PHOT 222: Quantum Photonics
LECTURE 11

Michaël Barbier, Spring semester (2024-2025)

OVERVIEW OF THE COURSE

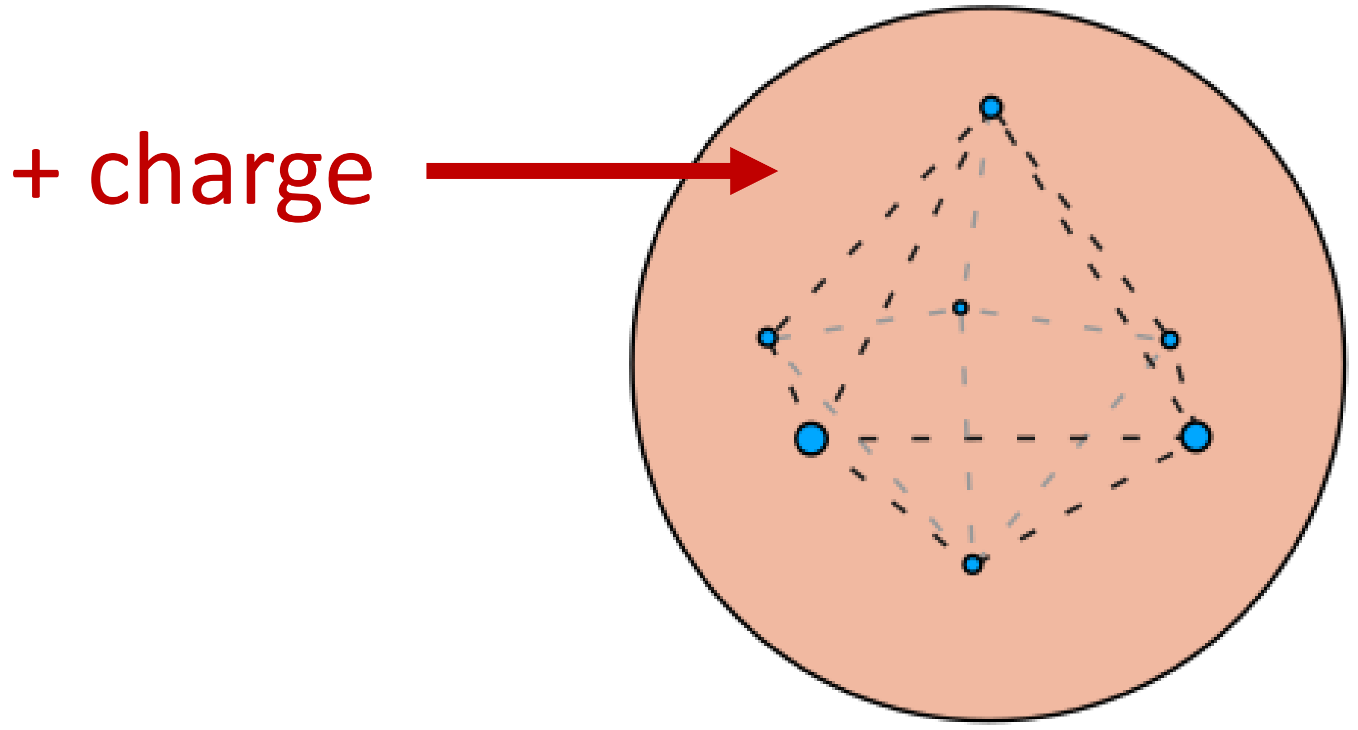
week	topic	Serway 9th	Young
Week 1	Relativity	Ch. 39	Ch. 37
Week 2	Waves and Particles	Ch. 40	Ch. 38-39
Week 3	Wave packets and Uncertainty	Ch. 40	Ch. 38-39
Week 4	The Schrödinger equation and Probability	Ch. 41	Ch. 39
Week 5	**Midterm exam 1**		
Week 6	Quantum particles in a potential	Ch. 41	Ch. 40
Week 7	Bayram		
Week 8	Harmonic oscillator	Ch. 41	Ch. 40
Week 9	Tunneling through a potential barrier	Ch. 41	Ch. 40
Week 10	**Midterm exam 2**		
Week 11	The hydrogen atom, absorption/emission spectra	Ch. 42	Ch. 41
Week 12	Many-electron atoms & Pauli-exclusion principle		
Week 13	Atomic bonds and molecules		
Week 14	Crystalline materials and energy band structure		

Early Models for the Atom

THOMSON MODEL FOR ATOMIC STRUCTURE

- **1897: J. J. Thomson** discovers **electron**
- **1904**: Atom plum pudding model
- Atom exists out of positive sphere
- Electrons embedded in sphere

  "Raisons in cake model"
- Electron oscillate with their own frequency
- Model explains:
  - Collisions with other atoms
  - Absorption specific frequencies light



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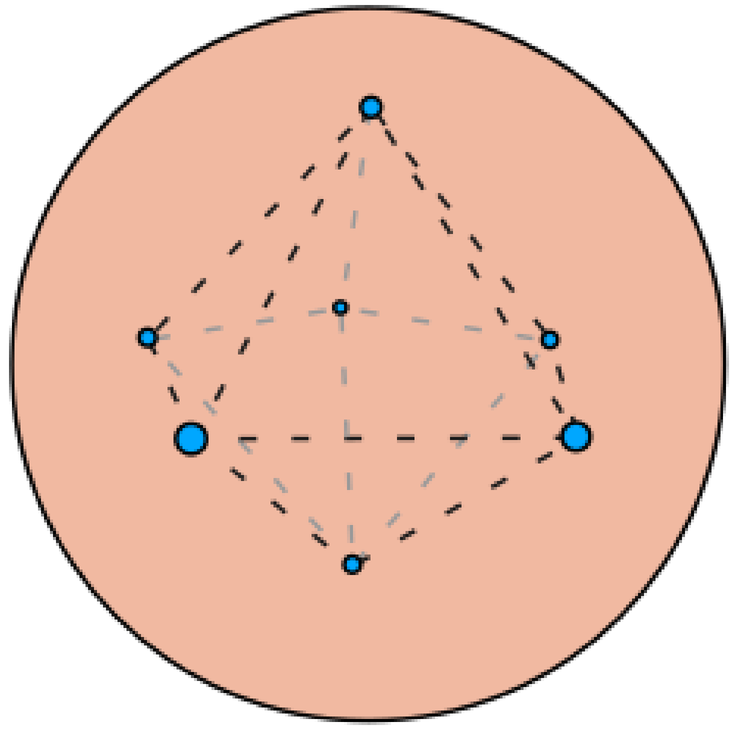

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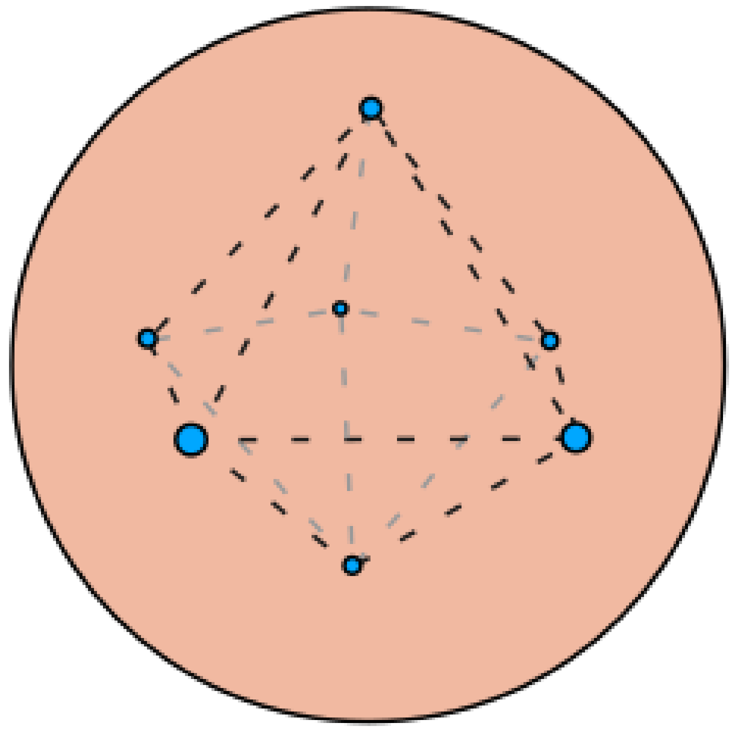
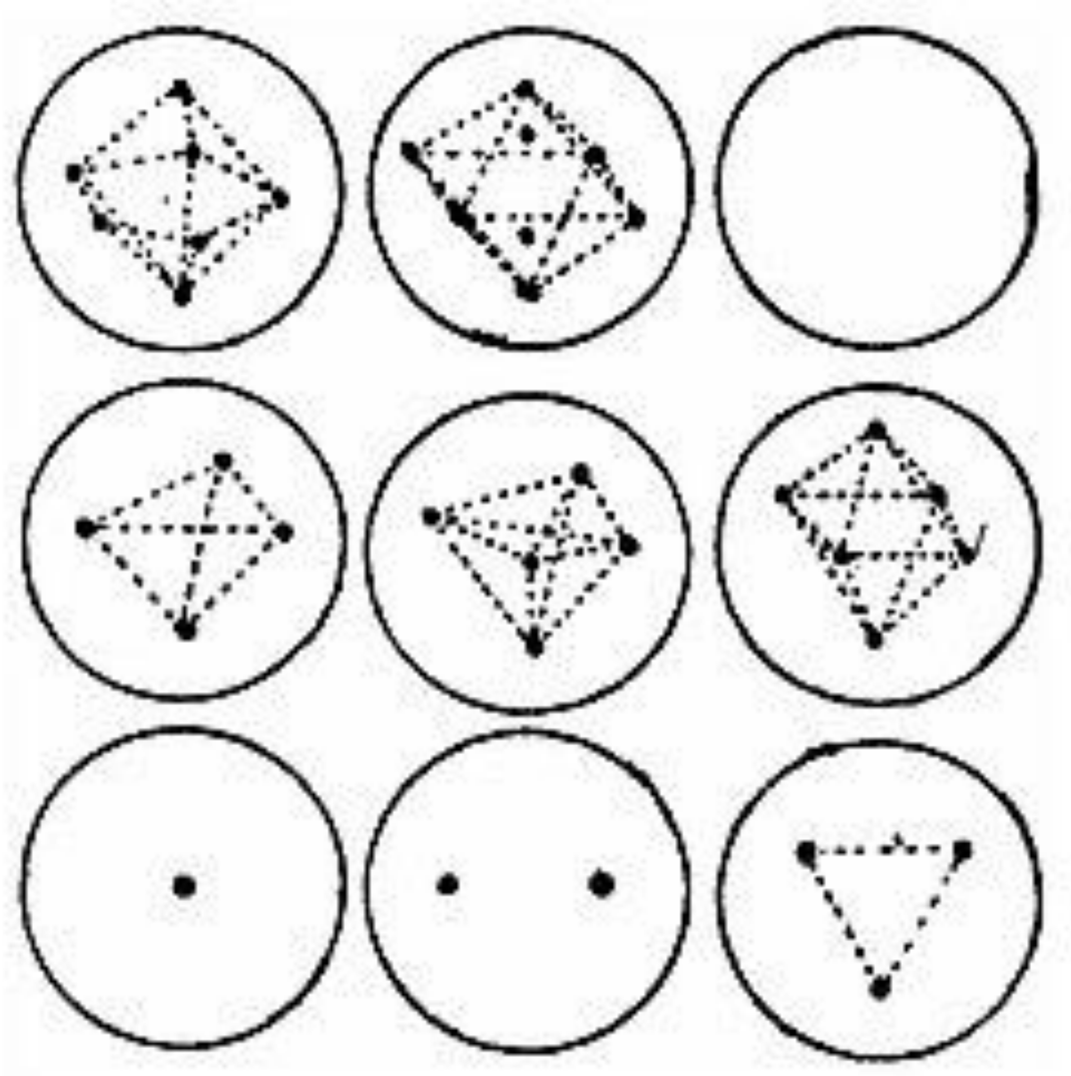




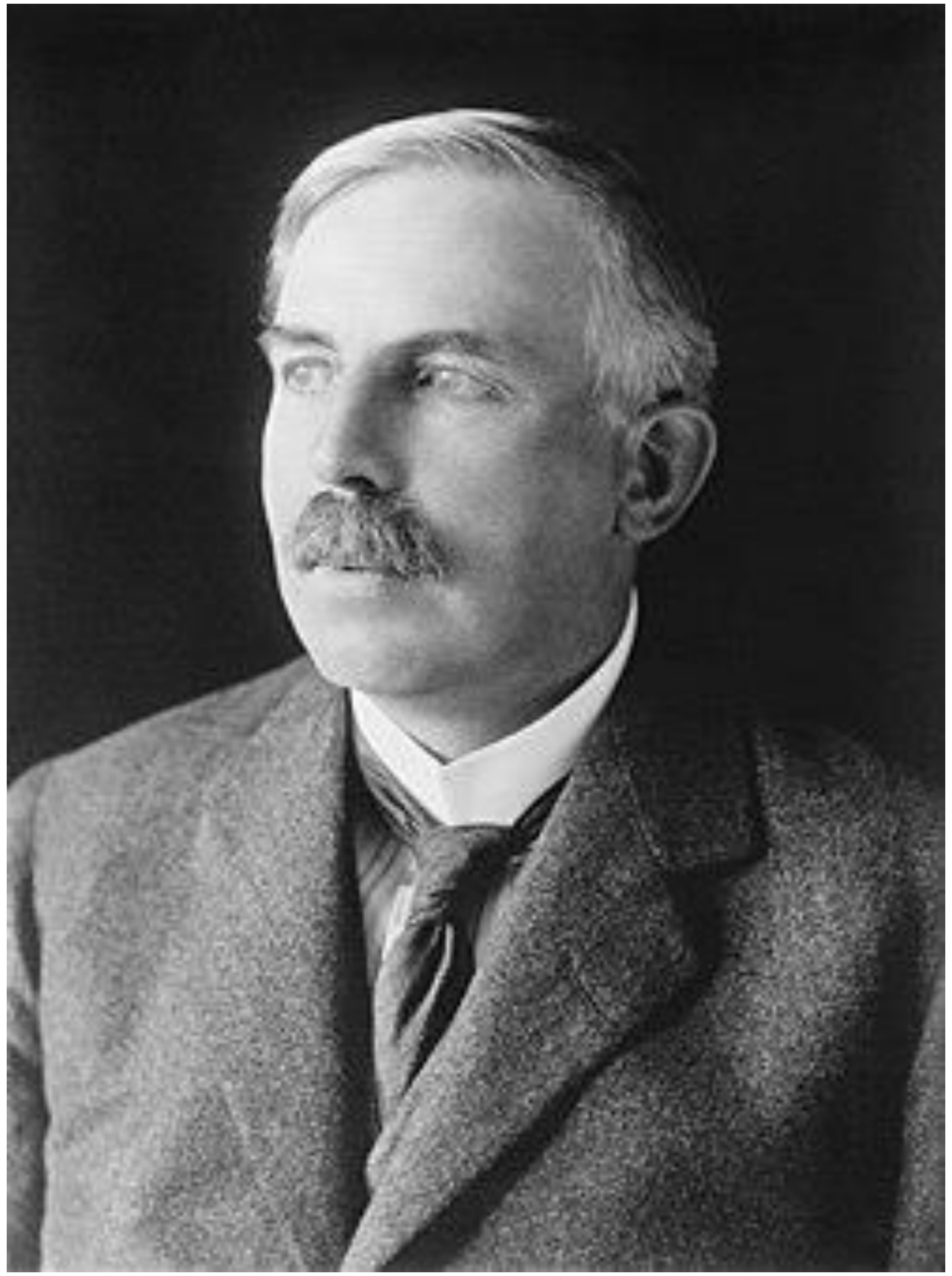
Adapted from Wikipedia

RUTHERFORD'S MODEL

- **1897: electron**
- **1904**: J. J. Thomson model
- **1911**: E. Rutherford

Scattering experiments:

- Nucleus is small < 10^{-14} m
- Gold atom $\approx 7 \times 10^{-15}$ m
- Contains all positive charge
- 99.75% of mass in nucleus



Lord Ernest Rutherford of Nelson

Taken from Wikipedia

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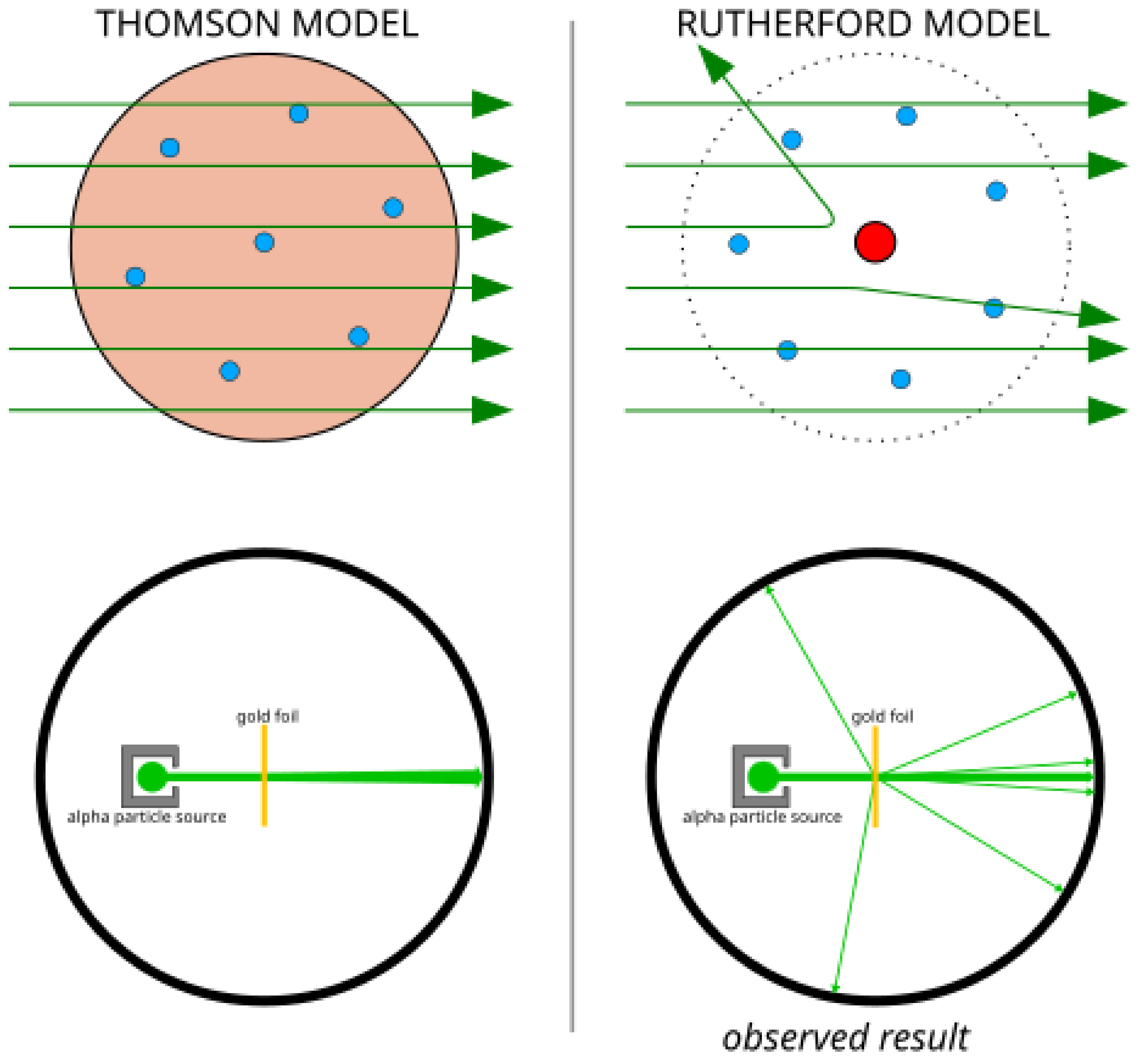


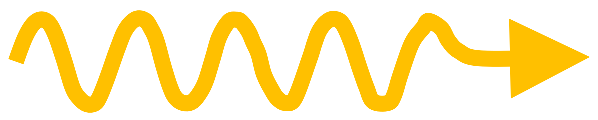
RUTHERFORD'S MODEL: SHORT-COMINGS

- Planetary model, electrons orbit nucleus due to Coulomb attraction:

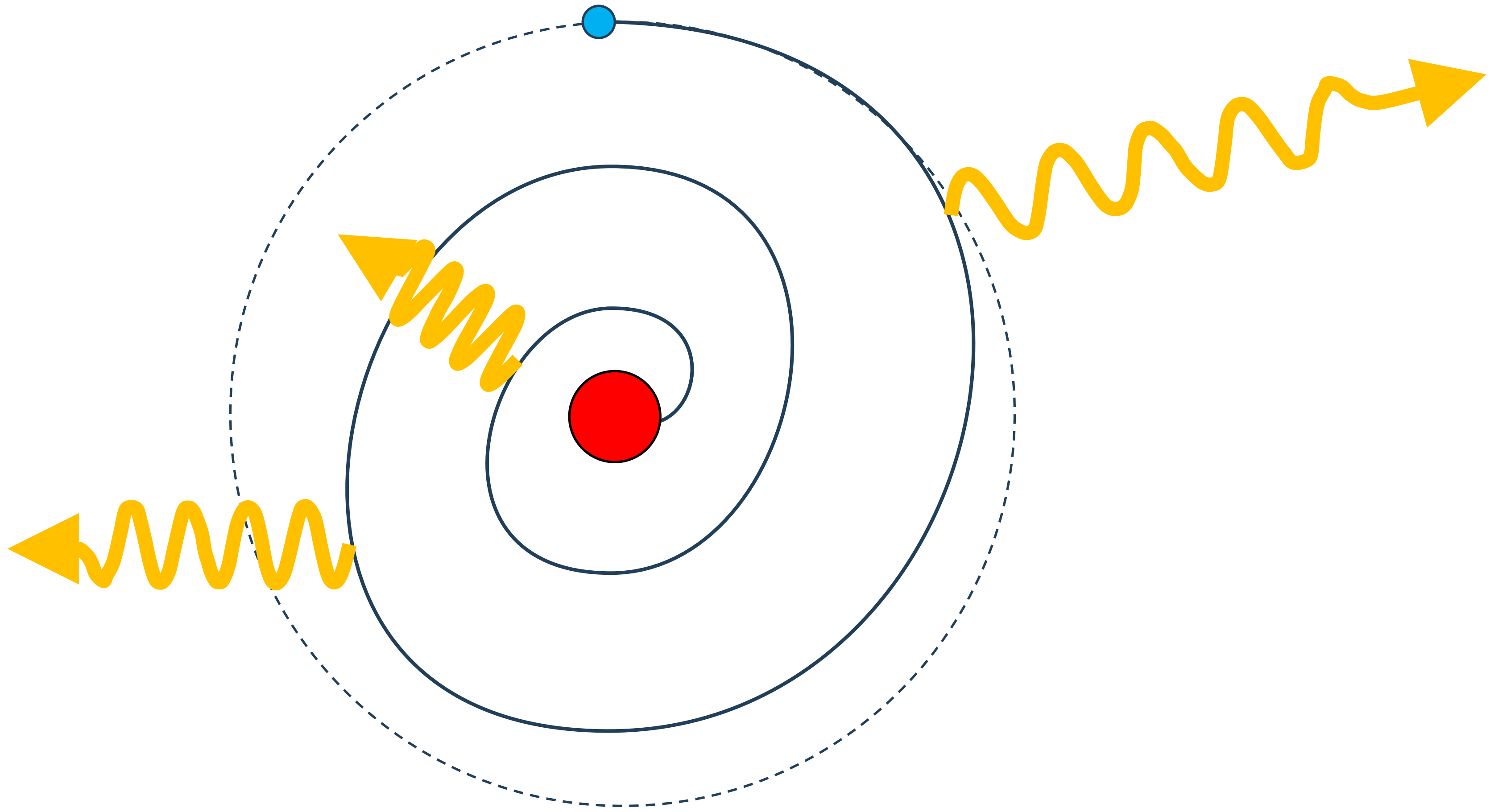
$$F(r) = \frac{1}{4\pi\epsilon_0}\frac{q_1 q_2}{r^2} = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r^2}$$

$$V(r) = \frac{1}{4\pi\epsilon_0}\frac{e}{r}, \qquad U(r) = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$$

$$E_{\text{photon}} = hf$$



$$\Delta K + \Delta U = E_{\text{photon}}$$



- Unlike planets: charge circulating at frequency f radiates light with f

  ➡ electron loses energy

- Closer to nucleus f increases
- Electron crashes into nucleus ?

BOHR MODEL OF THE HYDROGEN ATOM

- **1897:** electron
- **1904**: J. J. Thomson model
- **1911**: E. Rutherford
- **1913: Niels Bohr: Bohr model**

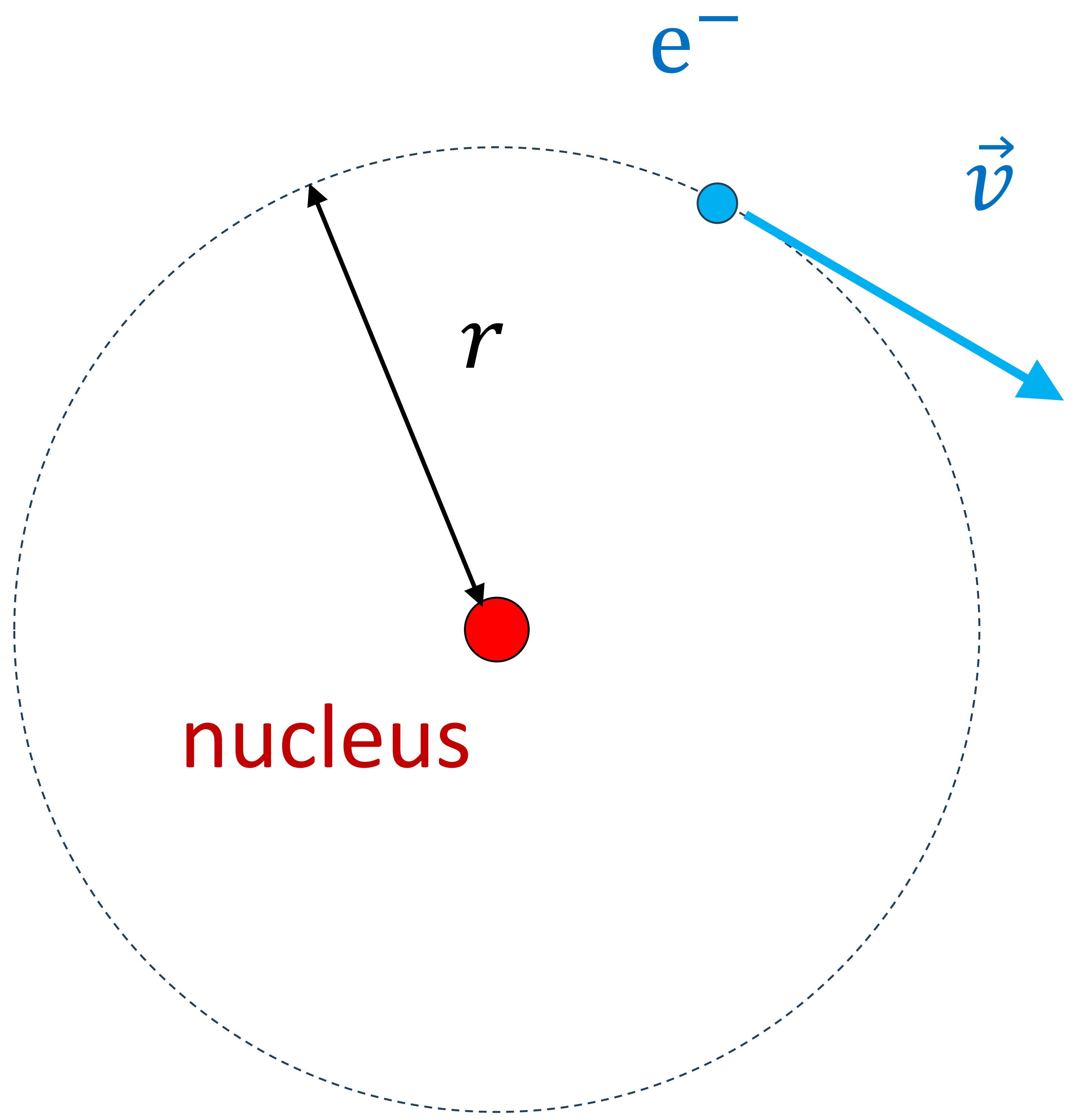
Niels Bohr (worked with Rutherford)
Taken from Wikipedia

BOHR MODEL: ENERGY LEVELS

Electron on circular orbits

1. Specific orbits are stable
2. **Angular momentum** quantized:

$$m_e v r = n\hbar = \frac{nh}{2\pi}$$



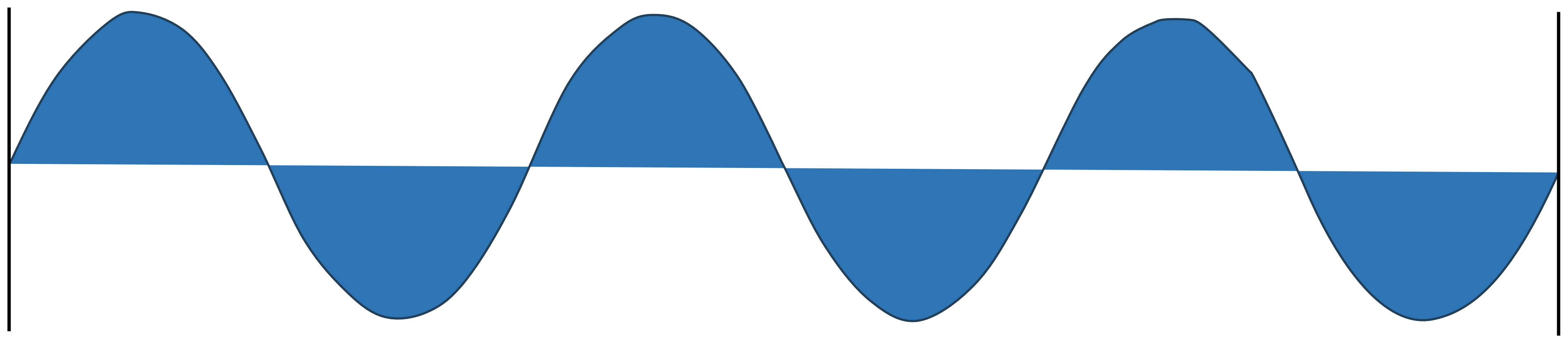
BOHR MODEL: ENERGY LEVELS

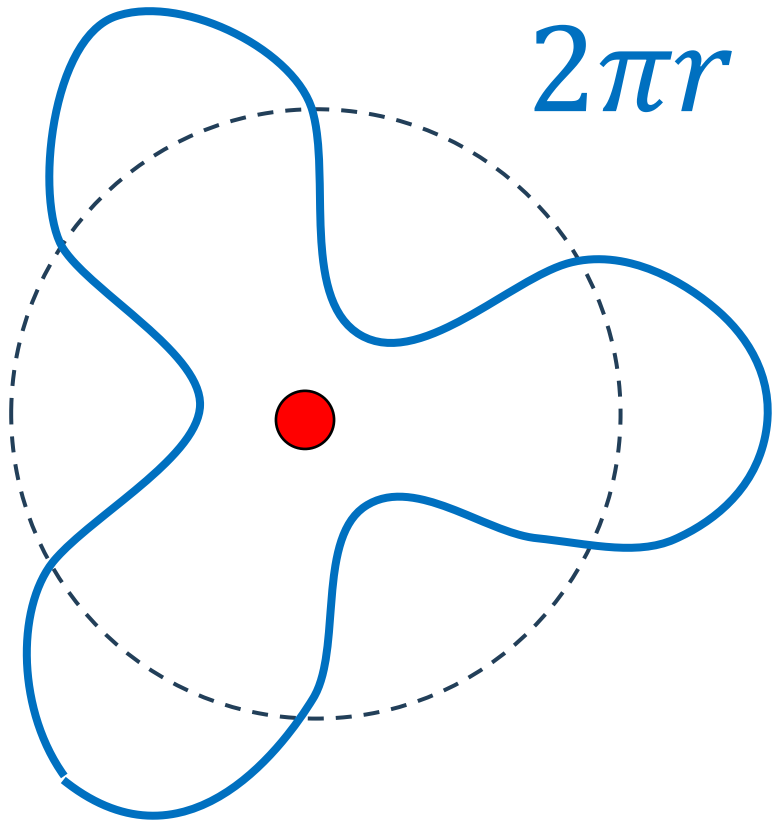
Electron on circular orbits

1. Specific orbits are stable
2. Angular momentum quantized:

$$m_e v r = n\hbar = \frac{nh}{2\pi}$$

$$L = 2\pi r = n\,\lambda, \qquad \lambda = \frac{h}{p} = \frac{h}{m_e v}$$





$$2\pi r = n\,\lambda$$

BOHR MODEL: ENERGY LEVELS

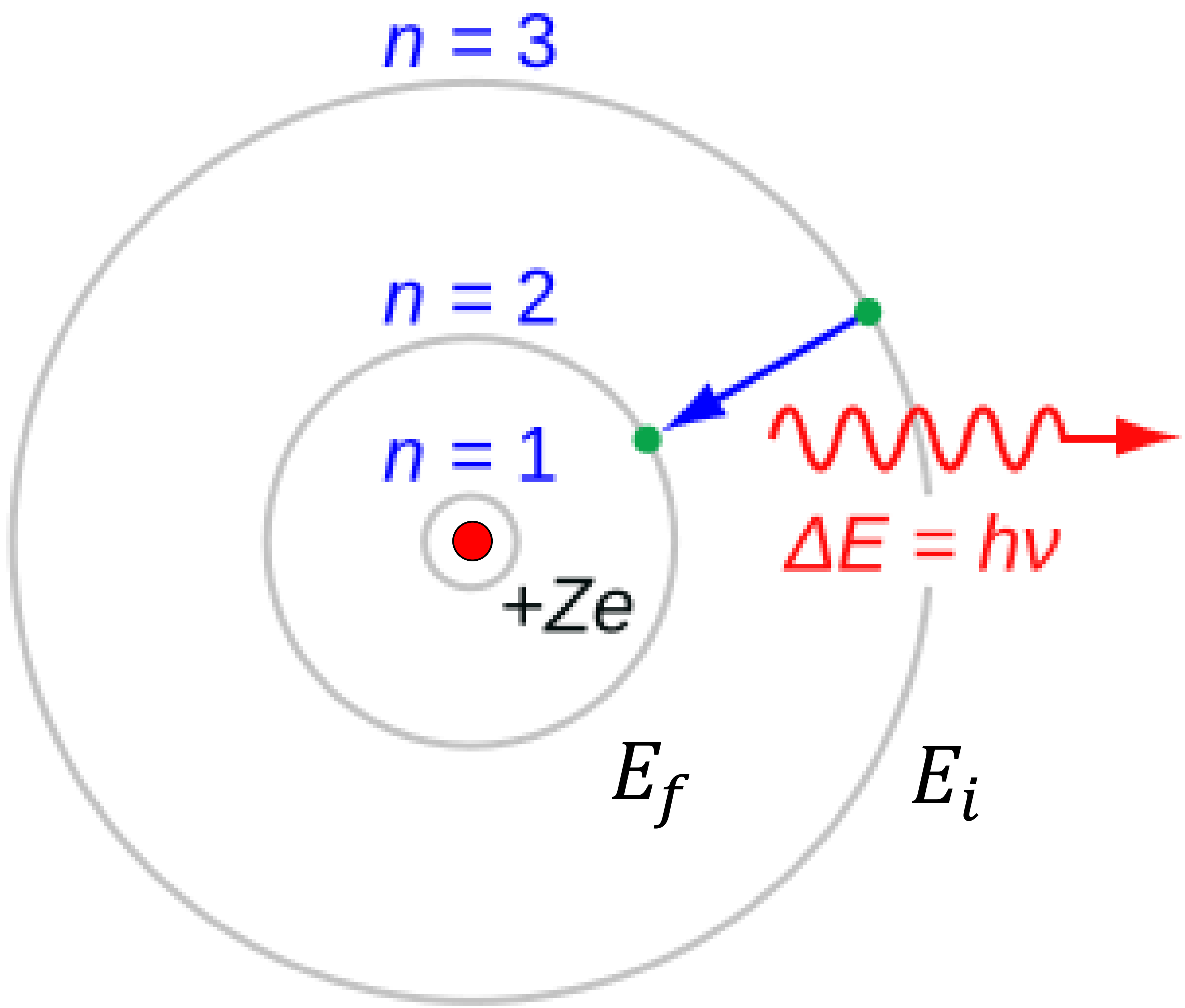
Electron on circular orbits

1. Specific orbits are stable
2. Angular momentum quantized:

$$m_e v r = n\hbar = \frac{nh}{2\pi}$$

3. Radiation depends on difference in energy levels NOT the electron circling frequency

$$hf = \frac{hc}{\lambda} = E_i - E_f$$

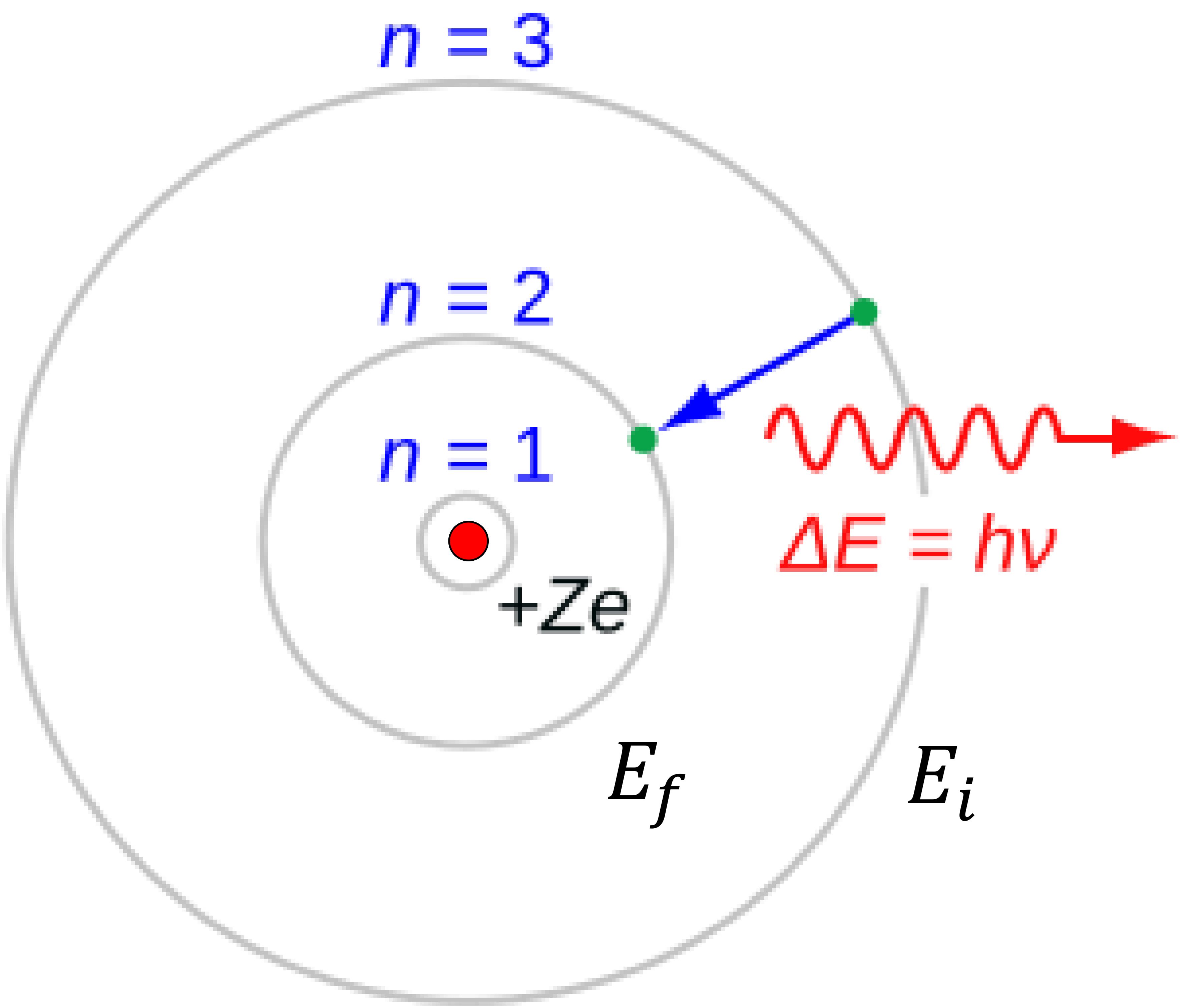


BOHR MODEL: ENERGY LEVELS

- Radius of the Bohr orbits?
- Discrete energy levels

$$E = K + U$$

$$\begin{cases} U = -\dfrac{1}{4\pi\epsilon_0}\dfrac{e^2}{r} \\ K = \dfrac{1}{2}m_e v^2 \end{cases}$$



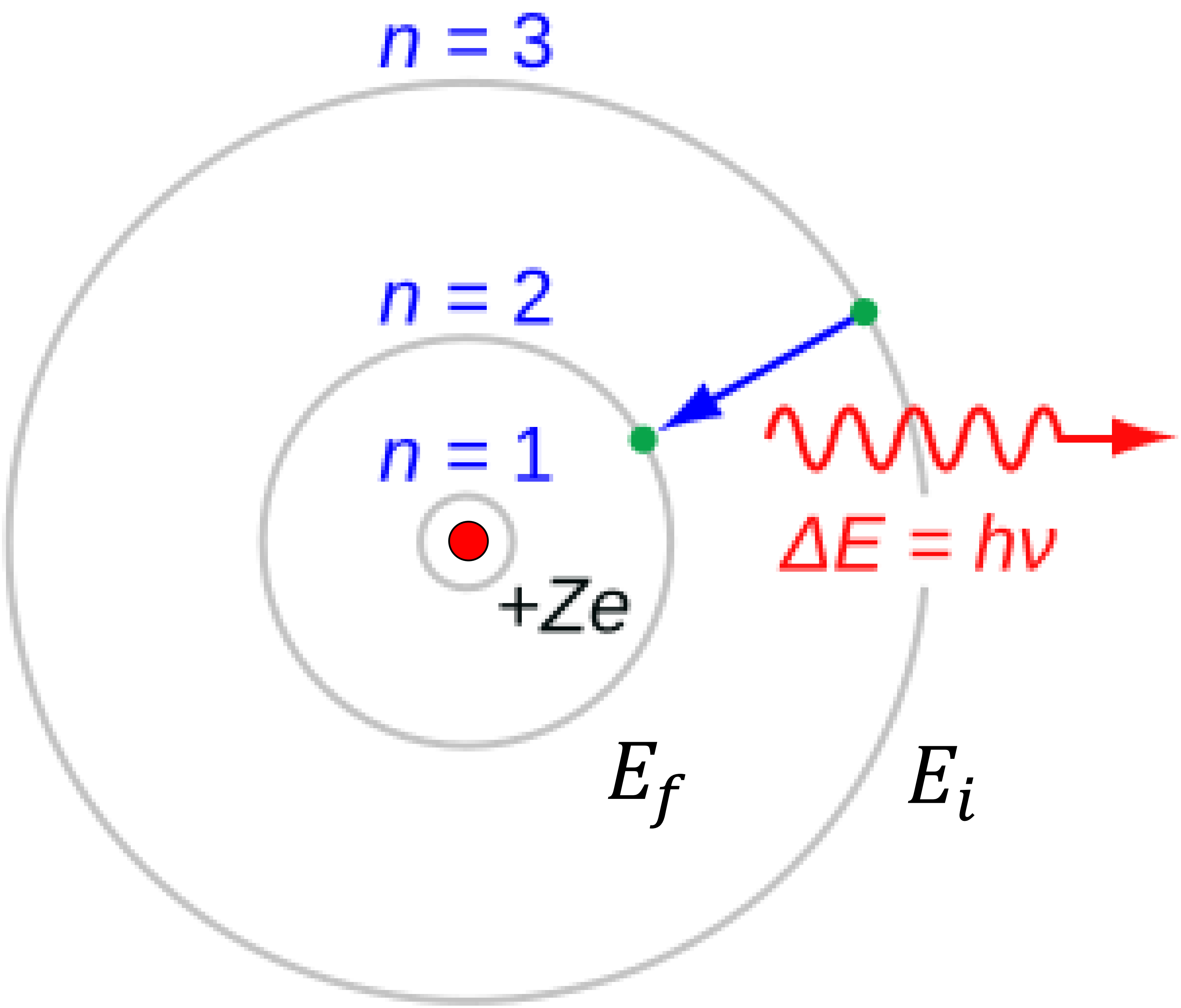
BOHR MODEL: ENERGY LEVELS

- Coulomb force F should equal mass times centripetal acceleration a_c:

$$\frac{1}{4\pi\epsilon_0}\frac{e^2}{r^2} = m_e a_c = \frac{m_e v^2}{r}$$

$$\Rightarrow \quad K = \frac{1}{2} m_e v^2 = \frac{1}{4\pi\epsilon_0}\frac{e^2}{2r}$$

$$m_e v r = n\hbar \Rightarrow v^2 = \frac{n^2\hbar^2}{m_e^2 r^2} = \frac{1}{4\pi\epsilon_0}\frac{e^2}{m_e r}$$



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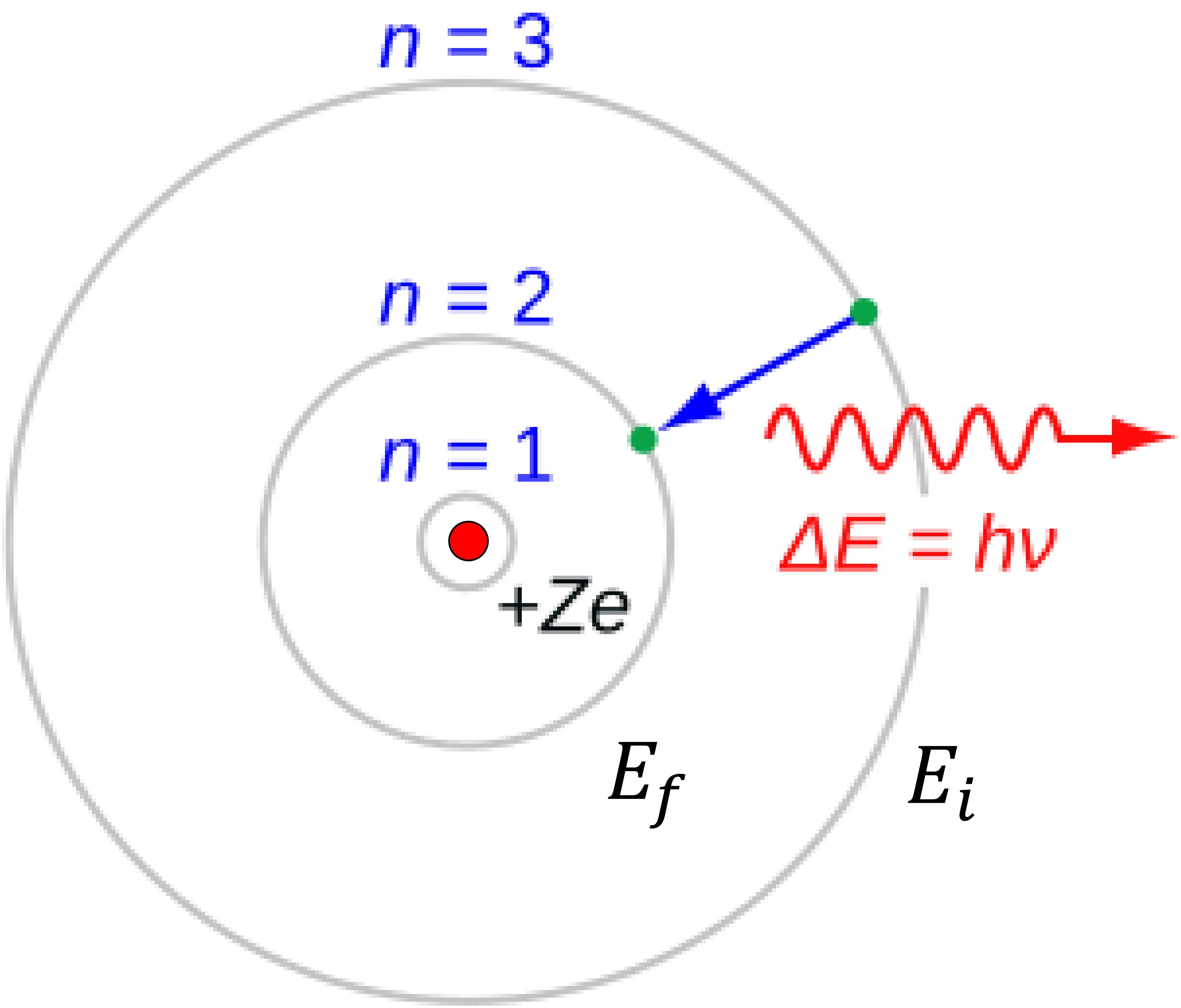
Extract radii r_n



BOHR MODEL: ENERGY LEVELS

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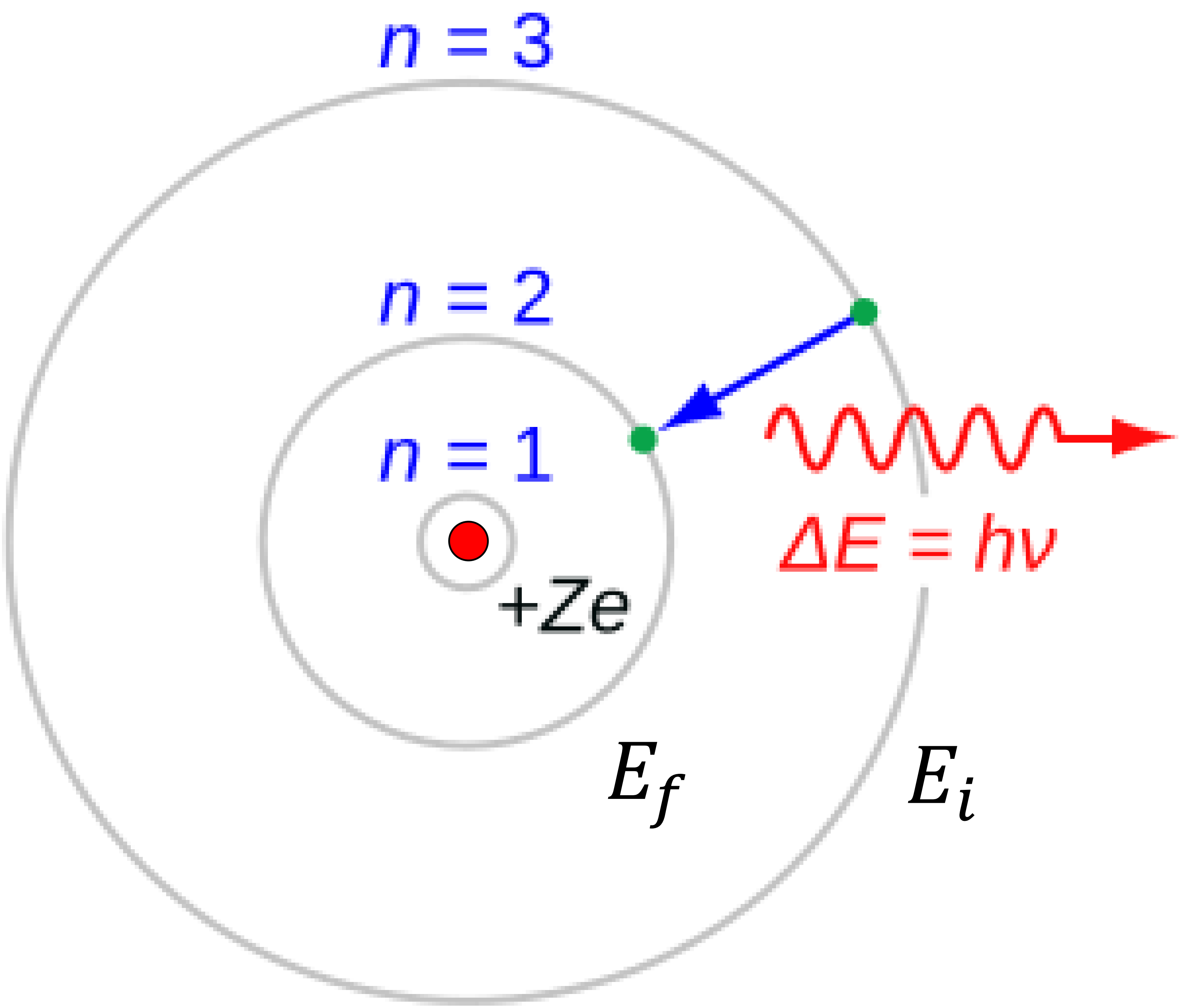
$$\frac{n^2\hbar^2}{m_e^2 r^2} = \frac{1}{4\pi\epsilon_0}\frac{e^2}{m_e r}$$

$$\Rightarrow \quad r_n = \frac{4\pi\epsilon_0\hbar^2}{m_e\, e^2} n^2 = \mathrm{a_0\, n^2}$$

Bohr radius: $\mathrm{a}_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e\, e^2} = 0.0529\ \mathrm{nm}$



BOHR MODEL: ENERGY LEVELS

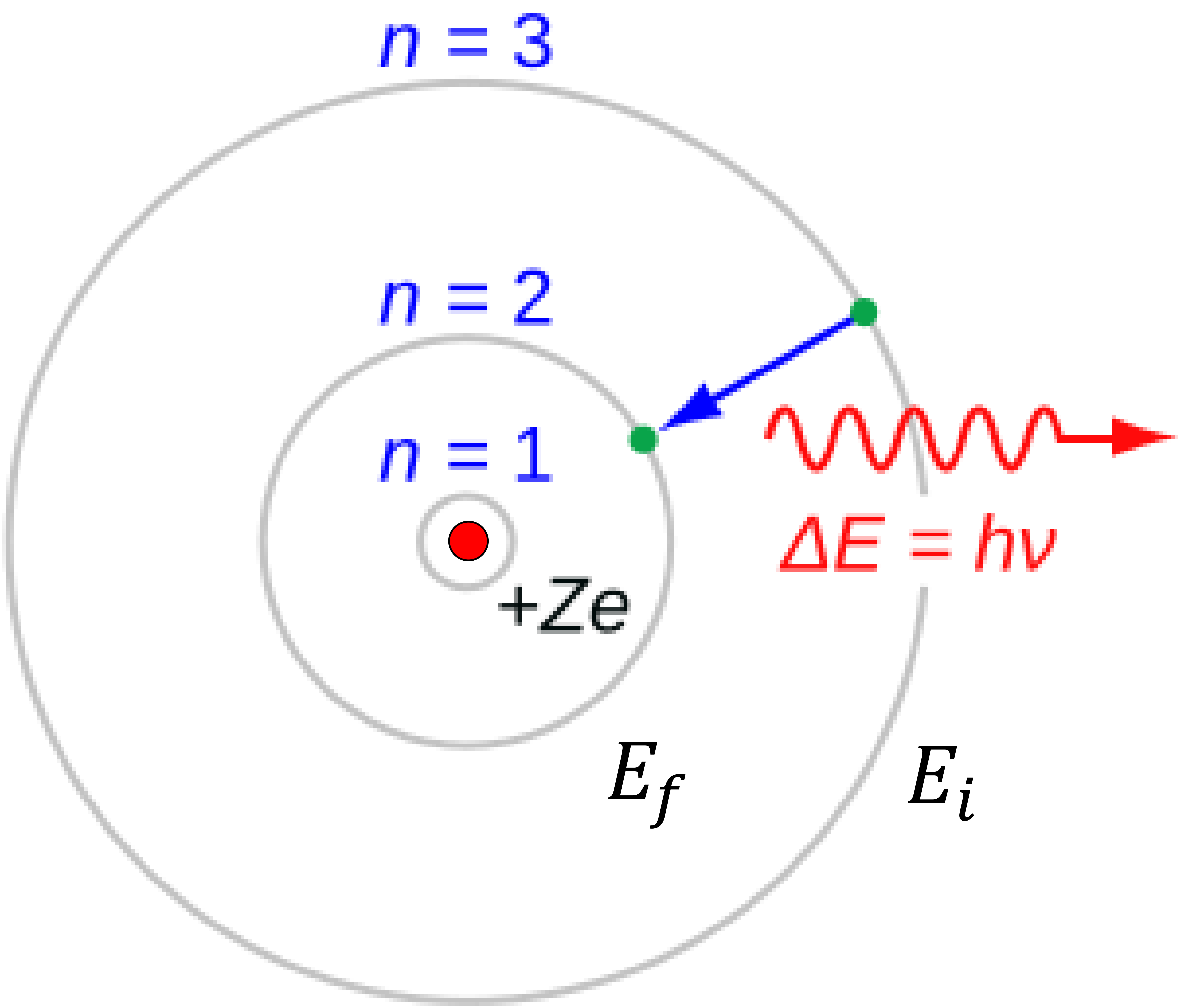
- What are the corresponding energies E_n?

$$\begin{cases} K = \frac{1}{2} m_e v^2 = \frac{1}{4\pi\epsilon_0} \frac{e^2}{2r} \\ U = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{r} \end{cases}$$

$$\Rightarrow \quad E_n = K + U = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{2a_0} \left(\frac{1}{n^2}\right)$$

$$E_n = -\frac{13.6}{n^2}\ \text{eV}$$

Rydberg energy: $Ry = \frac{1}{4\pi\epsilon_0} \frac{e^2}{2a_0} = 13.6\ \text{eV}$



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$$r_n = \frac{4\pi\epsilon_0\hbar^2}{m_e\, e^2} n^2 = \text{a}_0\ \text{n}^2$$

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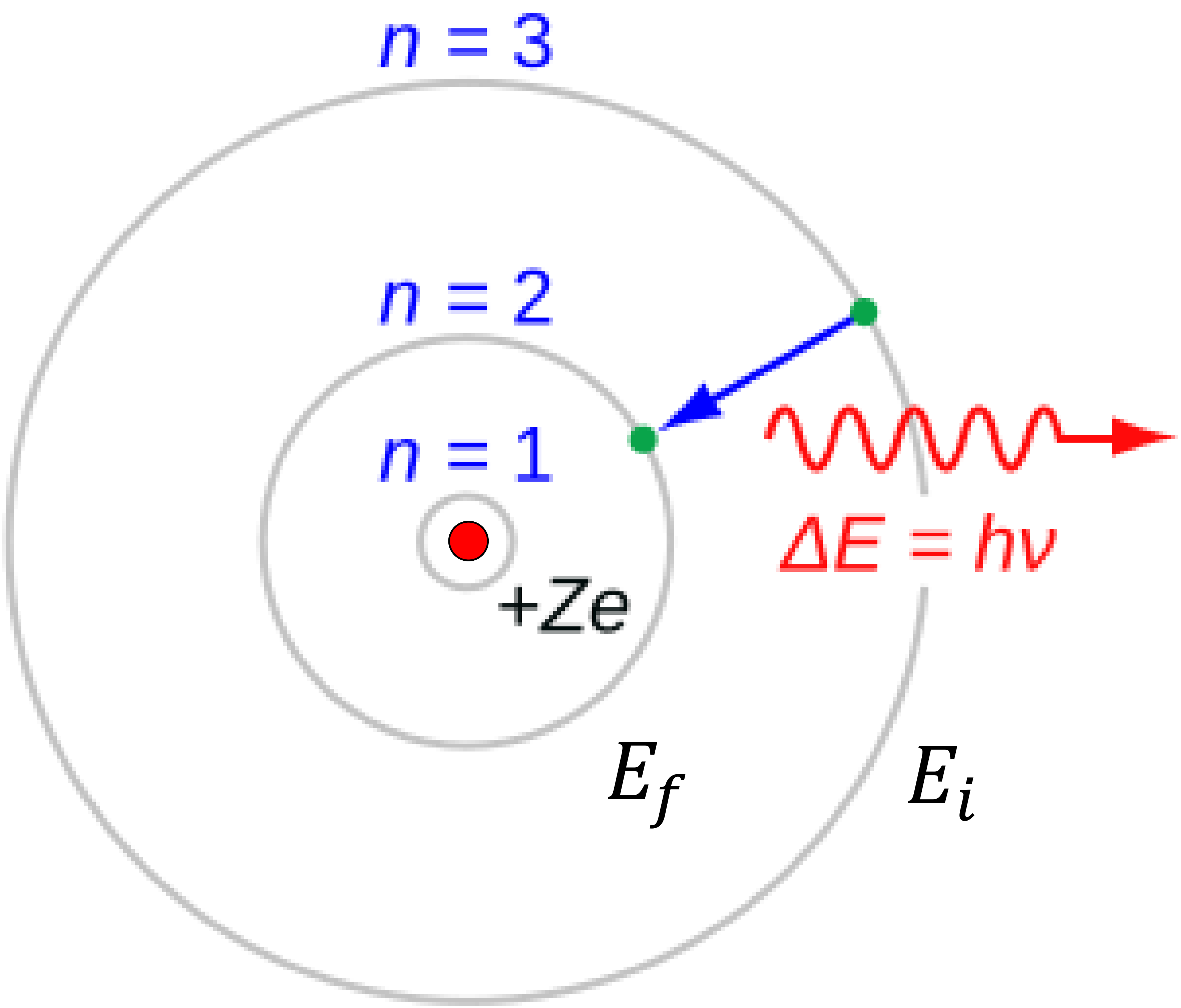
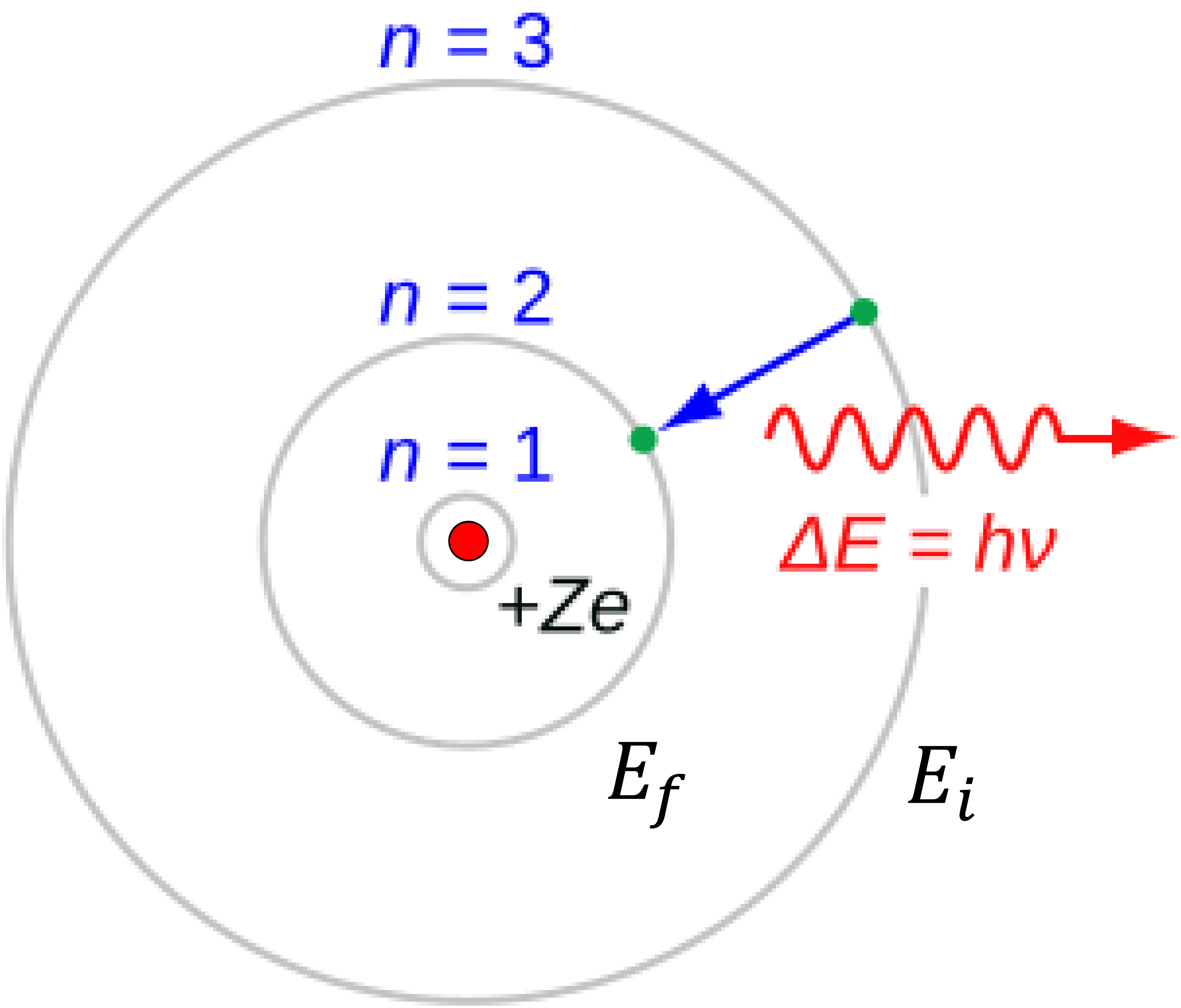


BOHR MODEL: ENERGY LEVELS

- Ionized atoms with only a single electron: $\mathrm{He}^{+}, \quad \mathrm{Li}^{2+}, \ \ldots$
- The atom has atomic number Z and its nucleus charge is $+Ze$

$$\boldsymbol{E_n} = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{2a_0}\left(\frac{Z^2}{n^2}\right) = -\frac{13.6\,Z^2}{n^2}\ \mathrm{eV}$$

$$\boldsymbol{r_n} = \frac{4\pi\epsilon_0\hbar^2}{m_e\,e^2}n^2 = \frac{\mathrm{a}_0}{Z}\ \mathrm{n}^2$$



BOHR MODEL: ENERGY LEVELS

Exercise: What is the radius of a highly exited hydrogen atom (a so-called Rydberg atom: if the atom is in the 167th energy level ? (remember that $r_n = n^2\, \mathrm{a}_0 = n^2\, 0.0529$ nm)

And what is its energy level? (Remember $E_n = -\frac{13.6}{n^2}$ eV)

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$$r_n = n^2\, \mathrm{a}_0 = n^2\, 0.0529\ \mathrm{nm} = 167^2\, 0.0529\ \mathrm{nm}$$
$$\approx (400 - 60 + 9) \times 100 \times 0.0529\ \mathrm{nm} \approx 1750\ \mathrm{nm}$$

And what is its energy level? (Remember $E_n = -\frac{13.6}{n^2}\ \mathrm{eV}$)

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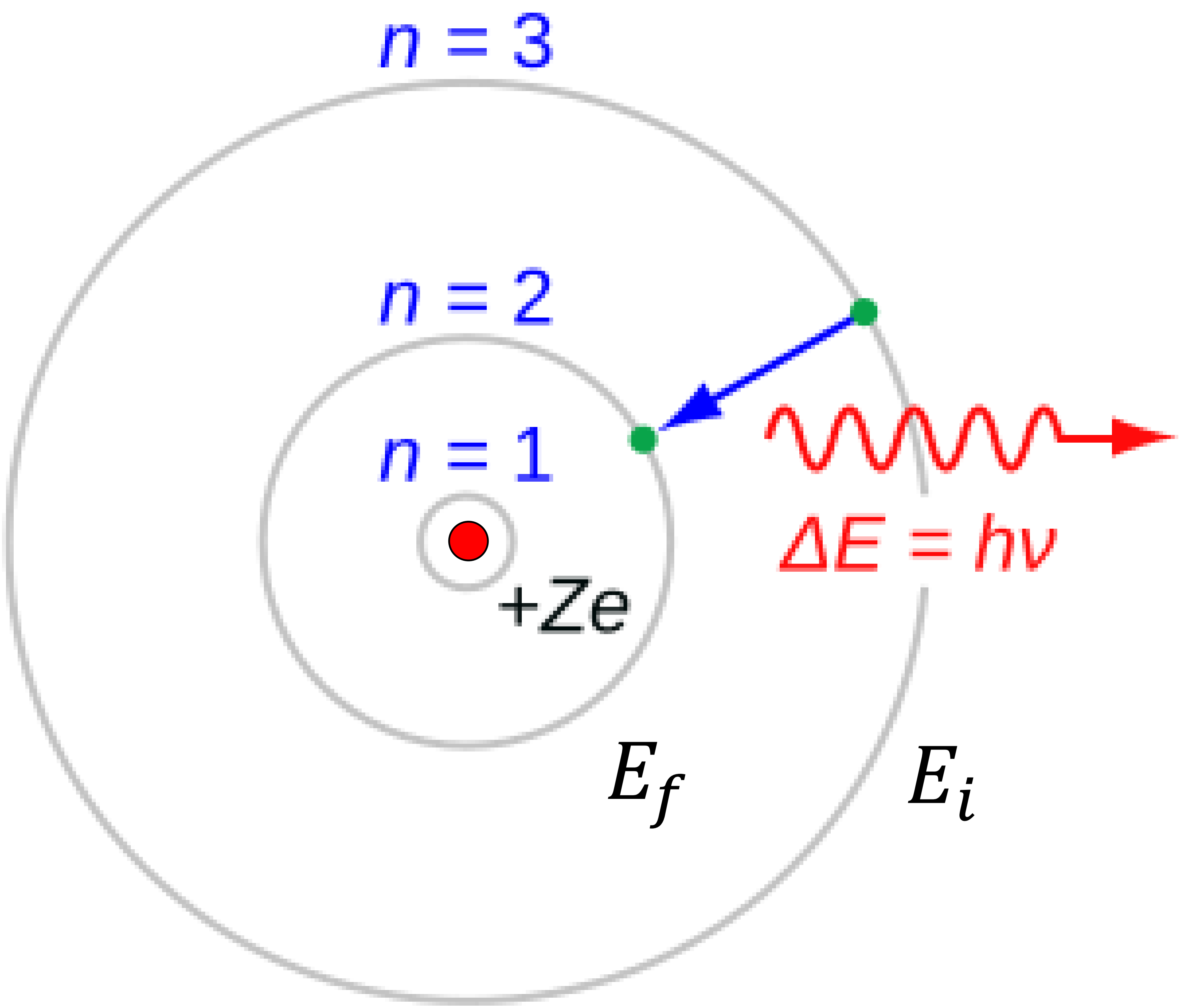
And what is its energy level? (Remember $E_n = -\frac{13.6}{n^2}$ eV)

$$E_n = -\frac{13.6}{n^2}\,\mathrm{eV} \approx -\frac{13.6}{35000}\,\mathrm{eV} \approx -4 \times 10^{-4}\,\mathrm{eV}$$

BOHR MODEL: ENERGY LEVELS

- Discrete energy levels
- Levels depend on atom type
- Electron on circular orbits
- Transitions by emitting/absorbing photons

- Minimum energy: **ground level or ground state**
- Higher energy levels: **excited levels or excited state**



BOHR MODEL: ENERGY TRANSITIONS

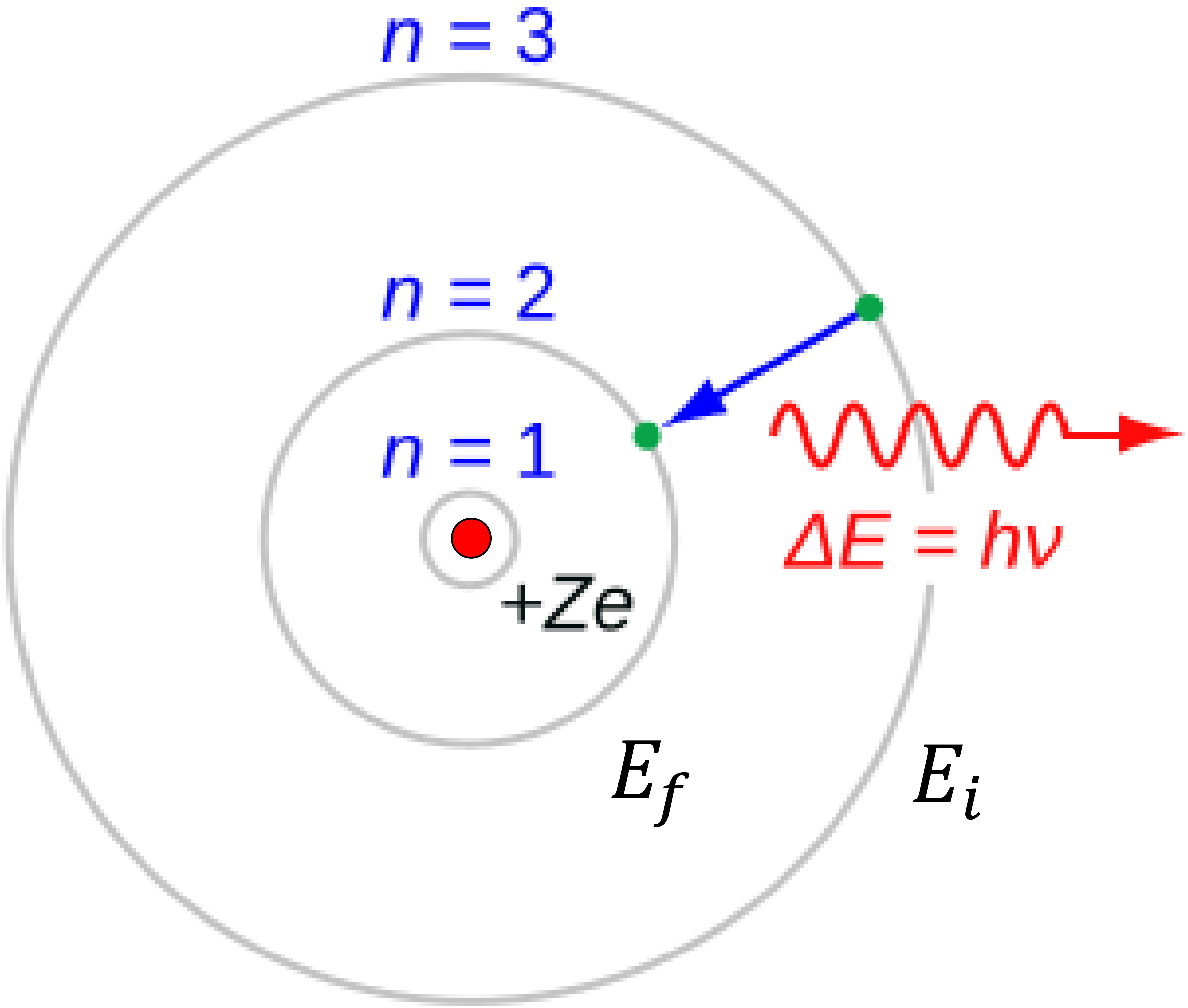
- Discrete energy levels
- Transitions between energy levels?

$$hf = \frac{hc}{\lambda} = E_i - E_f$$

$$\frac{1}{\lambda} = R_H \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

With Rydberg constant:

$$R_H = \frac{R_y}{hc} = 1.09737 \times 10^7 \text{ m}^{-1}$$



BOHR MODEL: SPECTRAL LINES

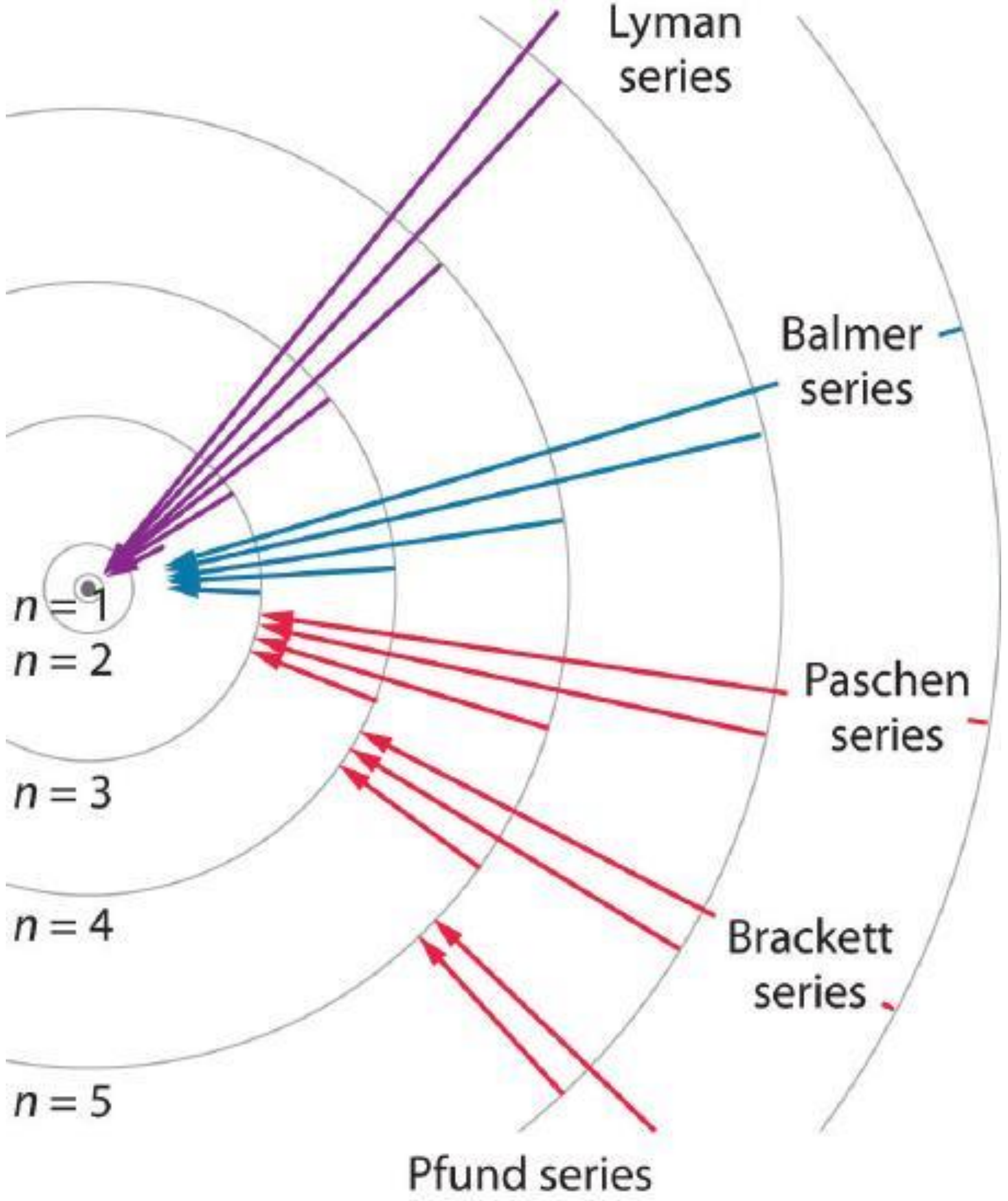
- Discrete energy levels
- Transitions between energy levels?

$$\frac{1}{\lambda} = R_H\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

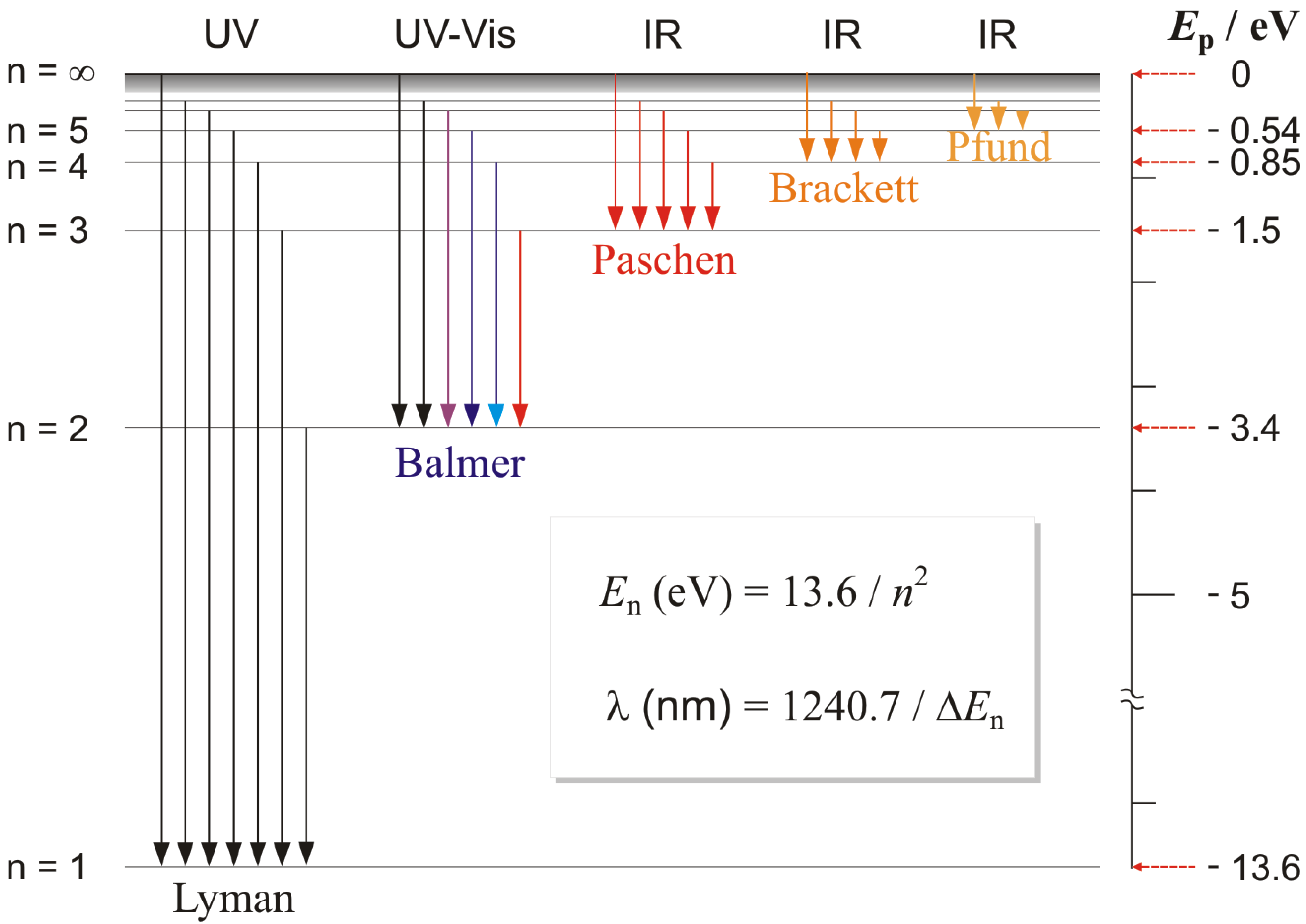
Lyman: $\frac{1}{\lambda} = R_H\left(1 - \frac{1}{n_i^2}\right)$

Balmer: $\frac{1}{\lambda} = R_H\left(\frac{1}{4} - \frac{1}{n_i^2}\right)$

Paschen: $\frac{1}{\lambda} = R_H\left(\frac{1}{9} - \frac{1}{n_i^2}\right)$



BOHR MODEL: SPECTRAL LINES



$$E_n\ (\text{eV}) = 13.6 / n^2$$

$$\lambda\ (\text{nm}) = 1240.7 / \Delta E_n$$

BOHR MODEL: ENERGY LEVELS

Exercise: Calculate the first wavelength of the Lyman, Balmer and Paschen series ($R_H = \frac{R_y}{hc} = 1.09737 \times 10^7$ m^{-1})

Remember: $\frac{1}{\lambda} = R_H \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$

BOHR MODEL: ENERGY LEVELS

Exercise: Calculate the first wavelength of the Lyman, Balmer and Paschen series ($R_H = \frac{R_y}{hc} = 1.09737 \times 10^7$ m^{-1})

Lyman: $\frac{1}{\lambda} = R_H\left(1 - \frac{1}{4}\right) = \frac{3}{4}R_H \Rightarrow \lambda = \frac{4}{3 \cdot 1.1} \times 10^2 \text{ nm} \approx 120 \text{ nm}$

Balmer: $\frac{1}{\lambda} = R_H\left(\frac{1}{4} - \frac{1}{9}\right) = \frac{5}{36}R_H \Rightarrow \lambda = \frac{36}{5 \cdot 1.1} \times 10^2 \text{ nm} \approx 650 \text{ nm}$

Paschen: $\frac{1}{\lambda} = R_H\left(\frac{1}{9} - \frac{1}{16}\right) = \frac{7}{144}R_H \Rightarrow \lambda = \frac{144}{7 \cdot 1.1} \times 10^2 \text{ nm} \approx 2 \times 10^3 \text{nm}$

BOHR MODEL: ENERGY LEVELS

Exercise: Calculate the energy difference corresponding to the second Balmer spectral line ($R_H = \frac{R_y}{hc} = 1.09737 \times 10^7$ m^{-1})

BOHR MODEL: ENERGY LEVELS

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Balmer: $\Delta f = \frac{hc}{\lambda} = R_y\left(\frac{1}{4} - \frac{1}{16}\right) = \frac{3}{16} R_y \approx \frac{3}{16}\ 13.6\ eV \approx 2.5$ eV

BOHR MODEL: VELOCITY OF THE ELECTRON

Exercise: Calculate the velocity of the electron for the first two energy levels: n = 1, 2 ($a_0 = 0.0529\ \mathrm{nm}$)

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$$v = \frac{n\hbar}{m_e r} = \frac{\hbar}{m_e\, n a_0} = \frac{1}{n} \times \frac{1.055 \times 10^{-34}\ \mathrm{J \cdot s}}{9.11 \times 10^{-31}\ \mathrm{kg} \times 0.0529\ \mathrm{nm}}$$

$$= \frac{1}{n} \times \frac{1.055}{9.11 \cdot 0.529} \times 10^{7} \times \frac{\frac{\mathrm{kg\ m^2}}{\mathrm{s^2}}\mathrm{s}}{\mathrm{kg\ m}} \approx \frac{2.2}{n} \times 10^{6}\ \mathrm{m/s}$$

$$\Rightarrow \qquad v_1 = 2.2 \times 10^{6}\, \frac{\mathrm{m}}{\mathrm{s}}, \qquad v_2 = 1.1 \times 10^{6}\, \frac{\mathrm{m}}{\mathrm{s}}$$

BOHR MODEL: VELOCITY OF THE ELECTRON

Exercise: Calculate the velocity of the electron for the first two energy levels: n = 1, 2 ($\mathrm{a}_0 = 0.0529\ \mathrm{nm}$)

Alternative approach :

$$v = \frac{n\hbar}{m_e r} = \frac{\hbar c^2}{m_e c^2\, n a_0} = \frac{1}{n} \times \frac{1240\ \mathrm{eV\ nm} \cdot c}{2\pi \cdot 0.511 \times 10^6\ \mathrm{eV} \times 0.0529\ \mathrm{nm}}$$

$$= \frac{1}{n} \times \frac{1.240}{2\pi \cdot 0.511 \cdot 0.529} \times 10^{-2} c \approx \frac{1}{n} \frac{5}{2\pi} \times 10^{-2}\ c \approx \frac{1}{n} \frac{5}{2} \times 10^6 \frac{m}{s}$$

$$\Rightarrow \qquad v_1 = 2.5 \times 10^6 \frac{\mathrm{m}}{\mathrm{s}}, \qquad v_2 = 1.25 \times 10^6 \frac{\mathrm{m}}{\mathrm{s}}$$

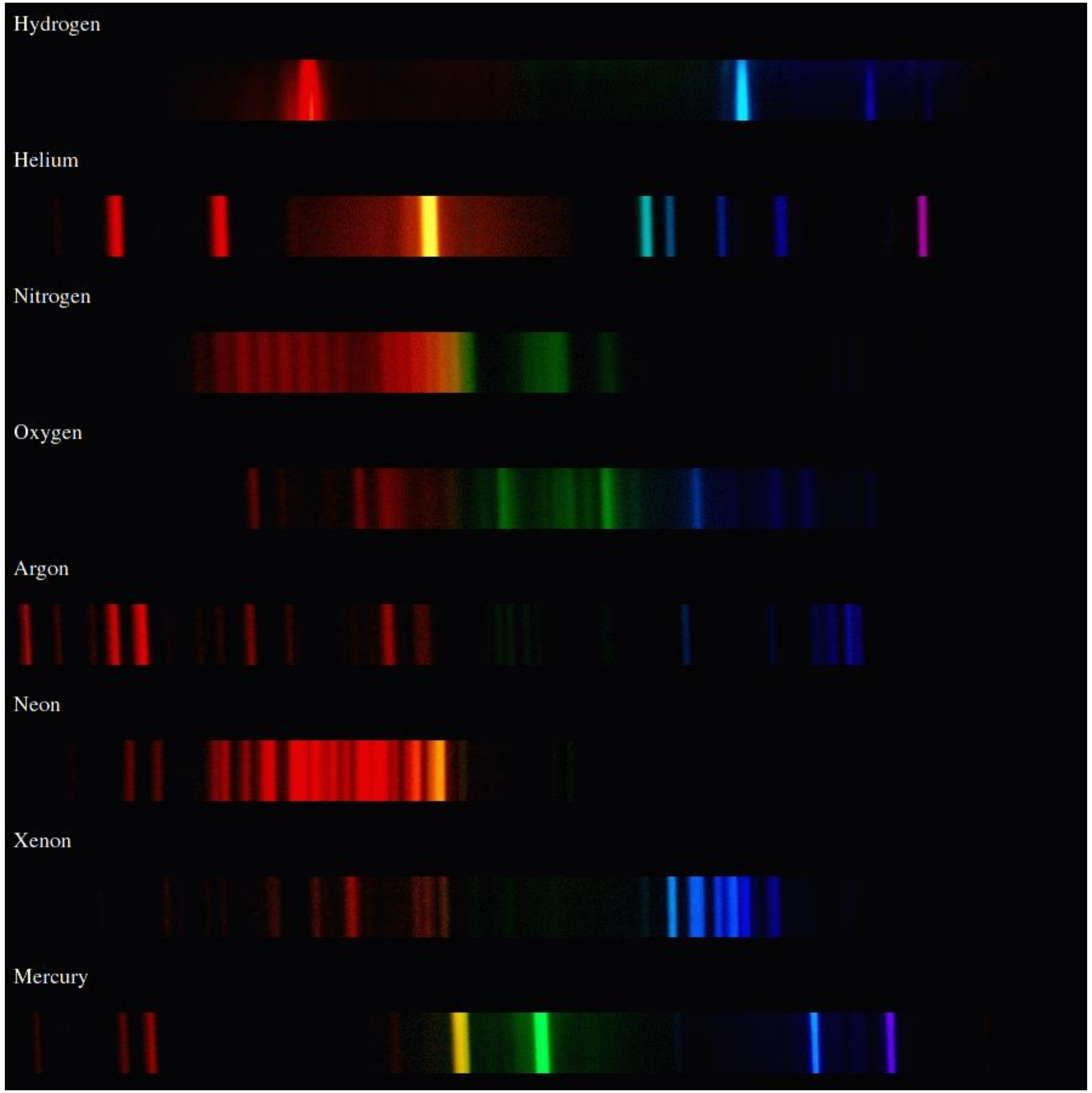
A rough approximation, actual value: $v_1 = 2.19 \times 10^6 \frac{\mathrm{m}}{\mathrm{s}}$

BOHR MODEL: ENERGY LEVELS

- Absorption and emission of light
- Transitions between energy levels

$$hf = \frac{hc}{\lambda} = E_i - E_f$$

- Different atoms have different levels



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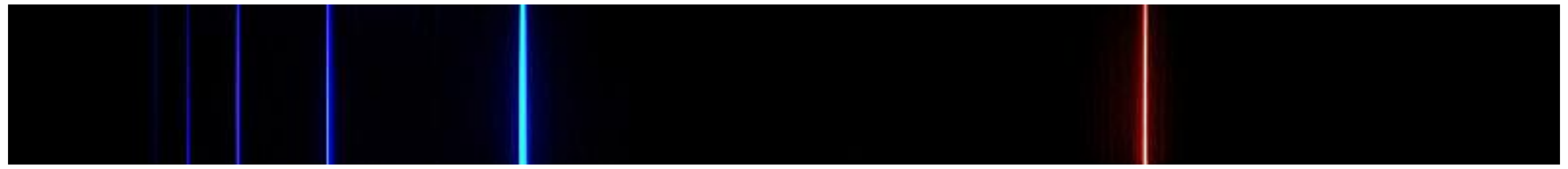
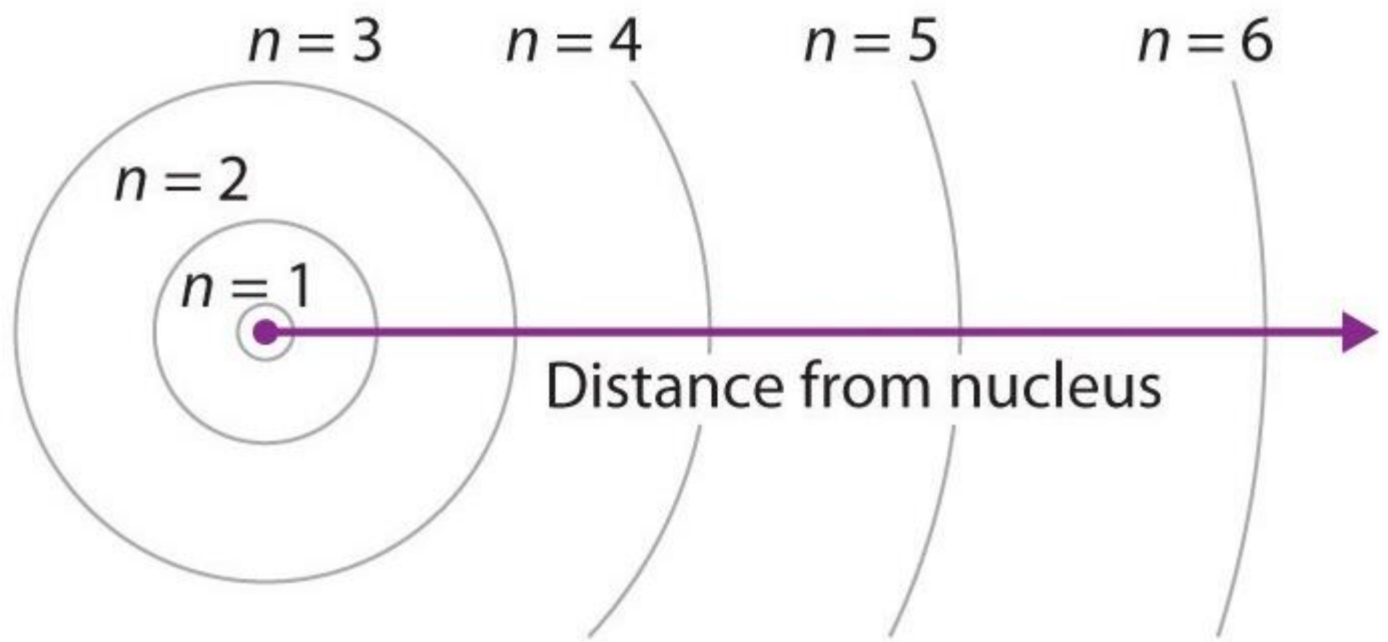




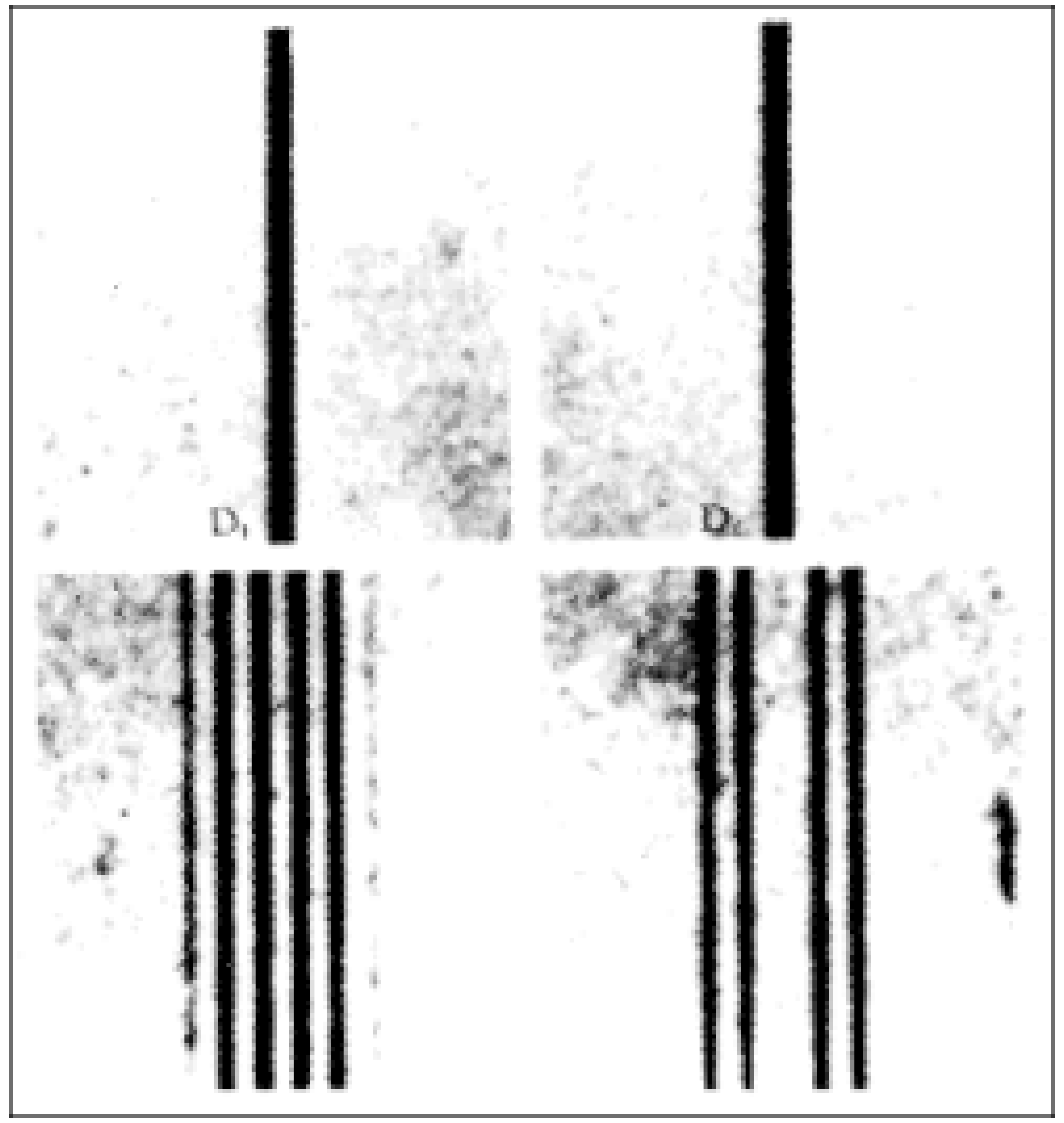
BOHR MODEL: SHORT-COMINGS

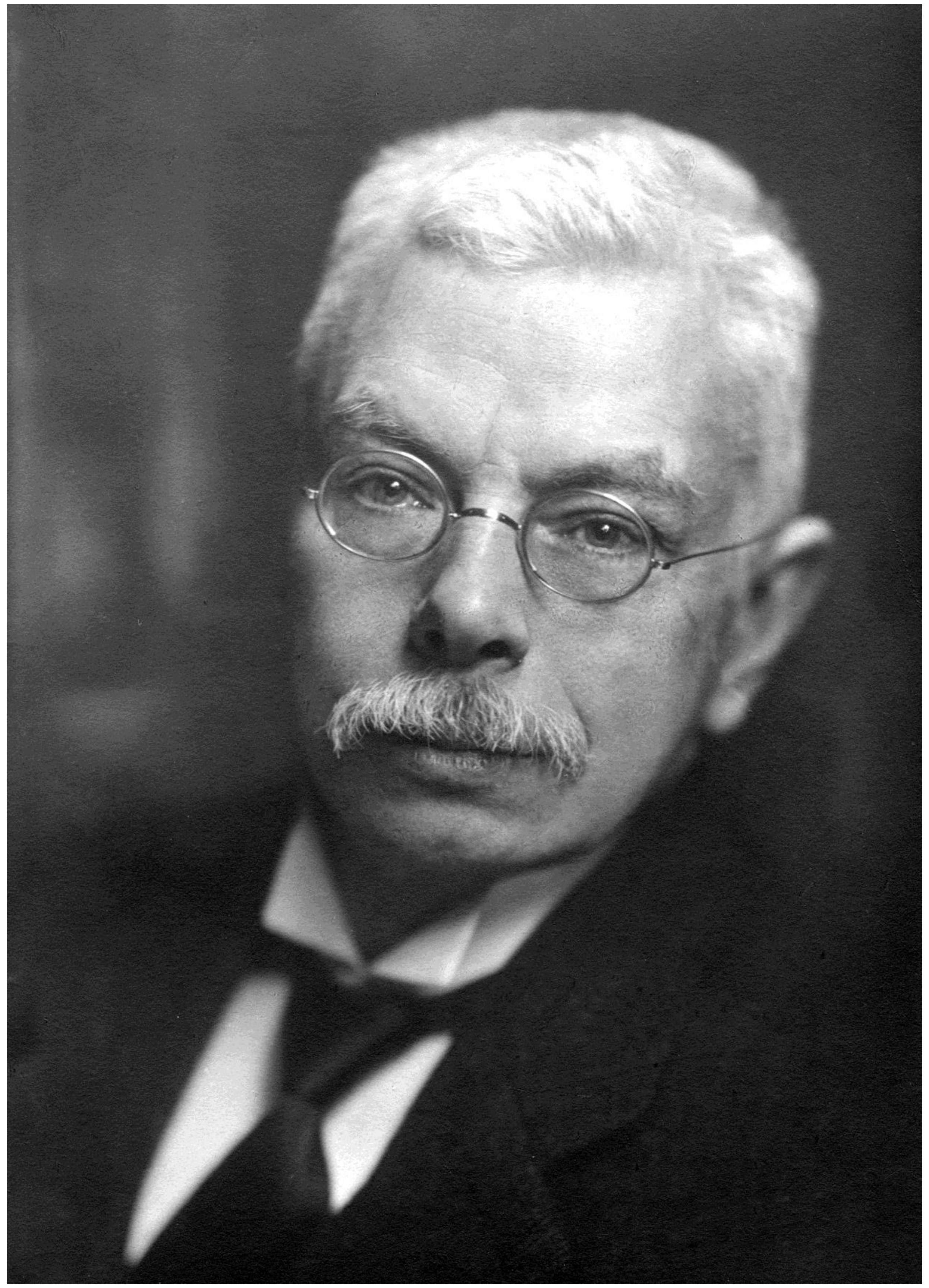
- Minimum angular momentum is nonzero? $= \hbar$
- Spectral lines can be split in experiments by a magnetic field

1896: Zeeman effect

No magnetic field

With magnetic field





Pieter Zeeman