

Solutions to paper 4B5 – Nanotechnology

1.

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

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

- The wave-particle duality. i.e. electrons in nm-sized devices can be described by QM, and have wave-functions, and exhibit interference and diffraction. E.g. electron waveguide experiments, tunnelling resonances.
- Tunnelling – when device dimensions are small enough, 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 of conventional transistors.
- Scanning-probe microscopy: essential tools in Nanotechnology. The operation of the STM is only explained by QM, due to tunnelling.
- Hot electron and resonant tunnelling devices which are complementing transistors are becoming widespread.
- Molecular electronics: the behaviour of devices using single molecules is governed by QM.

(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 started to penetrate the barrier region.

In the fourth figure, we see that more of the packet is in the barrier region.

In the fifth figure, we can see that the packet has reached the opposite side of the barrier, and some reflection has taken place there.

In figures 6-8, we see that the packet has become localised in the barrier region, the reflected packet is now distant and no longer interacting with the barrier, and there is evidence of a small amplitude, broad transmitted packet.

In the last figure, we can see that there are three distinct wave-packets, the reflected one, the transmitted one, and one which is localised in the barrier.

We can also see that the packet in the barrier region is bouncing around between the interfaces, and each time it does so, some of it is transmitted – the amplitude of this packet decays with time, as the packet “leaks out”.

By looking at the area under the incident and transmitted waves, we can see that the transmission probability is of the order 10-15%.

2.

(a) The wave-particle duality can be described as the fact that in certain situations, particles exhibit interference and diffraction behaviour, and similarly waves sometimes behave like discrete particles. This was first postulated by Louis de Broglie, who assigned a wavelength to particles, $\lambda = h/mv$, where m is the particle's mass, v is its velocity and h is Planck's constant.

Examples: (i) Photoelectric effect where light impinging on metal surfaces causes ejection of electrons, where (a) the kinetic energy of those electrons scales linearly with the frequency of the light, (b) no electrons are ejected below a threshold frequency and (c) the number of ejected electrons scales linearly with the light intensity. Classically, one would expect that the frequency plays no role, and that the kinetic energy should depend only on the light intensity.

(ii) Electron diffraction. Electrons are diffracted on passing through crystals, and double-slit experiment.

(b) (i) $\lambda = h/mv = (6.6 \times 10^{-34}) / (10^{-16} \text{ kg} \times 10^{-9} \text{ m}) = 6.7 \text{ nm}$.

(ii) $h/mv = (6.6 \times 10^{-34}) / (1500 \text{ kg} \times 160000 / 3600 \text{ m.s}^{-1}) = 9.9 \times 10^{-39} \text{ m}$.

(iii) $h/mv = (6.6 \times 10^{-34}) / ((2 \times 10^{-3} \text{ kg} / 6.02 \times 10^{23}) \times 1 \text{ m.s}^{-1}) = 198 \text{ nm}$.

Therefore, the first and last systems can be described by QM.

(c) Schrödinger's equation can be written in the regions to the left and right of the step as

$$(-\hbar^2/2m\partial^2/\partial x^2) \Psi_I(x) = E\Psi_I(x) \quad \text{Region I}$$

$$(-\hbar^2/2m\partial^2/\partial x^2 + V) \Psi_{II}(x) = E\Psi_{II}(x) \quad \text{Region II}$$

The solutions to these equations are:

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

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

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

$$A_1 + B_1 = A_2$$

$$ik_1A_1 - ik_1B_1 = -k_2A_2$$

$$\text{i.e. } B_1/A_1 = -(k_2+ik_1)/(k_2-ik_1)$$

Reflection probability = $|B_1/A_1|^2 = 1$ identically. If the step were replaced by a 1 nm barrier, then there is a probability that it will actually tunnel through. To see quantitatively, either use the transmission probability,

$$T = \left| \frac{A_3}{A_1} \right|^2 = \frac{1}{1 + \left(\frac{k_1^2 + k_2^2}{2k_1k_2} \right)^2 \sinh^2(k_2a)}$$

Or, more approximately, if we say that the amplitude of the incident wave is 1, then the wave-function in the barrier region is:

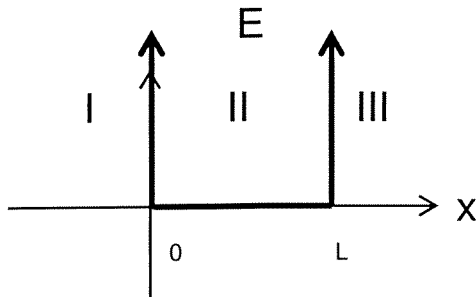
$$\psi = e^{-k_2 x}$$

Therefore, the transmission probability is $e^{-2k_2 a}$, where a is the width of the barrier.

For the situation shown here, this corresponds to $T \sim 0.0001$.

3.

(a)



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:

$$(-\hbar^2/2m\partial^2/\partial x^2)\Psi(x) = E\Psi(x)$$

The simplest solution of this equation is

$$\Psi(x) = Ae^{ikx} + Be^{-ikx} \quad \text{where } k = \frac{\sqrt{2mE}}{\hbar}$$

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 find the value of A, we need to normalise the function, i.e. $\int_{\text{allspace}} \Psi^* \Psi d^3r = 1$

$$\Rightarrow \int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

This gives us a value for $A = (2/L)^{1/2}$

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

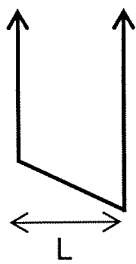
$$E = \hbar^2n^2/(8mL^2)$$

This spectrum of allowed energy levels is discrete – a common feature of quantum systems. The discretisation is due to the fact that the potential imposes certain restrictions on the allowed wave-functions, through the boundary conditions. The wave-function is sinusoidal, and is zero (has nodes) at the boundaries. This can only happen when an integer number of half wavelengths fit into the potential well. Therefore, only certain *modes* are allowed.

(b) Start with Schrödinger's equation:

$$((-\hbar^2/2m)\partial^2/\partial x^2)\Psi(x) = E\Psi(x)$$

(c) Triangular well:



In the well, $V(x) = -Cx/L$

Assuming that the perturbation is weak, we have that the energy correction is:

$$V_{kk} = -\frac{2}{L} \int_0^L Cx/L \sin^2\left(\frac{\kappa\pi x}{L}\right) dx$$

Using that $\sin^2(ax) = \frac{1}{2}(1 - \cos(2ax))$ and integrating by parts, we obtain:

$$\epsilon_1^k = -C/2$$

(d) Application of a voltage parallel to the interface will have no effect, and a voltage perpendicular to the interface will reduce the laser frequency, by shifting the states in the valence and conduction bands closer together.

4.

(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 α -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

extremely difficult to make in bulk quantities, and are not very reproducible. They are however, very fast, and because they exhibit NDR, they are useful as microwave sources.

(ii) hot-electrons are electrons which have excess kinetic energy, which they gain from passing from a region of high potential to a region of low potential. This essentially means a heterojunction, which is easy to fabricate. Unfortunately, these hot electrons lose their excess energy very quickly after scattering, so to utilise them in devices, the gate length must be shorter than the mean-free path. As they are travelling ballistically (at the Fermi velocity which is at least an order of magnitude faster than the drift velocity) devices using hot electrons are extremely fast.

(iii) In molecular electronic devices, the functional elements are molecules, which will be identical, so they should all have the same properties. As molecules are so small, they can conduct electric current extremely quickly. Also, they exhibit a vast range of transport phenomena. Answer should perhaps include a schematic of what such a device might look like.

5.

(a) This simple model assumes we can consider electrons in a solid as behaving like a gas. It is generally assumed that each atom contributes one electron to the gas, and the electrons obey Fermi-Dirac statistics. In the nearly-free electron model, it is assumed that the electrons are in a periodic potential. The general solution of the Schrödinger equation with a periodic potential is $\psi(x) = e^{ikx}u(x)$. This is a plane wave modulated by the function $u(x)$, where $u(x)$ is a periodic function with the periodicity of the lattice, i.e. $u(x)$ represents the influence of the crystal potential. This is known as **Bloch's theorem**, and $u(x)$ as a **Bloch function**.

In the same way as we expanded the potential as a Fourier series, we can now do the same for $u(x)$, to obtain:

$$u(x) = \sum_n C_n e^{iG_n x}$$

where $n = 0, \pm 1, \pm 2, \dots$ and $G_n = 2\pi n/a$

That gives for the total expansion of the wave function:

We now insert the Fourier expansions of both $\psi(x)$ and $u(x)$ into Schrodinger's equation,

$$\psi(x) = \sum_n C_n e^{i(\mathbf{k} + \mathbf{G}_n)x}$$

$$(-\hbar^2/2md^2/dx^2 + V) \Psi(x) = E\Psi(x)$$

We end up with a set of simultaneous equations in the unknown C_n . Note that the V_p are known, as the form of the crystal potential is assumed initially. There are an infinite number of terms, so to make the problem manageable, we artificially truncate the series and consider only the leading-order terms given by $n = 0, \pm 1$. This is justified for weak potentials such as those found in metals.

(b) We write $V(x)$ as:

$$\begin{aligned} V(x) &= V_0 + V_1 e^{iG_1 x} + V_{-1} e^{-iG_1 x} \\ &= V_0 + 2V_1 \cos(G_1 x) \end{aligned}$$

If we continue along the same lines, we can assume that the wave-function also only contains leading-order terms, i.e.

$$\psi(x) = [C_0 + C_1 e^{iG_1 x} + C_{-1} e^{iG_{-1} x}] e^{ikx}$$

$$(-\hbar^2/2md^2/dx^2 + V_0 + V_1 e^{iG_1 x} + V_{-1} e^{iG_{-1} x}) [C_0 + C_1 e^{iG_1 x} + C_{-1} e^{iG_{-1} x}] e^{ikx} =$$

$$E [C_0 + C_1 e^{iG_1 x} + C_{-1} e^{iG_{-1} x}] e^{ikx}$$

If we just consider a region where C_0 and C_{-1} dominate, we are left with the relationships (noting that $G_{-1} = -G_1$ etc.):

$$(-\hbar^2 k^2 C_0 / 2m + V_0 C_0 + C_0 V_1 e^{iG_1 x} + C_0 V_{-1} e^{iG_{-1} x} - \hbar^2 (k + G_{-1})^2 C_{-1} e^{iG_{-1} x} / 2m +$$

$$V_0 C_{-1} e^{iG_{-1} x} + V_1 C_{-1} + V_{-1} C_{-1} e^{2iG_{-1} x}) = E C_0 + E C_{-1} e^{iG_{-1} x}$$

Collecting terms in $e^{iG_{-1} x}$, we find that:

$$C_0 V_{-1} = [\hbar^2 (k + G_{-1})^2 / 2m + E - V_0] C_{-1}$$

Terms without any exponent give:

$$C_{-1} V_1 = [(\hbar^2 k^2 / 2m) + E - V_0] C_0$$

For a non-trivial solution, both ratios for C_{-1}/C_0 must be equal, i.e.

$$C_{-1}/C_0 = [(\hbar^2 k^2 / 2m) + E - V_0] / V_1$$

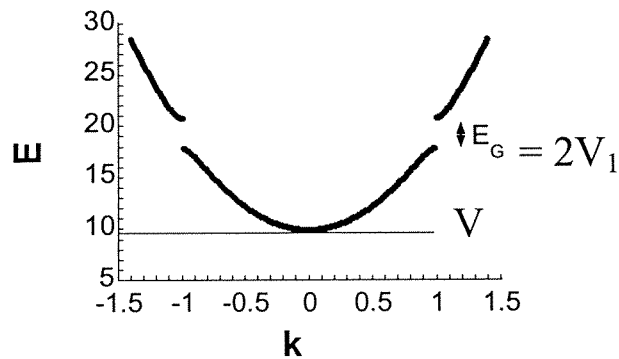
$$= V_{-1} / [\hbar^2 (k + G_{-1})^2 / 2m + E - V_0]$$

$$\text{or, } [E - V_0 + (\hbar^2 k^2 / 2m)] [E - V_0 + \hbar^2 (k + G_{-1})^2 / 2m]$$

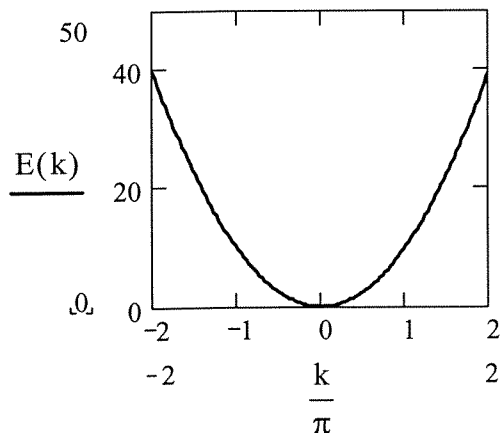
$$= V_1 V_{-1} = |V_1|^2 \quad (\text{Everything is symmetric})$$

(c) Dispersion relation:

(i)



(ii)



(d) Metals etc. In metals, the band gap is very small, and the upper band is half full. That means that there are plenty of available states around the Fermi energy, so electrons can move easily under the influence of an electric field.

Semiconductors have a larger band gap ($\sim 1-2$ eV), and states are filled all the way up to the top of the valence band. Therefore, there are no available states for electrons to go into. However, electrons can be thermally excited up into the conduction band, where they can conduct easily.

Insulators have a large band gap, > 5 eV. In this case, thermal excitation cannot provide enough energy to promote electrons from the valence band to the conduction band, and they are very poor conductors of electricity.