Solutions to paper 4B5 – Nanotechnology. 2004

1.

(a) We should use plane waves when dealing with a beam of particles, i.e. where there is no spatial localisation, and we should use wave packets when we are considering the behaviour of single particles.

(b) EM waves have the following E-k relationship: $E = \hbar ck$, whereas for matter waves: $E = \hbar^2k^2/2m$. As a result, the velocity of EM waves is a constant (speed of light), whereas the velocity of matter waves depends on k [Group velocity = $d\omega/dk$]. Therefore, EM wave packets retain their shape as they propagate through space, unless they are in a dispersice medium, whereas matter waves automatically spread out.

(c) Quantum factors which pose a problem to further miniaturisation of the transistor are **Tunneling** and **Coherence**.

(i) Tunneling is a purely quantum phenomenon whereby a particle of energy E can pass through (tunnel) a classically forbidden region, i.e. it can pass through a potential barrier with an energy greater than E. Tunneling is a problem as the gate oxide gets thinner, because it results in the leakage of signals from the gate, and hence reduces the transistor's gain. At the moment, the thickness of gate oxides is in the range 0.8 nm to a few nm. Further decreases in this dimension will increase tunnelling, and impair the gain of the transistor.

(ii) Coherence. As the electrons travel from the source to the drain in a conventional transistor, they are essentially incoherent as the distance they have to travel is significantly longer than the coherence length, so any quantum scattering is essentially smeared out. However, for 5 eV electrons, the de Broglie wavelength is $\sqrt{(\hbar^2/(2mE))}$, which is 0.55 nm. Thus, we can say that quantum coherence will give rise to interference effects which will alter the behaviour of the transistor once the gate length is comparable to 0.55 nm.

(d) (i) Quantum effects can be reduced by using a high-k dielectric as the gate oxide. This would mean lower gate voltages could be used for the same fields, and therefore there will be a lower probability of tunnelling.

(ii) Coherence effects cannot be overcome, so it makes more sense to try to use them to our advantage, eg in resonant tunnelling devices.

N.B. A number of answers here included a discussion on electromigration. It is true that this phenomenon degrades transistor performance at small length scales, but this has nothing to do with quantum mechanics!

2.

(a) Wave-functions represent the probability distribution of the quantum particles to which they pertain. If we have a particle described by the wave-function $\psi(\mathbf{r}, \mathbf{t})$, then $|\psi(\mathbf{r}, \mathbf{t})|^2$ is the probability of finding the particle at position r at time t. The rules for determining $\psi(\mathbf{r}, \mathbf{t})$ in boundary value problems are that $\psi(\mathbf{r}, \mathbf{t})$ and it's first derivative are continuous at all the boundaries. Physically this means that the wave-functions are single-valued, i.e. there is only one value for the probability of finding the particle at any point in space. Also, the energy of a quantum particle is proportional to $\delta^2\psi/\delta x^2$, so if there were any discontinuities, that would correspond to infinite energy, which is physically impossible.

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

$$(-\hbar^2/2m\partial^2/\partial x^2)\,\Psi_I(x) = E\Psi_I(x) \qquad \textbf{Region I}$$

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

The solutions to these equations are:

$$\Psi_I(x) = A_1e^{ik1x} + B_1e^{-ik1x} \text{ where } k_1 = \frac{\sqrt{2mE}}{\eta}$$

$$\text{and } \Psi_{II}(x) = A_2e^{-ik2x} \text{ where } k_2 = \frac{\sqrt{2m(E-V)}}{\eta}$$

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

$A_1 + B_1 = A_2$

$ik_1A_1 - ik_1B_1 = -ik_2A_2$

i.e. $B_1/A_1 = (k_1 - k_2)/(k_2 + k_1)$

Therefore, the probability of reflection, $R = |(k_1 - k_2)/(k_2 + k_1)|^2 = 0.03$. This means physically that on average, 3% of the beam will be reflected, or if we are looking at single electrons encountering the barrier, then if we observe the passage of many of them, then also on average 3% will be reflected.

(c) Now, we need to split space up into 3 regions, I, II & III, corresponding to the regions before, at and after the barrier, respectively. These three regions have the following wave-functions:

$$\Psi_I(x) = A_1e^{ik1x} + B_1e^{-ik1x} \text{ where } k_1 = \frac{\sqrt{2mE}}{\eta}$$

$$\Psi_{II}(x) = A_2e^{-ik2x} + B_2e^{-ik2x} \text{ where } k_2 = \frac{\sqrt{2m(E-V)}}{\eta}$$

and

$$\Psi_{III}(x) = A_3e^{ik3x} \text{ where } k_3 = k_1$$

We are looking for the reflection probability, which is $|B_1/A_1|^2$. After some algebra, we arrive at the following relationships:

At the left boundary, i.e. $x = 0$:

$$\frac{B_1}{A_1} = \frac{A_2(k_1 - k_2) + B_2(k_1 + k_2)}{A_2(k_1 + k_2) + B_2(k_1 - k_2)}$$

At the right boundary, i.e. $x = L$:

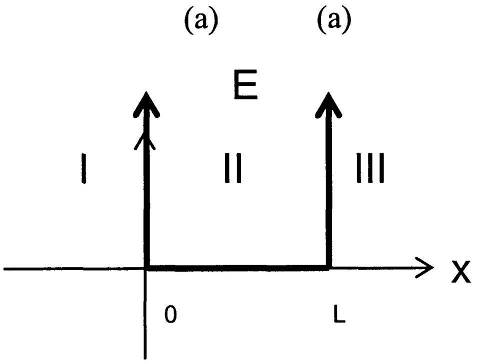
$$A_2 = \frac{A_3e^{ik1L}[k_2 + k_1]e^{-ik2L}}{2k_2} \quad \text{and} \quad B_2 = \frac{A_3e^{ik1L}[k_2 - k_1]e^{ik2L}}{2k_2}$$

This gives us the following: $R = \dfrac{(k_2^{\,2} - k_1^{\,2})Sinh(k_2L)}{2k_1k_2Cosh(k_2L) - (k_1^{\,2} + k_2^{\,2})Sinh(k_2L)}$

For our particular values, $R = 0.095$.

(d) For an incident wave on the barrier of amplitude 1, the approximate amplitude of the wave-function which reaches the right-hand-side of the barrier is $e^{-k_2 a}$, where a is the width of the barrier and $k_2 = \frac{\sqrt{2m(V-E)}}{\eta}$. Therefore, the transmission probability is approximately $e^{-2k_2 a}$. For the situation shown here, this corresponds to $T \sim 0$.

3.



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 it's configuration, i.e can the particle have any energy and sit in any position within the well?

The form of the potential is: **$V = 0$ for $0<x<L$**

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

Schrödinger's equation in region II is:

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

The simplest solution of this equation is

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

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 $\Psi(L) = 0 \Rightarrow A\sin(kL) = 0 \Rightarrow k = n\pi/L$, $n = 1,2\ldots..$

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. $\int_{allspace} \Psi^* \Psi d^3 r = 1$

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

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

Remember, Energy, $E = ½mv^2 = p^2/2m = \hbar^2 k^2/2m$

If $k = n\pi/L$, then the Energy levels of an electron confined in an infinite well are

$\mathbf{E = h^2 n^2/(8mL^2) = 9.5n^2}$ milli-electron volts.

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) Take the time-independent Schrodinger equation :

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

if x -> -x, then

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

Now, if $V(x) = \pm V(-x)$, => $\Psi(x) = \pm \Psi(-x)$.

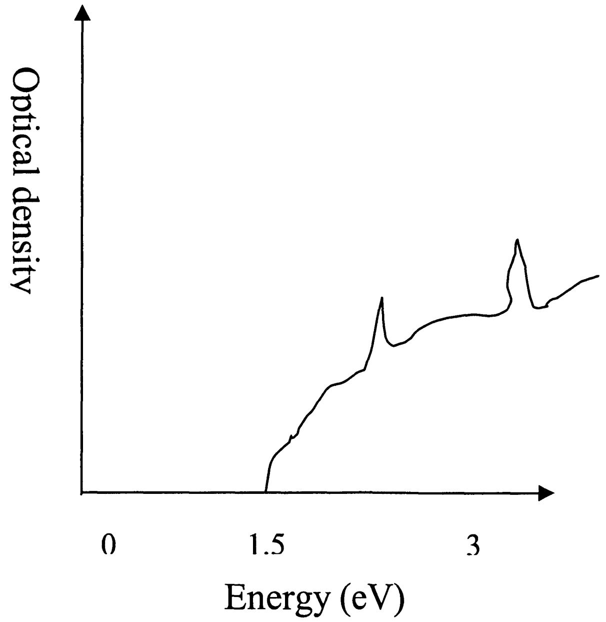
Therefore, a symmetric or antisymmetric potential means a symmetric or antisymmetric wave-function.

(c) Quantum wells are fabricated using band-gap engineering. The technique used to make them is generally MBE. The materials used are semiconductors, as they can be doped to produce specific band profiles.

In infinite wells, wave-functions only exist in the well, there is no probability of locating them outside the well. In finite wells, there is a probability of locating the particle outside. This probability increases as (i) the energy level increases, (ii) the well-width decreases or (iii) the confining potential (the depth of the well) decreases.

A finite well can be approximated as an infinite one if it is not too shallow, i.e. if the depth of the well is larger than the first bound state of the corresponding infinite well of the same width.

(d) The energy levels in the conduction band, using the formula from (a) are $149n^2$ mV in the conduction band (CB), and $249n^2$ mV in the valence band (VB). Therefore, the first transition which is from level 1 in the CB to level 1 in the VB is at an energy of (1.5 + 0.15 + 0. 25) eV = 1.9 eV. The second transition is at an energy of (1.5 + 0.56 + 1) eV = 3.06 eV. Therefore, the optical density looks like:



4

(a) The resolution limit is approximately λ/2. The Rayleigh criterion states that if there are two objects whose images in the image plane have a drop in intensity between them of less than 20%, then they are not resolved. This occurs when objects are closer together than 0.8λ. This limit to resolution is not fundamental but can be overcome by utilising the optical near-field.

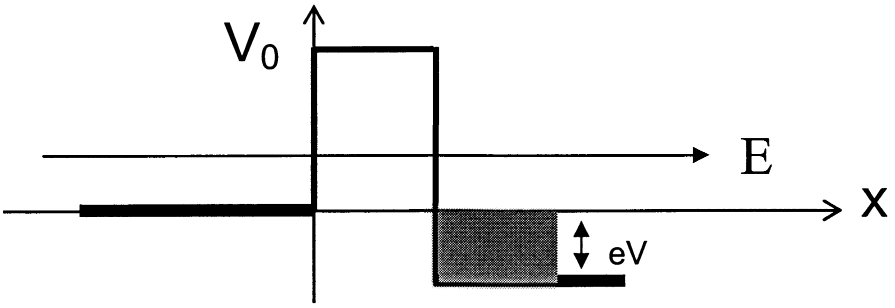
(b) The answer should include a description of tip-surface interactions, lengthscales, dependence of interactions on distance, feedback, distance control & scanning.

(c) The current I, for a voltage V between the tip and surface is, $I \propto \int_{eV}^{0} \rho_s \rho_t T(E,V) dE$

where ρ_s and ρ_t are the electronic density of states of the tip and sample, respectively.

We generally use a tip where the density of states is essentially a constant over the energy range of interest, and also T(E, V) is usually a smooth monotonic slowly varying function of E, then $I \propto \rho_s$. This means that the STM is measuring the density of states of the sample.

(d)



A number of assumptions have been made here:

(i) This is in 1-D

(ii) The top of the barrier is flat, in reality it will be tilted due to the applied voltage, V.

(iii) We have neglected the image potential.

$I \sim e^{-2k_2 x}$

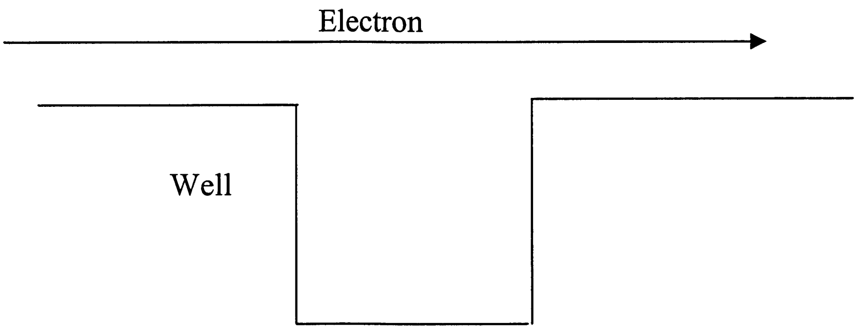
Therefore, I_2/I_1 which is current after/current before = $e^{-2k_2(x2 - x1)}$

= 0.04.

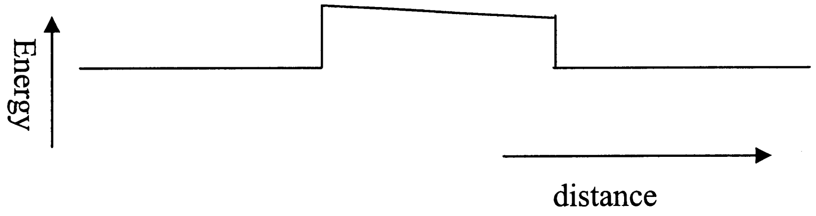
(e) STM is useful for atomic scale imaging, manipulation, magnetism, spectroscopy, etc of conductors and thin insulators.

5.

(a) Potential energy profile:

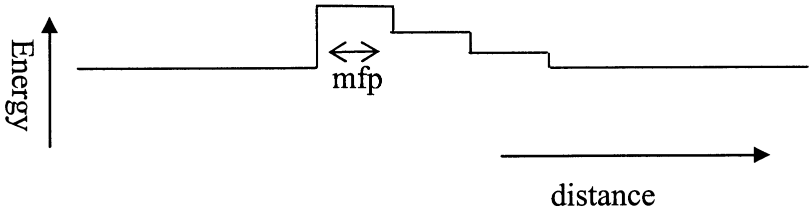


(a) Temp = 0, no defects, very few phonons



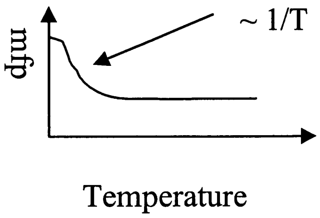
After passing the first interface, the electron is *hot.*

(b) At room temperature with defects, there will be scattering, so the particle will loose energy over distances comparable to the mean-free path (mfp).



For a conductor, the mfp is typically 10s of nm at room temperature.

(c) At room temperature with defects, there will be scattering, so the particle will loose energy over distances comparable to the mean-free path (mfp).

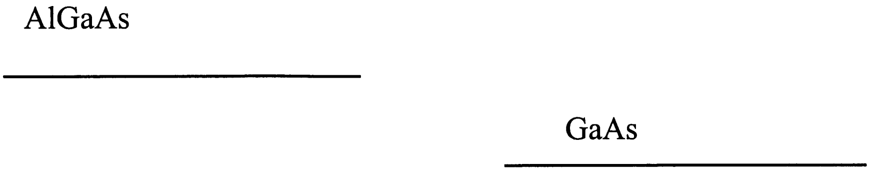


An important point to note here is that the mfp does not approach infinity as T approaches 0 K due to zero-point energy of lattice.

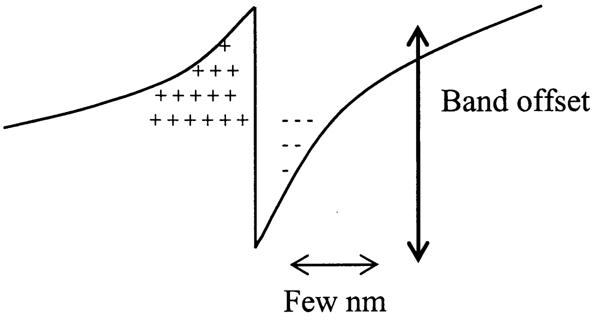
(d) The well width should be comparable to the mfp of the electrons. The well depth should not be too large, or electrons will get trapped.

(e) It can be created in an intrinsic semiconductor, so it is a way of having a large number of charge carriers with high mobility => fast operation. We can create a 2DEG by combining for eg GaAs with GaAlAs.

i.e. Conduction bands before contact:



In contact:



The electrons in the GaAs are in a triangular well, and are confined to a sheet parallel to the surface a few nm thick.

This will be fabricated by MBE, where the layers of semiconductor can be deposited with sub-monolayer precision, giving rise to extremely high quality interfaces. We would incorporate a 2DEG in the gate region of a transistor.