L04-Bohr's model of the atom

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* Review: Wave particle duality.

a) Planck/Einstein: $E = h\nu = \hbar\omega$ waves $\Rightarrow$ particles (photons)

b) de Broglie: $\lambda = h/p$ $p = \hbar k$ particles $\Rightarrow$ waves (matter waves)

Both of these concepts led to the discretization of energy states.

The quantization/dispersion table:
We will dive into dispersion next week.

E	ω
p	k

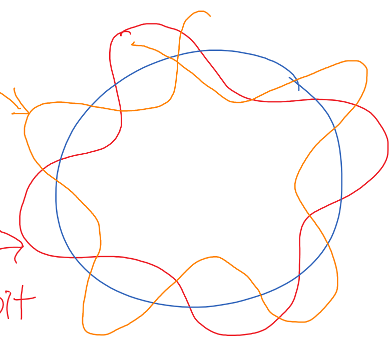
Bohr model of the atom:

* deBroglie's hypothesis also gave physical intuition to Bohr's quantum condition:
The wave must wrap around on itself for a stable orbit

$$2\pi r = n\lambda = nh/p$$
$$L = |\vec{r} \times \vec{p}| = \hbar n$$

unphysical: destructive interference

closed orbit



* Bohr's Postulates: over 10 years early, Bohr used both quantization of matter and radiation to explain the radiation spectrum of atomic hydrogen.

a) "stationary orbits": stable orbits of energy E_n satisfying the quantum condition: $L = n\hbar$

b) quantum transitions: "photon" $\frac{hc}{\lambda} = h\nu = E_{n_i} - E_{n_f}$

We will review the Bohr atom "old quantum theory" because it has most of the elements of any quantum problem.

For circular orbits, $F_c = \frac{mv^2}{r} = \frac{Ze^2}{4\pi\varepsilon_0 r^2}$

$$v_n = \frac{Ze^2}{4\pi\varepsilon_0} \frac{1}{m v_n r} = \frac{Z}{n} \frac{e^2}{4\pi\varepsilon_0 \hbar c} \cdot c = \frac{Z\alpha c}{n}$$ $Z < 137$!

$$v_n = \frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{m_e v r} = \frac{Z}{n}\frac{e^2}{4\pi\varepsilon_0\hbar c}\cdot c = \frac{Z\alpha c}{n}$$

$L = n\hbar$

$Z < 137$! otherwise relativistic)

$$r_n = \frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{m_e v^2} = \frac{n^2}{Z}\underbrace{\underbrace{\frac{\hbar c}{m_e c^2}}_{\lambda_c}\cdot\underbrace{\frac{4\pi\varepsilon_0\hbar c}{e^2}}_{1/\alpha}}_{a_0} = \frac{n^2}{Z}a_0$$

$$E_n = -\frac{Ze^2}{2\cdot 4\pi\varepsilon_0 r_n} = -\frac{Z^2}{n^2}\underbrace{\frac{m_e c^2}{2}\cdot\underbrace{\left(\frac{e^2}{4\pi\varepsilon_0\hbar c}\right)^2}_{\alpha^2}}_{E_0} = -\frac{Z^2}{n^2}E_0$$

Thus $\frac{1}{\lambda} = \frac{E_{n_f} - E_{n_i}}{hc} = R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$ $R = E_0/hc = 109737/\text{cm}$

* Fundamental constants in natural units: eV

kT	$= 25$ meV [300K]	thermal energy
$e^2/4\pi\varepsilon_0$	$= 1.44$ eV·nm	electric energy
$\hbar c$	$= 197$ eV·nm [GeV·fm]	quantum energy
$m_e c^2$	$= 0.511$ MeV	mass energy

$\alpha = e^2/4\pi\varepsilon_0\hbar c = 1/137$	electric/quantum ratio
$E_0 = \frac{1}{2}m_e c^2\cdot\left(e^2/4\pi\varepsilon_0\hbar c\right)^2 = 13.6\text{ eV}$	ionization energy.
$a_0 = \lambda_c/\alpha = \frac{\hbar c}{m_e c^2}\cdot\frac{4\pi\varepsilon_0\hbar c}{e^2} = 0.529\text{ Å}$	Bohr radius $10\text{ Å} = 1\text{ nm}$

* Correspondence Principle

Bohr did not have deBroglie's principle to use in quantizing the energy levels of the atom.

He solved for the energy levels that matched the Rydberg formula.

He formulated the correspondence principle to justify this selection of energy levels:

"The results of quantum physics match those of classical physics at large quantum numbers"

Ex: The orbital frequency $\approx$ radiation frequency as $n \to \infty$.

$$\omega_{cl} = \frac{v_n}{r_n} = \frac{Z\alpha c}{n} \cdot \frac{Z\alpha m_e c}{n^2 \hbar} = \frac{(Z\alpha)^2 \cdot m_e c^2}{\hbar \quad n^3}$$

classical radiation at the orbital freq.

$$\omega_q = \frac{\Delta E}{\hbar} = \frac{Z^2}{\hbar} \cdot \frac{m_e c^2}{2} \cdot \alpha^2 \underbrace{\left(\frac{1}{n^2} - \frac{1}{(n+1)^2}\right)}_{\frac{(n^2+2n+1) - n^2}{n^2 \cdot (n^2 + 2n+1)} \approx 2n} \xrightarrow{n \to \infty} \frac{(Z\alpha)^2 m_e c^2}{\hbar n^3}$$

Ex: Ehrenfest' theorem (expectation values classical)

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

We'll prove these using Schrödinger's equation.