4B5 solutions 2016

1.

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

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

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

The solutions to these equations are:

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

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

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

$A_1 + B_1 = A_2$

$ik_1 A_1 - ik_1 B_1 = -k_2 A_2$

i.e. $B_1/A_1 = -(k_2 + ik_1)/(k_2 - ik_1)$

The reflection probability is $|B_1/A_1|^2$, which in this case equals exactly 1. This represents the probability that a given particle will be reflected from the potential step, so must lie between 0 & 1. R does *not* represent the fraction of a particle which will be reflected. If we pass a large number of electrons over this potential step, then on average, a fraction R of them will be reflected, but any individual electron will either be totally reflected or totally transmitted.

(b)
 Schrodinger's equation is now

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

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

$$(-\hbar^2/2m\partial^2/\partial x^2 + V)\ \Psi_{III}(x) = E\Psi_{III}(x) \qquad \textbf{Region \textit{III}}$$
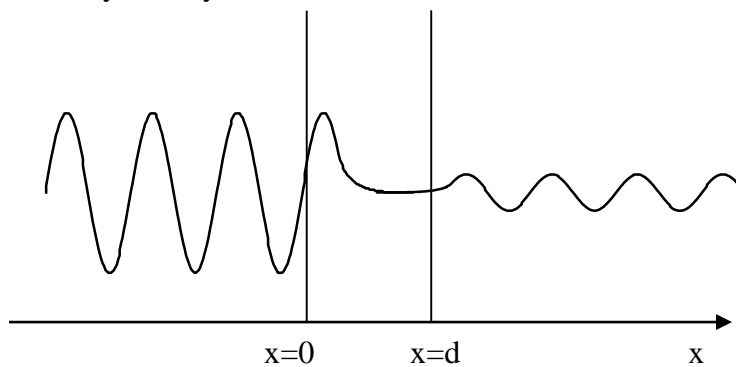
The solutions to these equations are:
$$\Psi_I(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x} \text{ where } k_1 = \frac{\sqrt{2mE}}{\hbar}$$

$\Psi_{II}(x) = A_2 e^{k_2 x} + B_2 e^{-k_2 x}$ where $k_2 = \dfrac{\sqrt{2m(V-E)}}{\hbar}$

And $\Psi_{III}(x) = A_3 e^{ik_1 x}$ where $k_3 = k_1$

Probability density:

If we say that the amplitude of the incident wave is 1, then the wave-function at the right hand edge of the barrier region is approximately: $\Psi_{II}(d) = e^{-k_2 d}$, so the transmission probability, T is roughly $e^{-2k_2 d}$. We are using the assumption that the coefficient $A_2 \sim 0$, as it is always $\ll B_2$.

Given the values of E, and V, we obtain a value for $k_2 = 3.25 \times 10^9$ m^{-1}.

Therefore, $T \sim 1.5 \times 10^{-3}$, which is vanishingly small.

Assumptions: (i) only an exponentially decaying term in barrier, (ii) effective mass of electron in each region is the same
To improve precision, would include full form of ψ_{II}, and would determine transmission probability for entire structure.

(c) This phenomenon is called *tunneling*, and is commonplace. It is used in the STM, happened across gate oxides in FETs, is the mechanism behind field emission and alpha-decay. Answer should include a brief discussion on one of these topics.
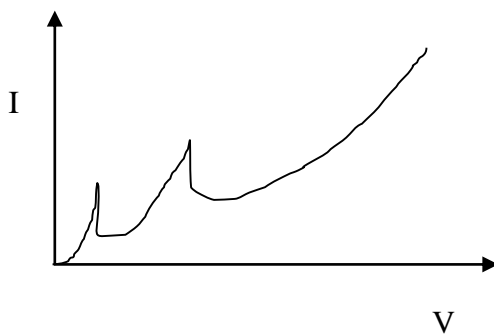
2.

(a) When a voltage is applied, the entire potential profile becomes sloped, and the conduction band edge on the left approaches bound state E_1.
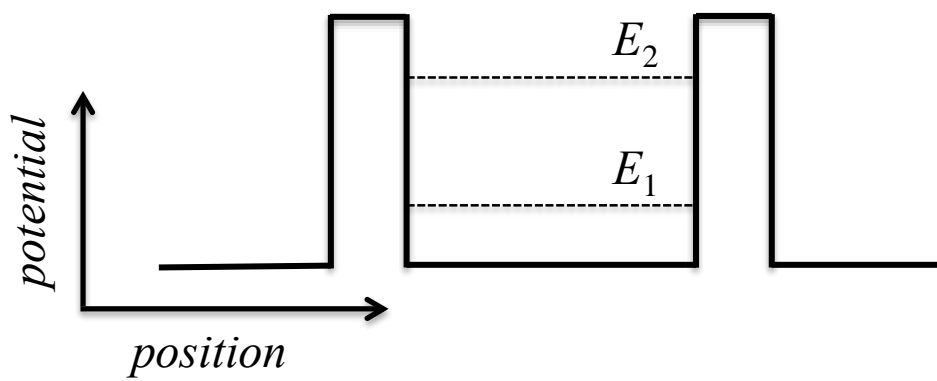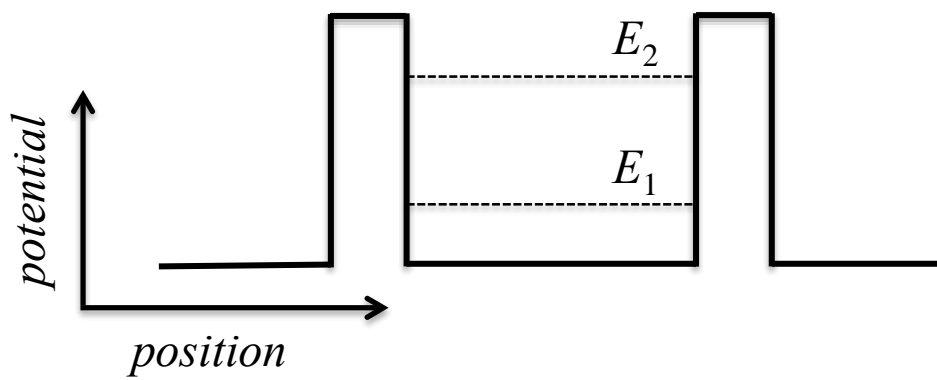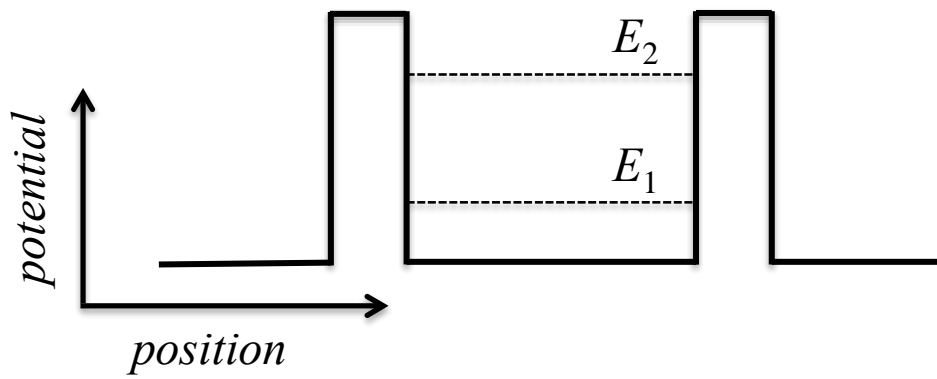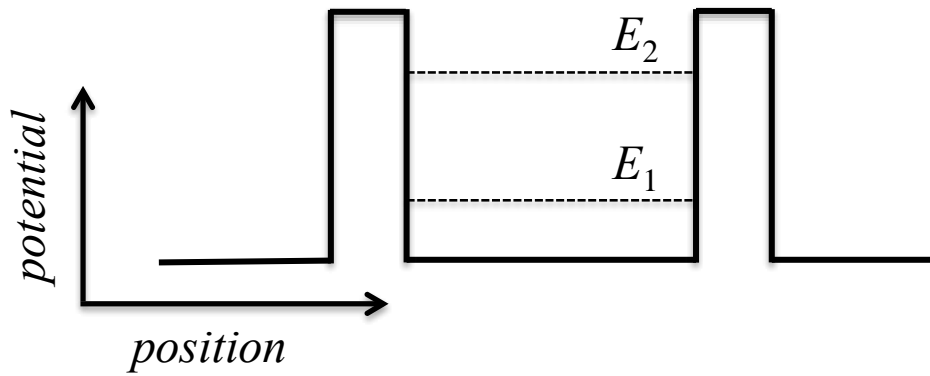

Filled states   Empty states
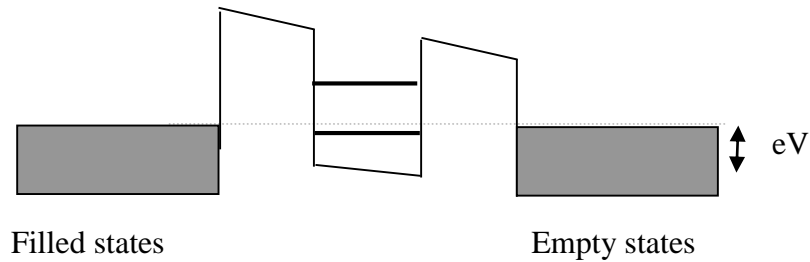
(b) The current, I depends on the transmission probability, T as follows:

As V is increased, the bound state energy E_1 starts below E_f, then when V is large enough they coincide, causing a peak in T. As V is further increased, there is no longer a match between E_1 and E_f, and T starts dropping. As we continue to increase V, E_2 starts to coincide with E_f, and we get another peak in T. further increasing V will cause T to drop again, and eventually Thermal current will start to dominate and the conventional exponential increase in current with applied voltage for a diode will be observed.

(c)

potential

position

E_2

E_1

potential

position

E_2

E_1

potential

position

E_2

E_1

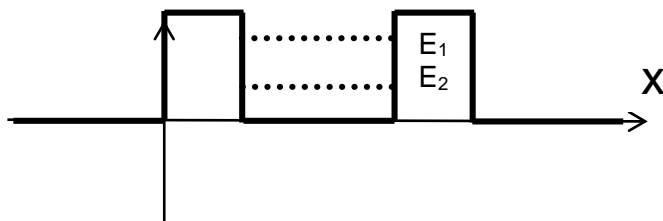*potential* vs *position*, with levels E_2 and E_1 marked.

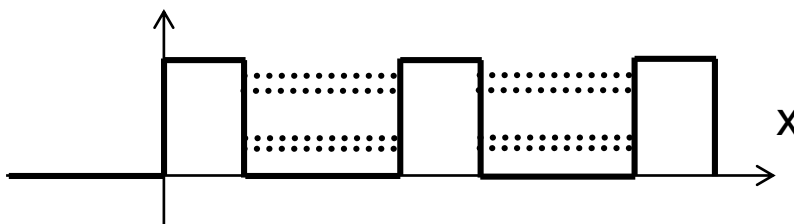(d)   Potential materials could be GaAs and GaAlAs. These can be deposited by MBE and will have typical layer thicknesses of the order 10 nm. GaAlAs has a larger bandgap than GaAs, and can be used for the barrier regions.
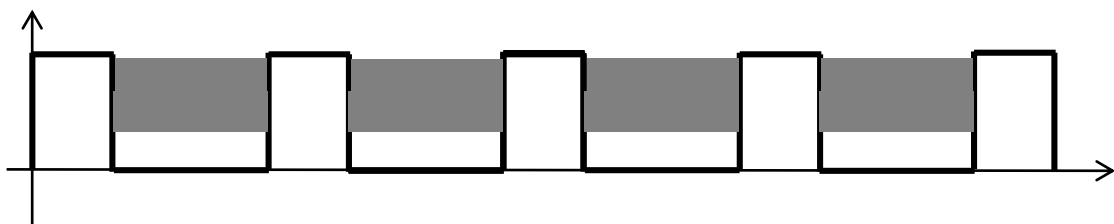
3.

(a)

Levels E_1 and E_2 shown in a well, axis labelled X.

Now add in another well:

Two wells with levels, axis labelled X.

Now for a very large number of wells:

Energy levels become bands.

If the wells are close enough, the tail of the wave-functions within each well can extend appreciably into neighbouring wells. This gives rise to a coupling between the wells, and generates new wave-functions which are combinations of the original ones. For two wells, those combinations are the sum and difference between the original functions. Hence, there will be two states instead of one. For N wells, each state will become N closely spaced states. The closer the wells are to each other, the larger will be the splitting in energy. This is similar to beats in the addition of waves: the closer the frequency, the more pronounced are the beats. As the wells are brought closer, the coupling increases and so therefore does the splitting of the energy levels.
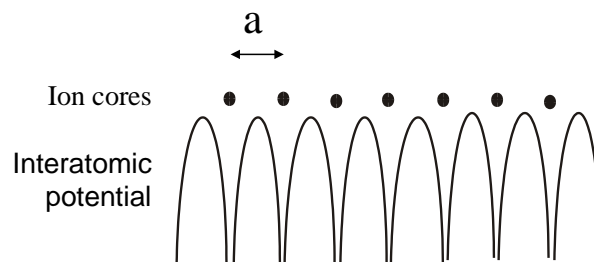
(b)   (i)   Assumptions in the nearly-free electron model:
      The electrons do not interact with each other
The electrons have *discrete* energy values
The electron gas follows Fermi-Dirac statistics

(ii)

a

Ion cores

Interatomic
potential

(iii)

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**.
If we expand the potential as a Fourier series, we can now do the same for $u(x)$, to obtain:

$$u(x) = \sum_{n} C_n e^{i\mathbf{G}_n x}$$

where $n = 0, \pm1, \pm2,\ldots$ and $\mathbf{G}_n = 2\pi n/a$
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,

$$y(x) = \sum_{n} C_n e^{\left(i\left(k+\frac{n\rho}{a}\right)x\right)}$$

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

We end up with a set of simultaneous equations in the unknown C_n. Note that the Vp 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, 1. This is justified for weak potentials such as those found in metals.

$$V(x) = V_0 + V_1 e^{i\pi x/a} + V_1 e^{-i\pi x/a}$$

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

$$\psi(x) = [C_0 + C_1 e^{i\pi x/a}] e^{ikx}$$

$$(-\hbar^2/2m \, d^2/dx^2 + V_0 + V_1 e^{i\pi x/a} + V_1 e^{-i\pi x/a})[C_0 + C_1 e^{i\pi x/a}] e^{ikx} \; =$$

$$E[C_0 + C_1 e^{i\pi x/a}] e^{ikx}$$

$$(- \hbar^2 k^2 C_0/2m + V_0 C_0 + C_0 V_1 e^{i\pi x/a} + C_0 V_1 e^{-i\pi x/a} - \hbar^2 (k + \pi x/a)^2 C_1 \, e^{i\pi x/a}/2m +$$

$$V_0 C_1 e^{i\pi x/a} + V_1 C_1 e^{2i\pi x/a} + V_1 C_1) = EC_0 + E_0 C_1 e^{i\pi x/a}$$

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:

$$V_1 C_1 = [(\hbar^2 k^2/2m) - E + V_0]C_0$$

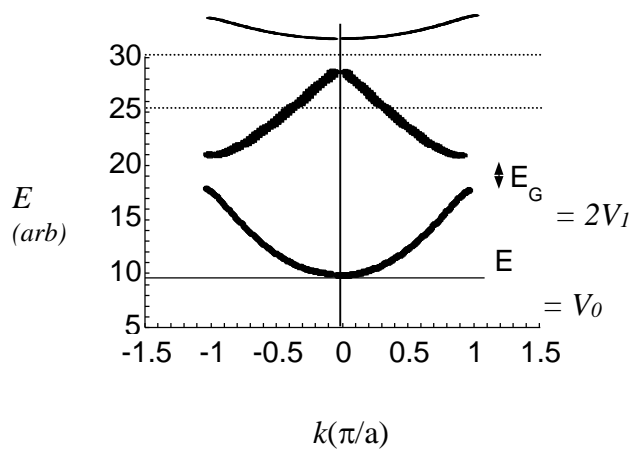For a non-trivial solution, both ratios for C_1/C_0 must be equal, i.e.

$$C_1/C_0 = [(\hbar^2 k^2/2m) + E - V_0]/V_1$$

$$= V_1/[\hbar^2 (k + \pi/a)^2/2m + E - V_0]$$

or, $[E - V_0 + (\hbar^2k^2/2m)] [E - V_0 + \hbar^2(k + \pi/a)^2/2m]$

$$= V_1^2 \quad \text{(Everything is symmetric)}$$

(c) Dispersion relation:

E *(arb)*

$k(\pi/a)$

4.

(a) The basic principle of STM is that a probe tip scans over a surface in close proximity to it (typically less than 1 nm), and we monitor the tunneling current between the two whilst scanning- maintaining a constant current and therefore a constant distance via a feedback loop. The information we can obtain from STM is the spacing between features at the atomic scale, variations in density of states, and overall, electronic density of states.

(b) Answer should include a discussion of vibration isolation, height resolution needing to be of order a few pm. Needs to be in a quiet environment, and requires ultrahigh vacuum (UHV). Samples and tips need to be prepared in UHV, and materials can be explored at atomic scale.

   (c)   Answer should touch on the fact that STM has atomic resolution, can only be used to look at conducting materials, and requires UHV. AFM can be operated in air, liquid or UHV, to perform measurements on conductors, nonconductors, hard materials, soft materials, living cells etc.   Under typical operating conditions, AFM has a resolution of a few nm, but under very special conditions it has demonstrated bond-level resolution.

(d) Video-rate AFM, multi-tip AFM, Quantitative mechanical measurements are now possible due to better calibration of cantilever stiffness, and closed-loop scanners in all 3 axes.

e.

5. (a) Nanotechnology is the ability to both fabricate and characterise structures with characteristic dimensions in the range 1-100 nm. Discussion should mention some of the following:

Electronic mean-free path

Magnetic domain size

Electron wavelength

Phase coherence length

Surface effects, surface area/volume ratio

(b) Discussion should contain elements on the following:

Wave-particle duality: electrons in devices have associated wave-packets, interference, resonant effects, tunneling, STM, nature of surface states.

(c) 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.

(d) This is resonant tunnelling, where the energy of the electrons is the same as that of a bound state within the well. The shape of the wave-function in the well is consistent with the ground state. Discussion should include notion of resonant tunnelling, excitation of meta-stable well state, relative amplitude of incident and transmitted waves, boundary conditions. Most accurate way to estimate electron

energy is to use wavenength, as an estimate using the infinite square well formula will be too innaccurate. From the graph, $\lambda = 1$ nm, from which we have

$$E = \frac{\hbar^2 k^2}{2m} = \frac{h^2}{8m\lambda^2} = 0.374 \text{ eV}.$$ Using the infinite well approximation, we get 1.04 eV.