4B5 2006 long Answers

1.

(a)   At the heart of quantum mechanics is the wave-particle duality, which is the fact that in certain situations, particles exhibit wavelike behaviour - interference and diffraction, and similarly waves sometimes behave like discrete particles – they come in discrete packets. 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 should include a discussion of two of the following:

(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, this is an analytical tool used to measure lattice periodicities.

(iii) electron coherence effects – quantum interference observed in transport measurements.

Plane waves can be used to represent a beam of electrons (as a plane wave has no localisation), whereas wave-packets should be used to represent individual electrons.

(b)   Matter waves have the dispersion relationship $E = \hbar^2 k^2 / 2m$, whereas for electromagnetic waves it is $E = \hbar k c$. This non-linearity for matter waves leads to dispersion even in the absence of a medium.

(c) $\psi(x, t)$ represents a particle in that $|\psi(x, t)|^2$ represents the probability of finding the particle at a position x at a time, t.

To obtain the momentum, p, if we differentiate with respect to x,

$$-i\hbar d\Psi/dx = p\Psi$$

Similarly, if we differentiate with respect to t,

$$i\hbar d\Psi/dt = E\Psi$$

Now, total energy is Kinetic + potential, i.e. E = K. E. + V. Kinetic energy is $mv^2/2$. If we remember that momentum, p is mv, then energy, $E = p^2/2m$. Combining this, we have:

$H = -(\hbar^2/2m)d^2/dx^2 + V$, where H is the Hamiltonian operator for E.
If we multiply across by $\psi(x, t)$, we obtain:

$-(\hbar^2/2m)d^2\psi(x, t)/dx^2 + V\psi(x, t) = i\hbar d\psi(x, t)/dt = E\psi(x, t)$

This is Schrodinger's equation

(d) Classical and quantum mechanics disagree as classical mechanics is only an approximation to quantum mechanics, valid for large-scale behaviour and large objects. They both tend to converge towards the same result if we apply quantum mechanics to macroscopic objects, or to highly excited states.

2.

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

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

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

The solutions to these equations are:

$\Psi_I(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}$ where $k_1 = \dfrac{\sqrt{2m(E-V)}}{\hbar}$

and $\Psi_{II}(x) = A_2 e^{ik_2 x}$ where $k_2 = \dfrac{\sqrt{2mE}}{\hbar}$

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

$A_1 + B_1 = A_2$

$ik_1 A_1 - ik_1 B_1 = ik_2 A_2$

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

The reflection probability is $|B_1/A_1|^2$. 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) $k_1 = 3.6 \times 10^9$, $k_2 = 1.2 \times 10^{10}$

=> R = 0.29

For R = 0, $k_1 = k_2$, i.e. there is no potential step!

For R = 1, either k_1 or $k_2 = 0$ or ∞, neither of which is physically reasonable, it would mean V is infinite or E is zero.

(c) Schrodinger's equation is now

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

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

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

The solutions to these equations are:

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

$$\Psi_{II}(x) = A_2 e^{ik_2 x} + B_2 e^{-ik_2 x} \text{ where } k_2 = \frac{\sqrt{2mE}}{\hbar}$$

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

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

$A_1 + B_1 = A_2 + B_2$

$ik_1 A_1 - ik_1 B_1 = ik_2 A_2 - ik_2 B_2$

matching at x = L gives:

$A_2 e^{ik_2 L} + B_2 e^{-ik_2 L} = A_3 e^{ik_1 L}$

$ik_2 A_2 e^{ik_2 L} - ik_2 B_2 e^{-ik_2 L} = ik_1 A_3 e^{ik_1 L}$
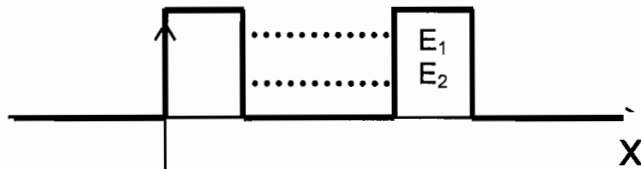
combining these equations, we eventually obtain for R:

$R = |B_1/A_1|^2 =$

$$\left\| \left[\frac{\left[\left(k_1^2 - k_2^2\right)\left(1 - e^{2ik_2 L}\right)\right]}{\left[\left(k_2 + k_1\right)^2 - \left(k_2 - k_1\right)^2 e^{2ik_2 L}\right]} \right] \right\|^2$$

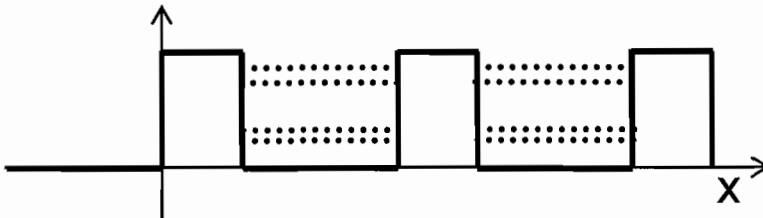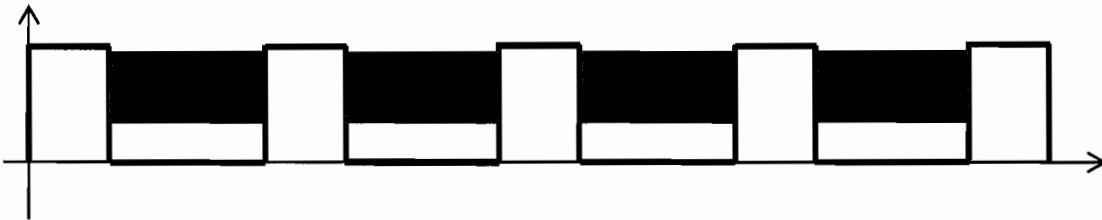$$= \left[1 + \frac{4k_1^2 k_2^2}{\left(k_1^2 - k_2^2\right)\sin^2 k_1 L} \right]^{-1}$$

$= 0.627$

3.

(a)

Now add in another well:

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.

(b)   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

        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:

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

where $n = 0, \pm1, \pm2,.....$ 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,

$$\psi(x) = \sum_n C_n e^{\left(i(k+G_n)x\right)}$$

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

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 $n = 0, \pm1$. This is justified for weak potentials such as those found in metals.

$$V(x) = V_0 + V_1 e^{iG_1 x} + V_{-1} e^{iG_{-1} x}$$

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

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

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

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

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.):

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

$$V_0 C_{-1} e^{iG_{-1} x} + V_1 C_{-1} + V_{-1} C_{-1} e^{2iG_{-1} x}) = EC_0 + EC_{-1} e^{iG_{-1} x}$$

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:

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

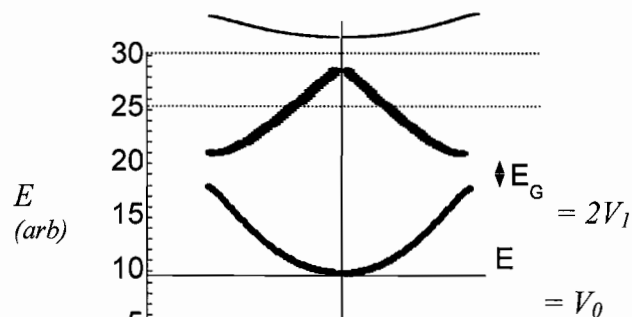For a non-trivial solution, both ratios for C_{-1}/C_0 must be equal, i.e.

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

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

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:
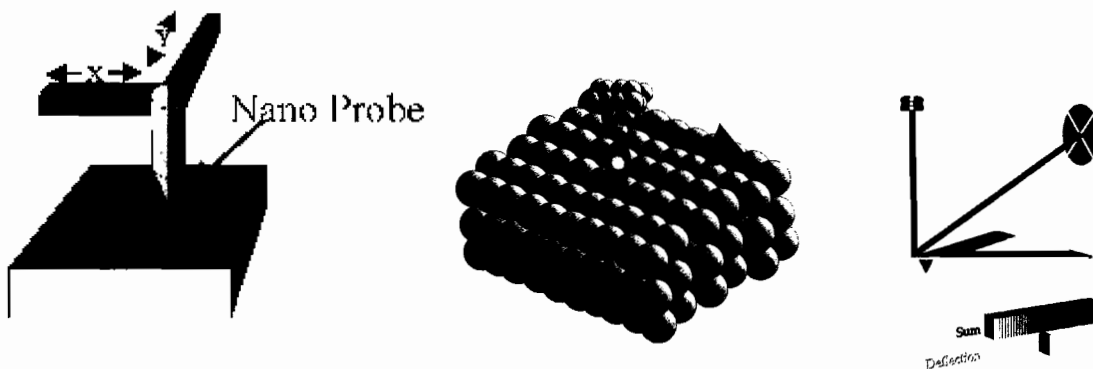
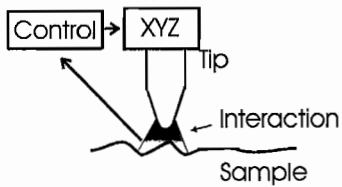The wave-functions at the valence and conduction-band edges can be written as:

$$\psi_v(x) = 2C_0 \cos\left(\frac{\pi x}{a}\right) \text{ and } \psi_c(x) = 2iC_0 \sin\left(\frac{\pi x}{a}\right)$$

These are standing waves which means electrons at these energies do not travel through the crystal, and hence do not contribute to conduction.
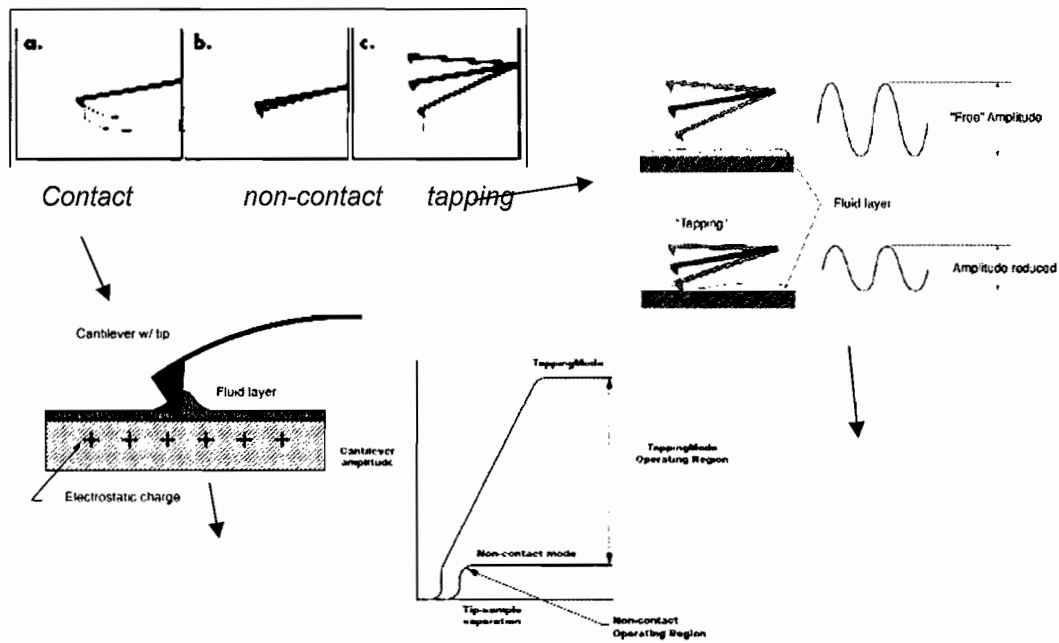
4

Answer should include a sketch of an AFM, along the following lines:

Most commonly used modes of AFM:

(b) answer should include a description of conducting AFM or MFM, types of tip used, method of imaging...
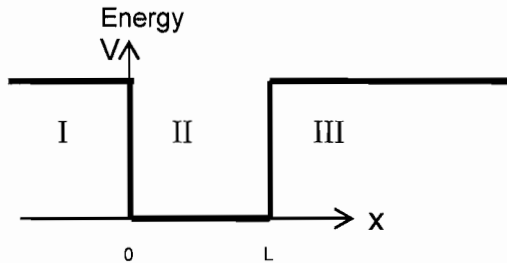
(c) limitations are scan area, scan speed, need for UHV for atomic resolution, sharpness of tips, sensitivity of force detection. Parallel AFM, video-rate AFM, millipede...

$\frac{1}{2} k_B T \sim \frac{1}{2} k x^2$, where k is cantilever stiffness, x is cantilever deflection. $\Rightarrow x \sim (k_B T/k)^{0.5}$
$= (1.38*10^{-23}*300/1)^{0.5} = 64$ pm.

5.

(a) A quantum well is a device which confines electrons in one direction.

Quantum wells are fabricated by MBE deposition of semiconductor layers.

(b)

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:

$$V = 0 \text{ for } 0<x<L$$

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

Schrödinger's equation in region II is:

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\Psi_x = E\Psi_x$$

The simplest solution of this equation is

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

Since the wave-function is zero outside the well, it must also be zero just at the boundaries (for continuity).

matching at left side $\quad \Psi(0) = A + B \Rightarrow A = -B$

i.e. $\quad \Psi(x) = A(e^{ikx} - e^{-ikx}) = A\sin(kx)$

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

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.

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

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

Remember, Energy, $E = \frac{1}{2}mv^2 = p^2/2m = \hbar^2 k^2/2m$
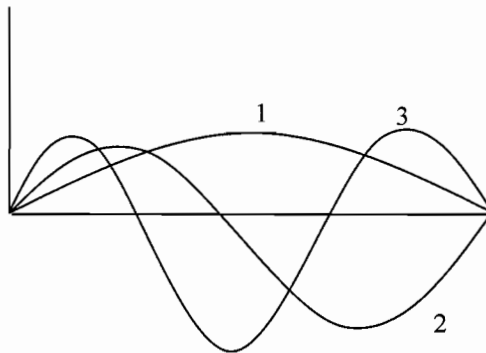
If $k = n\pi/L$, then the Energy levels of an electron confined in an infinite well are

$E = h^2 n^2/(8mL^2)$

The solutions are symmetric as the potential itself is symmetric

   (c) $E = 373n^2$ mV

   $\Rightarrow$ first three energy levels are at 373 meV, 1,492 meV and 3,357 meV

   (d)   If the well becomes finite, wave-functions will start to spread out into regions I & III. Energy levels will become lower. We should only approximate a finite well to an infinite one for the lower levels in the well, i.e. those that are below approximately 10% of the well's depth.