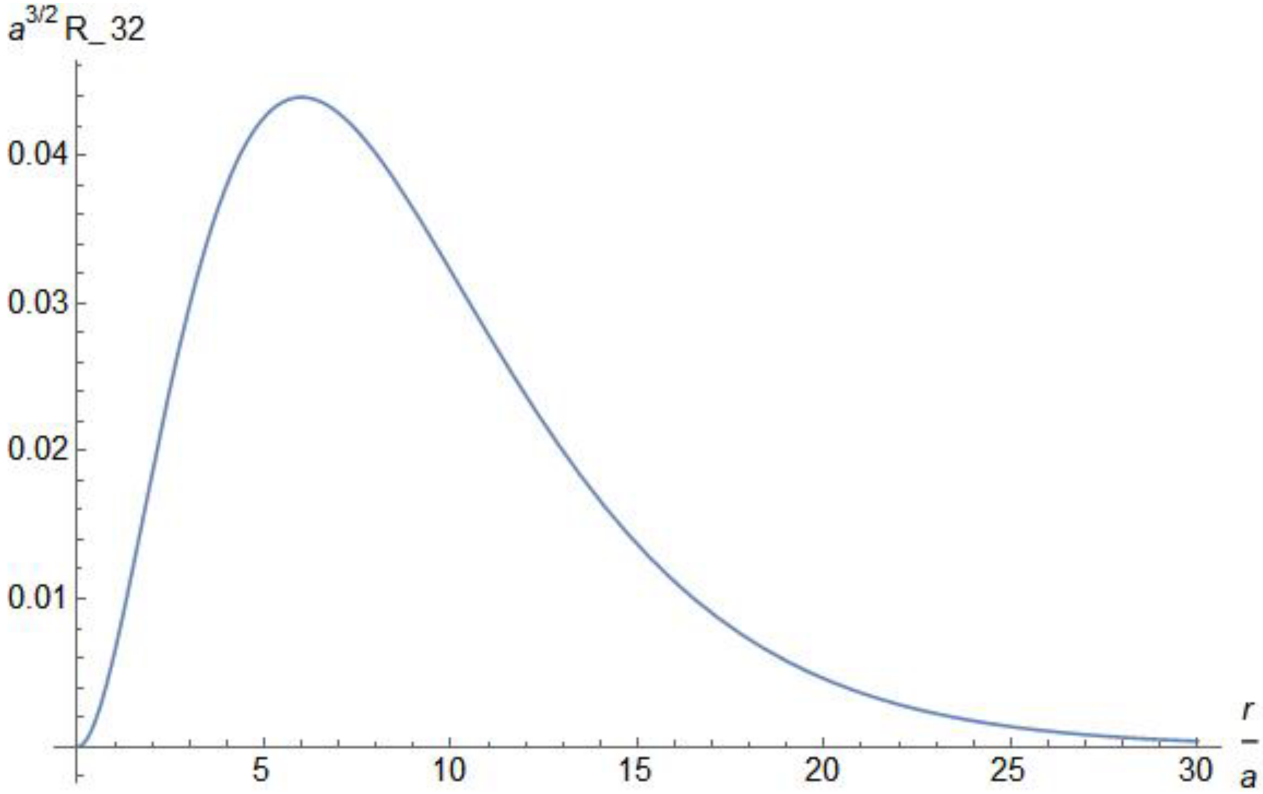
Note : the 2nd term is much smaller than the 1st term $\frac{p^2}{2m}$.

$\therefore$ We can treat the 2nd term as a perturbation on the original Hamiltonian.

You will learn it soon ...

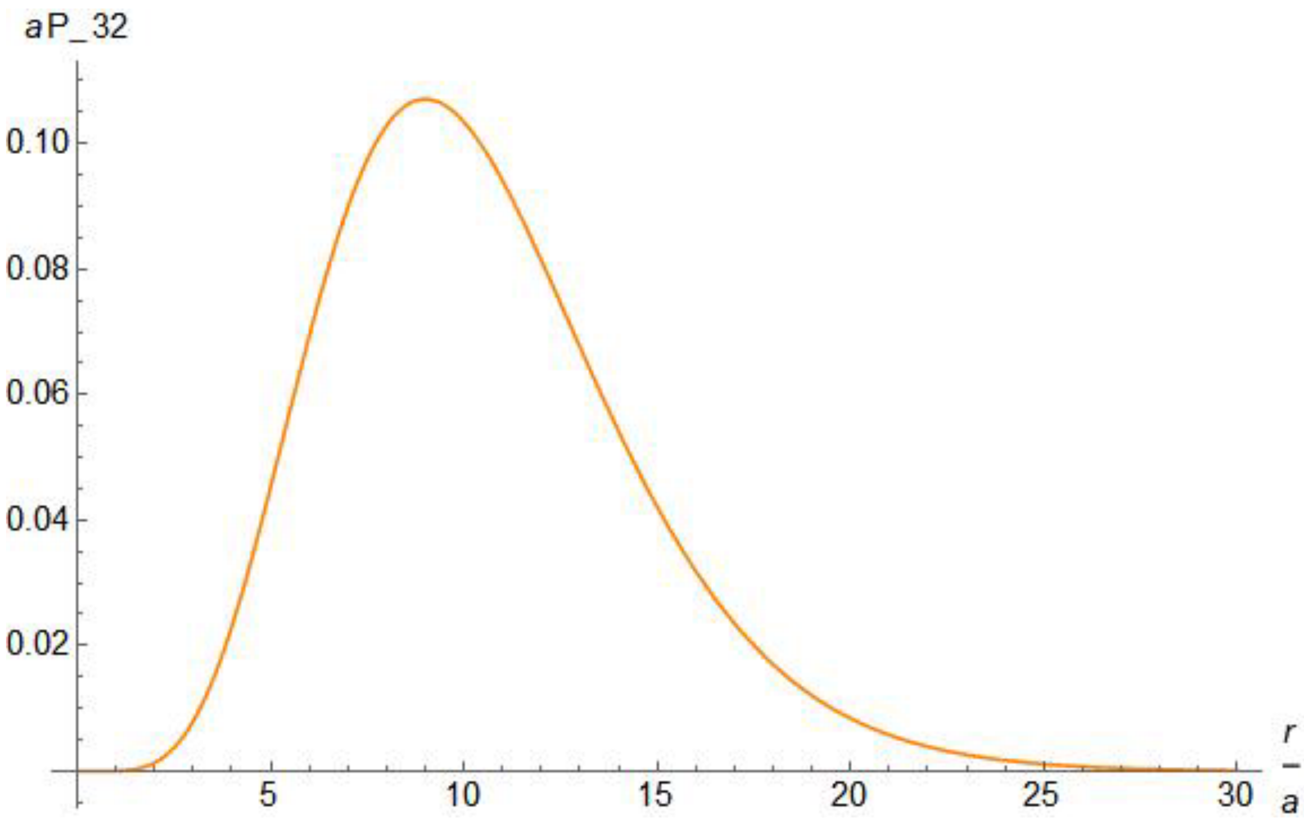
SQ5

$$R_{32}(r) = \frac{4}{81\sqrt{30}} a_0^{-3/2} \left(\frac{r}{a_0}\right)^2 e^{-r/3a_0}$$



$$P_{32}(r) = r^2 |R_{32}(r)|^2$$

$$= \frac{8r^2}{98415} a_0^{-3} \left(\frac{r}{a_0}\right)^4 e^{-2r/3a_0}$$



Let r_p be the most probable distance

$$\left.\frac{dP_{32}(r)}{dr}\right|_{r=r_p} = 0$$

$$\frac{8}{98415 a_0^7} e^{-2r_p/3a_0} \left(6r_p^5 - \frac{2r_p^6}{3a_0}\right) = 0$$

$$6r_p^5 - \frac{2r_p^6}{3a_0} = 0$$

$$r_p = 9a_0$$

According to Bohr's model, electron is in orbits with $r_n = n^2 a_0$
The orbits have fixed distances from the nucleus.

In QM, we showed that the most probable distance for the electron in 3d state is at $9a_0$ away from the nucleus, which matches the radius of Bohr's orbit $(n=3)$. However, the plot of $P_{32}(r)$ showed that the electron can be elsewhere, although with a lower probability. This is different from Bohr's model.

SQ6.

The model: we model a diatomic molecule as two balls connected by a string, where the masses of the balls are m_1 and m_2, the natural length of the string is r_0, the spring constant is K, and the coordinates of the two balls are x_1 and x_2.

(i) Firstly, we derive the equations of motion. The extension of the string from its natural length is $(x_2 - x_1 - r_0)$. Then by Newton's 2nd law,

$$m_1 \frac{d^2 x_1}{dt^2} = K(x_2 - x_1 - r_0) \quad (1)$$

$$m_2 \frac{d^2 x_2}{dt^2} = -K(x_2 - x_1 - r_0) \quad (2)$$

where the minus sign in the second equation is due to that the force on m_2 is in the opposite direction of the force on m_1.

(ii) We show that the Center of Mass (CM) moves in a constant momentum by finding its equation of motion. The Center of Mass of two masses m_1 and m_2 placed at x_1 and x_2 is defined as

$$X = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}$$

$\text{Eq.}(1) + \text{Eq.}(2)$ gives:

$$m_1 \frac{d^2 x_1}{dt^2} + m_2 \frac{d^2 x_2}{dt^2} = 0$$

which can be further written as

$$\frac{d^2}{dt^2}(m_1 x_1 + m_2 x_2) = 0$$

$$(m_1 + m_2)\frac{d^2}{dt^2}\left(\frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}\right) = 0$$

$$M \frac{d^2 X}{dt^2} = 0$$

where $M = m_1 + m_2$ is the total mass. We can see clearly that the acceleration of the CM is 0. Therefore we claim that the CM moves in a constant velocity or momentum, which means that there is no external force and the CM moves freely.

(iii) We derive the equation of motion for the relative coordinate $x = x_2 - x_1$, and compare it with the standard harmonic oscillator equation

$$\mu \frac{d^2 r}{dt^2} + Kr = 0 \quad (3)$$

where μ is the reduced mass.

$m_2 \cdot \mathrm{Eq.}\,(1) - m_1 \cdot \mathrm{Eq.}\,(2)$ gives,

$$m_1 m_2 \frac{d^2}{dt^2}(x_1 - x_2) = K(m_1 + m_2)(x_2 - x_1 - r_0)$$

Then we replace $(x_2 - x_1)$ by x,

$$m_1 m_2 \frac{d^2}{dt^2} x = -K(m_1 + m_2)(x - r_0)$$

$$\frac{m_1 m_2}{m_1 + m_2} \frac{d^2}{dt^2} x + (x - r_0) = 0 \quad (4)$$

Comparing equation (4) with the above standard harmonic oscillator equation (3), we find that the definition of the reduced mass is given by

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

or

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

and $r = (x - r_0)$ is the extension of the string from its natural length.

(iv) We derive the characteristic angular frequency ω, frequency ν and wavenumber $\bar{\nu}$. Recall that the angular frequency for a harmonic oscillator can be simply obtained from its equation of motion, i.e. from equation (3):

$$\omega = \sqrt{\frac{K}{\mu}}$$

The frequency

$$\nu = \frac{1}{T} = \frac{2\pi}{2\pi T} = \frac{\omega}{2\pi} = \frac{1}{2\pi}\sqrt{\frac{K}{\mu}}$$

The wavenumber

$$\bar{\nu} = \frac{1}{\lambda} = \frac{\nu}{c} = \frac{1}{2\pi c}\sqrt{\frac{K}{\mu}}$$

Conclusion: We transform the original problem into the CM motion plus the relative motion, i.e. the original equations of motion

$$m_1 \frac{d^2 x_1}{dt^2} = K(x_2 - x_1 - r_0)$$

$$m_2 \frac{d^2 x_2}{dt^2} = -K(x_2 - x_1 - r_0)$$

have been transformed into

$$M \frac{d^2 X}{dt^2} = 0$$

$$\mu \frac{d^2 r}{dt^2} + Kr = 0$$

where the CM motion is a free motion, as two-body problem under our consideration does not have an external force.