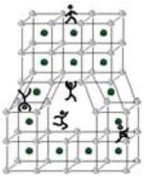
The Quantum World



- Introduction
- Four Important Solutions to the Schrödinger Equation
  - Free Electrons
  - Electron in a Well
  - Tunneling

Wednesday, Oct. 22, 2003

MATS275: INTRODUCTION TO MATERIALS SCIENCE

Photoelectric Effect

- When light strikes a solid, its energy can knock out an electron…so, if we increase the intensity, we should be able to knock out more electrons.
- BUT… this isn't true.

Planck's Constant

- The energy of a photon of light is proportional to the frequency:

$$E = hf = h\nu = \frac{hc}{\lambda}$$

$$h = 6.63\times10^{-34}\,J\cdot s \quad hc = 1240\,nm\cdot eV$$

- Or in angular frequency:

$$\omega = 2\pi f \quad E = hf = h\nu = \hbar\omega$$

$$\hbar = \frac{h}{2\pi} = 1.05\times10^{-34}\,J\cdot s$$

deBroglie Waves

- For light,

$$p = \frac{E}{c} = \frac{hf}{c} = \frac{h}{\lambda}$$

- DeBroglie said…same goes for particles:

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

- So by extension…

$$\vec{p} = \hbar\vec{k}$$
$$k = \frac{2\pi}{\lambda} \quad \Rightarrow \quad E = \tfrac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$
$$v = \frac{\omega}{k}$$

A Typical Wavelength

- An electron is accelerated through 5 kV, what is its wavelength?

$$p = \sqrt{2mE} = \sqrt{2\left(0.911\times10^{-30}\,\text{kg}\right)\left(5000\,\text{eV}\right)\left(\frac{1.602\times10^{-19}\,\text{J}}{1\,\text{eV}}\right)}$$

$$p = 3.82\times10^{-23}\,\frac{\text{kg}\cdot\text{m}}{\text{s}}$$

$$\lambda = \frac{h}{p} = \frac{6.626\times10^{-34}\,J\cdot s}{3.82\times10^{-23}\,\frac{kg\cdot m}{s}} = 0.017\,nm$$

A Typical Wavelength

- What about 2.5 V?

$$p = \sqrt{2mE} = \sqrt{2\left(0.911\times10^{-30}\,\text{kg}\right)\left(2.5\,\text{eV}\right)\left(\frac{1.602\times10^{-19}\,\text{J}}{1\,\text{eV}}\right)}$$

$$p = 8.54\times10^{-25}\,\frac{\text{kg}\cdot\text{m}}{\text{s}}$$

$$\lambda = \frac{h}{p} = \frac{6.626\times10^{-34}\,\text{J}\cdot\text{s}}{8.54\times10^{-25}\,\frac{\text{kg}\cdot\text{m}}{\text{s}}} = 0.78\,\text{nm}$$

What is a Wave?

- Simplest wave is called a "harmonic wave". It can be described by a wavefunction, Ψ, given by:

$$\begin{aligned}\Psi(x,t) &= \sin(kx-\omega t)\\ &= \sin[k(x-vt)]\\ &= \sin\left(\tfrac{2\pi}{\lambda}x-2\pi f\,t\right)\\ &= \sin\left(2\pi\tfrac{x}{\lambda}-2\pi\tfrac{t}{T}\right)\end{aligned}$$

- Any function can be made up of a combination of sines and cosines, so once we've learned this, we can apply it to any function we like…sort of

Superposition of Waves

- Add two waves, Ψ_1, and Ψ_2 having slightly different frequencies, ω and $\omega + \Delta\omega$

$$\Psi_1 = \sin(k_1x-\omega_1 t) \quad \Psi_2 = \sin(k_2x-\omega_2 t)$$

$$\Psi_1+\Psi_2 = \sin(k_1x-\omega_1 t)+\sin(k_2x-\omega_2 t)$$

$$= \sin\left[\left(k-\tfrac{\Delta k}{2}\right)x-\left(\omega-\tfrac{\Delta\omega}{2}\right)t\right]+\sin\left[\left(k+\tfrac{\Delta k}{2}\right)x+\left(\omega+\tfrac{\Delta\omega}{2}\right)t\right]$$

$$= \sin\left[(kx-\omega t)-\left(\tfrac{\Delta kx-\Delta\omega t}{2}\right)\right]+\sin\left[(kx-\omega t)+\left(\tfrac{\Delta kx-\Delta\omega t}{2}\right)\right]$$

$$= \sin(A-B)+\sin(A+B)$$

$$= \sin A\cos B+\sin B\cos A+\sin A\cos B-\sin B\cos A$$

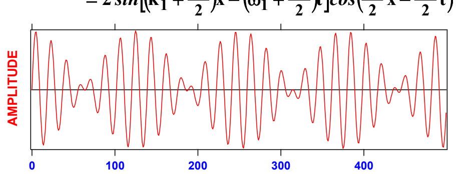
$$= 2\sin A\cos B$$

Superposition of Waves

- Add two waves, Ψ_1, and Ψ_2 having slightly different frequencies, ω and $\omega + \Delta\omega$

$$\Psi_1+\Psi_2 = 2\sin(kx-\omega t)\cos\left(\tfrac{\Delta kx-\Delta\omega t}{2}\right)$$

$$= 2\sin\left[\left(k_1+\tfrac{\Delta k}{2}\right)x-\left(\omega_1+\tfrac{\Delta\omega}{2}\right)t\right]\cos\left(\tfrac{\Delta k}{2}x-\tfrac{\Delta\omega}{2}t\right)$$



$k = \frac{2\pi}{20}$ $(\lambda = 20)$

$\Delta k = 0.05\,(\lambda_{beat} = 125)$

Heisenberg

- Notice, the better we know the momentum (k), the less we know the position (x).
- Heisenberg told us

$$\Delta x \Delta k = \frac{1}{2} \qquad \Delta\omega \Delta t = \frac{1}{2}$$

$$\text{or} \qquad\qquad \text{or}$$

$$\Delta x \Delta p = \frac{\hbar}{2} \qquad \Delta E \Delta t = \frac{\hbar}{2}$$

- These are the best we can ever do…

Implications of Uncertainty Principle

"The general implication of the U.P. is that there are two complimentary modes of describing the physical world: we can elect to discuss it in terms of the locations of the particles or in terms of their momenta. It was an error of classical physics to mix these descriptions. (my emphasis) Unfortunately, the conditioning of classical physics has been so great that many people still feel that the U.P. denies them complete knowledge of the world. I consider the correct attitude to be that classical physics unconsciously sought to be over complete. The U.P. reveals that there are alternative complete descriptions of the world; we should choose one description or the other, and not seek to mix them."

P.W. Atkins, Quanta

An Important Equation

- Let's take some d/dx's of our Ψ:

$$\Psi = \sin(kx - \omega t)$$

$$\frac{d\Psi}{dx} = k \cos(kx - \omega t)$$

$$\frac{d^2\Psi}{dx^2} = -k^2 \sin(kx - \omega t) = -k^2 \Psi$$

- Recall…

$$E = \frac{\hbar^2 k^2}{2m} \quad \Rightarrow \quad k^2 = \frac{2mE}{\hbar^2}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = \frac{\hbar^2 k^2}{2m}\Psi = (E + V)\Psi$$

Schrodinger Equation

- Time Independent (function of position and not time, ie: a vibration)

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (E+V)\psi$$

- Time Dependent (function of position and time, ie: a wave)

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$$

$$\nabla^2\Psi - \frac{2mV}{\hbar^2}\Psi - \frac{2mi}{\hbar}\frac{\partial\Psi}{\partial t}$$

What Does This Mean

- Boundary value problems lead to certain allowed energies known as eigenvalues. The equations which satisfy these are called eigenfunctions.
- The eigenfunctions represent probability density:

$$P(x) = \int_{x}^{x+\Delta x}\psi^*(x,t)\psi(x,t)dx$$

$$\int_{-\infty}^{\infty}P(x)dx = \int_{-\infty}^{\infty}\psi^*(x,t)\psi(x,t)dx = 1$$

Other Rules

- $\psi(x)$ must exist and satisfy Schrödinger
- $\psi(x)$ and $d\psi(x)/dx$ must be continuous
- $\psi(x)$ and $d\psi(x)/dx$ must be finite
- $\psi(x)$ and $d\psi(x)/dx$ must be single-valued
- $\psi(x)$ must go to 0 rapidly as x goes to infinity so that the function can be normalized.

Case I: Free Electron

- Free propagation in x direction (ie: V = 0)

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

- The solutions to this are known to be a harmonic oscillator given by:

$$\psi = Ae^{i\alpha x}$$

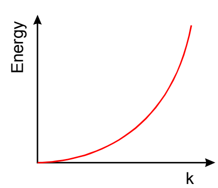
- where α is given by:

$$\alpha = \sqrt{\frac{2m}{\hbar^2}E} = k \quad \Rightarrow \quad E = \frac{\hbar^2 k^2}{2m}$$

E is Parabolic for a Free Electron

- This yields a new expression for the allowed energies in terms of the wave number

$$\boxed{E = \frac{\hbar^2}{2m}k^2}$$



Case II: Electrons in a Potential Well

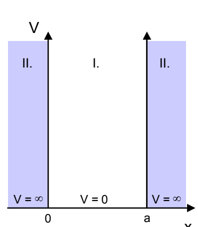
- There are now two regions to consider, Region I and Region II

- Region I (V = 0)

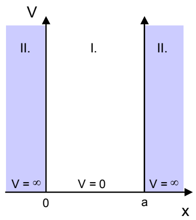
$$\frac{d^2\psi_I}{dx^2} + \frac{2m}{\hbar^2}E\psi_I = 0$$

- Region II (V =∞)

$$\psi_{II} = 0$$



Electrons in a Potential Well…continued

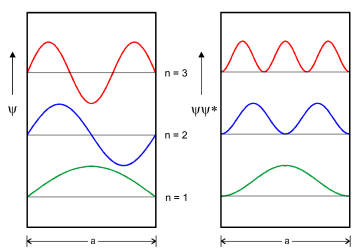


$$E_n = \frac{\hbar^2}{2m}k^2 = \frac{\hbar^2\pi^2}{2ma^2}n^2$$

- where n = 1, 2, 3, ...

$$\psi_I = \sqrt{\frac{2}{a}}\,\mathit{sin}\,\frac{n\pi}{a}x$$

Standing Waves



Case III: Electrons in a Finite Potential Well

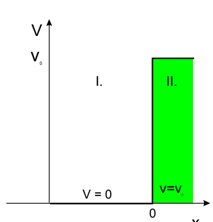
- Finite Energy Barrier, V_0
- Need two Schrodinger Equations for Region I and II
- Region I: Free Electron

$$\frac{d^2\psi_I}{dx^2} + \frac{2m}{\hbar^2}E\psi_I = 0$$

- Region II: Finite Barrier

$$\frac{d^2\psi_{II}}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_{II} = 0$$

$$\psi_{II} = Ce^{i\beta x} + De^{-i\beta x}$$



$$\beta = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$$

Apply Boundary Conditions

- Considering E<V…

$$\beta = \sqrt{\frac{2m}{\hbar^2}(E - V_0)} = i\sqrt{\frac{2m}{\hbar^2}(V_0 - E)} = i\gamma$$

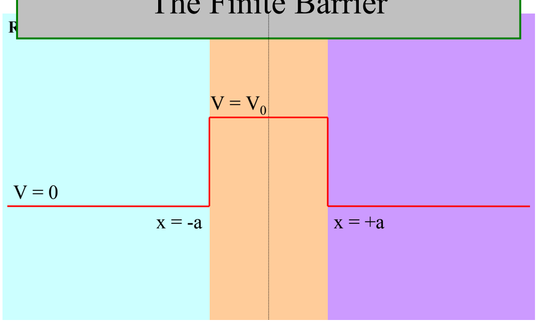
$$\psi_{II} = Ce^{\gamma x} + De^{-\gamma x}$$

- This must behave at ∞…

$$\psi_{II} = De^{-\gamma x}$$

- So it does exist inside the barrier!

The Finite Barrier



Solutions

- Region I

$$\psi_I(x) = e^{i\alpha x} + R\,e^{-i\alpha x}$$

- Region II

$$\psi_{II}(x) = Ae^{i\beta x} + Be^{-i\beta x}$$

- Region III

$$\psi_{III}(x) = Te^{i\alpha x}$$

$$\alpha = \sqrt{\frac{2m}{\hbar^2}E} \quad \beta = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$$

Applying the Conditions

- At x=-a

$$e^{-i\alpha a} + R\,e^{+i\alpha a} = Ae^{-i\beta a} + Be^{+i\beta a}$$

$$i\alpha e^{-i\alpha a} - i\alpha R\,e^{+i\alpha a} = i\beta Ae^{-i\beta a} - i\beta Be^{+i\beta a}$$

- At x=+a

$$Ae^{i\beta a} + Be^{-i\beta a} = Te^{i\alpha a}$$

$$i\beta Ae^{i\beta a} - i\beta Be^{-i\beta a} = i\alpha Te^{i\alpha a}$$

We want to solve this for R and T and leave out A and B

Solving for T

$$T = \frac{2\alpha\beta}{2\alpha\beta\,cos(2\beta a) - i(\alpha^2+\beta^2)sin(2\beta a)}e^{-i2\alpha a}$$

$$R = \frac{i(\beta^2-\alpha^2)sin(2\beta a)}{2\alpha\beta\,cos(2\beta a) - i(\alpha^2+\beta^2)sin(2\beta a)}e^{-i2\beta a}$$

- β<0 if we are below the barrier height…

$$T = \frac{2i\alpha\gamma e^{-i2\alpha a}}{(\alpha^2-\gamma^2)sinh(2\gamma a) + i2\alpha\gamma\,cosh(2\gamma a)}$$

The Tunneling Probability

- Find the magnitude squared of T:

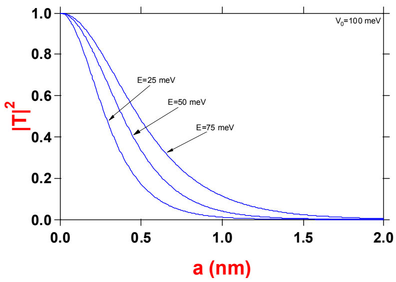
$$|T|^2 = T^*T = \frac{4\alpha^2\gamma^2}{(\alpha^2-\gamma^2)^2\,sinh^2(2\gamma a) + 4\alpha^2\gamma^2\,cosh^2(2\gamma a)}$$

- At large values of γa,

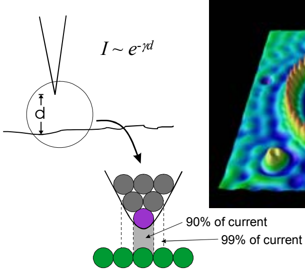
$$sinh^2(2\gamma a) \approx cosh^2(2\gamma a) = \left(\tfrac{1}{2}e^{2\gamma a}\right)^2 = \frac{e^{4\gamma a}}{4}$$

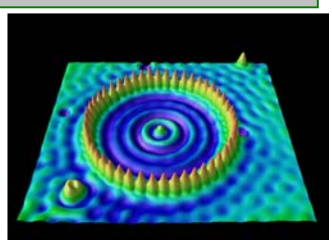
$$|T|^2 = \frac{16\alpha^2\gamma^2 e^{-4\gamma a}}{(\alpha^2+\gamma^2)^2}$$

The Tunneling Probability



Scanning Tunneling Microscope





Particle in a Square Well With Finite Barriers