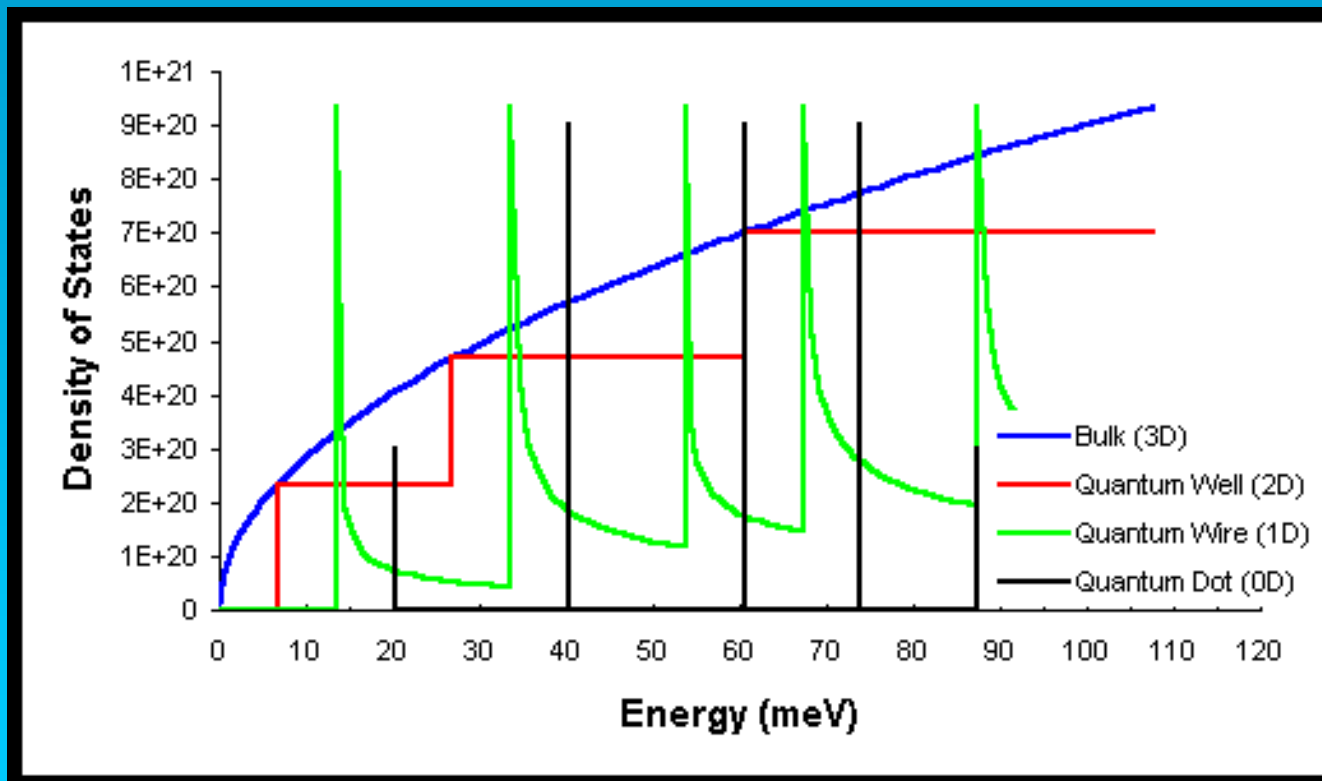
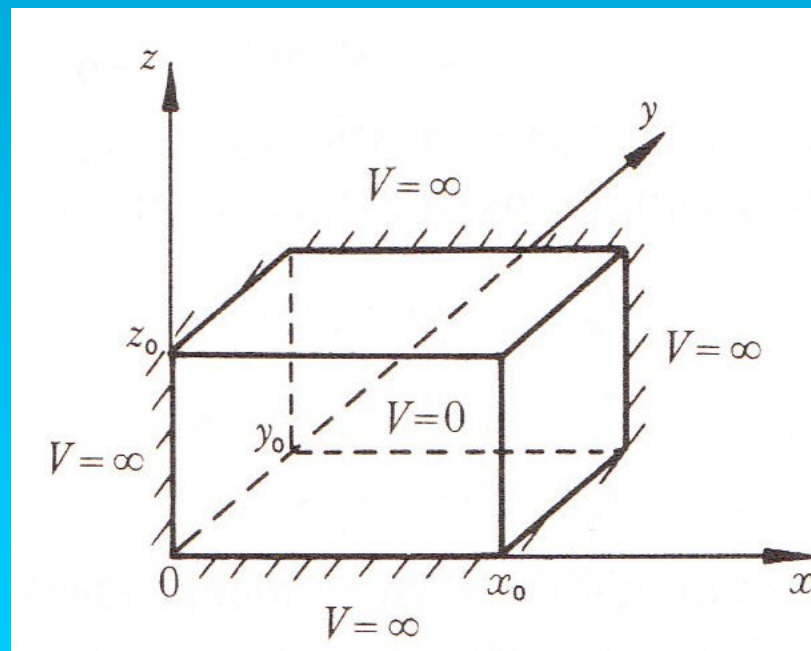


Density of states



Density of States

- For electrons trapped in a 3D potential box,



- The S equation is

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} + \frac{2m}{\hbar^2} E \Psi = 0 \quad (1)$$

- It can be shown that the wavefunction is:

$$\Psi_{n_x} \Psi_{n_y} \Psi_{n_z} = \sqrt{\frac{2}{x_o}} \sin\left(\frac{n_x \pi x}{x_o}\right) \sqrt{\frac{2}{y_o}} \sin\left(\frac{n_y \pi y}{y_o}\right) \sqrt{\frac{2}{z_o}} \sin\left(\frac{n_z \pi z}{z_o}\right) \quad (2)$$

- And substituting (2) back into (1) gives:

$$E_{n_x n_y n_z} = \frac{\hbar^2}{2m} \left[\left(\frac{n_x \pi}{x_o} \right)^2 + \left(\frac{n_y \pi}{y_o} \right)^2 + \left(\frac{n_z \pi}{z_o} \right)^2 \right]$$

- where $n_{x,y,z}$ are three quantum numbers that specify a particular energy state

If the volume is considered to be a cube of side d ,

$$E = \frac{h^2}{8md^2} (n_x^2 + n_y^2 + n_z^2)$$

Writing

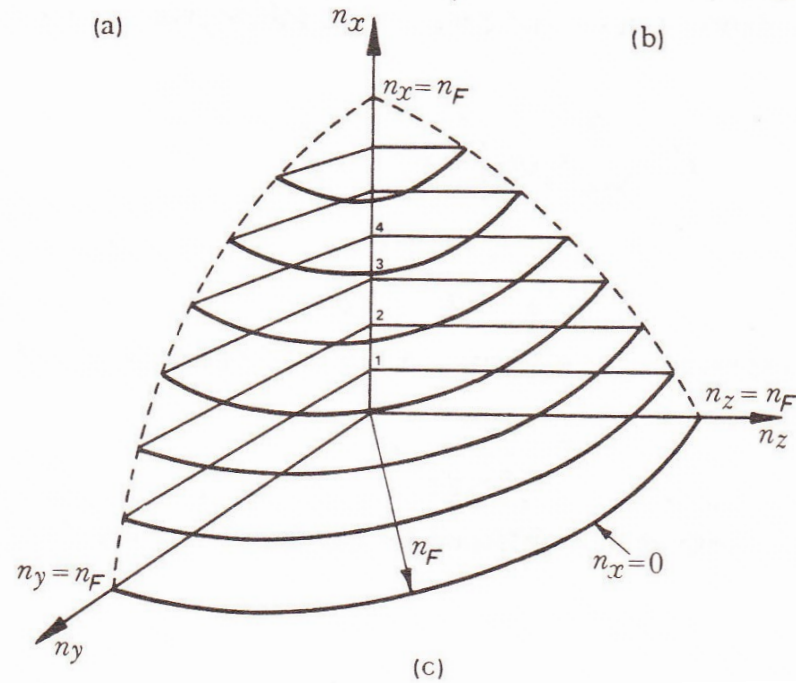
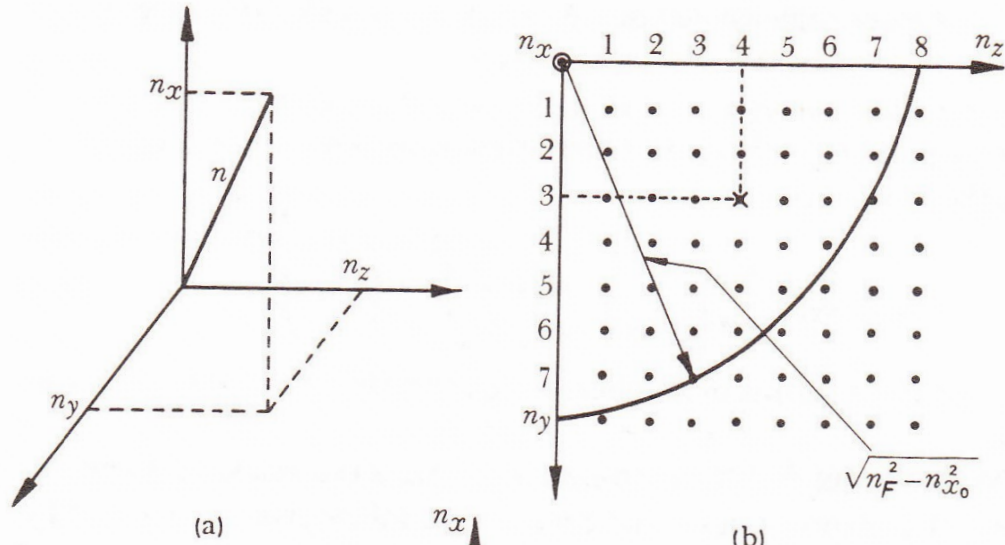
$$n^2 = (n_x^2 + n_y^2 + n_z^2)$$

The expression for eigenvalues of electrons in a cubical potential box is:

$$E = \frac{h^2}{8md^2} . n^2 \quad (3)$$

Maximum number of possible energy states

- It is instructive to find the maximum number of possible energy states for which n is less than some maximum value n_F .
- A particular value of n , which has components n_x, n_y, n_z all positive integers, can be visualised in n -space.



- In order to count the number of possible combinations of (n_x, n_y, n_z) up to a max. n_F , it is easier to assume first that n_x is fixed at some value n_{x0} , say and consider a plane which is a section through n -space. Each point in the diagram represents a particular combination of n_y and n_z . Make the area of this plane to be numerically equal to the number of possible combinations of n 's enclosed by the area.

$$n^2 - n_{x0}^2 = n_y^2 + n_z^2$$

Therefore, the total number of combinations of $(n_x, n_y, n_z) \leq n_F$, is numerically equal to that of a sphere of radius n_F which is contained in the 1st quadrant of n -space

$$= 1/8 (4/3 * \pi n_F^3) = \pi n_F^3 / 6$$

Including spin, \rightarrow 2 spin states for any combination of n quantum numbers

Total number of possible energy states

$$= 2 (\pi n_F^3 / 6) = \pi n_F^3 / 3$$

- This gives the total number of available energy levels. These are not in general necessarily all occupied by electrons. We shall assume, at this moment, all states are occupied up to max. energy state n_F . If the number density of electrons in the box is N
- $Nd^3 = \pi n_F^3/3$

Or

$$n_F = \left(\frac{3N}{\pi} \right)^{1/3} d$$

The energy of the highest occupied state is

$$E_{F_o} = \frac{h^2}{8m} \left(\frac{3N}{\pi} \right)^{\frac{2}{3}}$$

by substituting in (3)

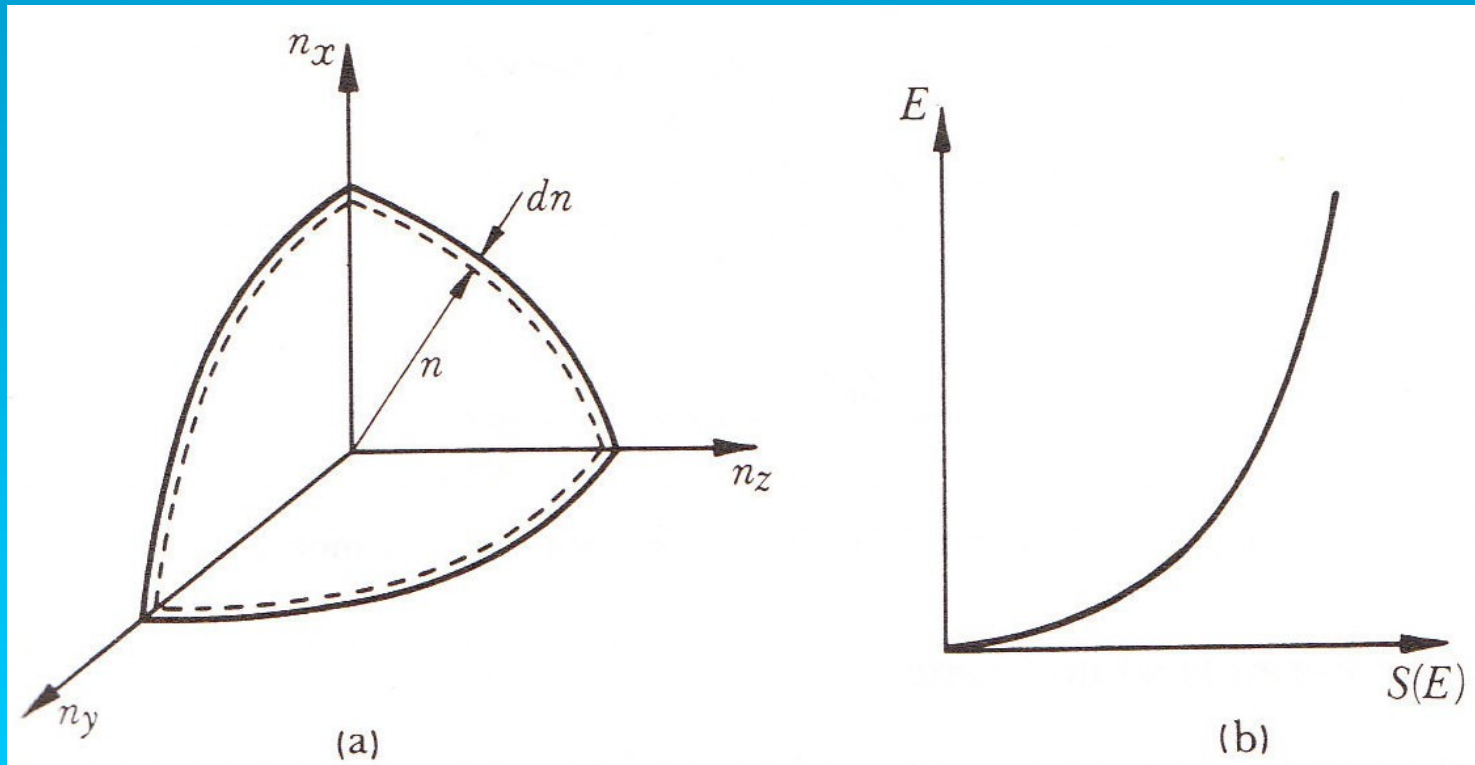
This maximum energy corresponds to the Fermi energy of a metal at 0K.

The energy distribution of electrons in a metal

In order to find out the energy *distribution* among the free electrons in a metal, it is necessary to determine the energy distribution of allowed energy levels which are available for occupation by the electrons. i.e. the number of available energy states lying in the range, say, between E and $E + dE$, is required.

- Define a function $S(E)$, called the density *distribution* of available states, so that $S(E)dE$ is the number of available states/unit volume in the energy range considered.
- In the energy range dE , there will be a corresponding range of quantum numbers dn .
- Therefore, consider a spherical shell in n -space of radius n and thickness dn , the number of states between n and $n + dn$ is equal to the volume of shell in 1st quadrant $\times 2$ (spin)

The distribution function $S(E)$



Therefore, the no. of available states in the range is

$$2(4\pi n^2 dn)/8 = \pi n^2 dn$$

$$\text{which} = S(E) dE \cdot d^3$$

$$\text{Therefore } S(E) = \pi n^2/d^3 \cdot dn/dE \quad (4)$$

Equ. (3) can be differentiated to give

$$n^2 \frac{dn}{dE} = \frac{8\sqrt{2} m^{\frac{3}{2}} d^{\frac{3}{2}} E^{\frac{1}{2}}}{h^3}$$

substituting in (4) gives

$$S(E) = \frac{8\sqrt{2}\pi m^{\frac{3}{2}}}{h^3} E^{\frac{1}{2}}$$

which is the density distribution of available states.

- The total number of available energy level/unit volume in a given energy range dE , is obtained by multiplying this distribution function $S(E)$, by the size of the range, to give, the number of available states/unit vol./unit of energy centred at E .

- However, not all the available energy states are filled \rightarrow determined by the probability that an electron can possess energy E .
- Such a probability is given by the Fermi-Dirac function $p(E)$
- Therefore, the number of electrons/unit volume in a given energy range depends not only on the number of available states in the range, but also on the probability the electrons can acquire sufficient energy to occupy the states.

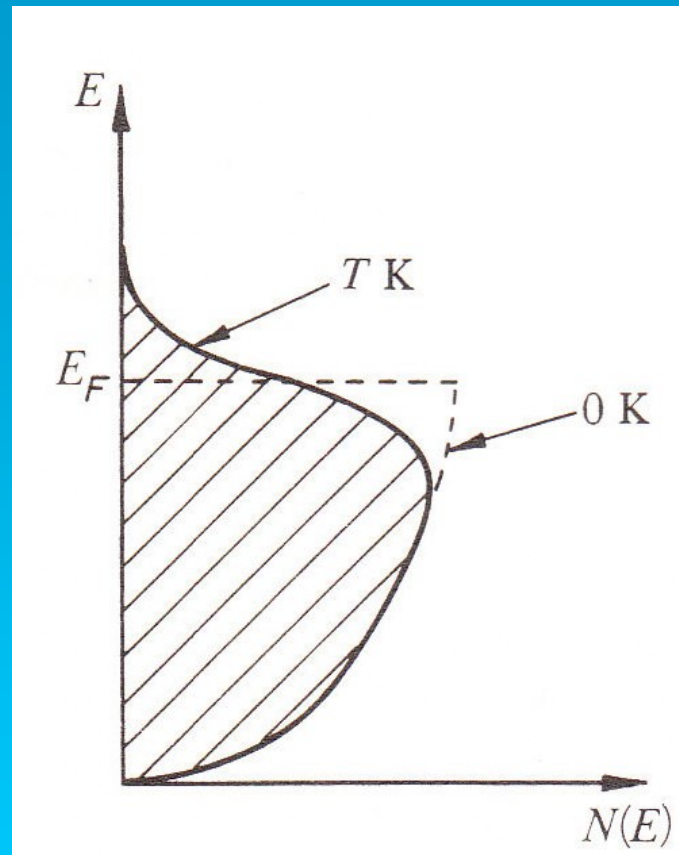
number of electrons/unit volume with
energies between E and $E + dE$

= (number of available states/unit volume in
the range E and $E + dE$) \times (the prob. that a
state of energy E is occupied)

$$N(E) dE = S(E) dE \cdot p(E)$$

where $N(E)$ is the number of electrons/unit
vol./unit of energy centred at E .

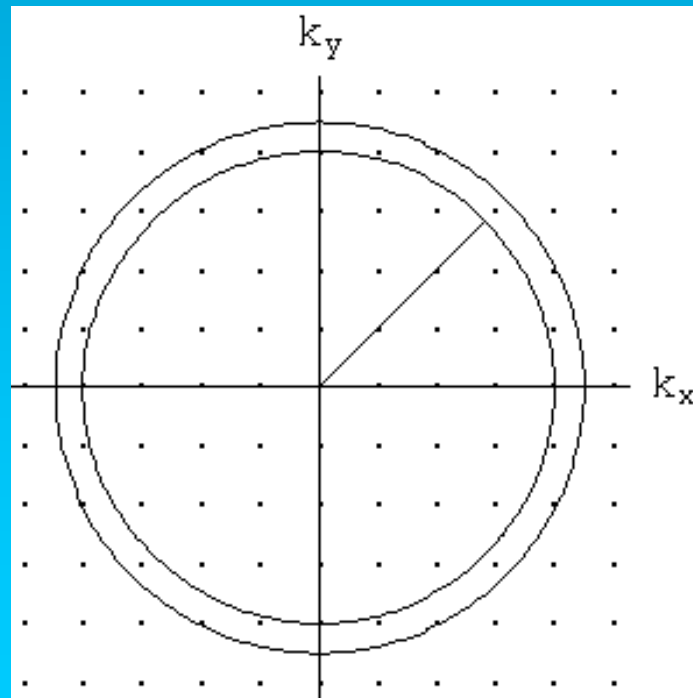
Therefore, $N(E) = S(E) \cdot p(E)$



At 0 K , states are filled up to E_F . At $T\text{ K} \rightarrow$ high energy tail with energy $> E_F$

2D density of states

In 2D, $S(E) dE \rightarrow$ number of states/unit area in the energy range considered.



2D density of states

In k-space, where $k = 2\pi/l$, ($k=2\pi$; area = k^2)

$$S(E) dE (2\pi)^2 = 2 \times 2\pi k dk$$

$$S(E) = (dk/dE) \cdot k / \pi$$

$$S(E) = \frac{m}{\hbar^2 \pi} \cdot n$$

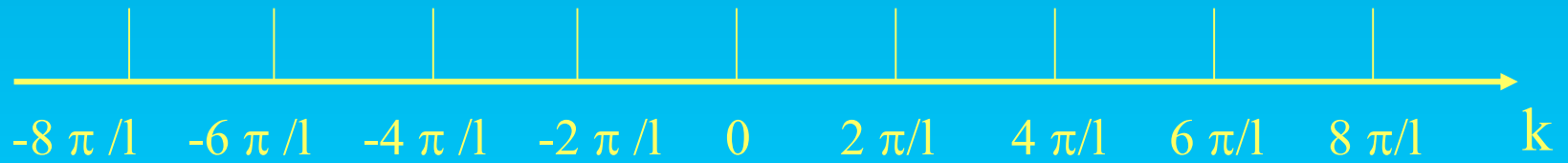
$$\left(E = \frac{\hbar^2 k^2}{2m} \right)$$

where $n = 1, 2, 3, \dots$

Density of states in 2D is independent of energy \rightarrow 2D subbands

1D density of states

In 1D, $S(E) dE \rightarrow$ number of states/unit length in the energy range considered.

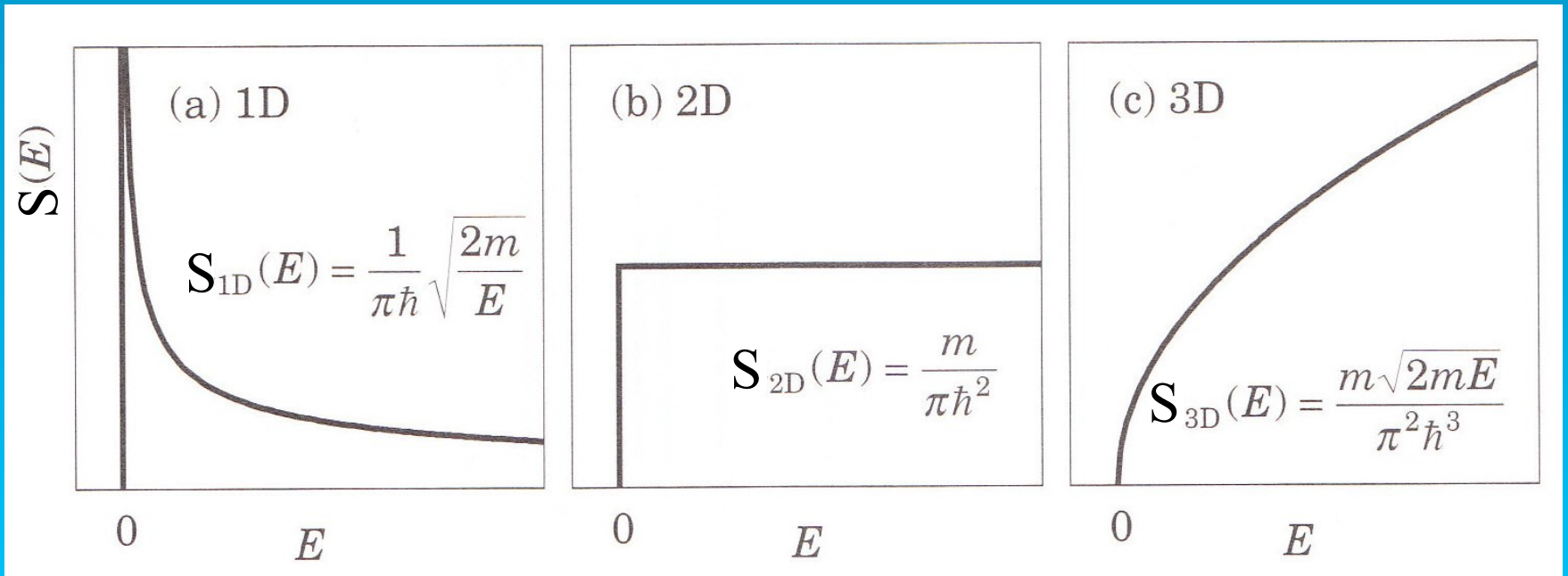


1D density of states

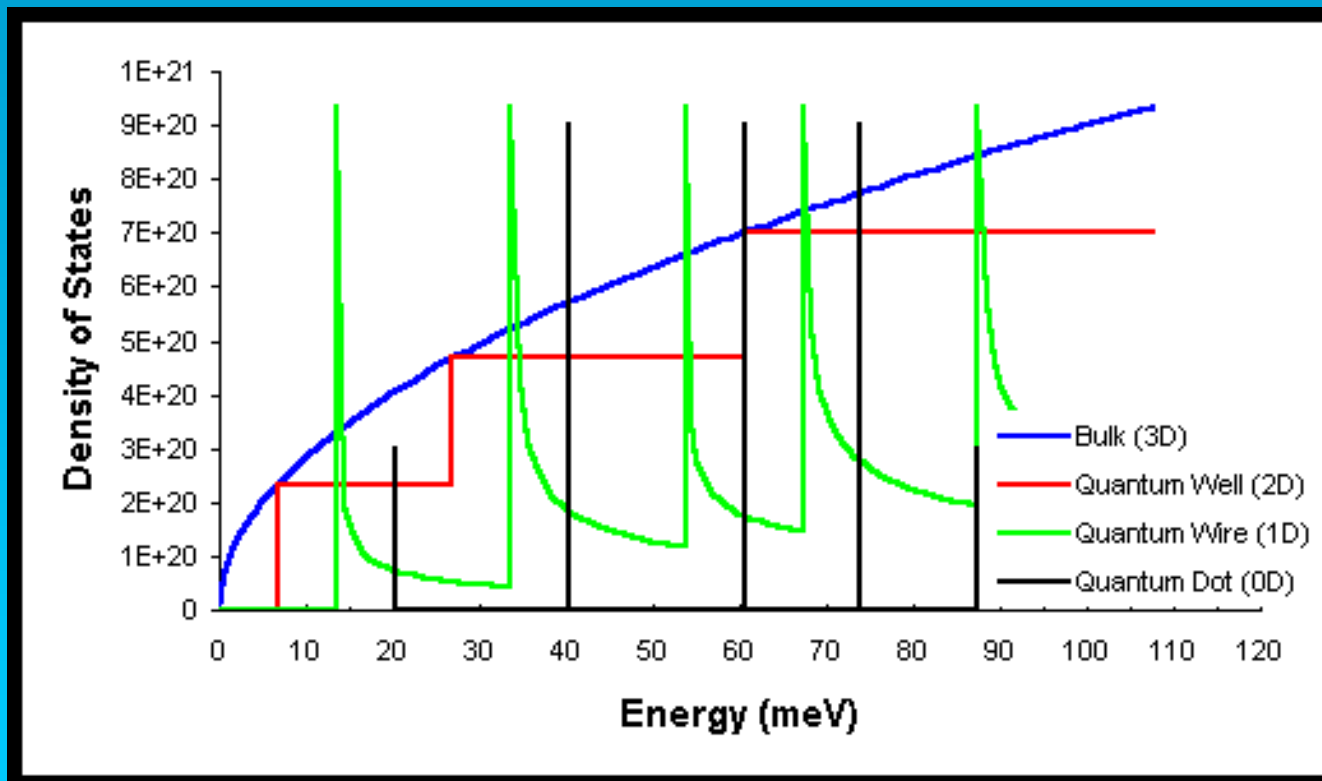
- In k-space, where $k = 2\pi/l$
- $S(E) dE (2\pi) = 2 \text{ (spin)} \times 2 \text{ (for } k>0 \text{ and } k<0) \times dk$
- $S(E) = (dk/dE) \cdot (2/\pi)$

$$= \frac{1}{\pi \hbar} \sqrt{\frac{2m}{E}} \quad \left(E = \frac{\hbar^2 k^2}{2m} \right)$$

Density of states in 1D \rightarrow 1D subbands



Density of states



quate generation of $(\text{CH}_3)_3$ species for reaction.

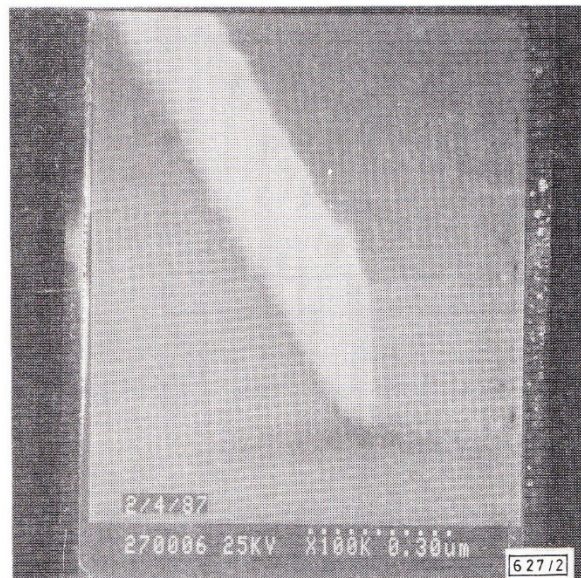
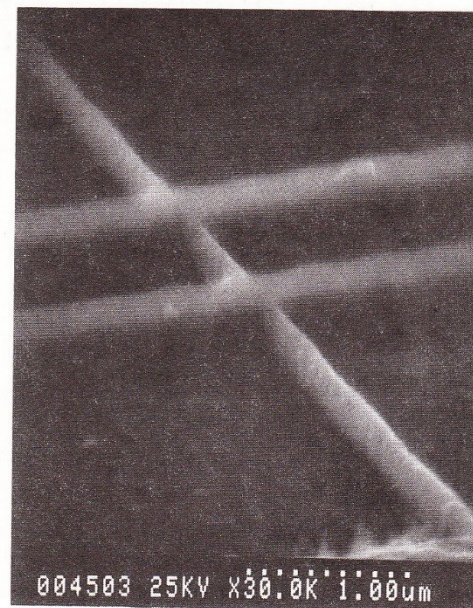
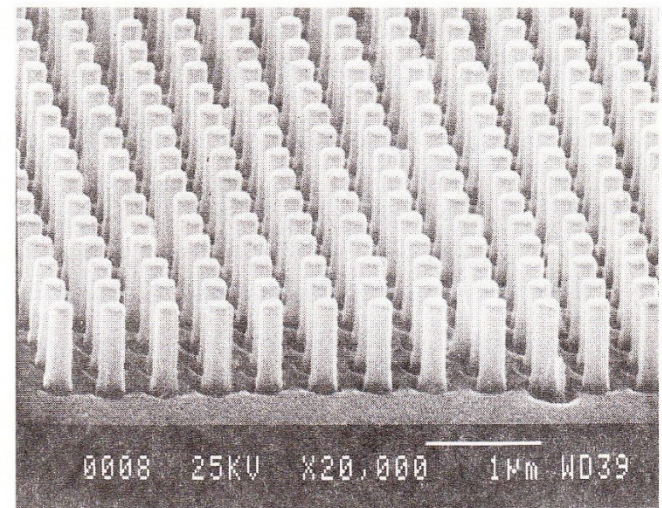
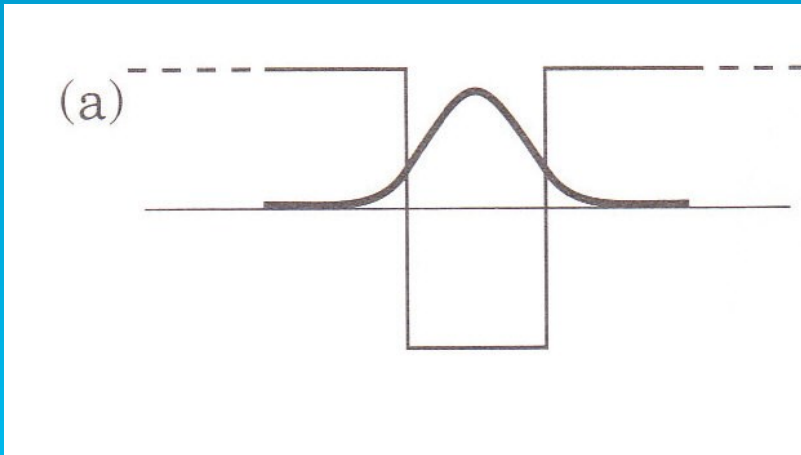


Fig. 2 SEM micrograph showing a 30 nm-wide wire after etching w

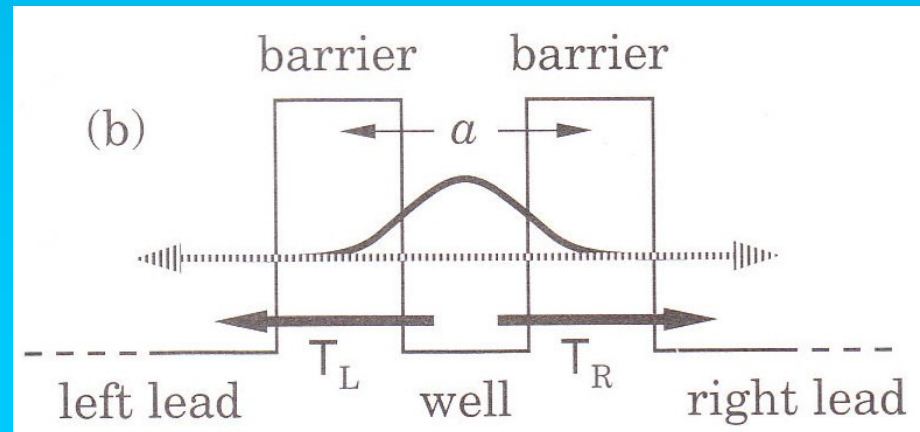


Resonant tunnelling

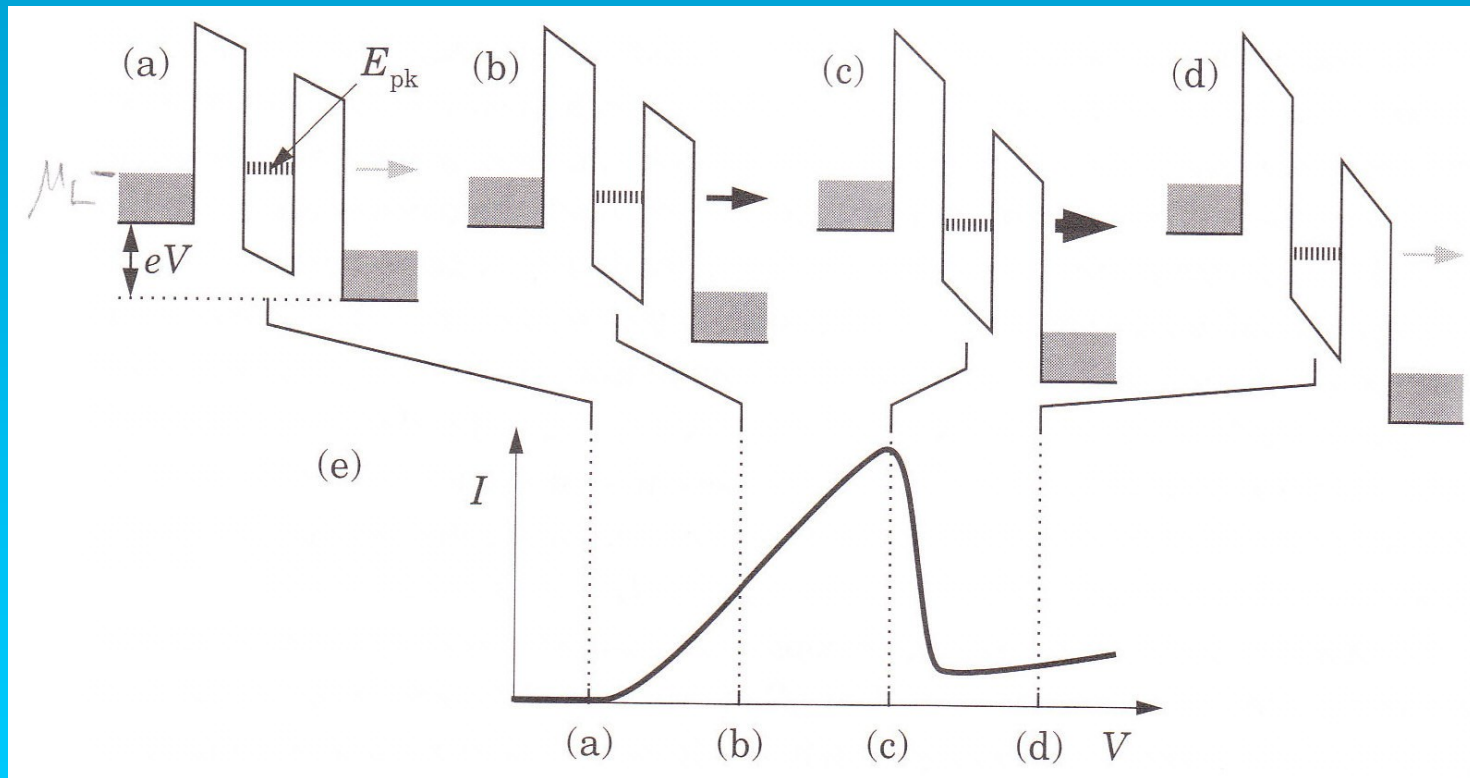


Leaky wavefunction in a finite 1D well

Wavefunction can tunnel through well into the next barrier – electron tunnelling



Resonant tunnelling devices



Tunnel current

$$I \propto \int_0^{\infty} T(E) f(E) S(E) dE$$



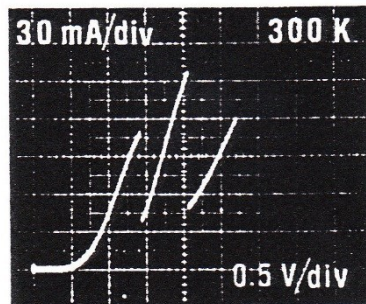
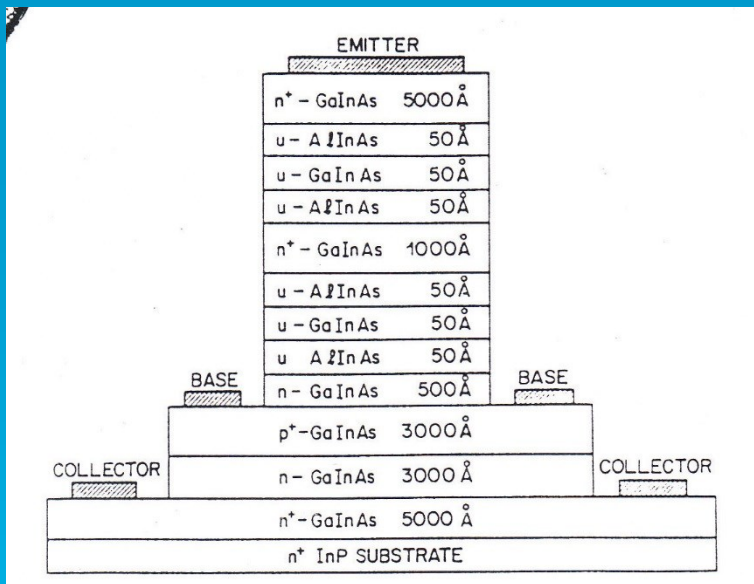
Tunnelling probability
for an electron with
energy E



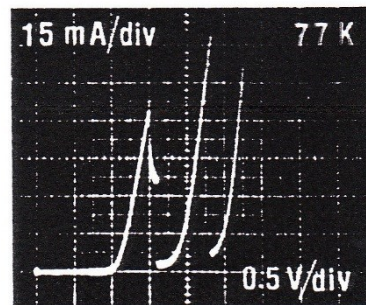
Fermi-dirac
distribution



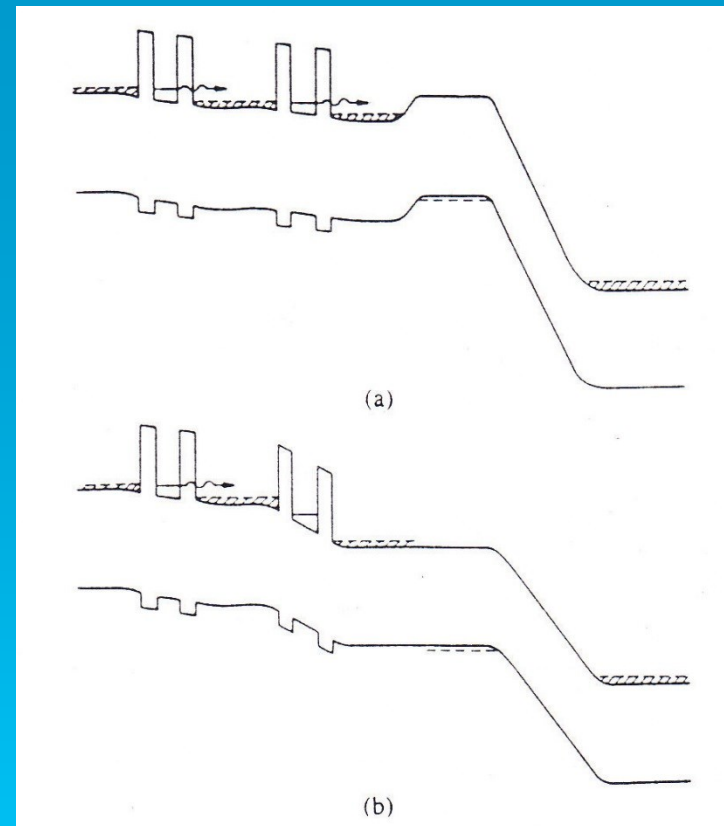
Density of states



(a)

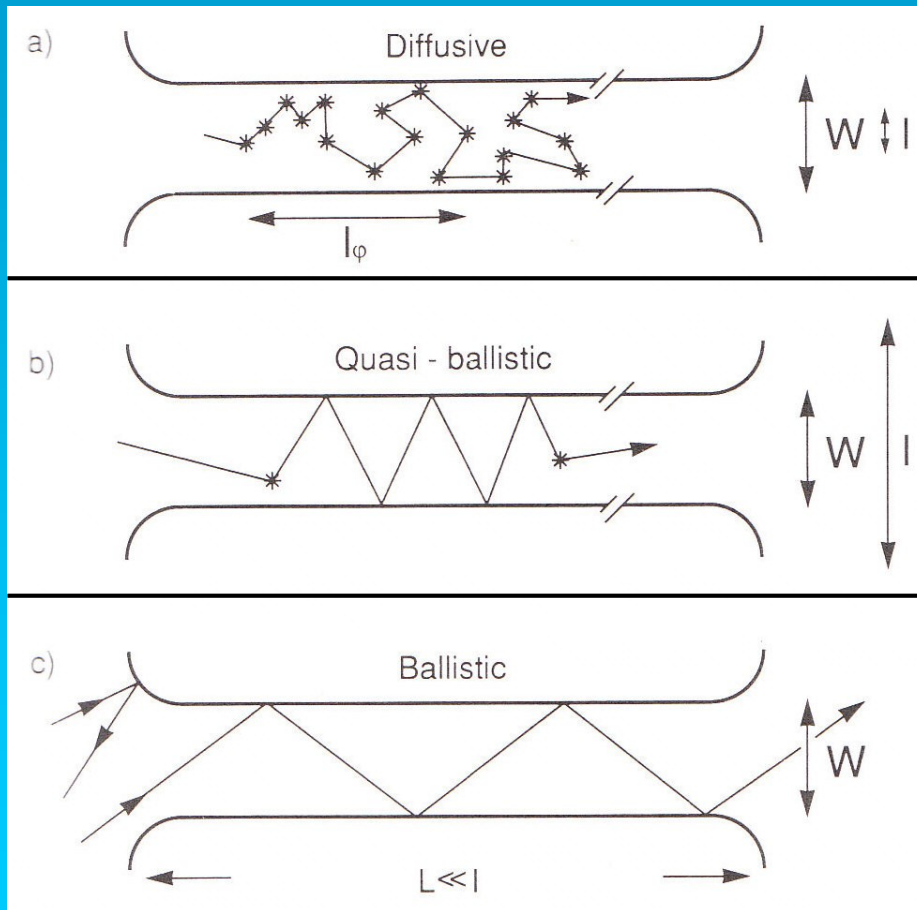


(b)



Multiple state resonant tunnelling BJT;
IEEE Trans. Elec. Dev.
(1989)

Low dimensional structures



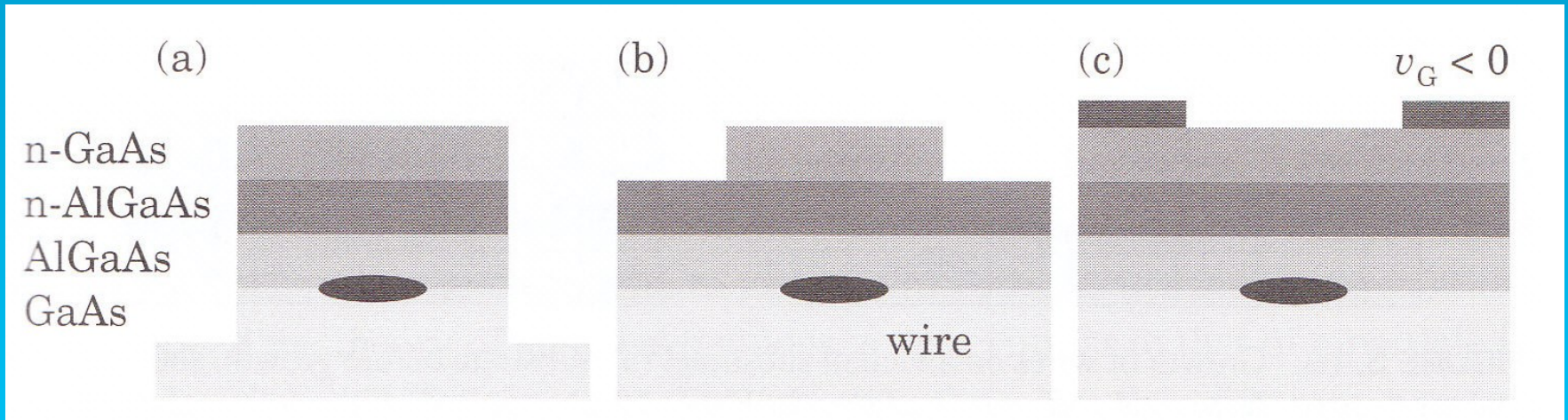
l is mean free path

l_ϕ is phase coherence length

w is width of the structure

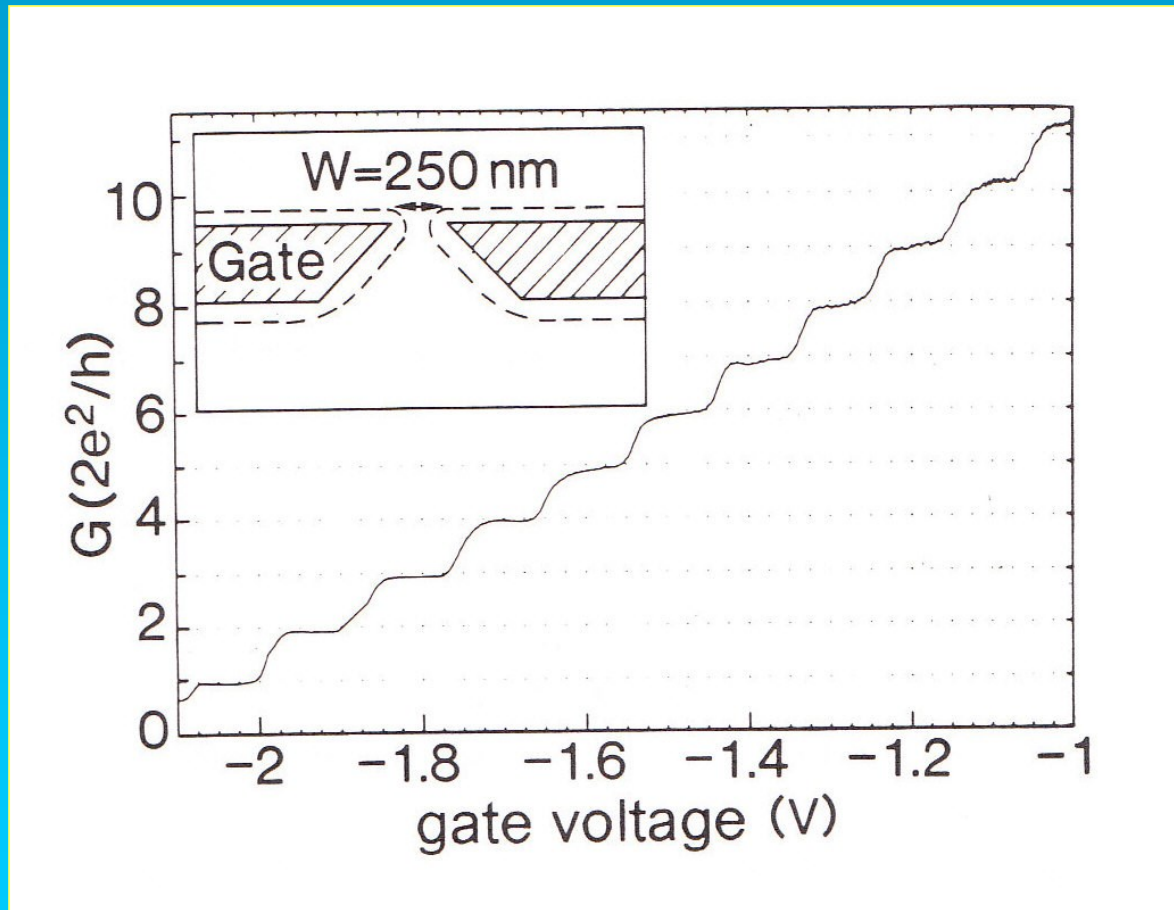
L is length of the structure

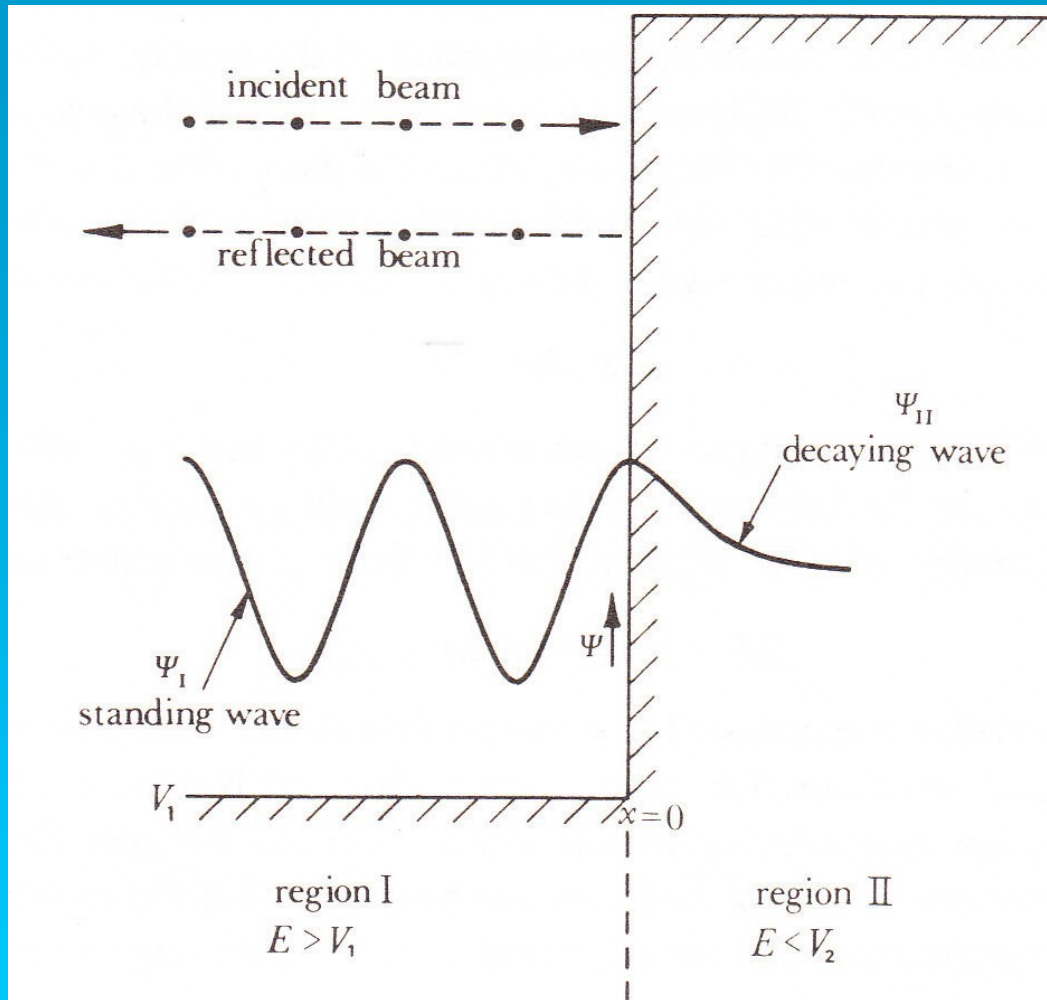
Confinement in one-dimension



Confinement to one-dimension wire structure from a 2DEG in
a) by deep etching; b) by shallow etching; c) by applying a
negative voltage onto split gates

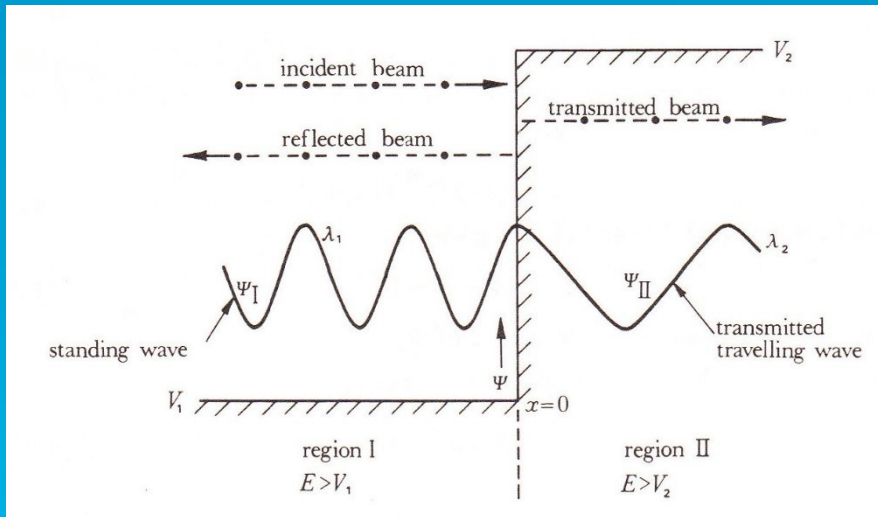
Quantised conductance





Tutorial 1

1st case

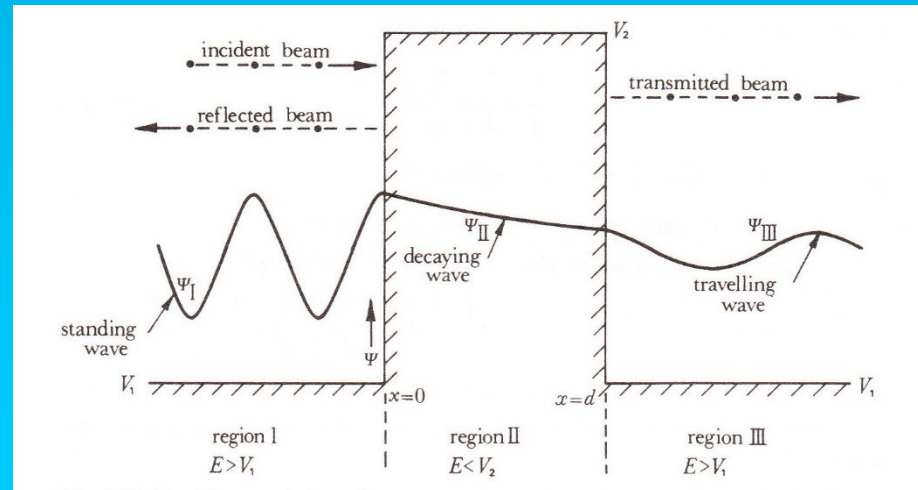


Tutorial 2

2nd case

Tutorial 2

3rd case



Single electron transistors



- when $E_{\text{ch}} = e^2/2C > kT/e$
- $C \sim \text{fF}$
- area of $C \sim \text{few nm}^2$

