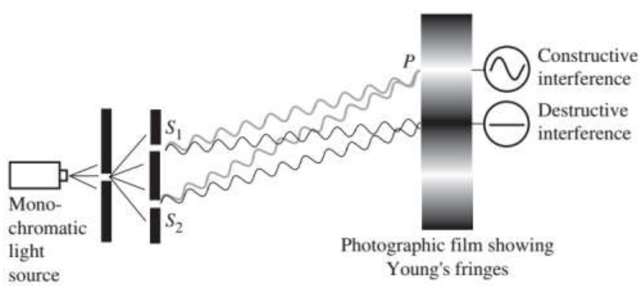
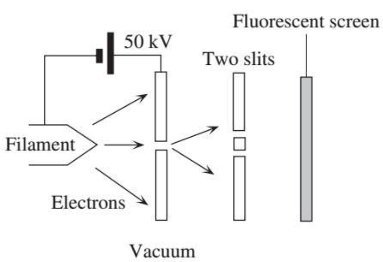
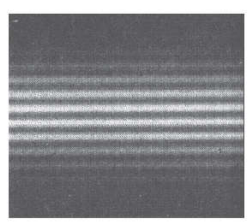
TIME-INDEPENDENT SCHRÖDINGER EQUATION

Young's Double Slit Experiments



Light Intensity





Electron diffraction fringes on the screen

Electron Probability

Copenhagen Interpretation of Quantum Mechanics

- A system is completely described by a wave function ψ, representing an observer's subjective knowledge of the system.
- The description of nature is essentially probabilistic, with the probability of an event related to the square of the amplitude of the wave function related to it.
- It is not possible to know the value of all the properties of the system at the same time; those properties that are not known with precision must be described by probabilities. (Heisenberg's uncertainty principle)
- Matter exhibits a wave–particle duality. An experiment can show the particle-like properties of matter, or the wave-like properties; in some experiments both of these complementary viewpoints must be invoked to explain the results.
- Measuring devices are essentially classical devices, and measure only classical properties such as position and momentum.
- The quantum mechanical description of large systems will closely approximate the classical description.

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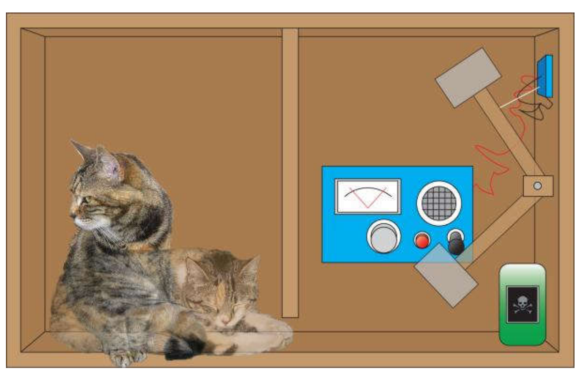
Schrodinger's Cat

"It is typical of these cases that an indeterminacy originally restricted to the atomic domain becomes transformed into macroscopic indeterminacy, which can then be resolved by direct observation. That prevents us from so naively accepting as valid a "blurred model" for representing reality. In itself, it would not embody anything unclear or contradictory. There is a difference between a shaky or out-of-focus photograph and a snapshot of clouds and fog banks."

-Erwin Schrodinger, 1935



SCHRÖDINGER'S CAT IS DEAD

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Heisenberg's Uncertainty Principle

- In the world of very small particles, one cannot measure any property of a particle without interacting with it in some way
- This introduces an unavoidable uncertainty into the result → One can never measure all the properties exactly

uncertainty in momentum (Δp)

$$\Delta x \Delta p \geq \frac{h}{4\pi} = \frac{\hbar}{2}$$

uncertainty in position (Δx)

- The more accurately you know the position (i.e., the smaller Δx is), the less accurately you know the momentum (i.e., the larger Δp is); and vice versa

Werner Heisenberg (1901-1976)

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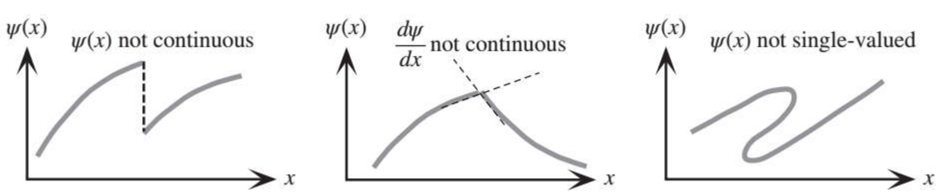
Electronic Wavefunctions

$$\Psi(x,t)$$

- A complex function of position x and time t.
- $|\Psi(x,y,z,t)|^2$: probability of finding the electron per unit volume at x, y, z at time t.
- If the potential energy of electron is time independent:

$$\Psi(x,t) = \psi(x)\exp(-j\omega t)$$

- $\psi(x)$ and $d\psi/dx$ must be continuous and single-valued.



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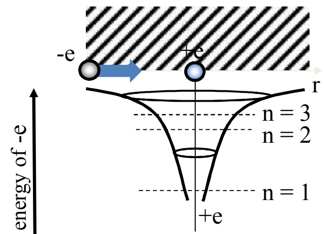
Atomic & Molecular Wavefunctions

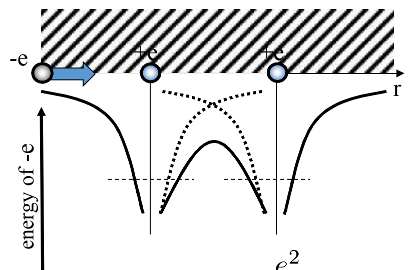
- Let's assume the case of hydrogen atoms.



Let' s represent the atom in space by its Coulomb potential centered on the proton (+e):

$$V(r) = -\frac{e^2}{4\pi\epsilon_o r}$$

Superposition of Coulomb potentials H_2:



$$V(r) = -\frac{e^2}{4\pi\epsilon_o |r - r_1|} - \frac{e^2}{4\pi\epsilon_o |r - r_2|}$$

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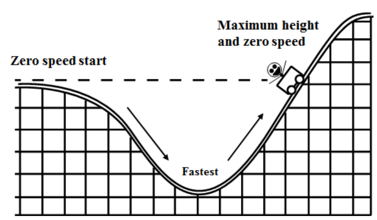
Time-Independent Schrödinger Equation

$$-\frac{\hbar^2}{2m_e}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} + \frac{2m_e}{\hbar^2}(E - V)\psi = 0$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m_e}{\hbar^2}(E - V)\psi = 0$$



Erwin Schrödinger (1887–1961)

- total energy = kinetic energy + potential energy
- In classical mechanics, $E = K + V$.
- V depends on the system
  - e.g., gravitational potential energy, electric potential energy

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The Free Electron

$$V = 0 \rightarrow \frac{d^2\psi}{dx^2} + \frac{2m_e}{\hbar^2}E\psi = 0$$

- **Solution:**

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

$$\psi(x) = A\exp(jkx), \quad \text{or} \quad \psi(x) = B\exp(-jkx)$$

$$\left.\begin{array}{l} \text{Quantum mechanics: KE} = E = \dfrac{(\hbar k)^2}{2m_e} \\ \text{Classical physics: KE} = \dfrac{p^2}{2m_e} \end{array}\right\} \quad p = \frac{h}{\lambda}$$

- The probability distribution for the electron is constant over the entire space.

$$|\psi(x)|^2 = |A\exp(jkx)|^2 = A^2$$

- **Uncertainties in position and momentum?**

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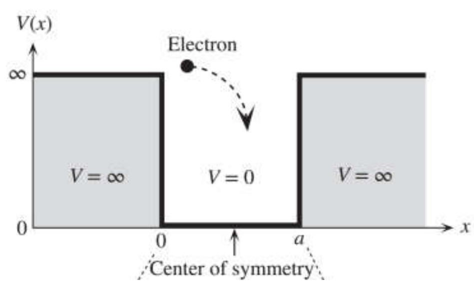
Infinite Potential Well

- $\psi = 0$ when $x \le 0$ and $x \ge a$, and ψ is determined by the Schrödinger equation in $0 < x < a$ with $V = 0$.



- Schrödinger equation:

$$\frac{d^2\psi}{dx^2} + \frac{2m_e}{\hbar^2}E\psi = 0$$

- Solution: $\psi(x) = A\exp(jkx) + B\exp(-jkx)$
- Boundary condition: $\psi(0) = 0$ at $x = 0$

$$\psi(x) = A\,[\exp(jkx) - \exp(-jkx)] = 2Aj\,\sin kx$$

- From S. E.: $-2Ajk^2\,(\sin kx) + \left(\frac{2m_e}{\hbar^2}\right)E(2Aj\sin kx) = 0 \rightarrow E = \frac{\hbar^2 k^2}{2m_e}$

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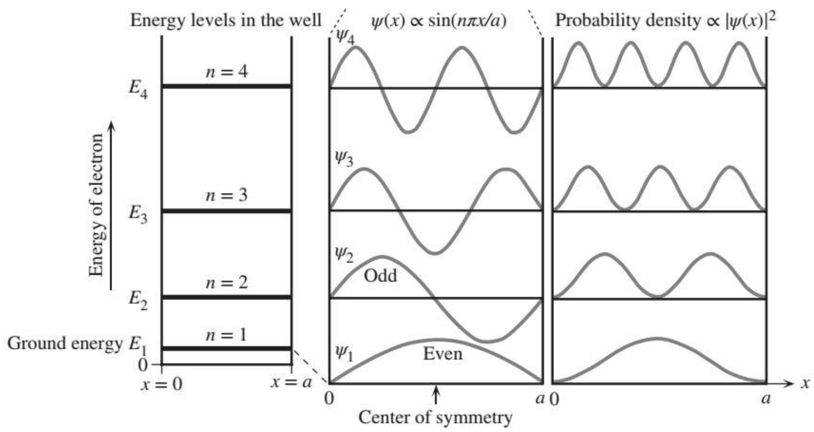
Infinite Potential Well

- $\psi(a) = 2Aj\,\sin ka = 0 \quad ka = n\pi$
- Solutions: $\psi_n(x) = 2Aj\,\sin\left(\frac{n\pi x}{a}\right) \qquad E_n = \frac{\hbar^2(\pi n)^2}{2m_e a^2} = \frac{h^2 n^2}{8m_e a^2}$



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Normalization

- ***A* =?**
- **Normalization:** The total probability of finding the electron in $0 < x < a$ is unity.

$$\int_{x=0}^{x=a} |\psi(x)|^2\,dx = \int_{x=0}^{x=a} \left|2Aj\,\sin\left(\frac{n\pi x}{a}\right)\right|^2 dx = 1$$

$$A = \left(\frac{1}{2a}\right)^{1/2}$$

$$\psi_n(x) = j\left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right)$$

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Class Test – 2

Day: 8 July 2019

Syllabus: Lectures 9–11

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