This note was written in "realtime" by Ingjald Pilskog. Edited by L. K.

Third lecture 29.08.06

Atomic world construction

a_0 - radius, length

$\Delta x \approx a_0$ $\Delta k \approx 1/a_0$

($\hbar \Delta k = \Delta p$ wavenumber

$\Delta E \approx \frac{(\Delta p)^2}{2m} = \frac{\hbar^2}{2ma_0^2} \approx \frac{\hbar^2}{ma_0^2}$ (kinetic energy T_0.) Potential energy V_0 $| - \frac{e^2}{a_0}$

Atomic unit of length

$a_0 = 0,529$ Å$= \frac{\hbar^2}{e^2 m}$ Lenght unit

Atomic unit of energy

Energy unit $\frac{e^2}{a_0} = \frac{\hbar}{ma_0^2} = 27,2$ eV

$< T_0 > = < V_0 >$ should be of the same order.

Atomic unit of velocity

$p_0 = \hbar k_0 = \frac{\hbar}{a_0}$ $\quad v_0 = \frac{p_0}{m} = \frac{\hbar}{m}\frac{1}{a_0} = \quad \frac{me^2}{\hbar^2}\frac{\hbar}{m} = \frac{e^2}{\hbar} \quad \frac{v_0}{c} = \frac{e^2}{\hbar c} = \alpha = \frac{1}{137}$

Atomic unit of time

$t_0 = \frac{a_0}{v_0} = (\frac{a_0}{e^2})\hbar = \frac{\hbar}{E_0}$

Alternative postulate $t_0 = \frac{\hbar}{E_0}$

(Statement a.u. $\longleftrightarrow e = m\hbar = 1$ is useless)

$\hbar = 0,66 \cdot 10^{-15}$ eVs $t_0 = \quad \frac{0,66 \cdot 10^{-15}}{27,2}s=0,24 \cdot 10^{-15}$

(2 π for angular freq.)

ν frequency $\quad$ ω - angular frequency

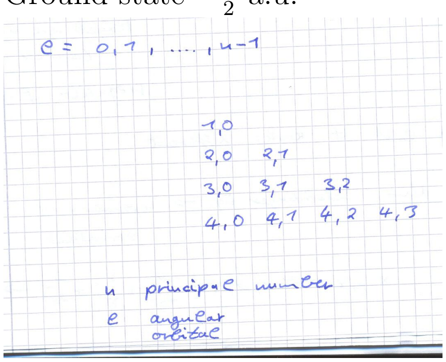
$k_0 T$ is the "physical temperature".

Room temperature is thus $\frac{1}{40}$eV or 25 meV

Atomic unit of energy $\longrightarrow$ VERY HOT

More about bound states in H

Ground state $-\frac{1}{2}$ a.u.



States characterized by n, l (m - magnetic)

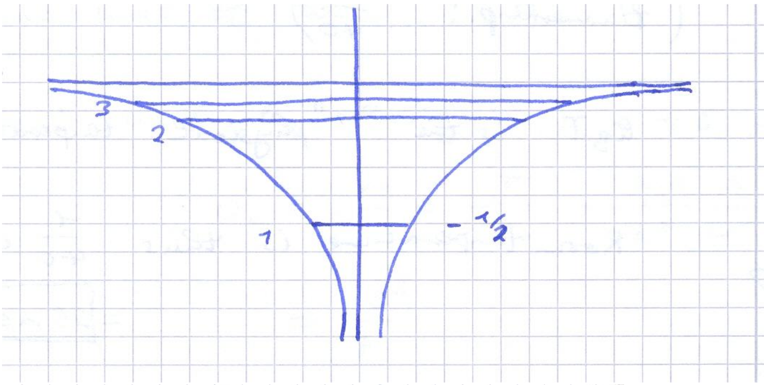
In H energies given by $\frac{1}{n^2}(-\frac{1}{2})$a.u.

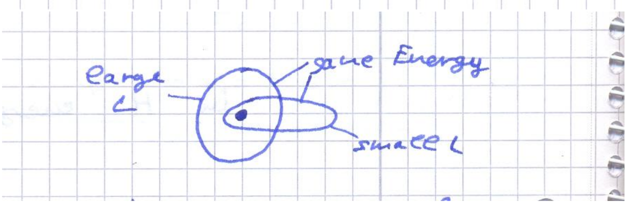
"Ladi says its nonsens to talk about m as a quantum number", wrote Ingjald. He did not write: "unless we have magnetic field on".

Angular momentum

$L = \omega \mathcal{I}$ $\quad T_{rot} = \frac{1}{2}\frac{L^2}{\mathcal{I}}$ $\quad T_{rot} = \frac{1}{2}\mathcal{I}\omega^2$ $\quad \mathcal{I}$ is the *moment of inertia*

$E = T + V$ is negativ .... T is kinetic energy





I_n QM it looks different
3-dim Schr.Eq. $\longrightarrow$ Seperation of variables
$x, y, z, \rightarrow r, \nu, \varphi$
$\frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2} \longrightarrow T_r + \frac{L^2(\theta,\varphi)}{r^2}$
$T_r \longrightarrow \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}$
L^2 is ugly (but can be made very elegant)
This is generally used in many fields.

$$\frac{L^2(\theta,\varphi)}{r^2} \longrightarrow \frac{1}{r^2}\frac{1}{sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2 sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}$$

Solutions of the above are $Y_l^m(\theta,\phi)$, known as the spherical harmonics. (The constants were not taken care of)

From the web ("stolen latex code")
`http://vergil.chemistry.gatech.edu/notes/quantrev/node25.html`

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)\frac{1}{r^2 sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2 sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right] - \frac{e^2}{4\pi\epsilon_0 r}\psi(r,\theta,\phi) = E\psi(r,\theta,\phi) \tag{1}$$

Exercise: Look on the separation of variables and how it's done.

(l=0) s-states,
(l=1) p-states,
(l=2) d-states,
(l=3) f-states, ... there are more, but it is not relevant in typical atoms