1.

(a)   The need for Quantum Mechanics arose around the turn of the 20th century, spurred on by a number of experimental irregularities. For instance, on the basis of the understanding of nature at the time, the very existence of atoms was puzzling. It was known that atoms consisted of negatively charged electrons "orbiting" positively charged nuclei. From conventional electromagnetism, we know that any accelerating charged particle will emit electromagnetic radiation, and hence lose energy. Therefore, if an electron orbits a nucleus, by the very fact that it is moving around the nucleus, it must be undergoing acceleration. One would expect then, that it would radiate, lose energy and spiral into the nucleus. This clearly doesn't happen, so a theory was needed to explain why not.

Another problem was the phenomenon of photoemission. This is the effect whereby electromagnetic radiation incident on a metal surface causes electrons to be ejected from it. It was observed that electrons are only ejected once the frequency of the light reaches some threshold value, their energy scales linearly with increasing frequency, and the number of electrons ejected increases as the intensity of light increases. This is at odds with classical electromagnetism which predicts that (i) the frequency should not make any difference whatsoever and (ii) the energy of the ejected electrons should only depend on the intensity of light (Energy per unit volume of light is $\frac{1}{2}\varepsilon E^2$, and Intensity is energy per unit area). There is no reason classically for the number of electrons ejected to depend on intensity. The explanation for this effect within the framework of Quantum mechanics is that light consists not only of waves, but also of particles called *photons*, which contain distinct amounts of energy, depending linearly on the frequency. The proportionality constant is Planck's constant, h. Electrons are bound to the metal by an energy called the work function, and until the frequency of light is high enough, individual photons don't have enough energy to free them. Above this threshold frequency then, electrons are emitted, and the excess energy is taken up as the electron's kinetic energy. The number of electrons ejected then scales as the number of photons, which depends on the intensity.

Another turning point was the observation of electron diffraction – clear evidence that particles have a wave-like character.

Other experimental evidence was for instance the inability of Physics to explain (i) why some materials are conductors and others insulators; (ii) the origin of electrical resistance; (iii) the observed dependence of specific heat on temperature and (iv) the origin of discrete spectra from heated materials, e.g the sun.

(b) Wave-packets are used to represent particles, eg. Electrons.

To construct a wave-packet, add two sinewaves:

$$E = E_0\{Cos(\omega t - kx) + Cos(\omega_2 t - k_2 x)\}$$

This can be re-written as $\quad E = 2E_0 sin(\omega_+ t - k_+ x)Cos(\omega_- t - k_- x)$

Where $\omega_\pm = (\omega \pm \omega_2)/2$ and $k_\pm = (k \pm k_2)/2$

This represents a sinewave of frequency ω_+ which has it's amplitude modulated at the frequency ω_-, to produce beats. This therefore exhibits localised areas of enhanced field strength which may be used to represent particles. These localised areas (which we call wave-packets) propagate through space at the group velocity $\delta\omega/\delta k = c$ (the speed of light). In the absence of dispersion, these wave-packets will propagate without changing shape, but if there is dispersion, they will spread out.

The phase velocity is $\omega/k = \omega_2/k_2 = c$. The group velocity can in principle vary, but up to a maximum limit of c. We could refine the wave-packet by summing together an infinite number of sinewaves, with for eg a Gaussian spectral function. This will increase the localisation.

(c) Construct a wave-packet as follows generally:

$$E = E_0 \int_{-\infty}^{\infty} f(k)e^{i(kx - \omega t)} dk \tag{1}$$

where f(k) is the spectral function, which is given here as being a gaussian of width δ:

$$f(k) = \frac{1}{\sqrt{2\pi}\delta} e^{-\frac{k^2}{2\delta^2}}$$

Therefore, we can write (1) as $\quad E = \frac{E_0}{\sqrt{2\pi}\delta} \int_{-\infty}^{\infty} e^{-\frac{k^2}{2\delta^2} + ik(x - ct)} dk$

Where we have used the relation that $\omega = ck$.

This is known as a Gaussian Integral, and the easiest way to solve is to change the variables to be more manageable: let x-ct -> x', k-ib/2a ->k', where a = $1/2\delta^2$ and b = x-ct. This gives us

$$E = \frac{E_0}{\sqrt{2\pi}\delta} e^{\frac{-b^2}{4a}} \int_{-\infty}^{\infty} e^{-ak^2} dk$$

The integral is just equal to $\sqrt{\pi/a}$

The net result then is that $E = E_0 \sqrt{\delta} e^{-\frac{\delta^2}{2}(x - ct)^2}$.

(d) Heisenberg's uncertainty principle states that $\Delta x \Delta p \geq \dfrac{\hbar}{2}$. To see where this comes from, consider the following:

The spectral function has a width $\Delta k = \delta$. By inspection, the solution for E(x) has a width $\Delta x = 1/\delta$. Therefore, $\Delta x \Delta k = 1$. Given that momentum, $p = \hbar k$, it follows that $\Delta x \Delta p = \hbar$. This is just a lower bound on the uncertainty, hence the inequality in Heisenberg's uncertainty principle. What this is saying is that we can never simultaneously know absolutely both the position and momentum of a particle, and the more accurately we know one, the less we can know about the other.

2.

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

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

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

The solutions to these equations are:

$$\Psi_I(x) = A_1 e^{ik1x} + B_1 e^{-ik1x} \quad \text{where } k_1 = \frac{\sqrt{2mE}}{\hbar}$$

$$\text{and } \Psi_{II}(x) = A_2 e^{-k2x} \quad \text{where } k_2 = \frac{\sqrt{2m(V-E)}}{\hbar}$$

Matching the wave-functions and their first derivatives at the boundary (x = 0) yields the following relationships:
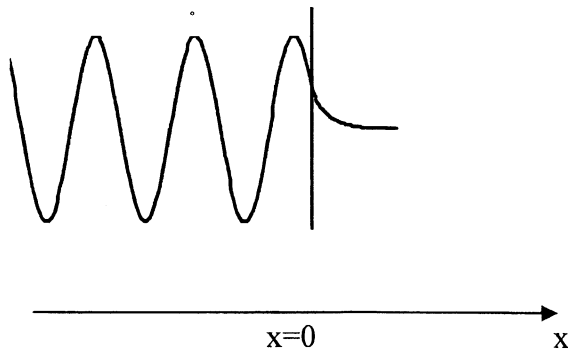
$A_1 + B_1 = A_2$

$ik_1A_1 - ik_1B_1 = -k_2A_2$

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

Reflection probability = $|B_1/A_1|^2 = 1$ identically.

(b) Probability density is defined as $|\psi(x,t)|^2$. This is the probability of finding the particle at position x, at time t.
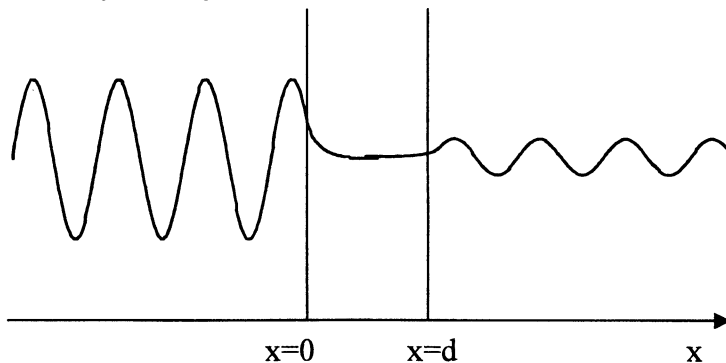
Probability density:

x=0   x

(c)

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

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

$$\Psi_{III}(x) = A_3 e^{ik_3 x} \text{ where } k_3 = k_1$$

Probability density:

x=0   x=d   x

If we say that the amplitude of the incident wave is 1, then the wave-function in the barrier region is:

$$\psi_{II} = e^{-k_2 x}$$

Therefore, the probability density, T at x=d is $e^{-2k_2 d}$. Taking the log of both sides

gives $\ln T = -2k_2 d \Rightarrow d = -\ln T/(2k_2)$ $\Rightarrow d = -\dfrac{\ln(\omega \cdot l)}{2\sqrt{2m(v \cdot e)}/\sqrt{\hbar}} =$

For the situation shown here, $\ln T = 1/e \Rightarrow d \sim 0.48$ nm

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.

(d) This phenomenon is called Tunneling. It is manifest in the following situations:
(1) α-decay of nuclei, (2) STM, (3) tunnelling diode, (4) gate oxide of transistors.

3.

(a)   This is a resonant tunnelling diode.
When a voltage is applied, the entire potential profile becomes sloped, and the Fermi Energy on the left approaches bound state E_1.
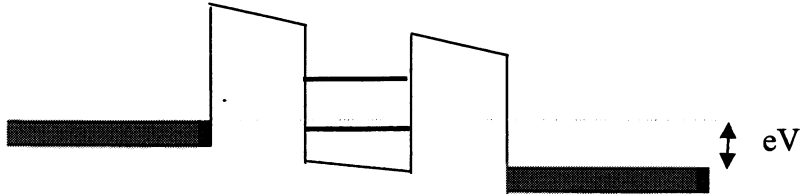
(b) As V is increased, the bound state energy E_1 starts below E_f, then when V is large enough they coincide, causing a peak in T. As V is further increased, there is no longer a match between E_1 and E_f, and T starts dropping. As we continue to increase V, E_2 starts to coincide with E_f, and we get 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.
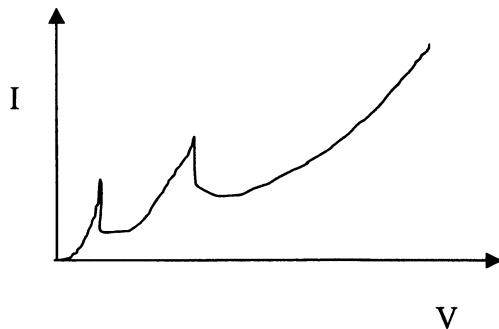

(c)
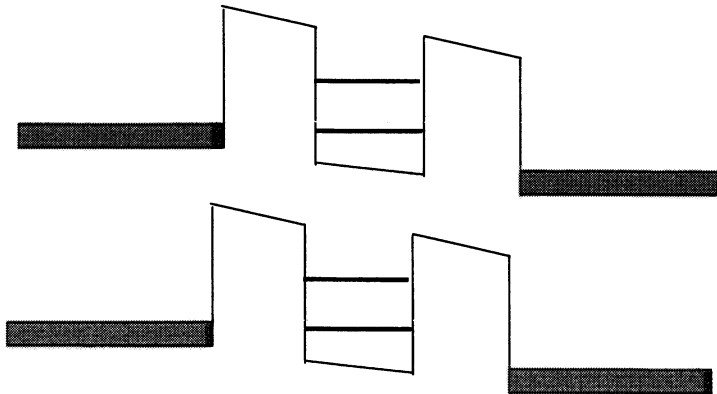
(d) If we had two wells close together, the tails of the bound state wave-functions would start to overlap, which would cause E_1 and E_2 each to split into two closely spaced levels, in accordance with the Pauli exclusion principle. This structure can contain a maximum of 8 electrons (4 levels, 2 possible values of electron spin).

   (i)   If we add more wells, then E_1 and E_2 will split further, and for n wells, they will split into n closely spaced levels. This is the origin of band structure, where instead of potential wells we have atoms, and there are so many atoms in a piece of bulk material that the n sublevels are too close together to be seen as distinguishable.

   (ii)   As we change the spacing between the wells, the sublevel spacing will change. The closer the wells are together, the larger this spacing:
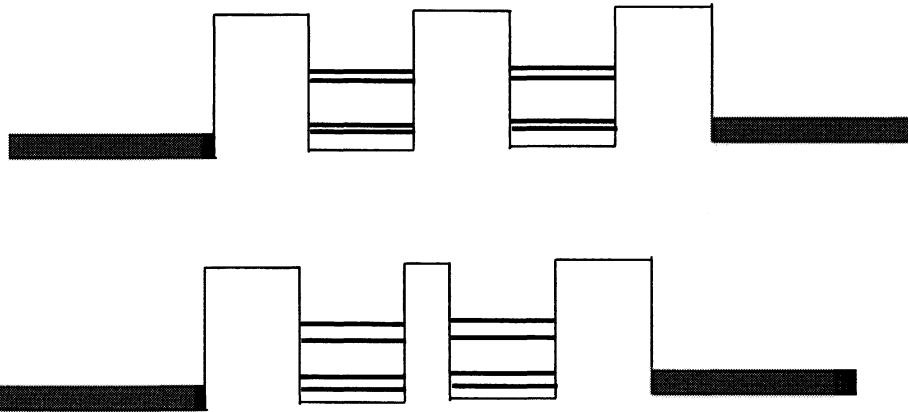
4.

(a) Schrödinger's equation: $-(\hbar^2/2m)\partial^2\psi/\partial x^2 + V\psi = E\psi$

The form of V is $V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega x^2$

Therefore, $\qquad\qquad -(\hbar^2/2m)\partial^2\psi/\partial x^2 + \frac{1}{2}m\omega x^2\psi = E\psi$

If we change variables to let $y = (m\omega/\hbar)^{0.5}x$, and $\alpha = 2E/\hbar\omega$, we can re-write the above equation as:

$$\partial^2\psi/\partial y^2 + (\alpha - y^2)\psi = 0$$

as required.

(b) Starting with the equation from above, i.e.

$$\partial^2\psi/\partial y^2 + (\alpha - y^2)\psi = 0$$

If we say that $\psi(y) = F(y)e^{-y^2/2}$ we get

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

If we assume that F(y) is a power series, i.e.

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

Then

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

Now, y can never have a negative power, as then the solution would have a singularity at y = 0. therefore, in the expansion for F'' we can let p -> p+2. That then gives us the following:

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

For a non-trivial solution then, we must have:

$$\frac{a_{p+2}}{a_p} = \frac{(2p+1-\alpha)}{[(p+1)(p+2)]}$$

Now, this series essentially goes as $1/p$, the sum of which diverges to infinity. Therefore, we must artificially truncate the power series at some value of p, say n. Because a_p is related to a_{p+2}, we can split the solution into two power series, one with even and the other with odd powers of y. Depending on whether n is even or odd, we then set the other power series equal to zero, so in other words, the solution is truncated at some value of p which we call n, and if n is even the series only contains even terms, and if n is odd, it only contains odd terms. Then that gives us the following relationship:

$$2n + 1 - \alpha = 0$$

which means $\alpha = 2n + 1$. But, $a = 2E/\hbar\omega$ which means :

$$E_n = (n + \tfrac{1}{2})\hbar\omega, \text{ as required.}$$

Only discrete values of energy are allowed as this is a quantum system which has *modes*. If we visualise the potential profile of a QSHO, it is a parabolic well, so only those quantum states whose wavelength is a half-integer divisor of the well length are allowed. This is not a discrepancy with classical mechanics, as for highly excited states, the Quantum and classical theories converge.

(c)
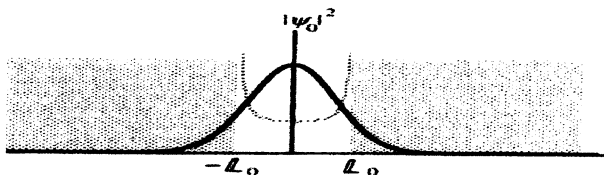
The solid curve is the Quantum probability density, and the dotted curve is the classically predicted one. They clearly predict the opposite behaviour: Quantum Mechanically, the ground state oscillator is most likely to be found at the centre position, whereas classically it is most likely to be found at the extremes.

(d) The QSHO is relevant for describing the vibration of atoms and molecules, and can be used to explain the temperature dependence of (i) specific heat and (ii) resistance of materials.

5

(a)

Band Engineering is essentially when you combine differently doped semiconductors of different band-gaps in multiplayer structures in order to create specific potential energy profiles, e.g a quantum well or a resonant tunnelling diode.

(b)

Consider what happens when we take a piece of GaAs and dope it on one side to make AlGaAs, which will be n-type. Due to the band offset (GaAs has a lower band-gap than AlGaAs), some electrons will flow from the n-type material into the GaAs. The AlGaAs and GaAs will then develop a slight positive and negative charge, respectively. This sets up a dipole layer of charge, and causes the bands to bend.

i.e. Conduction bands before contact:

AlGaAs

_____

GaAs

_____

In contact:

Band offset

Few nm
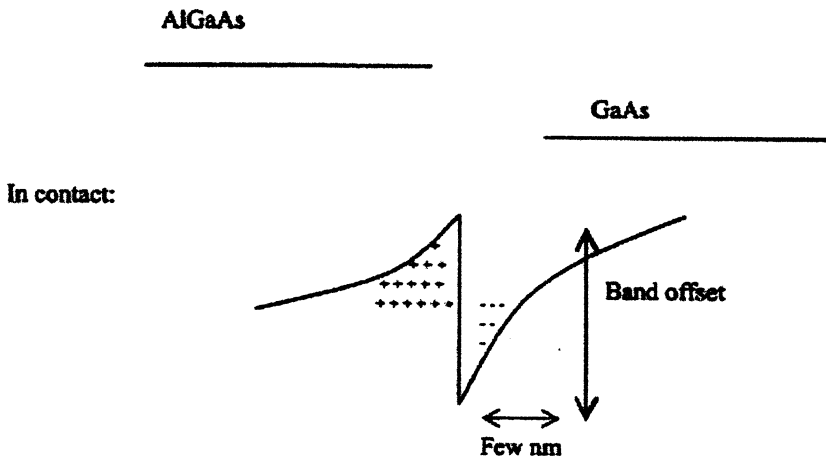
The 2-DEG is different in terms of its density of states:

3D
$E^{1/2}$

n(E)

E

Q2D
const.

n(E)

E
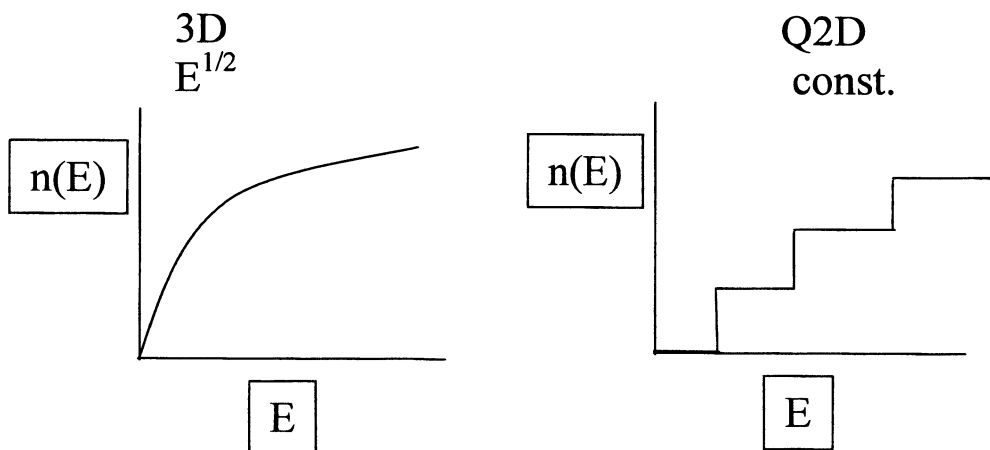
Electrons in a 2-DEG are confined in one direction (z), and free to move in the other two (x, y). To be general,.

$$E = E_{n,kx,ky} = E_n + \hbar^2 k_x^2/2m + \hbar^2 k_y^2/2m$$

Where the E_n are the discrete energy eigenvalues of the potential well. For most purposes, the triangular well can be approximated as a square well. The x, y components of energy are continuous, but the E_n are discrete, meaning that rather than have just one free electron parabola in the E-k diagram, we in fact have a number of sub-bands (as many as there are discrete states in the potential well). The form is like:
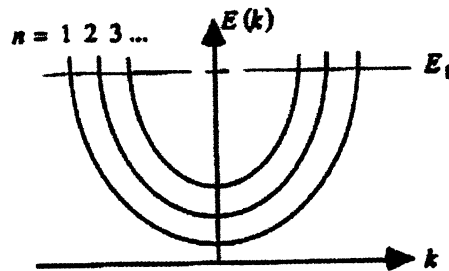
(c) Assume that well is infinitely deep (assumption 1) and square (assumption 2). Therefore, we can write energy eigenvalues as :

$$E_n = \frac{h^2 n^2}{8ml^2}$$ where l is the width of the well, and m is the electron mass within the well.

For the Valence band, then, E_{h1} = 0.05 eV, and for the Conduction band E_{e1} = 0.25 eV

⇨ emission wavelength of laser = 1.2 eV + 0.05 eV + 0.25 eV = 1.5 eV.

⇨ 1.5 eV = 2.4 x10^{-19} J = hc/λ => λ = 825 nm. The accuracy of this answer depends on the depth of the potential well, i.e. can we assume that it is infinitely deep? In reality, the well is probably 1-2 eV deep, so an energy level of 0.25 eV is relatively far below that, meaning the accuracy will be in the 10-20% range. In order to improve on the accuracy, we should calculate the bound state energies of the finite well.

(d) If we were to use a Quantum dot, the spread in laser wavelengths would be much smaller – it would be closer to monochromatic. Also, the threshold current would be lower.