

4B5 2010 Answers

1.

(a) Nanotechnology is the technology concerned with the controlled fabrication and characterization of structures with critical dimensions in the range 1-100 nm. There has been a high level of interest as it touches on many aspects of science & technology, and is based on the fact that the physical properties of matter can be altered simply by changing size. Many advances in technology and healthcare have been promised based on nanotechnology.

(b) The discussion should focus on the fact that as structures get smaller, the surface area to volume ratio increases, and this is important as surfaces have different atomic coordination and are therefore more reactive than bulk. Also, there is a size effect, described by quantum mechanics. Examples can include nanowires & resistance, color of colloids, quantum dots etc. Some candidates included the photoelectric effect which is nothing to do with this question.

(c) The answer should focus on existing products that we use and which contain nanostructures, e.g. sunscreen, anti-wrinkle cream, composites with enhanced mechanical properties, silver plasters, liposomes for drug delivery, small transistors, etc.

(d) The breakthrough that kick-started Nanotechnology as described in the context of this course was the STM. The reason for the impact is that it allowed us to visualize atoms on surfaces for the first time, and can be used to move single atoms around. It resolved the controversy regarding the reconstruction of the Si(111) surface. Some answers mentioned the development of Quantum mechanics, which certainly was a breakthrough, but did not start nanotechnology.

2.

Probability flux & quantum continuity equation

We could work out the Transmission probability from $R + T = 1$, or, recognize that momentum is different on both sides of step, so probability will flow at different rates..

$$\text{Probability, } P = \int |\psi|^2 d^3r$$

$$\begin{aligned} \text{Rate of change of probability, } \frac{dP}{dt} &= \int \frac{d}{dt} |\psi|^2 d^3r \\ &= \int d^3r \left\{ \psi^* \frac{d}{dt} \psi + \left(\frac{d}{dt} \psi^* \right) \psi \right\} \end{aligned}$$

But, we know from Schrodinger's equation that:

$$\begin{aligned} -i\hbar \frac{d\psi}{dt} &= \frac{-\hbar^2}{2m} \nabla^2 \psi + V\psi \Rightarrow \frac{dP}{dt} = \frac{i\hbar}{2m} \int d^3r \left[\left\{ \psi^* (\nabla^2 \psi) - (\nabla^2 \psi^*) \psi \right\} + \psi^* V\psi - V\psi^* \psi \right] \\ \Rightarrow \frac{dP}{dt} &= \frac{i\hbar}{2m} \int d^3r \nabla \cdot \left\{ \psi^* (\nabla \psi) - (\nabla \psi^*) \psi \right\} \\ \Rightarrow \frac{d|\psi|^2}{dt} &= \frac{i\hbar}{2m} \nabla \cdot \left\{ \psi^* (\nabla \psi) - (\nabla \psi^*) \psi \right\} = \frac{i\hbar}{2m} \nabla j, \text{ where } j \text{ is the probability flux} \\ \text{For plane waves, } j &= |\psi|^2 \frac{\hbar k}{m} \end{aligned}$$

To calculate T,

Schrodinger's equation has the following solution:

$$\text{Region I: } \psi_1(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}$$

$$\text{Region II: } \psi_2(x) = A_2 e^{ik_2 x}$$

$$\text{where } k_1 = \frac{\sqrt{2mV}}{\hbar} \text{ and } k_2 = \frac{\sqrt{2m(E-V)}}{\hbar}$$

$$\text{Matching } \psi_1 \text{ and } \psi_2 \text{ at the boundary } \Rightarrow A_1 + B_1 = A_2$$

$$\text{Matching } \psi_1' \text{ and } \psi_2' \text{ at the boundary } \Rightarrow A_1 k_1 - B_1 k_1 = A_2 k_2$$

$$\Rightarrow \frac{A_2}{A_1} = \frac{2k_1}{k_1 + k_2}$$



Transmission probability, $T = \frac{\text{Probability flux in Region II}}{\text{Probability flux in Region I}}$

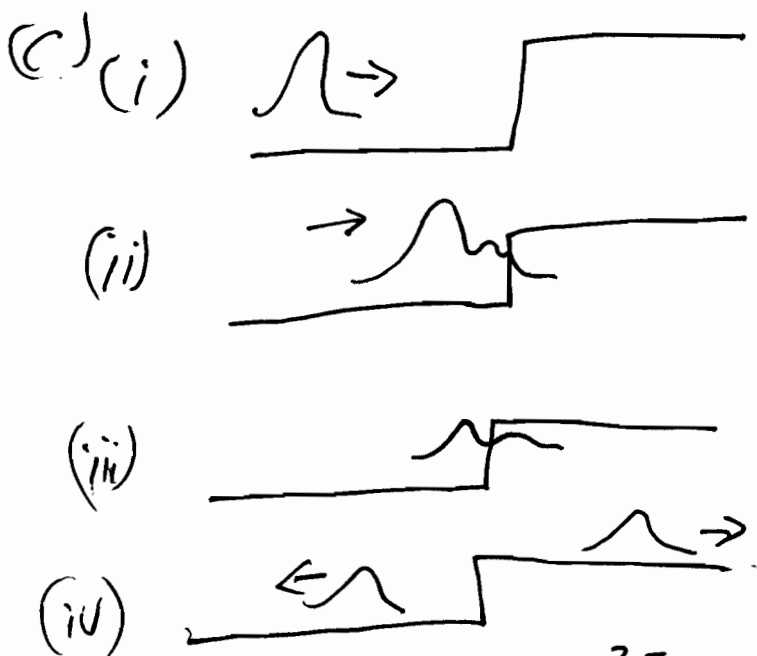
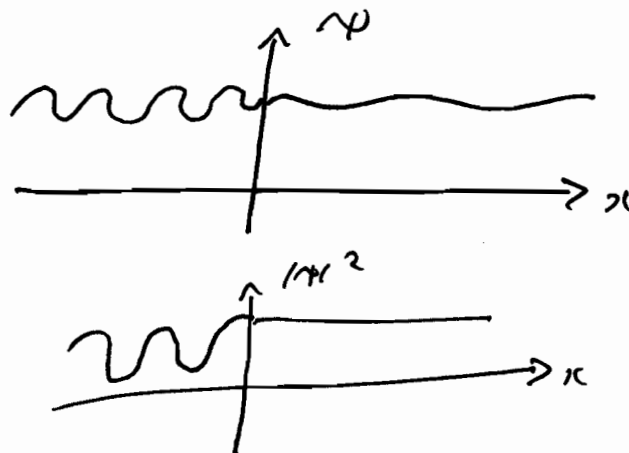
$$= \frac{|A_2|^2 \frac{\hbar k_2}{m}}{|A_1|^2 \frac{\hbar k_1}{m}} = \left(\frac{2k_1}{k_1 + k_2} \right)^2 \frac{k_2}{k_1}$$

Assuming the electron mass, m is the same in both regions and the electrons are described by plane waves.

T is the probability of transmission. For a beam of particles, it represents the proportion of the beam that is transmitted, whereas for a single electron, it represents the probability of transmission (NOT the proportion of the electron that is transmitted as some candidates suggested). For a single electron which will of course behave like a wave-packet rather than a plane wave, it will have a spread of energies around the mean E , so T will be slightly different.

Numerically, $k_1 = 5.14 \times 10^9 \text{ m}^{-1}$, $k_2 = 3.63 \times 10^9 \text{ m}^{-1}$

$\Rightarrow T = 0.97$



The dispersion rate \uparrow as initial width \downarrow . At the step, the packet interferes with reflected components, giving fine structure to the wavepacket.

A small proportion is transmitted as there will be some components with $E < V$.

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 $n = 0, \pm 1, \pm 2, \dots$ 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,

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

$$(-\hbar^2/2md^2/dx^2 + V) \Psi(\mathbf{x}) = E\Psi(\mathbf{x})$$

We end up with a set of simultaneous equations in the unknown C_n . Note that the V_p 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 $n = 0, \pm 1$. 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.

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

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

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

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.):

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

$$V_0 C_{-1} e^{iG_{-1} x} + V_1 C_{-1} + V_{-1} C_{-1} e^{2iG_{-1} x}) = E C_0 + E C_{-1} e^{iG_{-1} x}$$

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.

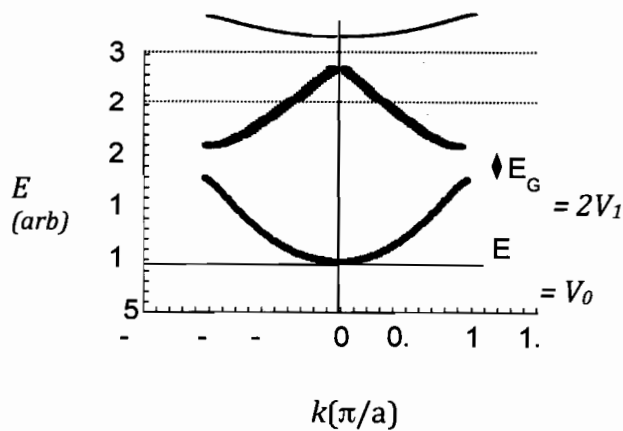
$$C_{-1}/C_0 = [-\hbar^2 k^2/2m + E - V_0]/V_1$$

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

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

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

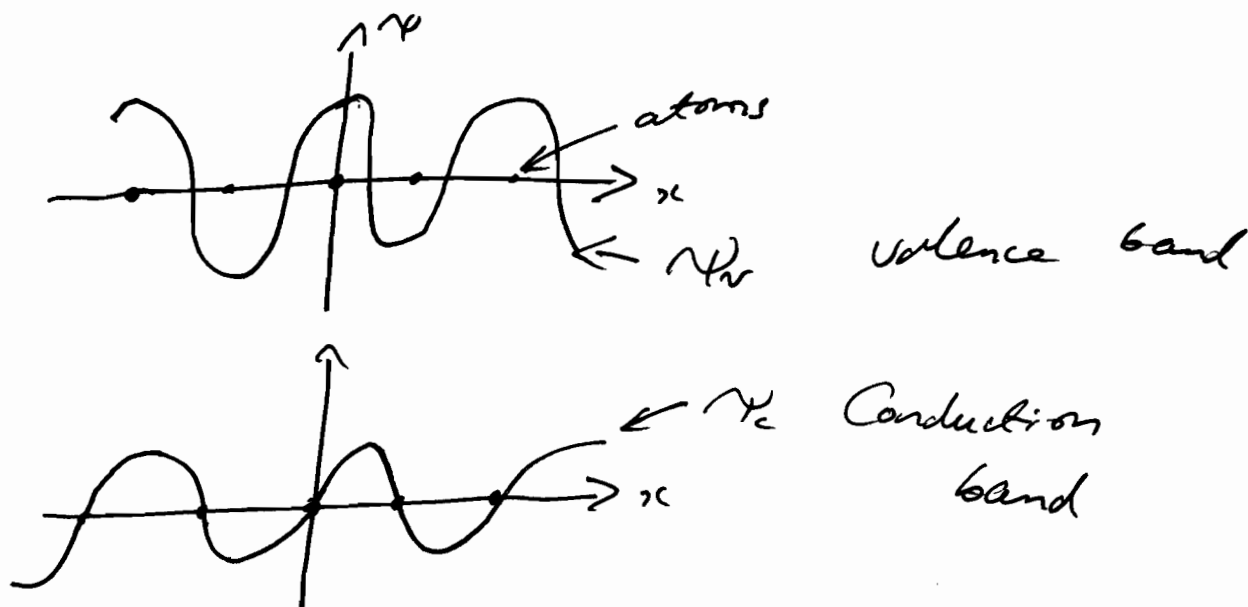
(c) Dispersion relation:



The 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.

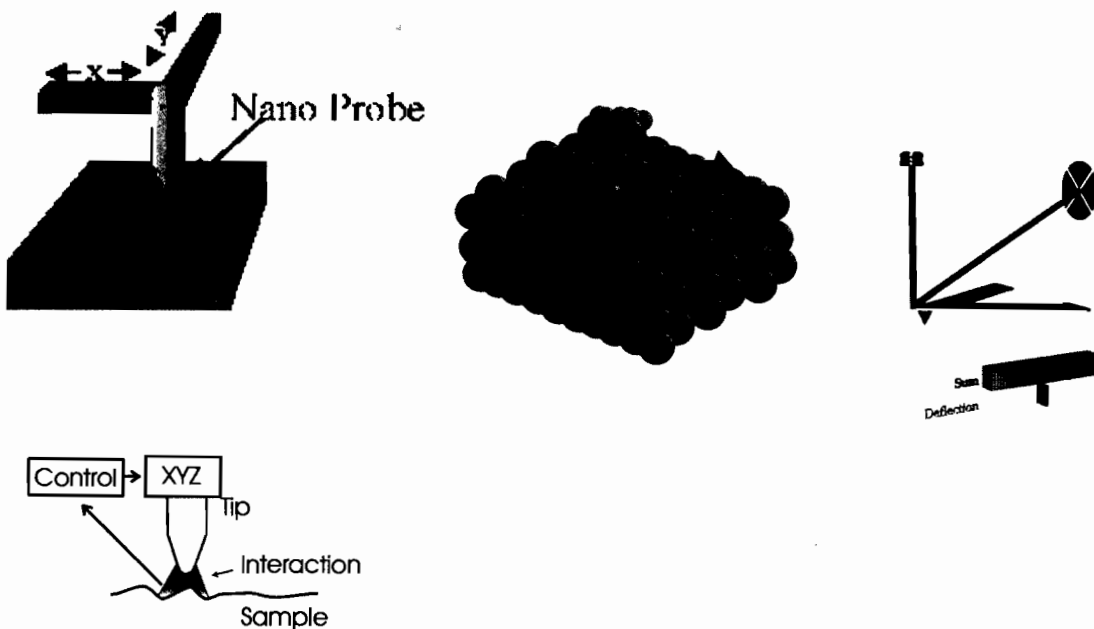


4.

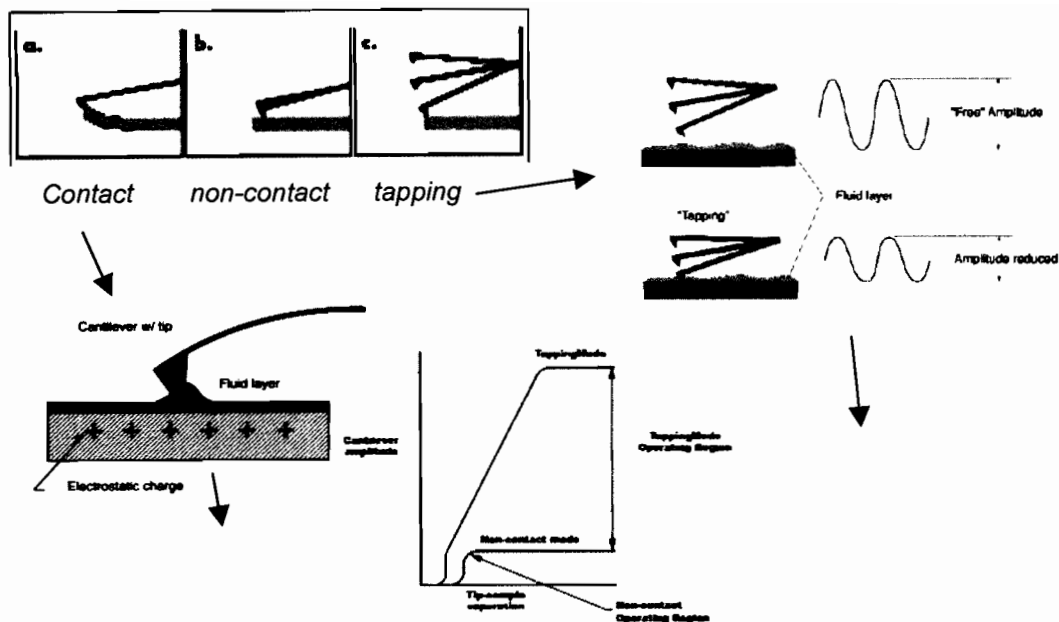
(a) Any feature can be observed, but the minimum size the image can have is $\sim \lambda/2NA$ – this is known as the *diffraction limit*. The minimum spacing between objects that can be resolved is 0.8λ , which happens when the central dip in intensity is $\geq 20\%$ of the maximum. This condition is known as the *Rayleigh criterion*. It can be overcome using evanescent waves. The reason for this is that the resolution depends on λ , which depends on $k (= 2\pi/\lambda)$. If k can be increased, the resolution will improve. As an example, if we want high resolution in the x -direction, we want to increase k_x . Now, $k_x = \sqrt{k^2 - k_y^2 - k_z^2}$ so if either k_y or k_z is complex (i.e. an evanescent wave such as you get under total internal reflection), then k_x can be greater than k , so the resolution in the x -direction can exceed the diffraction limit. The type of microscopy that attains this is the Scanning Near-field Optical Microscope, or SNOM.

(b) The answer should include a brief discussion about the probe tip, measurement of the interaction between it and the sample, the feedback loop, the actuator, different types of SPM etc.

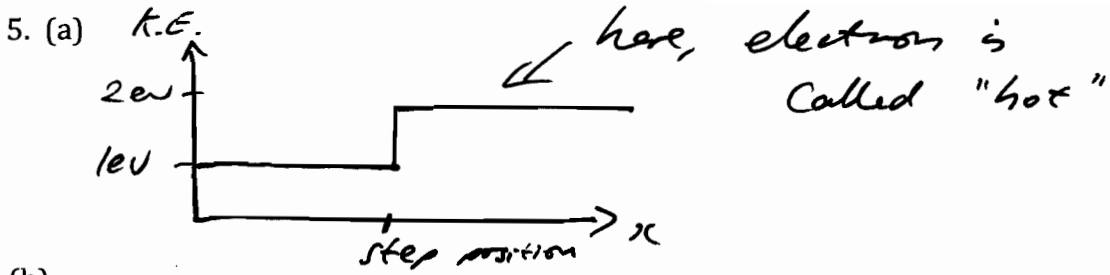
(c) The answer should include a sketch of an AFM, along the following lines:



Most commonly used modes of AFM:



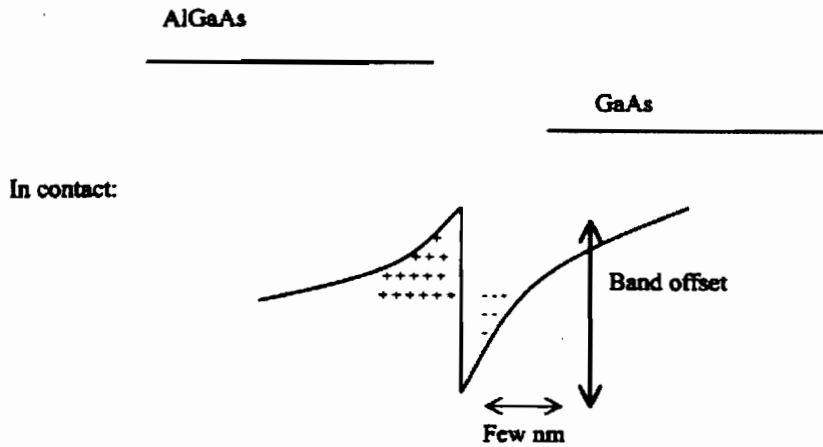
(d) The answer should include a description of conducting AFM- sources of current flow (Ohmic current, Tunneling current, field emission, and then time-dependent currents such as displacement current etc). This is a contact-mode technique whereby the tip is placed in mechanical and hopefully Ohmic contact with the sample of interest. A potential difference between the tip and sample causes a current to flow between the two, which can be measured, and the sample potential can be determined. This has a spatial resolution comparable with the tip contact radius, which is on the order 1 nm. The tip should be conductive and this can be achieved by coating a conventional tip with metal. One should be careful when scanning to not wear this coating off too quickly.



(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:



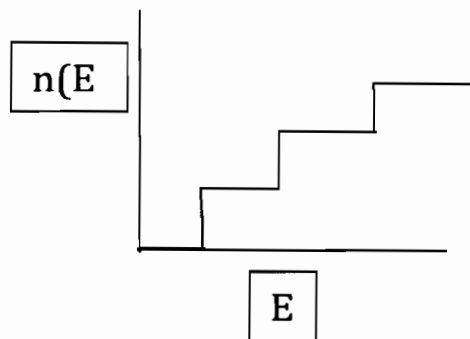
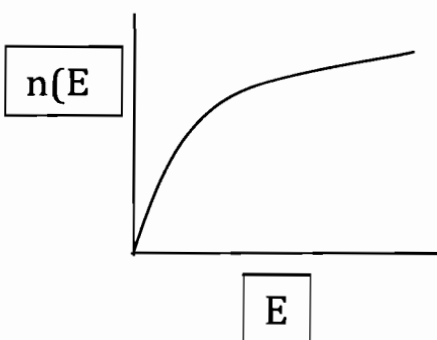
The 2-DEG is different in terms of its density of states:

3D

Q2D

$E^{1/2}$

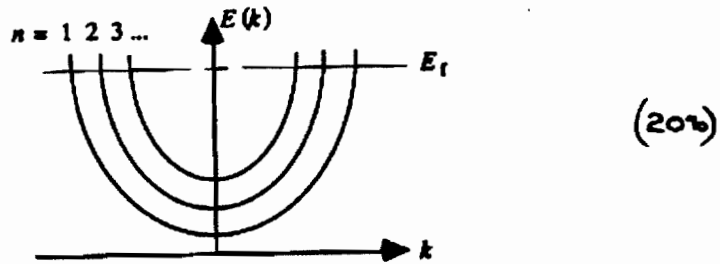
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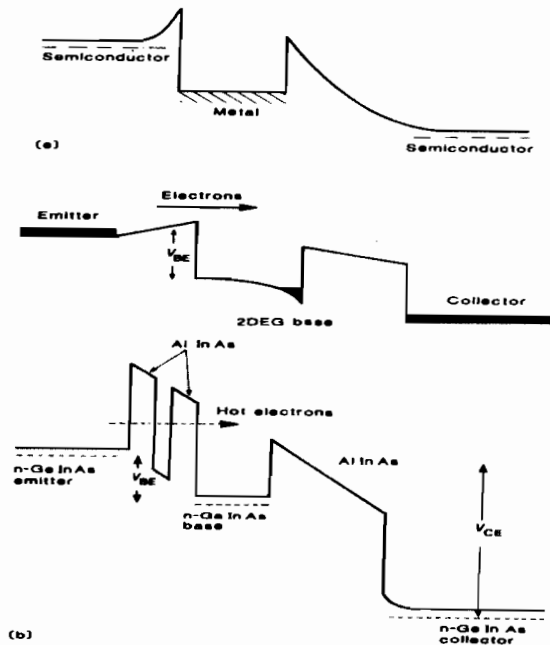
(e) Electrons in a 2-DEG are confined in one direction (z), and free to move in the other two (x, y). To be general,

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

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) The electrons in a 2DEG are essentially in an intrinsic (undoped) semiconductor, so experience very high mobility. This can be used to fabricate very high speed devices. A 2DEG can be incorporated in a device using one of the following concepts:



2DEGS are used to make quantum-well lasers, and to improve on transistor characteristics, in for example the HEMT.