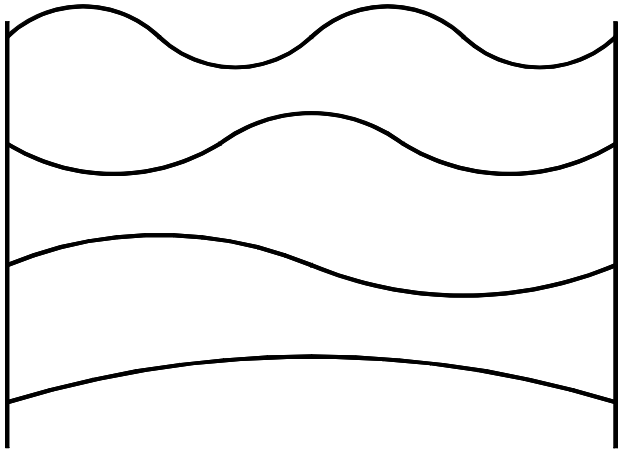
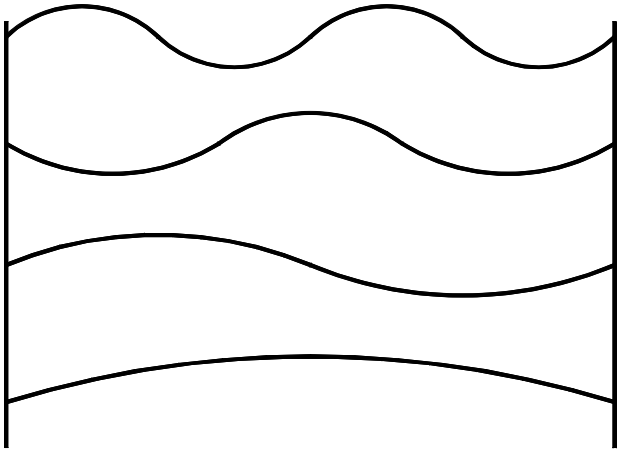


Vibrational modes on a stretched string.
The string is constrained so that it is fixed at each end.
The possible waves which can be present on the string correspond to an integral number of half wavelengths.

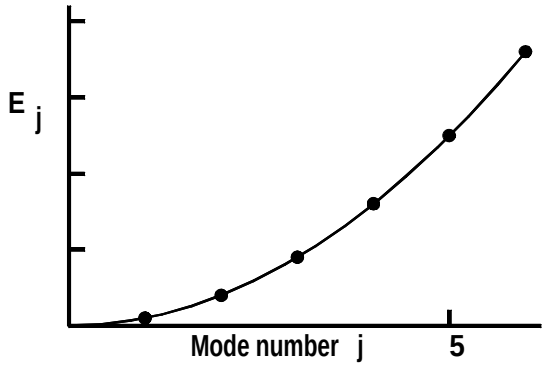
In quantum mechanics, a particle such as an electron is described by a wave function.
Electron constrained in a one dimensional box with rigid ends.
Solution of Schrödinger equation describes the system
similar mathematical form to the differential equation which describes the vibration of a string



Difference is that the vibrational modes of the string can have any energy
A particular mode for a particle in a box has an energy is given by

$$E_j = E_1 j^2$$

where
j is an integer,
E_1 is the energy of the lowest energy mode
E_j is the energy of the jth mode.

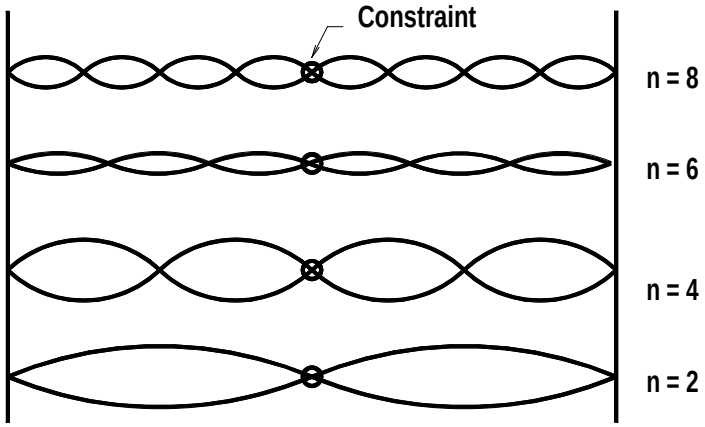


Plot of energy versus mode number.

The discrete modes lie on the parabola,

$$E_j = E_1 j^2$$

indicated by circles.



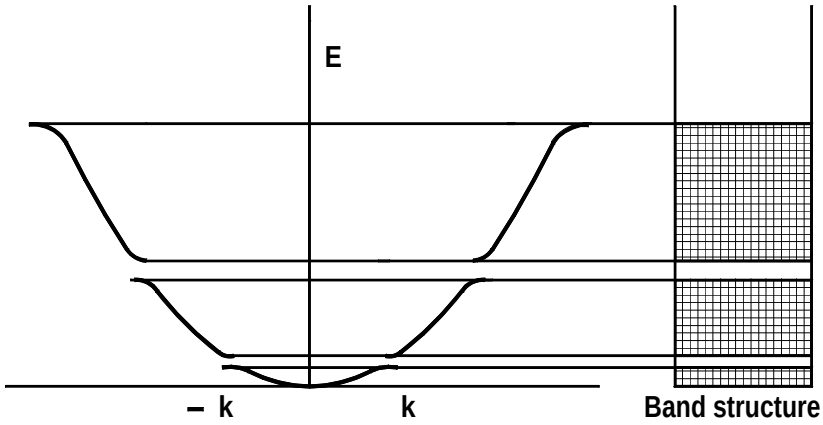
Loosely constrain the string at the centre
Vibrations of the odd numbered modes, for which $j = 1$, $j = 3$, $j = 5$ etc., are inhibited.
Constraint acts to 'forbid' a mode.

Electron in a one dimensional box.
Atoms regular intervals in the box form a one dimensional crystal
Some of the solutions or modes obtained for Schrödinger's equation are forbidden.
Within the crystal only electrons with certain wave vector values, k, can propagate through the crystal without being scattered by the atoms.

In a crystal, the quantized wave vector specifies the electron momentum, k,
Energy is given by

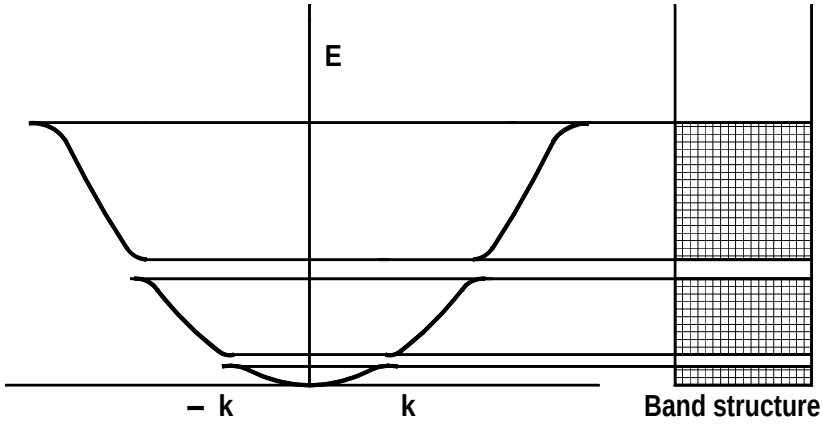
$$E(k) = \frac{h^2 k^2}{4\pi^2 2m^*}$$

where
h is Planck's constant
m^* is the effective electron mass.
Waves propagate in both directions,
k can have positive or negative values
N distinct modes or values of k
where $N = \frac{l}{a}$
a is the lattice size (lattice constant)
l is the length of the crystal.
Set of distinct modes called a Brillouin zone.

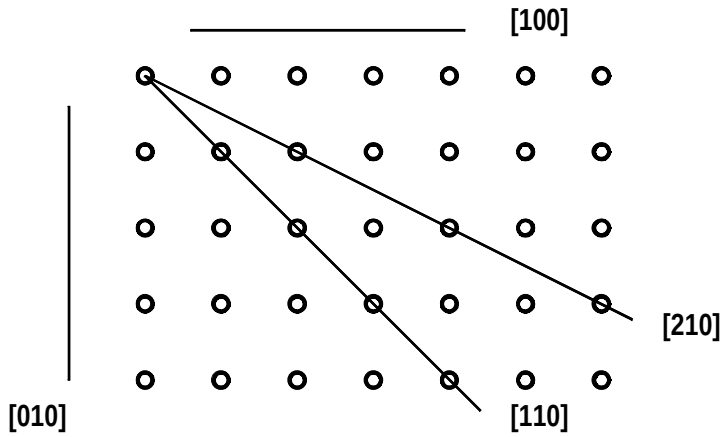


Energy levels and band structure.

When k exceeds the value of $\frac{\pi}{a}$
Momentum values differ by multiples of $\frac{2\pi}{a}$
Within the crystal multiples are indistinguishable due to interchanges of momentum between electrons and phonons



Energy continues to increase along the parabolic curve and moves into a new Brillouin zone.
It is possible to have electrons which have the same momentum within the crystal but have significantly different energies.
Localized bending of the E–k curve) at transition leaves a band gap where there are no energy states
Resulting in a forbidden band.



In a real three dimensional crystal the electron wave functions can propagate along each of the principal axes of the crystal in the [100], [010] and [001] directions.
Also propagation in diagonal directions
Spacing between the planes in the crystal is different for these diagonal directions, leading to different and distinct E–k curves.

Electrons in the lower atomic orbitals remain tightly bound to the individual atoms.
Outer shell valence electrons can no longer be considered to be attached to individual atoms
Delocalized throughout the crystal
Distribution corresponding to the amplitudes of the wave functions.

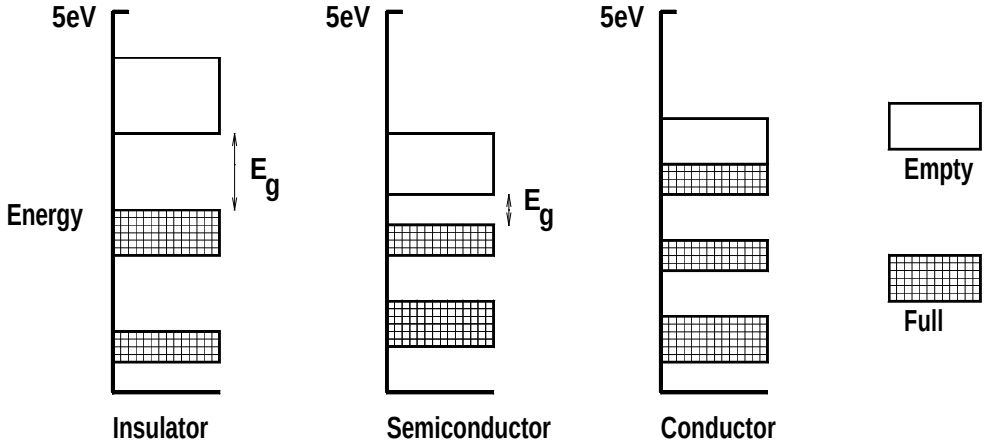
Since electrons are fermions, the Pauli exclusion principle applies

No two electrons can have the same set of quantum numbers

The available states fill up from the lowest energy states to a level called the Fermi level, E_F.

The probability of an electron having an energy E is given by:

$$P(E) = \frac{1}{1 + e^{\frac{(E-E_F)}{kT}}}$$



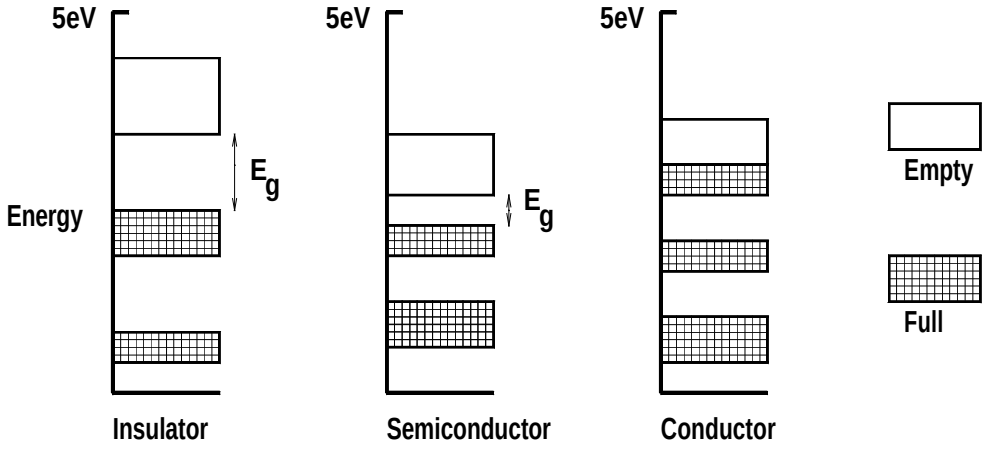
In insulators the available electrons fill lower valence bands completely

No electrons in the next band up in energy.

Energy gap or band gap between the highest full band and the lowest empty band is large, usually greater than 3 eV,

No mechanism for exciting significant numbers of electrons into the upper band

No electron movement.

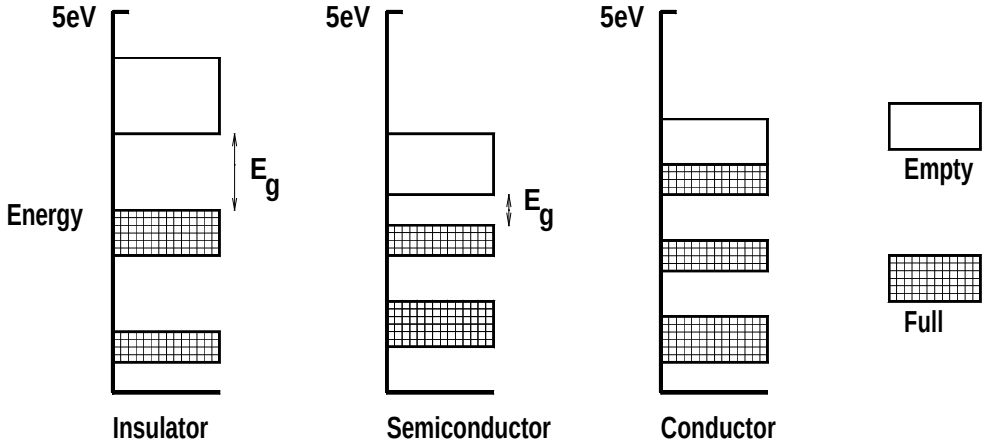


In semiconductors energy gap $\approx 1\,\text{eV}$.
Thermal vibrational modes or phonons

$$E_{Phonon} = kT = 1.38 \times 10^{-23} \times 293$$

$$= 4.04 \times 10^{-21}\,\text{joules} = \frac{4.04 \times 10^{-21}}{1.6 \times 10^{-19}} = 0.025\,\text{eV}$$

Phonon to electron energy transfer
Resistivity of a semiconductor decreases with increasing temperature
Negative temperature coefficient of resistance.



For conductors upper band partially filled
Free electron movement in crystal
High conductivity and a low resistivity.
Electric field accelerates electrons
Electrons collide with the vibrating atoms of the crystal via electron-phonon interactions.
Collisions randomize the imposed velocity
More collisions at higher temperature
Metallic conductors therefore have a positive temperature coefficient of resistance

Material	Resistivity, ρ, Ω m	Sign of TC of R
Glass	10^{10}	
Silicon	2000	$-$
Germanium	0.5	$-$
Copper	1.7×10^{-8}	$+$

There is a factor of $\approx 10^9$ change in the resistivity in going from one group to the next.

In a pure or intrinsic semiconductor material, if an electron is excited up into the conduction band, there will be electrical conduction due to this movable electron.
In semiconductors the hole left in the valence band by the excited electron can be considered as a positive charge carrier
An adjacent valence electron can hop into the hole to give an effective movement of the hole in a direction opposite to the direction of movement of the electron which hopped.
Therefore, we have p-type carriers or holes which can also move through the lattice.

Electrons and holes behave similarly and their behaviour is modelled using Fermi-Dirac statistics.

Consequence is that the probability that a particular energy level, E, is occupied is given by the Fermi-Dirac distribution function:

$$P(E) = \frac{1}{1 + e^{\frac{(E-E_F)}{kT}}} \approx 1 - \exp\left(\frac{E - E_F}{kT}\right)$$

where E_F is the Fermi level energy.

Exponential function leads to similar exponential functions appearing in the equation which describes variation of current as a function of applied voltage in a diode.

Extrinsic semiconductors

Silicon or germanium, doped with small quantities of either Group III (boron atoms) which act as acceptors for electrons

to reduce the free electron concentration and give p-type semiconductor material

OR

Group V (phosphorous atoms) which act as donors of electrons to increase the free electron concentration and give n-type semiconductor material.

If n is the electron concentration,
p is the hole concentration
and n_i is the carrier concentration in the intrinsic material

$n \times p = n_i^2$ (The semiconductor equation)

If n-type concentration goes up then p-type concentration goes down
In n-type material, n-type carriers (electrons) are the majority carriers and p-type carriers (holes) are the minority carriers and conversely for p-type material.

Concentrations other than those predicted by $n \times p = n_i^2$
got by injecting p-type holes into an n-type region
by applying appropriate voltages to some fabricated structure in the semiconductor crystal
Base region in a transistor.
Stop injection process and the system returns to thermal equilibrium
$n \times p = n_i^2$ applies once more.