4B5 (Nanotechnology) 2012

1.

(a) The discussion should include but is not restricted to the following points

- Nanostructures have a lot of surface area, and the ratio of surface area/volume is high. As the surface atoms aren't fully co-ordinated, they have higher free energy than bulk atoms, and are therefore more reactive.
- Quantum confinement – as the size of an object gets smaller, we enter a regime where the electrons "see" the boundaries, and this is manifested in the wavefunctions – this is why we look at the particle in a box (quantum well) problem. This leads to a spectrum of discrete energy levels, and is noticeable typically when an object is smaller than around 10 Fermi wavelengths.
- Defects – Nanostructures tend to have fewer defects than bulk structures, which leads to enhanced mechanical properties.

By controlling these properties, we can hope to improve/enhance the functionality of existing materials and generate new types of device.

(b) $|\psi(x)|^2$ is the probability of finding the quantum object at position x, so is physically significant. The Wavefunction encodes information about the position, energy, momentum and time evolution of a quantum system. Quantum systems display discretization and often differ from classical ones in that they are not deterministic, but are probabilistic. Mathematically, this arises due to the fact that the Schrodinger equation is only first order in time whereas the wave-equation is second order. In fact, the Schrodinger equation is like the diffusion equation (except that the time derivative has a complex part, i.e. it is id/dt in the Schrodinger equation), but it oscillates in time rather than decaying.

(c)

(i) The particle, which is localized and hence described by a wavepacket, is incident from the left, and has not encountered the barrier structure yet.

(ii) The leading edge of the wavepacket (which is made up of the higher momentum, shorter wavelength terms) has reached the first barrier and has been partially reflected. The transmitted wave is travelling towards the second barrier, with an increased kinetic energy (as the potential is lower in this middle region). There is interference between the incident wavepacket and the reflected components in the first region, leading to the formation of a partial standing wave.

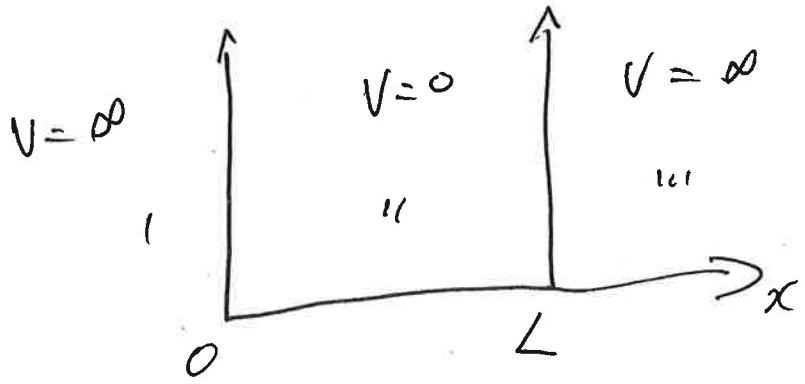
(iii) In the central region, the wavepacket has reached the second barrier, and has been partially scattered, so some of it is travelling backwards.

(iv) A standing wave has been formed in the central region due to the multiple reflections of the wavepacket between the two barriers. There is also a small transmitted wavepacket.

(v) The standing wave has dissipated and there is some transmission.

Overall, what this is telling us is that there is a small probability of the electron getting transmitted through the entire structure, and the electron will get trapped for a short time in the central region, which is essentially a quantum well. A common error was for people to not recognize that the wavepacket (and therefore the electron described by it) does not actually split up, and a part of it get transmitted. The wavepacket amplitude squared gives the *probability* of transmission.

2(a)



in regions I & III, $V = \infty \Rightarrow$ no probability of finding particle there $\Rightarrow \psi_I = \psi_{III} = 0$.

Schrödinger's equation:

$$\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

Simplest solution: $\psi(x) = Ae^{ikx} + Be^{-ikx}$

where $k = \frac{\sqrt{2mE}}{\hbar}$

At $\psi_I = \psi_{III} = 0 \Rightarrow \psi(0) = \psi(L) = 0$

$\Rightarrow \psi(0) = 0 \Rightarrow A = -B \Rightarrow \psi = C\sin kx$

$\psi(L) = 0 \Rightarrow C\sin(kL) = 0$

$\Rightarrow k = \frac{n\pi}{L}$ ... $n = 1, 2 \ldots$

i.e. $\psi(x) = C \sin\left(\frac{n\pi x}{L}\right)$

To normalise, $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$

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

$$\Rightarrow C = \sqrt{\frac{2}{L}}$$

$$\Rightarrow \psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

Now; Energy, $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$

$$= \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2 = \frac{h^2 n^2}{8mL^2}$$

Normalisation constant $= \sqrt{\frac{2}{L}} = \sqrt{\frac{2}{5 \times 10^{-9}}}$

$= 2 \times 10^4$

$$E_n = \frac{h^2 n^2}{8mL^2} \Rightarrow E_1 = \frac{h^2}{8 \times 0.067 \times 9.1\times10^{-31} \times (5\times10^{-9})^2}$$

$$= 0.223\, n^2\ eV$$

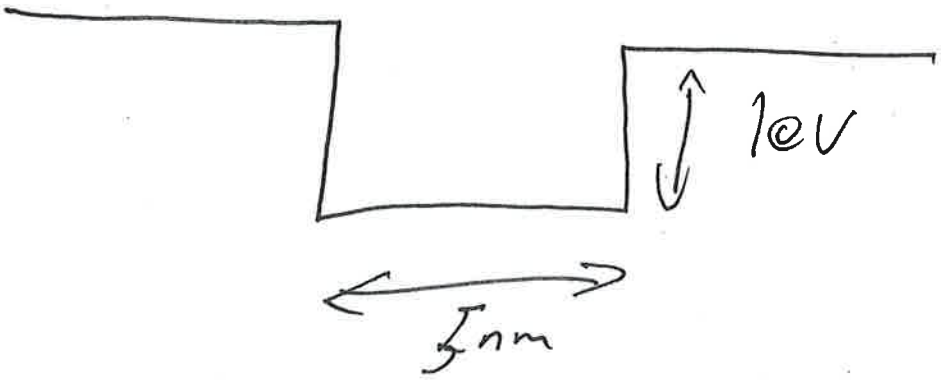
$$\frac{6.6\times10^{-68}}{8\times0.067\times9.1\times10^{-31}\times(5\times10^{-9})^2}$$

$$= \frac{8.43\times10^{-37}}{1.79\times10^{-19}}\ n^2$$

$$= 0.36\times10^{-19}\ n^2$$

$$=$$

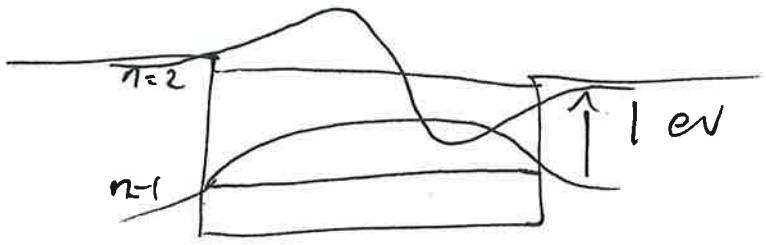
b)



Would expect $n=1$ always

$n=2$ = 0.892 eV

$\Rightarrow$



It is reasonable to approximate a well as ∞ when the energy level $< \frac{V}{10}$, where V is the depth of the well. Therefore, we expect the above estimate of the $n=2$ level to not necessarily be true.

(7)

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

if $x \to -x$

$$\Rightarrow \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\psi(-x) + V(-x)\psi(-x) = E\psi(-x)$$

Now, if $V_x = \pm V(-x) \Rightarrow \psi(x) = \pm\psi(-x)$

3 (a)

Pauli's exclusion principle: No two electrons can occupy the same state, so energy levels split when systems come close enough together to start coupling.

i.e. Two atoms far apart:

Close:

(b) solution:

In the free-electron model, electrons are represented as plane waves with no mutual interaction, no atomic cores and no surfaces, i.e. a non-interacting gas or sea of electrons. In the nearly-free electron model, the electrons are still plane waves, not interacting with each other and with no surfaces. There is however a periodic atomic potential that they see. 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 $n = 0, \pm1, \pm2, \ldots$ 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,

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

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

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.

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

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:

$$C_0V_{-1} = [-\hbar^2(k + G_{-1})^2/2m + E - V_0]C_{-1}$$

Terms without any exponent give:

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

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

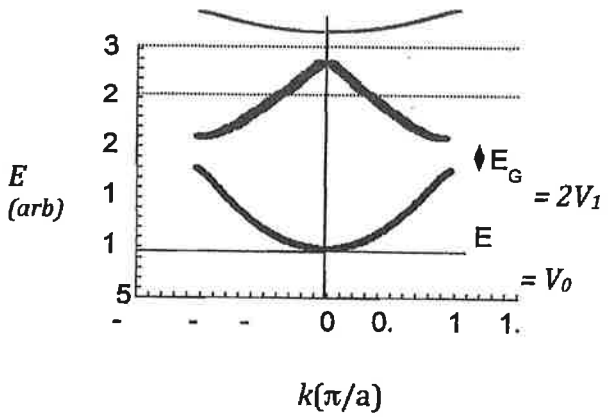
$$C_{-1}/C_0 = [-(\hbar^2k^2/2m) + E - V_0]/V_1$$

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

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

$$= V_1V_{-1} = |V_1|^2 \quad \text{(Everything is symmetric)}$$

(c) Dispersion relation:

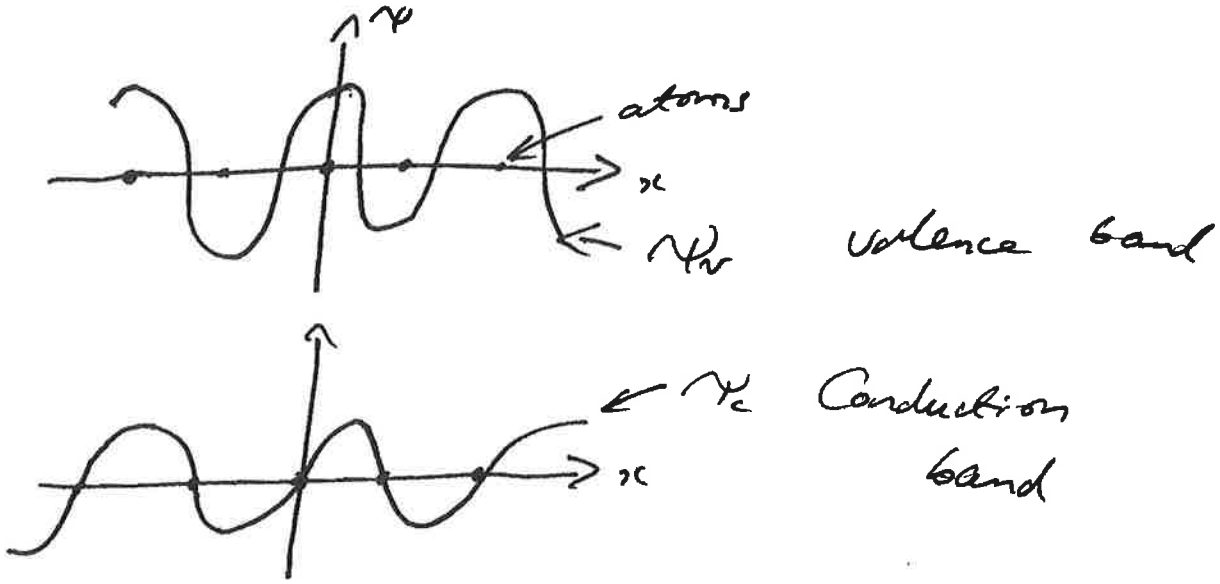


(10)

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

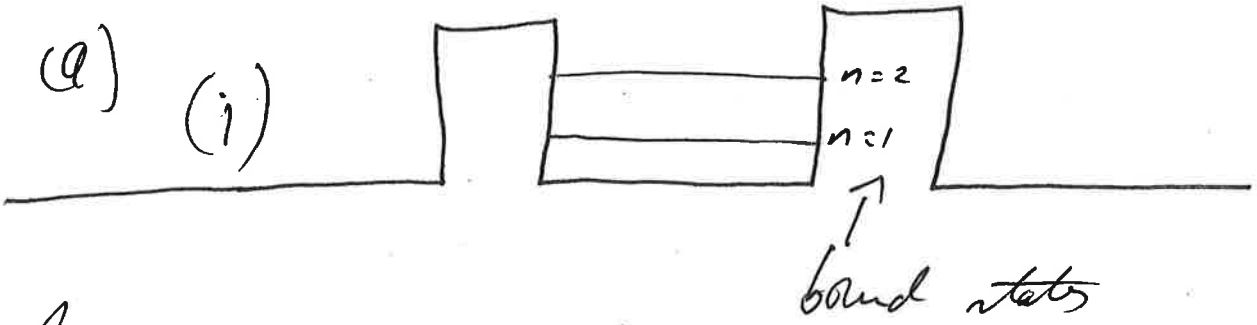
$E_{VB} = V_0 + (\hbar^2(\pi/a)^2)/2m - |V_1|$ $\quad$ $E_{CB} = V_0 + (\hbar^2(\pi/a)^2)/2m + |V_1|$

No, they do not contribute to conduction – they are described by standing waves.



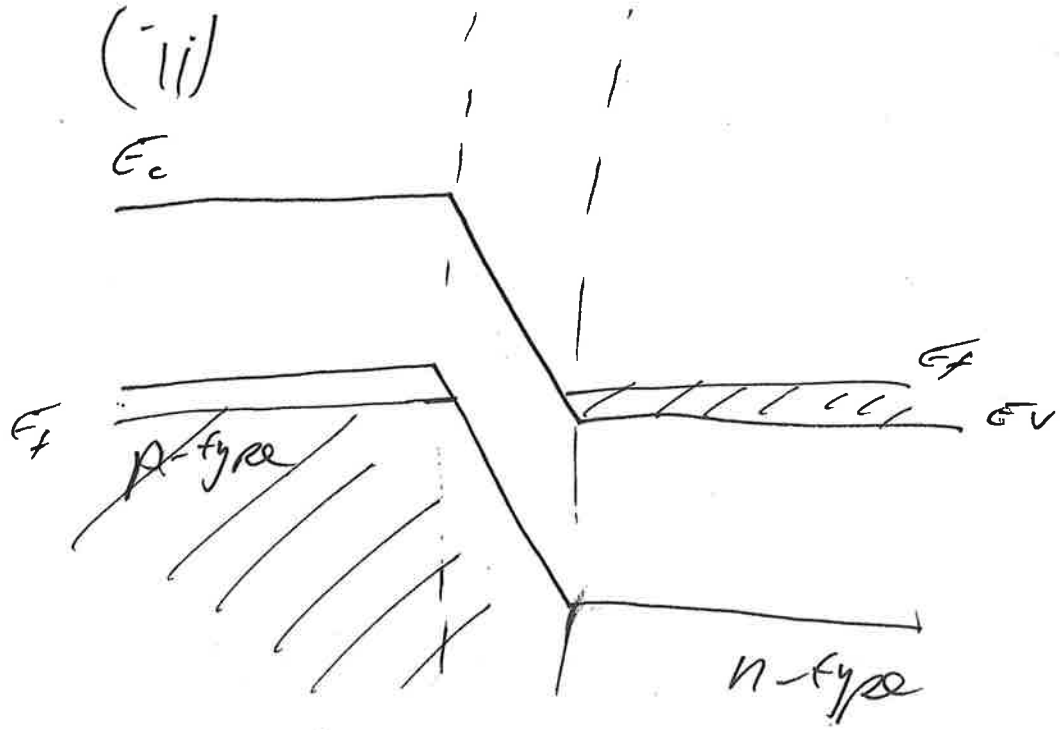
4.

(a) (i)



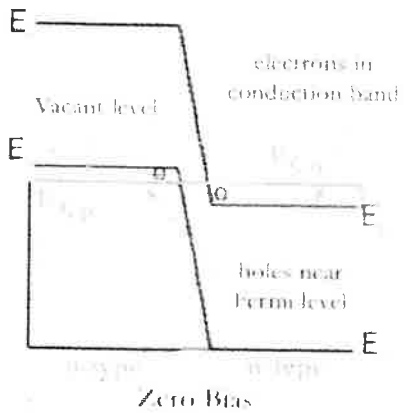
Resonant tunneling based on bound states between 2 barriers, created by band Engineering.

(ii)



Resonant tunnelling diode - created by highly doping a conventional p-n junction.

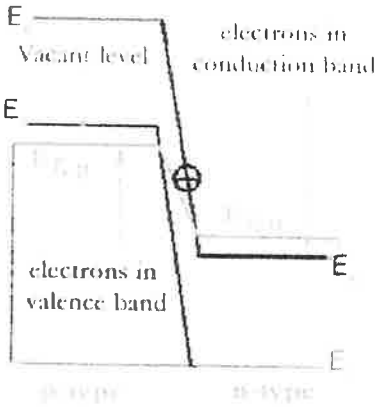
(i): Not a diode, harder to fabricate more complicated
(ii) Is a diode, simple to fabricate.



Zero Bias

Operating under *zero bias*

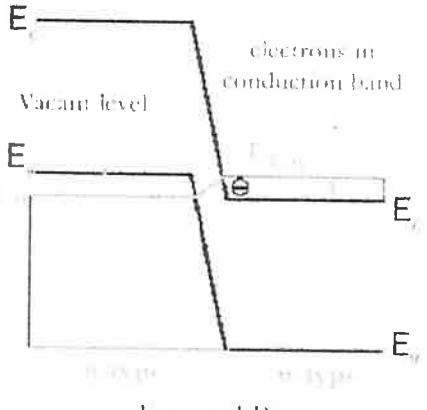
The electrons in the conduction band of the n-type side can tunnel into the p-type valence band if there are any holes just below $E_{F,p}$. Also electrons in valence band of p-type can tunnel into conduction band of n-type if there are holes just below the $E_{F,p}$. So, there is zero net current under zero bias.



Reverse Bias

Operating under *reverse bias*

Under reverse bias the bands are raised on the p-type side and lowered on the n-type side. This results in a large electron current flowing easily from p to n by tunnelling across the depletion region. Therefore, under reverse bias, there will be a net conventional current flow from n-type into p-type.

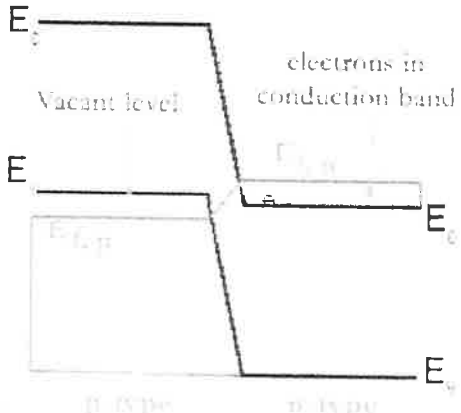


Forward Bias

Operating under *forward bias*
(1) small forward bias

Under low forward bias the bands are lowered on the p-type side and raised on the n-type side. The bias is so low (< 0.6 V) that there is no substantial thermal diffusion current.

(continued...)

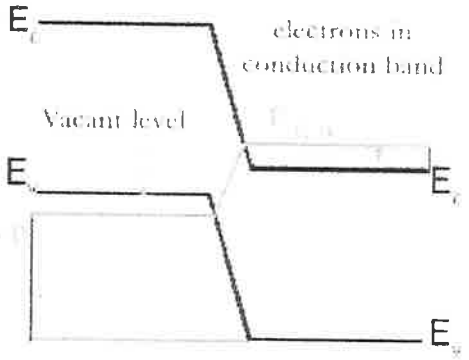


Forward Bias (increased)

Operating under *forward bias*
(2) increased forward bias

As the forward-bias voltage increases, more of the n-type conduction band electrons are facing the forbidden energy gap of the p-type side. So this reduces the conduction to valence band current.

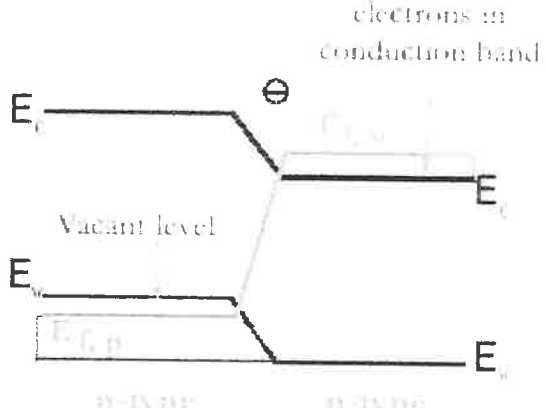
(continued...)



Forward Bias (at valley)

Operating under *forward bias*
= valley voltage

As the forward bias voltage continues to increase, it will reach a value where forward current has decreased to its minimum value (no tunnelling is possible as there are no vacant states into which the electrons can tunnel).



Forward Bias (Thermal Diffusion)

Operating under *forward bias*
> valley voltage

When the height of the barrier is reduced to a level that permits conventional (thermal diffusion) current to flow over the barrier, the forward current will increase as the thermal diffusion takes over as the main current carrying mechanism.

(c) Several reasons:

(i) Issues with reproducibility / tolerances in semiconductor processing → as transistors and other devices shrink, it is harder to produce them with an acceptable range of properties. This may be overcome using a bottom-up, or molecular approach. Key idea: many molecules that are identical can be fabricated easily.

(ii) Novel functionality, particularly quantum information processing.

(iii) Interesting new physics in the single molecule limit.

5(a)

The force on a spring extended by a distance x is

$F = -kx$

$\Rightarrow$ potential energy stored in spring $= \frac{1}{2}kx^2$

$= \frac{1}{2}m\omega^2 x^2$

Insert in Schrödinger's Equation:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + Vx = E\psi$$

i.e. $$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi$$

change variables : $y = \sqrt{\frac{m\omega}{\hbar}}\,x$, $\alpha = \frac{2E}{\hbar\omega}$

$$\Rightarrow \frac{d^2\psi}{dy^2} + (\alpha - y^2)\psi = 0$$

Trial solution is known to be $\psi(y) = F(y)e^{-y^2/2}$

where $F(y) = \sum_{p=0}^{\infty} a_p y^p$

Inserting solution into Schrödinger's equation gives:

$$F'' - 2yF' + (\alpha - 1)F = 0$$

$$F' = \sum_{p=0}^{\infty} p a_p y^{p-1} \qquad F'' = \sum_{p=0}^{\infty} p(p-1) a_p y^{p-2}$$

Problem arises when $\rho = 0$ or 1, as first two terms are then $F'' : \frac{0}{0} + \frac{0}{0}$: undefined!

To avoid this and without any loss of generality, we substitute $\rho \to \rho + 2$ in F''.

$$\Rightarrow F = \sum_{\rho=0}^{\infty} a_{\rho+2} y^{\rho}$$

$$F' = \sum_{\rho=0}^{\infty} (\rho+2) a_{\rho+2} y^{\rho+1}$$

$$F'' = \sum_{\rho=0}^{\infty} (\rho+2)(\rho+1) a_{\rho+2} y^{\rho}$$

$$\Rightarrow \sum_{\rho=0}^{\infty} (\rho+2)(\rho+1) a_{\rho+2} y^{\rho} - 2\sum_{\rho=0}^{\infty} \rho a_{\rho} y^{\rho} + (\alpha-1)\sum_{\rho=0}^{\infty} a_{\rho} y^{\rho} = 0$$

$$\Rightarrow \sum_{\rho=0}^{\infty} \left[(\rho+2)(\rho+1) a_{\rho+2} - 2\rho a_{\rho} + (\alpha-1) a_{\rho} \right] y^{\rho} = 0$$

$\Rightarrow$ term in brackets must equal zero for all ρ.

i.e. $$(\rho+2)(\rho+1) a_{\rho+2} - (2\rho + 1 - \alpha) a_{\rho} = 0$$

$$\Rightarrow \frac{a_{\rho+2}}{a_{\rho}} = \frac{2\rho + 1 - \alpha}{(\rho+2)(\rho+1)}$$

now; this tends towards $\frac{1}{\rho}$ as $\rho \to \infty$

and, the sum of $\sum_{\rho=1}^{\infty} \frac{1}{\rho} \to \infty$, so we need to truncate the series.

As it happens there is one value of ρ, which we will call n, where that value of $\frac{a_{\rho+2}}{a_\rho} = 0$

i.e. $$2n + 1 - \alpha = 0$$

$$\Rightarrow \alpha = 2n + 1$$

If n is even, then the power series has only even terms, and if n is odd, there are only odd terms.

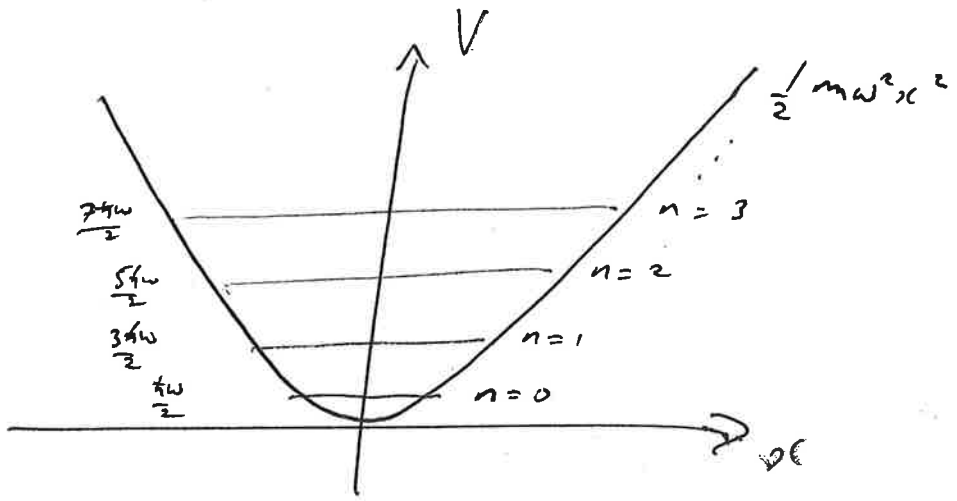
i.e. if n is even, $a_1 = 0$

if n is odd, $a_0 = 0$

Now; $\alpha = \frac{2E}{\hbar\omega} \Rightarrow E_n = (n + \frac{1}{2})\hbar\omega$.

i.e. the energy levels of the QSHO are quantized, and there is a zero-point energy when $n=0$, of $E_0 = \frac{\hbar\omega}{2}$.

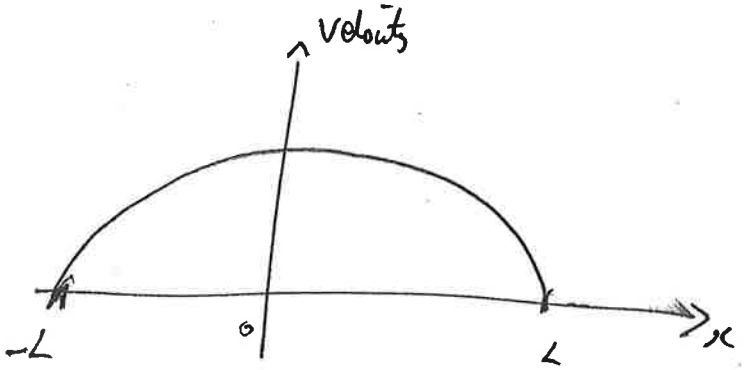
(5) (i) Discrete states:



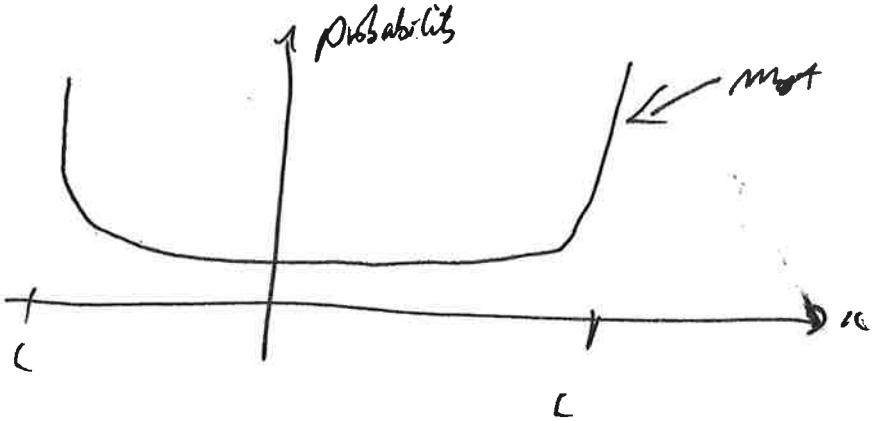
Classically, expect a SHO to spend most time at the extremes where velocity is slowest

i.e. if $x = L\sin\omega t$

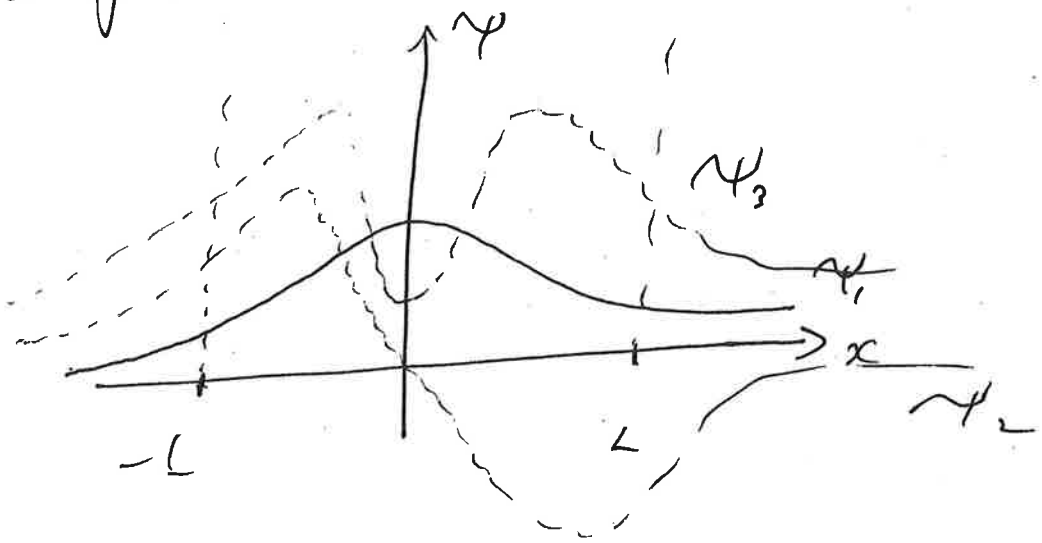
$\Rightarrow$ Velocity $= x' = \omega L\cos\omega t$



probability of finding particle $\propto \frac{1}{\text{Velocity}}$



Wave-functions:

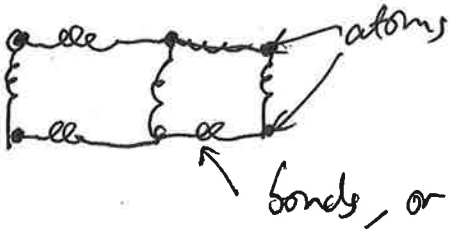


Points to note (i) $\psi \neq 0$ when $|x| \geq L$, i.e.

Q. Mechanically, particle can oscillate by a larger amount than it is excited by.

(ii) Ground state: probability is maximum at the centre, the opposite of what is seen classically. As we look at higher excited states, they approach the classical limit.

(C) (i) The motion of atoms in a crystal, as bonds can be considered as similar to springs, i.e.



Perhaps most important point is that atoms are never at rest. Heisenberg tells us that anyway as $\Delta x \Delta p \geq \frac{\hbar}{2}$; but Q.S.H.O tells us that minimum energy is $\frac{\hbar\omega}{2}$; so atoms are always moving. We can use it to describe phonons and then electrical resistance.