

Solutions to paper 4B5 – Nanotechnology, 2010/2011

1.

(a) Nanotechnology is the ability to both fabricate and characterise structures with characteristic dimensions in the range 1-100 nm.

The answer should include a discussion along the following lines:

- Tunnelling – when device dimensions are small enough (a few nm), electrons can tunnel from one part of a device to another. This is useful in single-electron devices, and a limiting factor in the reduction in size of conventional transistors, particularly in the case of the gate oxide. The answer may also mention field emission. Tunneling is one of the mechanisms for electron transport in molecules and is therefore relevant for an understanding of molecular electronics.
- Hot electron and resonant tunnelling devices that are complementing transistors are becoming widespread. Hot electrons are electrons that have excess kinetic energy after passing from a region of higher to lower potential (band-gap), and therefore travel faster than the drift velocity. Devices (eg HEMT) can be made that make use of this effect, and offer high speed operation. Resonant tunnelling is useful for the property of negative differential resistance.

(b) Briefly:

The first figure shows the packet as it approaches the barrier, no interaction yet.

The second figure shows that the packet has started to interact with the barrier, and we start to see interference between the incident and reflected waves.

The third figure shows that the packet has started to interact further with the barrier, and there is significant interference between the incident and reflected waves. The packet has also reached the opposite side of the barrier, and there is a small amplitude, transmitted packet.

In the last figure, we can see that there are two distinct wave-packets, the reflected one and the transmitted one.

The reason for the small, transmitted portion of the wave-packet is twofold: (i) there is tunnelling through the barrier and (ii) some components of the wave-packet will have energy greater than  $V$ , so will be transmitted. (ii) is expected to be the dominant influence.

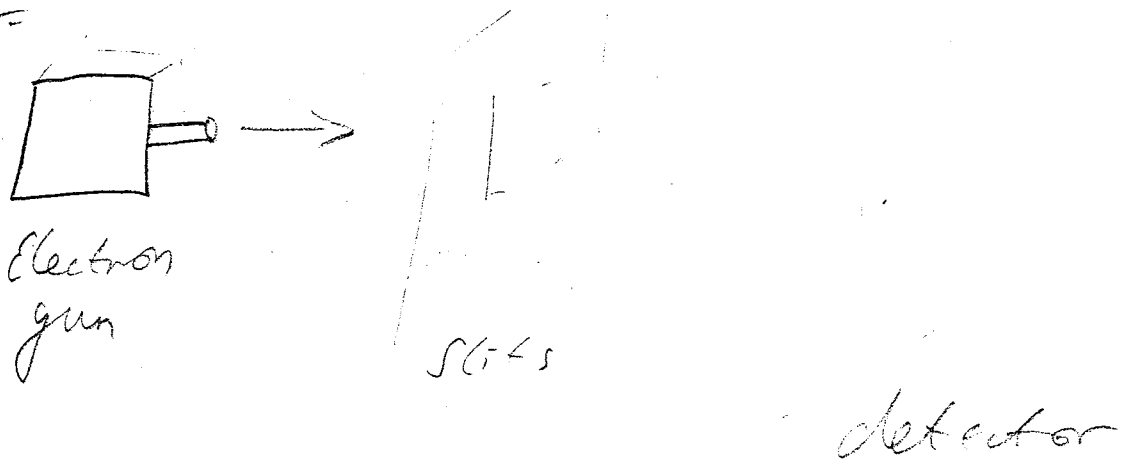
For the case of a plane wave, i.e. a beam of electrons, we would expect a lower transmission as there will not be any components with energy greater than  $V$ .

Should mention somewhere that the transmission probability,  $T$  is a probability, so if we have a single particle, or a wave-packet, the splitting into reflected and transmitted waves does not mean the particle is split, it just represents the probability of transmission. For a beam of particles,  $T$  represents the proportion of particles expected to pass the barrier.

### Examiner's comment:

Question 1: This question was a discussion question about the relevance of quantum mechanics to nanotechnology and involved an analysis of the interaction of a wavepacket with a barrier.

2.



The detector shows a periodic interference pattern. The distribution of electrons at it display clear interference. One would expect to see two bands of electrons one for each slit, in line with particle behaviour. Instead, the interference pattern demonstrates a wave-like nature of the electrons. Even in the case of anyone electron in the apparatus at a time, the pattern is found. This can only be explained using the concept of "sum over all possible paths" or superposition of all trajectories. This has been verified experimentally, and if one attempts to determine which slit the electron actually passes through, that causes collapse of the wave-function, rendering all other trajectories impossible, and the interference pattern disappears.

Consequence: electrons behave like waves. We don't

Often see this, as it is only noticeable when the electrons are confined in a structure of dimensions comparable to the electron wavelength. This is relevant to  $EE$  particularly as transistors are approaching these dimensions.

(6) Dust particle,  $m = 10^{-14} \text{ kg}$ ,  $v = 10 \text{ nm.s}^{-1}$

$$(i) \text{ K.E.} = \frac{1}{2}mv^2 = \frac{h^2/k^2}{2m} = \frac{h^2}{2m\lambda^2}$$

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

$$\Rightarrow p = 10^{-17} \text{ kg} \times 10^{-8} \text{ m.s}^{-1} = 10^{-25} \text{ kg.m.s}^{-1}$$

$$\lambda = \frac{h}{p} = \frac{6.6 \times 10^{-34}}{10^{-25}} = 6.6 \times 10^{-9} \text{ m} = 6.6 \text{ nm}$$

Dust particle  $\sim$  few  $\mu\text{m}$  across, so prob. not.

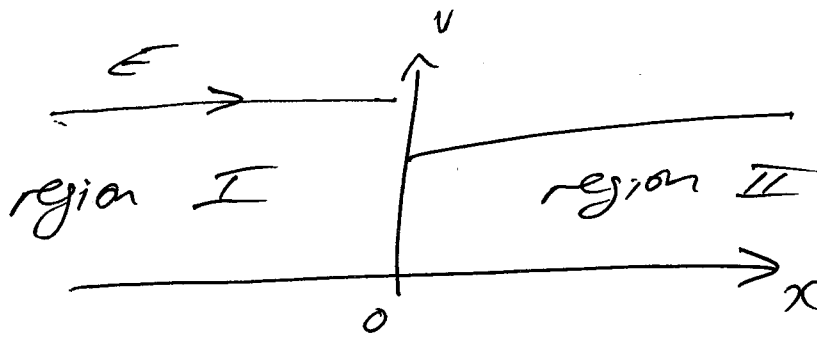
(ii)  $\text{H}_2$  moving @  $10 \text{ m.s}^{-1}$

$$m = \frac{\text{molar mass}}{\text{Avogadro's constant}} = \frac{29}{6.02 \times 10^{23}} = \frac{2 \times 10^{-2}}{6 \times 10^{23}}$$

$$\Rightarrow \lambda = \frac{6.6 \times 10^{-34}}{0.3 \times 10^{-26}} = 22 \times 10^{-8} = 220 \text{ nm}$$

Definitely need QM.

(c)



In region I: 
$$-\frac{\hbar^2}{2m} \frac{d^2 \Psi_I(x)}{dx^2} = (E - V) \Psi_I(x)$$

Region II 
$$-\frac{\hbar^2}{2m} \frac{d^2 \Psi_{II}(x)}{dx^2} + V \Psi_{II}(x) = (E - V) \Psi_{II}(x)$$

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

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

Transmission Coefficient = 
$$\frac{\text{prob. flux in II}}{\text{incident prob. flux}}$$

$$= \frac{|A_2|^2}{|A_1|^2} \times \frac{\hbar k_2 / m_2^*}{\hbar k_1 / m_1^*} = \frac{|A_2|^2}{|A_1|^2} \times \frac{k_2 m_1^*}{k_1 m_2^*}$$

$$m_2^* = 0.5 m_1^*$$

$$\Rightarrow T = \frac{|A_2|^2}{|A_1|^2} \times \frac{2k_2}{k_1}$$

# Boundary Conditions (Ben Daniel - Duke)

$$(i) \text{ @ } x=0, \quad \Psi_1(0) = \Psi_2(0)$$

$$(ii) \text{ @ } x=0, \quad \frac{1}{m_1^*} \frac{\partial \Psi_1(0)}{\partial x} = \frac{1}{m_2^*} \frac{\partial \Psi_2(0)}{\partial x}$$

$$(i) \Rightarrow A_1 + B_1 = A_2 \quad \dots (i)'$$

$$(ii) \Rightarrow \frac{ik_1 A_1 - ik_1 B_1}{m_1^*} = \frac{ik_2 A_2}{m_2^*}$$

$$\Rightarrow k_1 A_1 - k_1 B_1 = k_2 A_2 \frac{m_1^*}{m_2^*} = 2k_2 A_2 \quad \dots (ii)'$$

$$\times (i)' \text{ by } k_1 \Rightarrow \begin{aligned} A_1 k_1 + B_1 k_1 &= A_2 k_1 \\ k_1 A_1 - k_1 B_1 &= 2k_2 A_2 \end{aligned}$$

$$\Rightarrow 2k_1 A_1 = A_2 (k_1 + 2k_2)$$

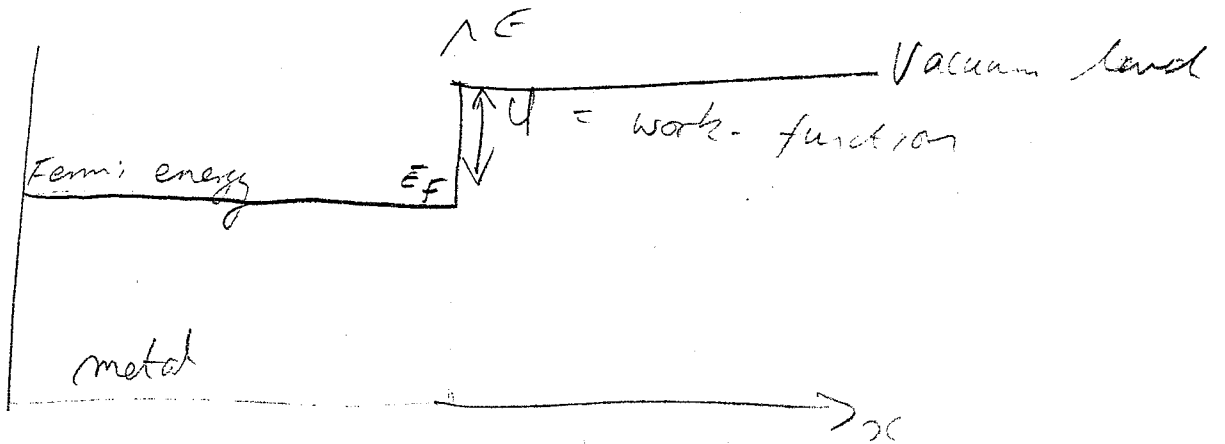
$$\therefore \frac{A_2}{A_1} = \frac{2k_1}{k_1 + 2k_2}$$

$$\Rightarrow T = \frac{4k_1^2}{(k_1 + 2k_2)^2} \times \frac{2k_2}{k_1} = \frac{8k_1 k_2}{(k_1 + 2k_2)^2} = 0.9898 \approx 0.99$$

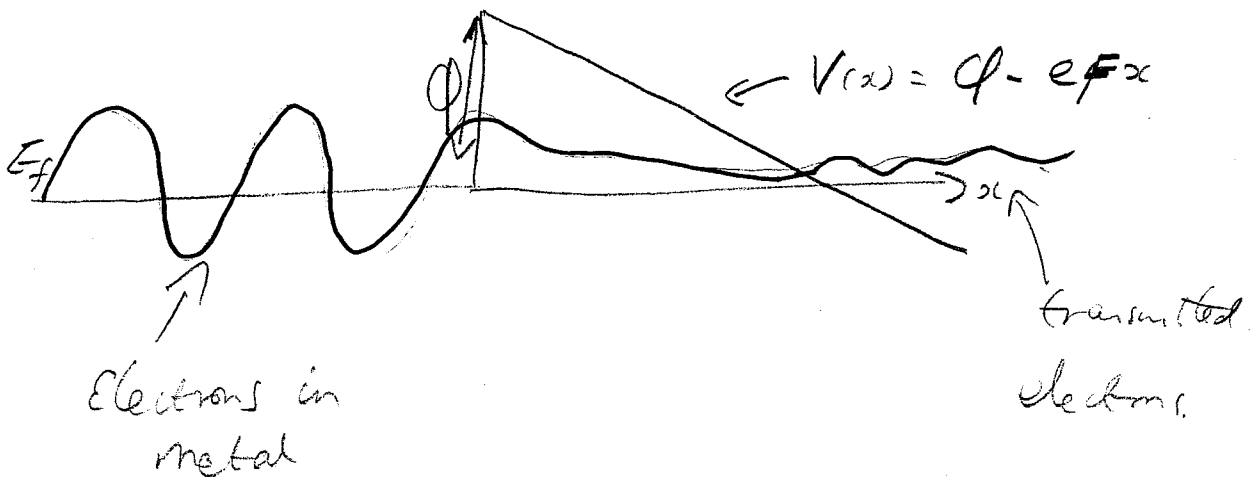
If have same electron, have wave-packet, T will be higher.

3. (a)

Field emission: Whereby electrons can be extracted from a metal by applying an electric field.



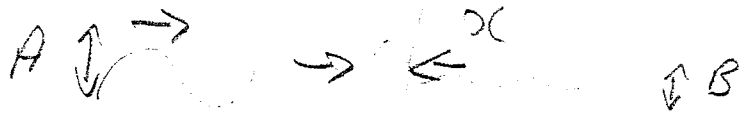
now apply a voltage, or electric field,  $E$



as  $E \uparrow$ , the tunneling barrier gets narrower and  $T \uparrow$ , with an exponential relationship.

⑤ WKB:

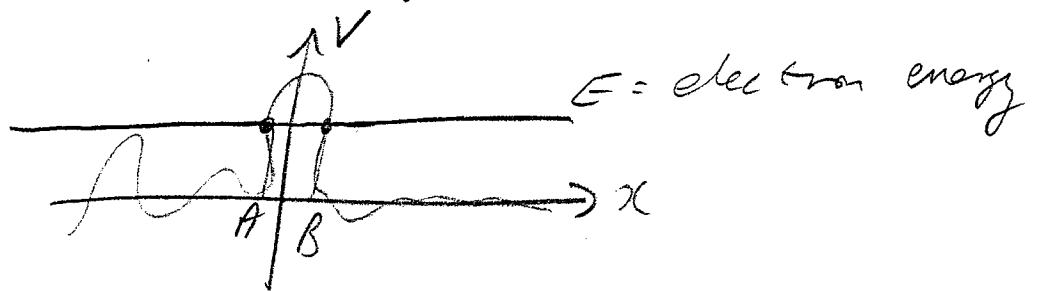
basic idea: wave-vector,  $k$



$$B \sim A e^{-kx}$$

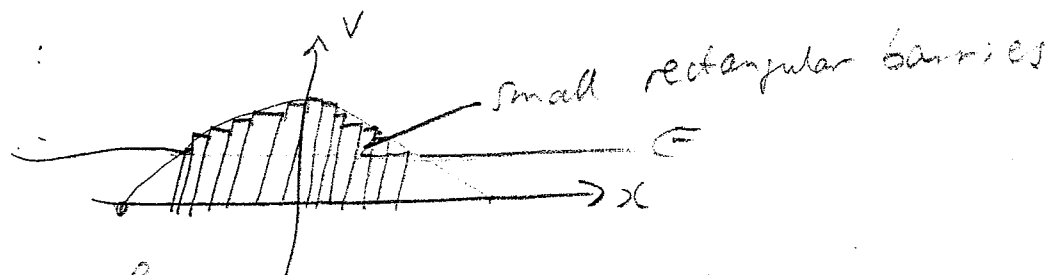
i.e.  $T \sim e^{-2kx}$ , as long as  $x$  is small, and the barrier is high.

Now for an arbitrary profile;



Between  $x=A$  &  $x=B$ , tunneling. These are the classical turning points, as here  $E=V$ .

zoom-in:



$$\text{total } T = e^{-\int_A^B 2k(x) dx}$$

$$k = \frac{\sqrt{2m(V-E)}}{\hbar}$$

$$\Rightarrow T = e^{-\frac{2}{\hbar} \int_A^B \sqrt{2m(V-E)} dx}$$



~~For field emission~~

$$T = e^{-\frac{2}{\hbar} \int_A^B \sqrt{2m(V-E)} dx}$$

(1) For field emission,  $V-E = \phi - eFx$

$$\text{i.e. } T = e^{-\frac{2}{\hbar} \int_A^B \sqrt{2m(\phi - eFx)} dx}$$

$$= e^{-\frac{2}{\hbar} \sqrt{2m\phi} \int \sqrt{1 - \frac{eFx}{\phi}} dx}$$

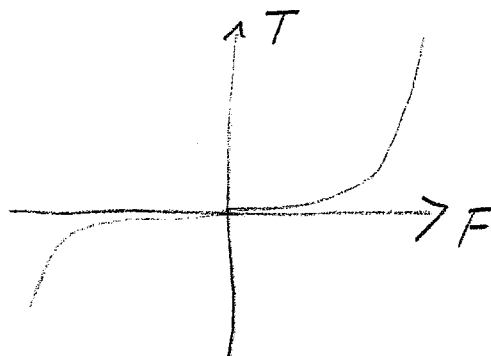
make the substitution  $eFx/\phi = \sin^2 \theta$

$$\Rightarrow dx = \frac{2\phi \sin \theta \cos \theta d\theta}{eF}$$

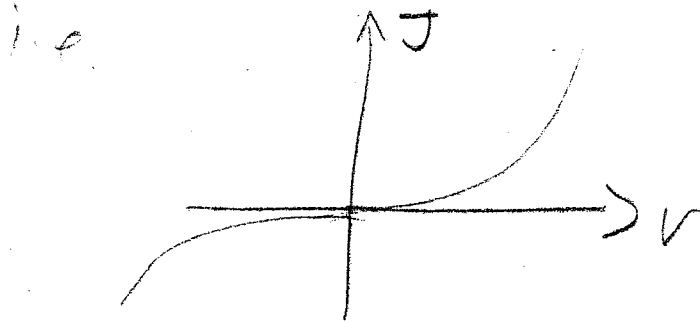
$$\Rightarrow T = e^{-\frac{4}{eF\hbar} \sqrt{2m\phi^3} \int \sin \theta \cos^2 \theta d\theta}$$

let  $\cos \theta = u \Rightarrow -\sin \theta d\theta = du$

$$\therefore T = e^{-\frac{4}{3F\hbar e} \sqrt{2m\phi^3}}$$



now:  $J$  (current density) =  $\int_{eV}^{\infty} T(V) dE$



Experimentally has been shown to be accurate, despite being 1-D.

(d) Used in displays as individual electron sources for each pixel.

4.

If a conventional p-n junction diode is doped heavily enough ( $\sim 10^{25}$  dopants  $m^{-3}$ ), it is possible to cause the Fermi levels in the n and p-type materials to be in the conduction and valence bands, respectively, as shown in the Figure below. Also, the effect of very high doping levels is to make the depletion region extremely thin, in the nm range, so appreciable tunnelling can occur.

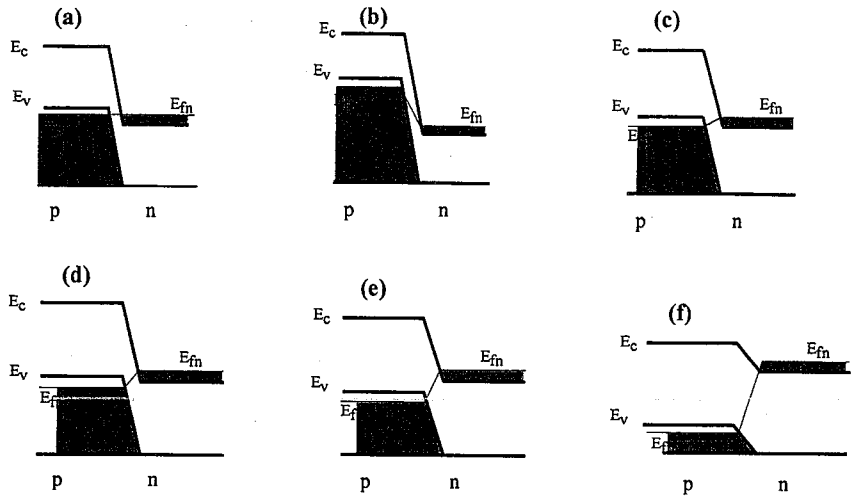
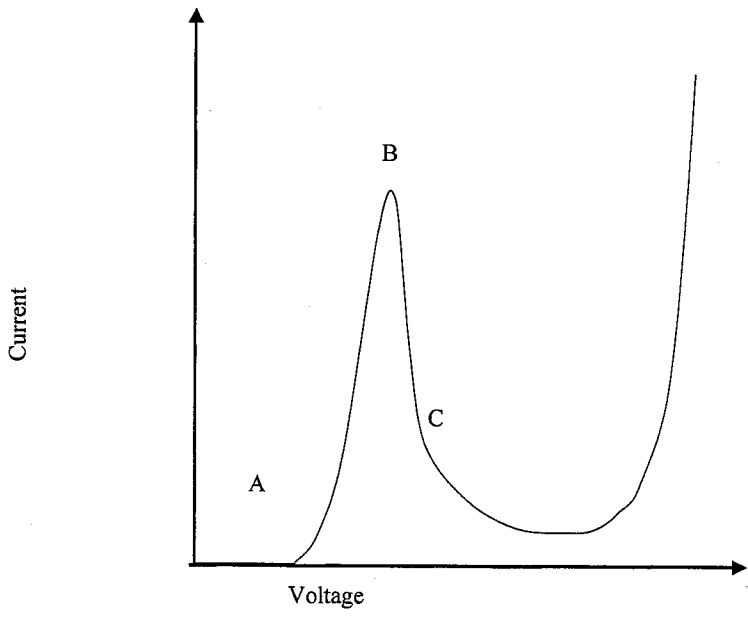


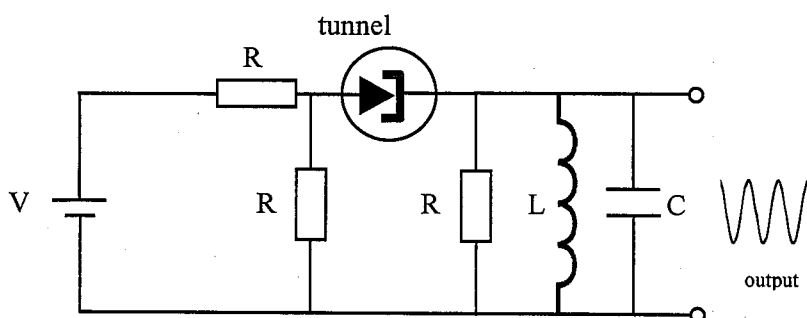
Fig. 2.37. Band diagram of tunnel diode.

(b)



In (a), i.e. under zero applied bias: there is no net current flow, as the electron current from the conduction band of the n-type into the valence band of the p-type is balanced by the electron current from the valence band of the p-type in to the conduction band of the n-type. In Fig. (b), under reverse bias conditions, the bands on the p-type side are raised relative to the n-type side, and electrons can flow from p to n, tunnelling across the depletion region. The width of this region will increase as the voltage is increased, so little current will actually flow. In Fig. (c), which is under a low forward bias, the electron-filled states in the n-type conduction band overlap with the holes in the p-type valence band and a significant current can tunnel across the depletion region, similar to Regime B in Fig. (b). In Fig. (d), as the forward bias is increased, the degree of overlap between the n-type conduction band electrons and the p-type valence band holes decreases, as more of them start to overlap with the band gap within the p-type. This has the effect of reducing the current across the depletion region as there are fewer states for the n-type electrons to tunnel into. In Fig. (e), similar to Regime (c) in Fig. (b), the current drops to its minimum value, as there is no longer any overlap between the conduction band electrons in the n-type and holes in the p-type: there are no available states for the electrons to tunnel into. The only current which can flow at this point is a small inelastic tunnel current and a small thermal diffusion current. In Fig. (f), when the applied forward bias is large enough, the height of the potential barrier between the n and p-type is low enough for a thermal diffusion current to flow over the barrier, and this becomes the dominant means of current flow.

(c) Resonant tunnelling diodes are made by heavily doping a p-n junction. They initially gained a lot in interest for their potential application in oscillator circuits, particularly ones operating at high (Microwave) frequencies. The reason for this can be seen by considering the simplest possible oscillator: an LC circuit (i.e. an inductor in parallel with a capacitor). Due to the phase difference of 180 degrees between the voltage dropped across each of these, energy is effectively continually transferred from one component to the other — the circuit is an oscillator. Once the oscillations begin, if we remove the voltage driving source, the oscillations would continue indefinitely in the absence of any resistance within the circuit. However, all circuits have some resistance, so real oscillator circuits have a finite Q-factor. In principle, if we could add a negative resistance into the circuit to counteract the stray resistance of the components, we could greatly increase the circuit's Q-factor. This is done by adding a resonant tunnelling diode into the LC circuit, and ensuring that it is operating in the middle of its NDR region. This is illustrated in the Figure below. In recent years, the tunnel diode has been replaced by digital components which are more reliable and which have significantly better performance.



Typical circuit utilising a tunnel diode. The voltage source  $V$  is used to set the diode operating in the NDR region (between A and B), and to start the oscillation. It also provides the energy to sustain the oscillation of the circuit.

5. Moore's law states that the number of transistors in a microprocessor is doubling every 16-18 months.

(a) Answer should include a discussion of several of the following topics:

- Better control of fabrication techniques and materials
- Vacuum devices to solid-state
- Increase in electron/hole mobility
- Reduction in size of transistors
- Band engineering, and novel device structures

The desire to have smaller transistors has two reasons: (i) smaller means faster, as electrons have shorter distances to travel, and there is less scattering, and (ii) smaller means higher density, so high performance devices can be made portable.

(b) **Quantum effect:** Tunnelling. Explain what tunnelling is. There is a finite probability that a particle of energy  $E$  striking a barrier of height  $V$  where  $V > E$ , will get through! This is non-classical behaviour. Classically, we expect that at the point where  $E = V$ , the particle will have zero kinetic energy, and will reverse its trajectory. Classically, you cannot have a situation where the particle has negative net kinetic energy, so the particle should not be able to penetrate the barrier. This purely quantum effect is called **tunnelling**, and is responsible for a number of effects, such as nuclear  $\alpha$ -decay and field emission.

Description should include some schematic of wave-function decay into "forbidden" regions. Then, tunnelling is a problem in transistors because gate oxides are becoming thinner, and are at the nm level. To continue reducing dimensions will lead to more tunnelling. This can be overcome by the use of high- $k$  dielectrics.

**Classical effect:** Electromigration. This is an effect whereby current flow causes atoms in wires to move to such an extent that the wires eventually fail. This affects all current-carrying wires. This limits the lifetime of interconnects in ICs, and as transistors and hence interconnects shrink, the lifetime will decrease further. This can be overcome by using materials which have low surface diffusion constants, and by coating the wires with a passivation layer.

(c) Reason: transistors cannot continue to shrink and get faster indefinitely, and as they get smaller, the reproducibility in properties will decrease due to the statistical spread in doping levels.

(i) Resonant tunnelling devices use band engineering to produce double-barrier structures a few nm apart, and rely on atomic-level manufacturing precision (MBE). Therefore, they are

(C) Answer should include mention of ~~nanoscale~~ break junctions, thin film devices, electron transport, localization. Should mention need for high reproducibility. Reproducibility is main concern why we don't have devices in common as yet.

5. Moore's law states that the number of transistors in a microprocessor is doubling every 16-18 months.

(a) Answer should include a discussion of several of the following topics:

- Better control of fabrication techniques and materials
- Vacuum devices to solid-state
- Increase in electron/hole mobility
- Reduction in size of transistors
- Band engineering, and novel device structures

The desire to have smaller transistors has two reasons: (i) smaller means faster, as electrons have shorter distances to travel, and there is less scattering, and (ii) smaller means higher density, so high performance devices can be made portable.

(b) **Quantum effect: Tunnelling.** Explain what tunnelling is. There is a finite probability that a particle of energy  $E$  striking a barrier of height  $V$  where  $V > E$ , will get through! This is non-classical behaviour. Classically, we expect that at the point where  $E = V$ , the particle will have zero kinetic energy, and will reverse its trajectory. Classically, you cannot have a situation where the particle has negative net kinetic energy, so the particle should not be able to penetrate the barrier. This purely quantum effect is called *tunnelling*, and is responsible for a number of effects, such as nuclear  $\alpha$ -decay and field emission.

Description should include some schematic of wave-function decay into "forbidden" regions. Then, tunnelling is a problem in transistors because gate oxides are becoming thinner, and are at the nm level. To continue reducing dimensions will lead to more tunnelling. This can be overcome by the use of high- $k$  dielectrics.

**Classical effect: Electromigration.** This is an effect whereby current flow causes atoms in wires to move to such an extent that the wires eventually fail. This affects all current-carrying wires. This limits the lifetime of interconnects in ICs, and as transistors and hence interconnects shrink, the lifetime will decrease further. This can be overcome by using materials which have low surface diffusion constants, and by coating the wires with a passivation layer.

(c) Reason: transistors cannot continue to shrink and get faster indefinitely, and as they get smaller, the reproducibility in properties will decrease due to the statistical spread in doping levels.

(i) Resonant tunnelling devices use band engineering to produce double-barrier structures a few nm apart, and rely on atomic-level manufacturing precision (MBE). Therefore, they are

(C) Answer should include mention of narrow band junction, thin film device, electron transport, localisation. Should mention speed can be less due to tunnelling. Reproducibility is main reason why we don't have devices in common use yet.