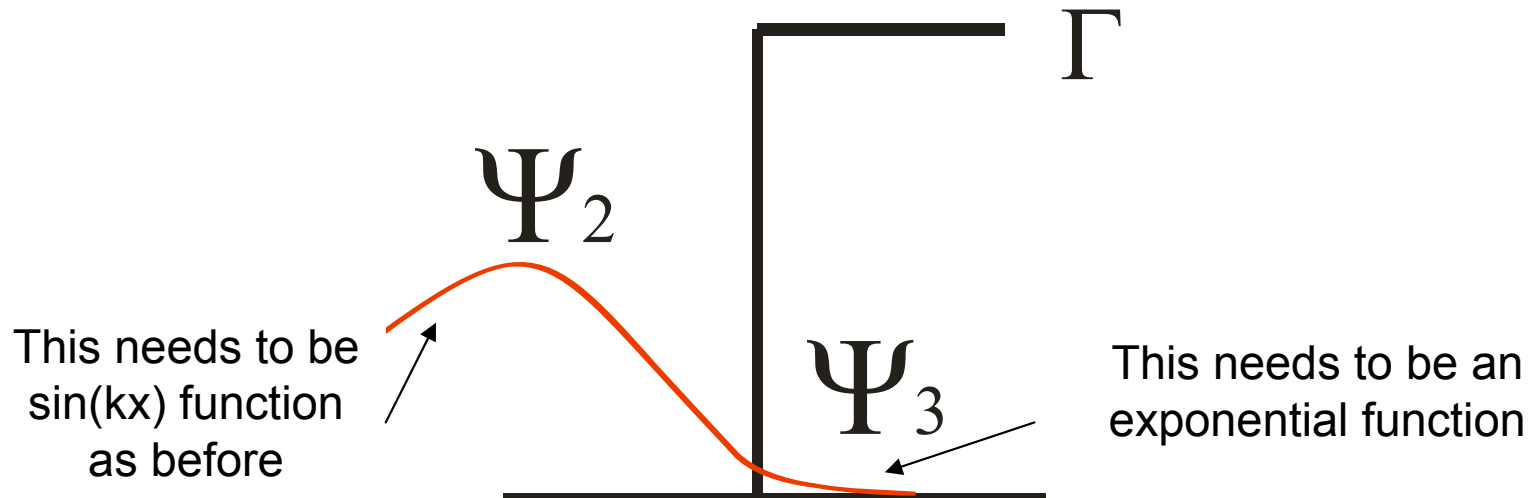


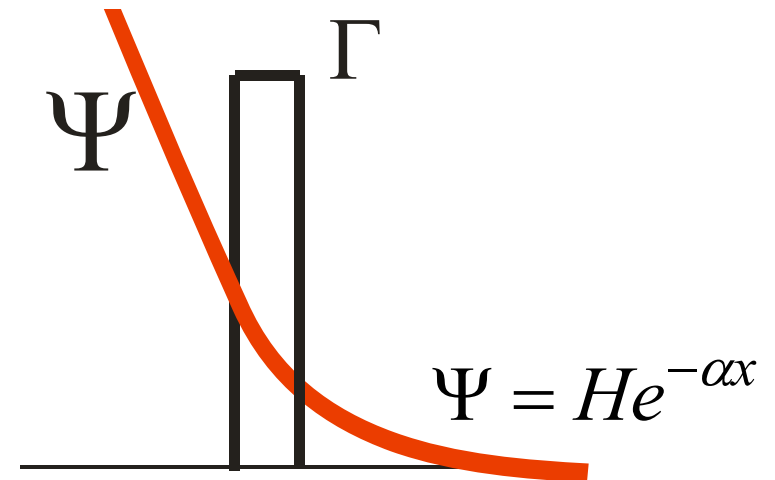


# Quantum Description of Semiconductors



Note the wavefunction is not zero in the barrier anymore. This means there is some probability of electrons in the barrier

For a thin barrier, the wavefunction can penetrate through, giving a good probability of electrons on the right hand side. The phenomenon is called **Tunneling**

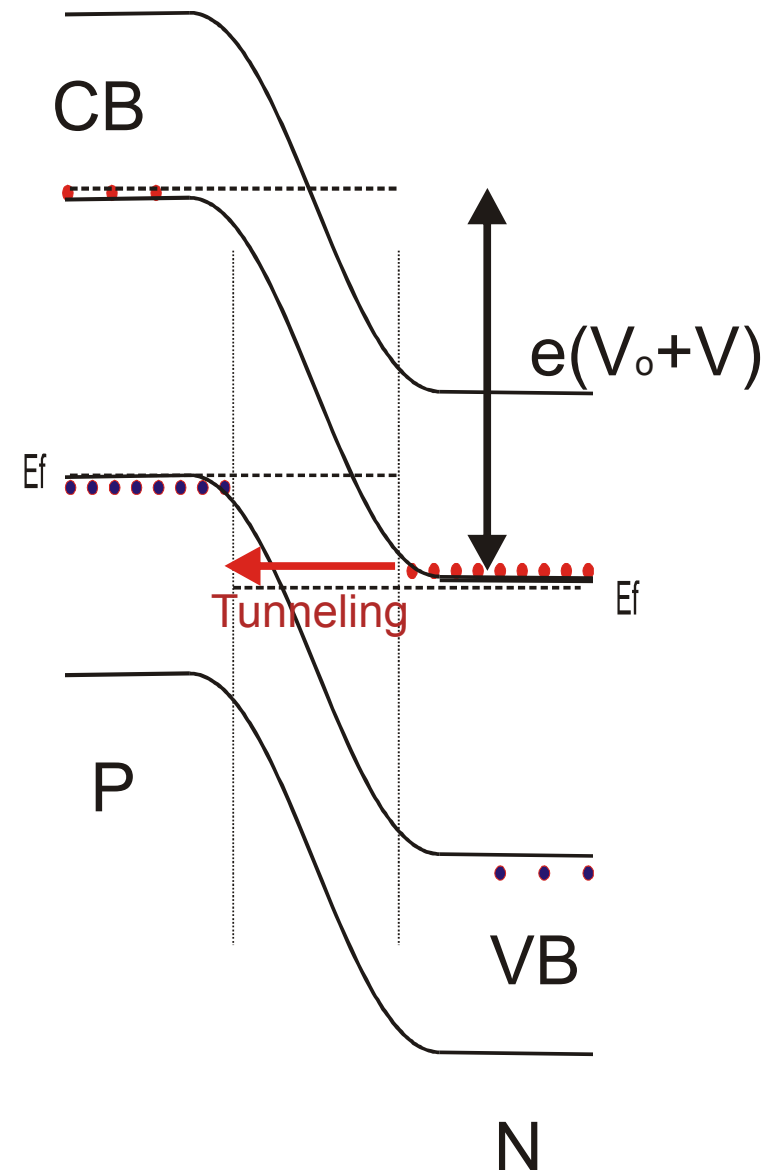


## Practical examples of tunnelling:

A **Zener diode** is a type of diode that permits current to flow in the forward direction like a normal diode, but also in the reverse direction if the voltage is larger than the rated breakdown voltage known as the "Zener voltage".

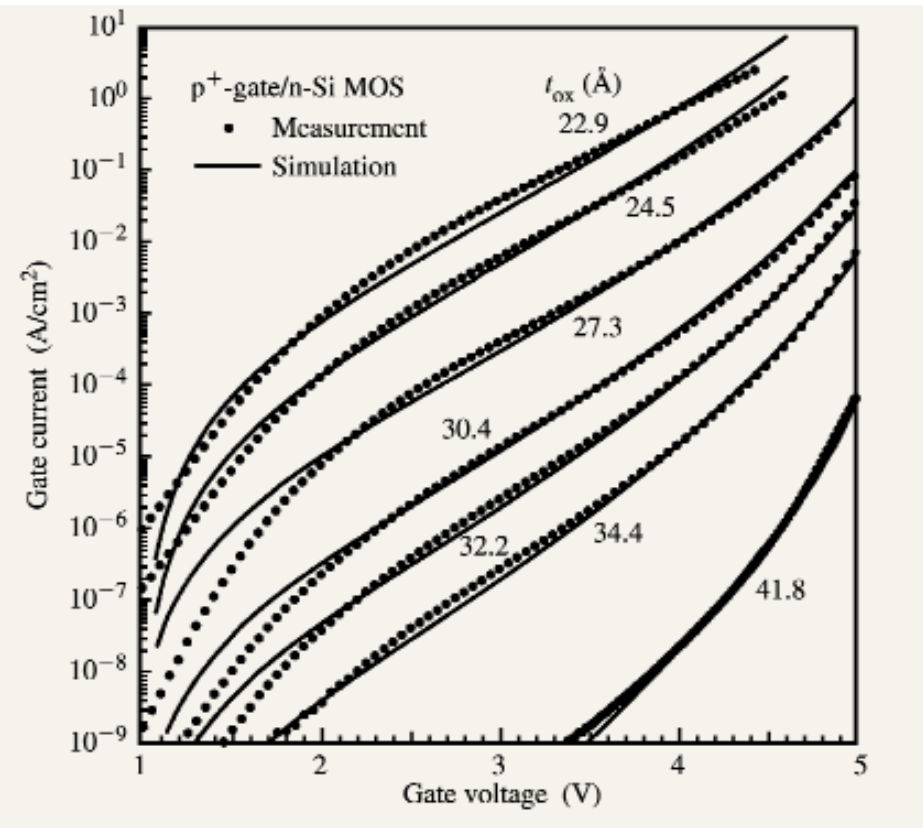
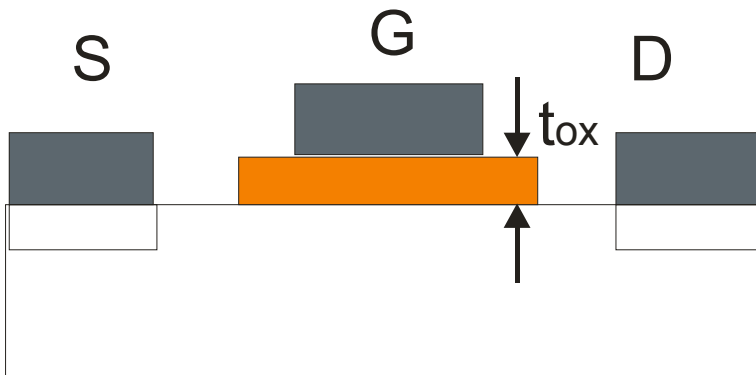
A conventional pn junction diode will not let significant current flow if reverse-biased below its reverse breakdown voltage. A **Zener diode** exhibits almost the same properties, except the device is especially designed so as to have a greatly reduced breakdown voltage, the so-called **Zener voltage**.

A Zener diode contains a heavily doped p-n junction allowing electrons to tunnel from the conduction band of the p-type material to the valence band of the n-type material. A reverse-biased Zener diode will exhibit a controlled breakdown and let the current flow to keep the voltage across the Zener diode at the Zener voltage. For example, a diode with a Zener breakdown voltage of 3.2 V will exhibit a voltage drop of 3.2 V if reverse biased..



## MOSFET Gate Leakage

Oxide layer between the gate and channel is very thin for modern devices as miniaturisation proceeds, resulting in tunnelling through the oxide as the gate voltage increases. Gives a leakage current



**Figure 14**

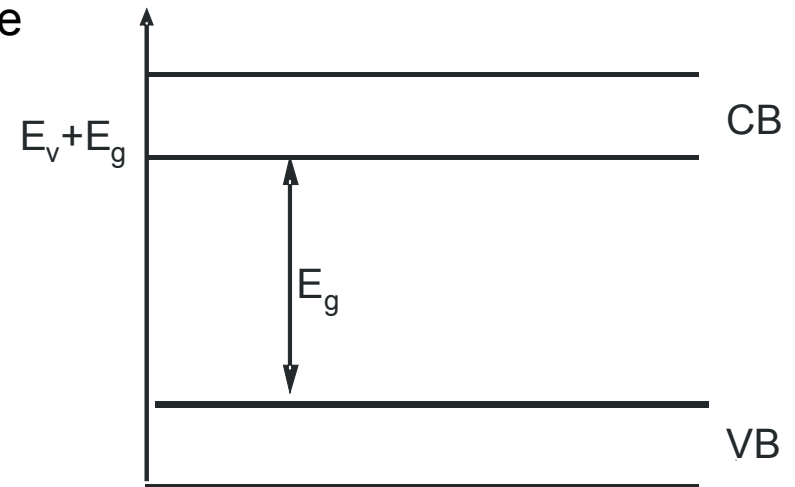
Measured and simulated  $I_G-V_G$  characteristics under accumulation conditions of  $p^+$ -gate/ $n$ -Si MOS devices with oxides ranging from 22.9 to 41.8 Å. The thickness is determined using the QM scheme.

# Quantum Description of Semiconductors

## Wave Picture of Forbidden Bandgaps in Semiconductors

Before we saw that electrons were 'not allowed' in the forbidden gap between the V.B. and C.B.

How does this arise?



## Classical Picture

Consider an electron in a vacuum

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} \quad (\text{since momentum } p = mv)$$

For an electron inside a semiconductor, the electron interaction with the lattice is taken into account by using an 'effective mass'  $m^*$  instead of  $m_0$  or  $m_e$ .

Differentiating  $E$  with respect to  $p$ ,

$$\frac{dE}{dp} = \frac{p}{m} \qquad \frac{d^2E}{dp^2} = \frac{1}{m}$$

i.e. the **mass** or effective mass is given by the **curvature** of the  $E$ - $p$  relationship

Since  $p = h/\lambda$  (de Broglie),  $E = hc/\lambda$ , i.e. relates energy and wavelength



# Quantum Description of Semiconductors

## Quantum Picture

Schrodinger Equation for a free particle

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V_0 \psi = E \psi$$

We can introduce a constant  $k$

$$\frac{\partial^2 \psi}{\partial x^2} = k^2 \psi$$

Rewrite E as a function of k  $E = V_0 + \frac{\hbar^2}{2m} k^2$

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

Differentiate twice and we get

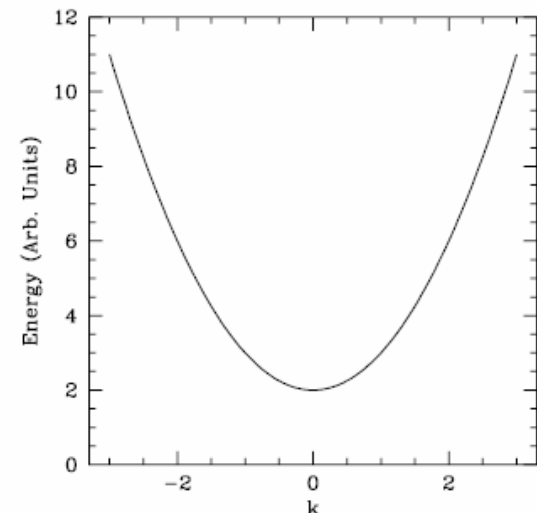
$$\frac{d^2 E}{dk^2} = \frac{\hbar^2}{m}$$

For a free electron

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

For an electron in any arbitrary  
crystal

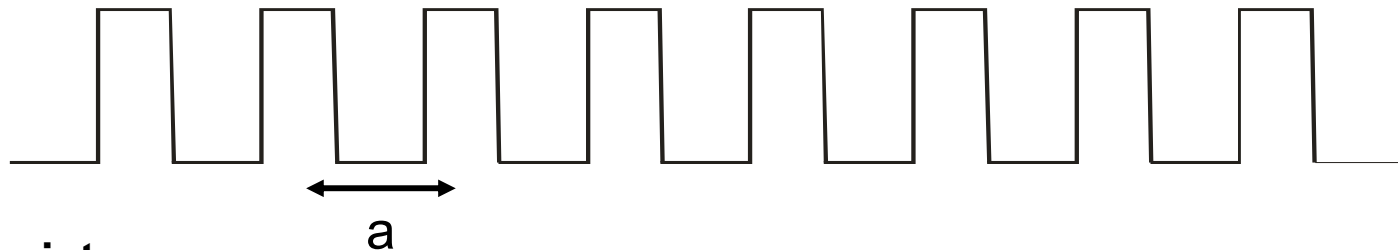
$$m_{eff} = \hbar^2 / \frac{\partial^2 E}{\partial k^2}$$





# Quantum Description of Semiconductors

Electron in a semiconductor crystal experiences a periodic potential caused by the atoms. This can be viewed as a 1 dimensional infinite series of quantum wells. This is known as the Kronig-Penney model of a crystal.



## Classical picture

$p = h/k$ , i.e. relates energy and wavelength.

As the electron energy increases from zero,  $E = hc/\lambda$ , so the wavelength decreases. Eventually the wavelength will be small enough to diffract (or reflect) from the crystal. This diffraction occurs when.

$$\frac{n\lambda}{2} = a \quad k = 2\pi p/h \quad \lambda = h/p \text{ so } \lambda = 2\pi/k \quad \frac{n2\pi}{2k} = a \quad \text{so } k = \frac{n\pi}{a}$$

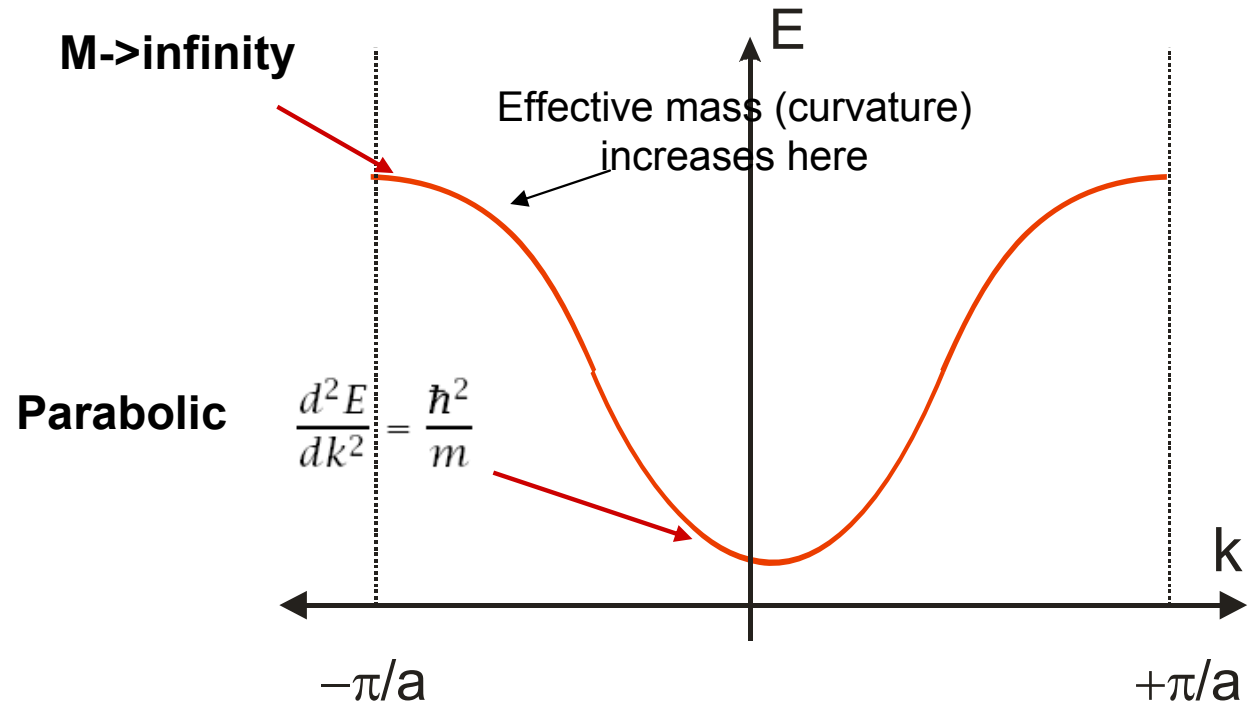
When this happens, a standing wave occurs and no propagation of the electron wave is possible. Hence we get forbidden energies when the above relation occurs.

Note  $k$  is proportional to the momentum ( $p$ ). That's why the  $k$ -axis is often called momentum space

# Quantum Description of Semiconductors

This equation only predicts discrete forbidden energies. In reality as the electron wave approaches this condition, more and more of the wave is reflected and the effective mass changes.

Electron behaves as a free electron with effective mass  $m^*$



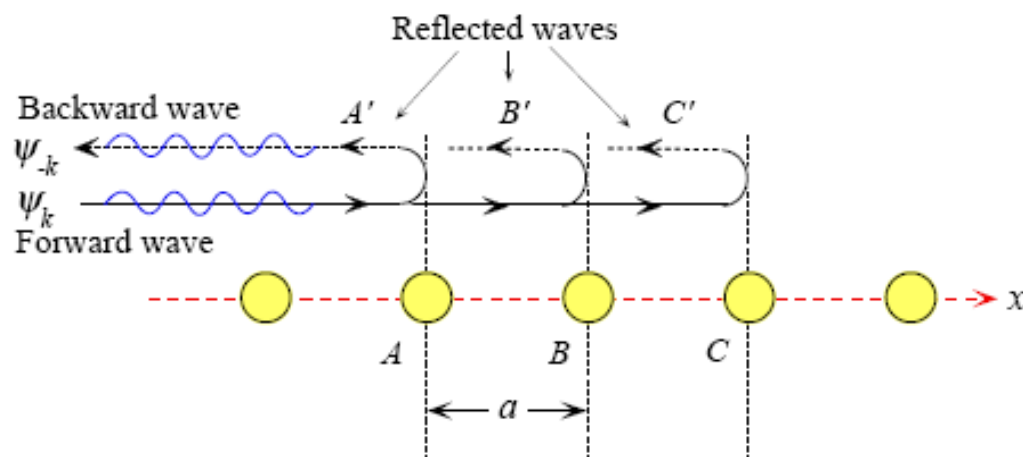
## Quantum mechanical description

Remember the solution to the Schrodinger equation for a free electron

$$\psi(x) = Ae^{jkx} = A_S \sin(kx) + A_C \cos(kx)$$



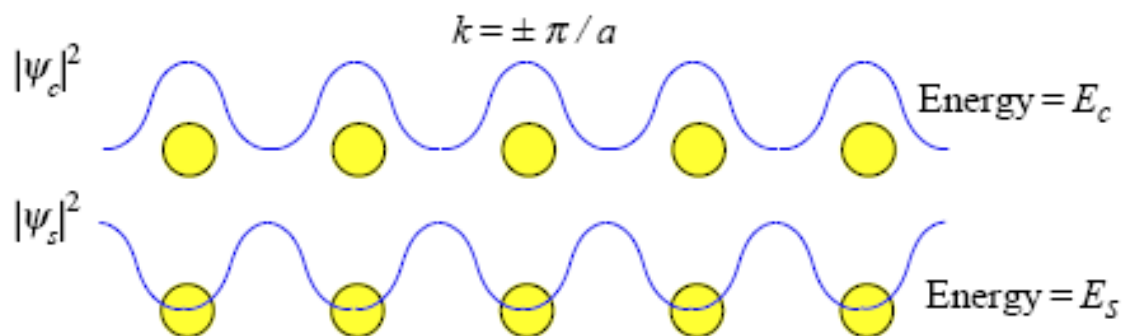
# Quantum Description of Semiconductors



Interference  
conditions:

$$2a = n\lambda \quad n=1,2,3 \dots$$

$$k = \frac{n\pi}{a}$$



$$\psi_c(x) = A_c \cos\left(\frac{n\pi x}{a}\right)$$

$$\psi_s(x) = A_s \sin\left(\frac{n\pi x}{a}\right)$$





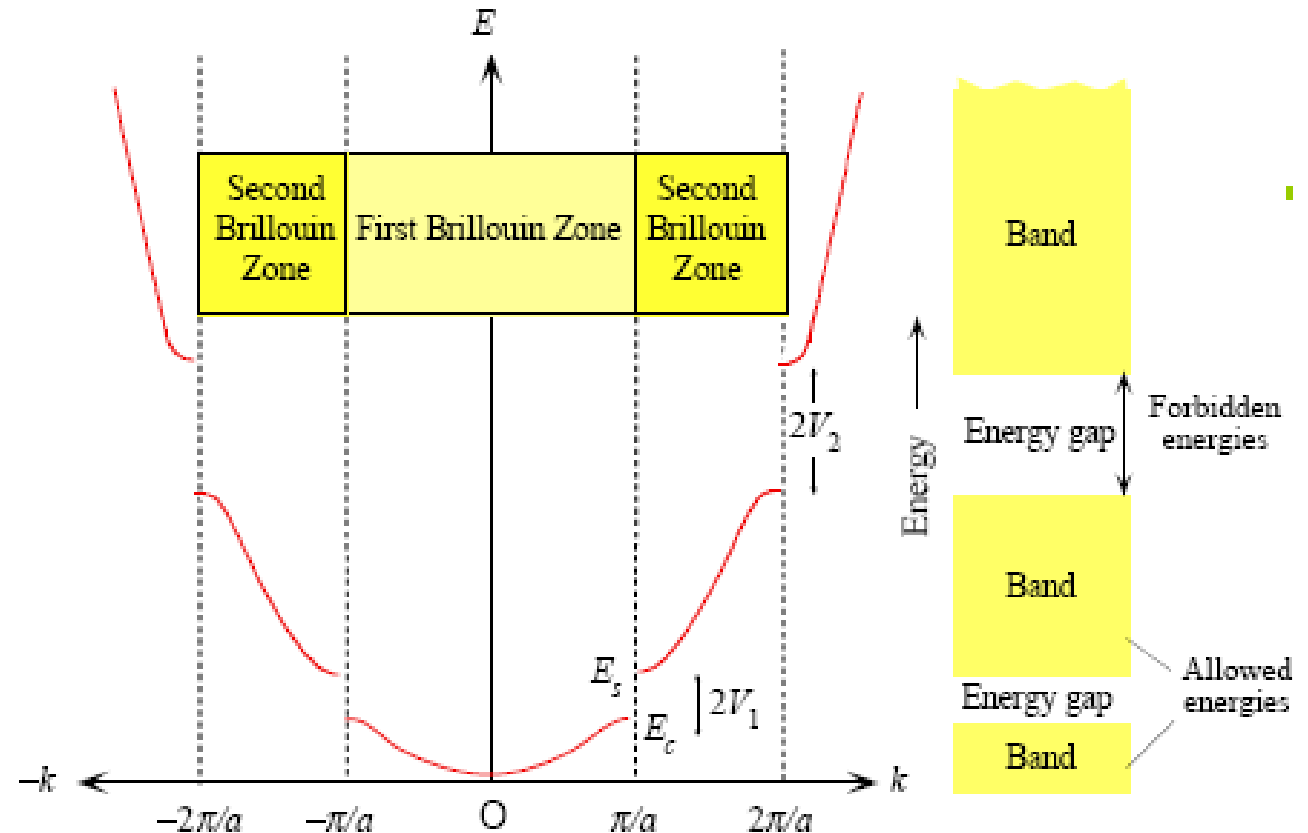
# Quantum Description of Semiconductors

away from  $k = \frac{n\pi}{a}$

$$E_k = \frac{(\hbar k)^2}{2m_e}$$

at  $k = \frac{n\pi}{a}$

$$E_k = \frac{(\hbar k)^2}{2m_e} \pm V_c$$



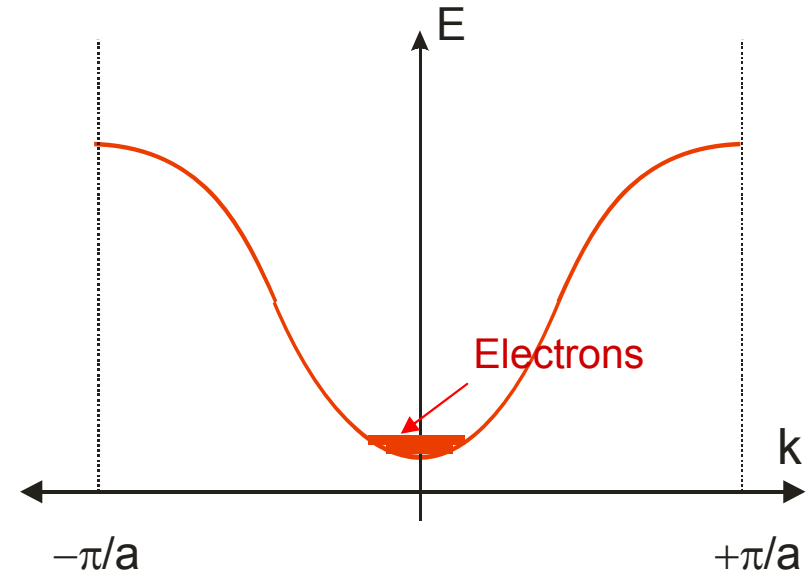
Energy 'jumps' at  $k=n\pi/a$ . Each group of  $n\pi/a$  is called a Brillouin zone eg::  
from  $-\pi/a$  to  $\pi/a$  is called the first Brillouin zone

# Quantum Description of Semiconductors

## Electrons in the conduction band

In most semiconductors electrons exist near the bottom of the conduction band where  $m^*$  is approximately constant (constant curvature).

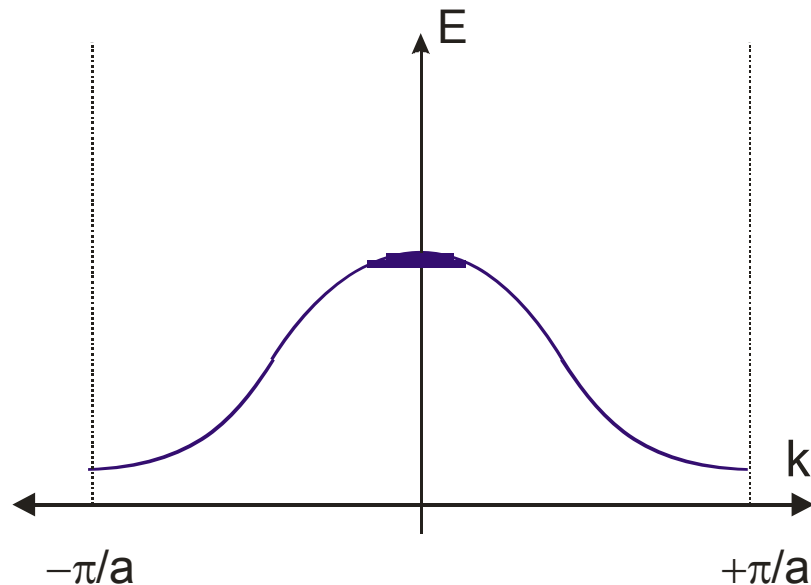
In this case we can use classical mechanics with  $m_e \rightarrow m_e^*$ .



## Holes in the valence band

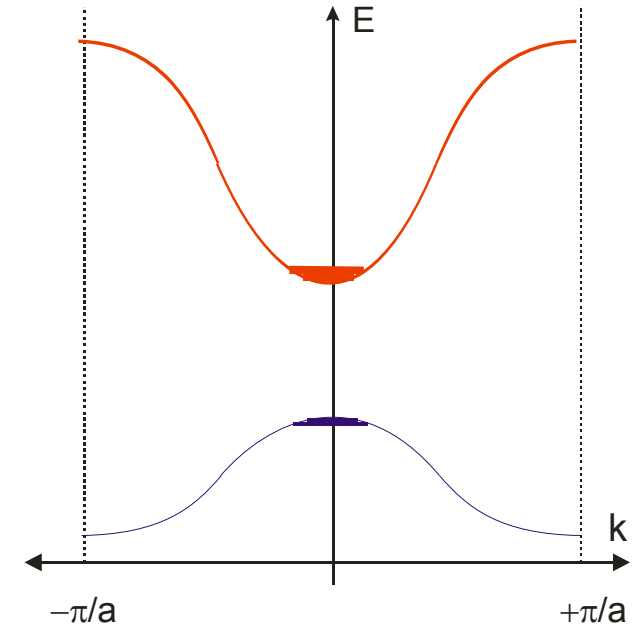
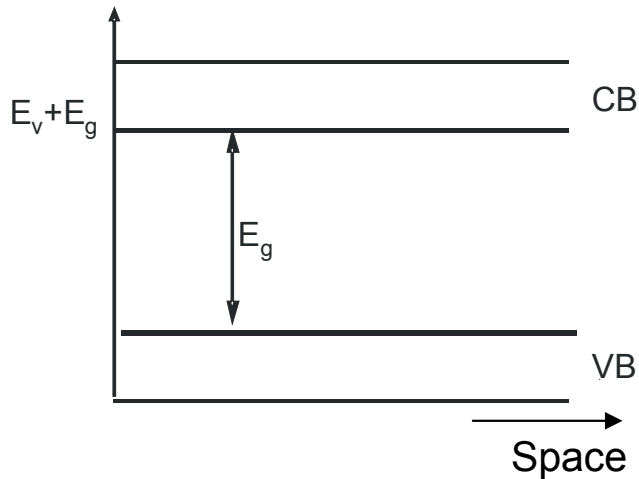
The valence band has opposite curvature, since  $m^*$  is 'negative' – this is allowed for by assuming holes are positively charged with an effective mass  $= m_h^*$ .

As with electrons, holes in a crystal lattice can be described by classical mechanics with  $m_e \rightarrow m_h^*$



# Quantum Description of Semiconductors

Before we drew a picture of the semiconductor band gap in space like this. Real picture is seen in 'k space' (momentum space). This is called a direct gap, where the maximum of the valence band lies directly below the minimum of the conduction band (where most electrons are).



What about optical transitions?

They must conserve momentum.  $p_e - p_h = p_p$

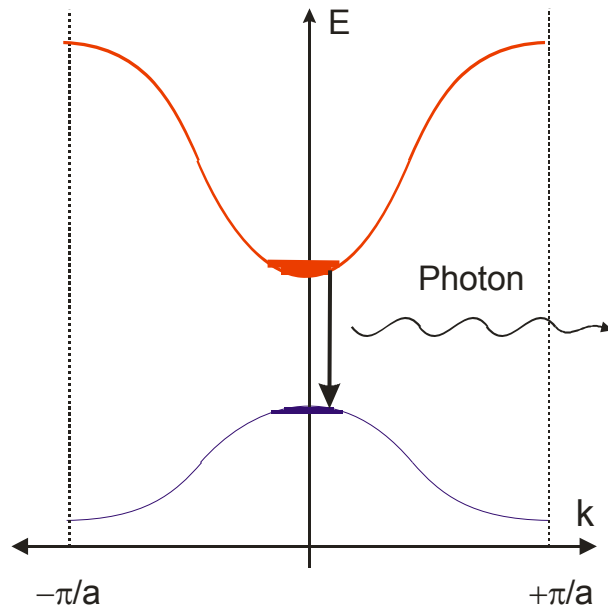
What is the typical momentum of an electron? Imagine an electron is moving under a potential of 1V. Its momentum  $p_e = mv = (2eVm)^{1/2} = 5 \times 10^{-25} \text{ Kg.m}^{-1}$

Momentum of a photon. Classically the photon has no mass. From de Broglie, anything which has a wavelength must have momentum. associated  $\lambda = h/p$ . Say  $\lambda = 500 \text{ nm}$ .  $p_p = 1 \times 10^{-27} \text{ Kg.m}^{-1}$

So  $P_e \gg P_p$  same for  $P_h$ . **Photons have insignificant momentum**



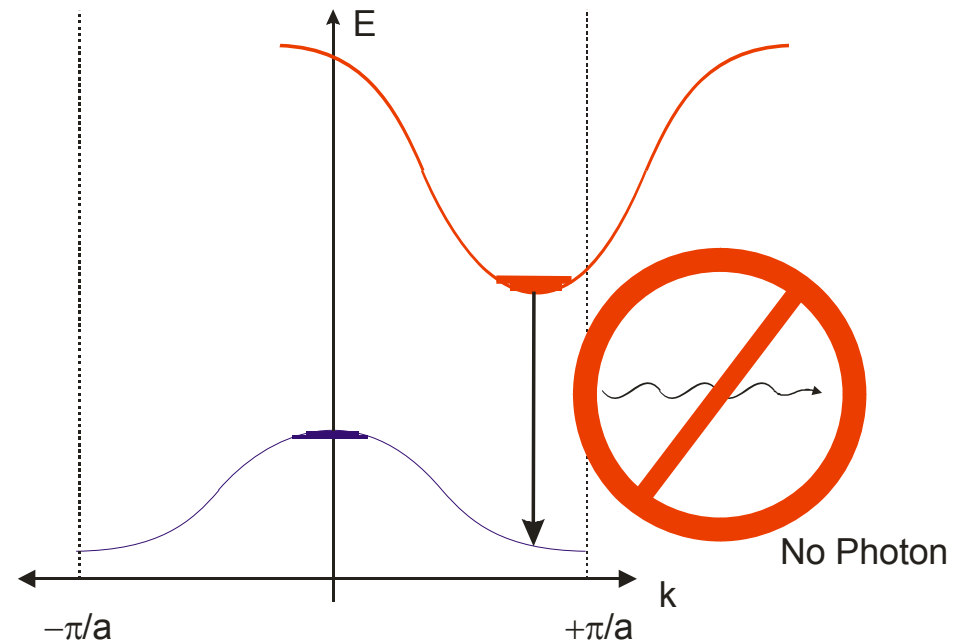
# Quantum Description of Semiconductors



Optical transitions occur with the same  $k$ ; they are vertical transitions. This type of **direct gap** semiconductor will have a strong recombination rate ( $\rightarrow$  a high efficiency for the emission of photons)

However this is not the only type of arrangement possible

In this Indirect gap semiconductor the vertical transition needed by a photon cannot occur (in the example shown there are no holes in the Valence band). The transition needs another particle to provide the momentum change. In a crystal, lattice vibrations have a high mass and a small velocity. They have momentum but not much energy. We call these lattice vibrations **phonons**.



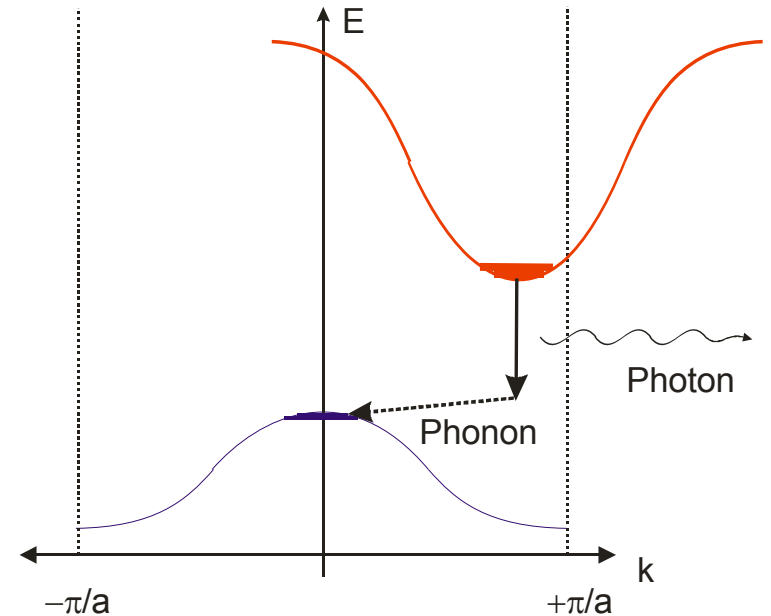


# Quantum Description of Semiconductors

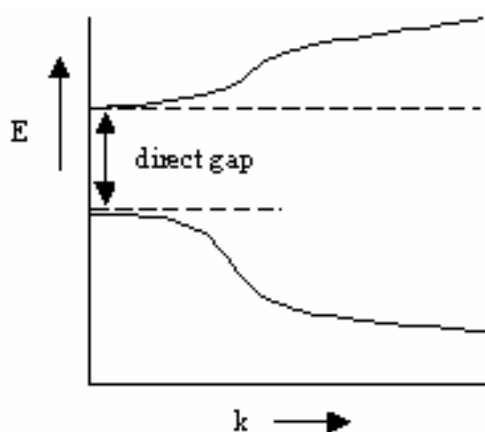
This requirement for a 4<sup>th</sup> particle (phonon) to provide the momentum change makes the transition less likely to happen compared to direct gap material.

So these **indirect band gap** materials are poor emitters of light compared to the direct gap ones.

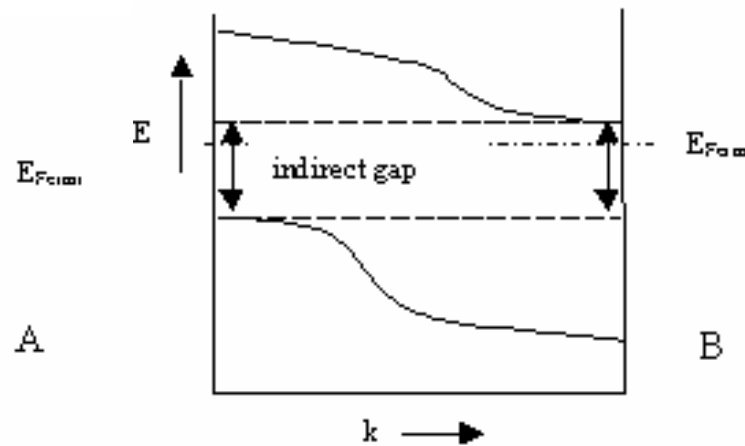
**Direct gap** materials are good for light emission, e.g. lasers, LEDs and light detection (reverse process).



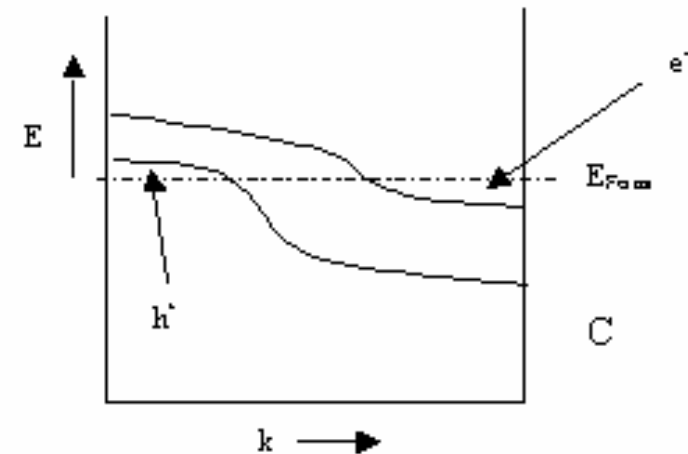
## Some 'real' band structures



Direct



Indirect

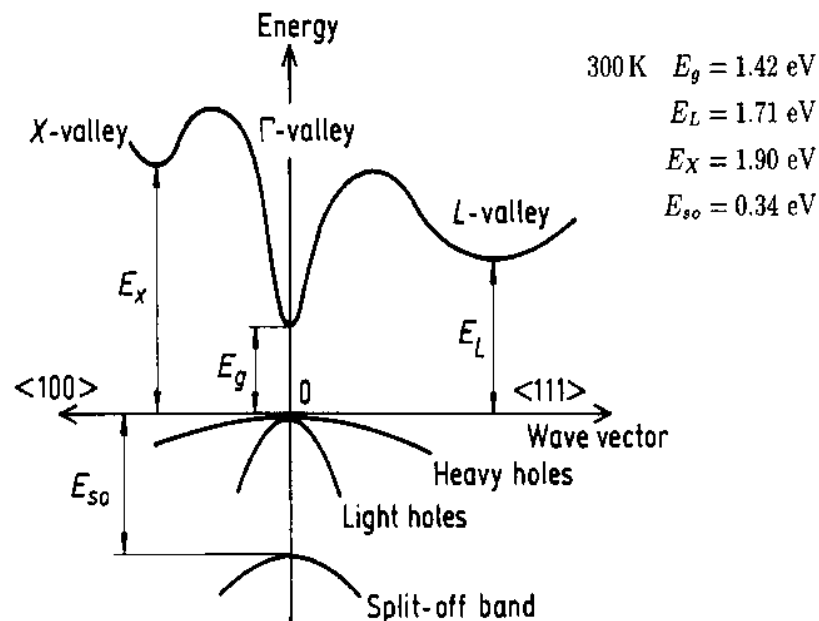
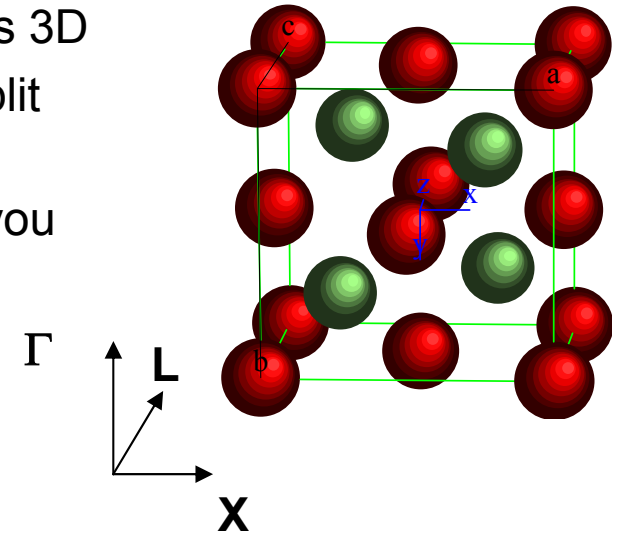


No band gap (semimetal)

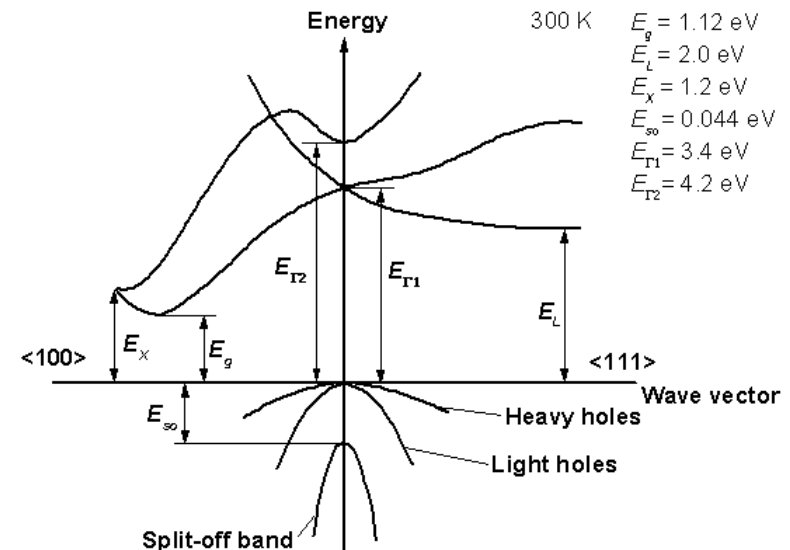
# Quantum Description of Semiconductors

A semiconductor crystal has 'directions'. Real band structure is 3D  
The holes split into 3 bands. So called heavy, light and spin-split bands.

Makes the real band structures a little complicated. However you can still easily see the direct/indirect nature



**GaAs (good light emitter)**



**Silicon (poor light emitter)**

## Schrodinger Derivation

### Wavepackets: group & phase velocities of particles

A wave travelling in the positive  $x$  direction may be represented by the expression :

$$A_o \cos(\omega t - \beta x)$$

where  $A_o$  is the amplitude of the wave,  $\omega$  is the angular frequency and  $\beta$  is the phase constant, which is related to the wavelength by,  $\beta = 2\pi/\lambda$ .

Mathematically, it is more convenient to represent the wave by an exponential function:

$$A_o \operatorname{Re} \exp[j(\omega t - \beta x)] \quad (1)$$

Most books omit the 'Re' part, but only the real part of a subsequent operation is valid.

The propagation of a wave is characterised by two velocities – the phase velocity,  $v_{ph}$  and group velocity,  $v_g$ . Phase velocity is defined as the velocity of planes of constant phase along the propagation direction of the waves.

Let us examine the motion of a point of constant phase, which is given by the condition:

$$\omega t - \beta x = \text{constant} \quad (2)$$

Phase velocity is obtained by differentiating this equation with respect to time:

$$\omega - \beta \delta x / \delta t = 0 \quad \text{or} \quad v_{ph} = \omega / \beta \quad (3)$$

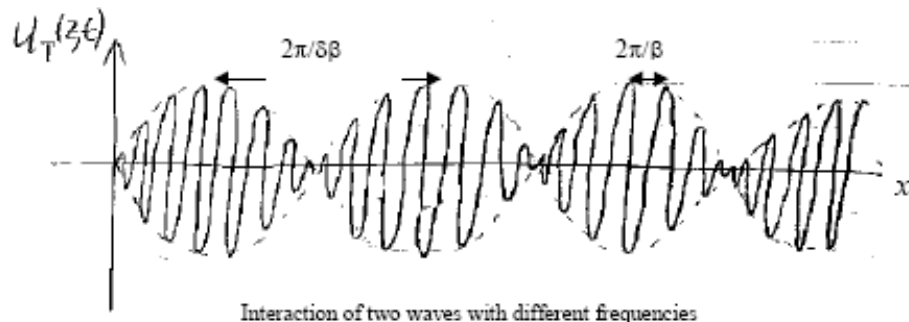
(this is the velocity with which the phase moves – nothing material propagates with this velocity – indeed  $v_{ph}$  can be greater than the speed of light without violating any physical laws.)

If we consider two waves with the same amplitude but small differences of  $\delta\omega$  and  $\delta\beta$  in wavelength propagating simultaneously in the  $x$  direction. The resultant wave can be represented by the sum:

$$\begin{aligned} & A_o \cos(\omega t - \beta x) + A_o \cos[(\omega + \delta\omega)t - (\beta + \delta\beta)x] \\ &= 2 A_o \left\{ \frac{1}{2} [\cos(2\omega + \delta\omega)t - (2\beta + \delta\beta)x] \cos[\frac{1}{2}(\delta\omega t - \delta\beta x)] \right\} \\ &\approx 2 A_o \cos[\frac{1}{2}(\delta\omega t - \delta\beta x)] \cos(\omega t - \beta x) \quad (4) \\ & \text{(since } \delta\omega \ll 2\omega \dots) \end{aligned}$$



# Quantum Description of Semiconductors



Interaction of two waves with different frequencies

Thus the resultant total wave consists of a high frequency wave varying as  $\cos(\omega t - \beta x)$ , whose amplitude varies at a slower rate given by  $\cos[\frac{1}{2}(\delta\omega t - \delta\beta x)]$ . The wave is modulated by constructive and destructive interference effects.

From (3), the high frequency wave has a phase velocity  $v_{ph} = \omega/\beta$ .

The envelope of the wavegroup varies sinusoidally with time and distance with a relatively long wavelength,  $2\pi/\delta\beta$ .

Group velocity is defined as the velocity of propagation of a plane of constant phase on the envelope. It corresponds to the velocity of the packet of waves along the direction of propagation. A plane of constant phase on the envelope is given as in (2) by:

$$\delta\omega t - \delta\beta x = \text{constant} \quad (5)$$

Doing the same thing as before, we see that the group velocity is given by:

$$v_g = \delta\omega/\delta\beta \quad (5a)$$

This velocity is the velocity with which energy is transmitted in the direction of propagation. (Think of AM of radio waves or modulation of light in an optical fibre).

We know that the momentum and kinetic energy (T) of a particle are given by:

$$\begin{aligned} p &= mv = h/\lambda \\ T &= \frac{1}{2}mv^2 = hf \end{aligned} \quad (6)$$

We know from (1) that an infinite plane wave travelling in x direction has the form:

$$A_0 \exp[-j(\omega t - \beta x)]$$

For the particle wave, using expression (6) above:

$$\beta = 2\pi/\lambda = 2\pi p/h = p/\hbar \quad (7)$$

$$\omega = 2\pi T/h = T/\hbar \quad (8)$$



# Quantum Description of Semiconductors

This suggests that it might be possible to represent a particle by a function  $\psi$  called a wavefunction, where

$$\psi = A_o \exp[-j(Tt - px)/\hbar] \quad (9)$$

Using (7) & (8),

$$v_{ph} = \omega/\beta = T/p = \frac{1}{2}mv^2/mv = v/2$$

(for photons travelling in a vacuum,  $v_{ph} = c$ )

This result is not valid for a single particle since this must be represented by a wavepacket and the concept of phase velocity is only applicable to infinite wavetrains.

From (6),

$$\begin{aligned} \frac{1}{2}mv^2 &= hf, \text{ or} \\ \omega &= \frac{1}{2}mv^2/\hbar \\ \delta\omega &= (mv/\hbar)\delta v \end{aligned}$$

From (7),

$$\begin{aligned} \beta &= p/\hbar = mv/\hbar \\ \delta\beta &= (m/\hbar)\delta v \end{aligned}$$

From (5a), and above,

$$v_g = \delta\omega/\delta\beta \quad (10)$$

Therefore a single electron can be represented by a wavepacket travelling at the same velocity as the electron. This is physically plausible as group velocity is defined as the rate at which energy (or information) is being transported by the wave.

(If the difference between  $v_p$  and  $v_g$  is still confusing, let us take something familiar. Think about how a caterpillar moves! Its 'group velocity' is much slower than its 'phase velocity'.)

## The Schrödinger wave equation

Erwin Schrödinger (1887-1961), placed Planck's quantum theory on a firm mathematical basis in 1926. (Nobel prize (with Dirac) in 1933).

The Schrödinger equation predicts  $\psi$  the wavefunction of a particle. There is no formal proof for the Schrödinger wave equation - same for Newton's laws. Agreement with experiment has been found to be valid in all circumstances, especially with microscopic particles, where relativistic effects can be significant. In the large size limit, it agrees with Newton.



# Quantum Description of Semiconductors

Equation (9) gave an expression for  $\psi$  including the K.E., T, of a particle. In general, the particle can also have P.E. due to the particle moving in a field in the crystal lattice.

$$E = \hbar\omega = K.E. + P.E. = T + V$$

$$\psi = A_0 \exp[-j(Et - px)/\hbar] \quad (11)$$

What equation does this generalised wavefunction satisfy?

Let us look at the magnetic field of a plane wave propagating in a medium with permittivity  $\epsilon$  and permeability  $\mu$ .

The solution for

$$\partial^2 H / \partial x^2 = \epsilon\mu \partial^2 H / \partial t^2 \quad (12)$$

is

$$H = H_0 \exp[-j(\omega t - \beta x)]$$

Let us try and find a wave equation similar to (12) for which the solution for  $\psi$  is given by (11).

If we differentiate (11) w.r.t.  $t$

$$\frac{\partial \psi}{\partial t} = -\frac{j}{\hbar} E \psi = -\frac{j}{\hbar} \left( V + \frac{1}{2} m v^2 \right) \psi \quad (13)$$

Let us also differentiate  $\psi$  w.r.t.  $x$ , twice

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{p^2}{\hbar^2} \psi = -\frac{m^2 v^2}{\hbar^2} \psi \quad (14)$$

Rearrange (13) to give:

$$-\frac{1}{2} m v^2 \psi = -j\hbar \frac{\partial \psi}{\partial t} + V \psi \quad (15)$$

Rearrange (14) to give:

$$-\frac{1}{2} m v^2 \psi = \frac{1}{2m} \hbar^2 \frac{\partial^2 \psi}{\partial x^2} \quad (16)$$

Equate (15) to (16) and rearrange to give:

$$\frac{\partial^2 \psi}{\partial x^2} - \frac{2m}{\hbar^2} V \psi + j \frac{2m}{\hbar} \frac{\partial \psi}{\partial t} = 0 \quad (17)$$

If the total particle energy is constant (as is normally the case), the Schrödinger equation can be simplified by separating out time and position dependent parts. Let us look at a 1-D problem for simplicity, and assume a solution of the form:



# Quantum Description of Semiconductors

$$\psi = \Psi(x)\Gamma(t) \quad (18)$$

where  $\Psi$  and  $\Gamma$  are respectively functions of position and time only.

By differentiating (18) w.r.t.  $x$  twice and w.r.t.  $t$ , and substituting into (17), you get:

$$\frac{\hbar^2}{2m\Psi} \frac{d^2\Psi}{dx^2} - V = -j\frac{\hbar}{\Gamma} \frac{d\Gamma}{dt} \quad (19)$$

Provided  $V$  is time independent, the L.H.S. is a function of position only and the R.H.S. is a function of time only. Thus each side must independently equal to some constant, say  $C$ .

$$C = -j\frac{\hbar}{\Gamma} \frac{d\Gamma}{dt}$$

$$\text{or } \Gamma(t) = \exp(jCt/\hbar)$$

If we compare this with (11), then the time dependent constant  $C$  must be  $-E$ , i.e.

$$\Gamma(t) = \exp(-jEt/\hbar)$$

Substitute this into (18) gives,

$$\psi = \Psi(x) \exp(-jEt/\hbar)$$

The L.H.S. of (19) is equal to  $-E$ , so substitution and rearranging gives,

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

This is the one dimensional time independent Schrödinger equation. It can be used to find the space-dependent part of the wavefunction, e.g. for bound particles.

## What is the wavefunction $\psi$ ?

What property of the particle is behaving like a wave?

For radio waves it is the oscillation of the electric and magnetic field vectors.

For sound waves it is varying pressure.

$\psi(x,y,z,t)$  is a function of position and time so we may expect that it represents the position of a particle at some time  $t$ . However we know from Heisenberg that it is impossible to locate a particle without there being some uncertainty in position and momentum.



# Quantum Description of Semiconductors

We can only consider the probability of the particle being at a particular point in space at a time  $t$ .

Another complication is that since  $\psi$  is a solution to Schrödinger's equation, it is usually a complex quantity.

Max Born overcame this problem in 1928 by showing that  $|\psi|^2$ , the square of the absolute magnitude, is proportional to the probability of a particle being in a unit volume of space, centred at the point where  $\psi$  is evaluated, at time  $t$ .

Although the *exact* position of the particle cannot be predicted, it is possible to find its most *probable* location.  $|\psi|^2 \Delta V$  is therefore *proportional* to the *probability* that a particle will be found in a volume element  $\Delta V$ . (V is volume here – not voltage)

$$|\psi(x,y,z,t)|^2 dx dy dz = \psi \psi^* dx dy dz$$

where  $\psi^*$  is the complex conjugate of the wavefunction.

If we solve Schrödinger's equation and obtain a wavefunction  $\psi$ , the probability density,  $|\psi|^2$ , can be used to predict accurately what the spatial distribution of particles will be at some time,  $t$ .

$$\iiint_{-\infty}^{+\infty} \psi \psi^* dx dy dz = 1$$

Such a wavefunction is said to be normalised. When this happens,  $|\psi|^2 \Delta V$  is now *equal* to the *probability* that a particle will be found in a volume element  $\Delta V$ .

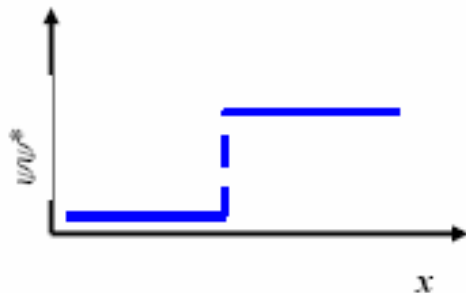
## Boundary conditions:

Before solving Schrödinger's equation, we need to know the boundary conditions to set on  $\psi$ . First,  $\psi$  must be continuous and a single-valued function of position. If not,  $\psi \psi^*$  would also be discontinuous. By similar reasoning the derivatives of  $\psi$ ,  $\partial \psi / \partial x$ ,  $\partial \psi / \partial y$  and  $\partial \psi / \partial z$  must be continuous and single-valued across any boundary.

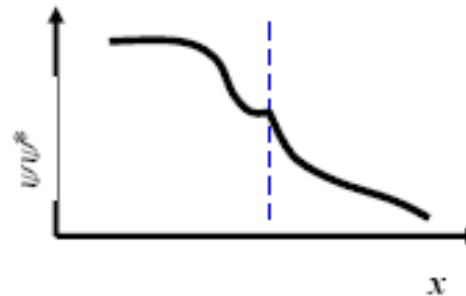


# Quantum Description of Semiconductors

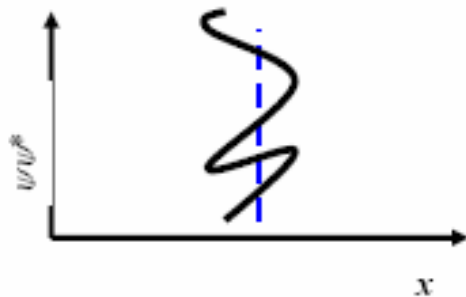
Some examples:



The probability,  $\psi\psi^*$ , is different, depending on whether we approach from the left or right – not physical to have a discontinuity in probability.



The gradient of the probability,  $\psi\psi^*$ , cannot be discontinuous – not physical.



The probability,  $\psi\psi^*$ , is multi-valued at a particular position – again not physical.



The  
University  
Of  
Sheffield.

# End of Lectures

- Summary

# Equations

## Basics

$$\begin{aligned} \text{Current density } (J) &= \frac{I}{A} & \text{Fermi-dirac } P(E) &= \frac{1}{1 + e^{\frac{E-E_f}{kT}}} & \text{Charge conservation } n + N_a &= p + N_d \\ J &= eE(n\mu_e + p\mu_h) = \sigma E & & & & \\ \text{conductivity } (\sigma) &= e(n\mu_e + p\mu_h) & & & \text{Intrinsic rule } np &= ni^2 \end{aligned}$$

## Diode

$$\text{Diode\_equation\_} J = J_o \left[ \exp\left(\frac{eV}{kT}\right) - 1 \right]$$

## MOS transistor

$$g_m = \frac{dI_d}{dV_{gs}} = \frac{C_G \mu_e V_{ds}}{l^2}$$

## Light emission

$$\begin{aligned} E_g &= \frac{hc}{\lambda} & \lambda &= \frac{c}{f} \\ \Delta\lambda &= \frac{c}{f^2} \Delta f \end{aligned}$$

$$C_g = \frac{\epsilon_r \epsilon_o l w}{t_{ox}}$$

$$\text{Internal\_Quantum.Eff } (\eta_{int}) = \frac{\text{number.of.photons}}{\text{number.of.injected.e-h.pairs}}$$

$$\begin{aligned} \text{Av.no.e-h.pairs} &= \frac{P}{\hbar\omega} x \eta & I_{photon} &= \frac{\eta e P}{\hbar\omega} \end{aligned}$$

## Q.Mechanics

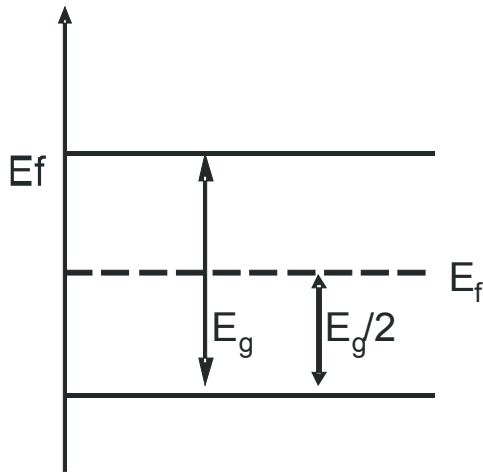
$$E_n = \frac{n^2 h^2}{8mL^2} \quad n = 1, 2, 3, \dots$$

$$\psi(x) = Ae^{jkx} = A_S \sin(kx) + A_C \cos(kx)$$

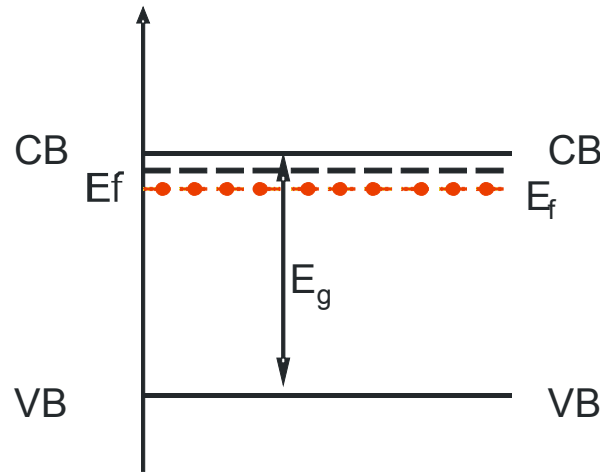




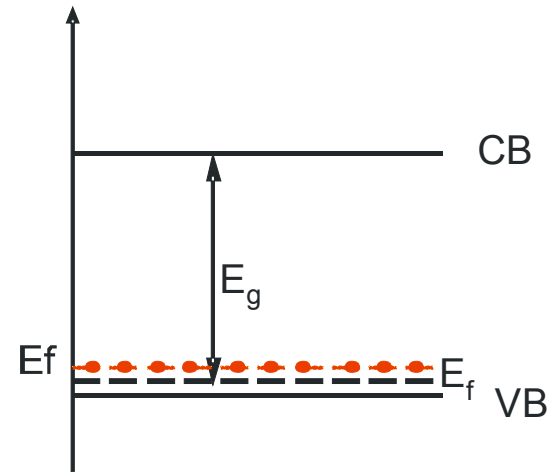
# Diagrams



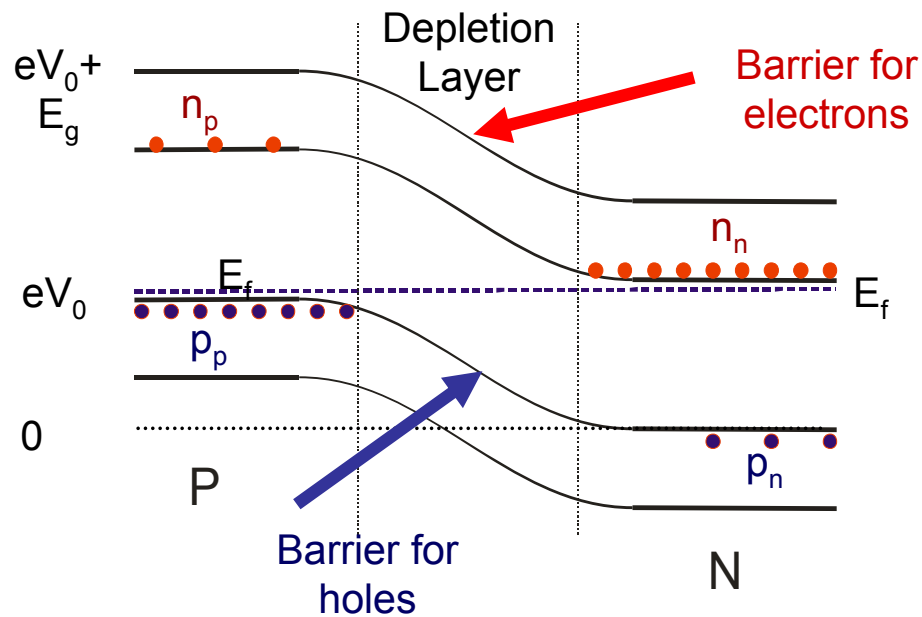
Intrinsic



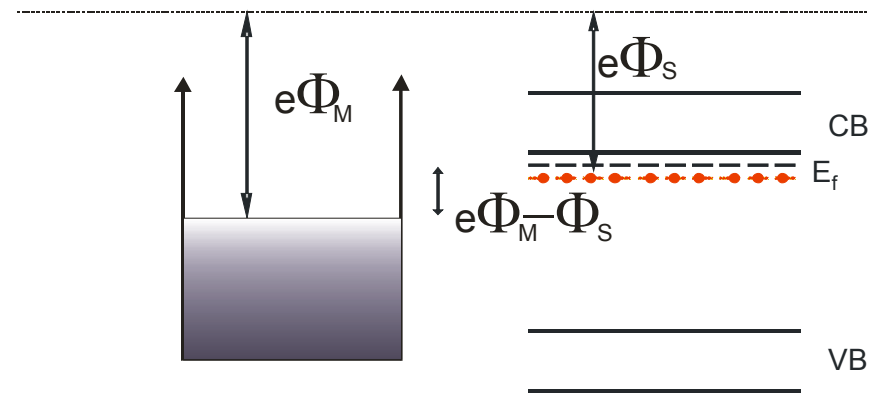
n-type



p-type



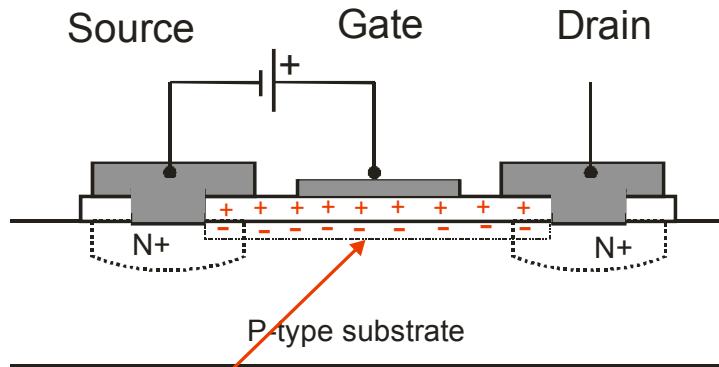
p-diode in equilibrium



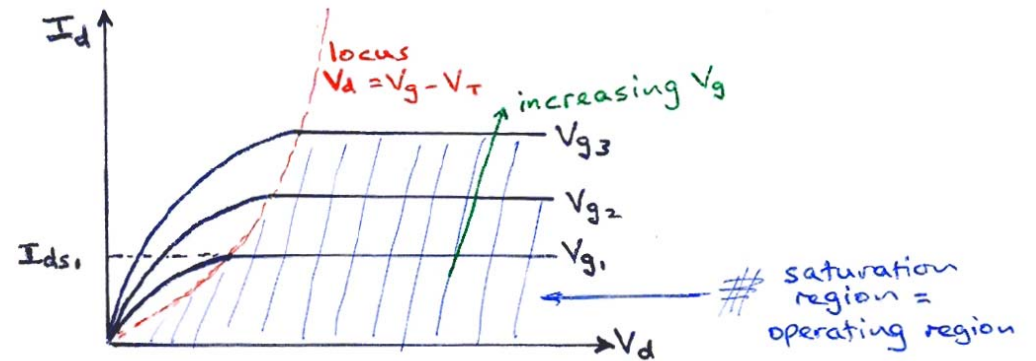
metal-semiconductor junctions



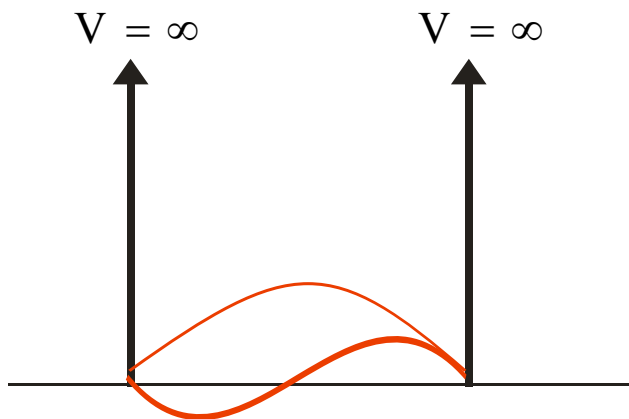
# Diagrams



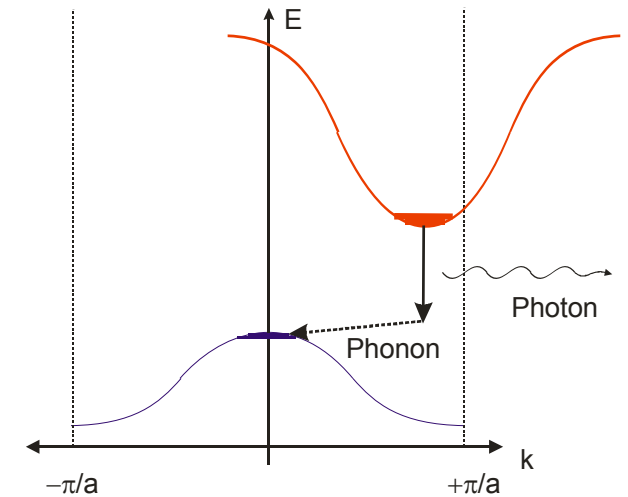
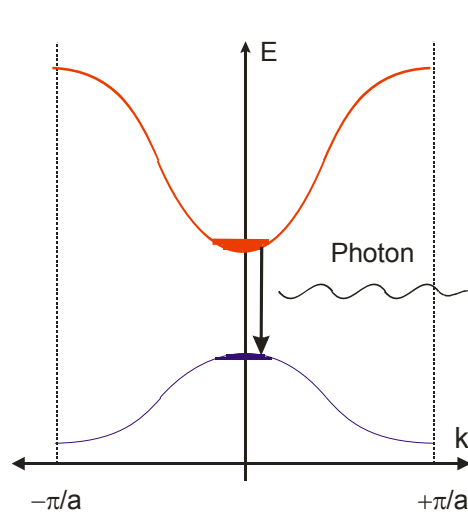
A negative conducting channel  
is formed under the gate



## MOS Transistor



QW wavefunctions



Difference between direct and indirect band gaps



## Exam Tips

- 1) Follow instructions on cover sheet
- 2) Read questions carefully. Decide which ones to do.
- 3) Check how many answers there should be in each section:  
e.g...calculate the minority and majority carrier concentrations at  $T=300\text{K}$ . Then later it might say “what happens to these if  $T=77\text{K}$ ?”
- 4) Give step by step working even if you think you can't get the correct answer– significant marks given for this
- 5) Spend 30min. **max.** on each question at 1st pass. Most questions can be done in ~20 min. Don't run out of time.
- 6) Questions are in several parts and get harder in the later parts. Try to answer all your 1st parts of every question and don't waste time struggling with part 4.