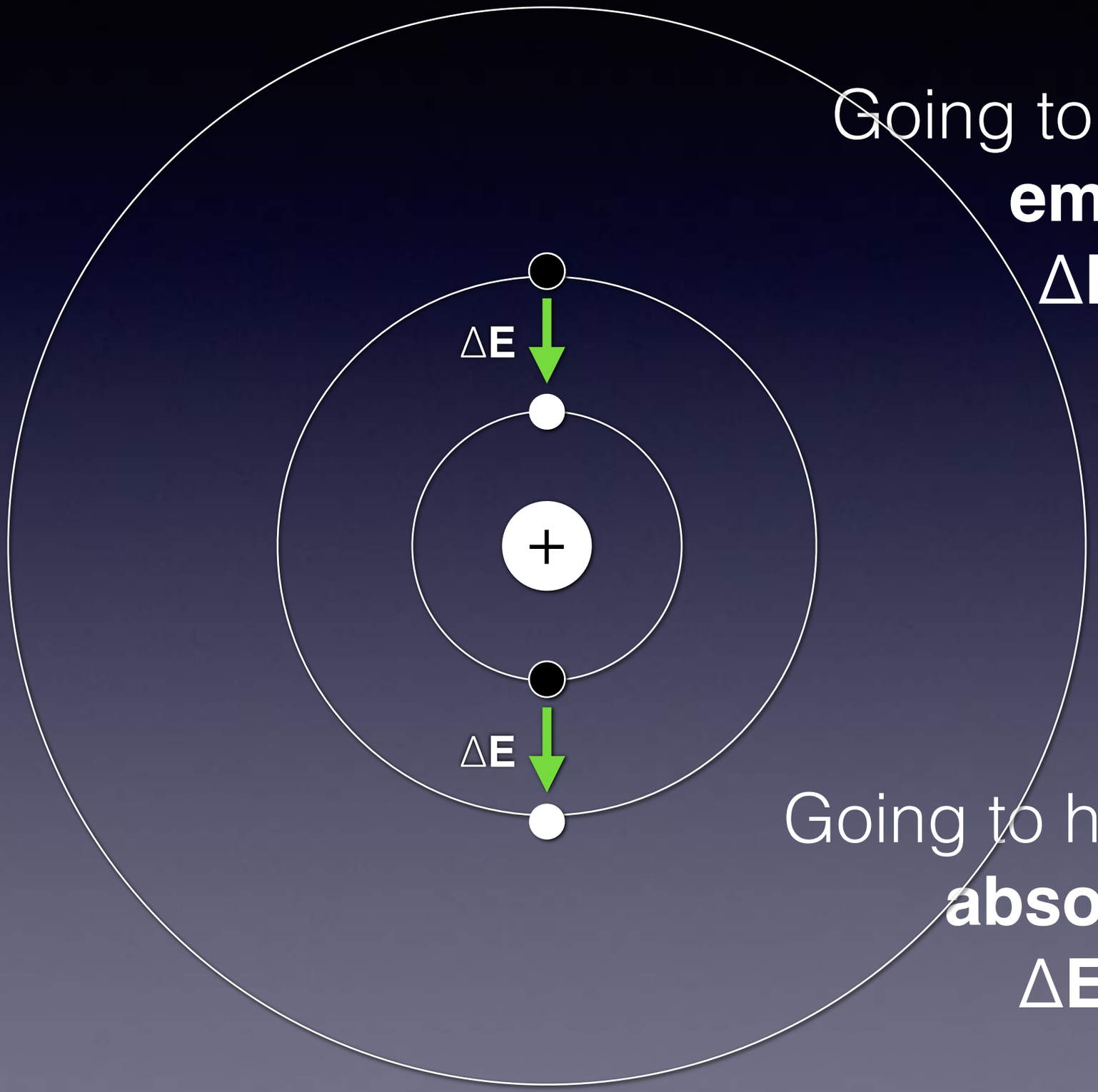
Previously in Molecularity…

Bohr's Theory:

- Atoms have well-defined e^- orbits.
- They don't radiate when in those orbits.
- Circular orbits: only specific orbits with specific angular momenta are allowed {quantization postulate}.
- Transitions in energy: electrons go from one orbit to the next.
- Absorption/emission of energy defined by quantized energy levels

Transitions: $\Delta \mathbf{E} = \mathbf{E}_{\text{final}} - \mathbf{E}_{\text{initial}}$

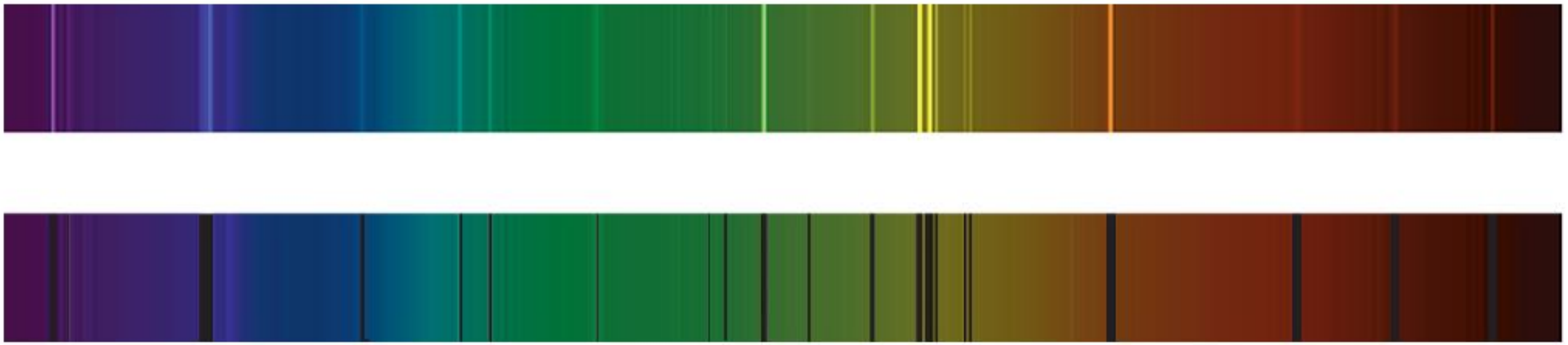


Going to lower energy level:
emitting energy
ΔE is negative

Going to higher energy level:
absorbing energy
ΔE is positive

Transitions: $\Delta \mathbf{E} = \mathbf{E}_{\text{final}} - \mathbf{E}_{\text{initial}}$

Going to lower energy level:
emitting energy
Δ**E** is negative



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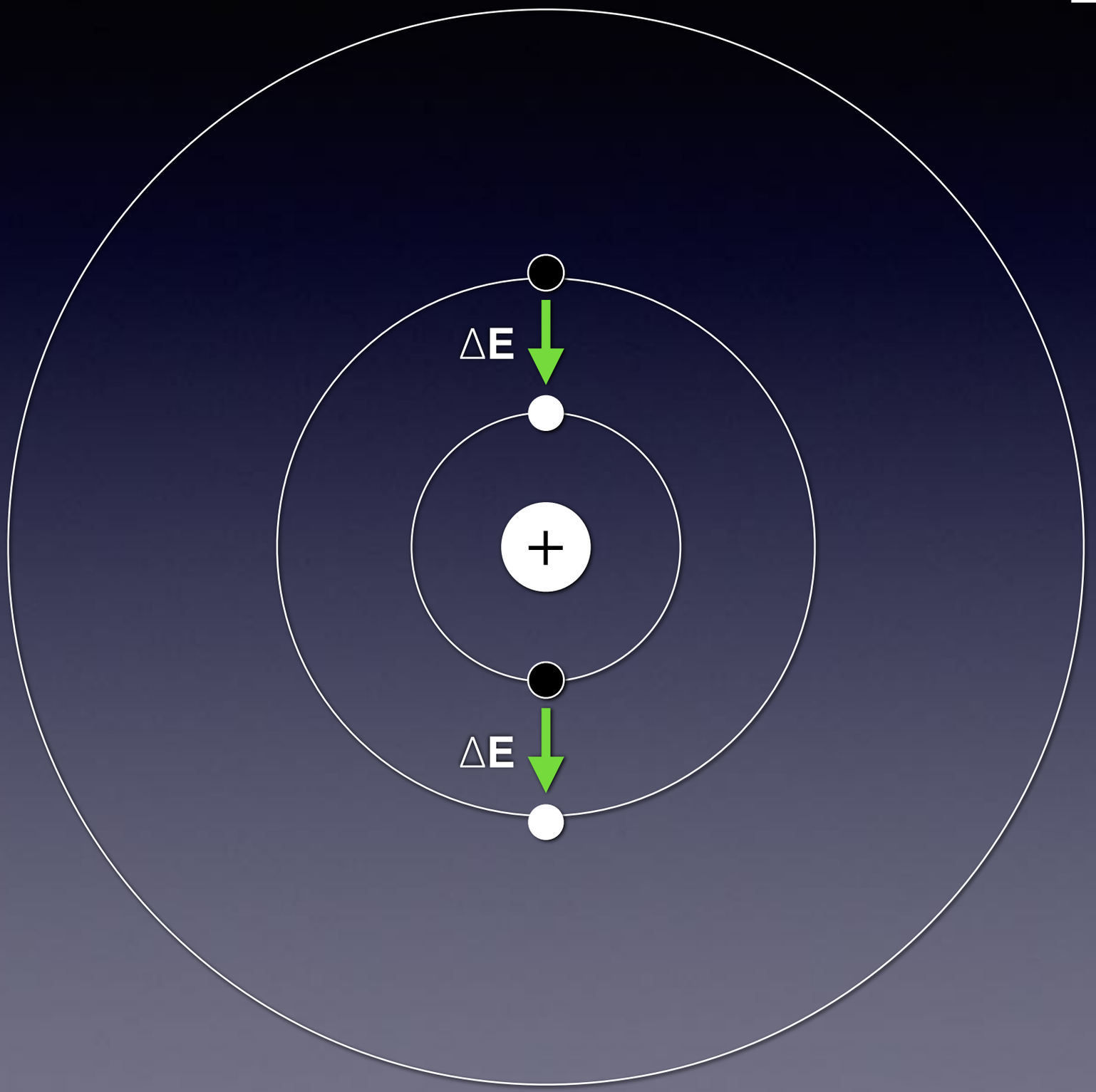
Going to higher energy level:
absorbing energy
Δ**E** is positive

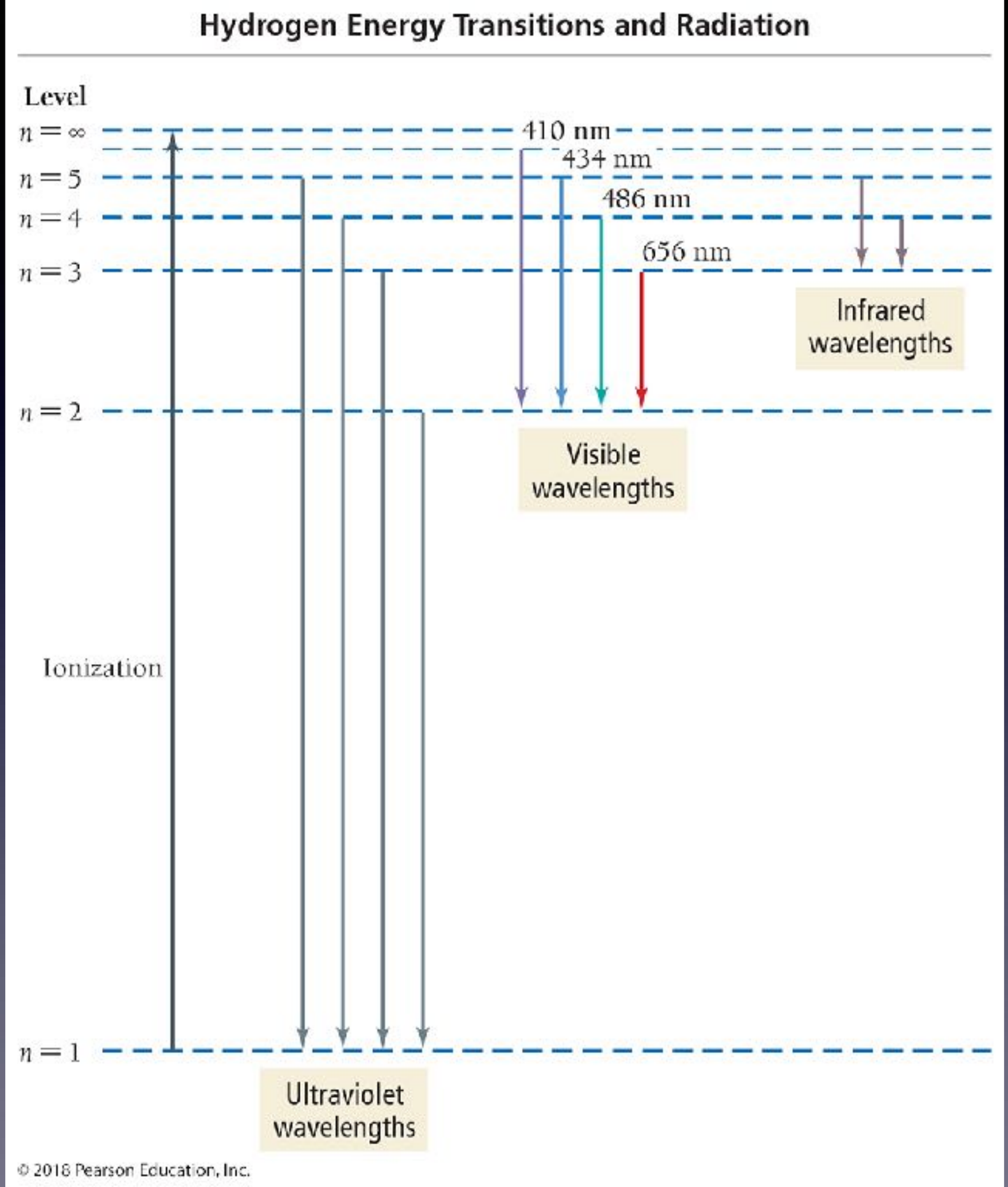
Interrogating the Bohr model…

- Do you understand:
  - How energy values differ for different values of n?
  - How energy values differ for different atoms (different Z)?
- Can you use the Bohr model to determine a particular spectroscopic line?
- Given a spectroscopic line, could you predict the atomic transition?

Bohr summary



- Know **E**, *r* for given *n*
- Positive vs negative **E**
- Ionization / leftover **E**
- Relationship with light λ, ν (nu), and color
- Other multi electron atoms (*Z*)



Series and ionization…

- Can you identify Lyman series, Balmer series, and Paschen series on this graph?
- Any extra energy in an ionization goes in to electron kinetic energy ($mv^2/2$)

Fig 2.22

Where are we going today?

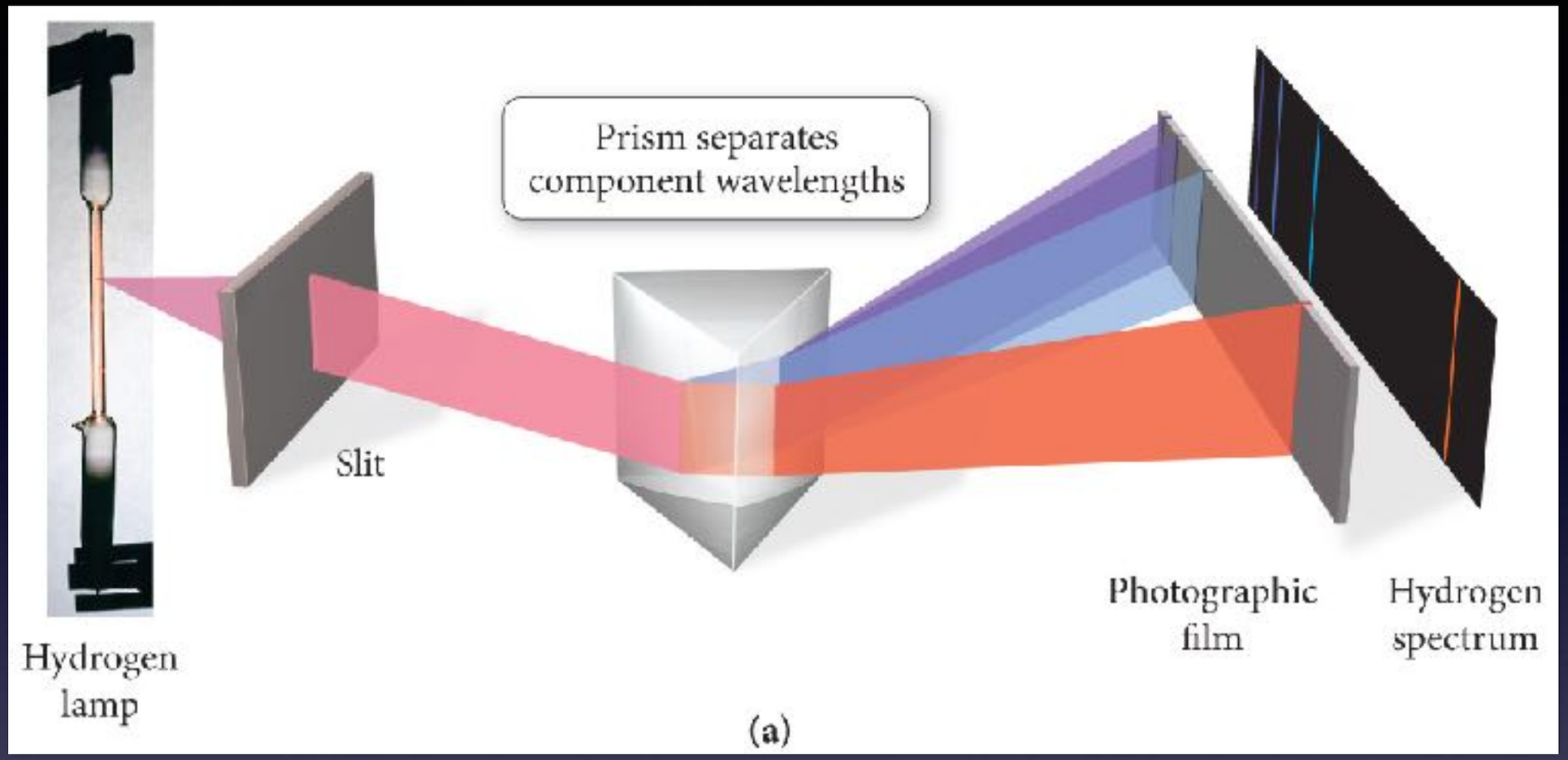
Ch1010-A17-A03 Lecture 4

- Chapter 2: Quantum chemistry (quantistry?)
- § 2.4 Matter as waves
- § 2.6 Waves, nodes, and gratuitous YouTube videos

http://stevedeace.com/wp-content/uploads/2012/11/

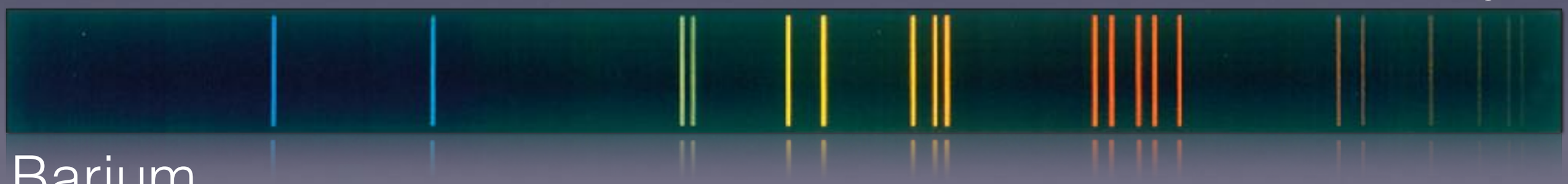
Success…

Tro, Fig 7.11a



…and failure

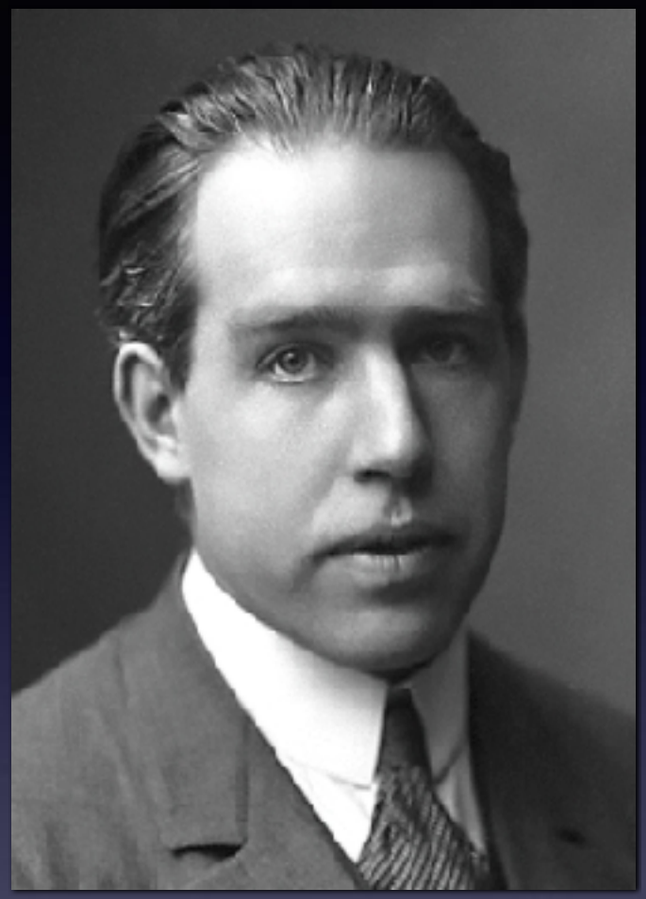
Tro, Fig 7.11b



Barium

Success of the theory…

www.papastravel.com
Stockholm.jpg



upload.wikimedia.org
Niels_Bohr.jpg

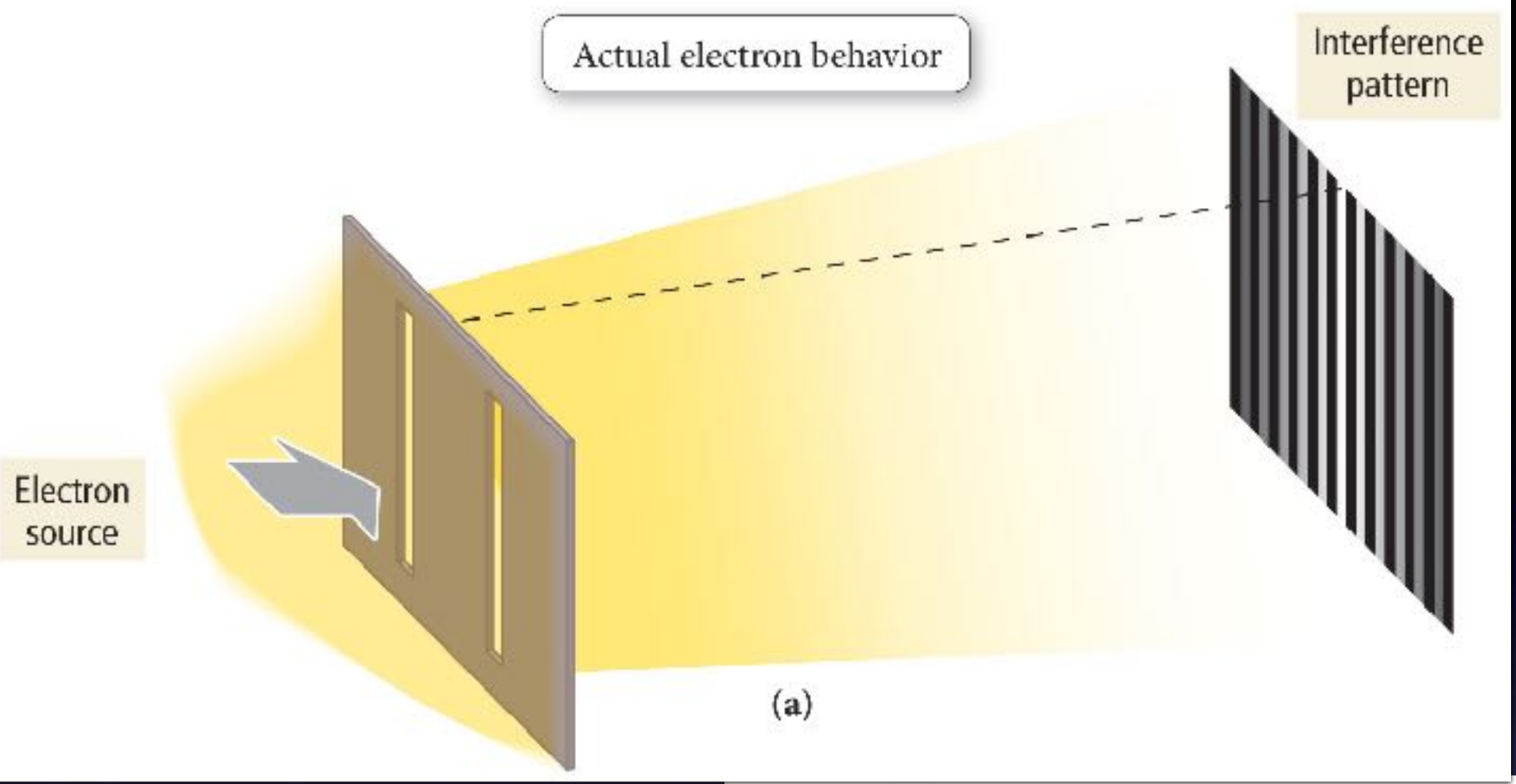
- Gets the spectroscopy of all $1e^-$ atoms right!
- So Bohr gets the hydrogen atom right!
- Go to Stockholm, Niels!

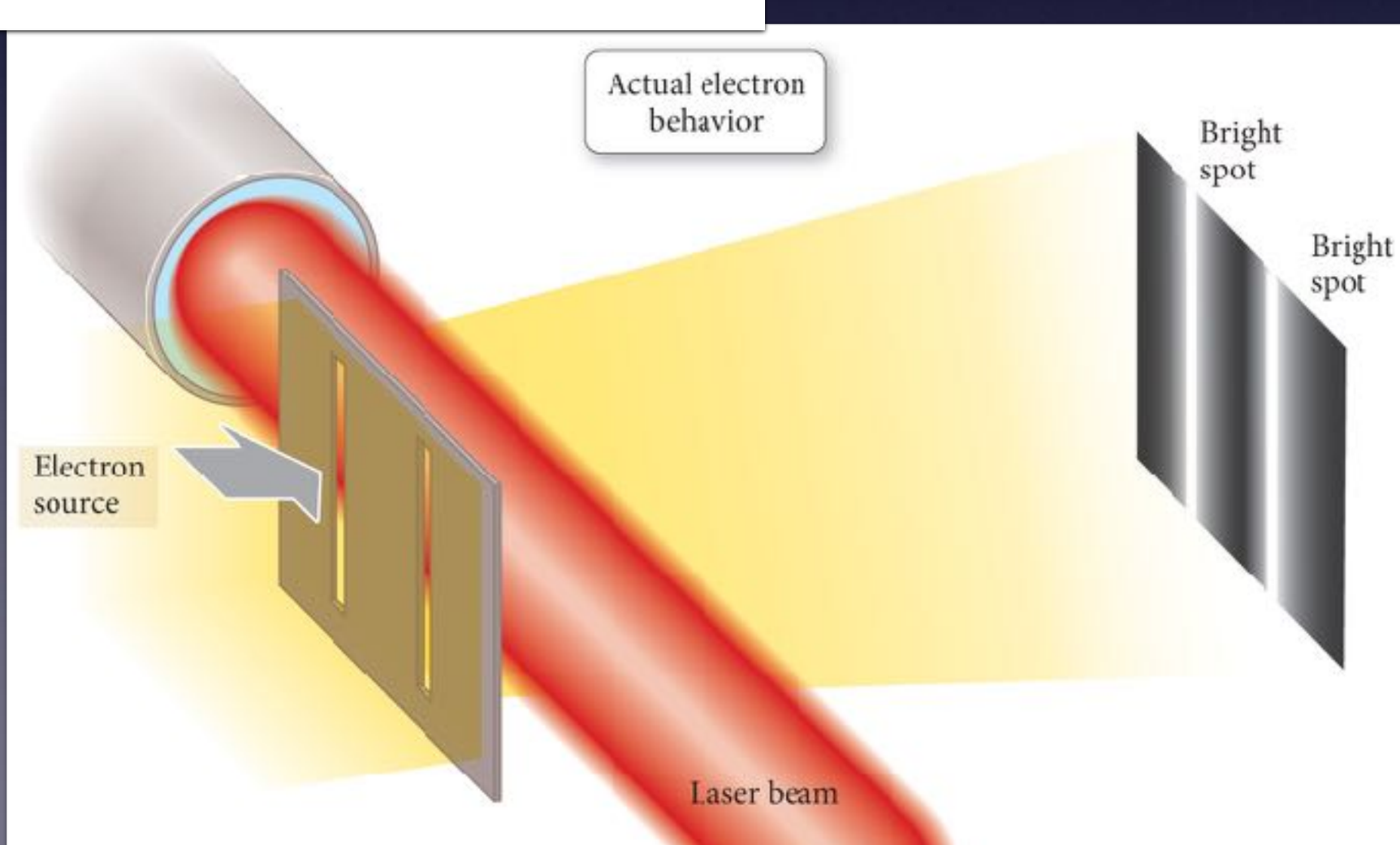
Failures of the theory…

- Can’t explain any multi-electron atoms!

- It’s completely wrong!
  (According to quantum mechanics)

Tro
Fig. 7.16A





Tro
pg 312

The uncertainty principle

- For complimentary properties, increasing accuracy in one value will lead to a decrease in accuracy in the other.

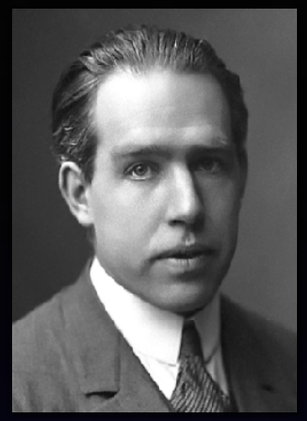
$$\Delta x \times \Delta p \geq \frac{\mathrm{h}}{4\pi}$$

$$\Delta x \times m\Delta v \geq \frac{\mathrm{h}}{4\pi}$$

$$\Delta \mathbf{E} \times \Delta t \geq \frac{\mathrm{h}}{4\pi}$$

www.nobelprize.org
heisenberg.jpg

Bohr vs Heisenberg



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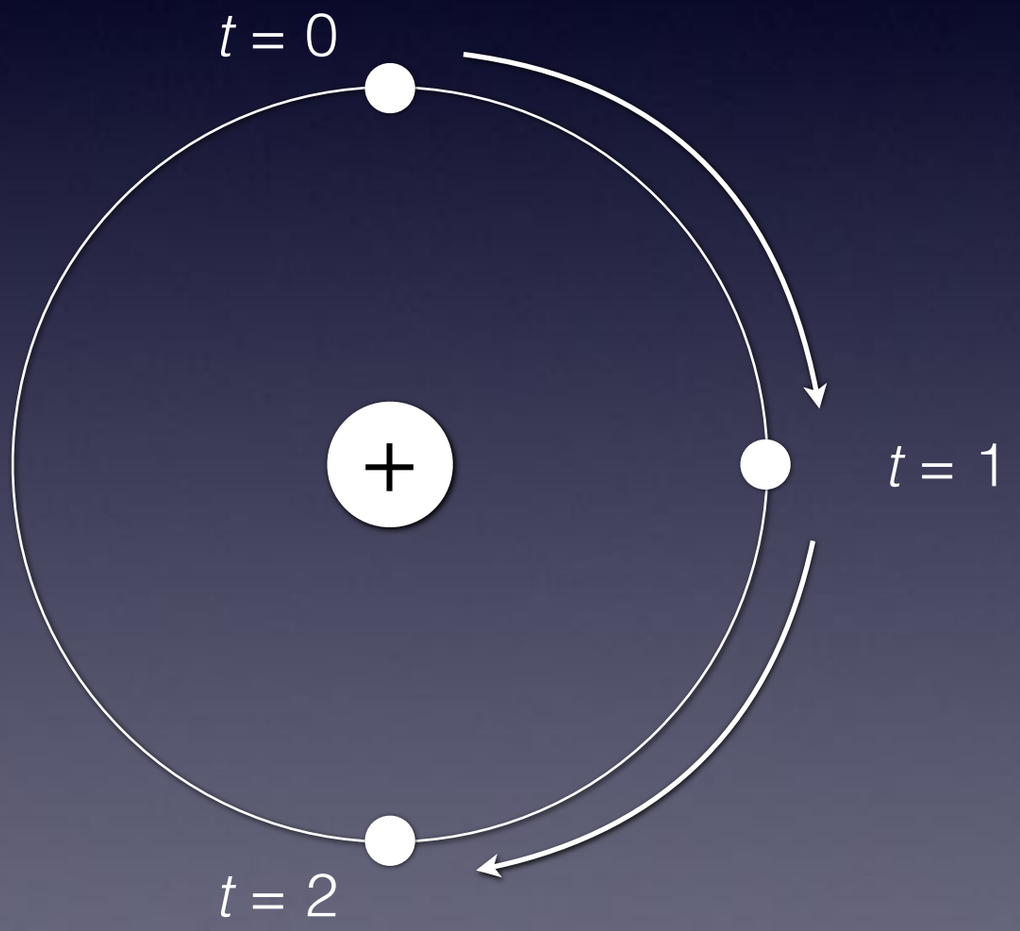
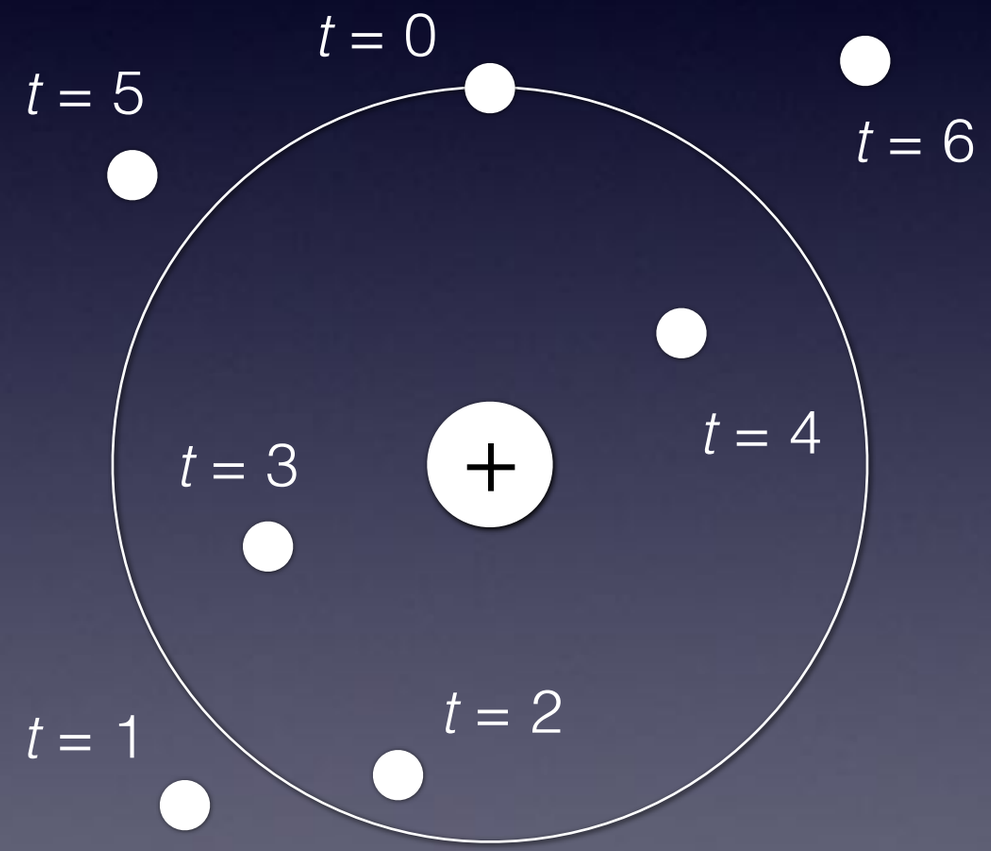
Niels_Bohr.jpg

www.nobelprize.org
heisenberg.jpg

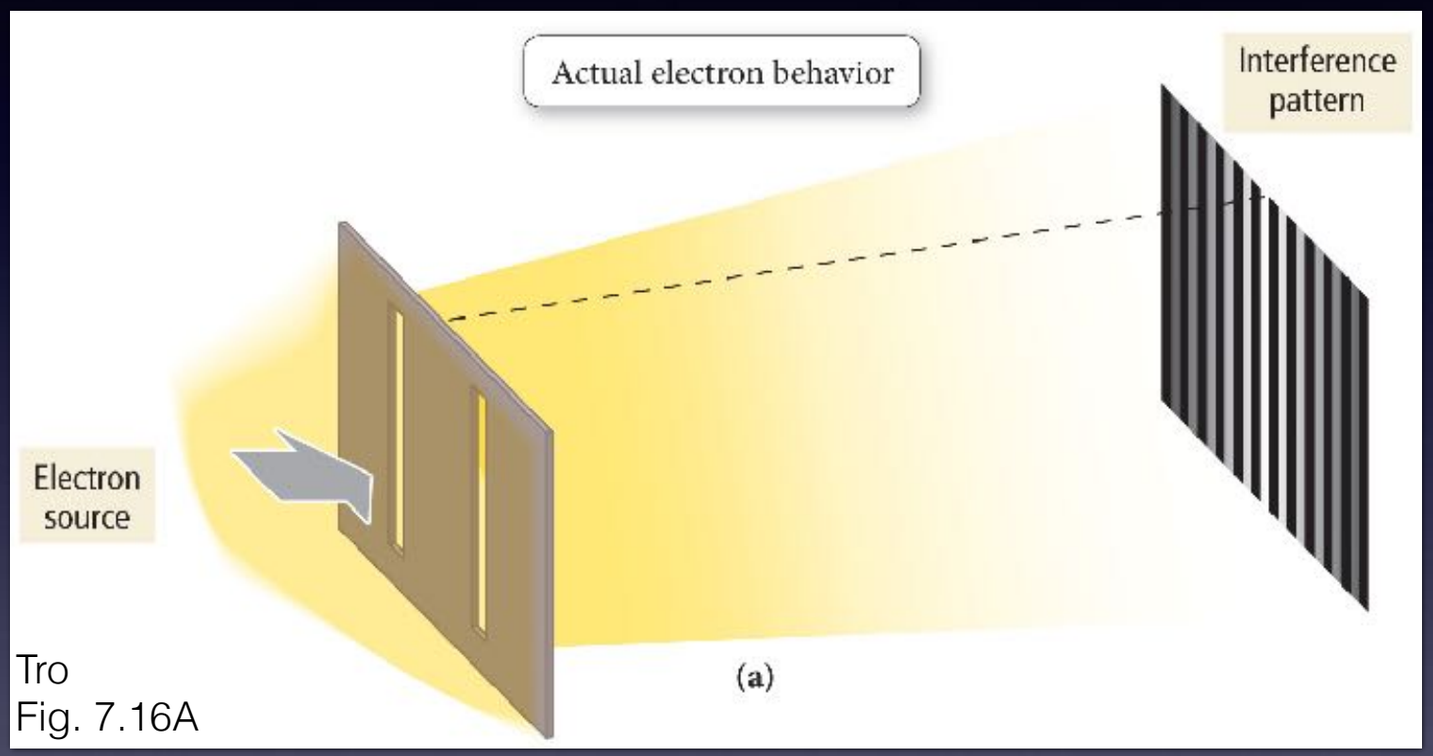


Violates uncertainty principle!

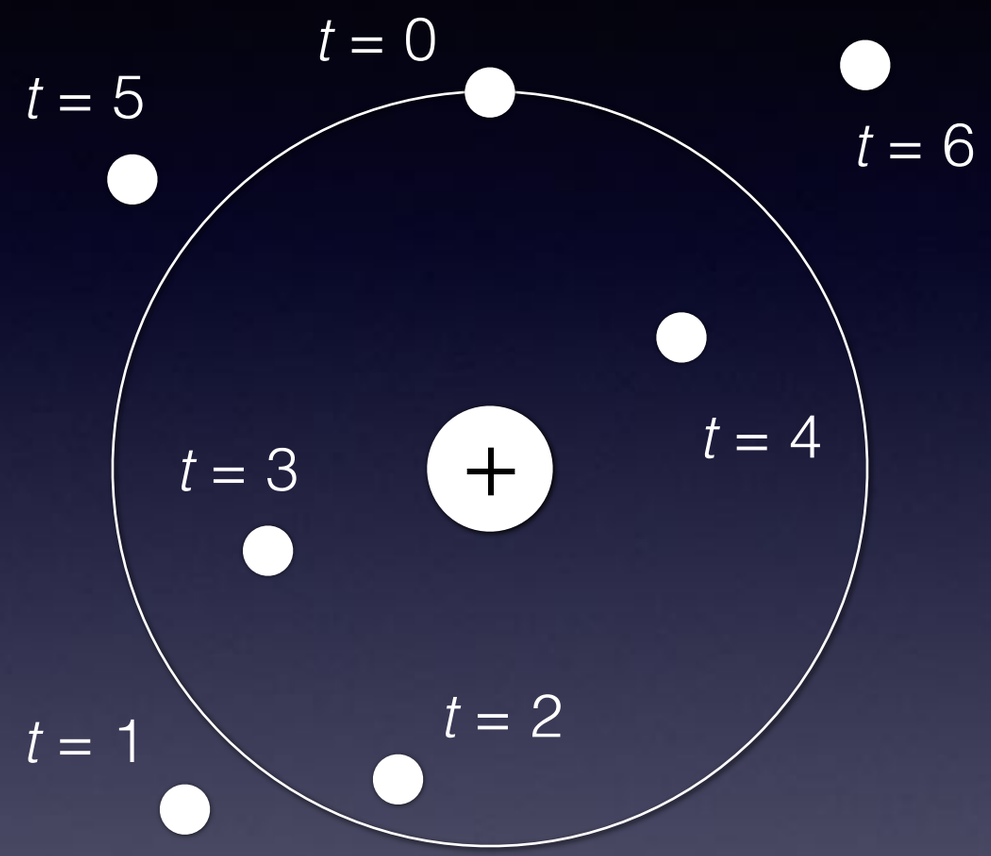


Uncertainty in position comparable to a_0!

Modern picture of the H atom



Tro
Fig. 7.16A

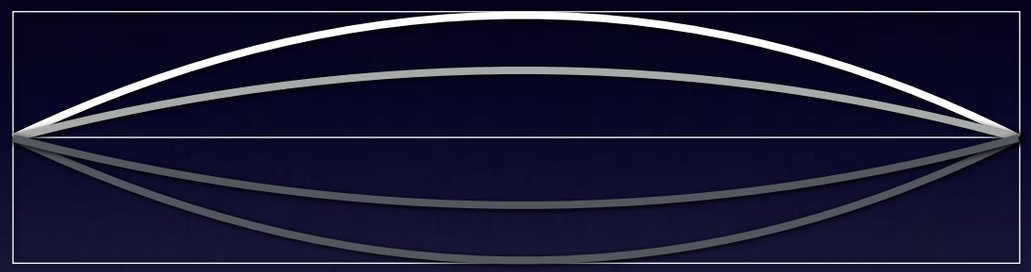


- Bound, 3 dimensional waves model electron behavior in atoms
- The best we can do is describe a probability of finding an electron
- Info is given by a function with properties of a wave, hence the term **wavefunction**.

Diversion #1: Standing waves

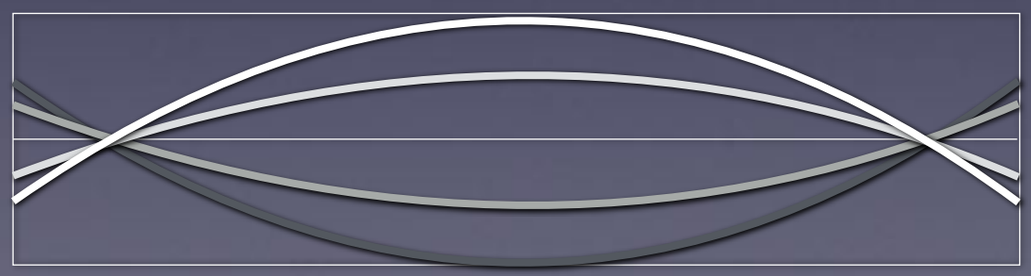
https://www.youtube.com/watch?v=efBUBvbsSYw

Standing wave boundary conditions

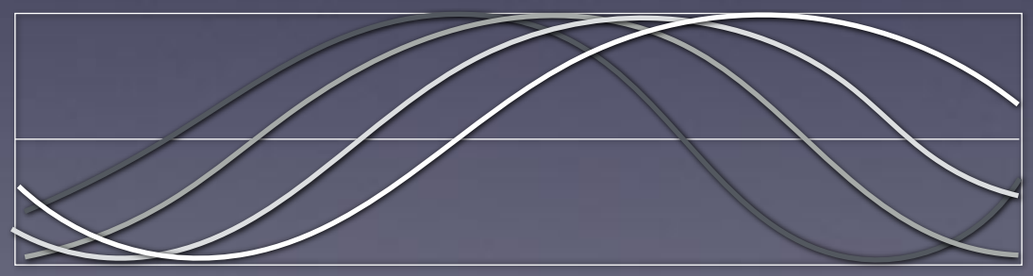


Allowed standing wave.
Endpoints are fixed. **Always**.

$$y = f(x,t) = A\sin\left(\frac{\pi x}{d}\right)\cos(\omega t)$$



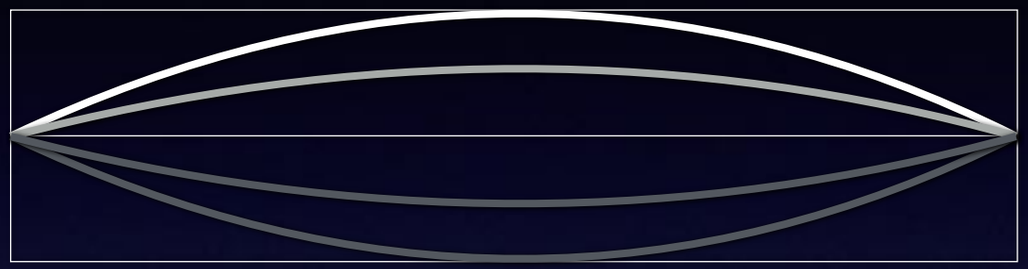
Not allowed. Endpoints aren't fixed.

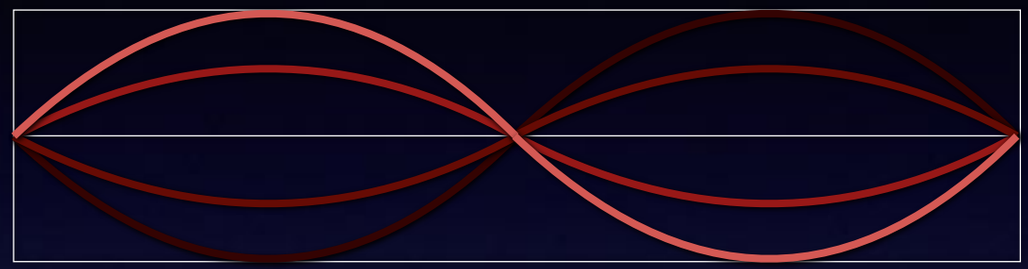


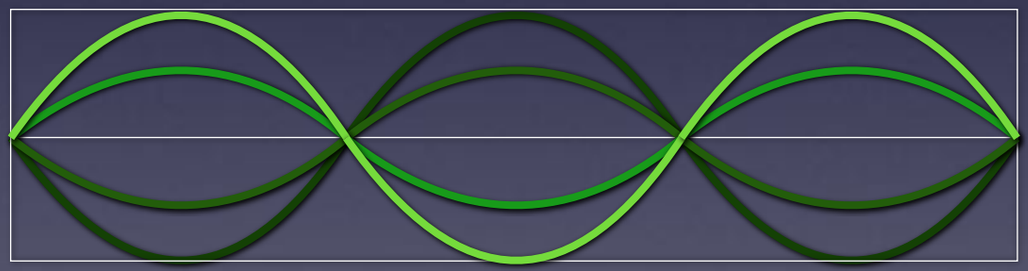
Not allowed. This is a traveling wave.

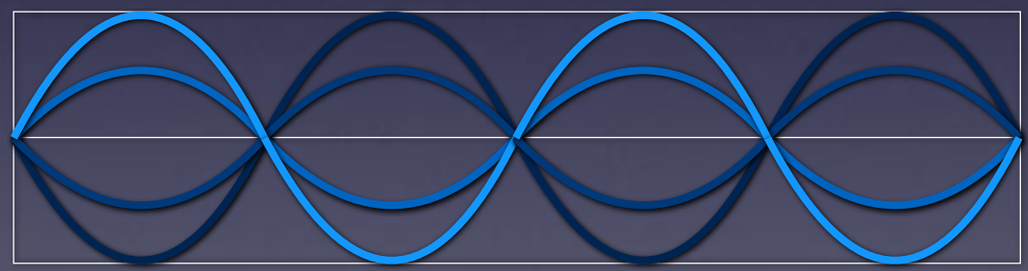
The boundary conditions for waves create quantum mechanics

Other allowed standing waves

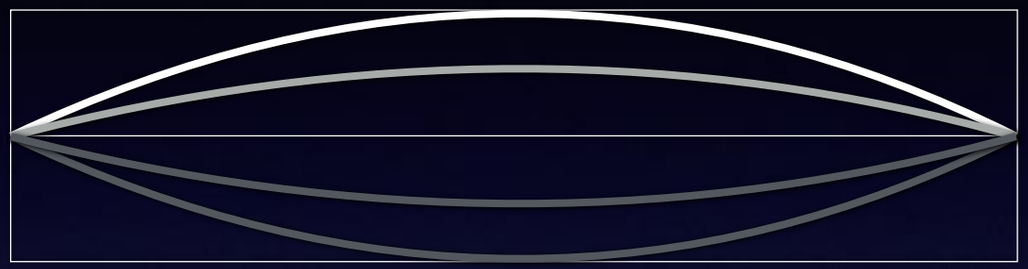




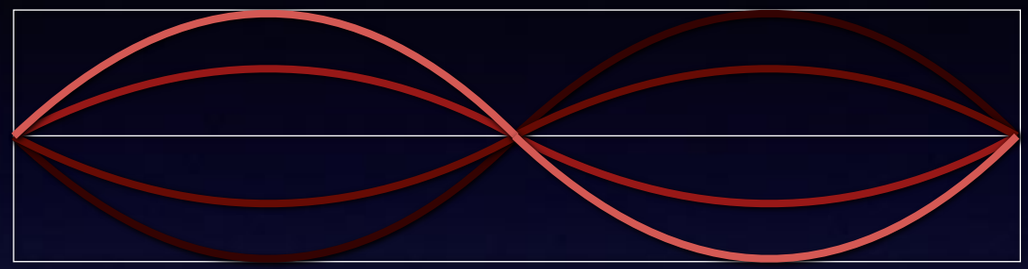




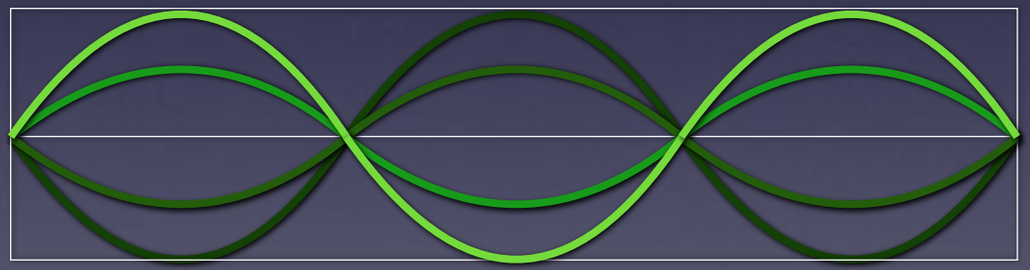
Other allowed standing waves



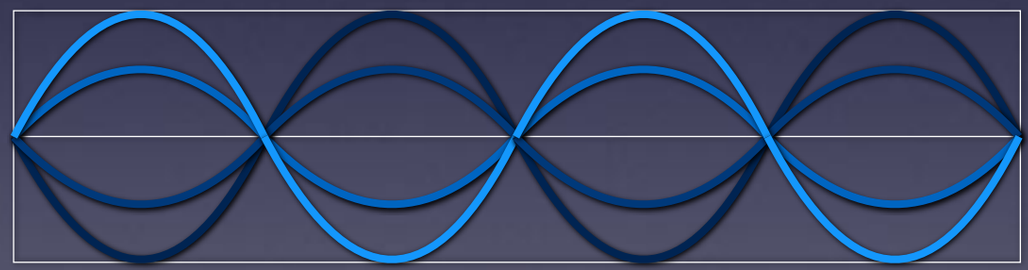
$$\sin\left(\frac{\pi x}{d}\right)$$



$$\sin\left(\frac{2\pi x}{d}\right)$$

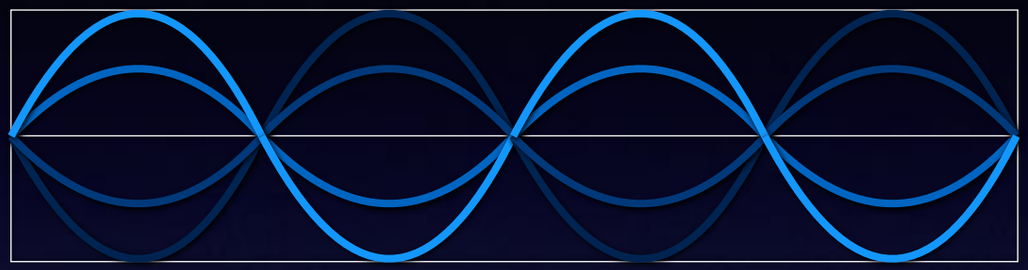


$$\sin\left(\frac{3\pi x}{d}\right)$$

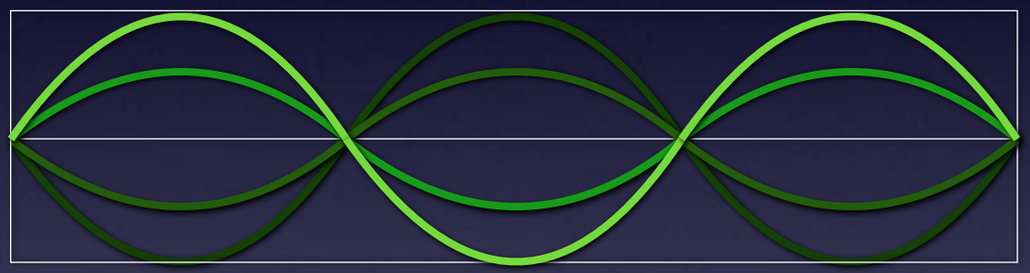


$$\sin\left(\frac{4\pi x}{d}\right)$$

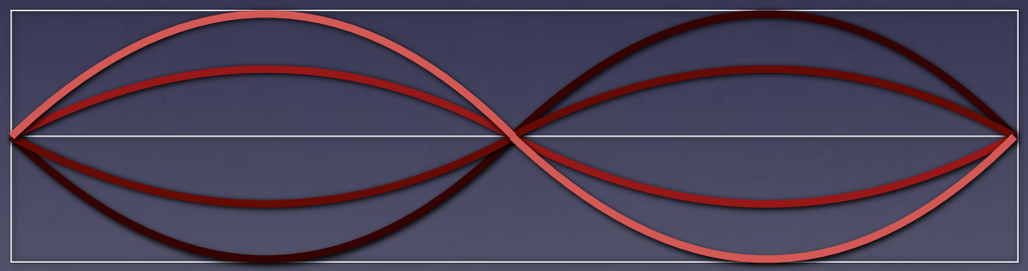
Other allowed standing waves



$n = 4$



$n = 3$



$n = 2$

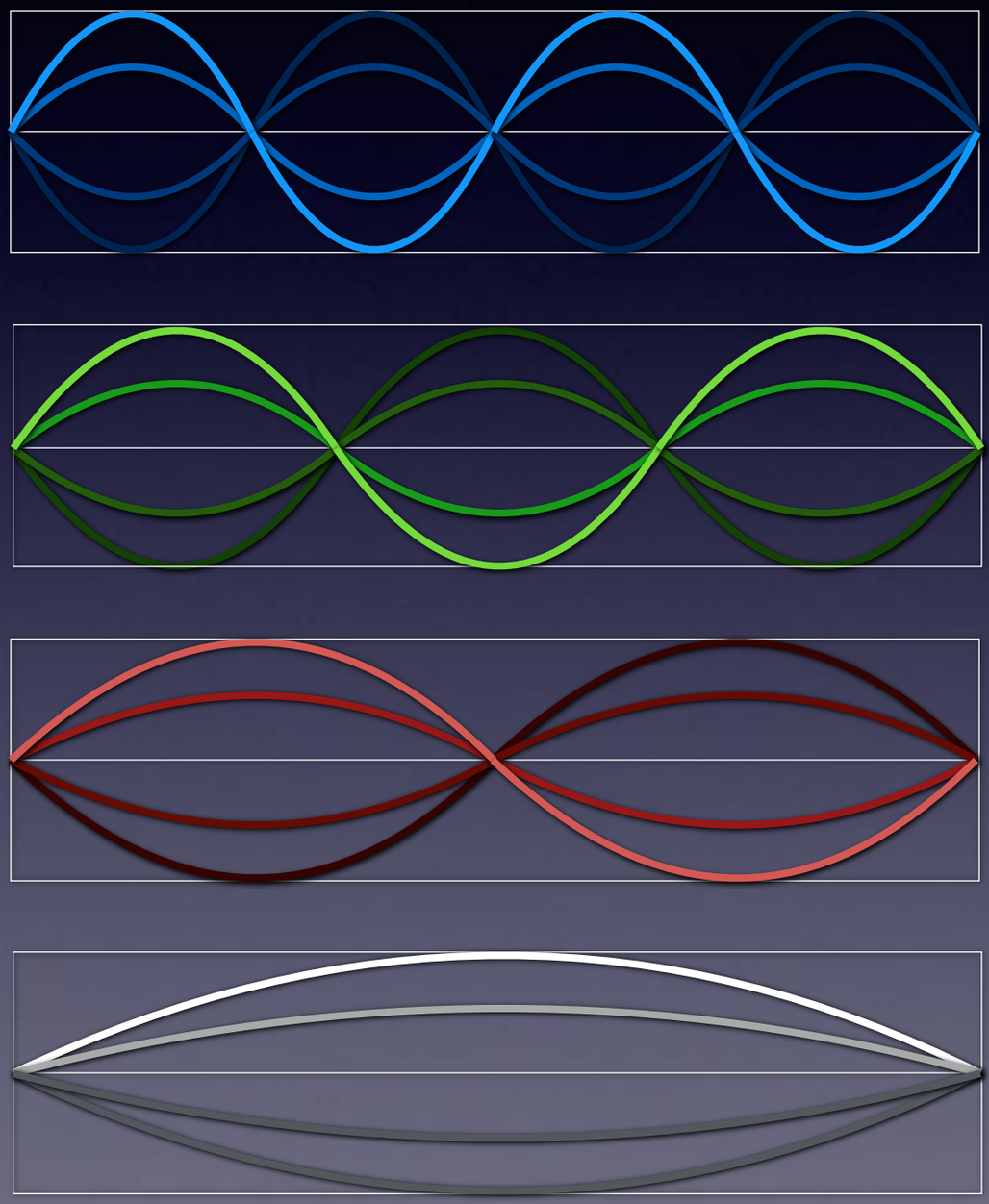
$n = 1$

General solution:

$$\sin\left(\frac{n\pi x}{d}\right)$$

n is the quantum number that describes this system

Relative energy of standing waves



$n = 4$

$n = 3$

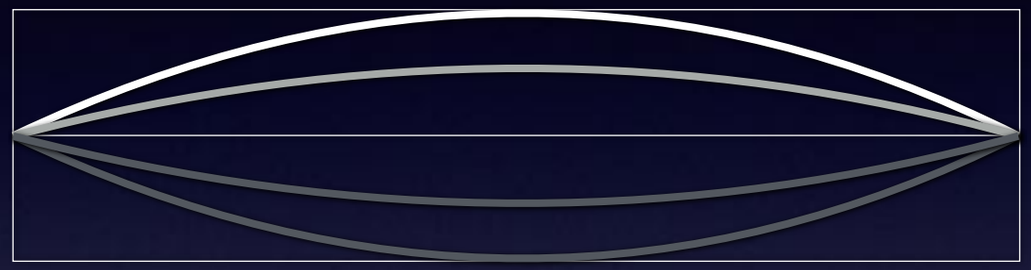
$n = 2$

$n = 1$

Higher energy

Lowest energy

Nodes



This wave has no nodes.

$$y = f(x,t) = A\sin\left(\frac{\pi x}{d}\right)\cos(\omega t)$$

- Nodes are points for which $\psi(x,t) = 0$ at all times
- Endpoints are fixed by boundary conditions so they don't count.

Diversion #2: Nodes

https://www.youtube.com/watch?v=rkeIubVQ0N8

Minute paper: waves in 1D…

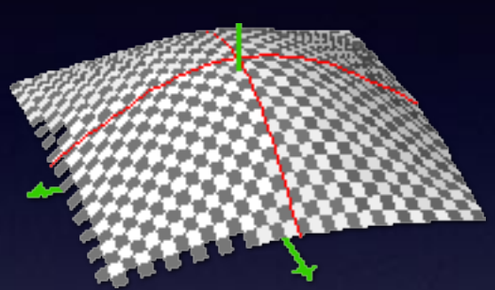
What is the relationship between:

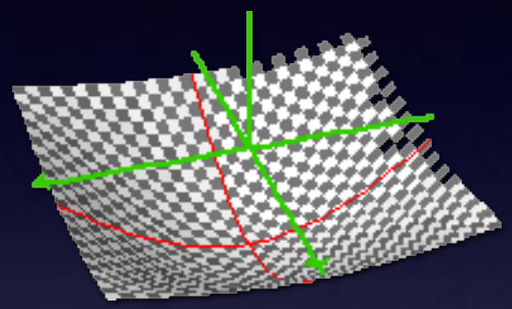
n, the quantum number

the number of nodes

the energy of the system

Waves in two dimensions





No nodes:
lowest in energy

Ernst Chladni
www.hps.cam.ac.uk
chladni.jpg

In two dimensions, nodes can be radial:
https://www.youtube.com/watch?v=CGiiSlMFFII

Or they can be more interesting geometries
with angular components:
https://www.youtube.com/watch?v=wMIvAsZvBiw

Where did we go today?

Ch1010-A17-A03 Lecture 4

- § 2.4 Matter as waves
- § 2.6 Waves, nodes, and gratuitous YouTube videos

Next time…

- §2.6 Quantum numbers
- §2.6 Atomic orbitals:

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Nathan S. Lewis
Professor, Caltech

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