3.021J / 1.021J / 10.333J / 18.361J / 22.00J Introduction to Modeling and Simulation
Spring 2008

It's A Quantum World: The Theory of Quantum Mechanics

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Class outline

theory

1. It's A Quantum World: The Theory of Quantum Mechanics
2. Quantum Mechanics: Practice Makes Perfect
4. From Atoms to Solids

practice

3. From Many-Body to Single-Particle; Quantum Modeling of Molecules
5. Quantum Modeling of Solids: Basic Properties
6. Advanced Prop. of Materials; What else can we do?

7. Review session

It's a quantum world!

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Motivation!

If we understand electrons, then we understand everything!!! (almost) ...

Lesson outline

- ☐ Why quantum mechanics?
- ☐ Wave aspect of matter
- ☐ Interpretation
- ☐ The Schrödinger equation
- ☐ Simple examples

Image of hydrogen orbitals removed due to copyright restrictions.
Please see:
http://www.kfunigraz.ac.at/imawww/vqm/images/qm/es421.jpg

Why quantum mechanics?

Classical mechanics

Newton's laws (1687) $$\vec{F} = \frac{d(m\vec{v})}{dt}$$

Problems?

Why quantum mechanics?

Problems in classical physics that led to quantum mechanics:

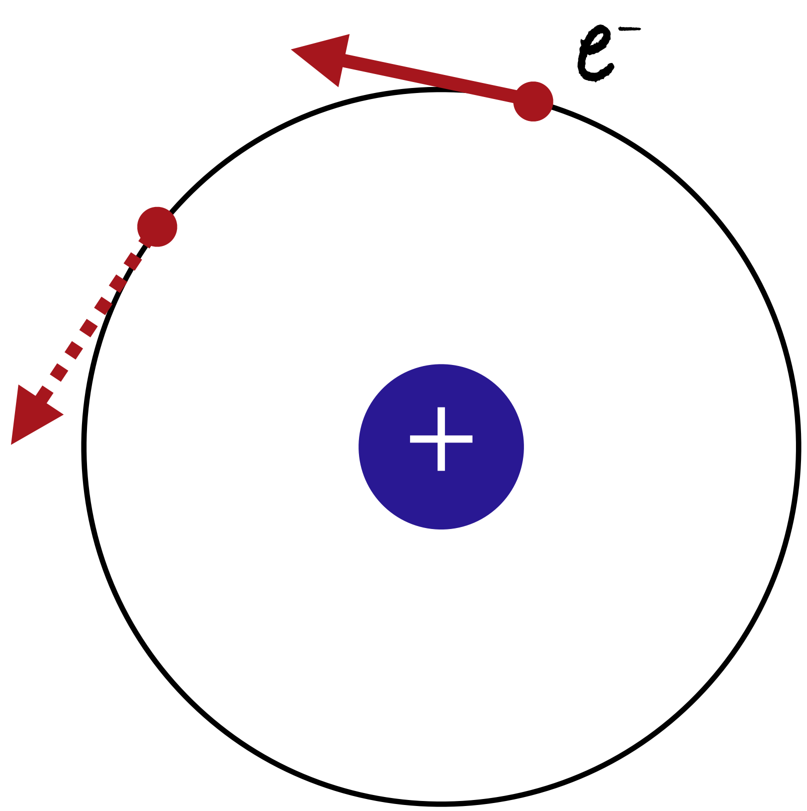
- ☐ "classical atom"
- ☐ quantization of properties
- ☐ wave aspect of matter
- ☐ (black-body radiation), ...

Quantum mechanics dudes!

Werner Heisenberg, Max Planck,
Louis de Broglie, Albert Einstein,
Niels Bohr, Erwin Schrödinger,
Max Born, John von Neumann,
Paul Dirac, Wolfgang Pauli
(1900 - 1930)

Photos of Werner Heisenberg, Louis de Broglie, Max Planck, Wolfgang Pauli, Erwin Schrodinger, and Paul Dirac removed due to copyright restrictions.

"Classical atoms"



hydrogen atom

problem:

accelerated charge causes radiation, atom not stable!

Quantization of properties

photoelectric effect

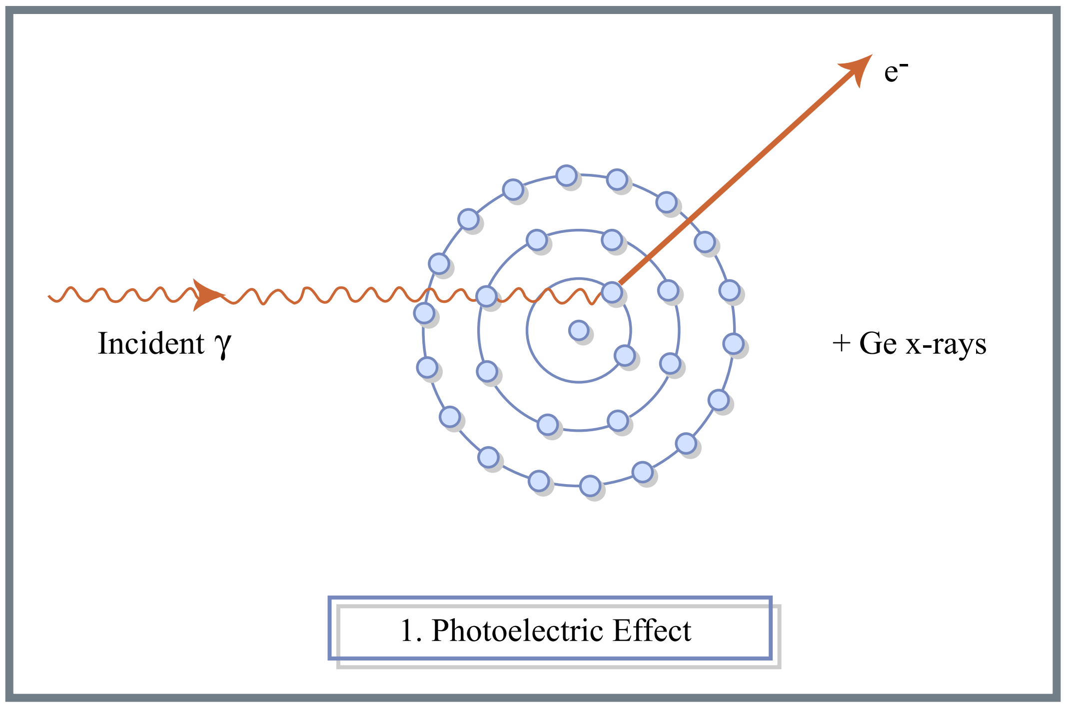
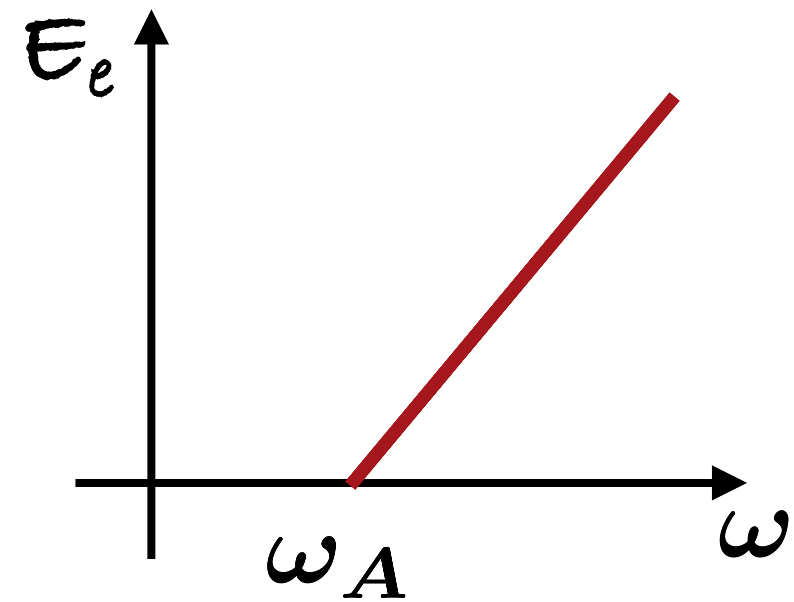


Figure by MIT OpenCourseWare.



$$E = \hbar(\omega - \omega_A) = h(\nu - \nu_A)$$

$$h = 2\pi\hbar = 6.6 \cdot 10^{-34} \text{ Wattsec.}^2$$

Einstein: photon $E = \hbar\omega$

Quantization of properties

atomic spectra

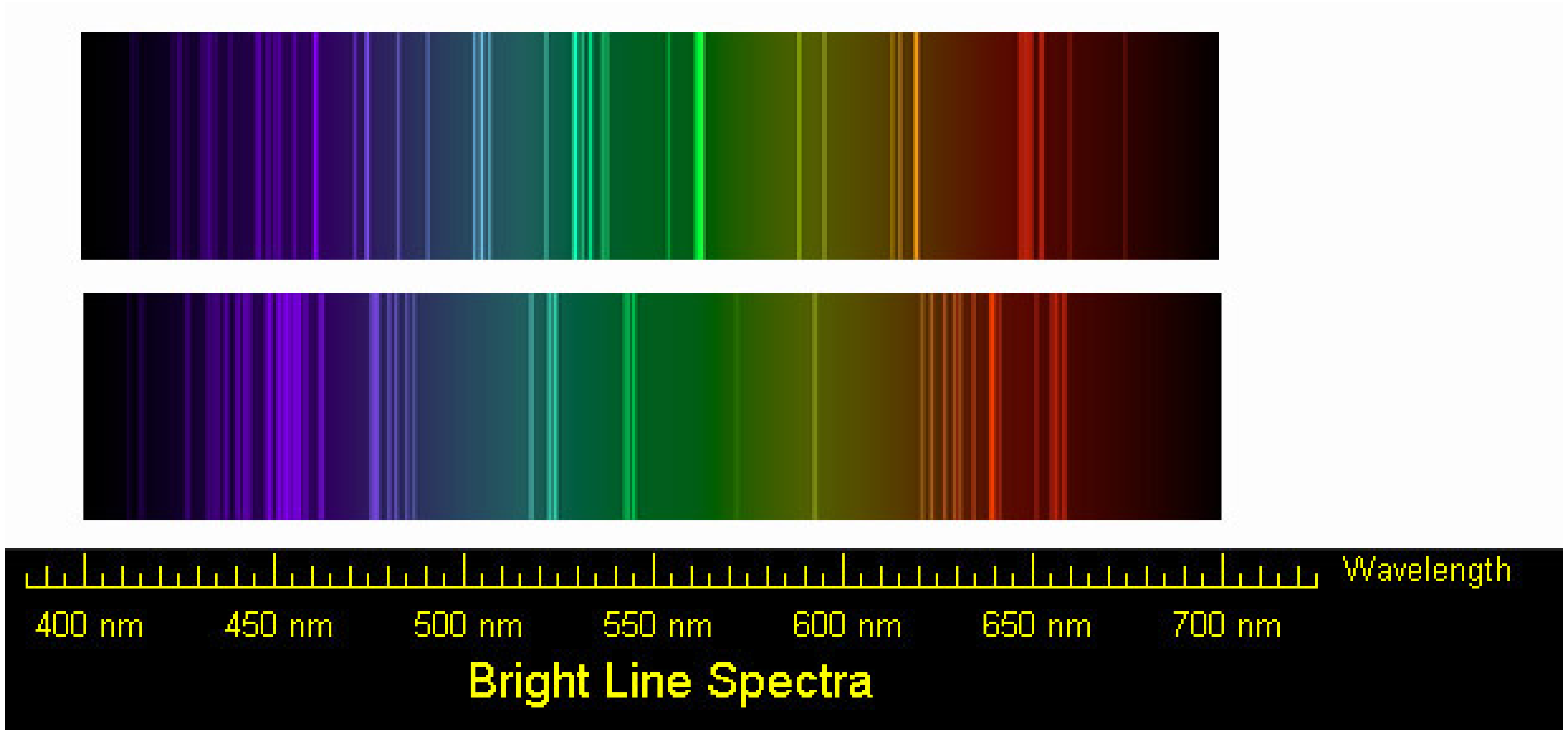
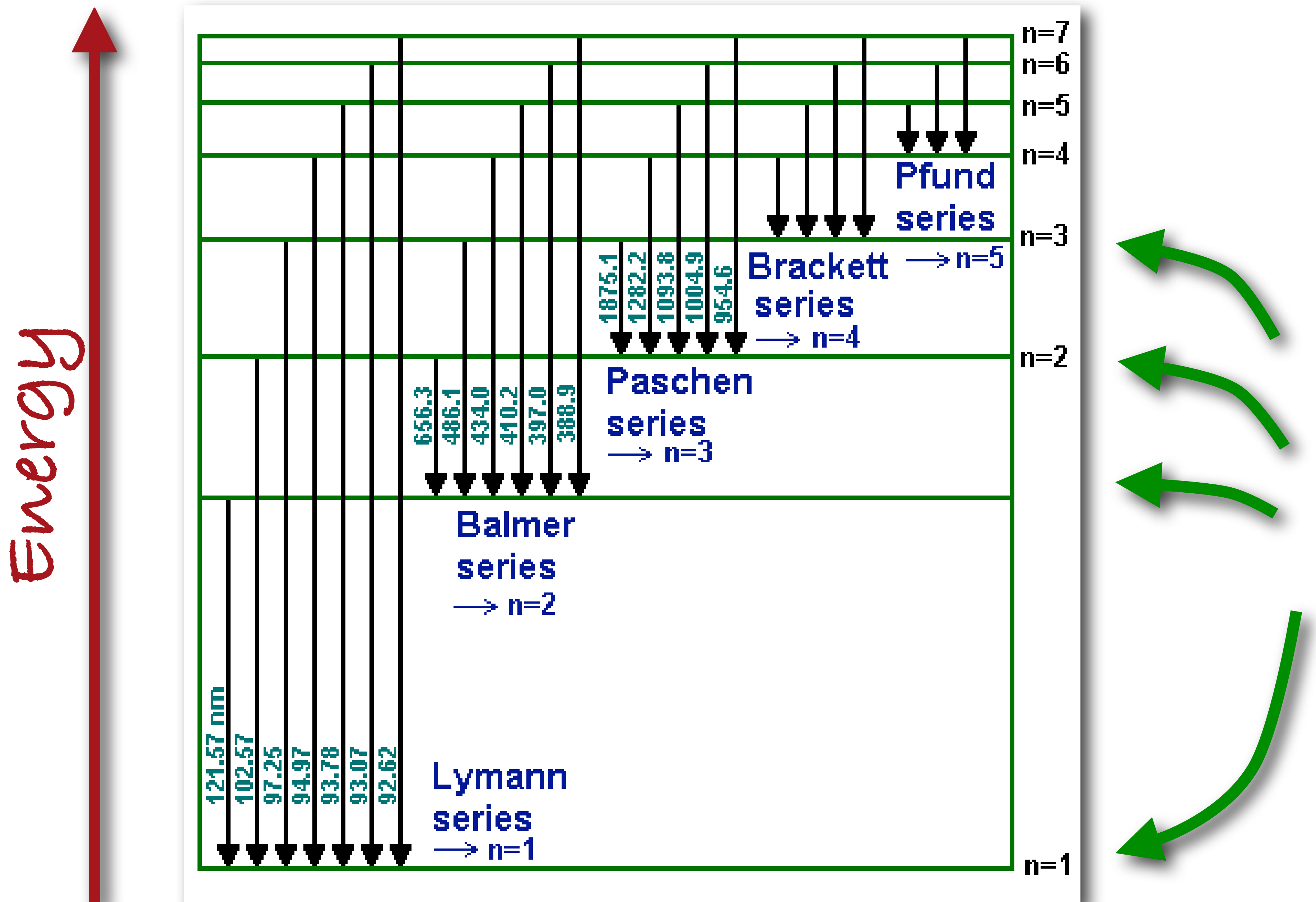


Image courtesy of NASA.

Quantization of properties



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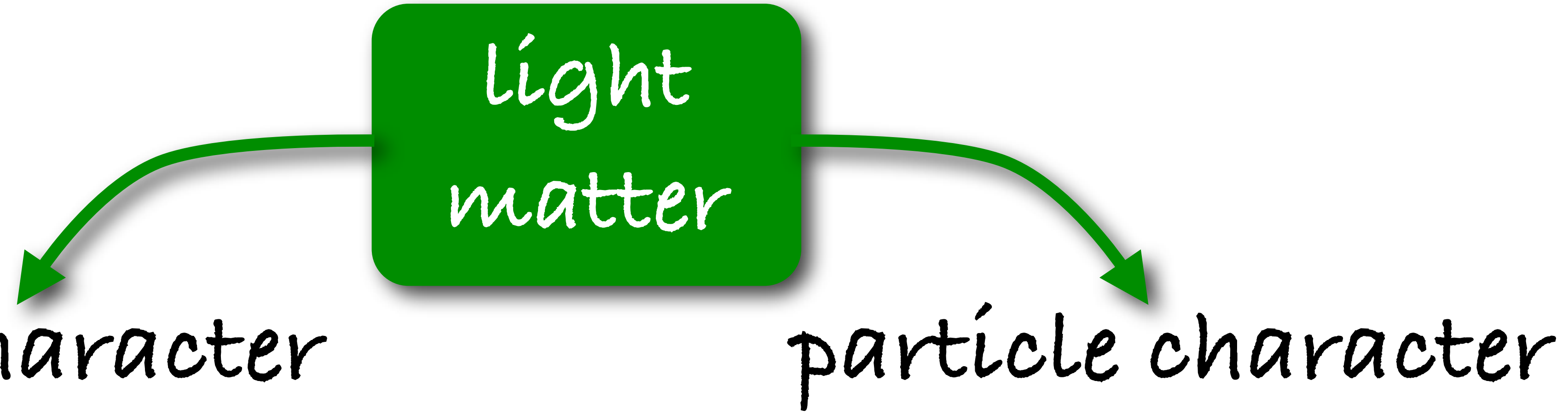
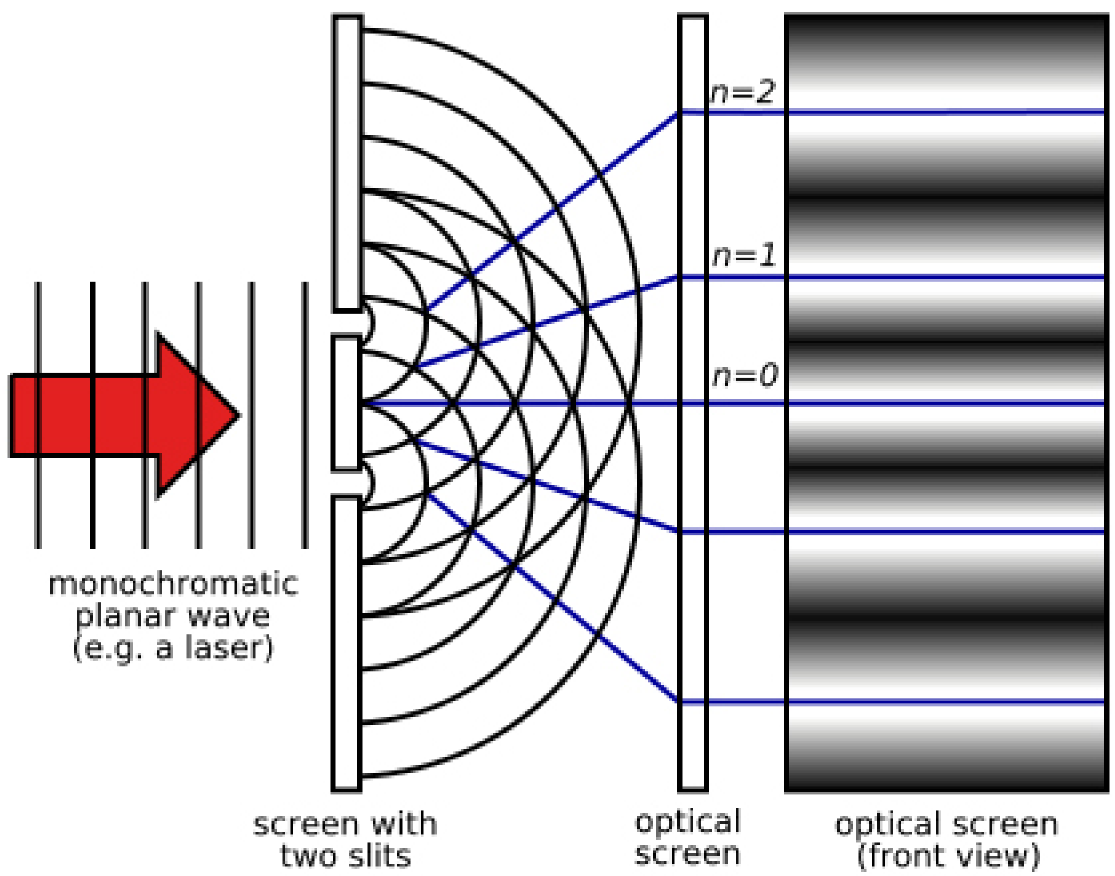
$E = \hbar\omega$

possible energy states

Wave aspect of matter





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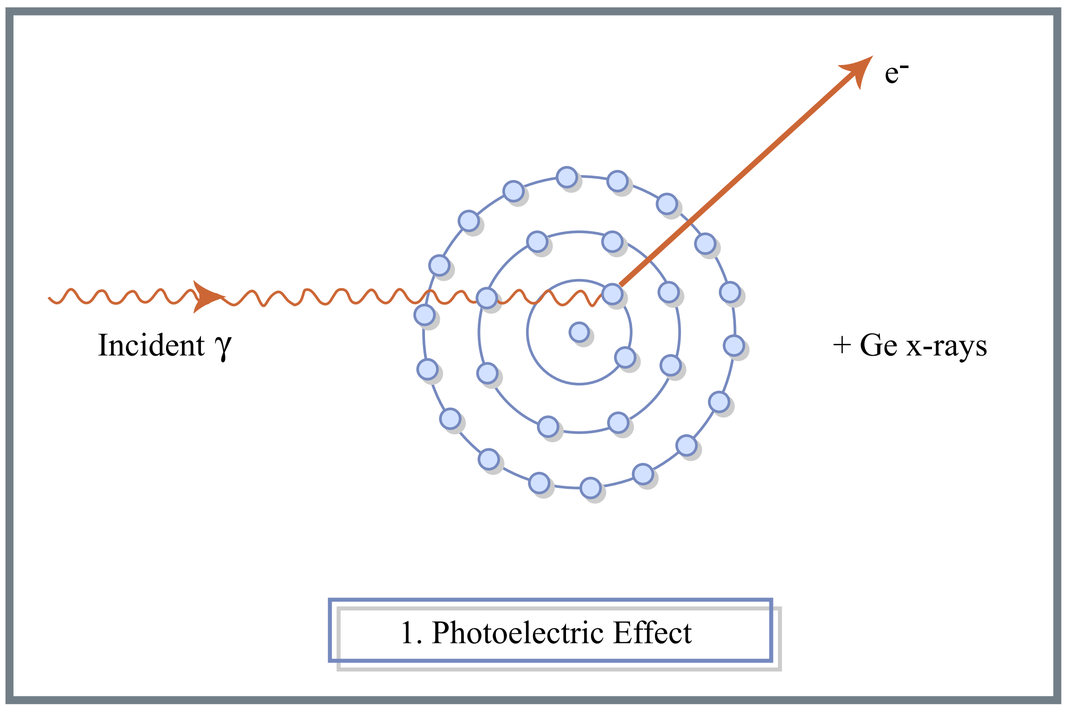

Figure by MIT OpenCourseWare.

Wave aspect of matter

particle: and momentum

wave: frequency and wavevector

$$E = h\nu = \hbar\omega$$

$$\vec{p} = \hbar\vec{k} = \frac{h}{\lambda}\frac{\vec{k}}{|\vec{k}|}$$

de Broglie: free particle can be described a as planewave $\psi(\vec{r},t) = Ae^{i(\vec{k}\cdot\vec{r}-\omega t)}$ with $\lambda = \dfrac{h}{mv}$.

Bucky- and soccer balls

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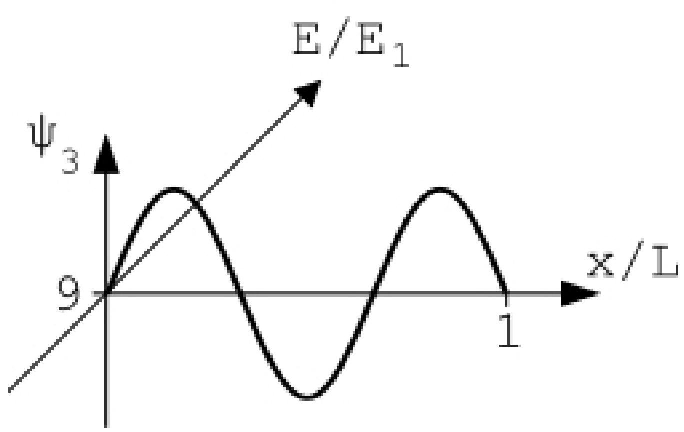
http://www.quantum.univie.ac.at/research/matterwave/c60/beam.jpg
http://www.quantum.univie.ac.at/research/matterwave/c60/c60beug.gif

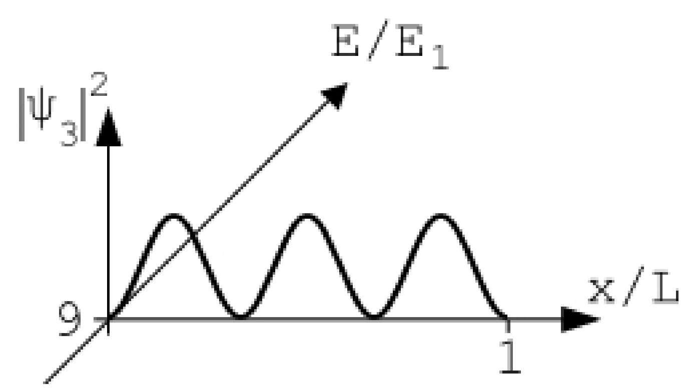
Interpretation of a wavefunction

$\psi(\vec{r}, t)$ → wave function (complex)

$|\psi|^2 = \psi\psi^*$ → interpretation as probability to find particle!



$\psi(\vec{r}, t)$



$|\psi(\vec{r}, t)|^2$

$$\int_{-\infty}^{\infty} \psi\psi^* dV = 1$$

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Classical vs. quantum

It is a mechanics of waves rather than classical particles!

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The Schrödinger equation

a wave equation: second derivative in space
first derivative in time

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)\right]\psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)$$

Hamiltonian

$$\begin{aligned} H &= -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t) = \\ &= \frac{p^2}{2m} + V = T + V \end{aligned}$$

$$\vec{p} = -i\hbar\nabla$$

Simple examples

Movies from:

Bernd Thaller, Visual Quantum Mechanics

In practice ...

H time independent: $\psi(\vec{r},t) = \psi(\vec{r}) \cdot f(t)$

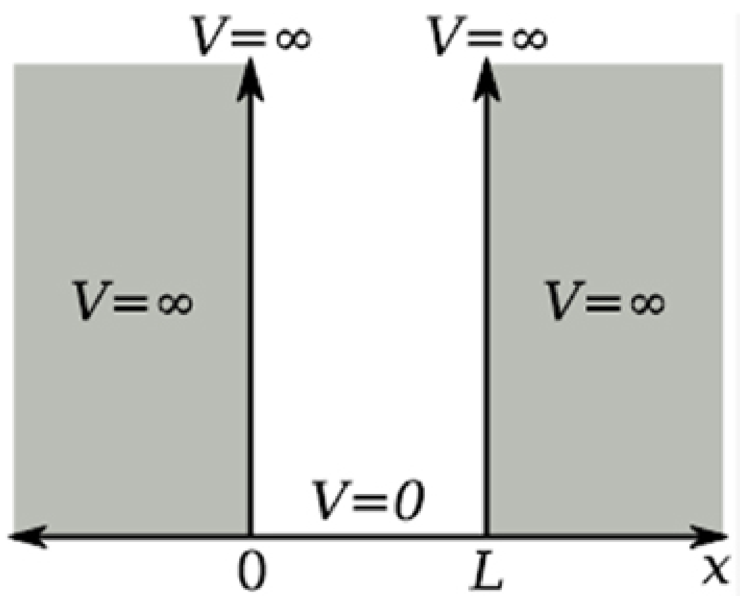
$$i\hbar \frac{\dot{f}(t)}{f(t)} = \frac{H\psi(\vec{r})}{\psi(\vec{r})} = \text{const.} = E$$

$$H\psi(\vec{r}) = E\psi(\vec{r})$$

$$\psi(\vec{r},t) = \psi(\vec{r}) \cdot e^{-\frac{i}{\hbar}Et}$$

time independent Schrödinger equation
stationary Schrödinger equation

Particle in a box



Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + V(x)\psi(x) = E\psi(x) \quad (1)$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = E\psi(x) \quad (2)$$

boundary conditions

$$\psi(0) = \psi(L) = 0 \quad (4)$$

$$\psi(x) = A\sin(kx) \quad (5)$$

$$\psi(L) = A\sin(kL) = 0 \quad (6)$$

general solution

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

$$E = \frac{k^2\hbar^2}{2m} \quad (3)$$

Particle in a box

quantization!

$$k = \frac{n\pi}{L} \quad \text{where} \quad n \in \mathbb{Z}^+ \quad (7)$$

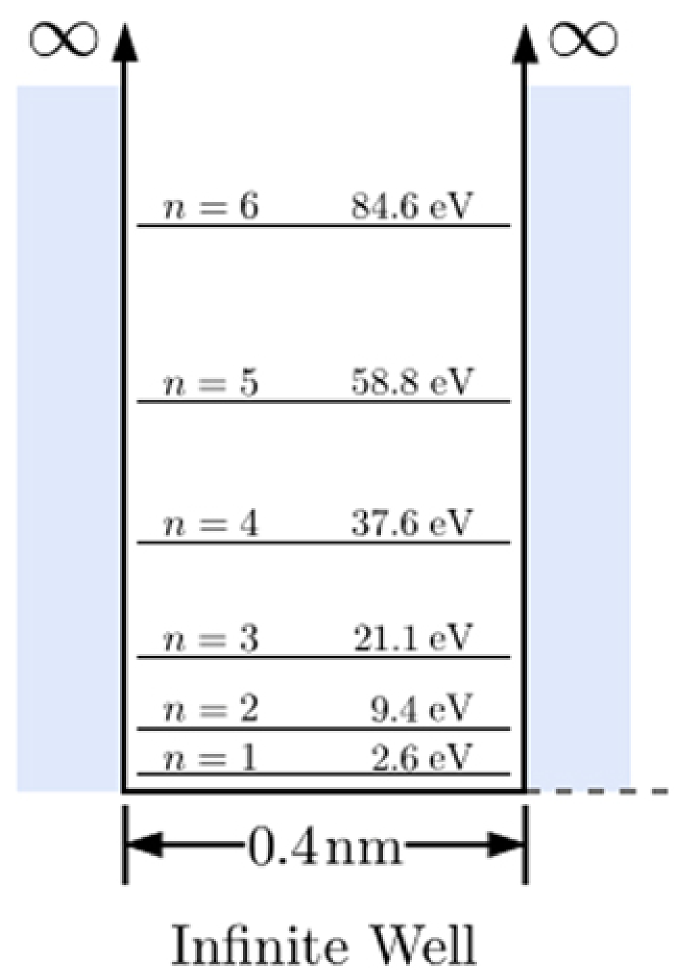
normalization

$$1 = \int_{-\infty}^{\infty} |\psi(x)|^2 \, \mathrm{d}x = |A|^2 \int_0^L \sin^2(kx) \, \mathrm{d}x = |A|^2 \frac{L}{2}$$

solution

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad (9)$$

$$E_n = \frac{n^2\hbar^2\pi^2}{2mL^2} = \frac{n^2h^2}{8mL^2} \quad (10)$$



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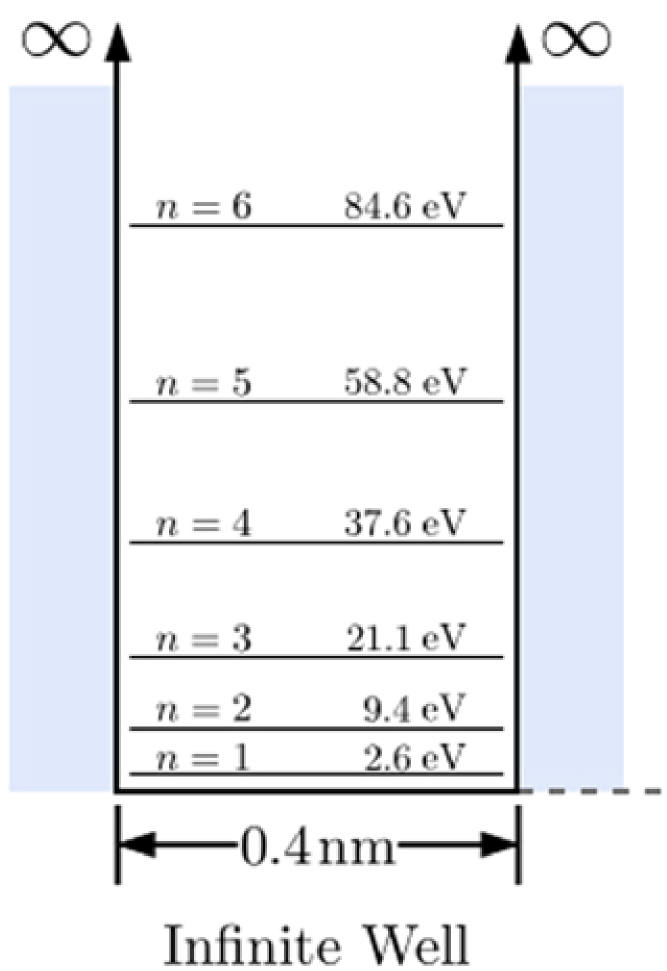
quantum number

Simple examples

electron in square well



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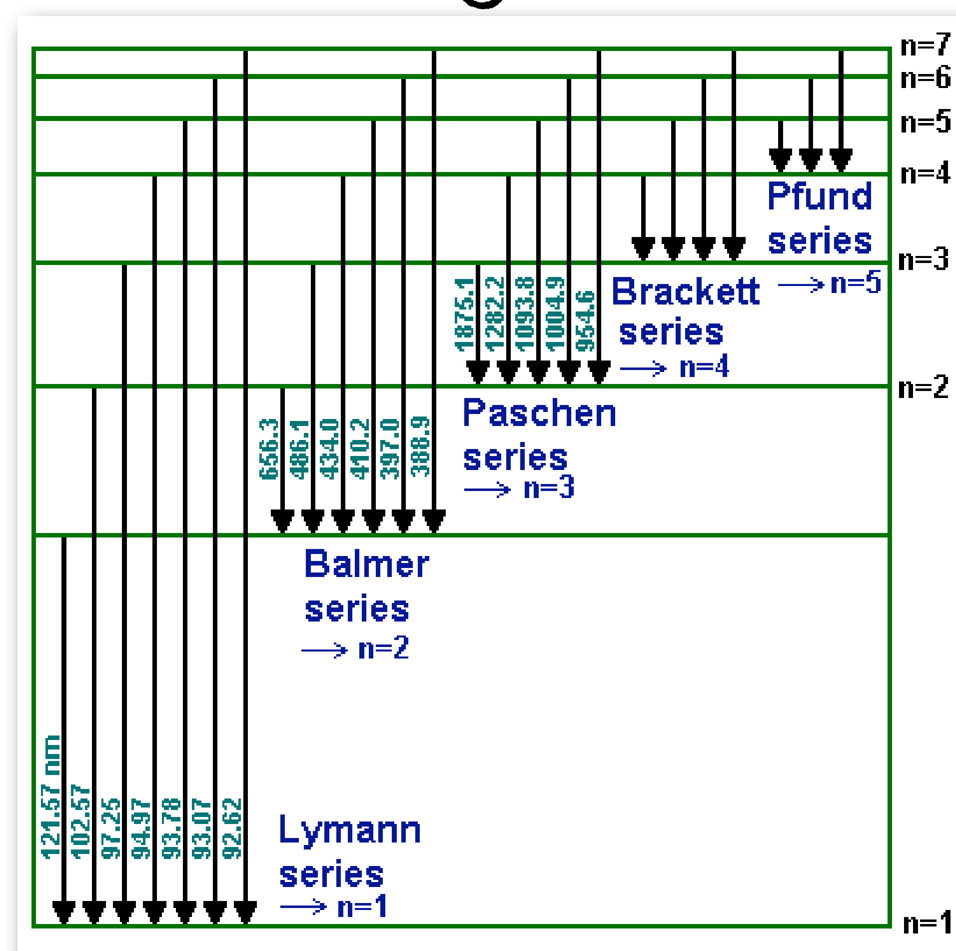
electron in hydrogen atom



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Harmonic oscillator

$$V(x) = \frac{1}{2} m\omega^2 x^2$$

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

solve Schrödinger equation

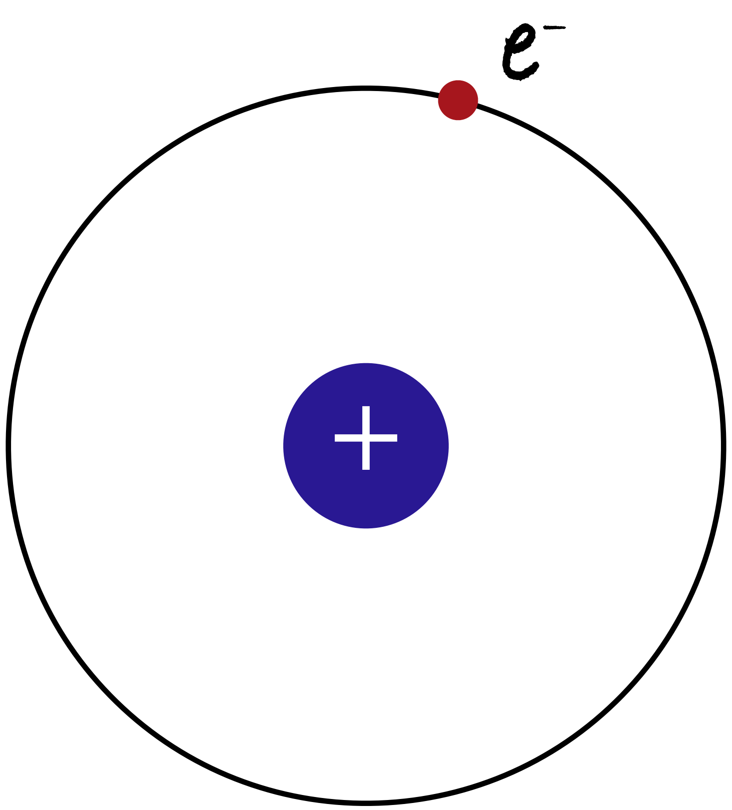
$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

$$\langle x|\psi_n\rangle = \sqrt{\frac{1}{2^n\, n!}} \cdot \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \cdot \exp\left(-\frac{m\omega x^2}{2\hbar}\right) \cdot H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)$$

Harmonic oscillator

Connection to reality?

potential: 1/r



hydrogen atom

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https://wiki.brown.edu/confluence/download/attachments/29471/HAtomOrbitals.png

Summary

Review

- ☐ Why quantum mechanics?
- ☐ Wave aspect of matter
- ☐ Interpretation
- ☐ The Schrödinger equation
- ☐ Simple examples

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Please see:
http://www.kfunigraz.ac.at/imawww/vqm/images/qm/es421.jpg

Literature

- Greiner, Quantum Mechanics: An Introduction
- Thaller, Visual Quantum Mechanics
- Feynman, The Feynman Lectures on Physics
- wikipedia, “quantum mechanics”, “Hamiltonian operator”, “Schrödinger equation”, ...

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