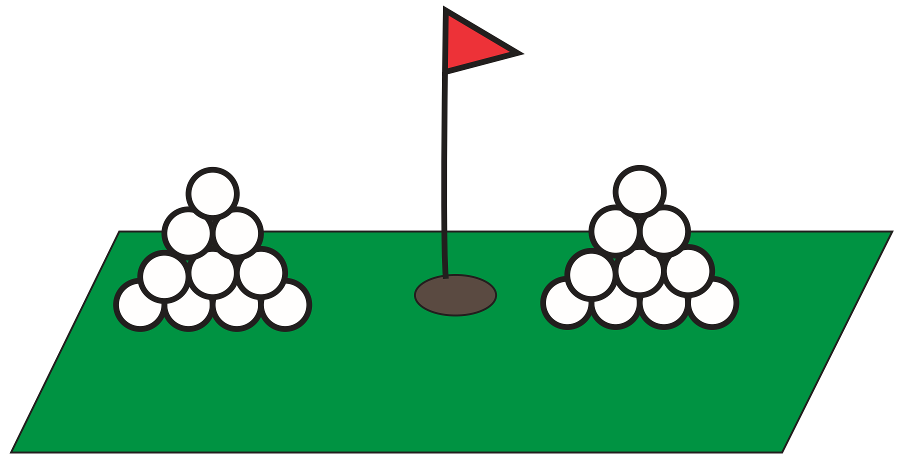
Schrödinger Equation

Reading - French and Taylor, Chapter 3



QUANTUM MECHANICS SETS PROBABILITIES

Outline

Wave Equations from ω-k Relations

Schrodinger Equation

The Wavefunction

TRUE / FALSE

1. The momentum p of a photon is proportional to its wavevector k. _____
2. The energy E of a photon is proportional to its phase velocity v_p. _____
3. We do not experience the wave nature of matter in everyday life because the wavelengths are too small. _____

Photon Momentum

IN FREE SPACE:

$$E = cp \Rightarrow p = \frac{E}{c} = \frac{\hbar\omega}{c} = \hbar k$$

IN OPTICAL MATERIALS:

$$E = v_p p \Rightarrow p = \frac{E}{v_p} = \frac{\hbar\omega}{v_p} = \hbar k_{vac} n$$

Heisenberg realised that …

- 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

Werner Heisenberg (1901-1976)

Image on the Public Domain

Heisenberg's Uncertainty Principle

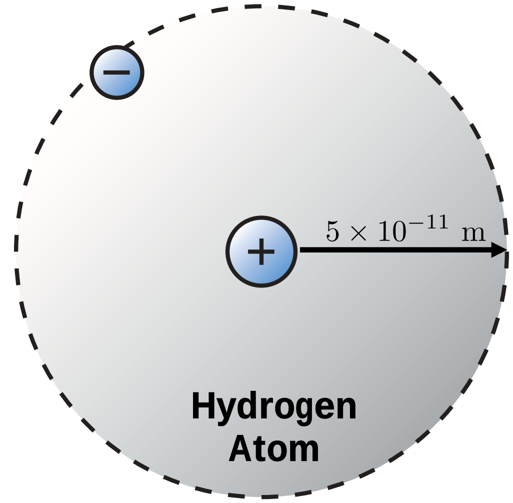
uncertainty
in momentum

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

uncertainty
in position

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

Consider a single hydrogen atom:



an electron of *charge* = -*e* free to move around in the electric field of a fixed proton of *charge* = +*e* (proton is ~2000 times heavier than electron, so we consider it fixed).

The electron has a potential energy due to the attraction to proton of:

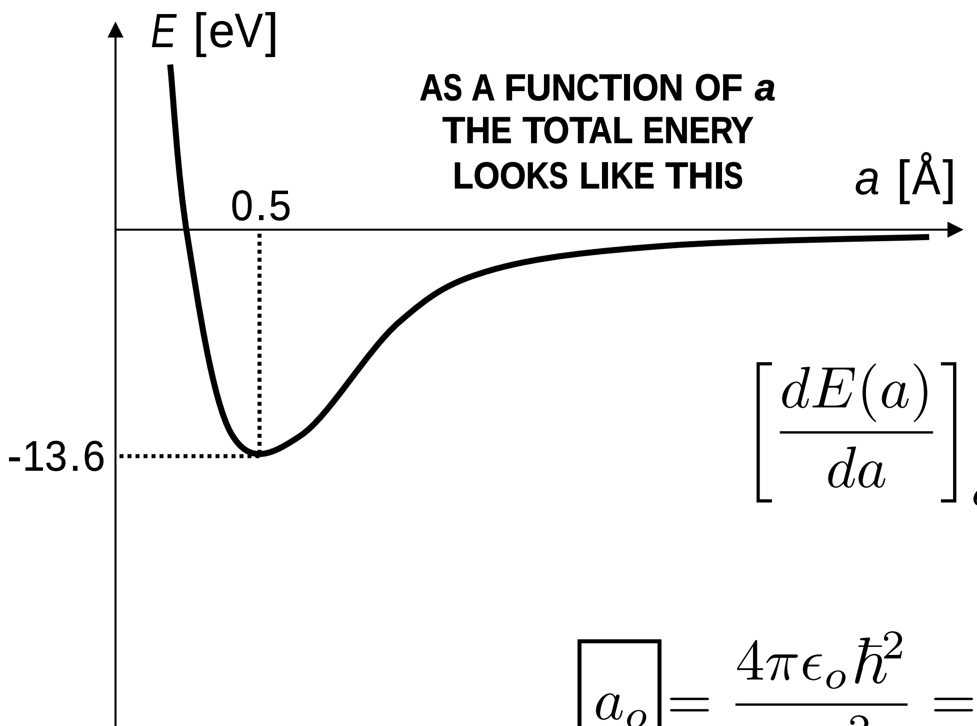
$$V(r) = -\frac{e^2}{4\pi\epsilon_o r}$$

where *r* is the electron-proton separation

The electron has a kinetic energy of $K.E. = \frac{1}{2}mv^2 = \frac{p^2}{2m}$

The total energy is then $E(r) = \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_o r}$

The minimum energy state, quantum mechanically, can be estimated by calculating the value of $a=a_o$ for which $E(a)$ is minimized:



$$E(a) = \frac{\hbar^2}{2ma^2} - \frac{e^2}{4\pi\epsilon_o a}$$

$$\left[\frac{dE(a)}{da}\right]_{a_o} = -\frac{\hbar^2}{ma_o^3} + \frac{e^2}{4\pi\epsilon_o a_o^2} = 0$$

$$\boxed{a_o} = \frac{4\pi\epsilon_o\hbar^2}{me^2} = \frac{10^{-10}\cdot 10^{-68}}{10^{-30}\cdot 2\cdot 10^{-38}} m \approx \boxed{0.5\ \mathring{A}}$$

By preventing localization of the electron near the proton, the Uncertainty Principle

RETARDS THE CLASSICAL COLLAPSE OF THE ATOM,

PROVIDES THE CORRECT DENSITY OF MATTER,

and YIELDS THE PROPER BINDING ENERGY OF ATOMS

One might ask:
"If light can behave like a particle, might particles act like waves"?

YES !
Particles, like photons, also have a wavelength given by:

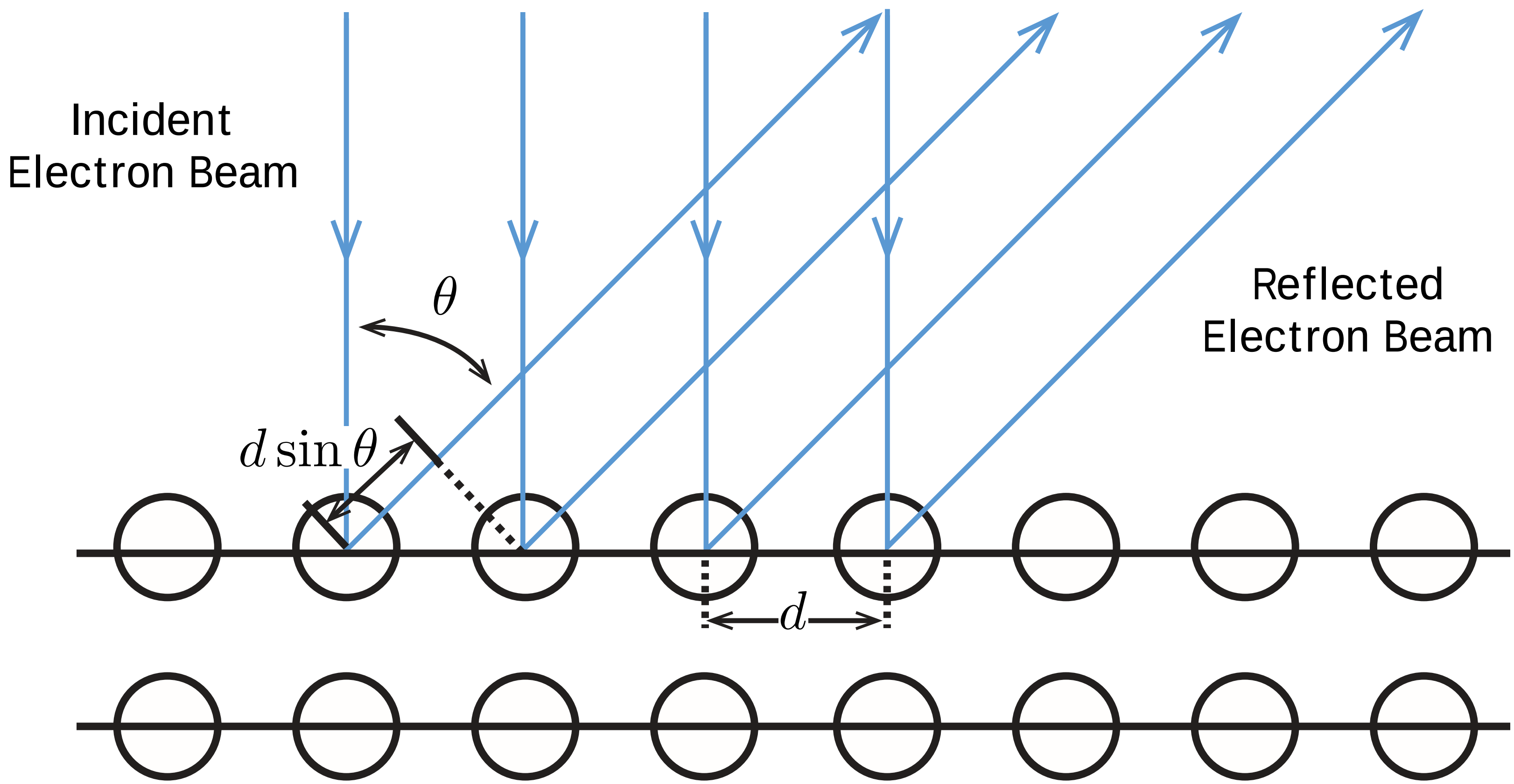
$$\lambda = h/p = h/mv$$

de Broglie wavelength

The wavelength of a particle depends on its momentum,
just like a photon!

The main difference is that matter particles have mass,
and photons don't !

Electron Diffraction – Simplified



Positive Interference: $d \sin\theta = n\lambda$

Electron diffraction for characterizing crystal structure

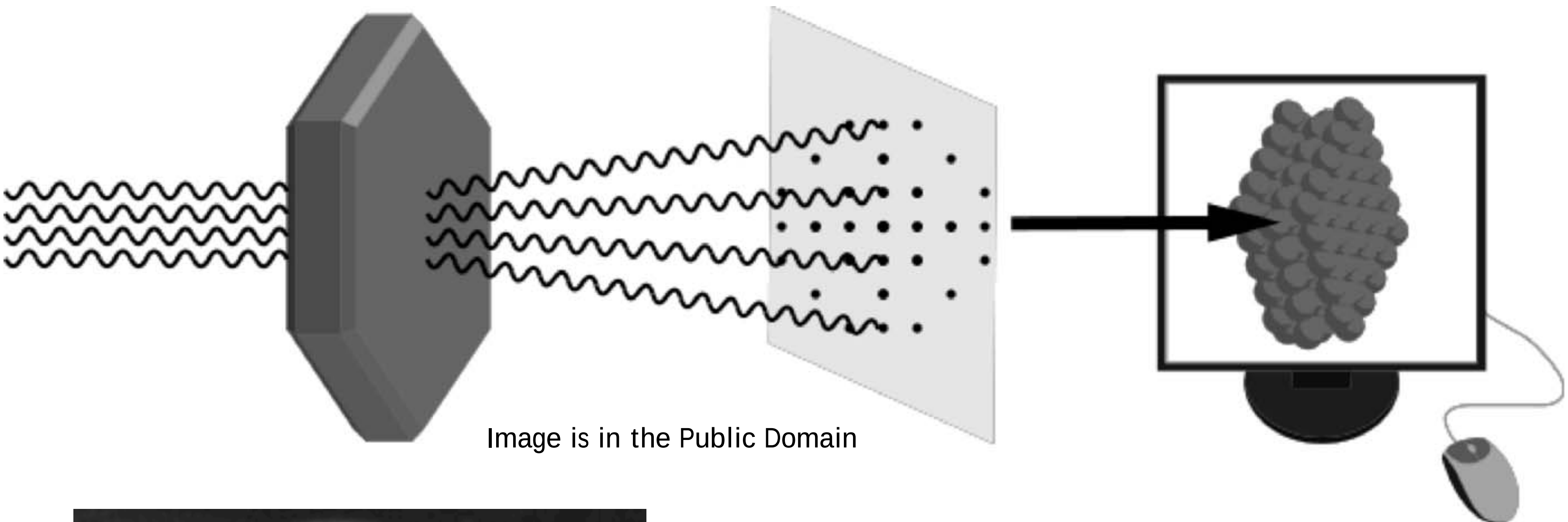


Image is in the Public Domain

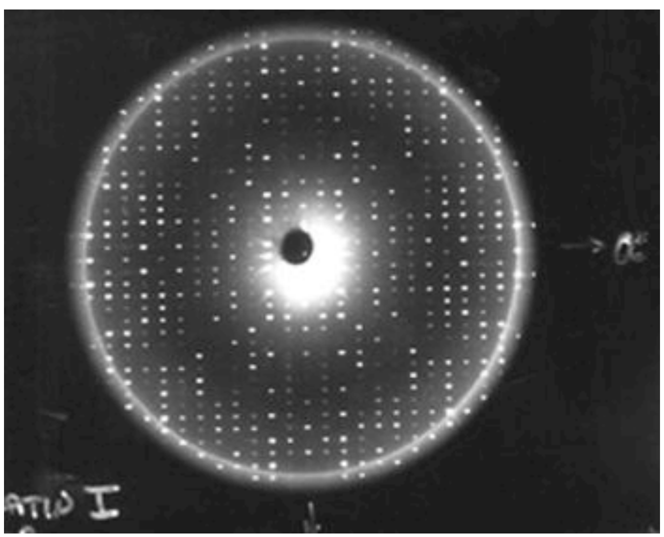


Image from the NASA gallery
http://mix.msfc.nasa.gov/abstracts.php?p=2057

From Davisson-Germer Experiment

Theory:

$E = 54$ eV

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$$

$$= \frac{6.626 \times 10^{-34}}{\sqrt{2 \times 9.109 \times 10^{-31} \times 54 \times 1.602 \times 10^{-19}}}$$

$= 0.167$ nm

Experiment:

$d = 0.215$ nm

$\theta = 50^\circ$

$\lambda = d \sin\theta = 0.165$ nm

Schrodinger: A prologue
Inferring the Wave-equation for Light

$$\psi \approx e^{j(\omega t - k_x x)}$$

$$\frac{\partial}{\partial t}\vec{E} = j\omega\vec{E}$$

$$\frac{\partial}{\partial x}\vec{E} = -jk_x\vec{E}$$

$$\omega = ck$$

⇓

$$\omega^2 = c^2 k^2$$

⇓

$$-\frac{\partial^2}{\partial t^2}\vec{E} = -c^2\frac{\partial^2}{\partial x^2}\vec{E}$$

… so relating ω to k allows us to infer the wave-equation

Schrodinger: A Wave Equation for Electrons

$$E = \hbar\omega \qquad\qquad p = \hbar k$$

Schrodinger *guessed* that there was some wave-like quantity that could be related to energy and momentum …

$$\psi \approx e^{j(\omega t - k_x x)}$$ wavefunction

$$\frac{\partial}{\partial t}\psi = j\omega\psi \quad \Rightarrow \quad E\psi = \hbar\omega\psi = -j\hbar\frac{\partial}{\partial t}\psi$$

$$\frac{\partial}{\partial x}\psi = -jk_x\psi \quad \Rightarrow \quad p_x\psi = \quad k_x\psi = j\hbar\frac{\partial}{\partial x}\psi$$

Schrodinger: A Wave Equation for Electrons

$$E\psi = \hbar\omega\psi = -j\hbar\frac{\partial}{\partial t}\psi \qquad p_x\psi = \quad k\psi = j\hbar\frac{\partial}{\partial x}\psi$$

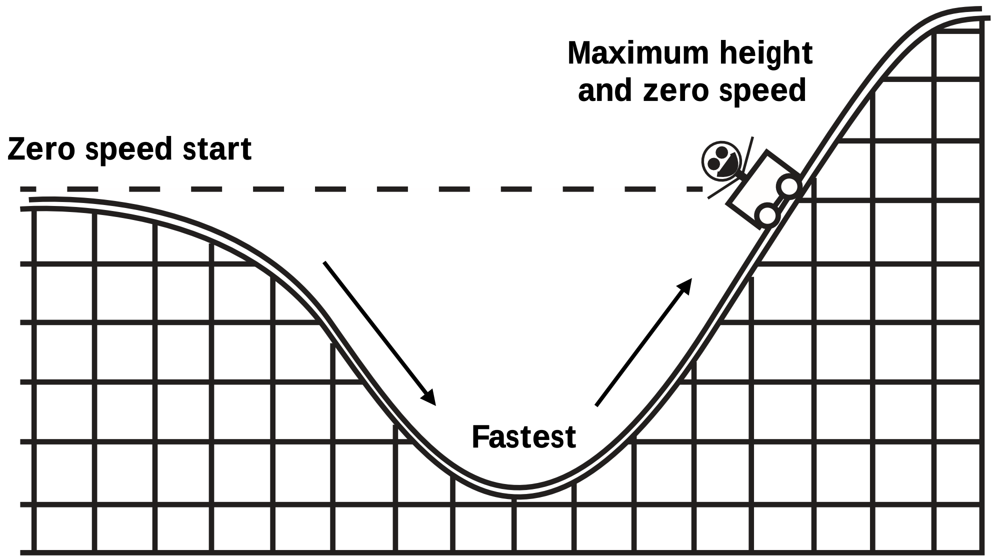
$$E = \frac{p^2}{2m}$$ (free-particle)

$$-j \quad \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$$ (free-particle)

..The Free-Particle Schrodinger Wave Equation !

Erwin Schrödinger (1887–1961)
Image in the Public Domain

Classical Energy Conservation



- 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

Schrodinger Equation and Energy Conservation

… The Schrodinger Wave Equation !

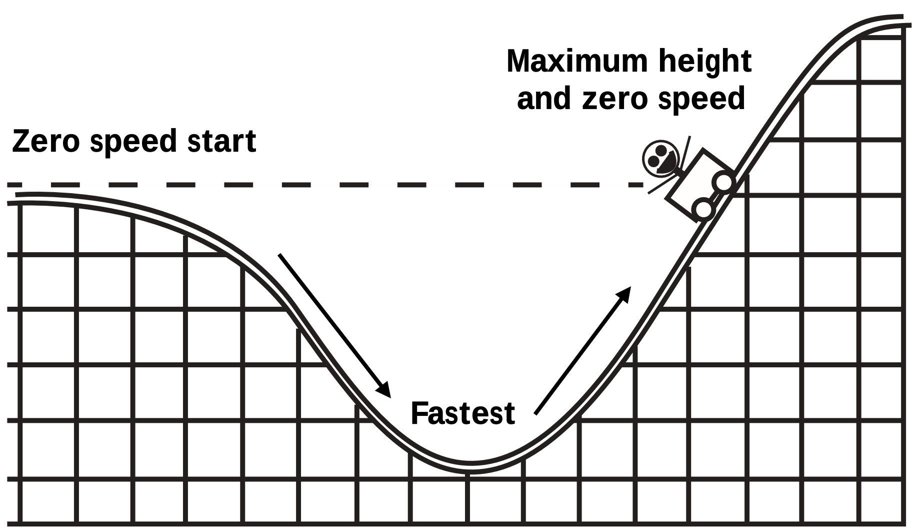
$$E = K + V$$

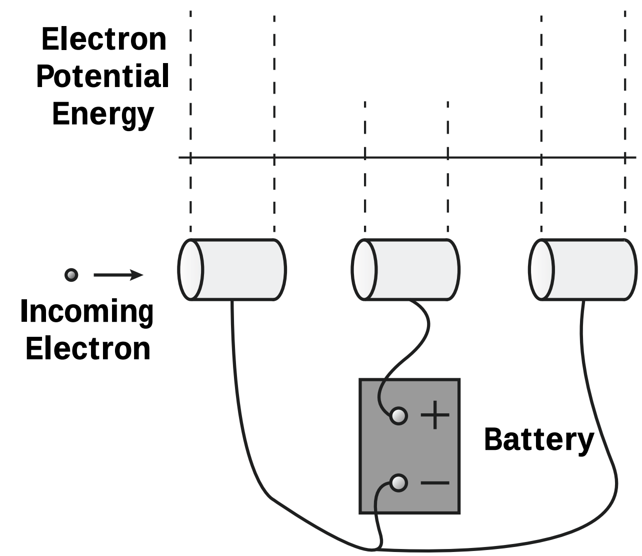
$$-j\hbar\frac{\partial}{\partial t}\psi = -\frac{{}^{2}}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$$

Total E term **K.E. term** **P.E. term**

… In physics notation and in 3-D this is how it looks:

$$i\ \frac{\partial}{\partial t}\Psi(\mathbf{r},t) = -\frac{{}^{2}}{2m}\nabla^2\Psi(\mathbf{r},t) + V(\mathbf{r})\Psi(\mathbf{r},t)$$





Time-Dependent Schrodinger Wave Equation

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t)$$

PHYSICS NOTATION

Total E term

K.E. term

P.E. term

$$\Psi(x,t) = e^{-iEt/\hbar}\psi(x)$$

Time-Independent Schrodinger Wave Equation

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x)$$

Electronic Wavefunctions

$$\psi(x) \approx e^{j(\omega t - k_x x)}$$ free-particle wavefunction

- Completely describes all the properties of a given particle
- Called $\psi = \psi(x, t)$ - is a complex function of position x and time t
- What is the meaning of this wave function?

- The quantity $|\psi|^2$ is interpreted as the probability that the particle can be found at a particular point x and a particular time t

$$P(x)dx = |\psi|^2$$

Image is in the public domain

Werner Heisenberg (1901–1976)
Image in the Public Domain

Copenhagen Interpretation of Quantum Mechanics

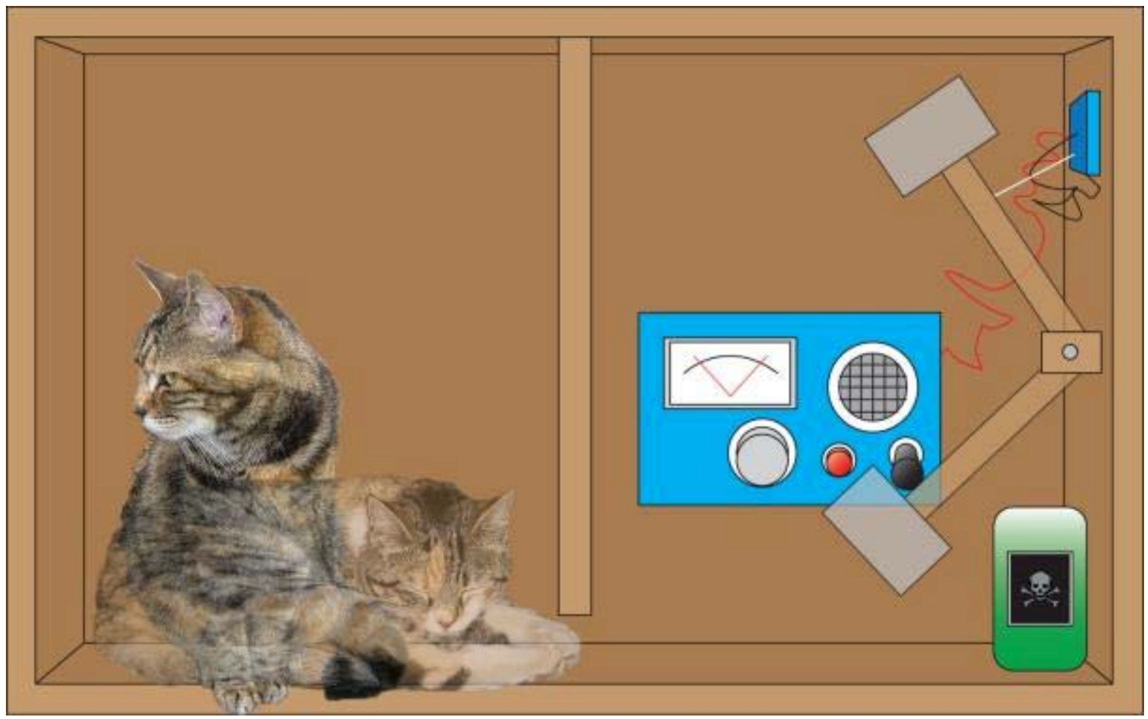
- A system is completely described by a wave function ψ, representing an observer's subjective knowledge of the system.
- The description of nature is essentially probabilistic, with the probability of an event related to the square of the amplitude of the wave function related to it.
- It is not possible 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.

Today's Culture Moment

Schrödinger'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

Comparing EM Waves and Wavefunctions

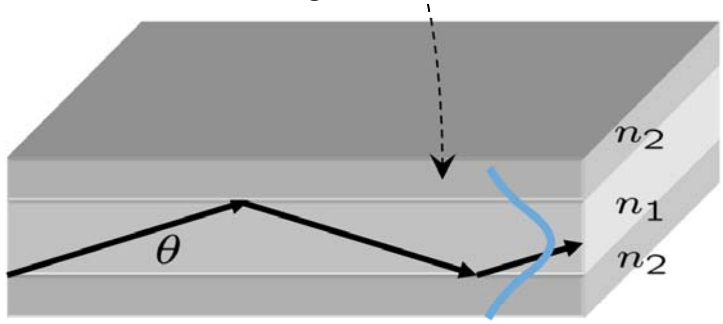
EM WAVES

$$\omega^2 = c^2 k^2$$

$$-\frac{\partial^2}{\partial t^2}\vec{E} = -c\frac{\partial^2}{\partial x^2}\vec{E}$$

$$I = \frac{|E|^2}{\eta}$$

waveguide



QM WAVEFUNCTIONS

$$E = \frac{p^2}{2m} + V(x)$$

$$-j\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi$$

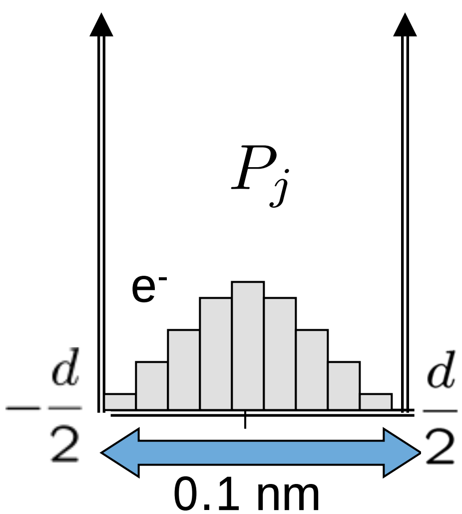
$$P(x)dx = |\psi|^2$$

Quantum well

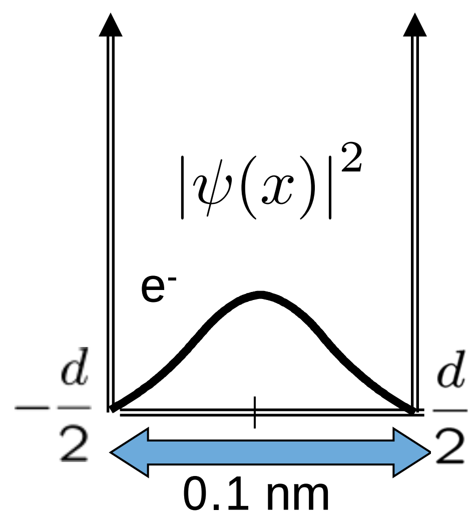
Expected Position

$$\langle x \rangle = \sum_{j=-\infty}^{\infty} x\, P_j$$

$$\langle x \rangle = \int_{-\infty}^{\infty} x|\psi|^2 dx$$



$$< x >= 0$$



$$< x >= 0$$

Expected Momentum

$$< p >= \int_{-\infty}^{\infty} p \left| \psi(x) \right|^2 dx$$

$$= \int_{-\infty}^{\infty} j\hbar \frac{\partial}{\partial x} \left| \psi(x) \right|^2 dx$$

imaginary real

Doesn't work !
Need to guarantee <p> is real

... so let's fix it by rewriting the expectation value of p as:

$$< p >= \int_{-\infty}^{\infty} \psi^*(x) \left(j\hbar \frac{\partial}{\partial x} \right) \psi(x) dx$$

free-particle wavefunction

$$\psi \approx e^{j(\omega t - k_x x)} \qquad < p >= \hbar k$$

Maxwell and Schrodinger

Maxwell's Equations

$$\oint_C \vec{E} \cdot d\vec{l} = -\frac{d}{dt}\left(\int_S \vec{B} \cdot d\vec{l}\right)$$

$$\oint_C \vec{H} \cdot d\vec{l} = \int \vec{J} \cdot d\vec{A} + \frac{d}{dt}\int_S \epsilon \vec{E} \cdot d\vec{A}$$

The Wave Equation

$$\frac{\partial^2 E_y}{\partial z^2} = \epsilon\mu \frac{\partial^2 E_y}{\partial t^2}$$

Dispersion Relation

$$\omega^2 = c^2 k^2$$

$$\omega = ck$$

Energy-Momentum

$$E = \hbar\omega = \hbar ck = cp$$

Quantum Field Theory

The Schrodinger Equation

$$-j\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi$$

(free-particle)

Dispersion Relation

$$\omega = \frac{\hbar^2 k^2}{2m}$$

Energy-Momentum

$$E = \frac{p^2}{2m}$$ (free-particle)

6.007 Electromagnetic Energy: From Motors to Lasers
Spring 2011