Quantum Mechanics

Understand how charge moves in semiconductors

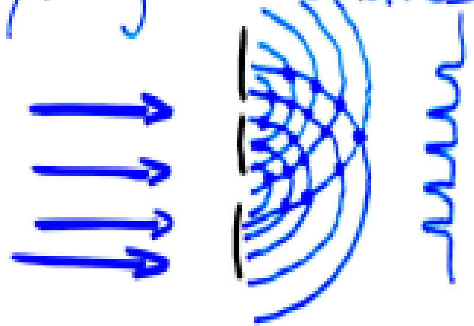
- on macroscopic scale, classical physics works just fine.
- on atomic scale, need QM to describe motion

Why?

Wave-Particle Duality

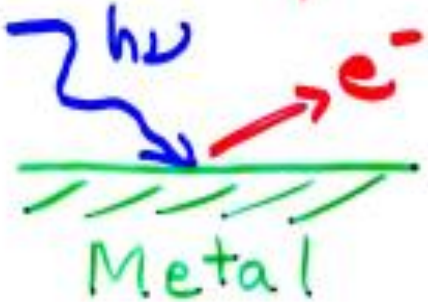
Light

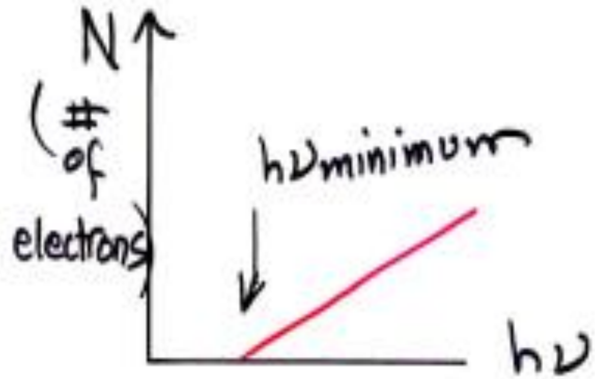
Classically, light behaves like waves



(diffraction intensities in real space)

Atomically, light behaves like particles (called "photons")





Photoemission

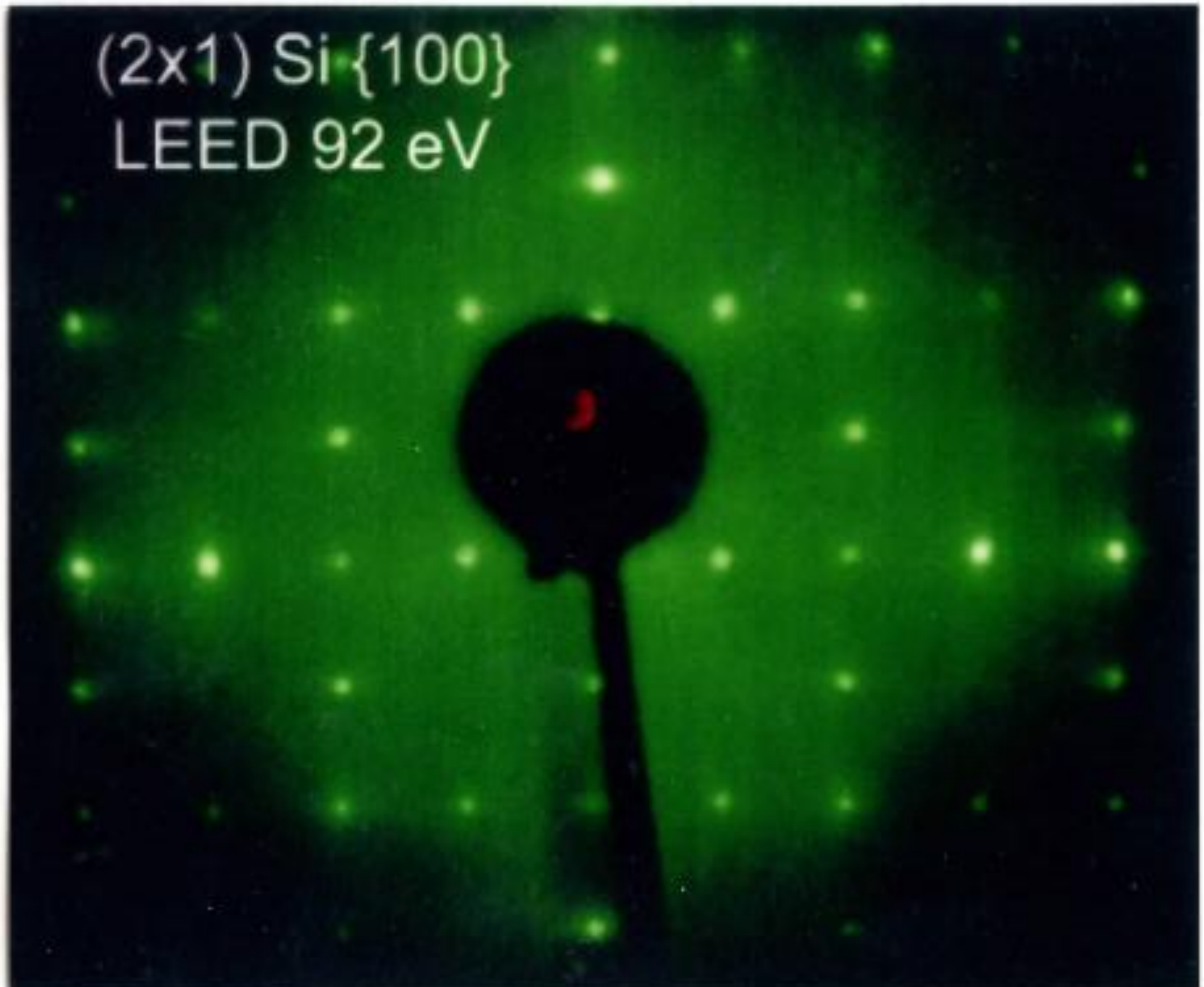
electron kicked out only if $E \geq h\nu$ minimum

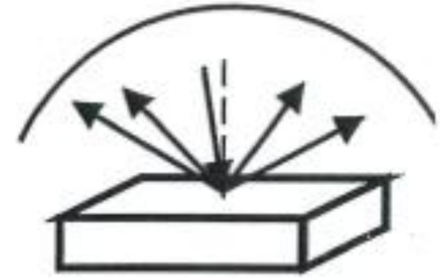
Lots of little $h\nu$'s don't do it!

(Note: A. Einstein got a Nobel Prize for this idea (1905))

So, light waves act as discrete units (particles).

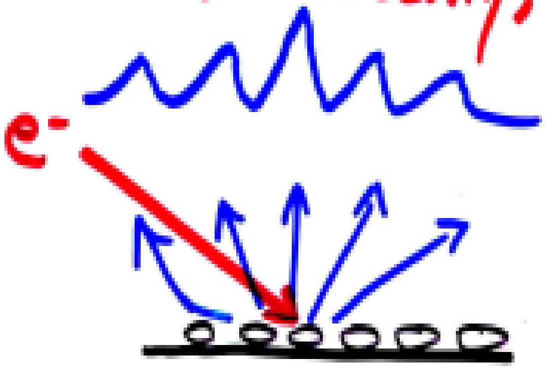
Electrons Can Diffract, Just Like Light Waves





Electrons – classically, electrons behave like particles.

– atomically, electrons behave like waves.



(Note: L. Germer got a Nobel Prize for observing this (1927))

Photons have particle momentum.

Particles have wavelength.

Photon: $\left(= \frac{1.24\,eV}{\lambda(\text{microns})} \right)$

ν = frequency (cycles/sec)

$h = 6.63 \times 10^{-34}$ J-sec (Planck's Constant)

$c = 3 \times 10^{10}$ cm/sec

Example: $5000\,\text{Å} = 0.5\,\mu m \Rightarrow 2.48\ eV$

$1\,\mu m \Rightarrow 1.24\,eV$

$1\,\text{Å} = 10^{-8}\,cm = 10^{-4}\,\mu m \Rightarrow 1.24 \times 10^{4}\,eV$

Particle: $p = mv = \dfrac{h}{\lambda}$ particle momentum (we'll see this later)

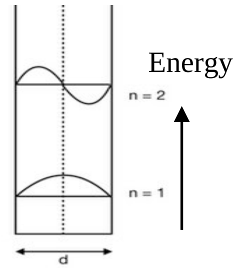
= De Broglie wavelength

Quantum Roadmap

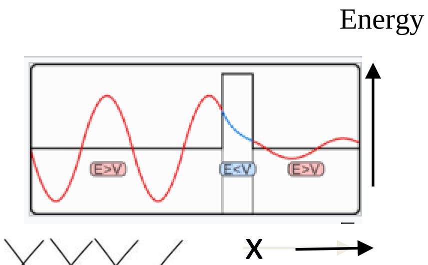
- **Electrons can act as particles but also as waves**

Electrons: $p = mv = h/\lambda$, Photons: $E = h\nu = hc/\lambda$

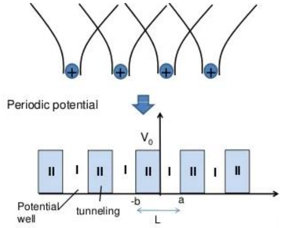
- **Quantum Mechanics can explain quantum wells**



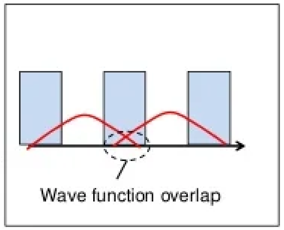
- **Quantum Mechanics can explain electron tunneling**



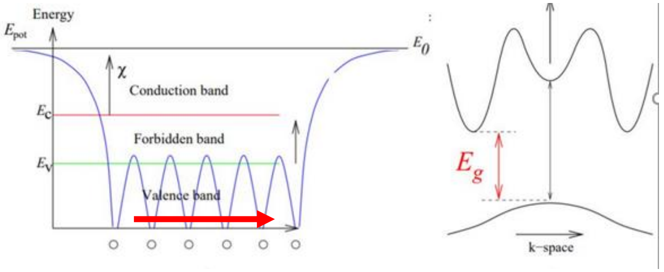
- **Atoms in semiconductor lattices behave like quantum wells**



- **Electrons can tunnel through closely spaced quantum wells**



- **Energy bands form that include conduction & valence band**



Example: Electron λ for $v = 10^7$ cm/sec
(close to saturation velocity in a semiconductor)

$$p = mv = (9.11 \times 10^{-28}\ \text{gm})\left(10^7\ \frac{\text{cm}}{\text{sec}}\right)$$
$$= 9.11 \times 10^{-21}\ \text{gm}\cdot\frac{\text{cm}}{\text{sec}}$$

$$\lambda = \frac{h}{p} = \frac{6.625 \times 10^{-27}\ \text{erg-sec}}{9.11 \times 10^{-21}\ \text{gm}\frac{\text{cm}}{\text{sec}}}$$

(If semiconductor features are comparable or smaller in size, can have diffraction effects!)

$$\lambda = \frac{h}{p}$$

Small mass, small p, "large" λ → quantum (e's, n's, p's)
Large mass, large p, small λ → classical (cars, trucks, pizzas)

Wave - Particle Duality - basis for using "wave theory" to describe motion/energy of electrons in crystal

▷ Uncertainty Principle (Heisenberg's)

$\left(\hbar = \frac{h}{2\pi}\right)$

The basic idea: Can't know x and p both exactly at the same time. The act of measuring one will change the other.

also.

Everything has a probability

Multiply $\int P(x)dx$ times a function to get the function's average (expectation) value

▷ Average (Expectation) Value of a Function or Property

$$\langle f(x) \rangle = \frac{\int f(x)\, P(x)\, dx}{\int P(x)\, dx}$$

← Normalization

▷ Schroedinger Wave Equation

Apply quantum concepts to classical equations of mechanics $\longrightarrow$ "quantum mechanics"

Basic Postulates

(1) Each particle described by a wave function

$\psi(x,y,z,t)$: ψ and $\nabla\psi$ continuous, finite, single -valued

(2) Classical Variable $\longleftrightarrow$ Quantum "operator"

$$x \longrightarrow x$$

$$f(x) \longrightarrow f(x)$$

$$p(x) \longrightarrow \frac{\hbar}{j}\frac{\partial}{\partial x}$$

$$E \longrightarrow \frac{-\hbar}{j}\frac{\partial}{\partial t}$$

(3) $\int_{-\infty}^{\infty} P(x)\,dx = 1 \longrightarrow \int_{-\infty}^{\infty} \psi^* \psi \,dx\,dy\,dz = 1$

(4) $\int_{-\infty}^{\infty} Q(x) P(x)\,dx = \langle Q \rangle \longrightarrow \int_{-\infty}^{\infty} \psi^* Q_{op} \psi \,dx\,dy\,dz = \langle Q \rangle$

ψ^* is complex conjugate of ψ

example: $(e^{jx})^* = e^{-jx}$

$j^2 = -1$

$\left(\frac{\partial}{\partial x}\right)^2 \equiv \frac{\partial^2}{\partial x^2}$

Probability Density Function $= \psi^* \psi = |\psi|^2$

$$\langle x \rangle = \int \psi^* x \, \psi \, dx \, dy \, dz \, dt$$

$$\langle p(x) \rangle = \int \psi^* \frac{\hbar}{j} \frac{\partial}{\partial x} \psi \, dx \, dy \, dz \, dt$$

$$\langle E \rangle = \int \psi^* \left(-\frac{\hbar}{j} \frac{\partial}{\partial t} \right) \psi \, dx \, dy \, dz \, dt$$

$$\langle p(x)^2 \rangle = \int \psi^* \left(-\hbar^2 \frac{\partial^2}{\partial x^2} \right) \psi \, dx\, dy\, dz\, dt$$

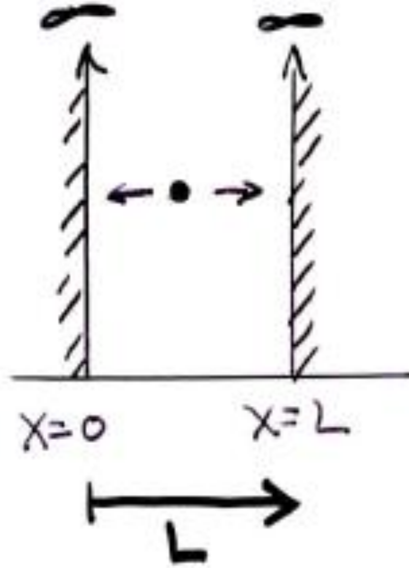
$$\langle v(x)^2 \rangle = \int \psi^* \left(\frac{-\hbar^2}{m^2} \frac{\partial^2}{\partial x^2} \right) \psi \, dx\, dy\, dz\, dt$$

$$\langle E_k \rangle = \int \psi^* \left(\frac{1}{2} m v^2 \right) \psi \, dx\, dy\, dz\, dt$$

$$= \int \psi^* \left(-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi \, dx\, dy\, dz\, dt$$

$$= \int \psi^* \left(-\frac{\hbar^2}{2m} \nabla^2 \right) \psi \, dx\, dy\, dz\, dt$$

Example: Particle in a Potential Well



Accept: that $\psi(x,t) = C\sin\left(\frac{\pi x}{L}\right) e^{-j\frac{Et}{\hbar}}$

inside well $(0 \le x \le L)$ $\qquad V = E_p = E_0$

and $\psi(x,t) = 0$ everywhere else.

The particle must be in the well. So $\int \psi^* \psi \, dx = \int_0^L \psi^* \psi \, dx = 1$

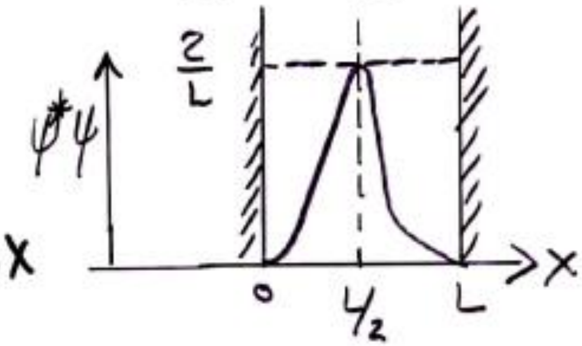
$$\int_0^L \psi^* \psi \, dx = \int C^* \sin\left(\frac{\pi x}{L}\right) C \sin\left(\frac{\pi x}{L}\right) dx = 1$$

substitute variables to simplify: $y = \frac{\pi x}{L}$

so $C^* \frac{CL}{\pi} \int_0^{\pi} \sin^2 y \, dy = 1$

so $C^* \frac{C L}{\pi} \int_0^{\pi} \sin^2 y \, dy = 1$

$\int_0^{\pi} \sin^2 y \, dy = \frac{\pi}{2}$ so $C^* C = \frac{2}{L}$ or $C = \sqrt{\frac{2}{L}}$



Maximum value of $\psi^* \psi = \frac{2}{L}$

$\psi^* \psi = |\psi|^2 = \sin^2\left(\frac{\pi x}{L}\right)$ at position x

since $\int_0^L |\psi|^2 dx = 1$ over distance L, average value per unit distance $= \frac{1}{L}$. ← $|\psi|^2 L = 1$

Average Position: $\langle x \rangle = \int \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) x \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) dx$

Again simplify with $y = \frac{\pi x}{L}$.

$$\langle x \rangle = \frac{2}{L} \frac{L^2}{\pi^2} \int_0^{\pi} y \sin^2 y \, dy = \frac{2L}{\pi^2} \cdot \frac{\pi^2}{4} = \frac{L}{2}$$

So average position is in center of well.

Probability Density Function $= \psi^* \psi \equiv |\psi|^2$

$$\langle x \rangle = \int \psi^* x \psi \, dx \, dy \, dz \, dt$$

$$\langle p(x) \rangle = \int \psi^* \frac{\hbar}{j} \frac{\partial}{\partial x} \psi \, dx \, dy \, dz \, dt$$

$$\langle E(x) \rangle = \int \psi^* \left(-\frac{\hbar}{j} \frac{\partial}{\partial t} \right) \psi \, dx \, dy \, dt \, dz$$

Classical Energy Equation

Kinetic Energy + Potential Energy = Total Energy

$$\frac{1}{2m} p^2 \quad + \quad V \quad = \quad E$$

"Plug in" Ψ's. In one-dimension,

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

In three-dimensional case,

(*)

where $\nabla^2 \Psi \equiv \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2}$

Separate time and space dependencies:

$$\Psi(x,t) = \psi(x)\,\phi(t)$$

Schroedinger equation in one dimension becomes:

Time-Dependent Equation

Time-Independent Equation

Each side of (*) equation = constant

$= E$

All functions of x are on the left.

" " " time " " " right.

so can make 2 equations.

Note: $\psi(x)$ and E describe electron energy and motion.

$V(x)$ describes the surroundings (lattice, atoms..)

So for all QM problems, come up with reasonable V, then solve for ψ and E.

Why Bother? QM determines properties of electrons in crystal lattice. Then can determine statistical characteristics of large numbers of electrons in the crystal.

Discrete Energies -> Bands -> <u>Explains</u> <u>Semiconductor</u> <u>Behavior</u>