

IB Paper 8: Electrical Elective

Easter term

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2. Semiconductors – an introduction to Quantum Mechanics

Introduction & Contents

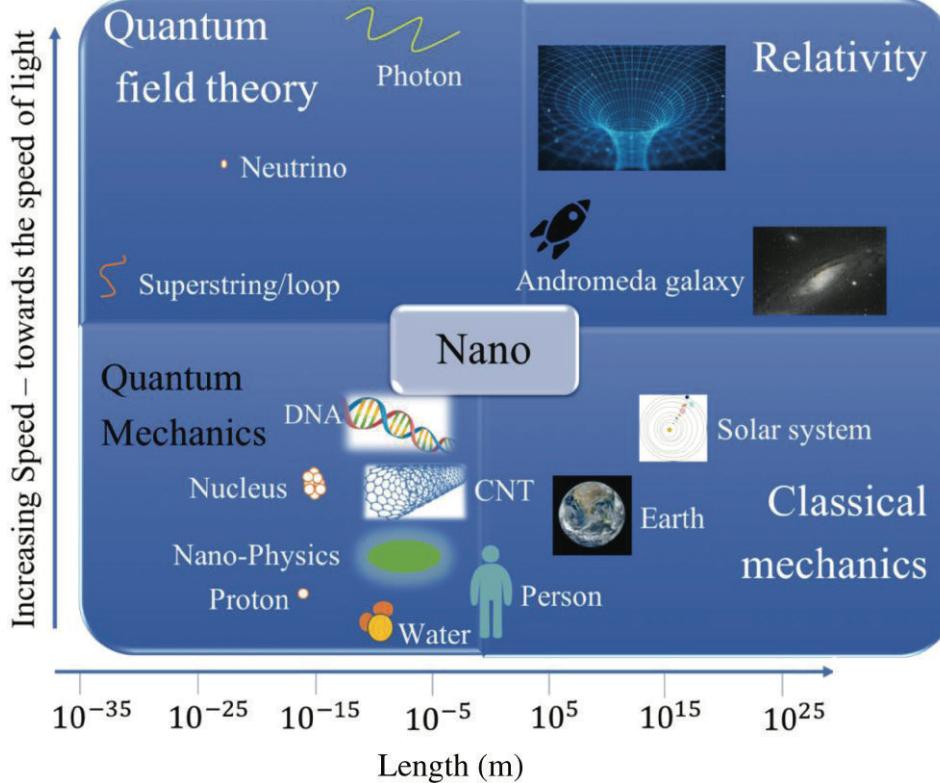
In this part of the course, which is Lectures 2-8 + examples class, we look at the origin of the charge transport characteristics of semiconductor devices, so we can understand the operation of a MOSFET, and its fundamental limitations. We also apply the same approach to understand the operation of the light-emitting elements in displays.

Our starting point is an introduction to the concepts underlying the quantum nature of charge carriers and materials at the atomic scale, the nature of bonding in materials, and how this is related to electronic structure. We then consider how free charges move throughout a material, and then (from section 7 onwards) how electric fields and voltages are distributed inside materials that contain charges (both free charges and fixed ones (dopants)) – this will allow us to predict current-voltage characteristics.

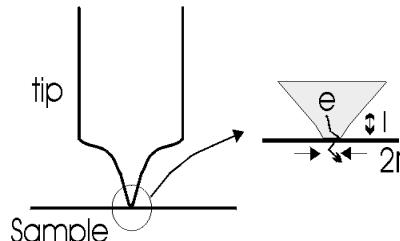
Contents

- Section 2 – An introduction to Quantum Mechanics
- Section 3 – Wavefunctions & Schrödinger's equation with examples
- Section 4 – Atomic Structure & Atoms to Solids
- Section 5 – Charge Carriers & Carrier Concentration
- Section 6 – Motion of Charge Carriers

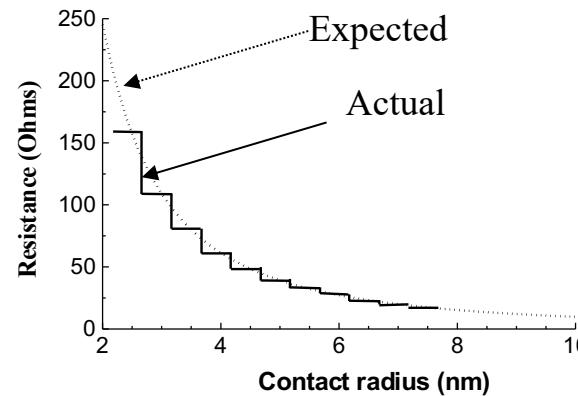
Lengthscales in Physics



Eg, point contact:
how does
resistance
change as it
gets
smaller?



e: electron
l: mean free path



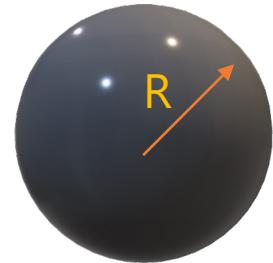
- When the dimensions of a conductor shrink below the electronic mean free path, electrical resistivity starts to change – it's not a material constant
- Dimensions below $\sim 5\text{nm}$, Quantum effects start to come to the fore

Quantum effects:

- Fundamental (i.e. we can't get rid of them)**
- Discrete – properties no longer change smoothly, but occur in jumps**

A major factor
Making nanostructures so
novel is to do with
surfaces: they have
different properties than
bulk. Nanostructures
have a lot of surface!

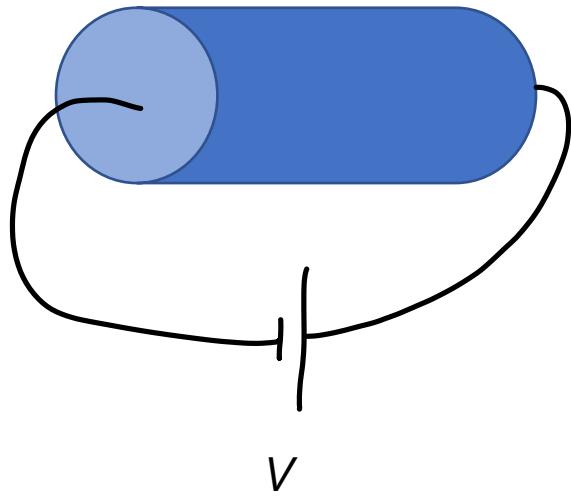
What is an electron.....?



Is it a ball? Is it a wave? No- it's a wave-packet.....

- Electrostatic potential a distance r away from a charge q is $V(r) = \frac{q}{4\pi\epsilon_0 r}$
- To first order, the energy associated with this is $qV = \frac{q^2}{4\pi\epsilon_0 r}$

Equate to relativistic rest-mass energy $mc^2 \Rightarrow r = \frac{q^2}{4\pi\epsilon_0 mc^2} = 2.82 \times 10^{-15} \text{ m}$

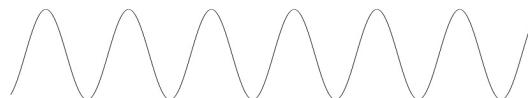


How do electrons move through a system?

1. A stream of particles?



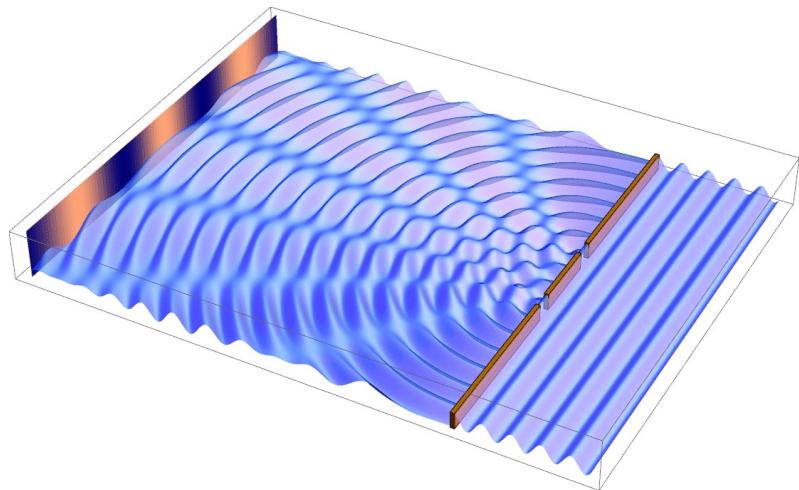
2. A wave?



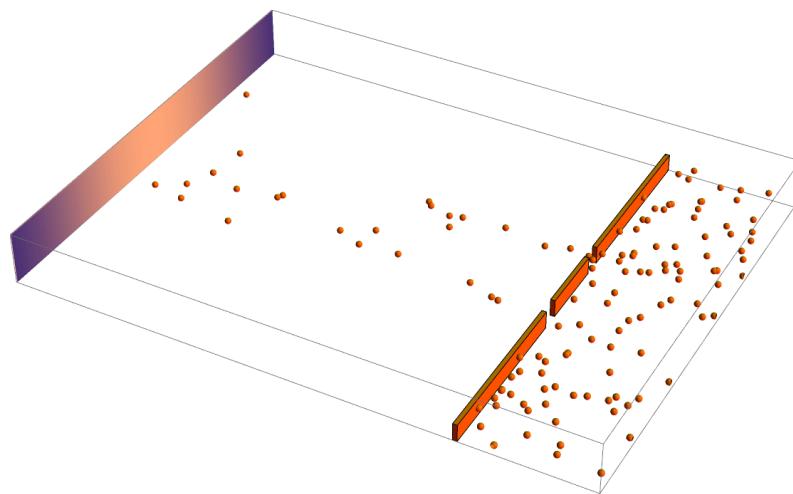
3. A wave-packet?



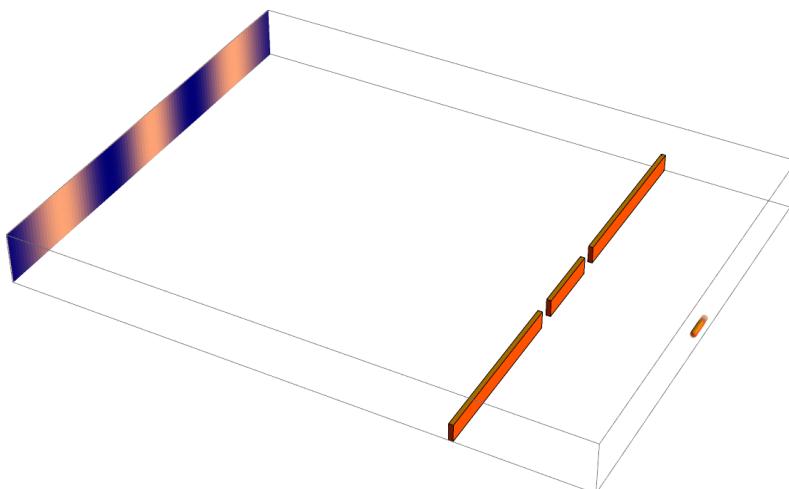
The double slit experiment & the interpretation of QM



Waves



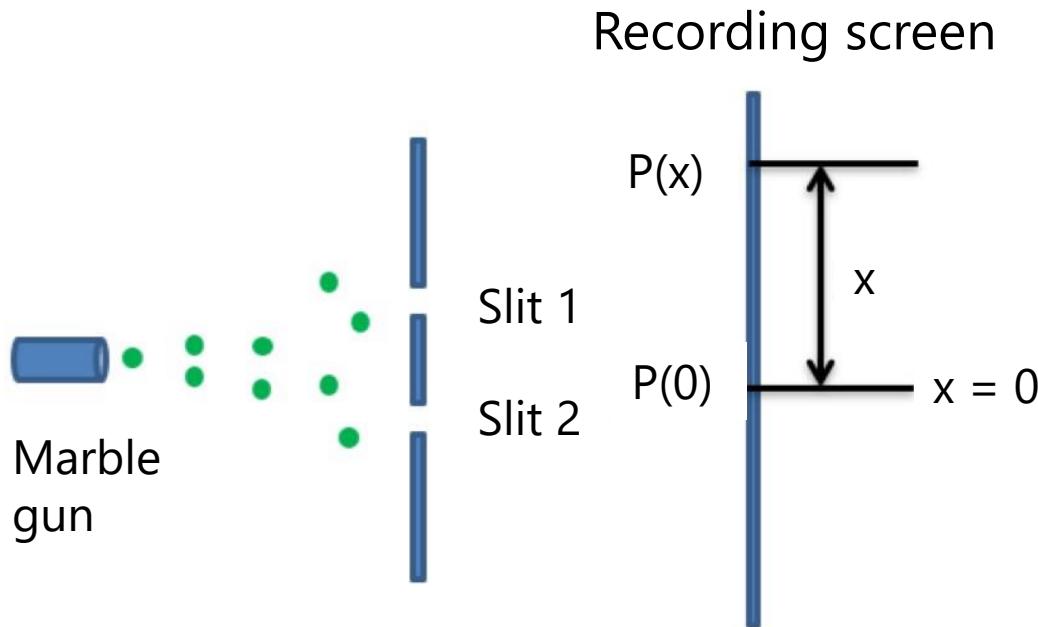
Particles



Wave-particles, e.g. electrons

Quantum Mechanics

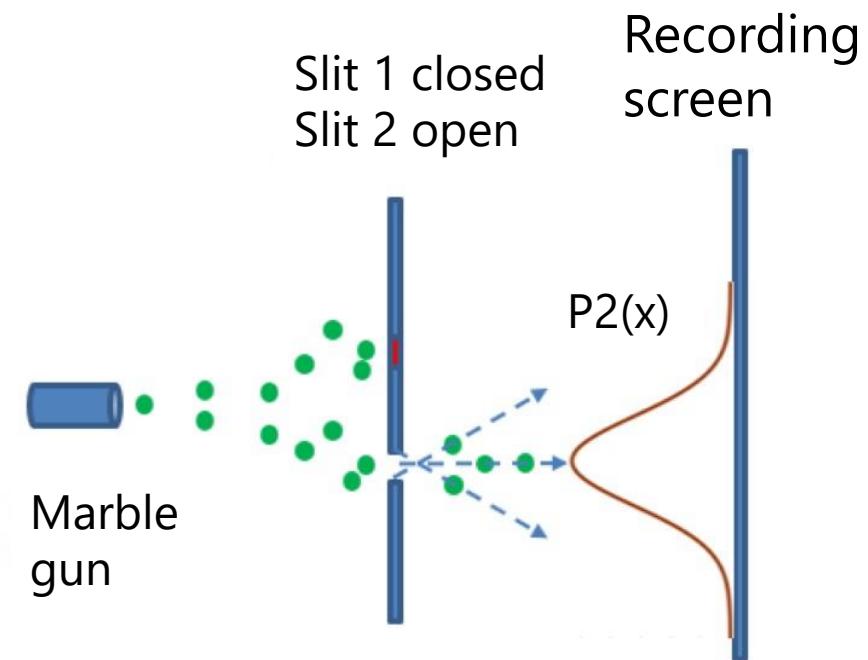
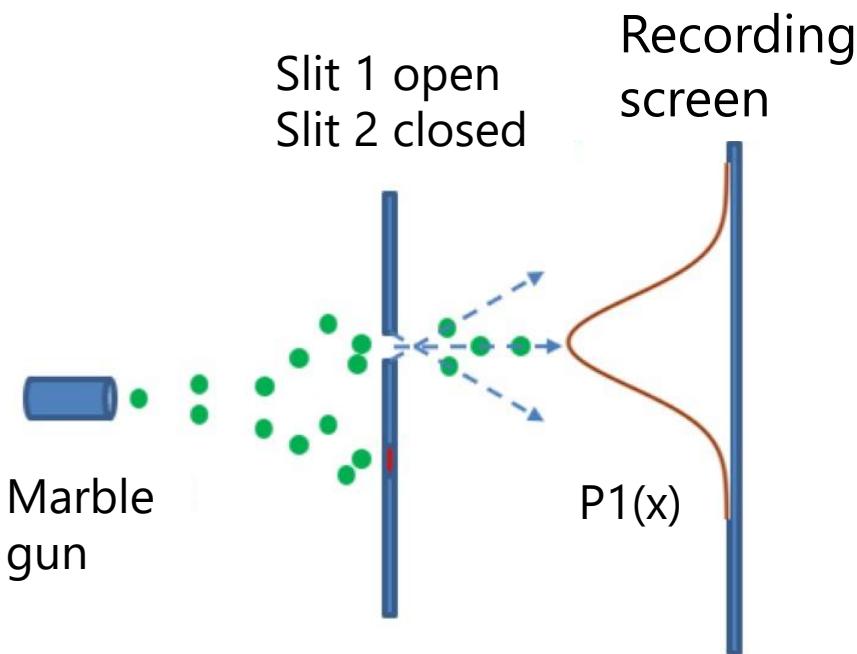
Feynman's thought experiment



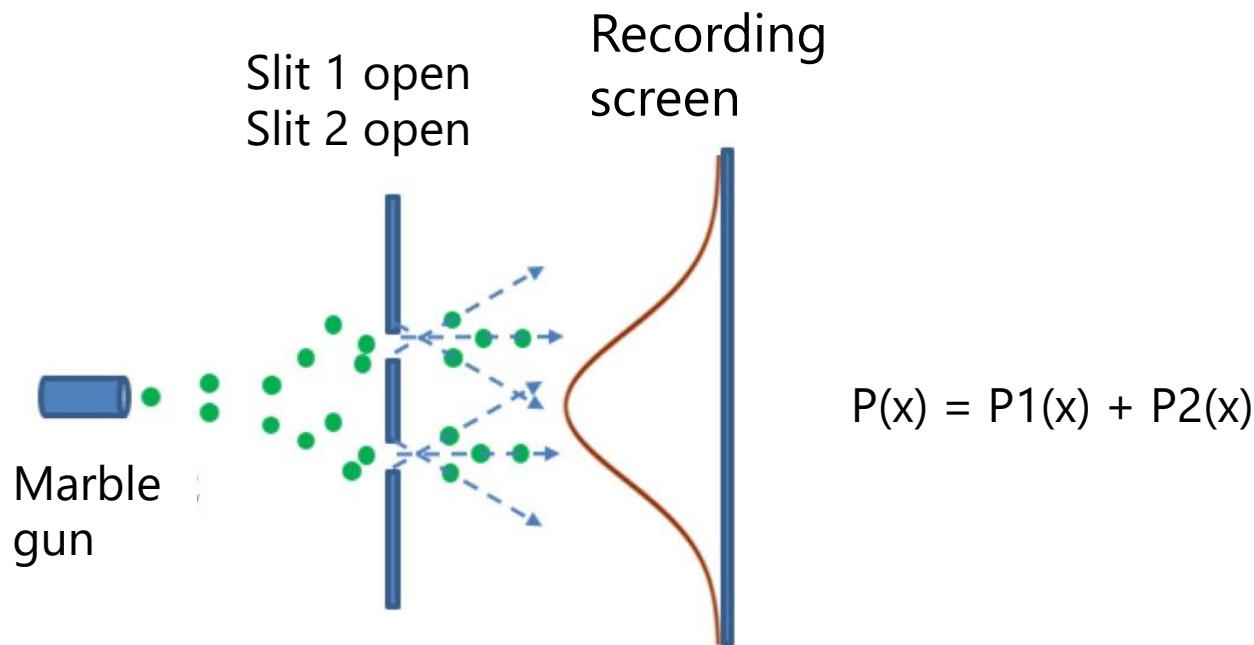
Probability, $P(x) = ?$

$$P(x) = \frac{\text{Number of marbles arriving at } x}{\text{Total number of marbles fired}}$$

Quantum Mechanics

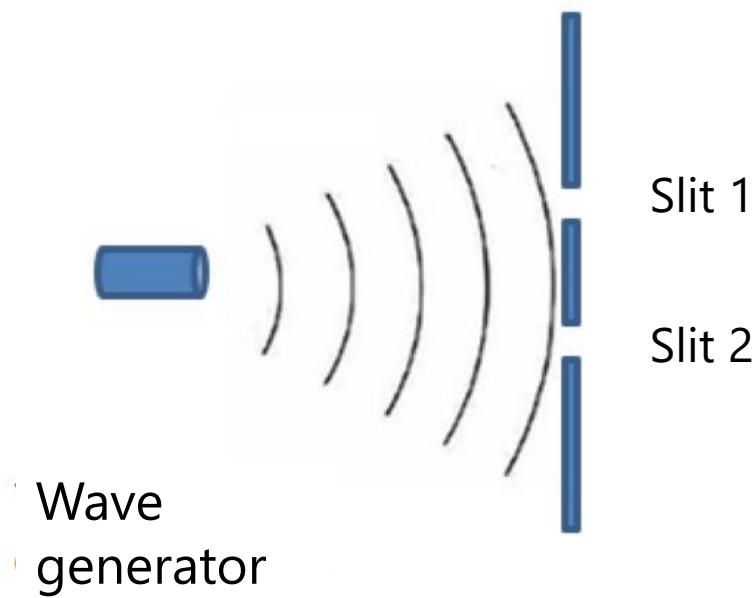


Quantum Mechanics

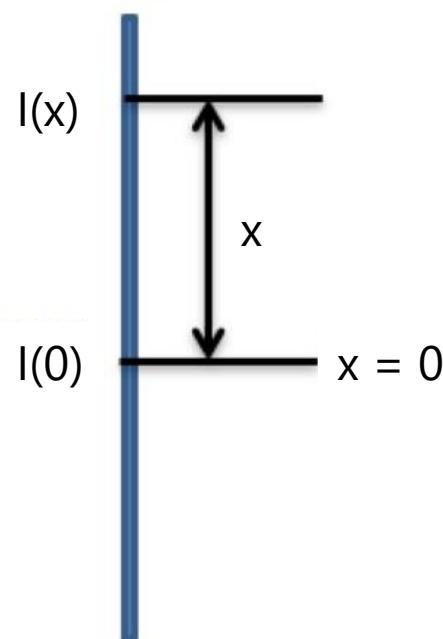


Classical mechanics : surely a marble can only go through one of the slits?

Now try with waves

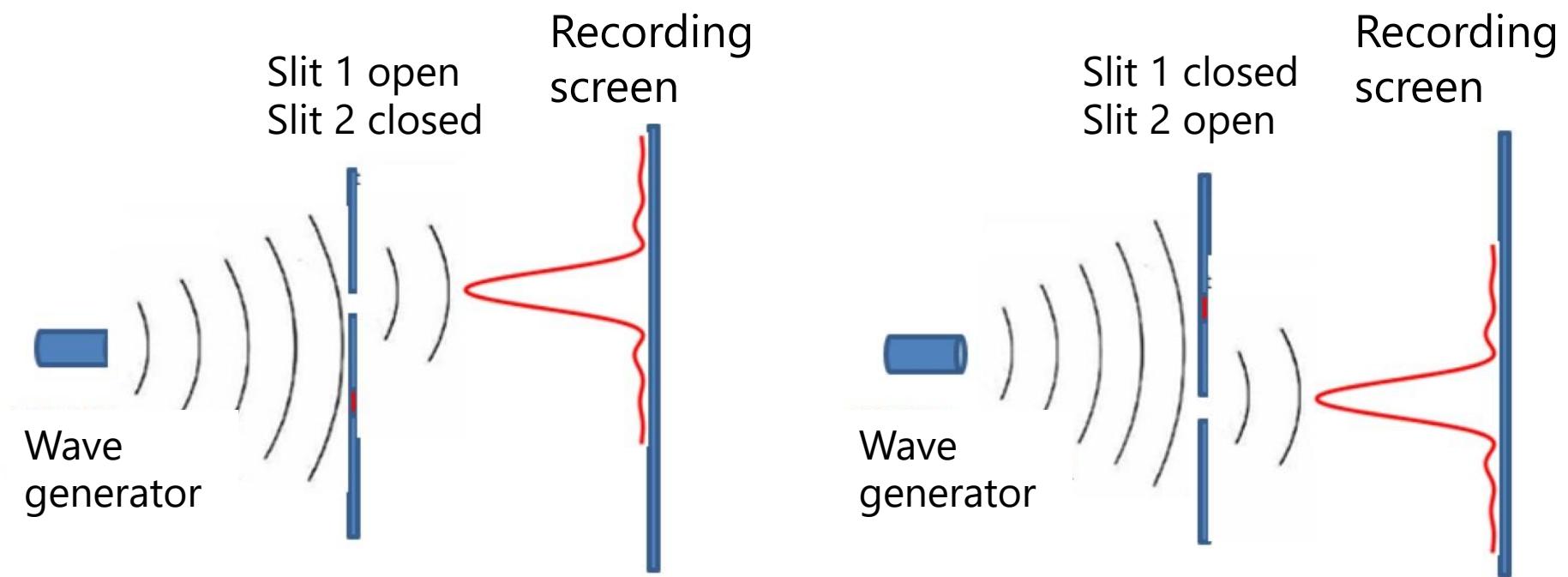


Recording
screen

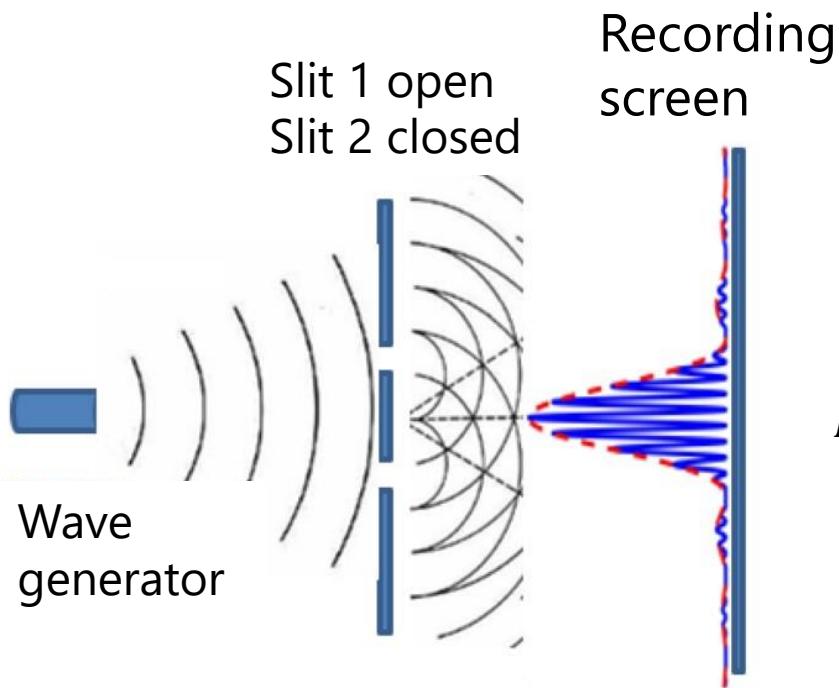


Intensity, $I(x) = ?$

One slit open at a time



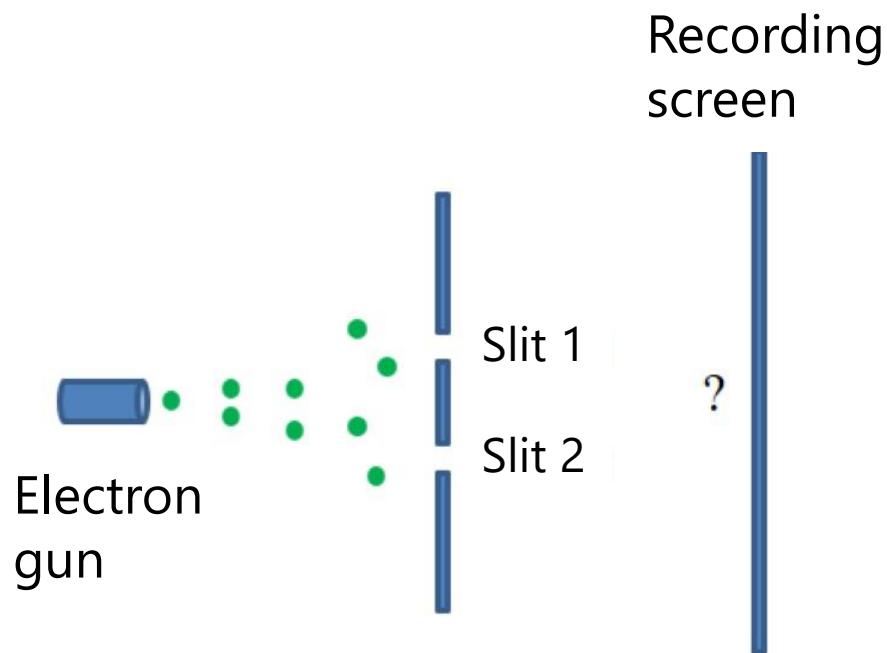
Both slits open



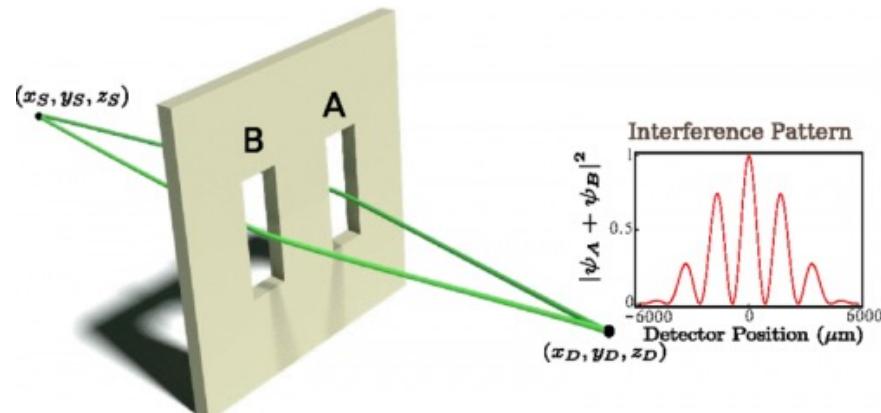
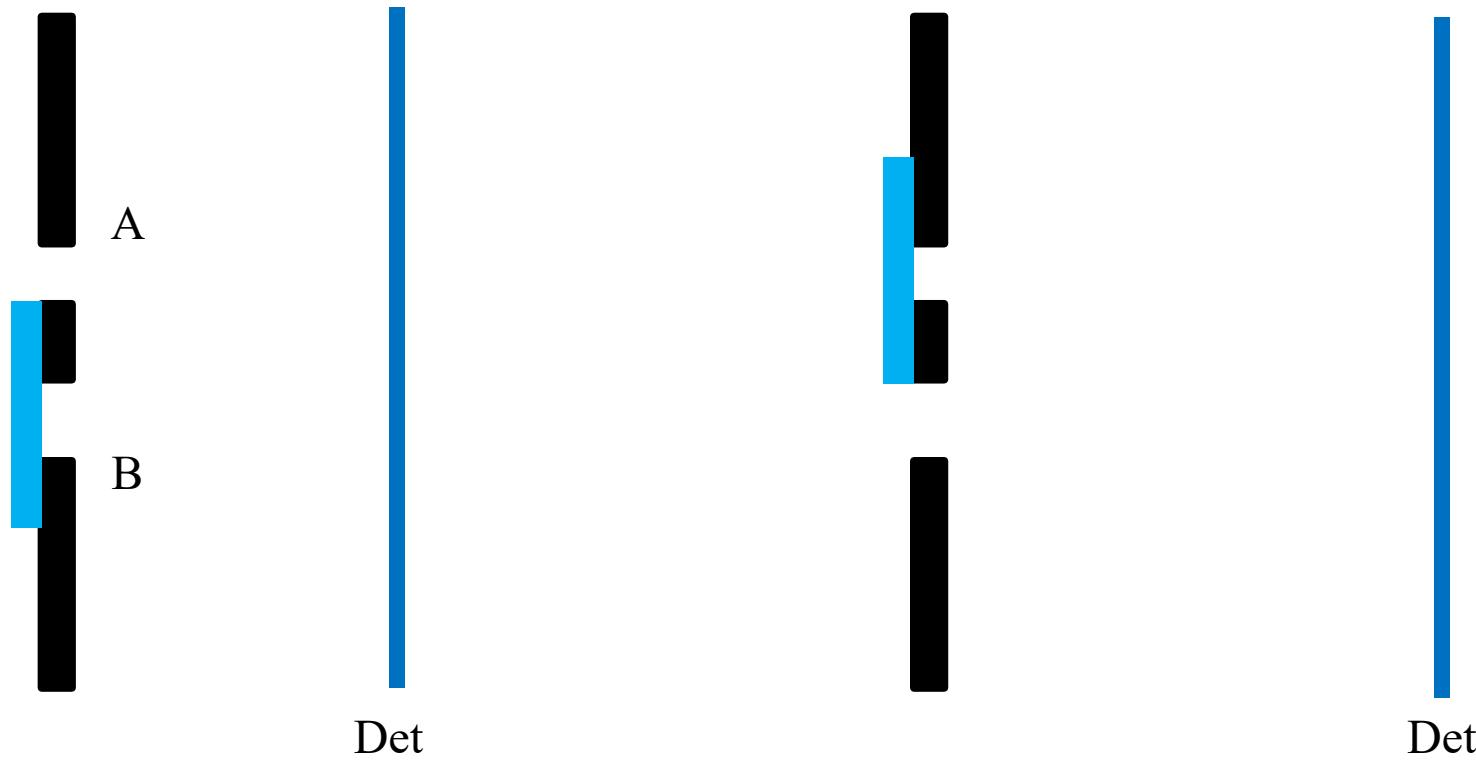
$$I(x) = I_1 + I_2 + 2\sqrt{I_1 I_2} \cos\theta$$

Classical mechanics : Wavefronts go through both slits simultaneously and we have diffraction & interference

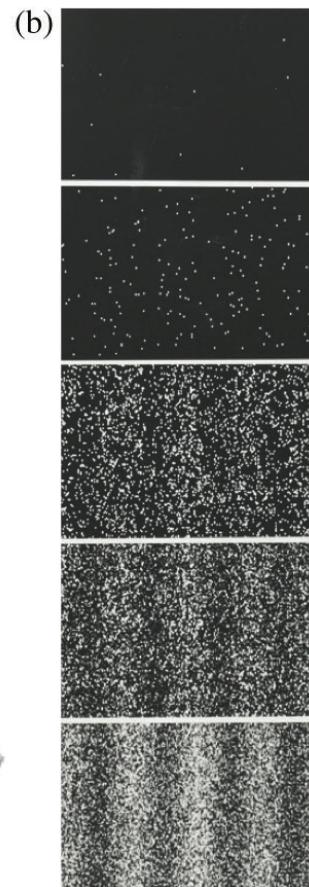
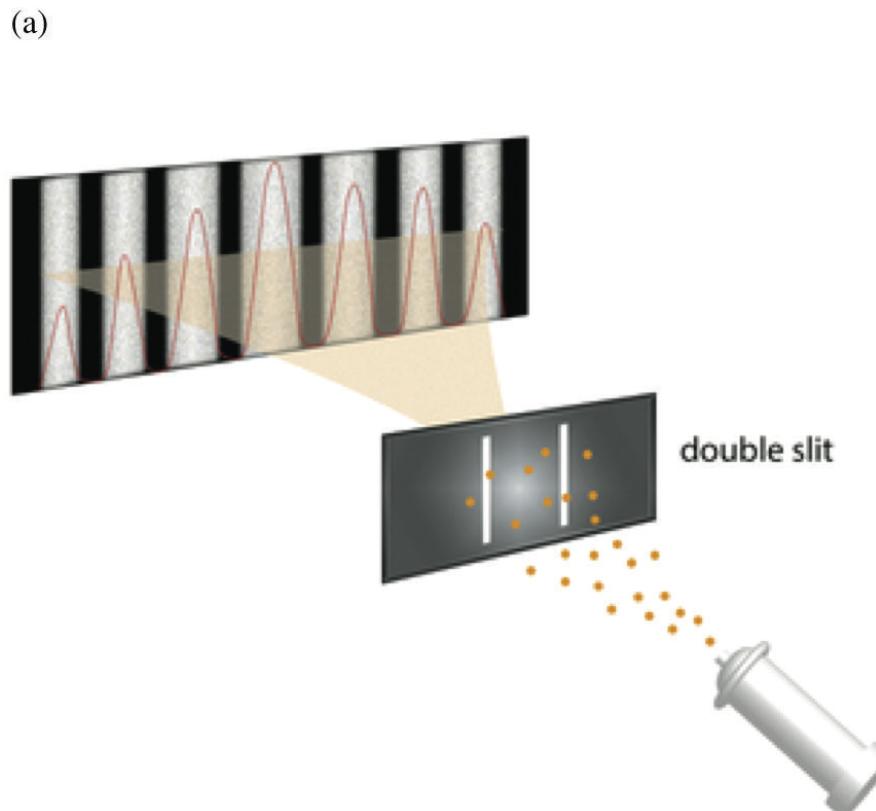
Now try with electrons



One slit at a time vs both slits simultaneously...

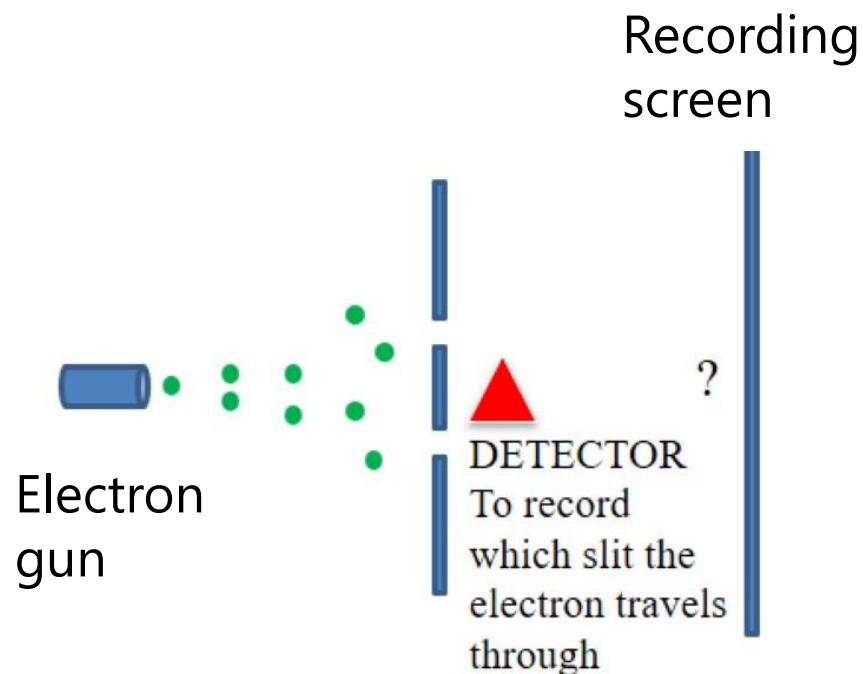


Double-slit experiment with electrons



Even with intensity so low that only 1 electron is in the system at a time, interference is still observed...

The effect of observation....



Explanation: The particle-wave duality

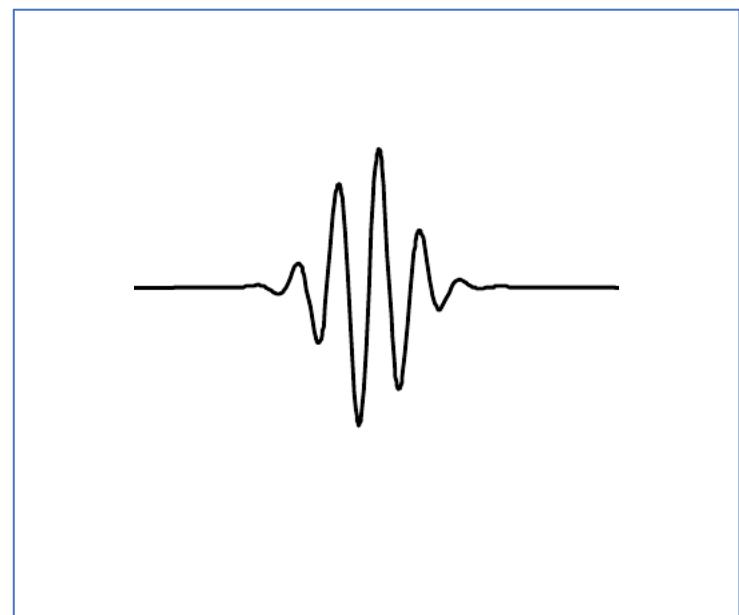
Light sometimes behaves as particles, and other times as waves.

Louis de Broglie (in 1923) postulated the converse, i.e. that particles will sometimes behave as waves.

- The exact relationship between the two came from relativity, where total energy, $E = mc^2$
- If we equate this to the Planck energy of a quantum, we have $E = mc^2 = h\nu$
- deBroglie then said, let $c \rightarrow v$, the velocity of a particle $\Rightarrow mv^2 = h\nu$
- Now, the relationship between frequency, ν & wavelength, λ of a wave travelling with speed, v is:



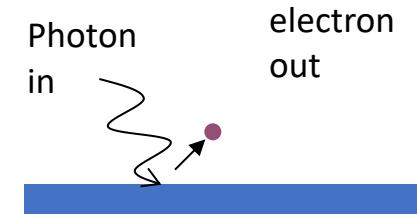
Wavepacket



E.g. for 1 keV electrons, $E = \frac{1}{2}mv^2 \Rightarrow v = 1.9 \times 10^7 \text{ m.s}^{-1}$ (5 % of c , so non-relativistic) $\Rightarrow \lambda \sim 4 \times 10^{-11} \text{ m}$. (compare to inter-atomic spacing in a crystal $\sim 2 \times 10^{-10} \text{ m}$). If indeed particles sometimes behave as waves, then should be able to observe diffraction and interference.

The Photoelectric effect

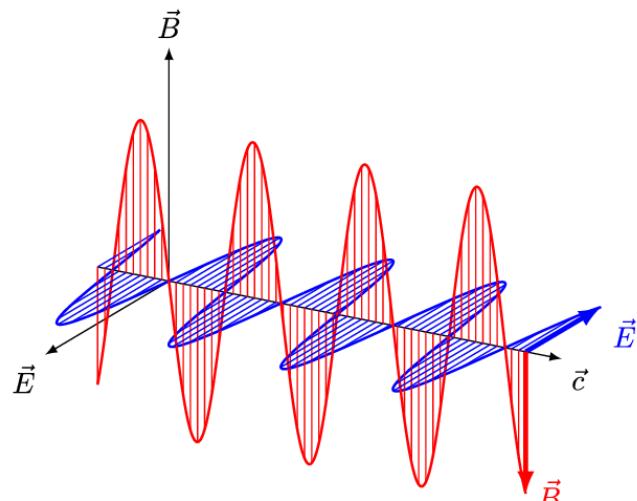
This is a process whereby electromagnetic radiation (light) impinging on a surface can cause ejection of electrons. Electrons are bound to the solid with an average binding energy known as the work function, usually denoted by ϕ . If energy of radiation is E , then from energy conservation, expect K.E. (Kinetic energy) of ejected electron to be:



$$\text{K.E.} = E - \phi \quad (1)$$

Classical electrodynamics $\Rightarrow E \propto \text{Intensity (I)}$

Poynting vector – Intensity of an EM wave



The Wave-Particle Duality

We Need both the Wave and Particle-like treatment to explain Experiments.

Photons, electrons etc have both characteristics.

DeBroglie's hypothesis – if waves behave like particles (e.g. photoelectric effect), then particles *may* behave like waves. If so, they will have a wavelength $\lambda = h/p$ p = momentum.
 h = Planck's constant, with the value 6.6×10^{-34} Js

Example : Electron, travelling at 1×10^5 m/s - determine its momentum, Kinetic energy and wavelength

$$\text{Momentum, } p = mv = 9.1 \times 10^{-31} \times 1 \times 10^5 \text{ kg m/s} = 9.1 \times 10^{-26} \text{ kg m/s}$$

$$\text{Kinetic Energy} = \frac{1}{2}mv^2 = p^2/2m = 4.55 \times 10^{-21} \text{ J. In Electron Volts (eV)} = \frac{4.55 \times 10^{-21} \text{ J}}{1.6 \times 10^{-19} \text{ C}} = 28.4 \text{ meV}$$

$$\text{Wavelength} = \lambda = h/p = \frac{6.6 \times 10^{-34}}{9.1 \times 10^{-26}} = 7.2 \text{ nm } (1 \text{ nm} = 10^{-9} \text{ m})$$

Example : Tennis ball, mass 58 g, travelling at 50 m/s - determine its momentum, Kinetic energy and wavelength

$$\text{Momentum, } p = mv = 2.9 \text{ kg m/s}$$

$$\text{Kinetic Energy} = \frac{1}{2}mv^2 = p^2/2m = 72.5 \text{ J. Doesn't make sense to convert to Electron Volts!}$$

$$\text{Wavelength} = \lambda = h/p = \frac{6.6 \times 10^{-34}}{72.5} = 9.1 \times 10^{-32} \text{ m}$$

* You can now try Questions 1 & 2 on Examples paper 1 *

The Wave-Particle Duality

Summary of useful relationships

Wavelength of a particle = $\lambda = \frac{h}{p}$ *deBroglie*

$k = \text{wave-vector} = \frac{2\pi}{\lambda}$

$p = \text{momentum} = mv = \frac{h}{\lambda} = \frac{h}{2\pi} \times \frac{2\pi}{\lambda} = \hbar k$ *h bar* is called the
reduced Plank Constant

Energy of a Photon: $E = hf = \hbar\omega$

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Topic 3. *Wavefunctions & Schrödinger's equation*

The wave equation

- Second - order linear differential equation

- $\frac{\partial^2 F(x,t)}{\partial t^2} - c^2 \frac{\partial^2 F(x,t)}{\partial x^2} = 0$

- Solutions are sinusoidal and of the form:

$A\sin(x - ct) + B\sin(x + ct)$ Both directions

Or $Ae^{i(wt - kx)} + Be^{i(wt + kx)}$

Quantum Mechanics

The wave-function, ψ

The wave-function, ψ contains information about all measurable parameters of the system.

In 1D, say the x -direction, the wave-function will be $\psi(x, t)$

The physical meaning is that $\psi^* \psi$ represents the probability of finding the object (particle or wave) between x and $x + dx$

More generally, the probability of finding the object between $x = a$ and $x = b$ is $\int_a^b |\psi|^2 dx$

Schrodinger's Equation

Kinetic Energy + Potential Energy = Total Energy

Kinetic Energy : $\frac{p_x^2}{2m} = \frac{1}{2m} \frac{\hbar}{i} \frac{\partial}{\partial x} \left(\frac{\hbar}{i} \frac{\partial \psi}{\partial x} \right) = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$

Potential Energy: Depends on the potential terrain the particle is placed in = $V\psi$

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

Time independent Schrodinger Equation, Total Energy = Constant = $E\psi$

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

Important constraint on the Wave function: ψ must be a solution of Schrodinger's Equation

Solving Schrödinger's equation: If V(x) is constant

V(x): Potential energy profile.

If V(x) is constant, we can write the time independent Schr Equation as:

$$\frac{\partial^2 \psi}{\partial x^2} = -\alpha^2 \psi$$

Where the constant $\alpha^2 = \frac{2m}{\hbar^2}(E - V)$

General Solution $\psi = Ae^{i\alpha x} + Be^{-i\alpha x}$

To find the coefficients, we make use of properties of the wavefunction:

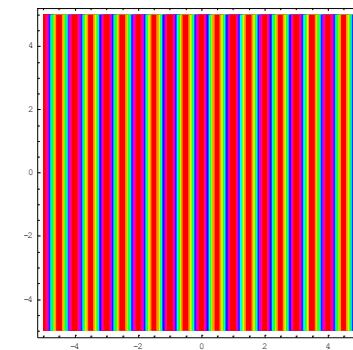
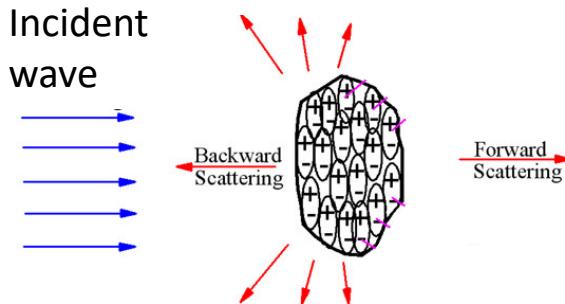
ψ must be continuous

$d\psi/dx$ must be continuous

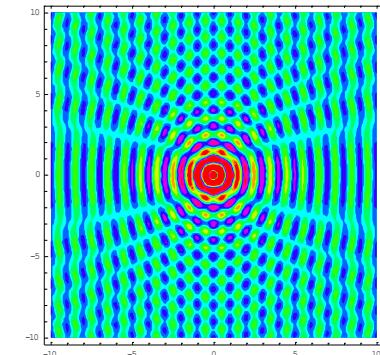
Probability of finding the particle somewhere is 1 .

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

Whenever a quantum particle encounters any discontinuity in potential, it will be scattered. (This is a characteristic of **all** waves.)

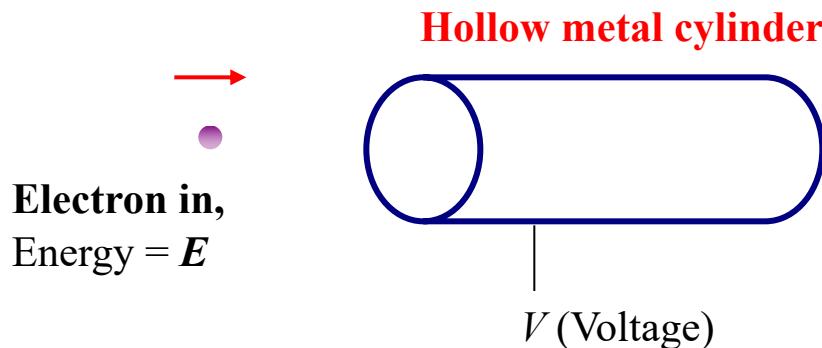


Plane wave

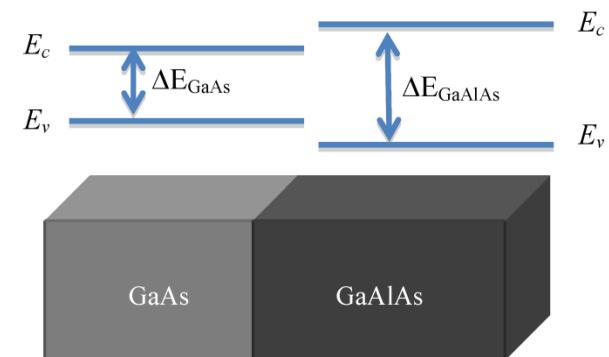


Plane wave after encountering point scatterer

1. Scattering by a 1-D potential step:

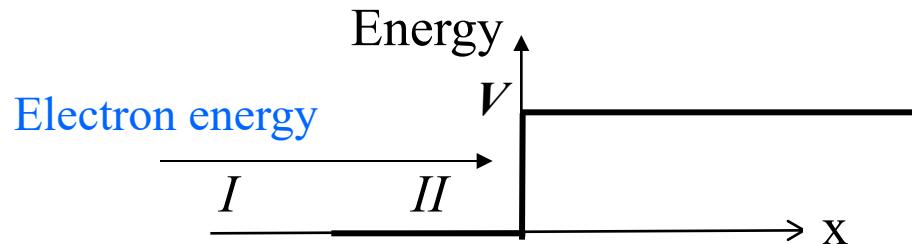


In reality:



Classically, expect electron to pass if $E > V$.

If we draw the potential as seen by the electron, it looks like:



Case 1: $E < V$ (i.e. when electron has less energy than step).

We can split the solution into two regions of space, I & II as shown. The equations to solve are:

Region I $-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_I(x) = E\psi_I(x)$

Region II $\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi_I(x) = E\psi_I(x)$

The solutions are of the form:

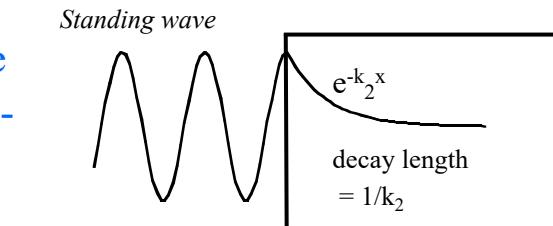
$$\psi_I(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x} \quad \text{where } k_1 = \frac{\sqrt{2mE}}{\hbar}$$

(which consists of left- and right- travelling waves)

$$\psi_{II}(x) = A_2 e^{-k_2 x} \quad \text{where } k_2 = \frac{\sqrt{2m(V-E)}}{\hbar}$$

Which only has an exponentially decaying part. Why?

Approximate
form of wave-
function:



To find the reflection/transmission coefficients of this system, we need to know the relationship between the coefficients A_i & B_i , i.e. what are the relative strengths of the incident and reflected waves?
 Matching the wave-functions and their first derivatives at the boundary ($x = 0$) yields the following relationships:

$$\psi_I(0) = \psi_{II}(0) \Rightarrow A_1 + B_1 = A_2$$

$$\psi_I'(0) = \psi_{II}'(0) \Rightarrow ik_1 A_1 - ik_1 B_1 = -k_2 A_2$$

$$\Rightarrow \frac{B_1}{A_1} = -\frac{k_2 + ik_1}{k_2 - ik_1}$$

Reflection probability = $|B_1/A_1|^2 = 1$ identically.

There is zero probability of the electron passing through this potential step.

Case 2: $E > V$ (i.e. the total energy of the electron is greater than the potential energy of the step)

$$\psi_I(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x} \quad \text{where } k_1 = \frac{\sqrt{2mE}}{\hbar}$$

$$\psi_{II}(x) = A_2 e^{ik_2 x} \quad \text{where } k_2 = \frac{\sqrt{2m(E-V)}}{\hbar}$$

i.e. the wave-function is a STANDING WAVE on the left side of the barrier, and a TRAVELLING WAVE on the right side.

There is no left-travelling wave after the step, because there is no reason for one: it would only be generated by another scatterer, which we don't have.

Matching the wave-functions and their first derivatives at the boundary yields:

$$A_1 + B_1 = A_2$$

$$ik_1 A_1 - ik_1 B_1 = ik_2 A_2$$

$$\psi_I(0) = \psi_{II}(0) \Rightarrow A_1 + B_1 = A_2$$

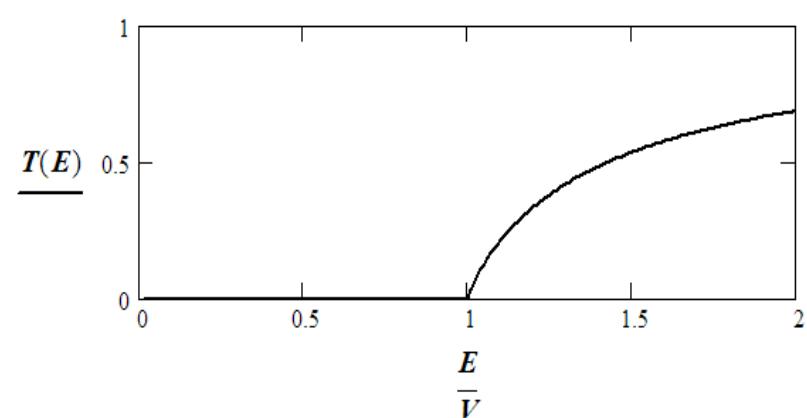
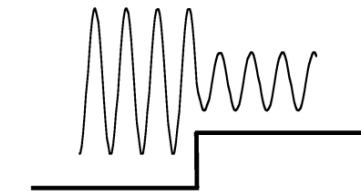
$$\psi_I'(0) = \psi_{II}'(0) \Rightarrow ik_1 A_1 - ik_1 B_1 = ik_2 A_2$$

$$\Rightarrow \frac{B_1}{A_1} = \frac{k_1 - k_2}{k_1 + k_2}$$

$$\Rightarrow \text{Reflection probability, } R, \left| \frac{B_1}{A_1} \right|^2 = \left| \frac{k_1 - k_2}{k_1 + k_2} \right|^2$$

$$\text{Transmission probability, } T = 1 - R$$

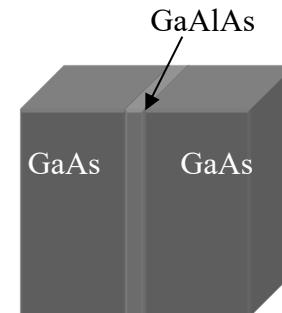
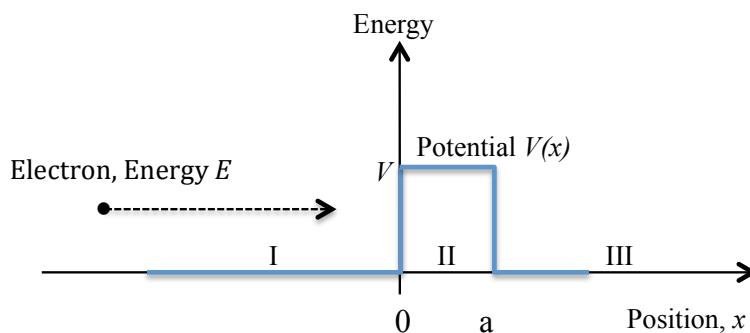
Approximate form of wave-function:



i.e. any time a particle experiences a potential discontinuity, there is a finite probability that it will be reflected. The larger the discontinuity, the greater the probability of reflection. Classically, this can only happen when the potential discontinuity is larger than the particle's starting energy. However, this is something which happens to all waves

2. Scattering by a 1-D potential barrier:

We are interested in solutions when $E < V_0$



We can split the solution into three regions of space, I , II & III as shown.
The equations to solve are:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_I(x) = E\psi_I(x) \quad \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi_{II}(x) = E\psi_{II}(x) \quad -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{III}(x) = E\psi_{III}(x)$$

$$\psi_I(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x} \quad \text{where } k_1 = \frac{\sqrt{2m(E)}}{\hbar}$$

$$\psi_{II}(x) = A_2 e^{k_2 x} + B_2 e^{-k_2 x} \quad \text{where } k_2 = \frac{\sqrt{2m(V-E)}}{\hbar}$$

$$\psi_{III}(x) = A_3 e^{ik_3 x} \quad \text{where } k_3 = k_1$$

Matching the wave-functions and their first derivatives at the boundaries ($x = 0$ & a) yields the following relationships:

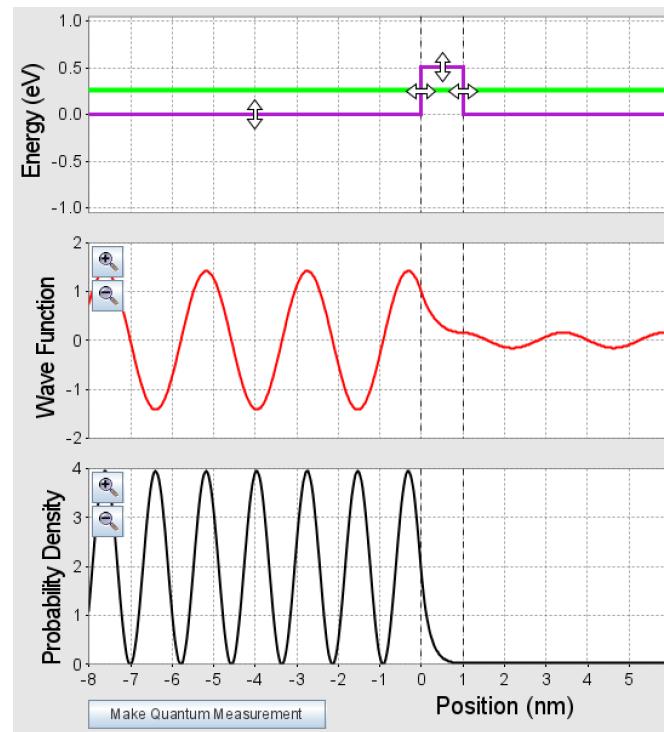
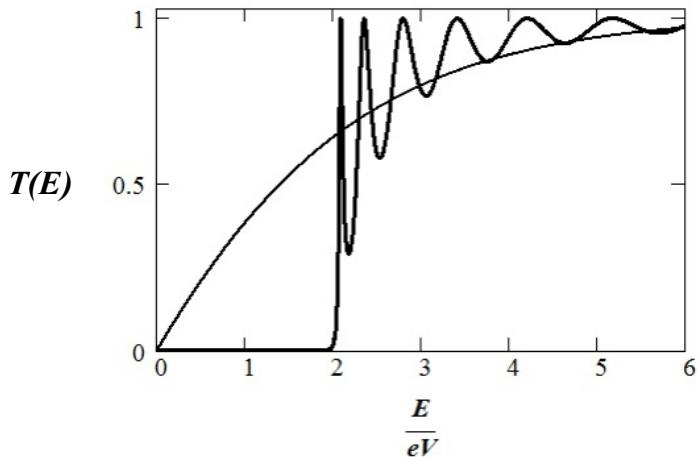
$$\psi_I(0) = \psi_{II}(0) \Rightarrow A_1 + B_1 = A_2 + B_2$$

$$\psi_I'(0) = \psi_{II}'(0) \Rightarrow ik_1 A_1 - ik_1 B_1 = k_2 A_2 - k_2 B_2$$

$$\psi_{II}(a) = \psi_{III}(a) \Rightarrow A_2 e^{k_2 a} + B_2 e^{-k_2 a} = A_3 e^{-ik_1 a}$$

$$\psi_{II}'(a) = \psi_{III}'(a) \Rightarrow k_2 A_2 e^{k_2 a} - k_2 B_2 e^{-k_2 a} = ik_1 A_3 e^{-ik_1 a}$$

Solving simultaneously, we get the transmission coefficient

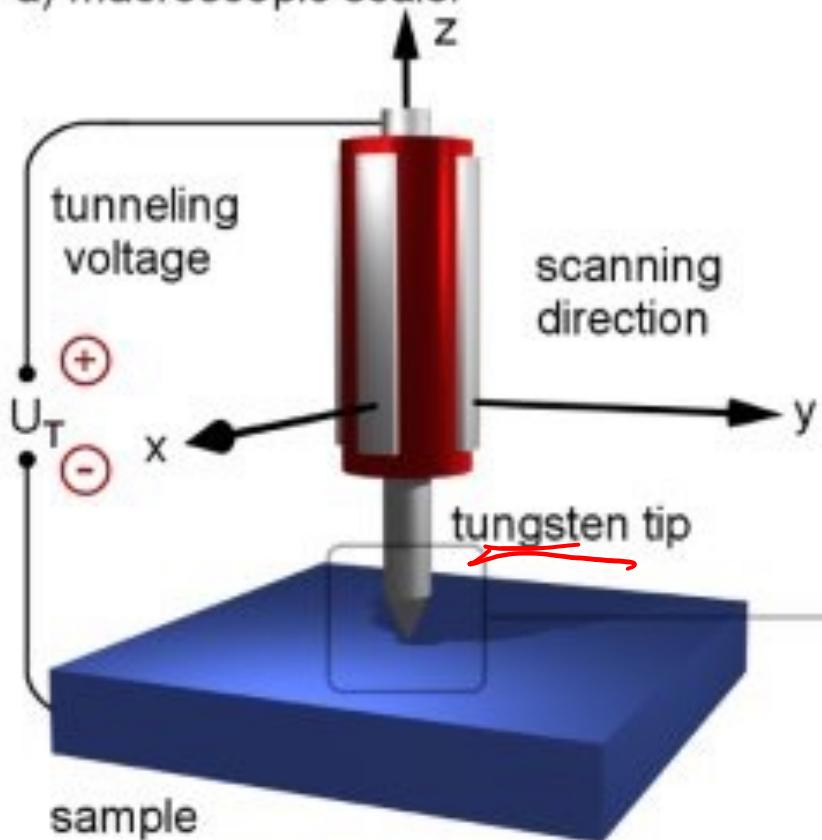


$$T = \left| \frac{A_3}{A_1} \right|^2 = \frac{1}{1 + \left(\frac{k_1^2 + k_2^2}{2k_1 k_2} \right)^2 \sinh^2(k_2 a)}$$

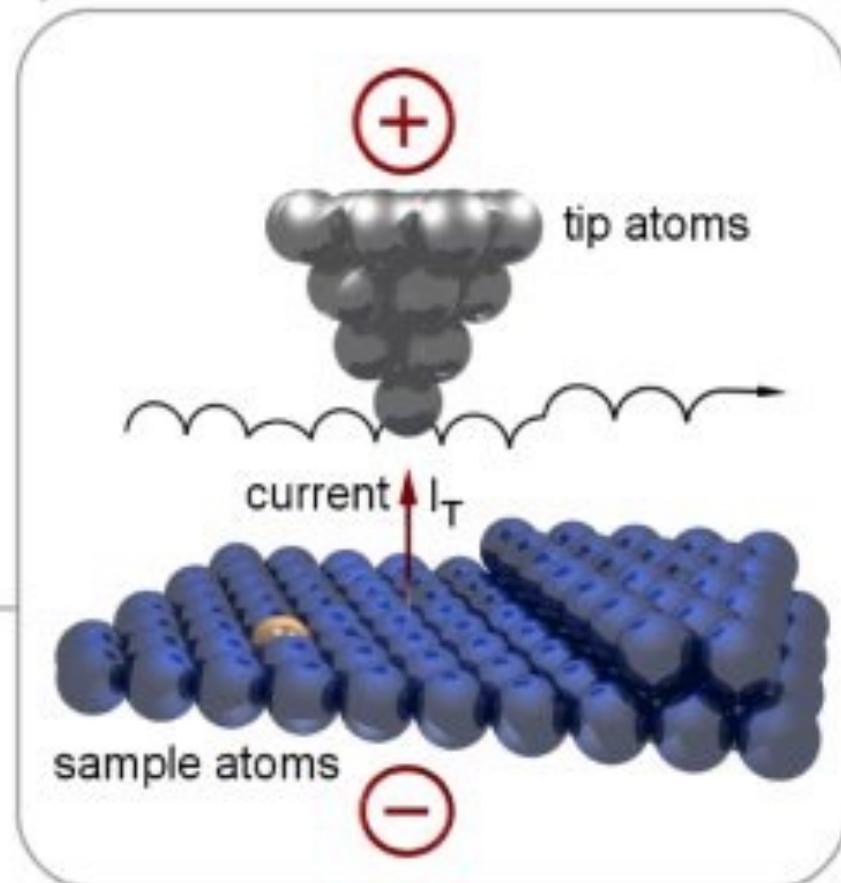
N.B. Classically, we would expect **zero** probability of passing through (because the Electron doesn't have enough energy to overcome the barrier).

Scanning tunneling microscope

a) macroscopic scale:



b) atomic scale:



Depending on whether the tip is positively or negatively biased w.r.t. the sample, we are imaging either filled or empty states of the sample. i.e. electrons will flow from filled states into empty states

Example:

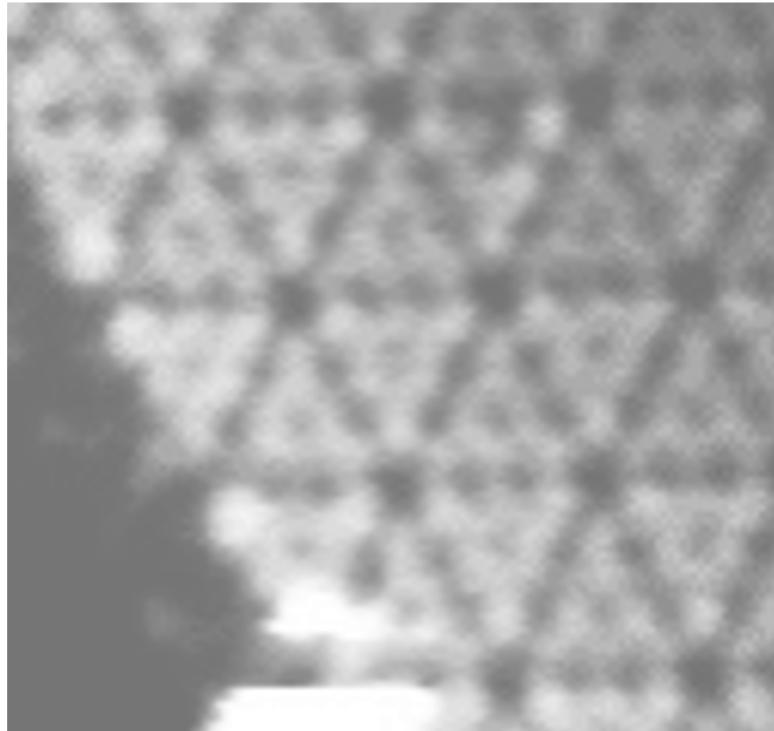
Si(111)



3 nm

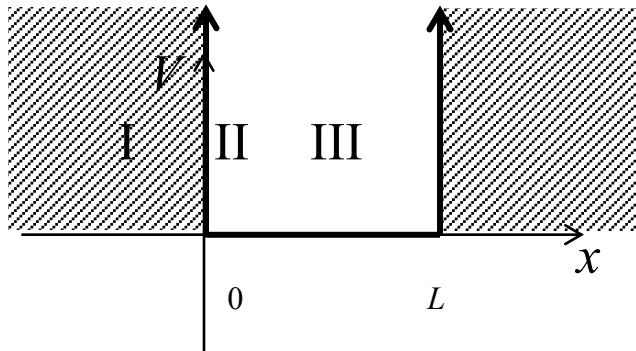
**Empty
States**
(Valence band)

**Filled
States**
(conduction band)



Example 3. Bound states – electron in an infinite potential well

Consider the situation whereby the electron is in a “Potential well” of infinite height, i.e.:



In regions I & III, the potential is infinite. That means there is no possibility of finding the particle there, so it must be confined to region II. What is its configuration, i.e. can the particle have any energy and sit in any position within the well?

The form of the potential is:

$$V = 0 \text{ for } 0 < x < L$$

$$V = \infty \text{ for } x < 0, x > L$$

Schrödinger's equation in region II is:

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

$$\psi(x) = A e^{ikx} + B e^{-ikx} \quad \text{where } k = \frac{\sqrt{2mE}}{\hbar}$$

Since the wave-function is zero outside the well, it must also be zero just at the boundaries (for continuity).

matching at left side

$$\psi(0) = A + B \Rightarrow A = -B$$

i.e.

$$\psi(x) = A(e^{ikx} - e^{-ikx}) = A\sin(kx)$$

Matching at right side

$$\psi(L) = 0 \Rightarrow A\sin(kL) = 0 \Rightarrow k = n\pi/L, \quad n = 1, 2, \dots$$

In other words, the wave-function for an electron in an infinite potential well is of the form

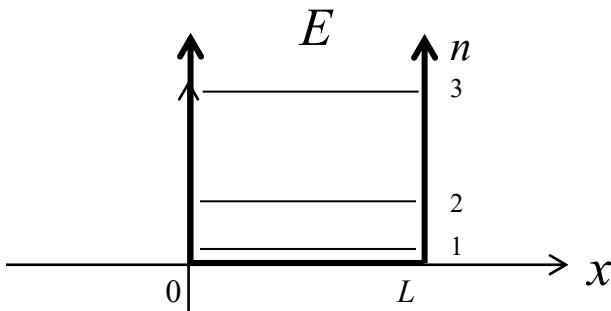
$$\psi(x) = A\sin(n\pi x/L)$$

To determine A , we need to normalise the function, i.e. $\int \psi^* \psi d^3r = 1 \Rightarrow \int_0^L A^2 \sin^2(\frac{n\pi x}{L}) dx = 1$

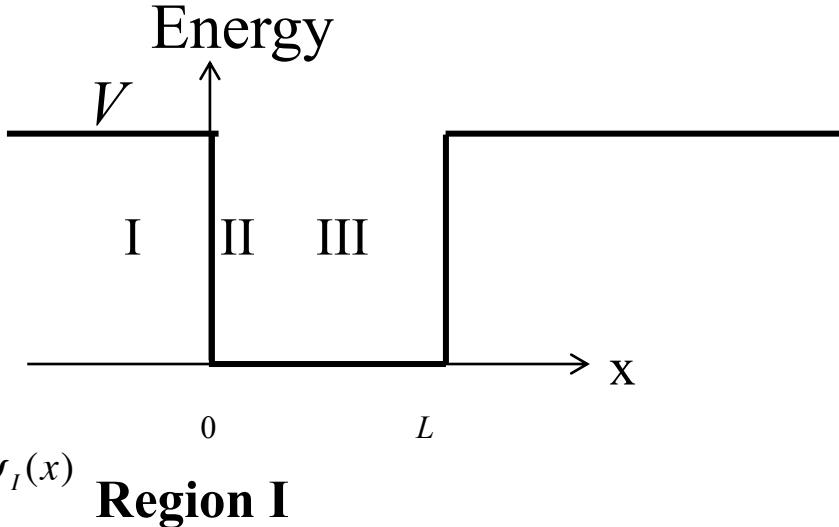
This gives us a value for $A = \sqrt{\frac{2}{L}}$

Remember, Energy, $E = \frac{1}{2}mv^2 = p^2/2m = \hbar^2k^2/2m$
 If $k = n\pi/L$, then the Energy levels of an electron confined in an infinite well are

$$E = \hbar^2 n^2 / (8mL^2)$$



Bound states – electron in a finite potential well



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

Region II

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{II}(x) = E \psi_{II}(x)$$

Region III

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi_{III}(x) = E \psi_{III}(x)$$

The solutions are of the form:

$$\psi_I(x) = A_1 e^{k_1 x} \text{ where } k_1 = \frac{\sqrt{2m(V-E)}}{\hbar}$$

$$\psi_{II}(x) = A_2 e^{ik_2 x} + B_2 e^{-ik_2 x} \text{ where } k_2 = \frac{\sqrt{2mE}}{\hbar}$$

$$\psi_{III}(x) = A_3 e^{-k_3 x} \text{ where } k_3 = k_1$$

There are discrete energy values allowed. The particle cannot sit just anywhere in well - see wave-functions.

N.B. for reference, the electron in this case is confined in one direction, and the energy expression has one state variable, n. This number is called a “Quantum number”, and the more directions of confinement, the more quantum numbers define the system. Electrons in atoms also have quantum numbers: n, l and m.

Matching the wave-functions and their first derivatives at the boundaries ($x = 0$ & L) yields the following relationships:

$$A_1 = A_2 + B_2$$

$$k_1 A_1 = ik_2 A_2 - ik_2 B_2$$

$$A_2 e^{ik_2 L} + B_2 e^{-ik_2 L} = A_3 e^{-k_1 L}$$

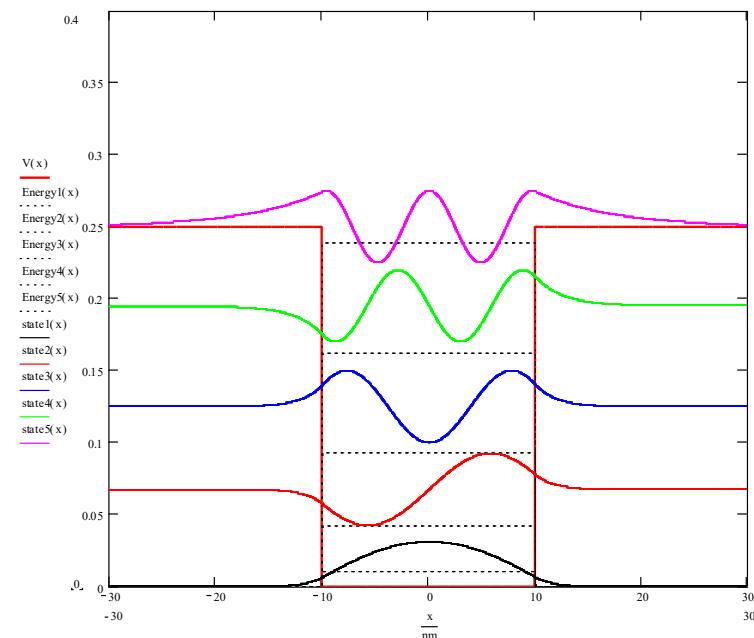
$$ik_2 A_2 e^{ik_2 L} - ik_2 B_2 e^{-ik_2 L} = -k_1 A_3 e^{-k_1 L}$$

Solving simultaneously, we end up with Transcendental relationships, which can only Be solved graphically or numerically:

$$k_1 \tan(k_1 L) = k_2 \quad A_1 = A_3, \text{ and } B_2 = 0$$

$$k_1 \cot(k_1 L) = -k_2 \quad A_1 = -A_3, \text{ and } A_2 = 0$$

N.B. solutions alternate in symmetry



Example, 0.25 eV deep well,
20 nm wide in GaAs: has 5
energy levels



UNIVERSITY OF
CAMBRIDGE



IB Paper 8: Electrical elective

Easter term

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Topic 4. *Atomic Structure*

Heisenberg's Uncertainty Principle

Cannot measure position and momentum – both – absolutely accurately.

(Equivalently, error in energy and error in time of measurement)

If Δx is the error in determining position and Δp the error in determining momentum, $\Delta p \Delta x \geq \hbar / 2$

In general a signal in time/space \leftrightarrow frequency will have this restriction

Atoms

(This page is not for examination)

Atoms are more complicated than a ‘box’. But same ideas.

The potential energy term will have to account for electron-proton and electron-electron interactions.

Intuitive ideas for a hydrogen atom:

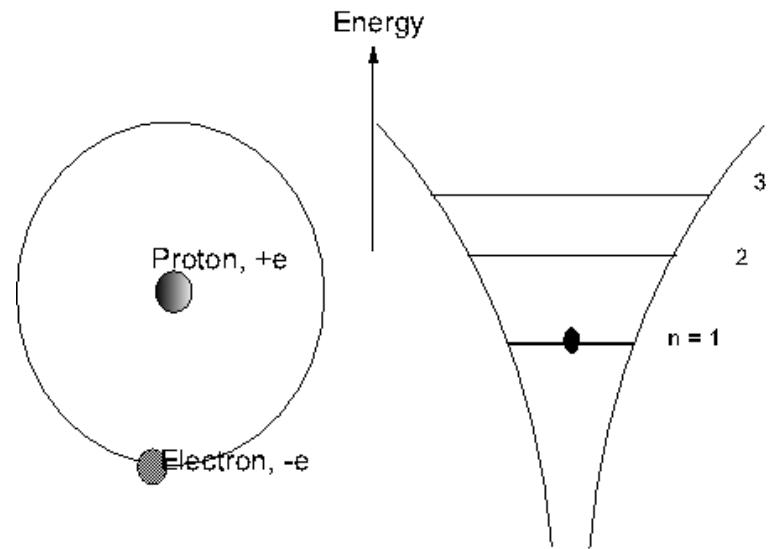
Electron bound by a coloumbic potential well
(particle in a box, but the box is not rectangular)

Centrifugal force=Electrostatic Attraction

$$F = \frac{mv^2}{r} = \frac{q^2}{4\pi\epsilon_0 r^2} \Rightarrow mv^2 = \frac{q^2}{4\pi\epsilon_0 r}$$

Total Energy = K.E + P.E

$$E = KE + PE = \frac{1}{2}mv^2 - \frac{q^2}{4\pi\epsilon_0 r} = -\frac{q^2}{8\pi\epsilon_0 r}$$



Atoms

(This page is not for examination)

Waves must interfere constructively around the orbit.

$$2\pi r = n\lambda$$

Use this idea to replace r in the total energy

$$r = n\lambda / 2\pi$$

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

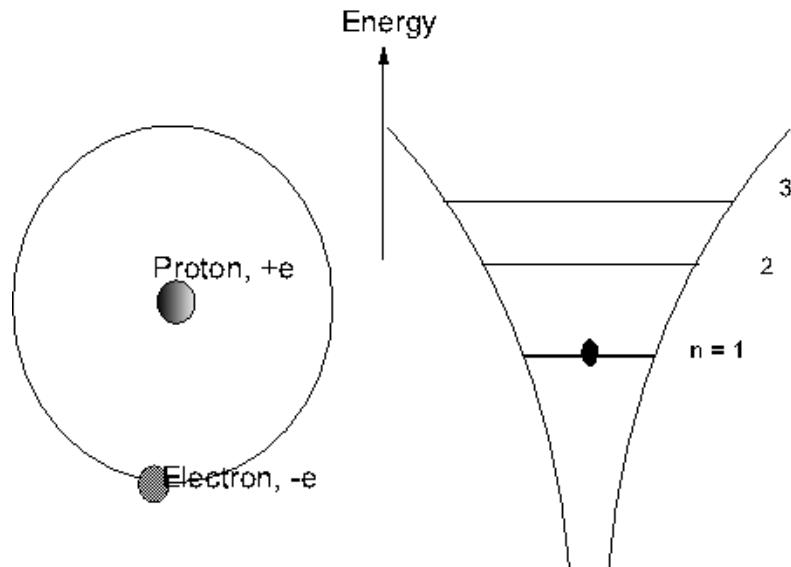
$$mv r = n\hbar$$

$$mv^2 = \frac{q^2}{4\pi\epsilon_0 r} \Rightarrow mv r = \left(\frac{mq^2}{4\pi\epsilon_0} \right)^{1/2} r^{1/2} = n\hbar$$

$$\Rightarrow r = (n\hbar)^2 / \left(\frac{mq^2}{4\pi\epsilon_0} \right)$$

Therefore

$$E = KE + PE = \frac{1}{2}mv^2 - \frac{q^2}{4\pi\epsilon_0 r} = -\frac{q^2}{8\pi\epsilon_0 r} = \frac{-mq^4}{32\pi^2\epsilon_0^2(n\hbar)^2}$$



Energy is Quantized.

There are more quantum numbers.

Atoms to Solids: Chemical Bonding

The difference between metals, semi-conductors and insulators arises from their different atomic bonding

core - tightly bound – atomic character – unaffected by their bonding

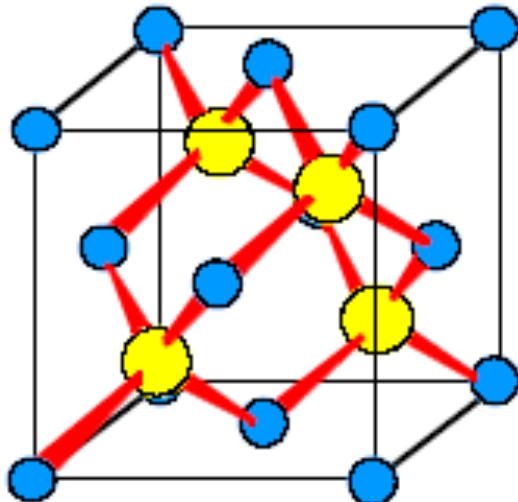
valence - loosely bound, large size - only these orbitals form the chemical bonds

Valence electrons form the bonds of an atom – hence its chemistry - hence the Periodic Table – the periodicity of chemical behaviour. They determine atomic size in a solid or molecule.

Atoms to Solids: Chemical Bonding

Three main types of bonds

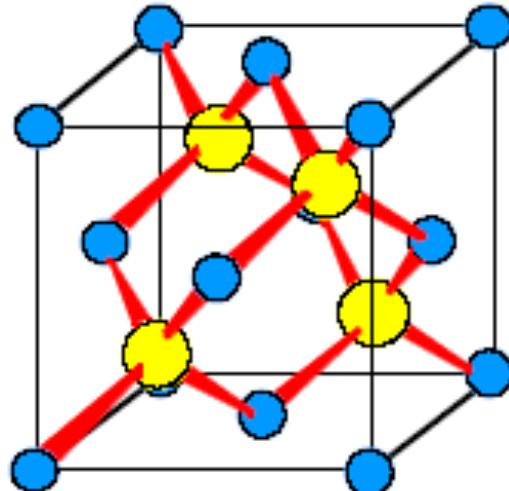
- Metallic – valence electrons are shared between all atoms
 - Ionic - electrons are transferred between atoms to form ions, eg Na^+ Cl^-
 - Covalent – bonds consist of electron pairs, shared between 2 atoms. eg Silicon, Si. Also in molecules like H_2
 - Elements of column 4 of Periodic Table have 4 valence electrons. They can make 4 bonds – the diamond structure as in Si



Chemical Bonding: Diamond and Zinc Blende

Carbon, Si and Ge are each from column 4, with 4 valence electrons. All form *diamond-structure* solids. Each atom forms 4 bonds with its four valence electrons. Each bond consists of an electron pair, one from each of the 2 atoms in each bond.

We can also form compounds with an *average* of 4 electrons per atom. For example GaAs, where Ga has 3 electrons and As has 5. This has the same structure as diamond, with alternate atoms Ga and As. This lattice is called *zincblende*. Other examples are AlAs, GaP, ZnSe, ZnS



Atoms to Solids: Si Crystal

Number of atoms of Si per unit cell?

- Cell = Face-Centred Cubic (FCC) symmetry
- FCC has 4 symmetry points, 2 atoms per symmetry point = 8 atoms per cell
- L = 5.43 Angstrom, Avogadro's number A = $6 \times 10^{23} / \text{cm}^3$, Atomic weight M = 28.1

$$N = \frac{8}{(5.43 \times 10^{-8})^3} = 5 \times 10^{22} \text{ atoms/cm}^3$$

$$\rho = \frac{N \cdot M}{A} = \frac{5 \times 10^{22} \times 28.1}{6 \times 10^{23}} = 2.33 \text{ gm/cm}^3$$

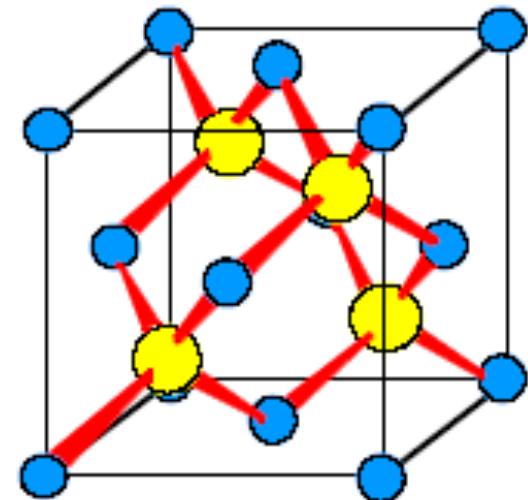
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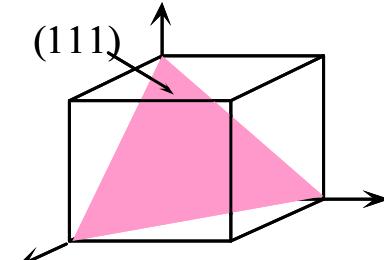
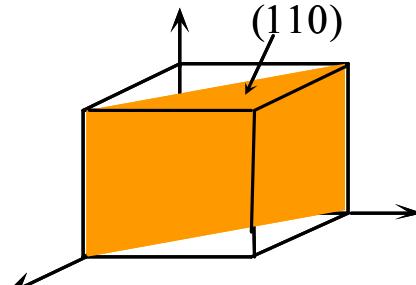
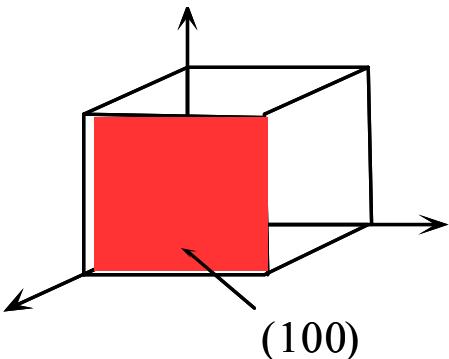
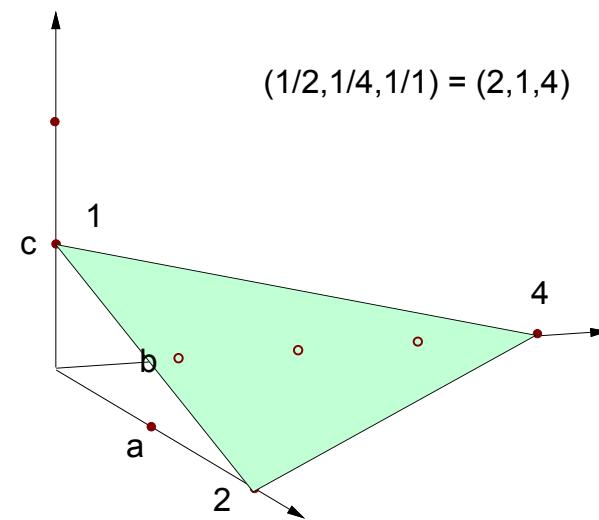


Atoms to Solids: Crystal Planes

- Crystal planes are defined Miller Indices
- Miller Indices are integers (h, k, l)
- The plane will cut the x, y and z axis at integer multiple of $(1/h, 1/k, 1/l)$

Cubic example

- The plane cuts axes at 2,4,1
- Take reciprocals, $\frac{1}{2}, \frac{1}{4}, 1/1$.
- Multiply through by 4 to give integers,
- gives $(h, k, l) = (2, 1, 4)$ plane

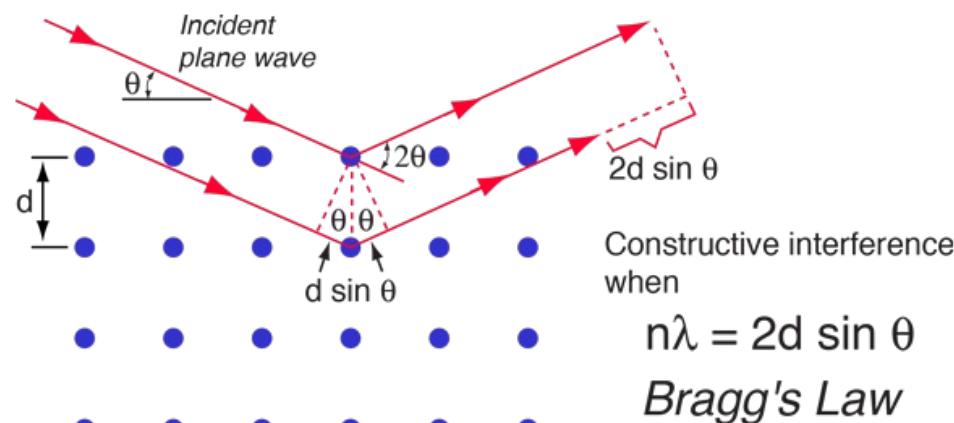


Bragg's Law: Electron Diffraction from a Crystal (or x-ray)

The diffraction of electrons can be used to identify properties of a crystal.

Experiment:

- 1.) Impinge a beam of high energy electrons (x-rays – we will see why ‘high energy’ soon) on a crystal at an angle θ
- 2.) Measure the intensity pattern of electron strikes on a screen as shown.



Constructive interference when
 $n\lambda = 2d \sin \theta$
Bragg's Law

Observed: Diffraction pattern

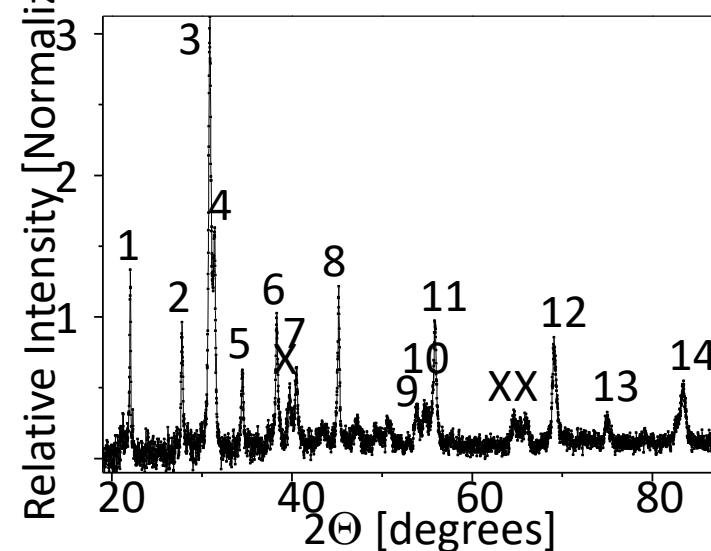
Path difference = $2d \sin \theta$

Constructive Interference when $2d \sin \theta = n\lambda$

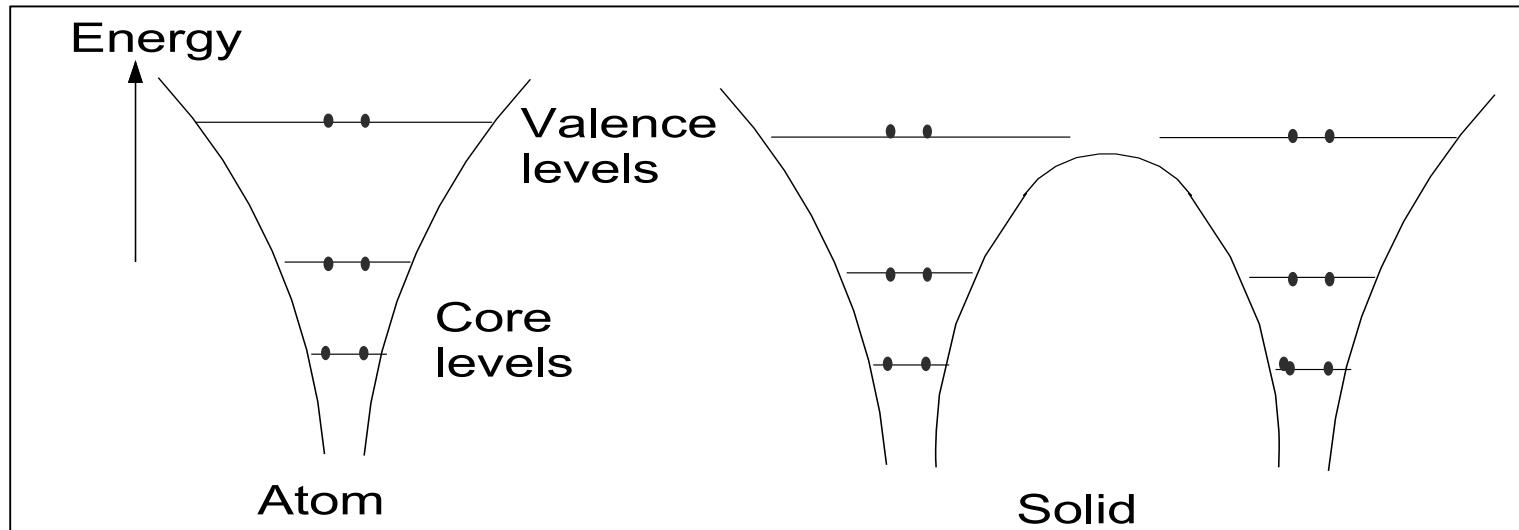
$n = \text{integer}$

$\lambda = \text{wavelength of electrons.}$

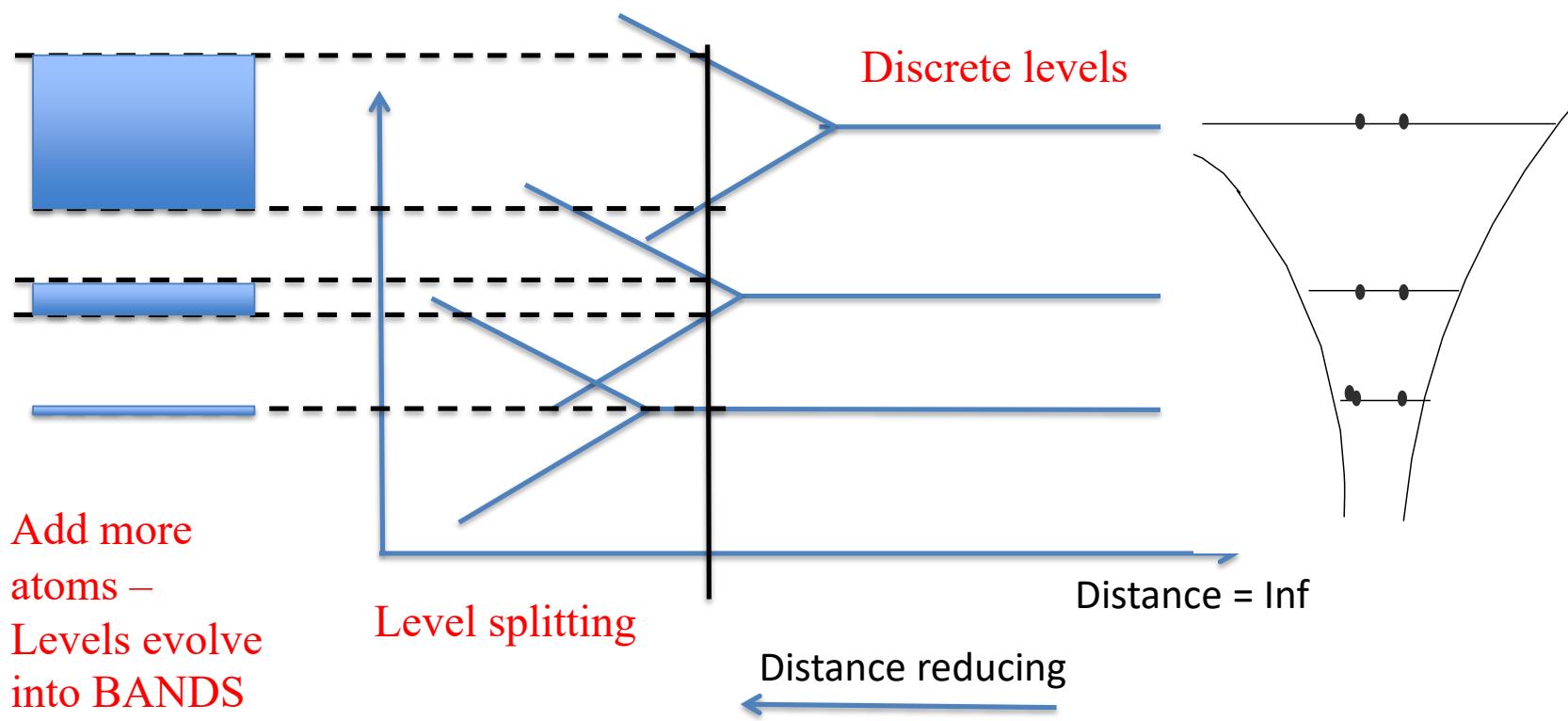
Can be used to identify d .



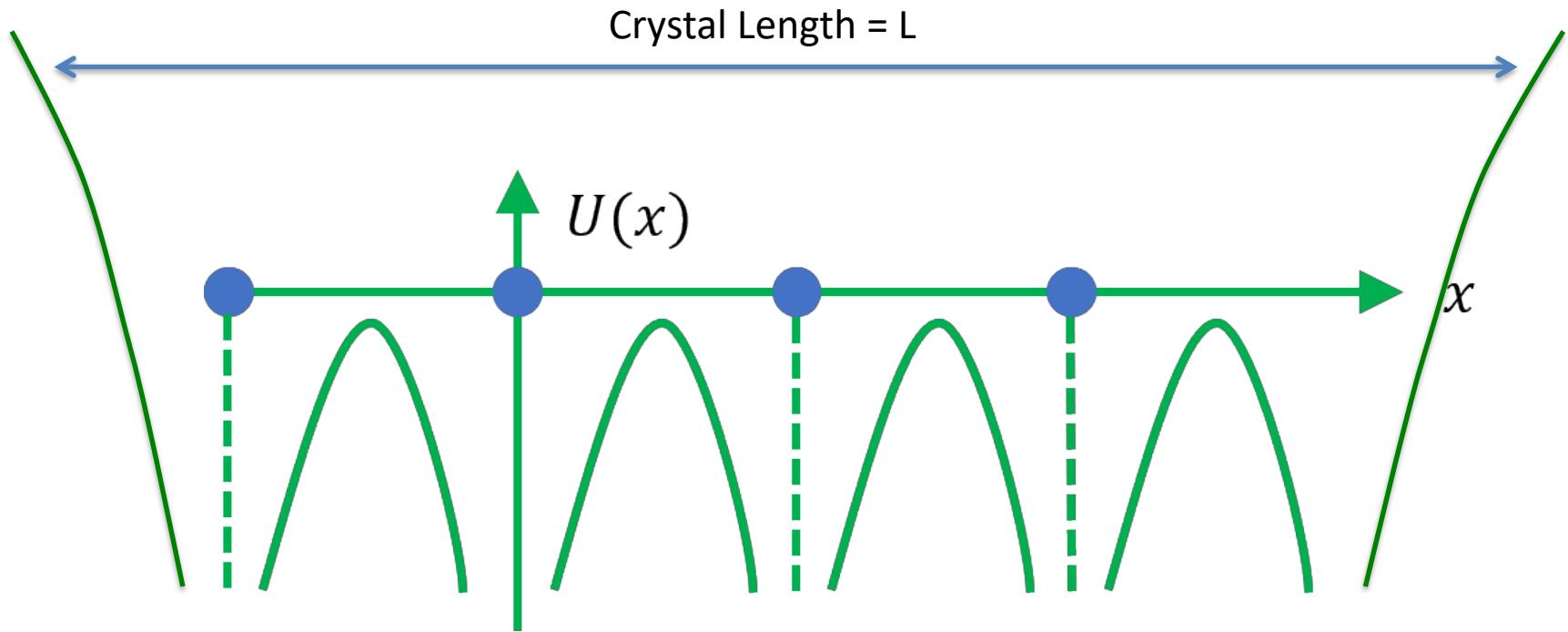
Atoms to Solids: Formation of Bands



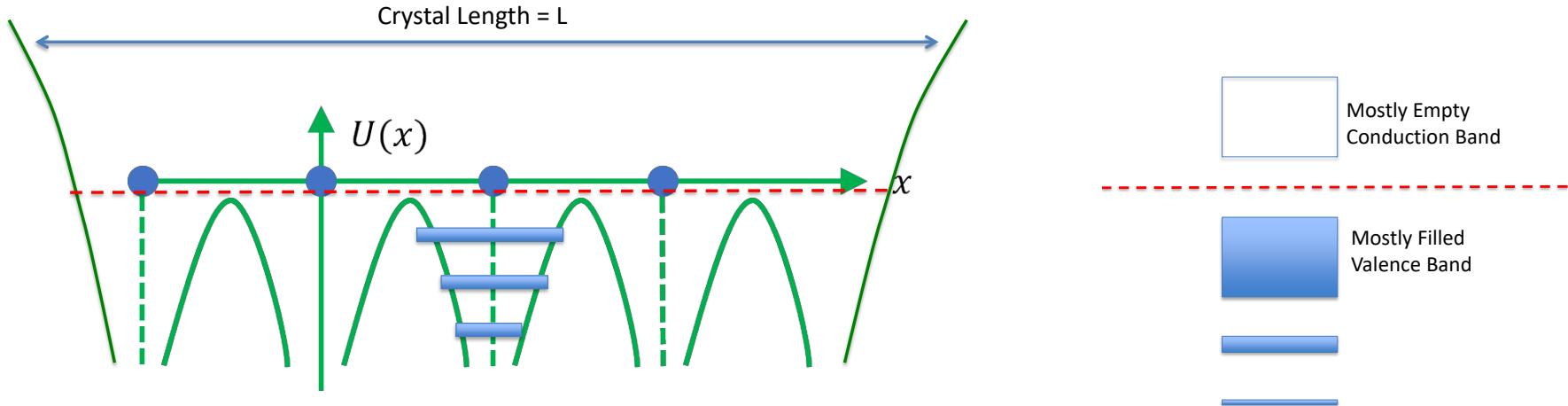
Atoms to Solids: Formation of Bands



Atoms to Solids: Formation of Bands



Atoms to Solids: Formation of Bands



Metals, Insulators and Semiconductors

Decided by how tightly bound the electrons are. This decides the energy gap.

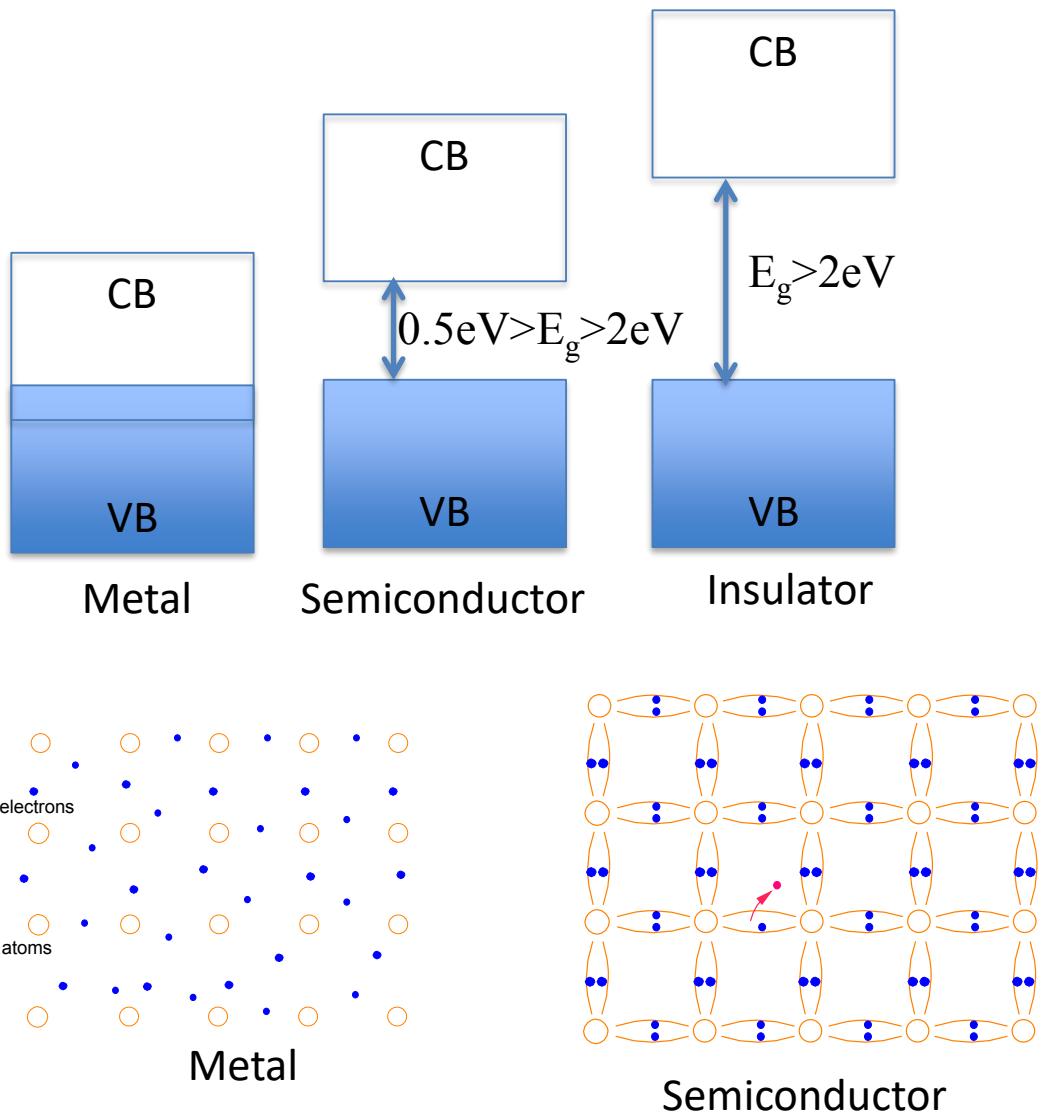
$$\text{Energy gap} = E_g$$

$$\text{Metal: } E_g = 0\text{eV}$$

Semiconductor: $E_g > 0\text{eV}$ to about 2eV (typically)
This is not a strict rule— In practice, the key parameter is how many free carriers are available at room temperature.

$$\text{Insulator: } E_g > 2\text{eV}$$

The energy gap is also temperature dependent.



IB Paper 8: Electrical elective

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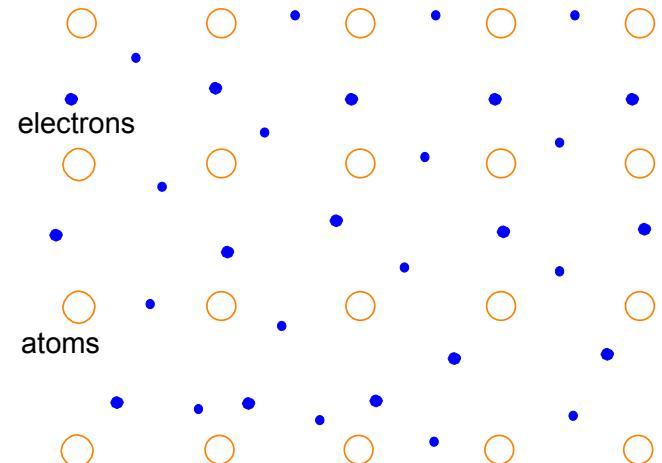
Topic 5. *Charge carriers in metals & Semiconductors*

Conduction in a Metal

A metal's outer electrons are shared between bonds, and run around between all atoms as free electrons.

The free electrons are available for conduction while core electrons stay fixed to their atoms.

- The free electrons are like a gas confined to the volume of material, and move randomly around, colliding with vibrating host atoms with their net positive charge.
- Good metallic conductors are gold, copper, silver, aluminium



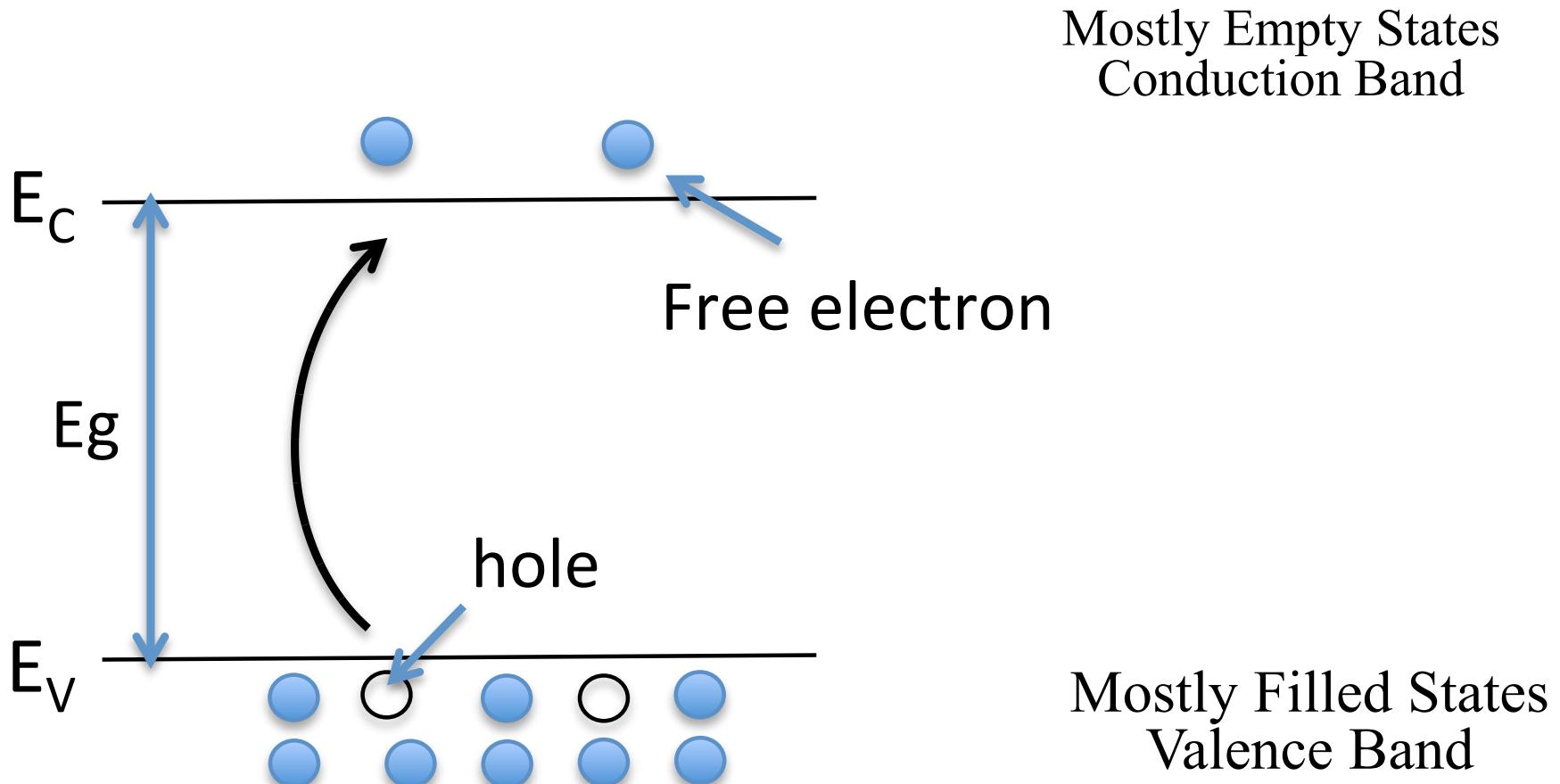
Two parameters are important to determine conductivity:

Electron concentration i.e. number of electrons/unit volume

Drift velocity of electrons to an applied field

We will discuss them shortly.

Band Diagram: Electrons and Holes



Conduction in a Semiconductor

Depends on

1.) Free electron concentration

i.e. number of electrons/volume in the conduction band, n

Depends on thermal energy

Can be influenced by *doping*

2.) Hole concentration in the valence band

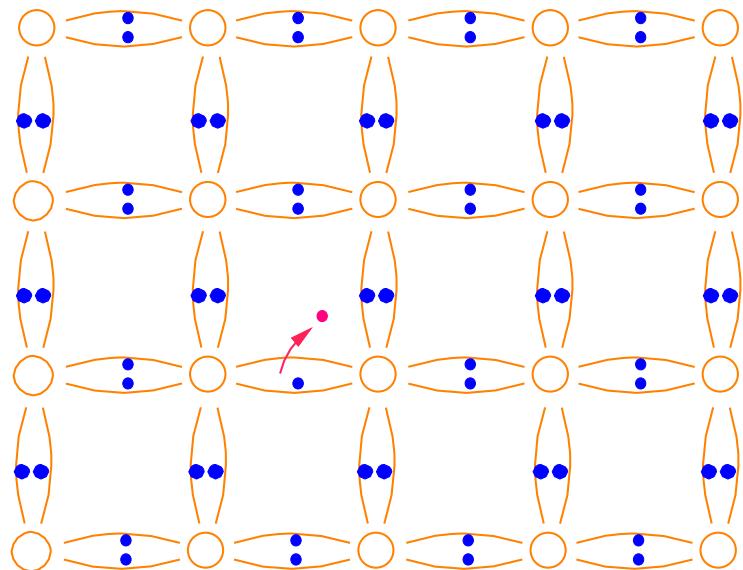
i.e. number of electrons/volume in the conduction band, p

Depends on thermal energy

Can be influenced by *doping*

3.) Velocity of electrons when a field is applied.

4.) Velocity of holes when a field is applied.



Carrier Concentration in a Semiconductor

How many carriers are available for conduction?

Intrinsic semiconductor = pure material

Thermal equilibrium implies the material is kept in the dark, no electrical bias applied. The only source of energy for electrons is thermal due to ambient temperature.

Electron in valence band gets excited by thermal energy and jump to the conduction band. They leave behind vacancies called holes. Both electrons in the conduction band and holes in the valence band can contribute to current. Holes can be considered to have +ve charge of $1.6e-19$ C.

Number of free carriers/unit volume available for conduction at *thermal equilibrium* in intrinsic semiconductor = **Intrinsic carrier concentration** = n_i

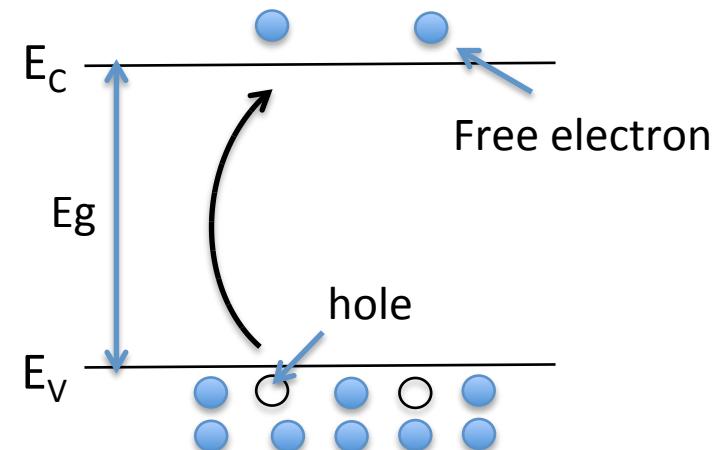
In Si, $n_i \sim 1.05 \times 10^{10}/\text{cc}$ (average at 300K).

n_i is temperature dependent. Proportionality relation:

$$n_i \propto T^3/2 e^{-\frac{E_g}{2k_B T}}$$

T is the temperature

k_B is Boltzmann's constant = $1.38 \times 10^{-23} \text{ J/K}$



E_V = Top of valence band

E_C = Bottom of conduction band

E_g = Energy Gap

n = number of electrons in the conduction band (i.e. above E_C) / unit volume

p = number of holes in the valence band (i.e. below E_V)/unit volume

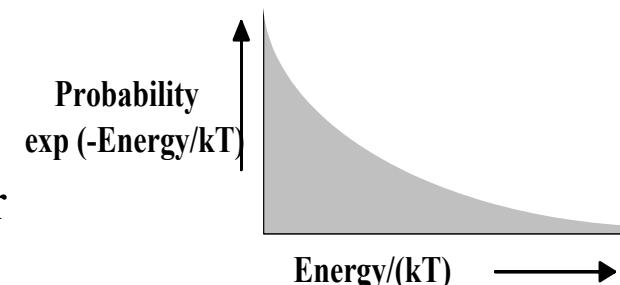
At thermal equilibrium, in an intrinsic semiconductor $n=p=n_i$

Carrier Concentration in a Semiconductor

(This slide is not for examination)

The carrier concentration in a semiconductor is counted as follows:

1.) Determine the ‘density of states’ , $g(E)$, i.e. the number of states available per unit volume per unit energy



2.) Determine the probability that an electron occupies these states. This is given by the Fermi Function, $f(E)$

The Fermi Function can be approximated as the Boltzmann distribution.
i.e. the probability that a state at energy E is occupied by an electron is $\exp(-(E-E_f)/kT)$
Here E_f is the Fermi level (you will learn more about it in 3B5) k_B is Boltzmann’s constant= 1.38×10^{-23} J/K , T is the temperature

Number of electrons/unit volume between E and $E+dE$ = $n(E)=g(E)f(E)dE$
Number of holes/unit volume between E and $E+dE$ = $p(E) = g(E)(1-f(E))dE$

Number of electrons/unit volume in the conduction band = integrate $n(E)$ over energies from E_c to infinity

Number of holes/unit volume in the valence band = integrate $p(E)$ over energies from E_v to -infinity

Current depends on :

- # of electrons, n
- # of holes, p
- Mobility of carriers
- Density of states
- Fermi function

Carrier Concentration in a Semiconductor: Doping

Electron and Hole concentration can be shifted from intrinsic concentrations by adding impurities to the semiconductor i.e. doping it. The semiconductor now becomes *extrinsic*. But always, at equilibrium: $np = n_i^2$

n-type doping:

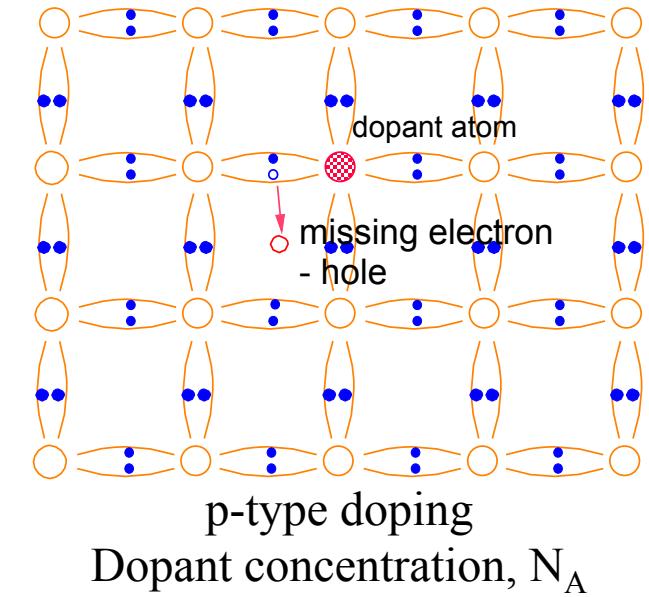
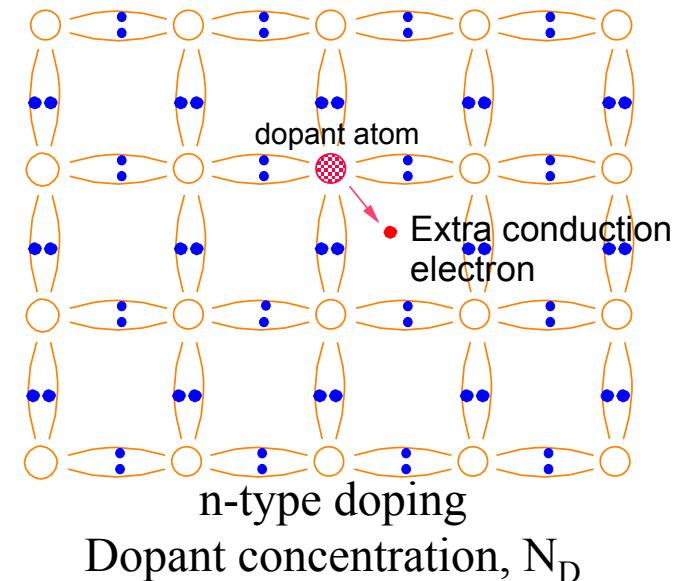
Adding impurity atom with 5 valence electrons (e.g. P), into a Si lattice. 4 participate in bonding. 1 escapes the dopant and is free to conduct. **This is n-type doping** (increases electrons). Dopants are **donors**, because they **donate electrons**. When dopant concentration, $N_D \gg n_i$

$$n \approx N_D \text{ and } p = n_i^2 / n = n_i^2 / N_D$$

p-type doping:

Adding impurity atom with 3 valence electrons (e.g. B), into a Si lattice. 4 needed to participate in bonding. 1 pulled in from the lattice i.e. a hole escapes the dopant and is free to conduct. **This is p-type doping** (increases holes). Dopants are **acceptors**, because they **accept electrons**. When dopant concentration, $N_A \gg n_i$

$$p \approx N_A \text{ and } n = n_i^2 / p = n_i^2 / N_A$$



Velocity of Carriers

When an electric field E is applied, electrons start moving to the +ve electrode, Holes start moving to the -ve electrode.

(Hole movement = electron filling vacancies and moving towards the +ve electrode)

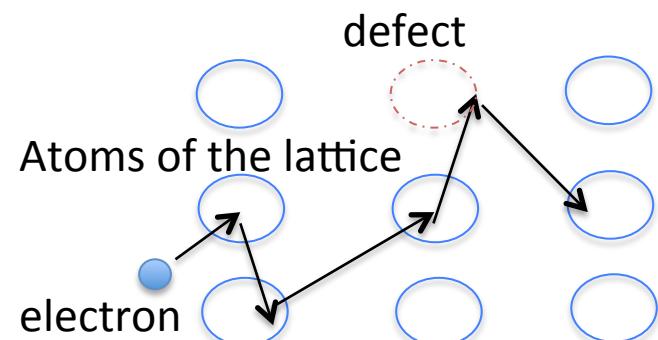
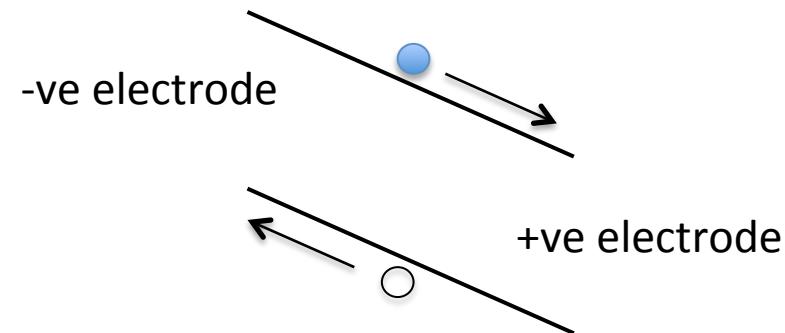
How quickly do they move?

In vacuum, electron will accelerate in an electric field.

In the semiconductor/metal it accelerates and immediately scatters (collides with the lattice, defects or each other). Thus the motion is intermittent bursts of speed and fall to low velocity. (Random walk – drift + diffusion).

At low electric fields, the velocity (called **drift velocity**, v_d) is proportional to the electric field.
Constant of proportionality = Mobility, μ

$$v_d = \mu E$$



Scattered movement of the electron in response to an applied electric field.

Velocity of Carriers

Understanding mobility better

Change of momentum of the electron = force

Let τ = mean time between collisions

m_n^* =effective mass of electron

Concept of Effective Mass: In vacuum, the mass of an electron = 9.1×10^{-31} kg

In a crystal lattice, the electron interacts with the lattice – it polarises the neighbouring atoms and moves through the lattice. We can continue using Newton's laws if we model its mass as different from 9.1×10^{-31} kg. This is the effective mass.

$$\frac{m_n^* v_d}{\tau} = qE$$

$$\Rightarrow v_{dn} = \frac{q\tau}{m_n^*} E = \mu_n E$$

$$\text{i. e. } \mu_n = \frac{q\tau}{m_n^*}$$

Similarly we can define an effective mass of holes, m_p^* and a mobility for holes μ_p

$$\mu_p = \frac{q\tau}{m_p^*}$$

Velocity of Carriers

Understanding Drift Velocity better

At low electric fields, drift velocity of electrons,

$$v_{dn} = \mu_n E$$

At low electric fields, drift velocity of holes,

$$v_{dp} = \mu_p E$$

Typical electron mobility in Si = $1500 \text{ cm}^2/\text{Vs}$

Typical hole mobility in Si = $500 \text{ cm}^2/\text{Vs}$

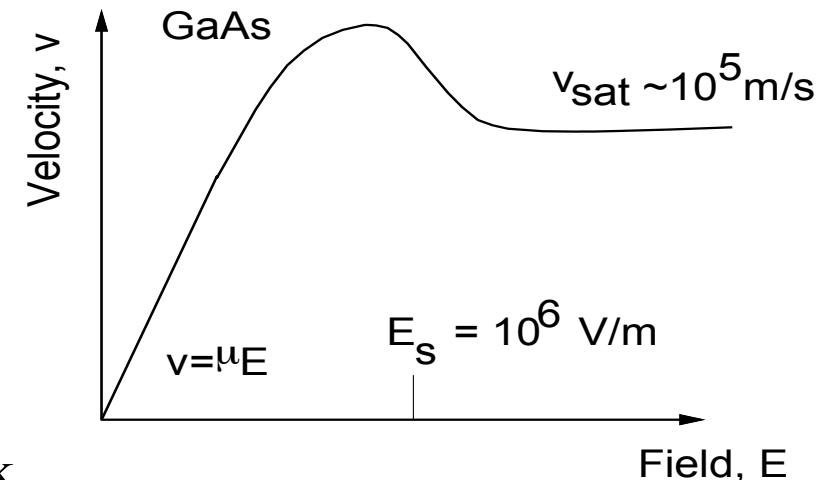
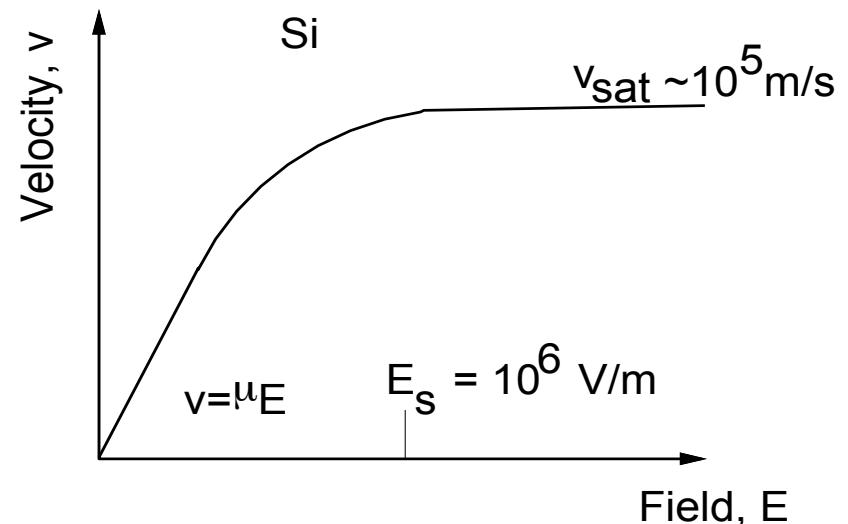
At high electric field, the drift velocity depends on the semiconductor

In most semiconductors, including Si, the velocity saturates at high fields.

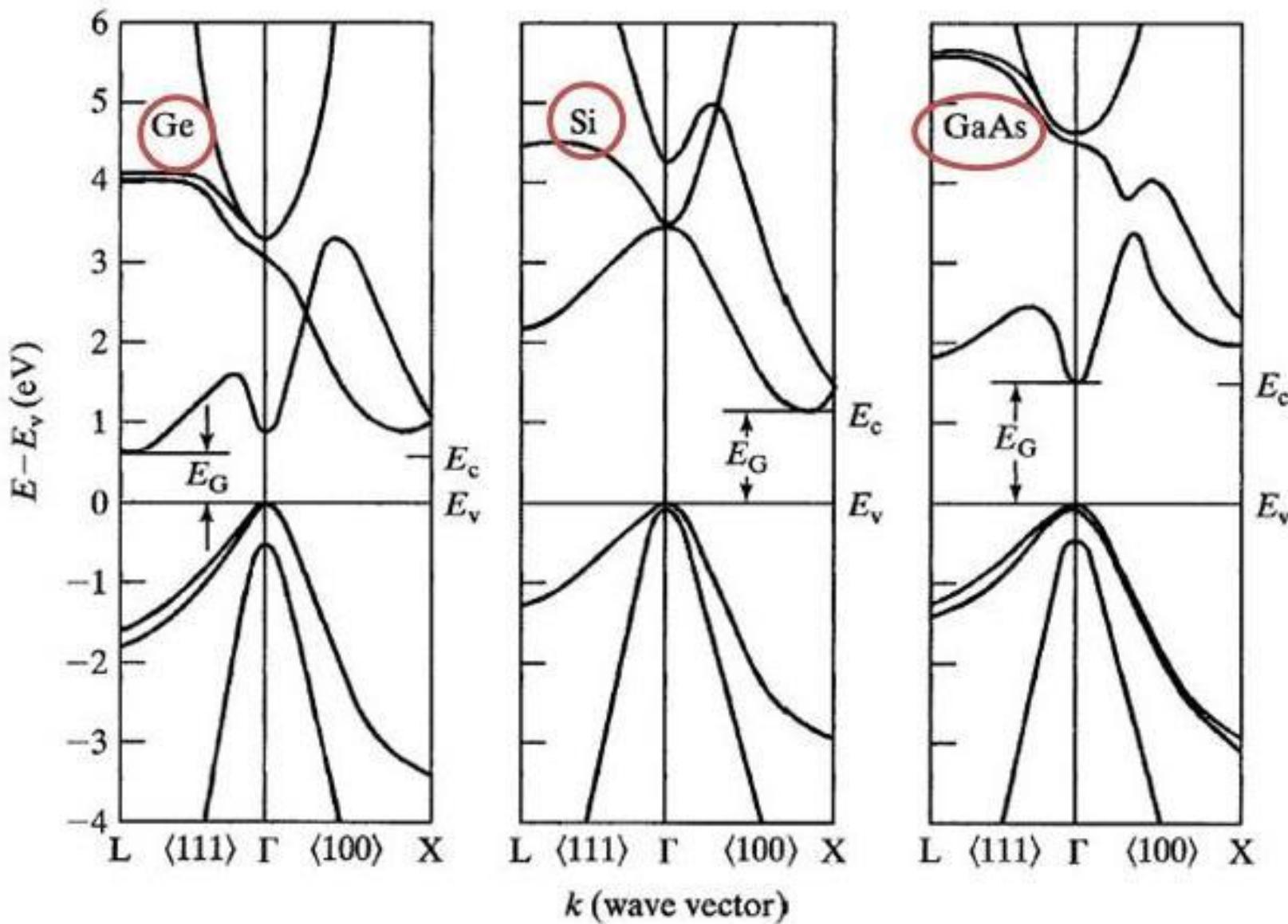
However, in GaAs, we see the Gunn Effect.

The velocity initially increases and then reduces due to the effective mass of the carriers increasing and reducing mobility.

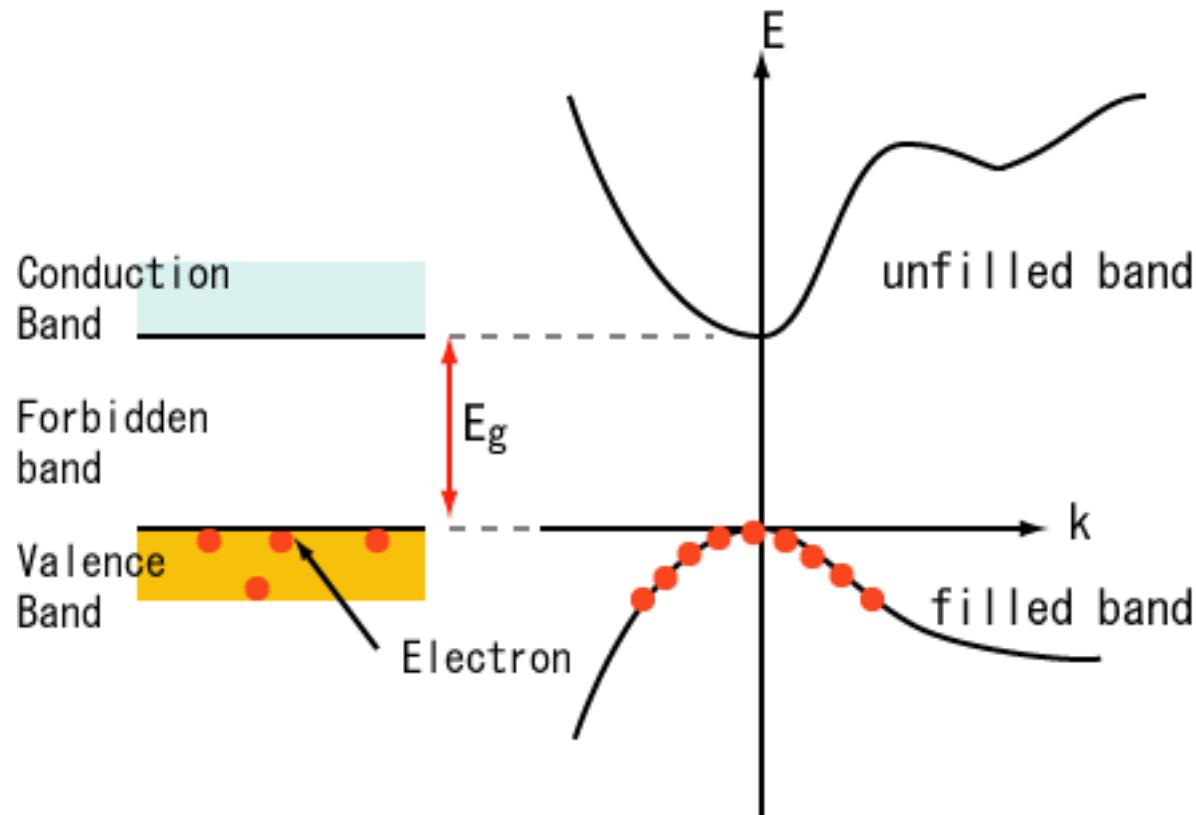
(This is due to inter-valley transfer in the E-k diagram - you will study this in 3B5)



E-k Diagram: Direct and Indirect Band Gap



Effective Mass



$$m^* = \frac{\hbar^2}{d^2E / dk^2}$$

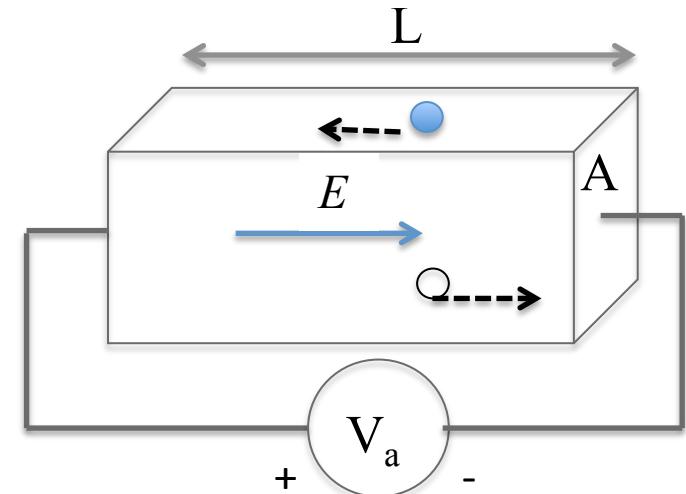
Calculating Drift current in a semiconductor

- We now know the number of carriers/unit volume
- We also know their velocity
- Then we can calculate the current due to an electric field (known as the *Drift Current*)

Drift current density = J_{dr}

Where J_{dr} = charge per unit volume x drift velocity

$$J_{dr} = qn v_{dn} + qp v_{dp} = qn \mu_n E + qp \mu_p E = q(n\mu_n + p\mu_p)E$$



V_a = Applied voltage

E = electric field due to the applied voltage

A = Area of cross section

L = length of the semiconductor

$$I = J_{dr}A = q(n\mu_n + p\mu_p)AE = q(n\mu_n + p\mu_p)A \frac{dV}{dx}$$

$$\Rightarrow \int_0^L I dx = \int_0^{V_a} q(n\mu_n + p\mu_p)AdV$$

$$\Rightarrow V_a = \frac{1}{q(n\mu_n + p\mu_p)} \frac{L}{A} I$$

$$\Rightarrow \text{Resistivity, } \rho = \frac{1}{q(n\mu_n + p\mu_p)}$$

IB Paper 8: Electrical elective

Easter term

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6.2 *Some examples*

Resistance of a Semiconductor

Resistance of a Semiconductor

$$J_{dr} = qn\nu_{dn} + qp\nu_{dp} = qn\mu_n E + qp\mu_p E = q(n\mu_n + p\mu_p)E$$

$$\text{Resistance} = \frac{1}{q(n\mu_n + p\mu_p)} \frac{L}{A}$$

$$\text{Resistivity} = \rho = \frac{1}{q(n\mu_n + p\mu_p)}$$

If the semiconductor is intrinsic

$$n = p = n_i$$

n_i is the intrinsic carrier concentration. For Si it is about $1.05 \times 10^{10}/\text{cm}^3$ @ 300K.

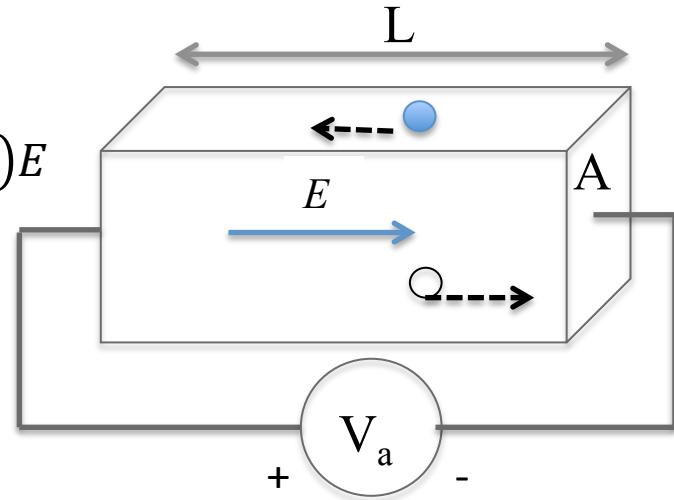
Note: $np = n_i^2$ (called Mass Action Law). This holds true only at equilibrium but is true even after doping

If the semiconductor is doped with donor dopants of concentration $N_D \gg n_i$

$$n = N_D \text{ and } np = n_i^2 \Rightarrow p = n_i^2 / N_D$$

If the semiconductor is doped with acceptor dopants of concentration $N_A \gg n_i$

$$p = N_A \text{ and } np = n_i^2 \Rightarrow n = n_i^2 / N_A$$



Example 1: Resistance of a Semiconductor

What is the resistance of a 10μm by 10μm by 10μm block of intrinsic silicon when the resistance is measured across two opposite faces? The electron and hole mobilities are 1000 cm²/Vs and 500 cm²/Vs, respectively. The intrinsic carrier concentration is 1x10¹⁰/ cm³

Answer:

$$n = p = n_i = 1 \times 10^{10} / \text{cm}^3$$

$$\mu_n = 1000 \text{cm}^2 / \text{Vs}$$

$$\mu_p = 500 \text{cm}^2 / \text{Vs}$$

$$q(\mu_n n + \mu_p p) = qn_i(\mu_n + \mu_p)$$

$$= (1.6 \times 10^{-19}) \times (1 \times 10^{10}) \times (1000 + 500)$$

$$= 2.4 \times 10^{-6} (\Omega \text{cm})^{-1}$$

$$L = 10 \times 10^{-4} \text{cm} = 1 \times 10^{-3} \text{cm}$$

$$A = (10 \times 10^{-4}) \times (10 \times 10^{-4}) \text{cm}^2 = 1 \times 10^{-6} \text{cm}^2$$

$$\text{Resistivity} = \rho = \frac{1}{q(n\mu_n + p\mu_p)}$$

$$= \frac{1}{2.4 \times 10^{-6}} = 4.16 \times 10^5 \Omega \text{cm}$$

$$\text{Resistance} = \frac{1}{q(n\mu_n + p\mu_p)} \frac{L}{A}$$

$$= \rho \frac{L}{A} = (4.16 \times 10^5) \times \frac{1 \times 10^{-3}}{1 \times 10^{-6}}$$

$$= 4.16 \times 10^8 \Omega$$

Example 2: Resistance of a Semiconductor

What is the resistance of a 10μm by 10μm by 10μm block of n-doped silicon when the resistance is measured across two opposite faces? The donor dopant density is $N_D = 1 \times 10^{15}/\text{cc}$. The electron and hole mobilities are 1000 cm²/Vs and 500 cm²/Vs, respectively. The intrinsic carrier concentration is $1 \times 10^{10}/\text{cm}^3$

Answer:

$$N_D = 1 \times 10^{15} / \text{cc} \gg n_i$$

$$n \approx N_D = 1 \times 10^{15} / \text{cm}^3$$

$$p = n_i^2 / n = (1 \times 10^{20}) / (1 \times 10^{15}) = 1 \times 10^5 / \text{cm}^3$$

$$\mu_n = 1000 \text{ cm}^2 / \text{Vs}$$

$$\mu_p = 500 \text{ cm}^2 / \text{Vs}$$

$$q(\mu_n n + \mu_p p) \approx q(\mu_n n) \text{ Since } n \gg p$$

$$= (1.6 \times 10^{-19}) \times (1 \times 10^{15}) \times (1000)$$

$$= 1.6 \times 10^{-1} (\Omega \text{cm})^{-1}$$

$$L = 1 \times 10^{-3} \text{ cm}$$

$$A = 1 \times 10^{-6} \text{ cm}^2$$

$$\text{Resistivity} = \rho = \frac{1}{q(n\mu_n + p\mu_p)}$$

$$\approx \frac{1}{1.6 \times 10^{-1}} = 6.25 \Omega \text{cm}$$

$$\text{Resistance} = \frac{1}{q(n\mu_n + p\mu_p)} \frac{L}{A}$$

$$= \rho \frac{L}{A} = 6.25 \times \frac{1 \times 10^{-3}}{1 \times 10^{-6}}$$

$$= 6.25 k\Omega$$

Example 3: Resistance of a Semiconductor

What is the resistance of a 10μm by 10μm by 10μm block of p-doped silicon when the resistance is measured across two opposite faces? The acceptor dopant density is $N_A = 1 \times 10^{15}/\text{cc}$. The electron and hole mobilities are 1000 cm²/Vs and 500 cm²/Vs, respectively. The intrinsic carrier concentration is $1 \times 10^{10}/\text{cm}^3$

Answer:

$$N_A = 1 \times 10^{15} / \text{cc} \gg n_i$$

$$p \approx N_A = 1 \times 10^{15} / \text{cm}^3$$

$$n = n_i^2 / p = (1 \times 10^{20}) / (1 \times 10^{15}) = 1 \times 10^5 / \text{cm}^3$$

$$\mu_n = 1000 \text{ cm}^2 / \text{Vs}$$

$$\mu_p = 500 \text{ cm}^2 / \text{Vs}$$

$$q(\mu_n n + \mu_p p) \approx q(\mu_p p) \text{ Since } p \gg n$$

$$= (1.6 \times 10^{-19}) \times (1 \times 10^{15}) \times (500)$$

$$= 0.8 \times 10^{-1} (\Omega \text{cm})^{-1}$$

$$L = 1 \times 10^{-3} \text{ cm}$$

$$A = 1 \times 10^{-6} \text{ cm}^2$$

$$\text{Resistivity} = \rho = \frac{1}{q(n\mu_n + p\mu_p)} \\ \approx \frac{1}{0.8 \times 10^{-1}} = 12.5 \Omega \text{cm}$$

$$\text{Resistance} = \frac{1}{q(n\mu_n + p\mu_p)} \frac{L}{A} \\ = \rho \frac{L}{A} = 12.5 \times \frac{1 \times 10^{-3}}{1 \times 10^{-6}} \\ = 12.5 k\Omega$$