

L05-Bohr Model: Correspondence

Principle

Friday, September 4, 2015 10:07 AM

* classical Rutherford model:

- atomic spectra
- J.J. Thompson "plumb pudding" model
modes of vibration
- "radiation catastrophe"

* problems with Bohr model

- only: H + H-like atoms, K, L series X-rays.
- wrong angular momentum
- ad-hoc quantization
- no prediction of spectral intensity.
- no description of radiative process

* Fundamental constants

$$kT = 25 \text{ meV } [300 \text{ K}]$$

$$e^2/4\pi\epsilon_0 = 1.44 \text{ eV}\cdot\text{nm}$$

$$\hbar c = 197 \text{ eV}\cdot\text{nm } [\text{GeV}\cdot\text{fm}]$$

"electric" energy
"quantum" energy

$$\alpha = e^2/4\pi\epsilon_0\hbar c = 1/137$$

$$m_e c^2 = 0.511 \text{ MeV}$$

$$E_0 = \frac{1}{2} m_e c^2 \cdot (e^2/4\pi\epsilon_0\hbar c)^2 = 13.6 \text{ eV}$$

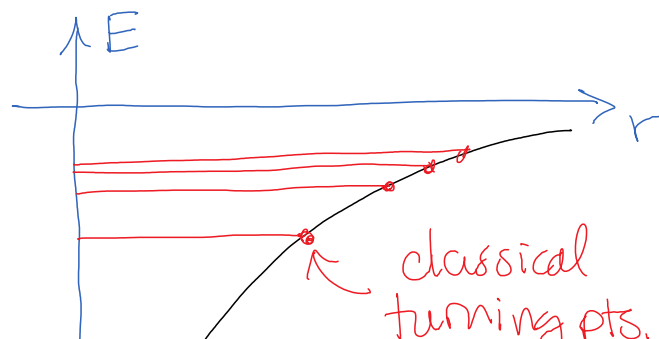
— ratio —
mass energy
ionization energy.

* Virial Theorem $\langle T \rangle$ vs $\langle V \rangle$

$$V = kr^n$$

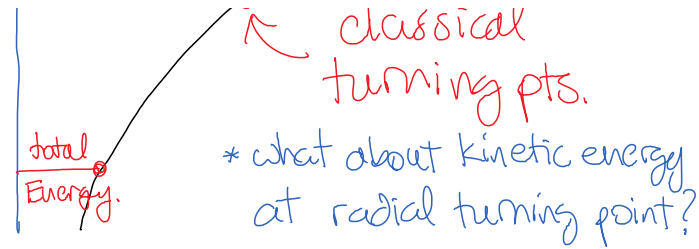
$$\vec{F} = -\nabla V = -knr^{n-1} \hat{r}$$

$$= -\frac{mv^2}{r} \hat{r} \text{ centripetal}$$



$$= -\frac{mv^2}{r} \hat{r} \text{ centripetal}$$

$$n\langle V \rangle = 2\langle T \rangle$$



$$\text{Hydrogen: } n=1 \quad \langle T \rangle = -\frac{1}{2}V \quad E = \langle T \rangle + \langle V \rangle = \frac{1}{2}V$$

$$V = -\frac{Ze^2}{4\pi\epsilon_0 r} \quad T = \frac{1}{2}mv^2 = -\frac{1}{2}V \quad v^2 = \frac{Ze^2}{4\pi\epsilon_0} \frac{1}{mr}$$

$$\ast \text{ Rydberg formula: } \frac{1}{\lambda} = R \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right) = \frac{\nu}{c}$$

$\ast$ Bohr's Postulates

- a) "stationary orbits" stable orbits energy E_n
- b) quantum transitions - "photon" $E = h\nu = E_{n_i} - E_{n_f}$
- c) quantum condition - $L = n\hbar$

$$\nu_n = \frac{Ze^2}{4\pi\epsilon_0} \frac{1}{\underbrace{mvr}_{L=n\hbar}} = \frac{Z}{n} \frac{e^2}{4\pi\epsilon_0\hbar c} \cdot c = \frac{Z\alpha c}{n} \quad Z < 137!$$

$$r_n = \frac{Ze^2}{4\pi\epsilon_0} \frac{1}{mv^2} = \frac{n^2}{Z} \underbrace{\frac{\hbar c}{m_e c^2}}_{\alpha_c} \cdot \underbrace{\frac{4\pi\epsilon_0 \hbar c}{e^2}}_{1/2} = \frac{n^2}{Z} a_0$$

$$E_n = -\frac{Ze^2}{2 \cdot 4\pi\epsilon_0 r_n} = -\frac{Z^2}{n^2} \frac{m_e c^2}{2} \cdot \underbrace{\left(\frac{e^2}{4\pi\epsilon_0 \hbar c} \right)^2}_{2^2} = -\frac{Z^2}{n^2} E_0$$

$\ast$ correspondence principle:

- frequency of orbital $\cong$ frequency of emission
as $n \rightarrow \infty$ (classical)

- Ehrenfest's theorem (expectation values classical)

$$\frac{d\langle x \rangle}{dt} = \left\langle \frac{\partial H}{\partial p} \right\rangle = \frac{\langle p \rangle}{m} \quad \frac{d\langle p \rangle}{dt} = -\left\langle \frac{\partial H}{\partial x} \right\rangle = -\left\langle \frac{\partial V}{\partial x} \right\rangle$$