# Band Theory of Solids

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# Syllabus

**Electrical and magnetic materials**: Conducting and resistor materials, and their engineering application; Semiconducting materials, their properties and applications; Magnetic materials, Soft and hard magnetic materials and applications; Superconductors; Dielectric materials, their properties and applications. Smart materials: Sensors and actuators, piezoelectric, magnetostrictive and electrostrictive materials.

CLO: Classify engineering materials based on its structure.

# Materials Based on electrical resistivity

Resistivity range in Ohm m ⇨ *25 orders of magnitude*

Metallic materials

Semi-conductors

| $10^{-9}$ | $10^{-7}$ | $10^{-5}$ | $10^{-3}$ | $10^{-1}$ | $10^{-1}$ | $10^{3}$ |
|---|---|---|---|---|---|---|
| Ag<br>Cu Al<br>Au | Ni<br>Pb | Sb Bi<br>Graphite | Ge<br>(doped) | Ge | | Si |

Insulators

| $10^{5}$ | $10^{7}$ | $10^{9}$ | $10^{11}$ | $10^{13}$ | $10^{15}$ | $10^{17}$ |
|---|---|---|---|---|---|---|
| Window glass<br>*Ionic conductivity* | | Bakelite | Porcelain<br>Diamond<br>Rubber<br>Polyethylene | Lucite<br>Mica | PVC | $SiO_2$<br>(pure) |

# Electrical conductivity



For many solids, conductivity depends on number of electrons participating in conduction process.

No. of participating electrons is related to

1. Arrangement of electron states or levels with respect to energy,
2. The manner in which these states are occupied by electrons.

# Free electron theory

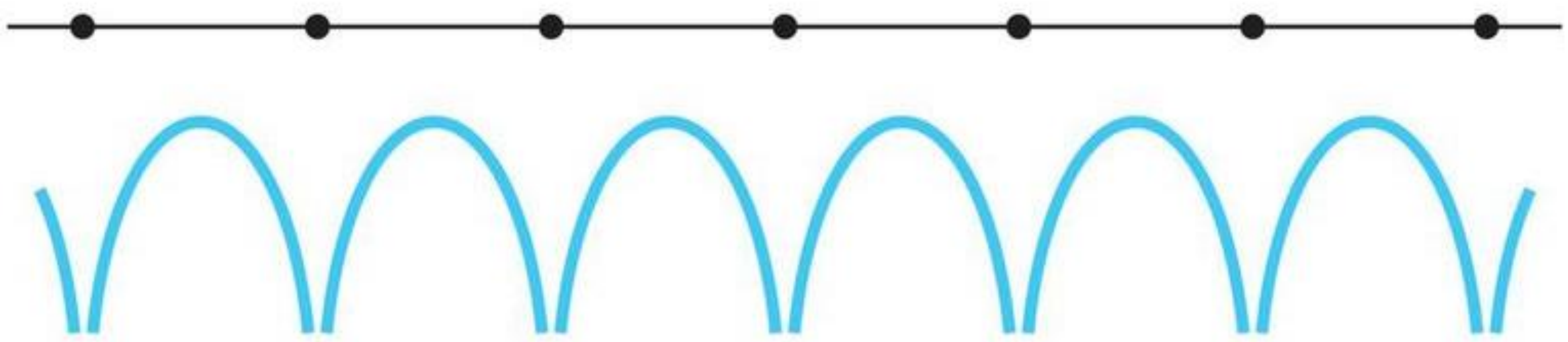


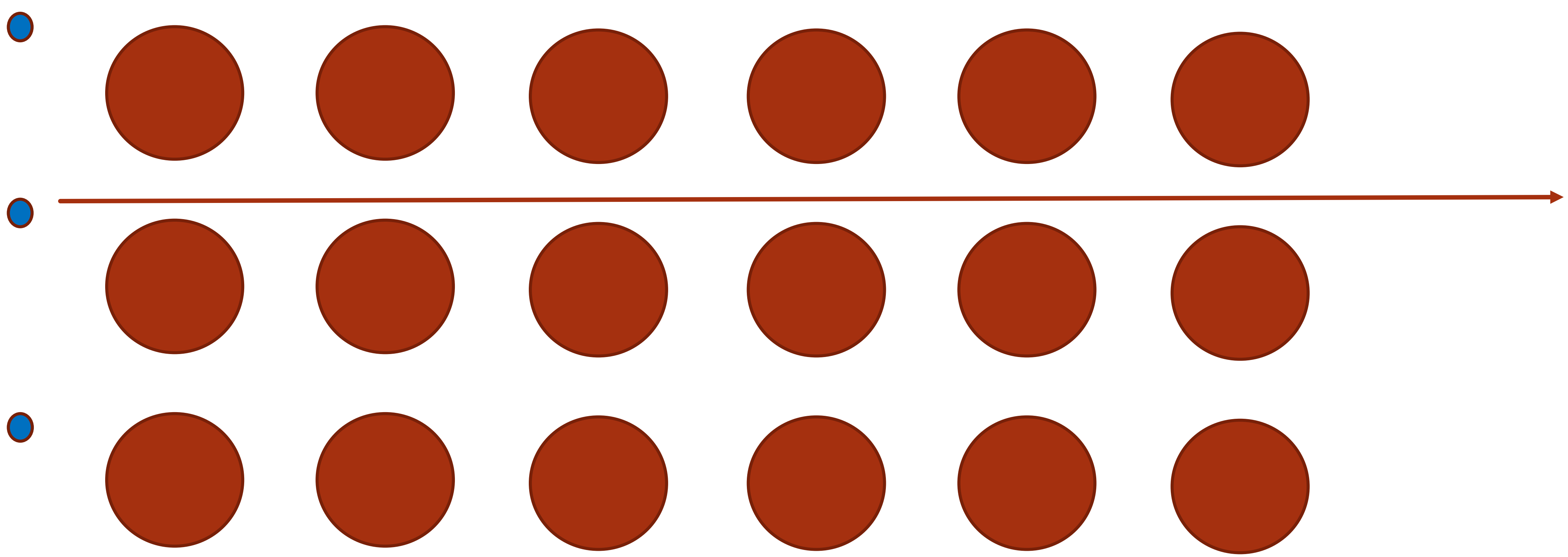
1. Outermost electrons of the atoms take part in conduction.
2. These electrons are assumed to be free to move through the whole solid ➔ Free electron cloud / gas, Fermi gas.
3. Potential field due to ion-cores is assumed constant $\Rightarrow$ potential energy of electrons is not a function of the position (constant negative potential).
4. The kinetic energy of the electron is much lower than that of bound electrons in an isolated atom.

# Free electron theory



Electron experiences periodic potential of positive ion core





# Electronic configuration



## In individual atoms

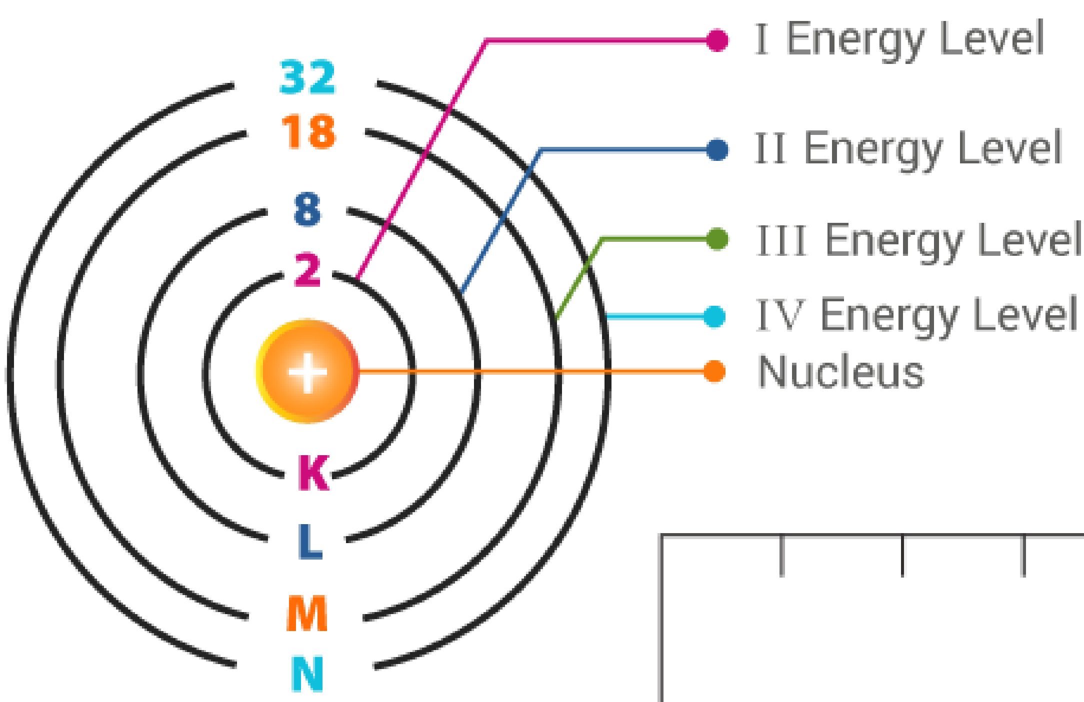
Discrete energy levels that may be occupied by electrons, arranged into shells and subshells.

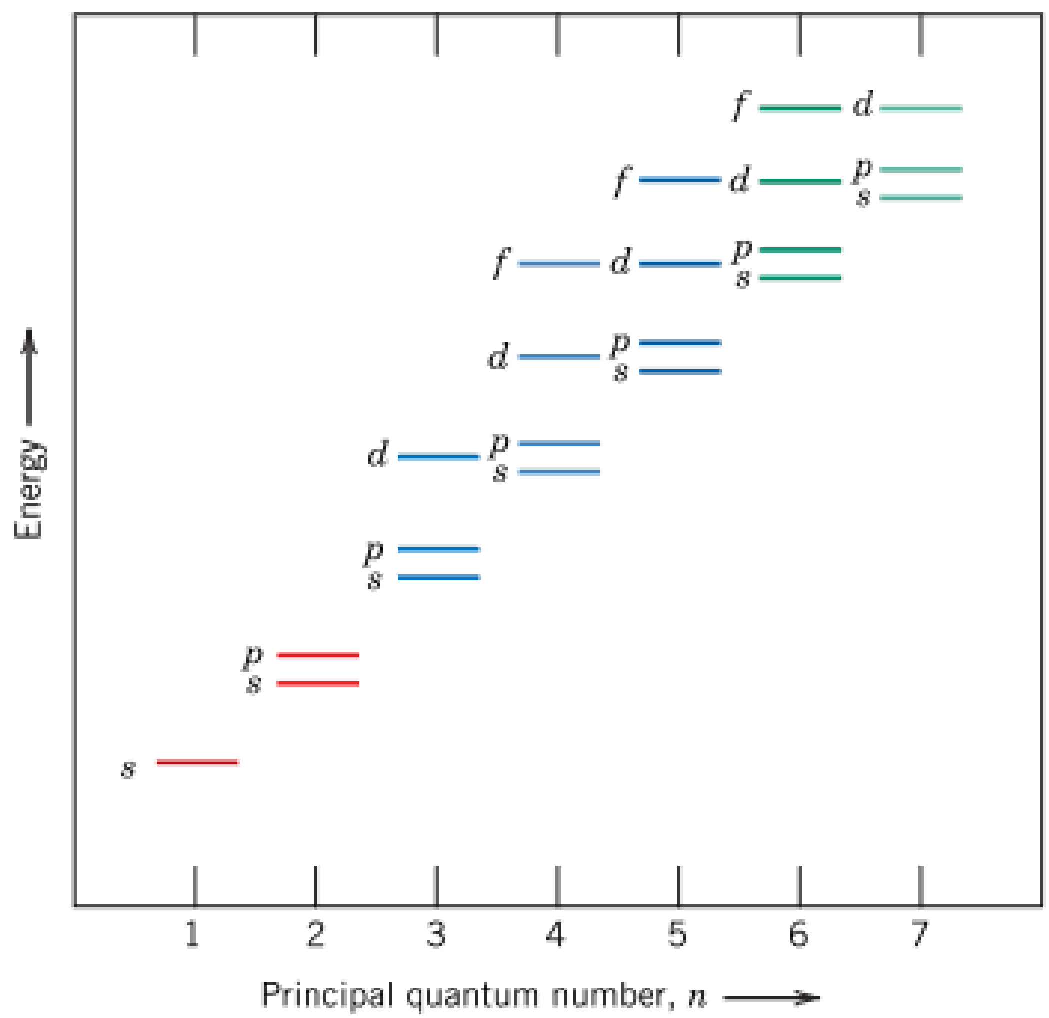
| Shell | Sub-shell | No. of States | | | |
|---|---|---|---|---|---|
| | | *s* | *p* | *d* | *f* |
| K, L, M, ….. | *s, p, d, f* | 1 | 3 | 5 | 7 |

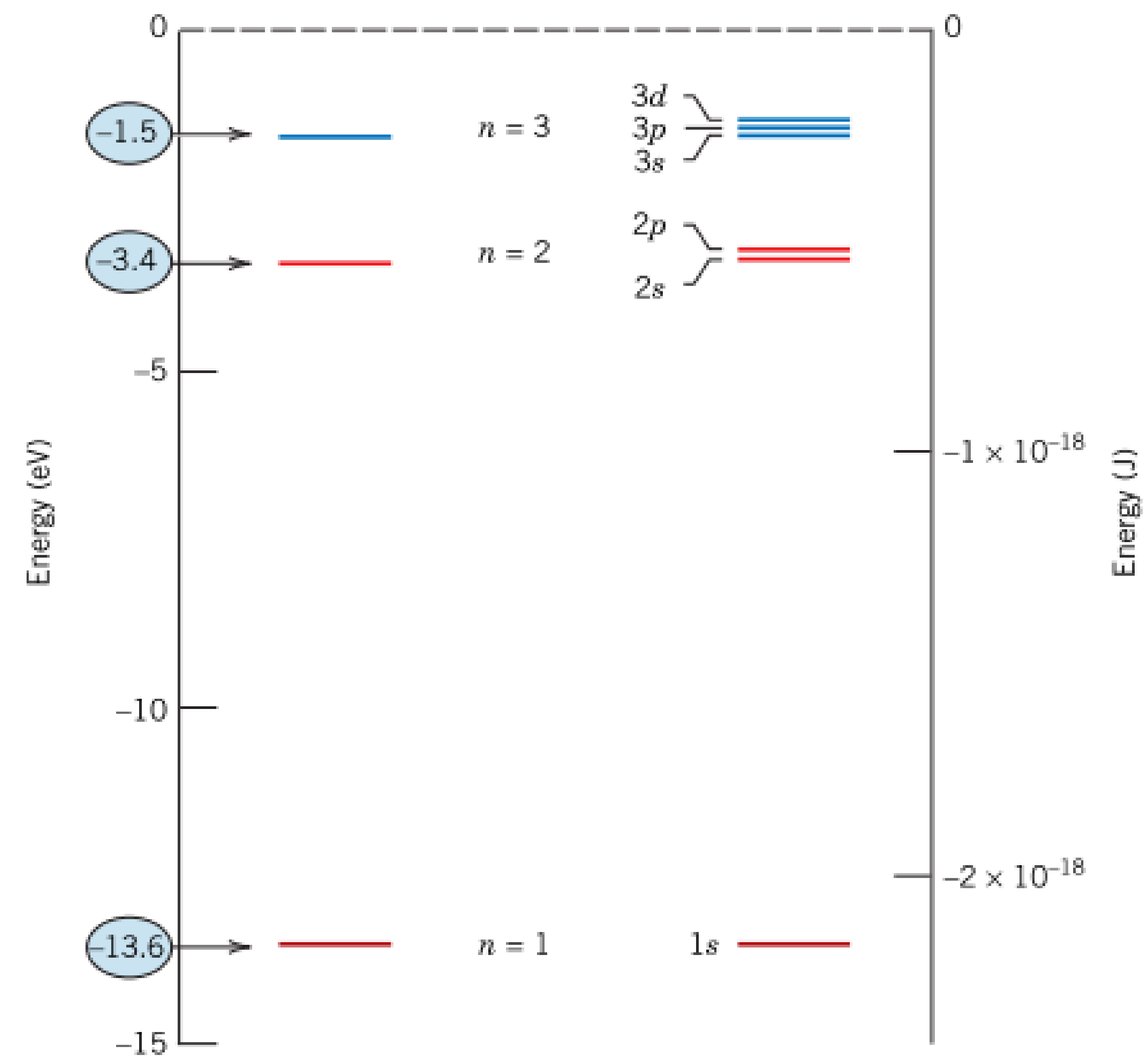
Electrons fill only the states having the lowest energies, two electrons of opposite spin per state, in accordance with Pauli exclusion principle.

Electron configuration of an isolated atom represents the arrangement of the electrons within the allowed states.

# Energy levels in an atom

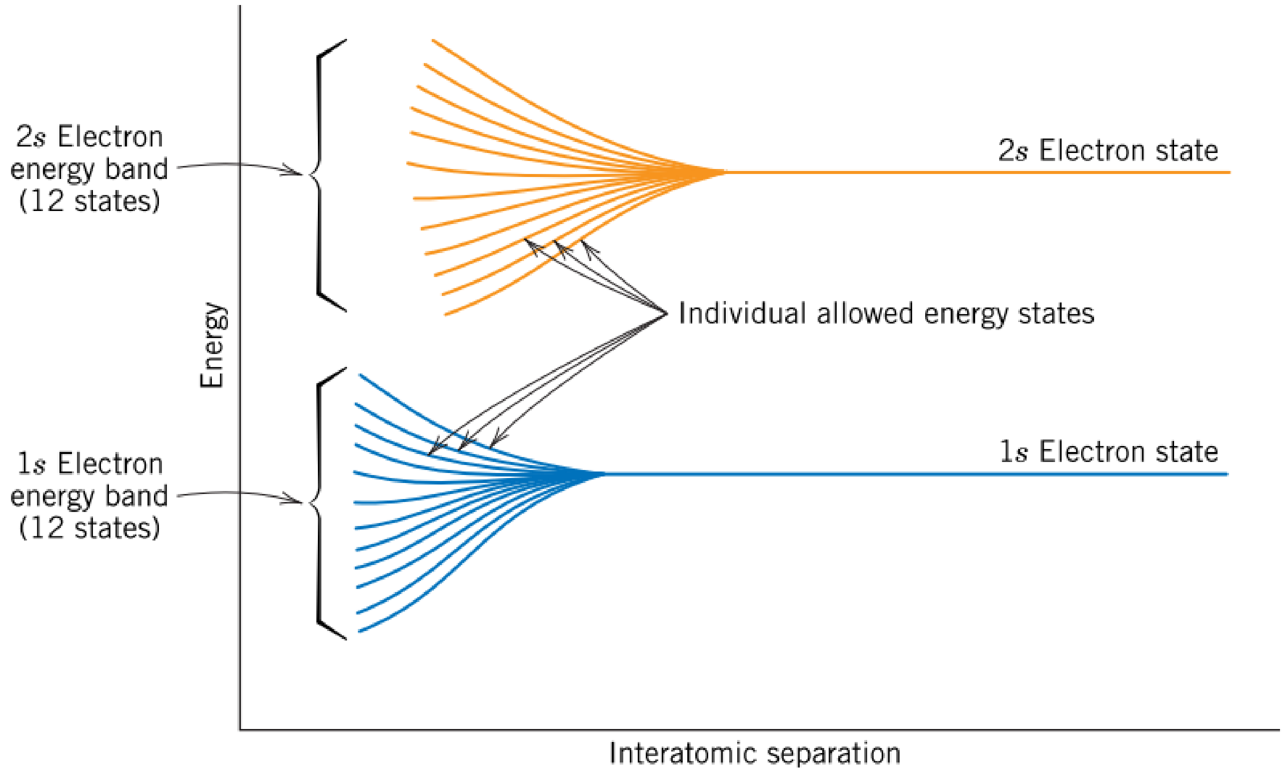


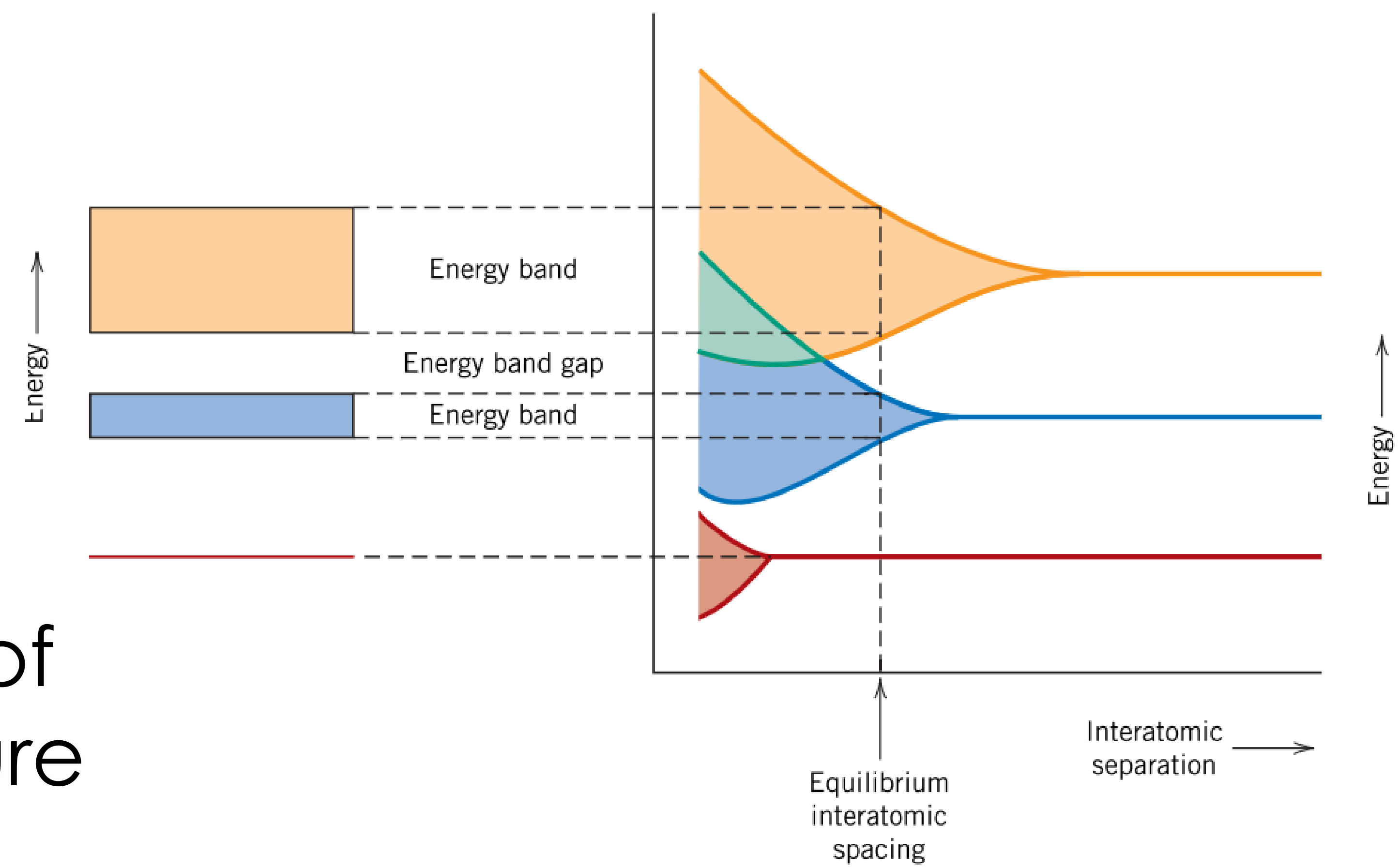



# Band formation in solids





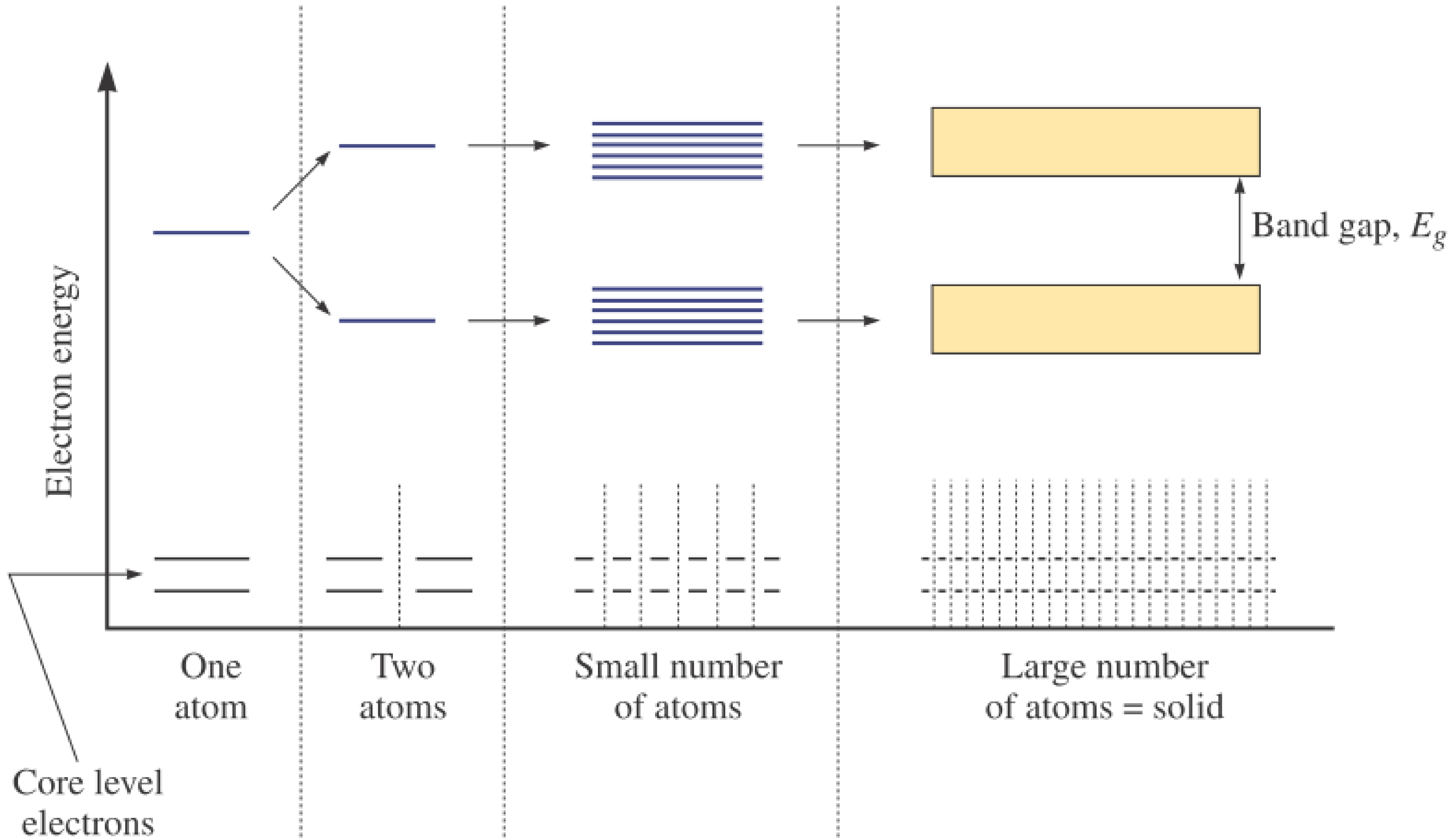

Schematic of electron energy levels for 12 atoms




Conventional representation of electron energy bands structure

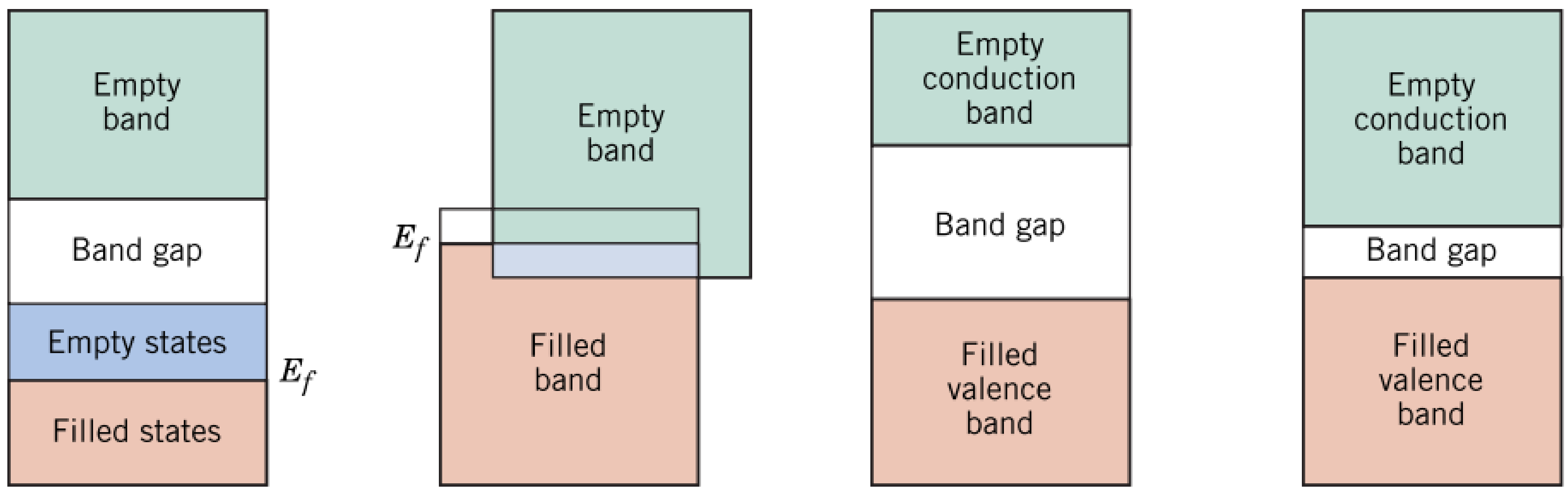
# Band formation in solids





# Band formation in solids

Various possible electron band structures in solids at 0 K




Conductors

Conductors
$E_g = 0$ eV

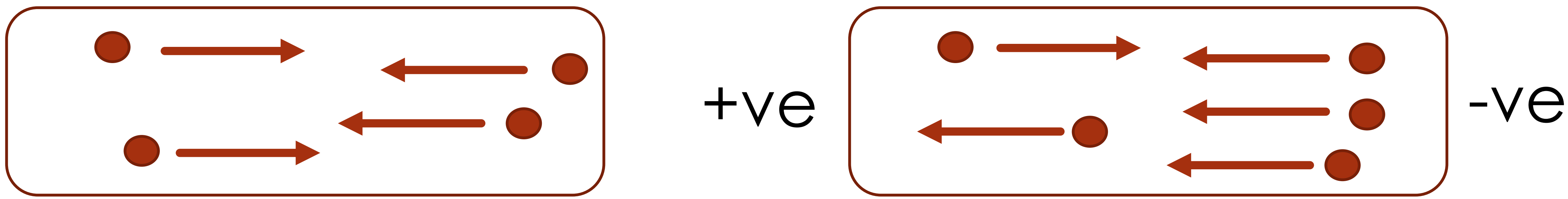
Insulators
$E_g > 2$ eV

Semiconductors
$E_g < 2$ eV

# Conduction by electron



For each electron moving with some velocity in certain direction, there is another electron moving with same speed but in opposite direction.




No Field

With Field

- Applied electric field $\rightarrow$ net velocity in a particular direction.
- Electrons are accelerated towards +ve end.
- Velocity of fastest moving electron towards +ve end is higher than velocity of fastest moving electron towards -ve end
- This is possible only when there are empty states available just above the Fermi level.

Example: metals

# Wave particle duality

## Electron can behave as a particle and wave

Particle $$E = \frac{1}{2}mv^2$$

Wave $$\lambda = \frac{h}{mv}$$

λ → de Broglie wavelength
v → velocity of the electrons
h → Planck's constant

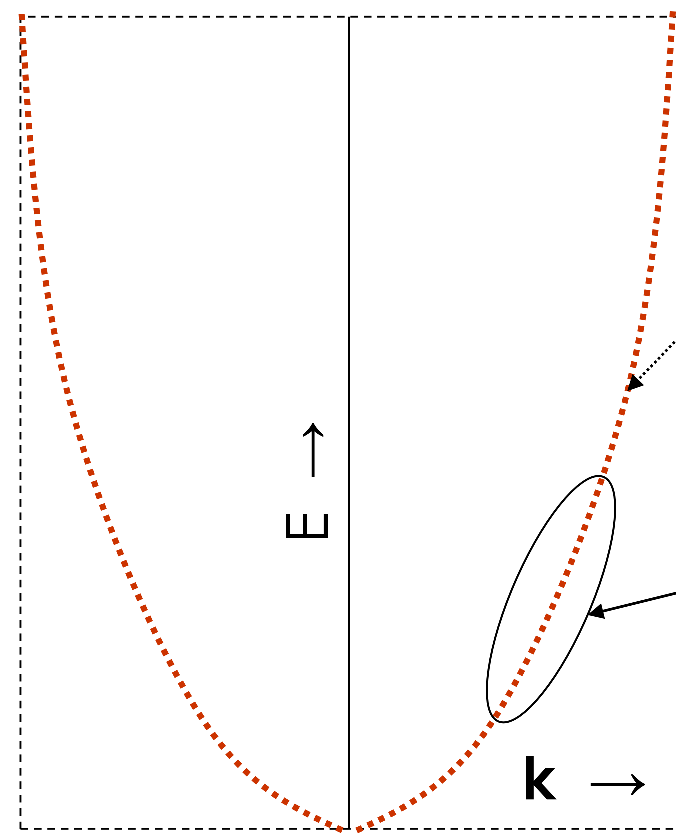
- *k is a vector in 2D/3D and is represented as a scalar in 1D*
- *k represents spatial representation of a wave*

Wave number vector (**k**)

$$k = \frac{2\pi}{\lambda}$$

$$k = 2\pi\frac{mv}{h} \rightarrow \frac{kh}{2\pi m} = v$$

$$E = \left(\frac{h^2}{8\pi^2 m}\right)k^2$$




$$E = \left(\frac{h^2}{8\pi^2 m}\right)k^2$$

λ ↑ → k ↓ → E ↓

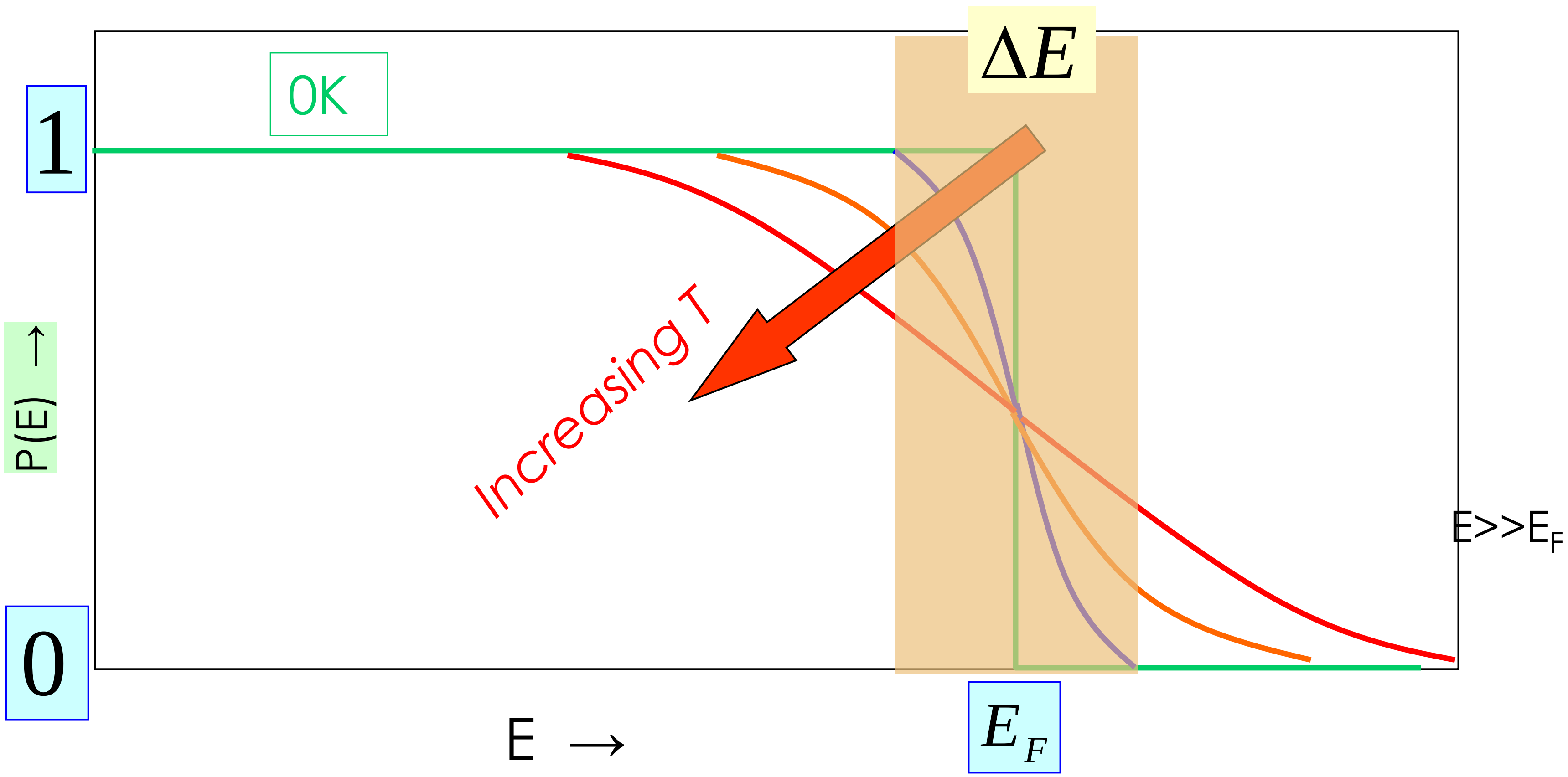
*Free electrons*

Discrete energy levels
*(Pauli's exclusion principle)*

# Fermi Level



- At zero K the highest filled energy level ($E_F$) is called the Fermi level.
- If $E_F$ is independent of temperature (valid for usual temperatures) Fermi level is that level which has 50% probability of occupation by an electron.




$T > 0\ K$

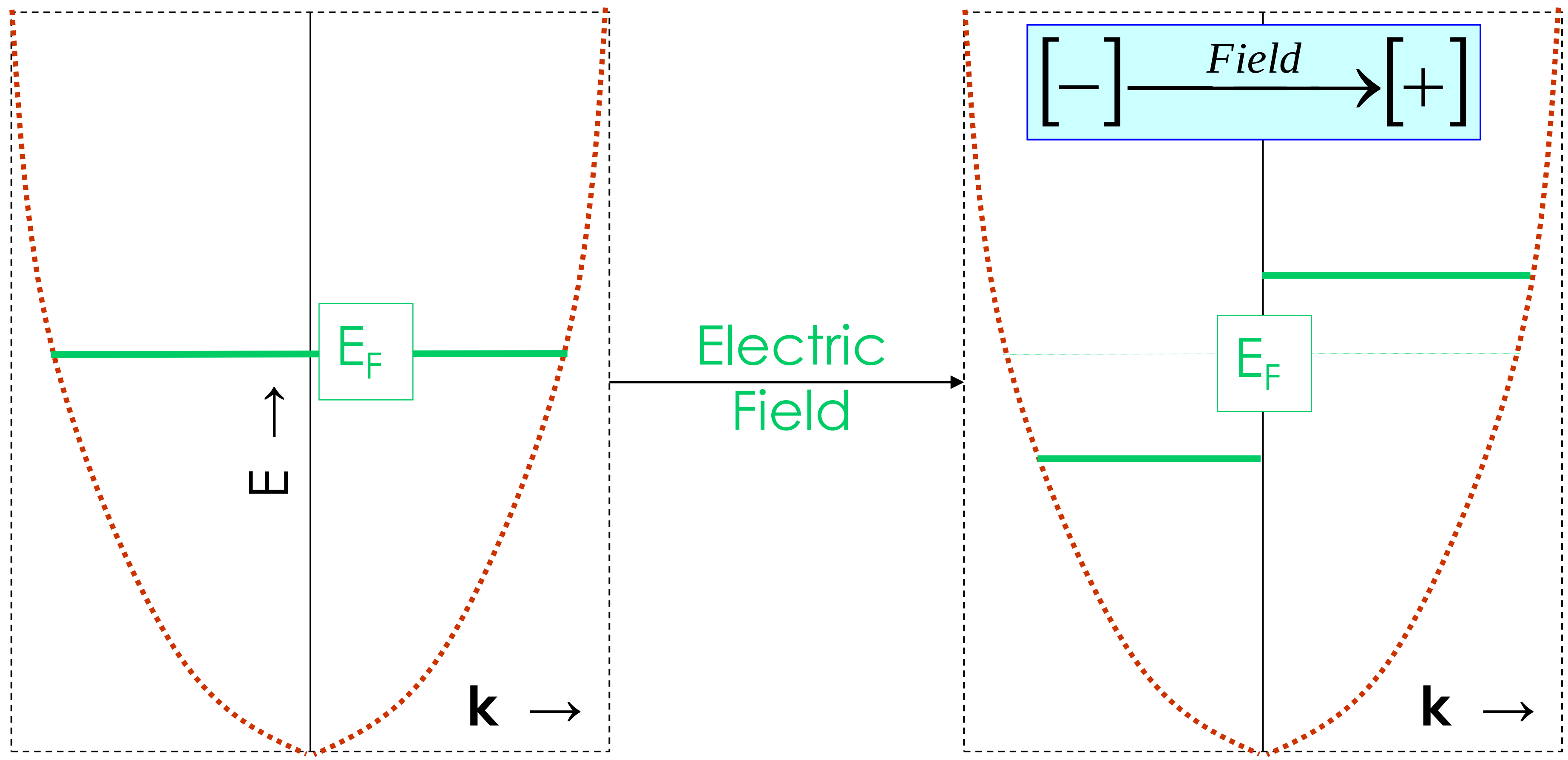
$$P(E) = \frac{1}{1 + \exp\left[\frac{E - E_F}{kT}\right]}$$

$$P(E) \approx \exp\left[-\left(\frac{E - E_F}{kT}\right)\right]$$

# Conduction by electron



If there are empty energy states above the Fermi level then in the presence of an electric field there is a redistribution of the electron occupation of the energy levels.



# Summary



1. The electron is assumed to be free and available for conduction.
2. The electrons has dual nature and can behave like a wave and a particle at a same time.
3. Fermi energy is the highest occupied energy level at zero Kelvin temperature.
4. The electrons in the Fermi level shifts on applications of electric field for redistribution to the higher energy levels.