

# Solid State Physics

**Condensed Matter = liquids and solids**

**Solid State = Solids**

**Solids may be crystalline, polycrystalline, amorphous, etc...**

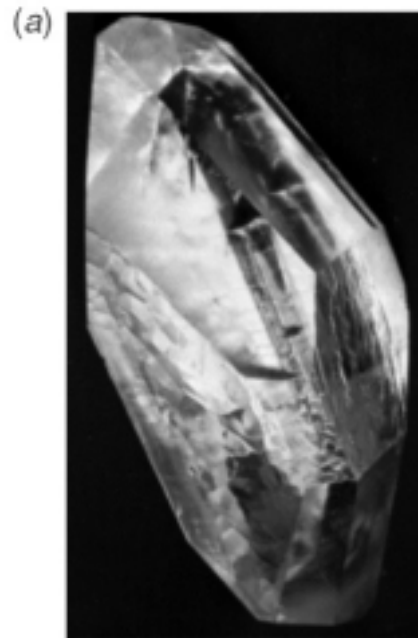
**We will focus on crystalline solids.**

**Crystalline solids have a large variety of structures;**

**fcc, hcp, bcc, sc, zincblende, wurtzite, perovskite, chalcogenides, etc...**

**Crystalline structures are characterized by their unit cell, the smallest repeating unit.**

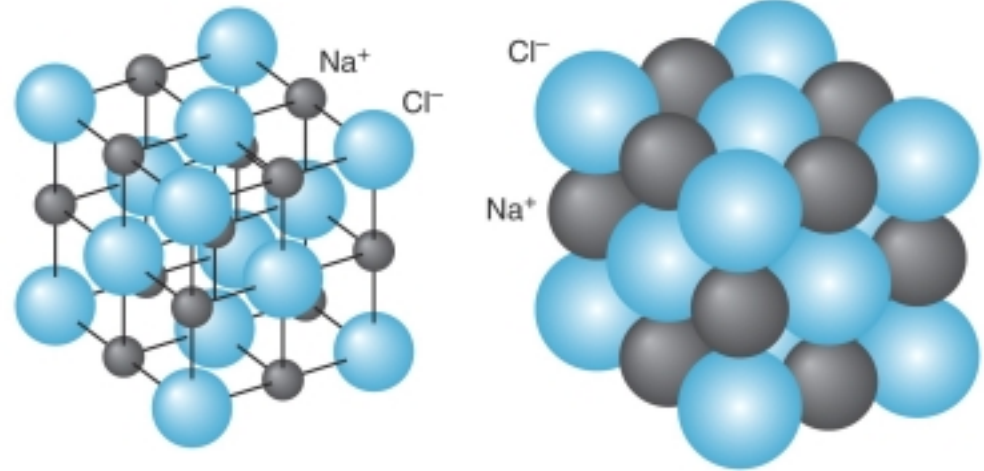
**We will focus on the most common ones and the general consequences.**



## Ionic Solids

The Coulomb interaction of one ion with all the other ions in a crystal can be calculated by an infinite series.

For instance, for the crystals with the face-centered cubic structure, like NaCl:



$$U_{Coulomb} = -\frac{6ke^2}{r} + \frac{12ke^2}{\sqrt{2}r} - \frac{8ke^2}{\sqrt{3}r} + \frac{6ke^2}{2r} - \frac{20ke^2}{\sqrt{5}r} + \dots$$

$$U_{Coulomb} = -\frac{ke^2}{r} \left( 6 - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} - \frac{6}{2} + \frac{20}{\sqrt{5}} - \dots \right) = -\alpha \frac{ke^2}{r}$$

The constant alpha is called the Madelung constant of the crystal structure. Alpha is positive and the Coulomb energy is negative.

**As we saw for ionic molecules, the potential energy of the crystal compared to the constituent ions has a term from the exclusion principle repulsion.**

$$U(r) = U_{Coulomb} + E_{ex} = -\alpha \frac{ke^2}{r} + \frac{A}{r^n}$$

$$F = -\frac{dU}{dr} = \alpha \frac{ke^2}{r^2} - \frac{nA}{r^{n+1}}$$

**At equilibrium,**

$$F = 0 = \alpha \frac{ke^2}{r_0^2} - \frac{nA}{r_0^{n+1}} \qquad \alpha \frac{ke^2}{r_0^2} = \frac{nA}{r_0^{n+1}} \qquad A = \frac{\alpha ke^2 r_0^{n-1}}{n}$$

**Substituting back into the potential energy we get**

$$U(r) = -\frac{\alpha ke^2}{r} + \frac{\alpha ke^2 r_0^{n-1}}{nr^n} = -\frac{\alpha ke^2}{r_0} \left[ \frac{r_0}{r} - \frac{1}{n} \left( \frac{r_0}{r} \right)^n \right]$$

**and at equilibrium we have**

$$U(r_0) = -\frac{\alpha ke^2}{r_0} + \frac{\alpha ke^2 r_0^{n-1}}{nr_0^n} = -\frac{\alpha ke^2}{r_0} \left[ 1 - \frac{1}{n} \right]$$

The dissociation or lattice energy is minus this potential energy at equilibrium.

Since this potential energy with respect to ions, the dissociation or lattice energy is the energy required to break the crystal up into ions.

To break the crystal into atoms requires an amount of energy called the cohesive energy, which is lower than the lattice energy by an amount equal to the energy needed to form the ions,

$$E_{ion}$$

TABLE 10-1 Properties of selected crystalline solids

Solid	Bonding	Equilibrium separation (nm)	Crystal symmetry	Madelung constant	Cohesive energy (eV/atom)	Melting point (K)
NaCl	ionic	0.282	fcc	1.7476	3.19	1074
LiBr	ionic	0.275	fcc	1.7476	3.10	823
KCl	ionic	0.315	fcc	1.7476	3.24	1043
RbF	ionic	0.282	fcc	1.7476	3.55	1068
CsCl	ionic	0.348	sc	1.7627	3.27	918
ZnO	ionic	0.222	hcp	1.4985	7.22	2248
Li	metallic	0.302	bcc	—	1.63	454
Fe	metallic	0.248	bcc	—	4.28	1811
Au	metallic	0.288	fcc	—	3.81	1338
Zn	metallic	0.266	hcp	—	1.35	693
C	covalent	0.154	fcc	—	7.37	†
Si	covalent	0.235	fcc	—	4.63	1687
Ge	covalent	0.245	fcc	—	3.85	1211
H <sub>2</sub> O	dipole-dipole	0.367	hcp	—	0.52*	273
C <sub>60</sub>	dipole-dipole	1.00	fcc	—	1.5*	?
Ne	dipole-dipole	0.313	fcc	—	0.020	24

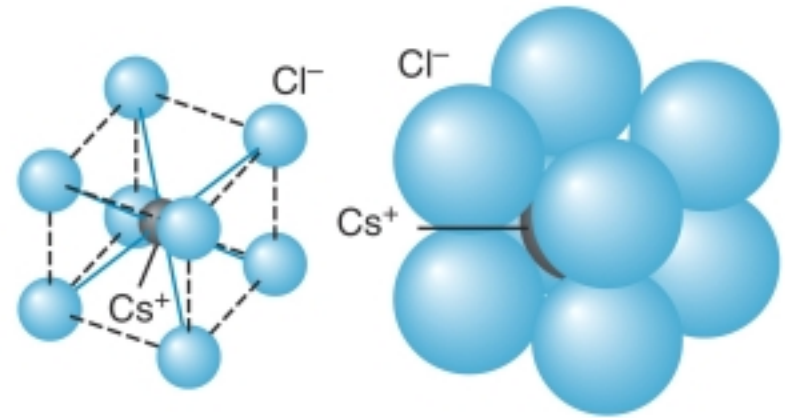
\*eV/molecule.

† Diamond transforms to graphite at high temperature. The latter then sublimates at about 3800 K.

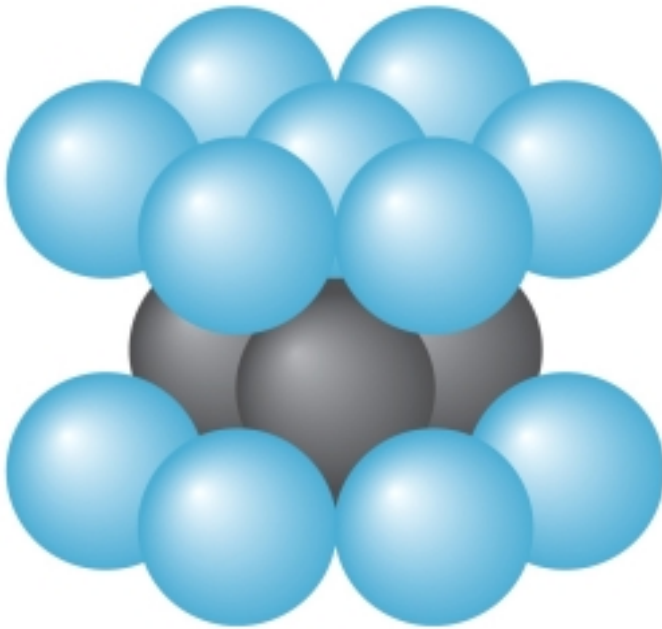
## Other crystal structures

### Body-Centered Cubic

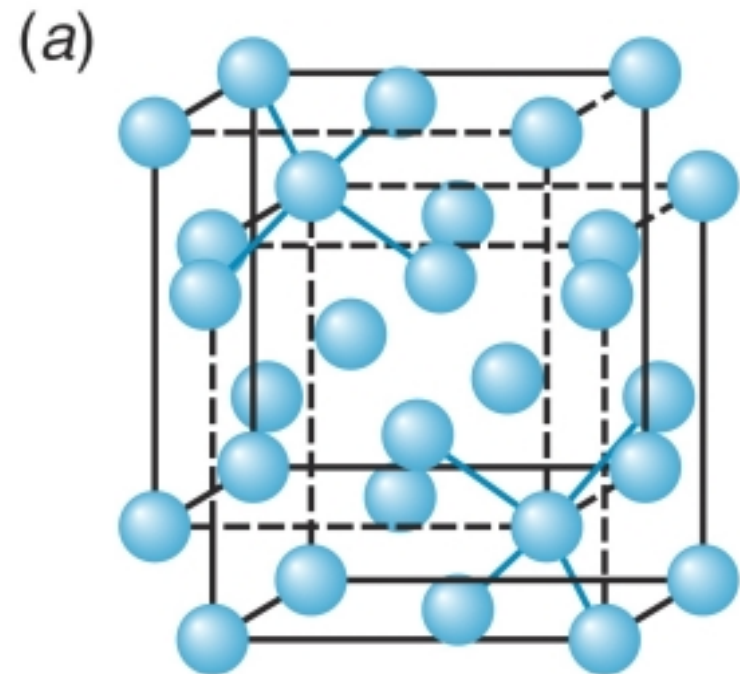
### Simple Cubic



### Hexagonal Close Packed



### Diamond/Zincblende



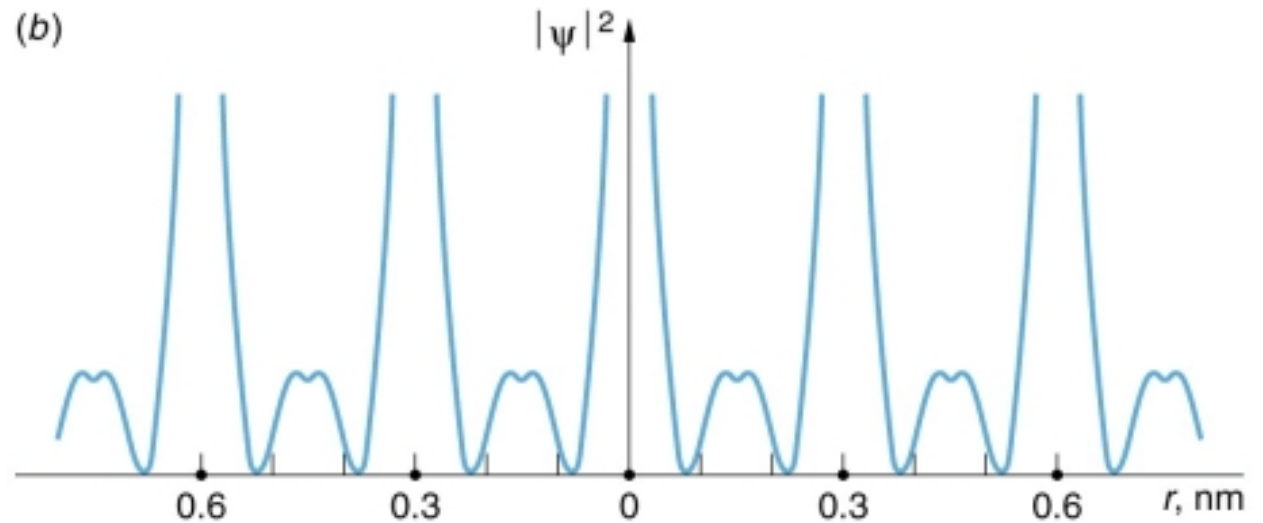
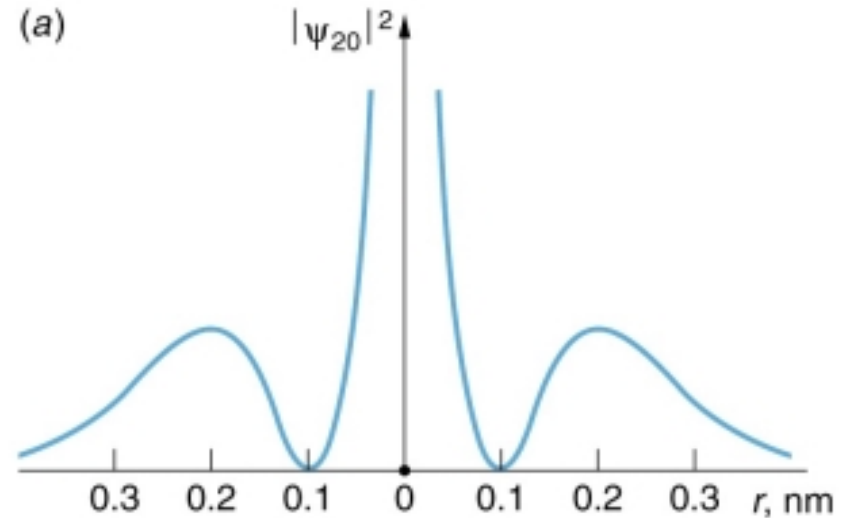
# Metallic Bonding

**Electrons shared by all atoms**

**Lithium shares its 2s electrons**

$$\psi_{20} = C_{20} \left( 2 - \frac{r}{a_0} \right) e^{-r/2a_0}$$

**Sharing of the electrons increases the Coulomb attraction, but it also increases the kinetic energy due to confinement.**



# Electric Current

**Drude Model of Conduction (1900).**

**Conduction is due to free electrons in material, which behave similar to an ordinary gas.**

$$\langle v \rangle = \sqrt{\frac{8kT}{\pi m_e}}$$

**The current through a surface is the rate at which charge flows through the surface.**

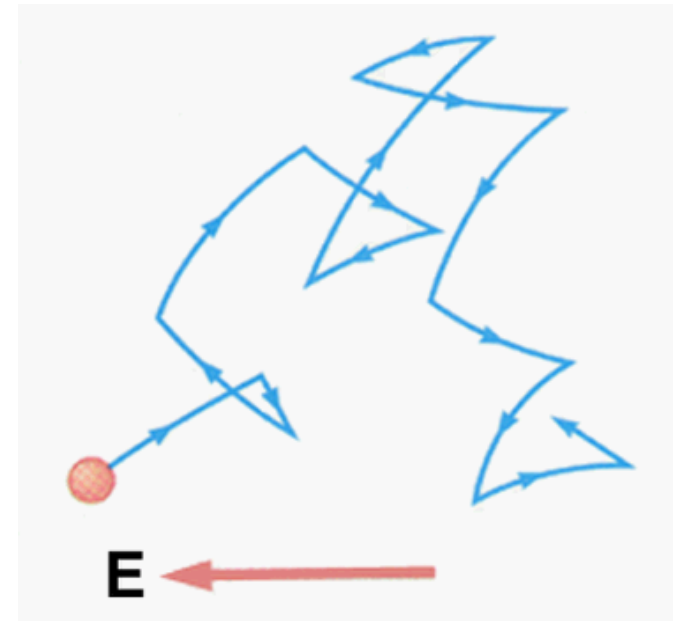
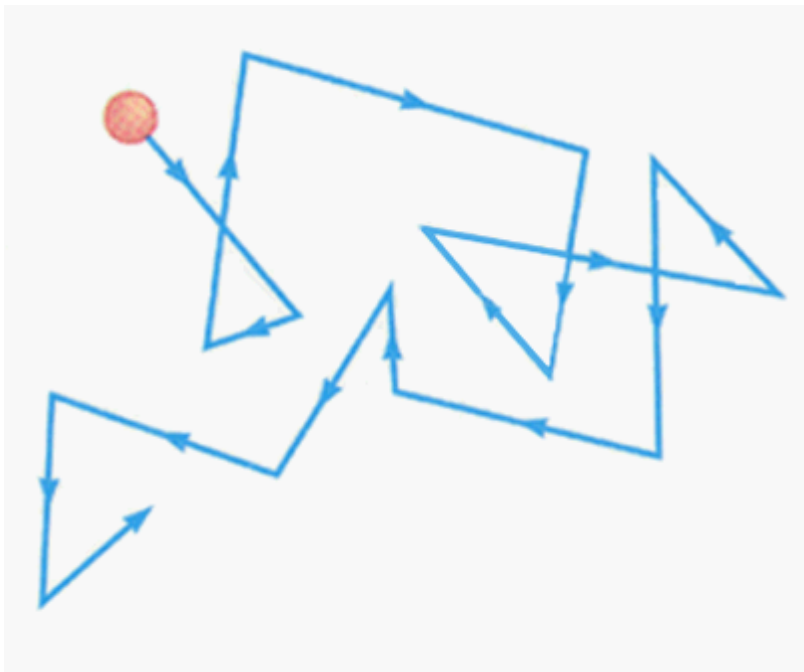
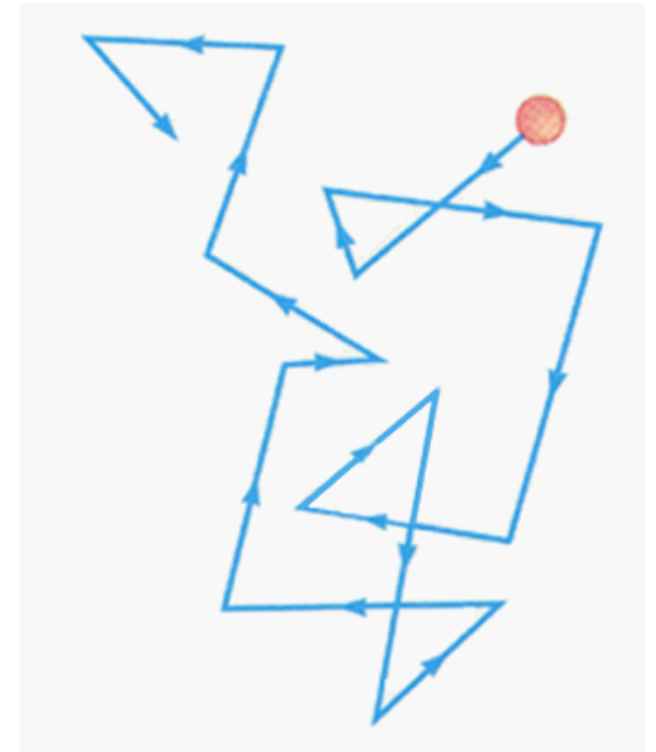
$$I_{avg} = \frac{\Delta Q}{\Delta t}$$

$$I = \frac{dQ}{dt}$$

The mobile charged particles are called the **charge carriers**.

The number of charge carriers per unit volume is called the **charge carrier density,  $n$** .

The average speed of the charge carriers is called their **drift speed,  $v_d$** .



In a time  $\Delta t$ , charge carriers move an average distance

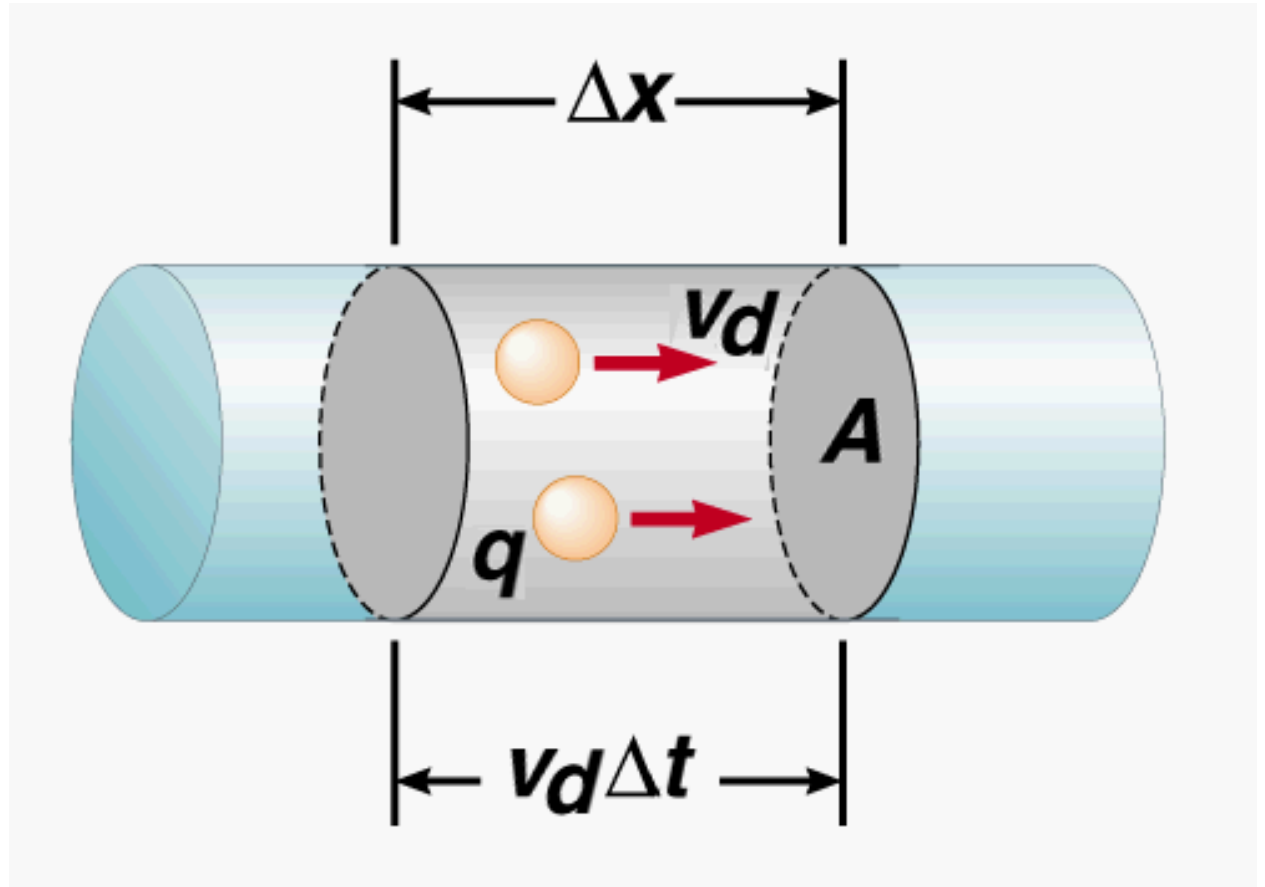
$$\Delta x = v_d \Delta t$$

Therefore the charge which passes through area  $A$  in time  $\Delta t$  is

$$\Delta Q = n(A\Delta x)e$$

$$\Delta Q = n(Av_d \Delta t)e$$

$$I_{av} = \frac{\Delta Q}{\Delta t} = nAv_d e$$



The current density,  $J$ , is the current per unit area.

$$j = \frac{I}{A}$$

Units: A/m<sup>2</sup>.

$$j = \frac{nAev_d}{A} = nev_d$$

The carrier density  $n$  is a property of the material.

The drift velocity is produced by an Electric Field,  $E$ .

**Electric fields produce current.**  $\vec{j} = \sigma \vec{E}$

**Conductivity,  $\sigma$ , is a property of a material.**

$$\text{Units: } \frac{A}{Vm} = \frac{1}{\Omega m} .$$

**Resistivity,  $\rho = 1 / \sigma$ , is also a property of a material.**

$$\vec{j} = \vec{E} / \rho$$

$$\vec{E} = \rho \vec{j}$$

$$\text{Units: } \frac{Vm}{A} = \Omega m .$$

**If  $\sigma$  (or  $\rho$ ) is a constant, the material is said to obey  
“Ohm’s Law” or to be ohmic.**

# Resistance

A wire of length  $\ell$  and cross-sectional area  $A$  has a potential difference  $\Delta V$  across it. The wire material has resistivity  $\rho$ .

$$E = \rho J$$

$$\frac{\Delta V}{\ell} = \rho J$$

$$\frac{\Delta V}{\ell} = \rho \frac{I}{A}$$

$$\Delta V = I \frac{\rho \ell}{A} = IR$$

$$R = \frac{\rho \ell}{A} = \frac{\ell}{\sigma A}$$

**Resistance,  $R$ , is a property of the material and the size and shape of the conductor.**

**Units: Ohms,  $\Omega$ .**

## Mean Free Path

The electrons are accelerated in the electric field and gain energy. But collisions between electrons and the ion cores in the lattice cause its energy to be thermalized and its direction randomized.

Let's call the average time since an electron's last collision  $\tau$ .

$$v_d = a\tau = \frac{eE}{m_e} \tau$$

The average distance the electron traveled since its last collision is called the mean free path,  $\lambda$ ,

$$\lambda = \langle v \rangle \tau.$$

So we can write the drift speed in terms of the mean free path

$$v_d = \frac{eE\lambda}{\langle v \rangle m_e}$$

$$I = nAv_d e = \frac{ne^2 \lambda EA}{m_e \langle v \rangle}$$

$$j = \frac{I}{A} = nv_d e = \frac{ne^2 \lambda E}{m_e \langle v \rangle} = \sigma E$$

$$\sigma = \frac{ne^2 \lambda}{m_e \langle v \rangle} \quad \rho = \frac{1}{\sigma} = \frac{m_e \langle v \rangle}{ne^2 \lambda}$$

## Mean Free Path

Classically, we can calculate the mean free path.

In a time  $t$ , an electron moves a distance  $vt$ .

The number of collisions the electron has is equal to the number of ions centered within the volume

$\pi r^2 vt$ , where  $r$  is the radius of the ion.

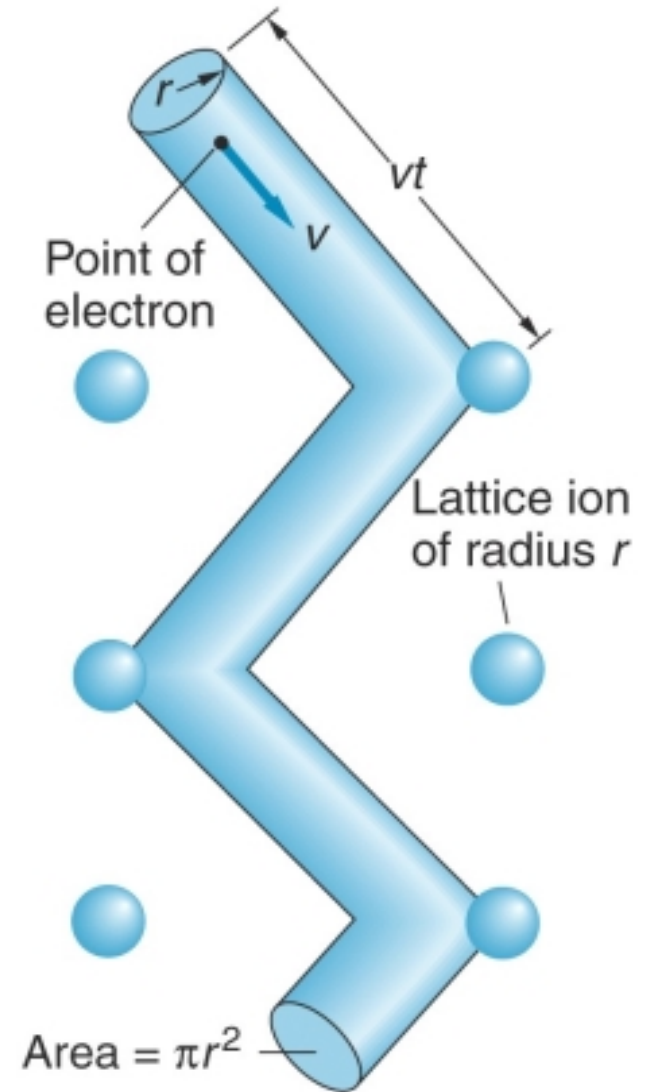
The number of ions in that volume is

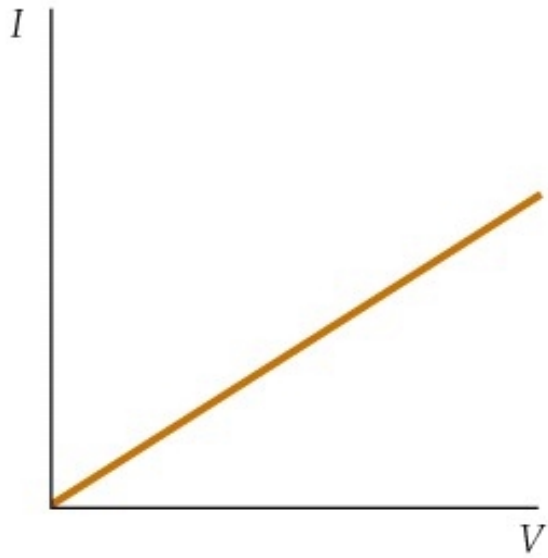
$$n_a \pi r^2 vt$$

where  $n_a$  is the density of ions.

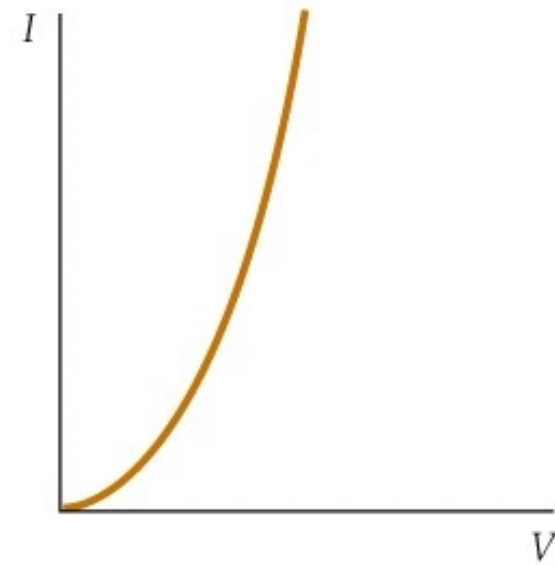
So the mean free path between collisions is

$$\lambda = \frac{\text{distance}}{\# \text{collisions}} = \frac{vt}{n_a \pi r^2 vt} = \frac{1}{n_a \pi r^2}.$$

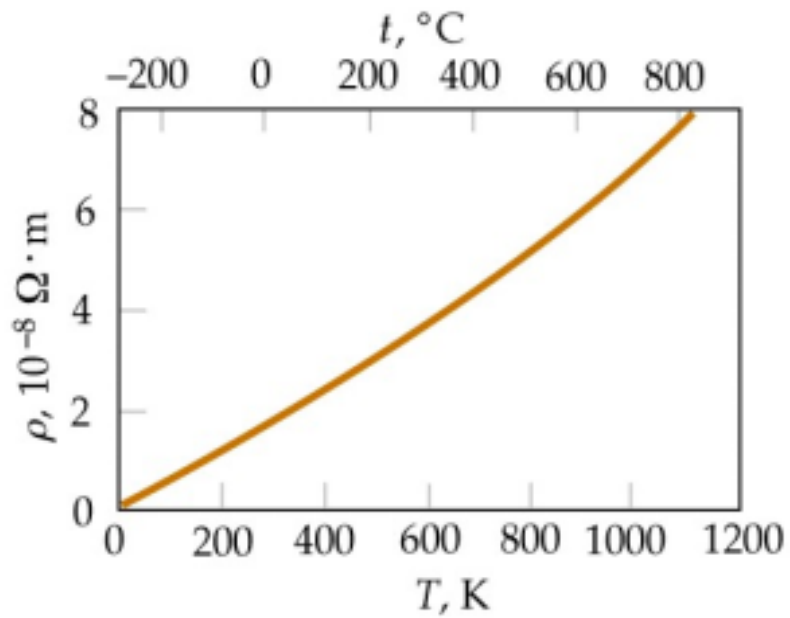




(a)



(b)



$$\rho = \frac{1}{\sigma} = \frac{m_e \langle v \rangle}{ne^2 \lambda}$$

$$\langle v \rangle = \sqrt{\frac{8kT}{\pi m_e}}$$

## Free Electron Gas in Metals

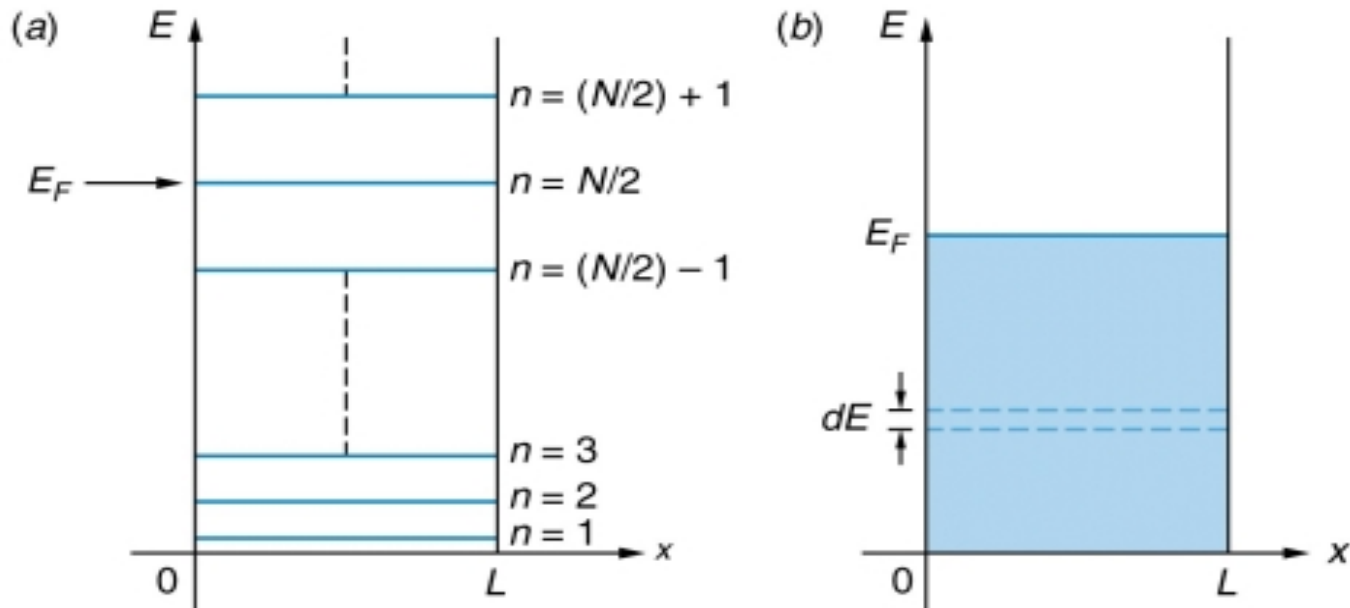
We must treat electrons as fermions, not classical particles.  
So we have zero-point energy and exclusion principle in effect.

The energy levels for a particle in a one dimensional box are

$$E_n = \frac{n^2 h^2}{8mL^2} = n^2 E_1.$$

At  $T=0$ , the  $N$  electrons will fill the first  $N/2$  levels so that

$$E_F = E_{N/2} = \frac{N^2 h^2}{32mL^2} = \frac{h^2}{32m} \left( \frac{N}{L} \right)^2.$$



The average energy of the electrons in this box can be calculated by

$$\begin{aligned} \langle E \rangle &= \frac{1}{N} \sum_{n=1}^{N/2} 2n^2 E_1 = \frac{1}{N} \int_0^{N/2} 2n^2 E_1 dn \\ \langle E \rangle &= \frac{2E_1}{N} \frac{n^3}{3} \Big|_0^{N/2} = \frac{2E_1}{N} \frac{(N/2)^3}{3} = \frac{E_1}{3} \left( \frac{N}{2} \right)^2 \\ \langle E \rangle &= \frac{E_F}{3} \end{aligned}$$

The number of electrons with each energy can also be calculated:

$$\begin{aligned} n(E)dE &= g(E) f_{FD}(E) dE \\ g(E) &= 2 \frac{dn}{dE} = 2 \frac{d}{dE} \left( \frac{E}{E_1} \right)^{1/2} = \left( \frac{1}{E_1 E} \right)^{1/2} \end{aligned}$$

At  $T = 0K$ ,  $f_{FD}(E) = 1$  for  $E < E_F$  and

$f_{FD}(E) = 0$  for  $E > E_F$ , so

at  $T = 0K$ ,  $n(E) = (E_1 E)^{-1/2}$  for  $E < E_F$  and

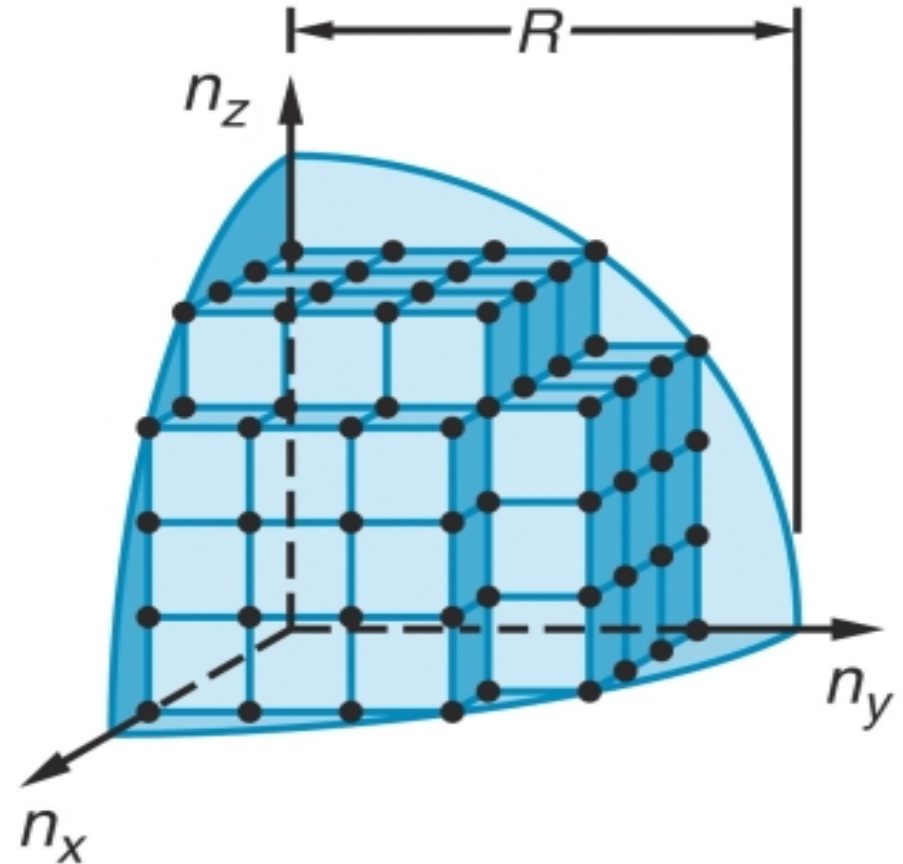
$n(E) = 0$  for  $E > E_F$ .

## Three-Dimensional Electron Gas

We can extend this to a three-dimensional electron gas using results from chapter 8.

Equation 8-63 gave us the number of states within energy of E or less:

$$n = \frac{\pi}{6} \left( \frac{E}{E_0} \right)^{3/2} = \frac{\pi}{6} \left( \frac{2mL^2 E}{\hbar^2 \pi^2} \right)^{3/2} .$$



From this we calculated the density of states in equation 8-64 (with the extra 2 for fermions):

$$g(E) = 2 \frac{dn}{dE} = \frac{2(2m)^{3/2} L^3}{4\pi^2 \hbar^3} E^{1/2} = \frac{2(2m)^{3/2} V}{4\pi^2 \hbar^3} E^{1/2} .$$

The number of electrons can be used to normalize, but this is a difficult integral.

$$N = \int_0^{\infty} g(E) f_{FD}(E) dE = \int_0^{\infty} \frac{2(2m)^{3/2} V E^{1/2}}{4\pi^2 \hbar^3} \frac{1}{e^{(E-E_F)/kT} + 1} dE$$

Since the Fermi-Dirac distribution function takes a simple form at  $T = 0 K$ , we can evaluate it:

$$N = \int_0^{E_F} g(E) dE = \int_0^{E_F} \frac{2(2m)^{3/2} V}{4\pi^2 \hbar^3} E^{1/2} dE = \frac{2(2m)^{3/2} V}{4\pi^2 \hbar^3} \frac{2}{3} E_F^{3/2}$$

The Fermi energy can then be expressed as

$$E_F = \left( \frac{3\pi^2 \hbar^3 N}{(2m)^{3/2} V} \right)^{2/3} = \frac{\hbar^2}{2m} \left( 3\pi^2 \frac{N}{V} \right)^{2/3} .$$

**TABLE 10-3** Free-electron number densities, Fermi energies, and Fermi temperatures for selected elements

Element	$N/V$ ( $\times 10^{28} \text{ m}^{-3}$ )	Fermi energy (eV)	Fermi temperature ( $\times 10^4 \text{ K}$ )
Al	18.1	11.7	13.6
Ag	5.86	5.53	6.41
Au	5.90	5.55	6.43
Cu	8.47	7.06	8.19
Fe	17.0	11.2	13.0
K	1.40	2.13	2.47
Li	4.70	4.77	5.53
Mg	8.61	7.14	8.28
Mn	16.5	11.0	12.8
Na	2.65	3.26	3.78
Sn	14.8	10.3	11.9
Zn	13.2	9.50	11.0

$$T_F = \frac{E_F}{k}$$

We can express the density of states in terms of the Fermi energy as

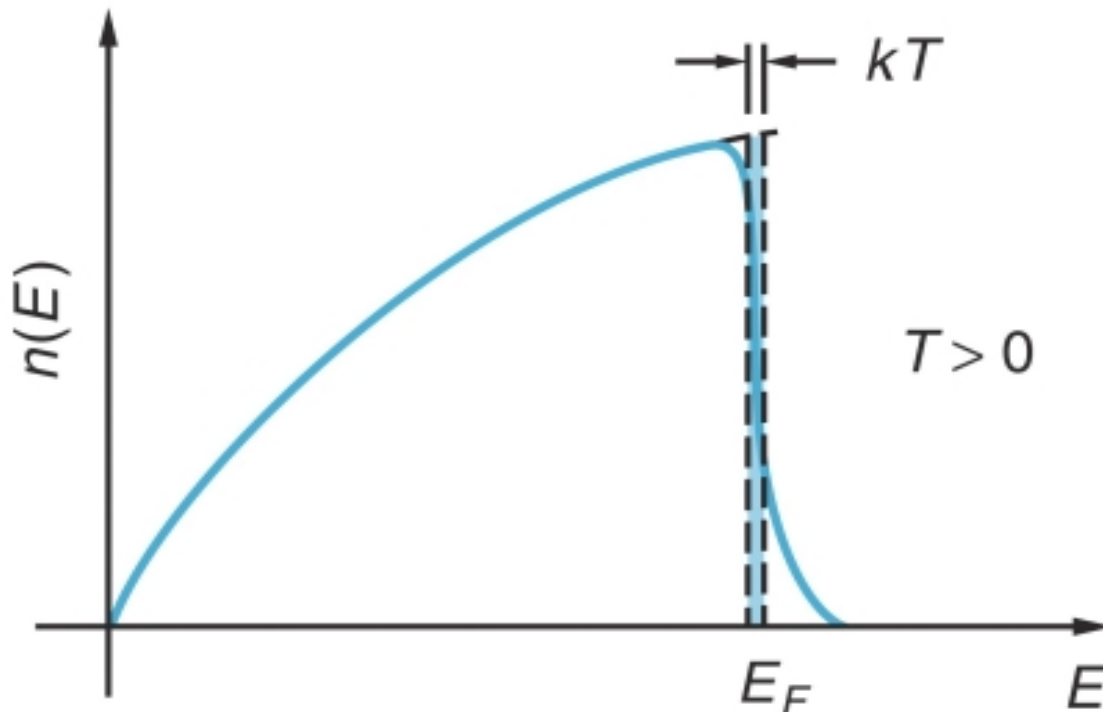
$$g(E) = \frac{2(2m)^{3/2}V}{4\pi^2\hbar^3} E^{1/2} = \frac{3NE^{1/2}}{2E_F^{3/2}}.$$

Remember that at  $T = 0\text{ K}$ ,  $n(E)=g(E)$  for  $E < E_F$  and  $n(E)=0$  for  $E > E_F$ .

So the average energy at  $T = 0\text{ K}$  is

$$\langle E \rangle = \frac{1}{N} \int_0^\infty E n(E) dE = \frac{1}{N} \int_0^{E_F} E \frac{3N}{2E_F^{3/2}} E^{1/2} dE$$

$$\langle E \rangle = \frac{3}{2E_F^{3/2}} \int_0^{E_F} E^{3/2} dE = \frac{3}{2E_F^{3/2}} \frac{2}{5} E_F^{5/2} = \frac{3}{5} E_F$$



At temperatures above 0 K, only the populations of states with energies near the Fermi energy are changed.

Collisions with lattice ions can't deliver enough energy to most of the electrons to bump them up into any of the unoccupied states as long as the temperature is far below the Fermi Temperature.

# Quantum Theory of Conduction

The classical theory of conduction gave the resistivity of our electron gas as  $\rho = \frac{1}{\sigma} = \frac{m_e \langle v \rangle}{ne^2 \lambda}$ .

Quantum theory uses the same expression, but the average velocity and mean free path change.

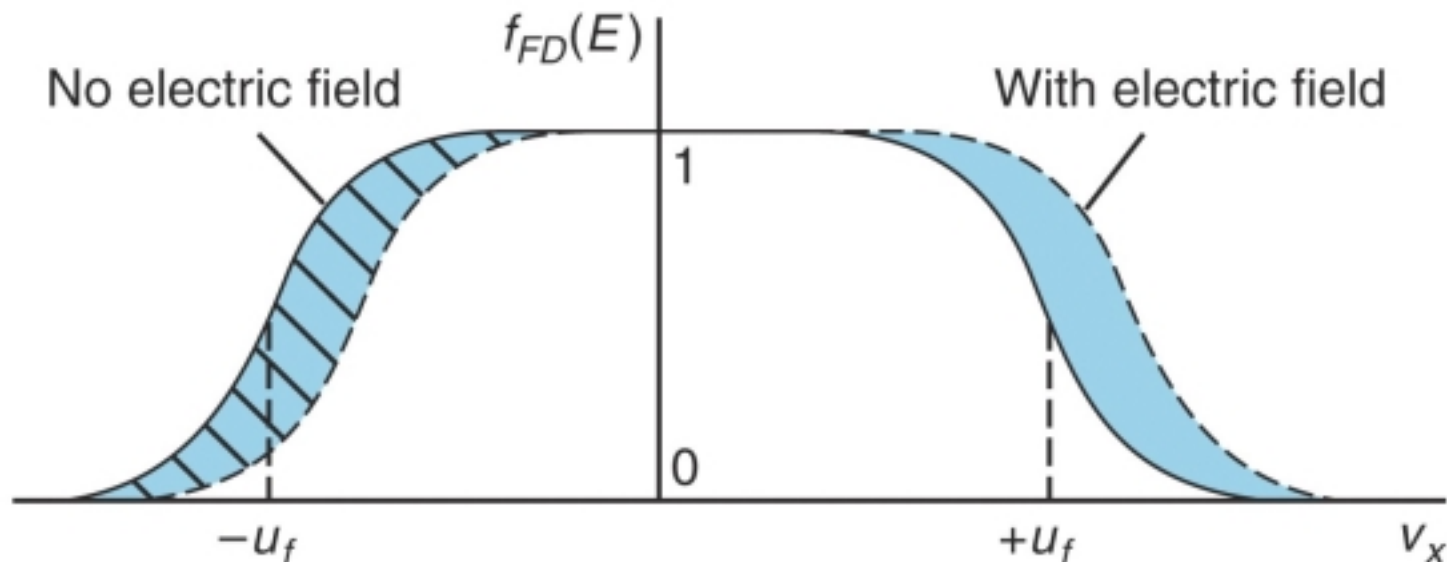
If we express the kinetic energy of the electrons in terms of a velocity,  $u = \sqrt{\frac{2E}{m_e}}$ ,

the velocity of the electrons at the Fermi energy will be,  $u_F = \sqrt{\frac{2E_F}{m_e}}$ , called the Fermi velocity.

We can express the Fermi-Dirac distribution function in terms of velocity as well.

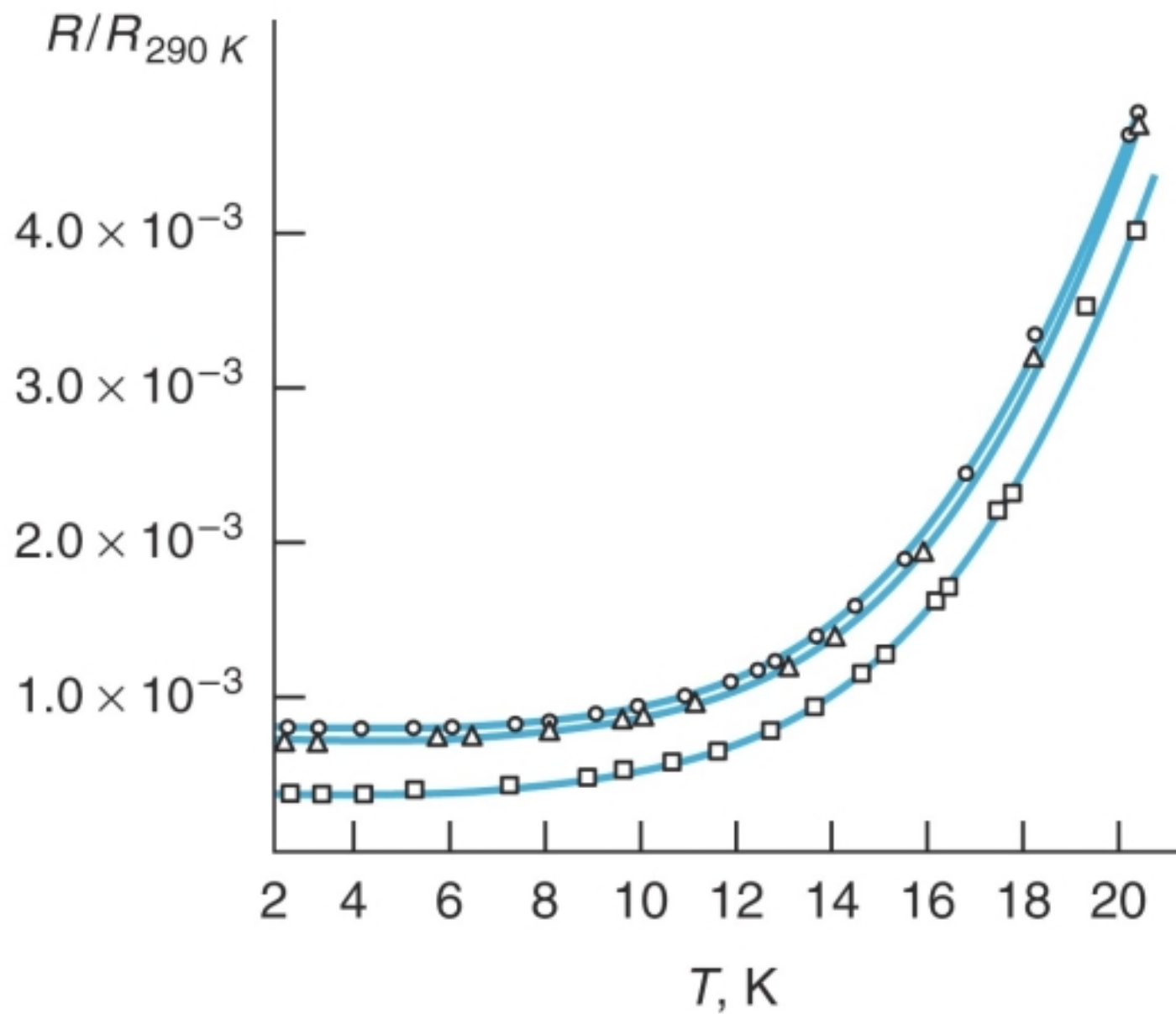
Application of an electric field imposes a shift in the distribution of velocities, making it no longer symmetric about zero.

So it's the electrons near the Fermi energy that result in conduction,  $\langle v \rangle = u_F$ .





Several samples of solid sodium (a good free-electron metal) with different levels of impurities.



## Heat Capacity

Since only the electrons within about  $kT$  of the Fermi energy are affected by changes in temperature, only those electrons contribute to the heat capacity.

The density of states is given by 
$$g(E) = \frac{2(2m)^{3/2} V}{4\pi^2 \hbar^3} E^{1/2} = \frac{3NE_F^{1/2}}{2E_F^{3/2}} .$$

The number of states within an energy of  $kT$  of the Fermi energy is about

$$g(E_F)\Delta E = \frac{3NE_F^{1/2}}{2E_F^{3/2}} kT = \frac{3NkT}{2E_F} .$$

So the fraction of free electrons that are affected by changes in temperature is of the order  $kT/E_F$ .

Since these electrons are changing their energy by an amount of the order of  $kT$ ,

the increase in kinetic energy per electron is of the order  $(kT)^2/E_F$  or  $kT^2/T_F$ .

The increase in energy per mole of ions is then of the order of  $RT^2/T_F$

and the molar heat capacity associated with this energy is of the order  $2RT/T_F$ .

Since  $T/T_F$  is very small, this contribution is small compared with the lattice heat capacity.

# Magnetism in Solids

Electron Spin (unpaired spins)  $\Leftrightarrow$  Magnetic Moment

$$\mu_z = -m_s g_s \mu_B$$

where  $m_s = \pm \frac{1}{2}$ ,  $g_s$  is the g-factor for the electron, and  $\mu_B$  is the Bohr magneton.

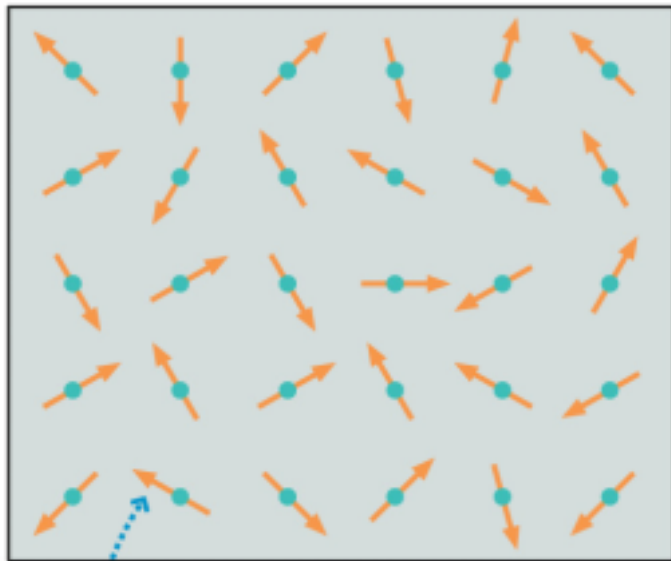
In an applied magnetic field, the atoms will have energy  $U = -\mu_z B = m_s g_s \mu_B B$ .

The lower energy state is the  $m_s = -\frac{1}{2}$  state, called spin down since  $\vec{S}$  is anti-parallel to  $\vec{B}$ .

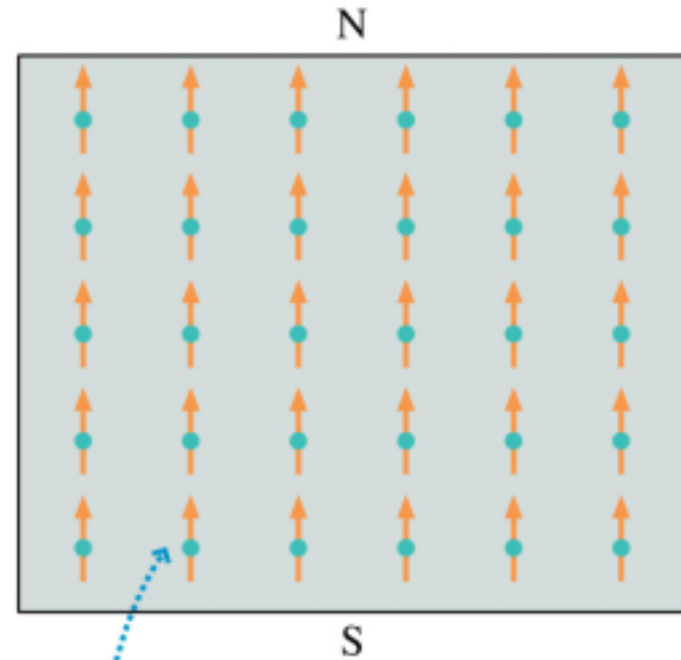
The higher energy state is the  $m_s = +\frac{1}{2}$  state, called spin up since  $\vec{S}$  is parallel to  $\vec{B}$ .

# Paramagnetism

No magnetic interaction between atoms, so no magnetic energy or net magnetic moment in the absence of an applied magnetic field. But atomic magnetic moments will be affected by an applied magnetic field.



The atomic magnetic moments due to unpaired spins point in random directions. The sample has no net magnetic moment.



The atomic magnetic moments are aligned. The sample has a north and south magnetic pole.

A thermal distribution will result in more spin-down than spin-up and a net magnetic moment.

$$M = \mu(\rho_+ - \rho_-) > 0$$

For small fields, M is proportional to B,  $\mu_0 \vec{M} = \chi \vec{B}$ , where  $\chi$  is the magnetic susceptibility.

For high temperatures where  $\mu B \ll kT$ , 
$$\chi = \frac{\mu_0 M}{B} = \frac{(\rho_+ + \rho_-)\mu^2}{kT} = \frac{\rho\mu^2}{kT}.$$

This is Curie's law.

At low temperatures where  $\mu B \gg kT$ ,  $M \approx \mu\rho$   
since all the spins will be aligned with the applied magnetic field.

Curie's law applies to electrons bound to atoms in a solid but not to the free electrons in a metal. The free electrons are almost all in doubly occupied states and the energy cost of increasing the population of spin down is quite large.

# Diamagnetism

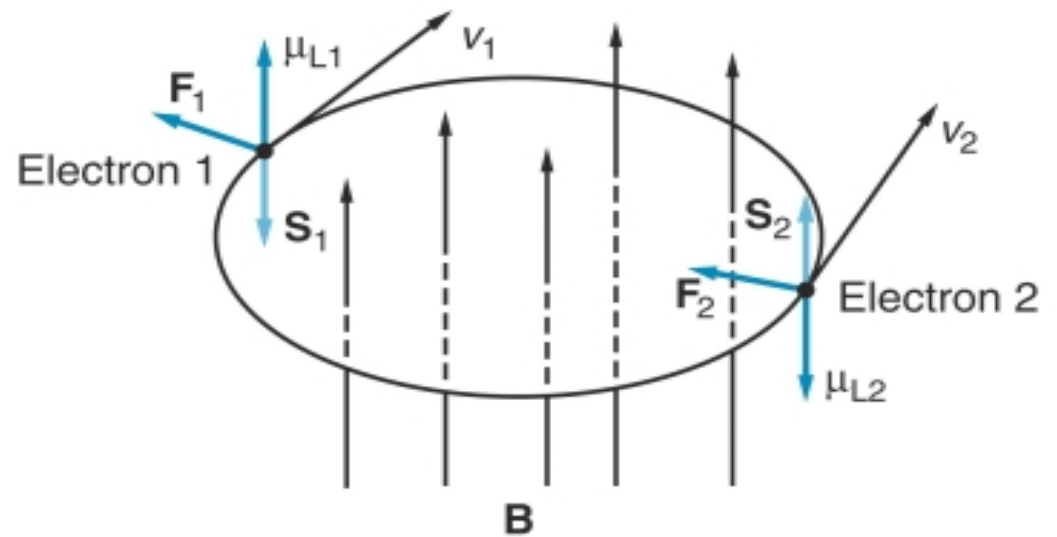
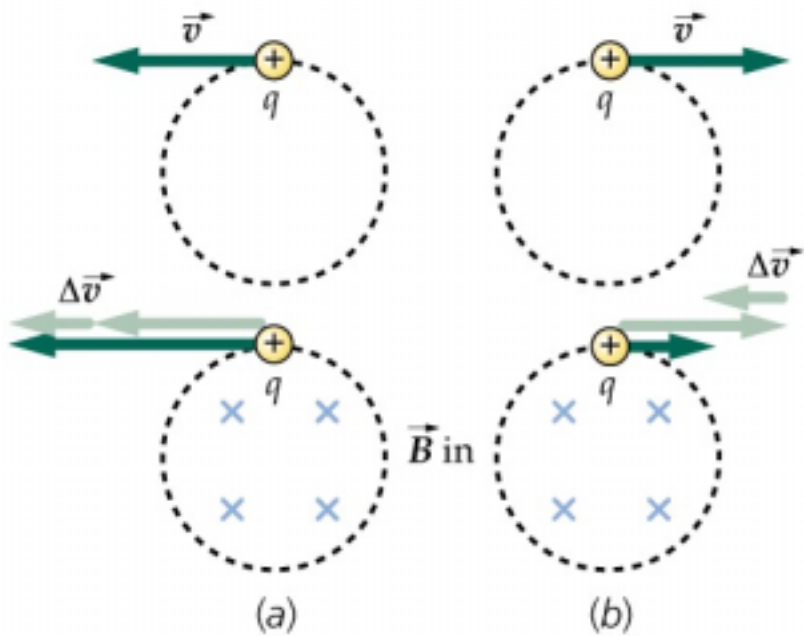
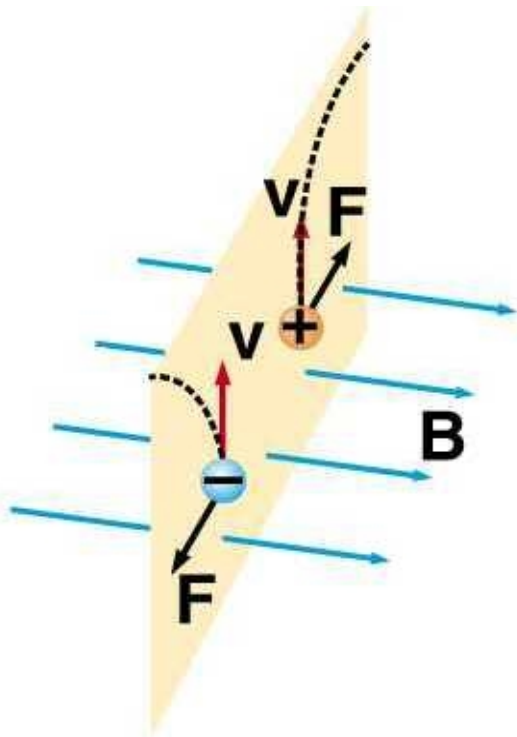
Free electrons will spiral or circle in a magnetic field.

The magnetic moment of the circling electron is opposite that of the applied field.

This reduces the magnetic field in the material.

Just like dielectric reduce an applied electric field, diamagnets reduce an applied magnetic field.

This is observed in materials where all the electrons are paired.

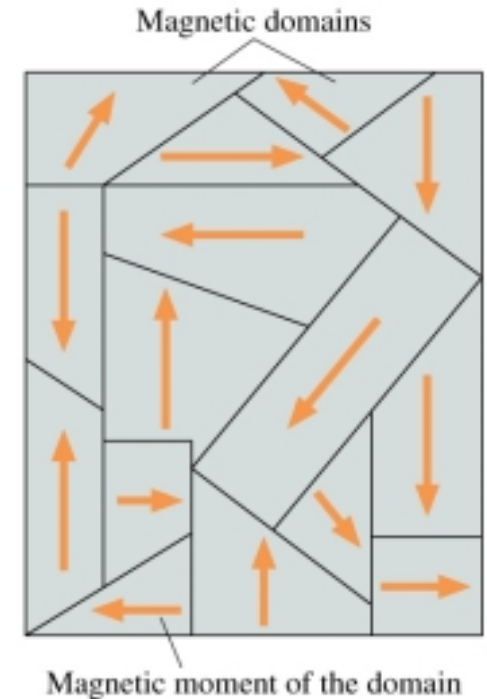


# Ferromagnetism

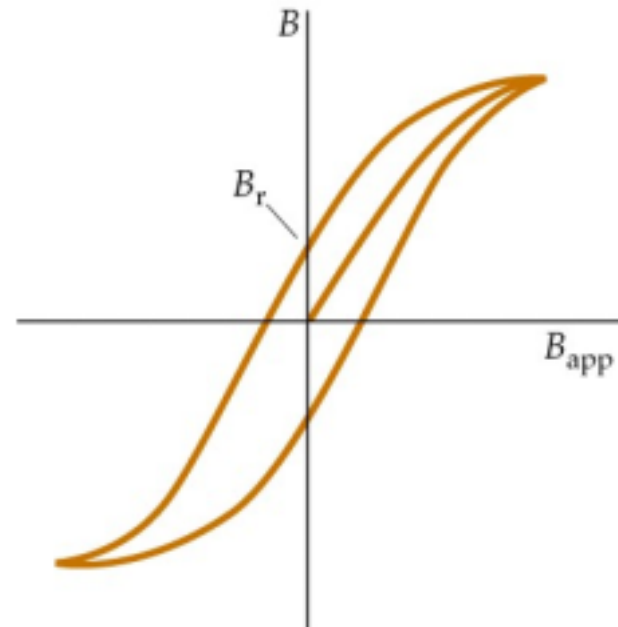
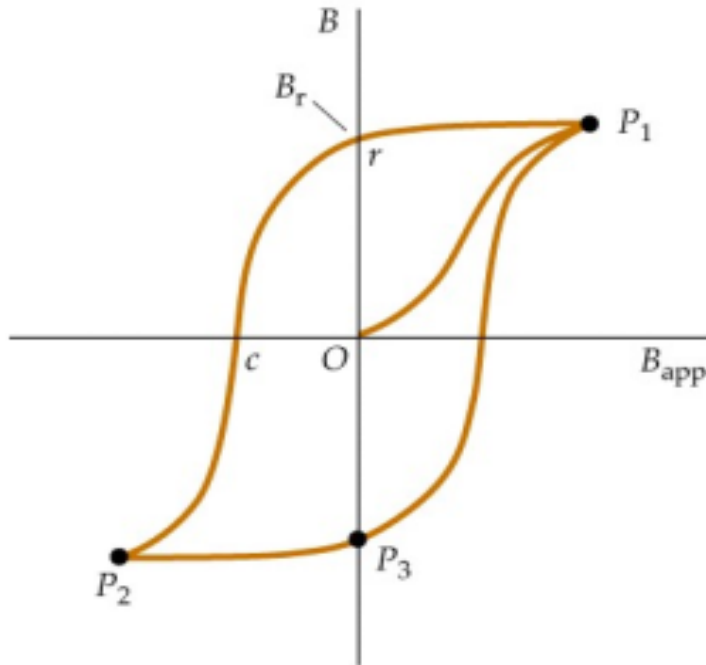
The atomic magnetic moments will be randomly oriented at high temperatures. An applied magnetic field will cause some preferential orientation, thus paramagnetism.

As the temperature is lowered below some critical temperature (the Curie temperature), a strong magnetic interaction between the atoms will cause the spins to align within magnetic domains. If the material is cooled within a magnetic field, the domains may be aligned.

This spontaneous alignment is due to a phase transition. This results in creating a permanent magnet where there is a net magnetic moment in the absence of an applied magnetic field.



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<b>Material</b>	<b>Curie temperature (K)</b>
<b>Fe</b>	<b>1043</b>
<b>Co</b>	<b>1388</b>
<b>Ni</b>	<b>627</b>
<b>Gd</b>	<b>293</b>
<b>Dy</b>	<b>85</b>
<b>CrBr<sub>3</sub></b>	<b>37</b>
<b>Au<sub>2</sub>MnAl</b>	<b>200</b>
<b>Cu<sub>2</sub>MnAl</b>	<b>630</b>
<b>Cu<sub>2</sub>MnIn</b>	<b>500</b>
<b>EuO</b>	<b>77</b>
<b>EuS</b>	<b>16.5</b>
<b>MnAs</b>	<b>318</b>
<b>MnBi</b>	<b>670</b>
<b>GdCl<sub>3</sub></b>	<b>2.2</b>
<b>Fe<sub>2</sub>B</b>	<b>1015</b>
<b>MnB</b>	<b>578</b>

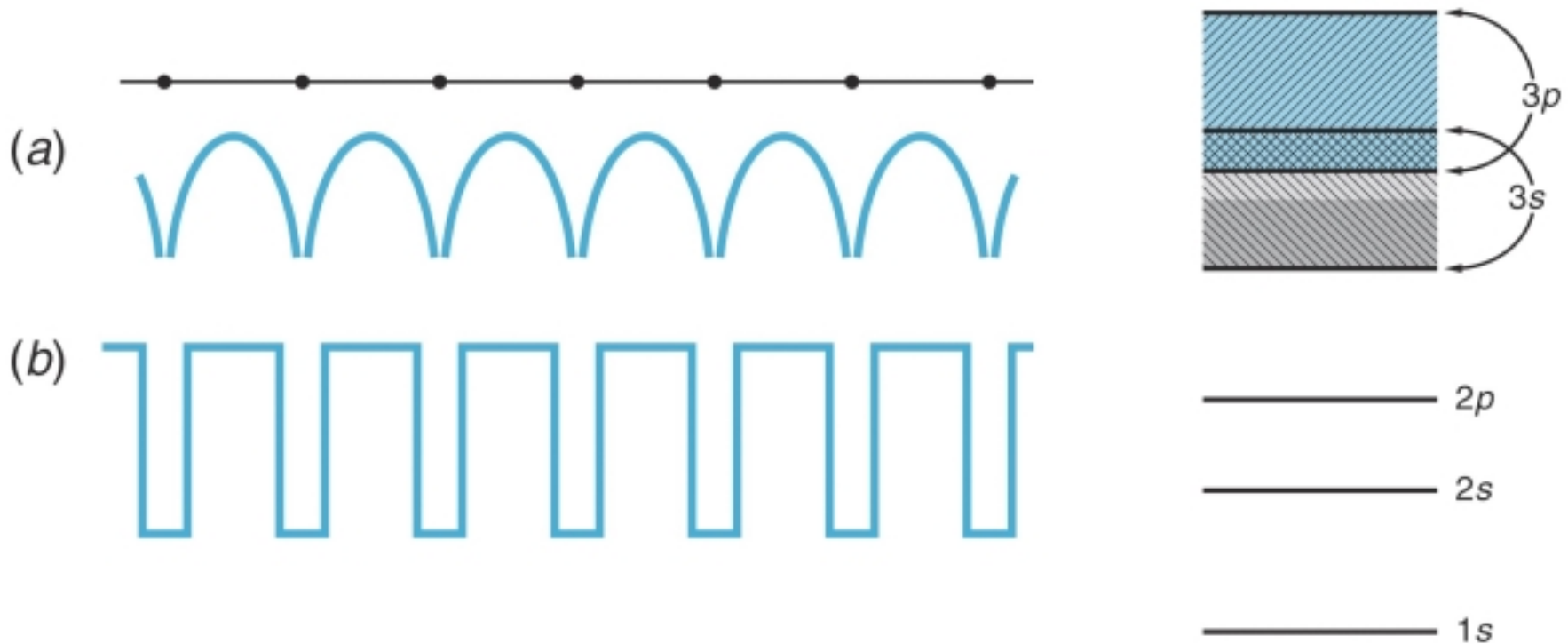
## **Anti-Ferromagnetism**

Transition below the Neel Temperature where adjacent spins align anti-parallel.

# Band Structure

First iteration: Electrons in a three-dimensional well, i.e. a free electron metal.  
Explains some important characteristics of metals.  
Ignores the fact that ion cores are localized and potential is not a constant.  
Doesn't explain insulators and semiconductors.

Second Iteration: Add effect of ion cores localized at particular locations, i.e. electrons are moving in a periodic potential  
Need to determine potential and solve Schrodinger Equation.  
We'll start with a simplified potential energy function in one-dimension.



Felix Bloch showed that solutions to Schrodinger's equation for a one-dimensional periodic potential,  $U(x)$ ,

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x)$$

must have the form

$$\psi(x) = u_k(x)e^{ikx}$$

where  $u_k(x) = u_k(x + L) = u_k(x + nL)$

and  $k = 2\pi / \lambda$ .

This form (called Bloch states) is the wave function for a free electron,  $e^{ikx}$ , times a periodic modulation,  $u_k(x)$ .

$$\psi(x + nL) = u_k(x + nL)e^{ik(x+nL)}$$

$$\psi(x + nL) = u_k(x)e^{ikx} e^{iknL}$$

$$\psi(x + nL) = \psi(x)e^{iknL}$$

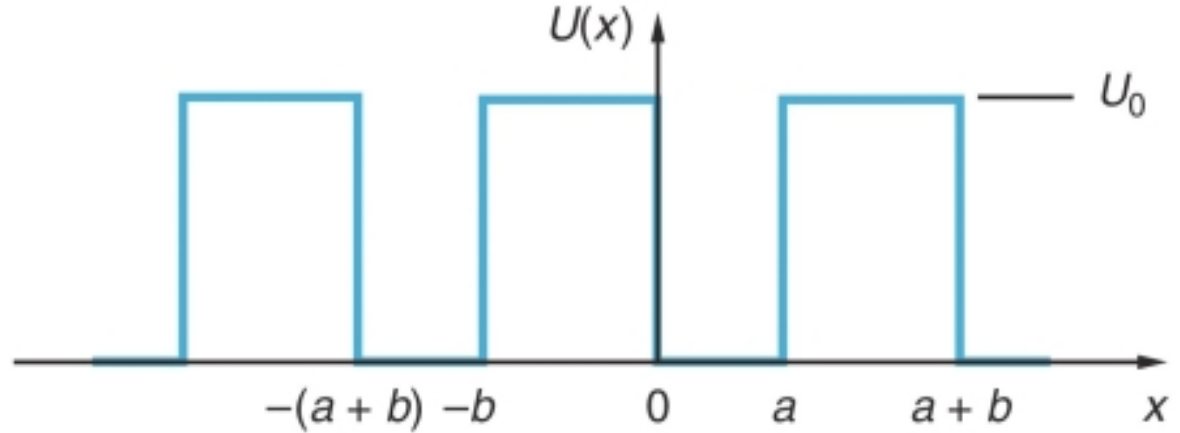
We'll look at the solutions for the simplest periodic potential, the Kronig-Penney potential.

$$U(x) = 0$$

for  $0 < x < a$

$$U(x) = U_0$$

for  $a < x < a + b = L$



$$\psi(x) = A_1 e^{ik'x} + A_2 e^{-ik'x} \text{ for } 0 < x < a$$

$$\text{with } k' = 2\pi / \lambda = \sqrt{2mE} / \hbar$$

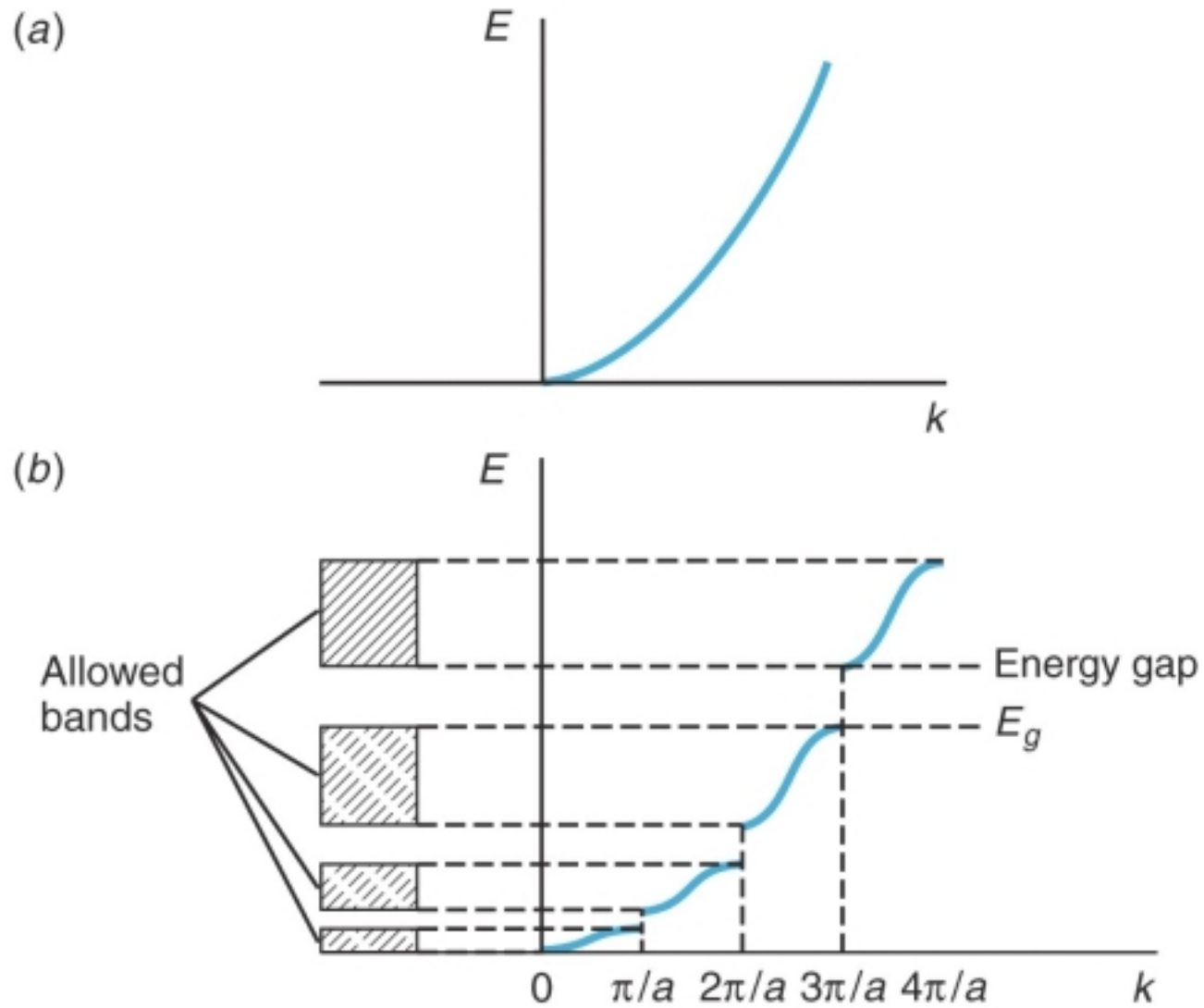
$$\psi(x) = B_1 e^{\alpha x} + B_2 e^{-\alpha x} \text{ for } a < x < a + b = L$$

$$\text{with } \alpha = \sqrt{2m(U_0 - E)} / \hbar$$

We can solve for the constants  $A_1$ ,  $A_2$ ,  $B_1$ , and  $B_2$  as we did in chapter 6.

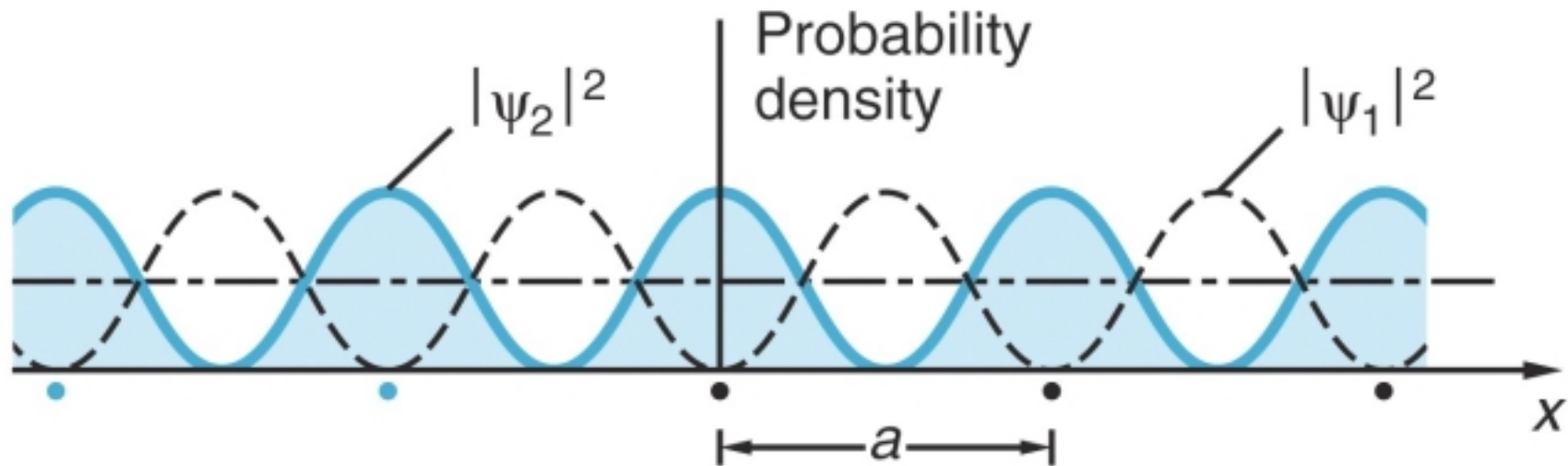
Solving gives a relationship between  $k$ ,  $k'$ ,  $a$ ,  $b$ , and  $\alpha$ .

There are only solutions for some values of  $E$ , but instead of discrete values, there are ranges of allowed energies (called bands) and ranges of forbidden energies (called energy gaps).



Within each band there are  $N$  states, where  $N$  is the number of atoms in our one-dimensional chain. For large values of  $N$ , we can take the energy states to be continuous.

The energy gaps occur at  $kL = \pm n\pi$  .  
 At these values of  $k$  only standing waves occur.



Two standing waves for  $kL = \pi$  .  
 The one with higher electron density at the ion cores has lower energy  
 than the wave with no electron density at the ion cores.

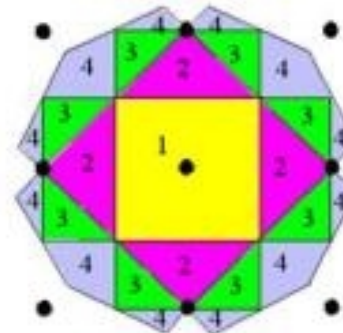
The energy difference is the first energy gap.

The ranges of  $k$ -values,  $0 < k < \pi / L$  ,  $\pi / L < k < 2\pi / L$  , and  $2\pi / L < k < 3\pi / L$  ,  
 are called the first, second, and third Brillouin zones.



## Bloch Waves and Brillouin Zones

- Brillouin Zones defined in Reciprocal Space around lattice point
  - › First Brillouin Zone defined as the volume encompassed around a lattice point without crossing any Bragg planes
  - › Second Brillouin Zone is the volume obtained by crossing only one plane
  - › Continue on to higher orders
- Periodicity of wavefunction mandates all unique information is contained within the first Brillouin zone
  - › Wave-functions in higher zones can be obtained by translating the "pieces" back through the Bragg planes to the First Brillouin Zone.



**Brillouin Zones for  
2-D Square Lattice**

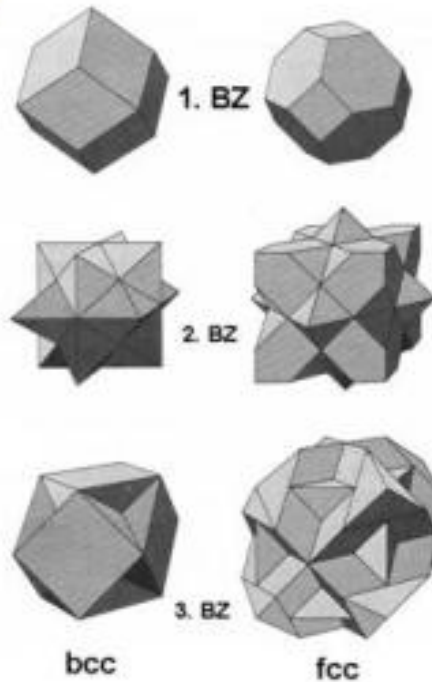


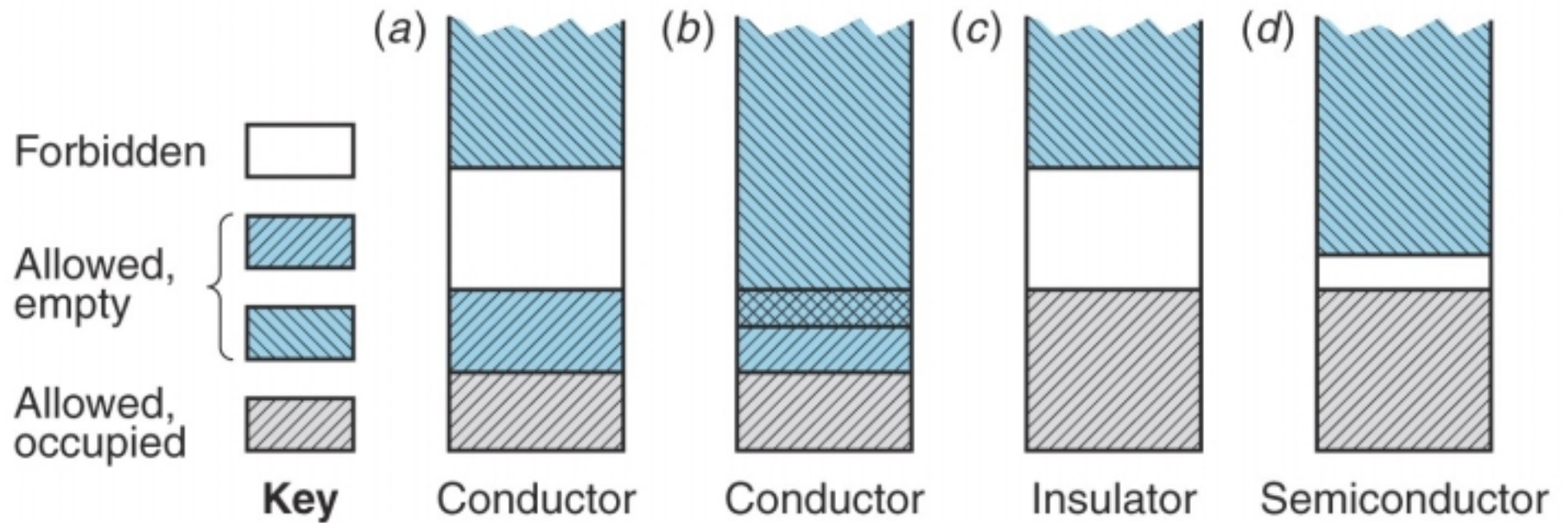


## Brillouin Zones in



- Brillouin zones for three-dimensional solids can be **very** complex, as illustrated here for the 'simple' cases of BCC and FCC lattices.
- Pictures from Ashcroft/Mermin, taken from doctoral dissertation of R. Lück in 1965 (before computer graphics).
- Demonstrates the importance of determining these Brillouin Zones.





Filled or empty bands do not conduct. Electrons have no place to go.

If an allowed band is partially filled, an electric field can easily excite an electron to an unfilled part of the band where conduction can occur.

Partially filled band = conductor

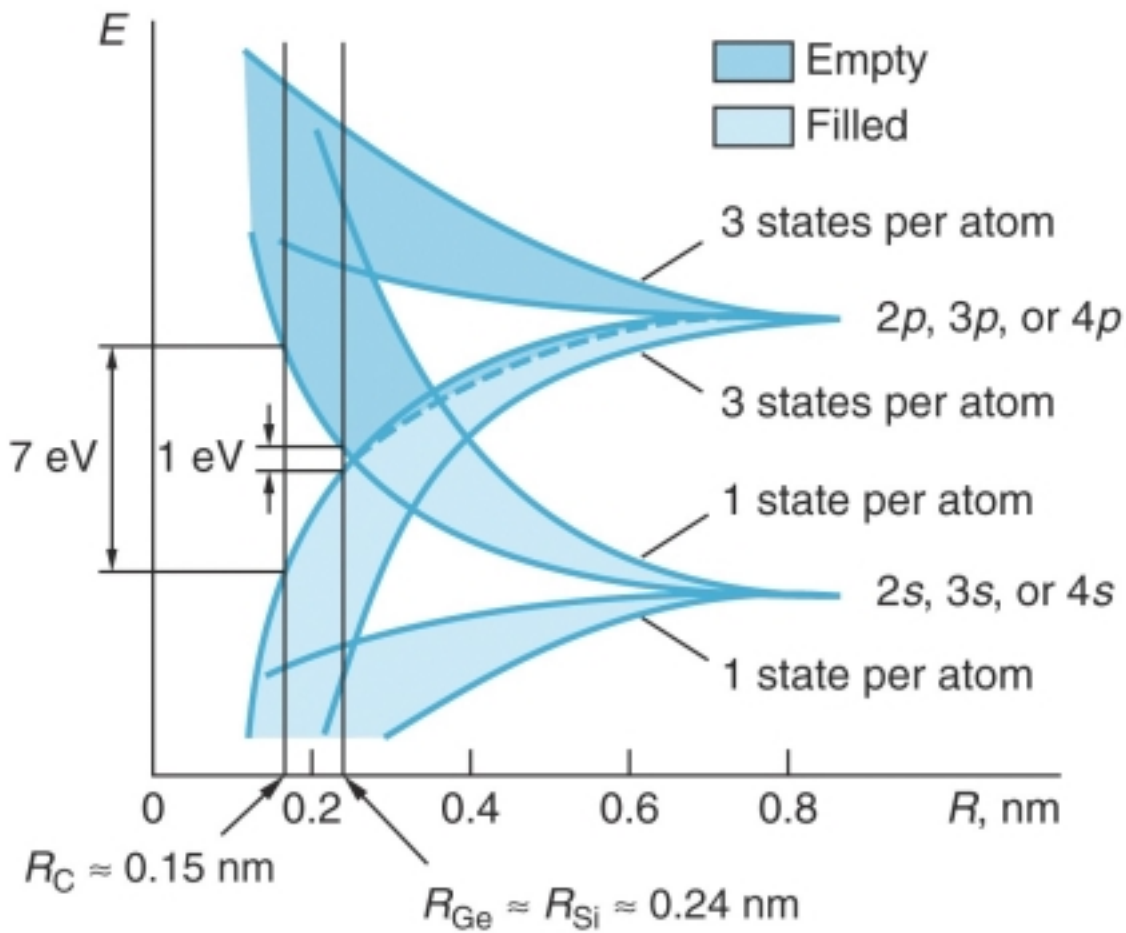
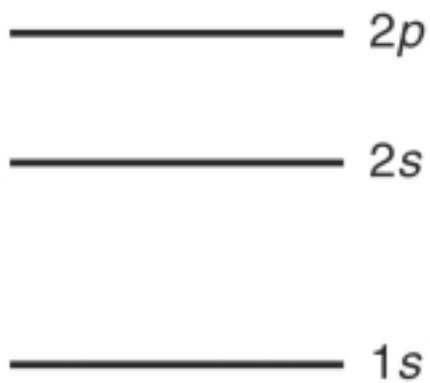
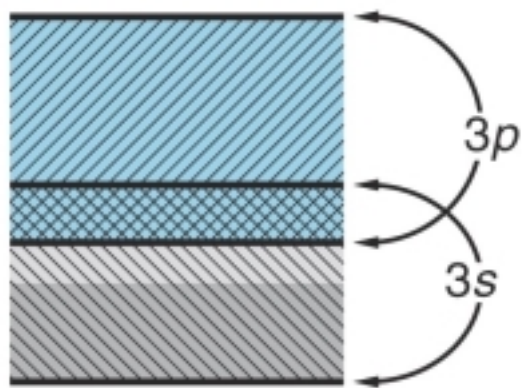
Overlapping filled and empty bands = conductor

Large gap between filled band and empty band = insulator

Small gap between filled band and empty band = semiconductor

The highest filled band is called the valence band.

The lowest unfilled band is called the conduction band.



The Fermi level for an intrinsic semiconductor (no impurities or defects) is mid-gap. The number of electrons we expect to find in the conduction band due to thermal excitation can be calculated from the Fermi-Dirac distribution.

**TABLE 10-4** Values of  $f_{FD}(E)$  for  $T = 293$  K

$E - E_F$ (eV)	0.05	0.10	0.25	1.0	2.5	7.5
Multiple of $kT$	2	4	10	40	100	300
$f_{FD}(E)$	0.12	0.019	$5.1 \times 10^{-5}$	$6.5 \times 10^{-18}$	$1.1 \times 10^{-43}$	$1.3 \times 10^{-129}$

We will have the same number of holes created in the valence band. Both the electrons and the holes contribute to the conduction.

As the temperature of a semiconductor is increased, resistivity goes down, in contrast to a metal. This is because the increase in free carriers more than compensates for the increased scattering.

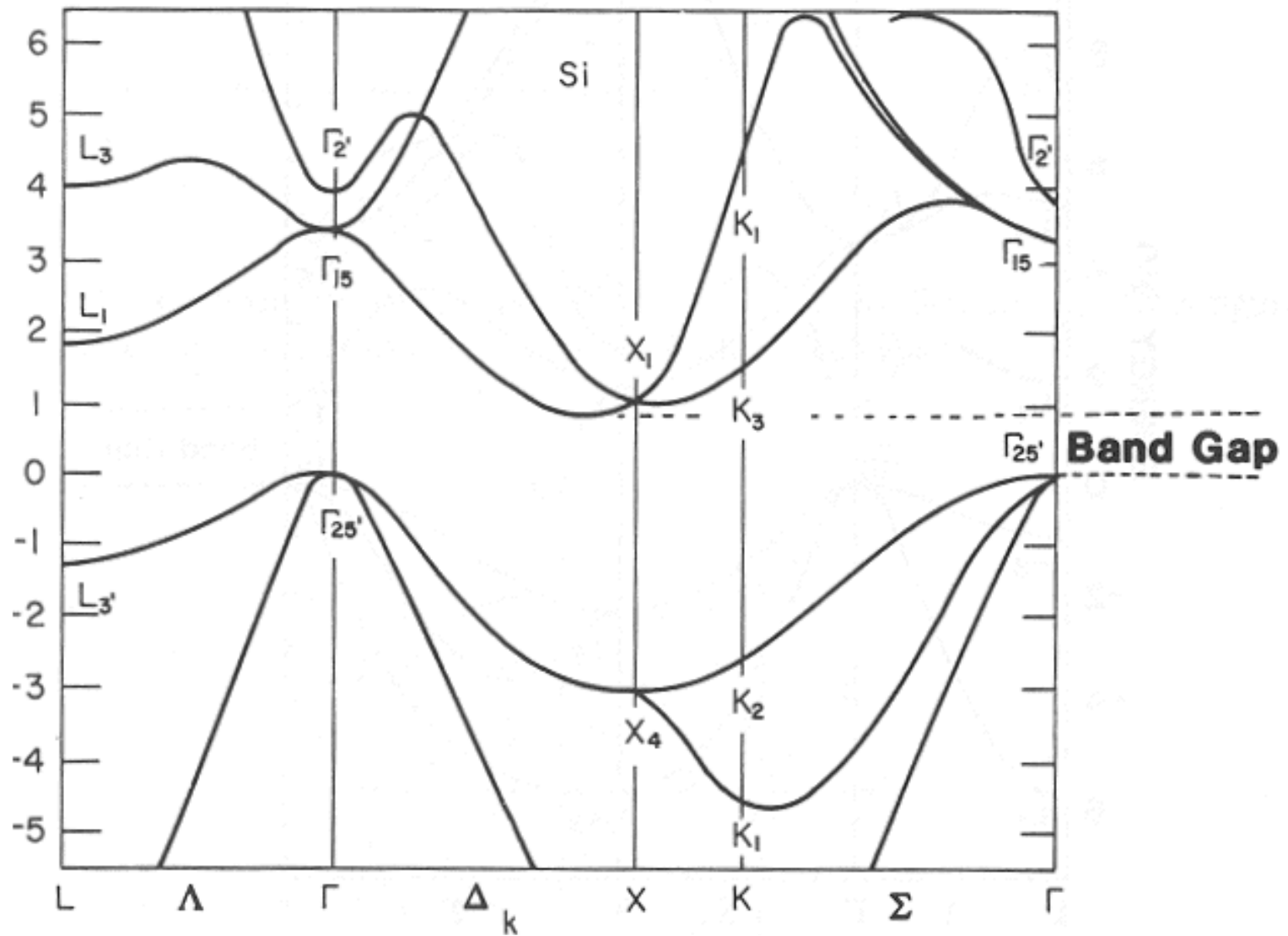
The electrons at the bottom of the conduction band can be characterized by an effective mass. For a free electron  $E = \hbar^2 k^2 / 2m_e$  or  $d^2 E / dk^2 = \hbar^2 / m_e$ .

Because the band is not parabolic at the edge of the Brillouin zone, but has a larger curvature, the effective mass of the electrons in the conduction band is lower,  $d^2 E / dk^2 = \hbar^2 / m^*$ .

**TABLE 10-5** Energy gap  $E_g$  and dielectric constant  $\kappa$  for selected semiconductors

Material	$E_g$ (eV)		$\kappa$	Material	$E_g$ (eV)		$\kappa$
	0 K	293 K			0 K	293 K	
Si	1.15	1.11	11.8	CdTe	1.56	1.44	10.2
Ge	0.74	0.67	15.9	PbS	0.28	0.37	17.0
Te	—	0.33	—	InP	1.41	1.27	12.4
GaAs	1.53	1.35	13.1	CdSe	1.85	1.74	10.1
InSb	0.23	0.16	17.8	GaP	2.40	2.24	11.1
ZnS	—	3.54	5.2	PbTe	0.19	0.25	30.1

E [eV]

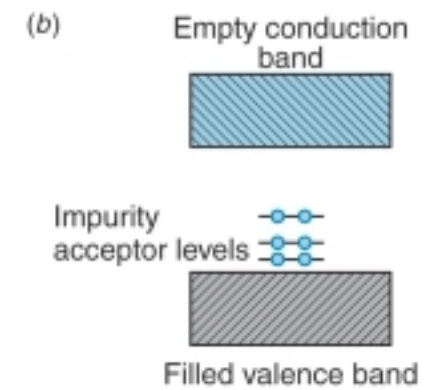
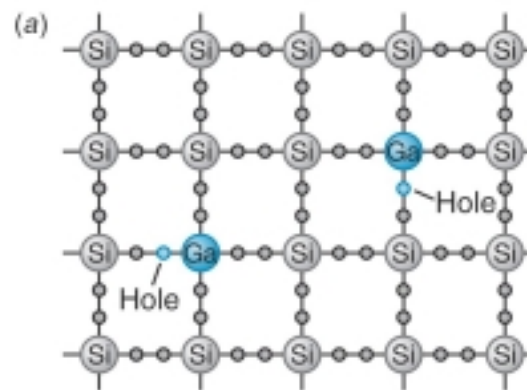
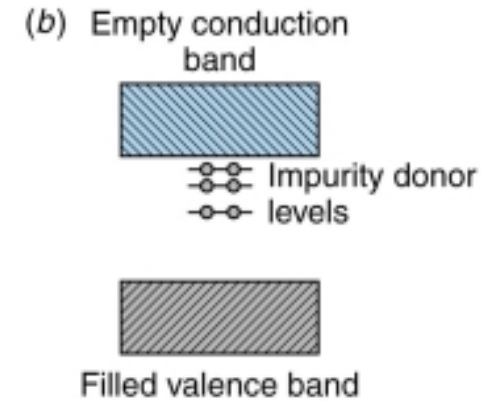
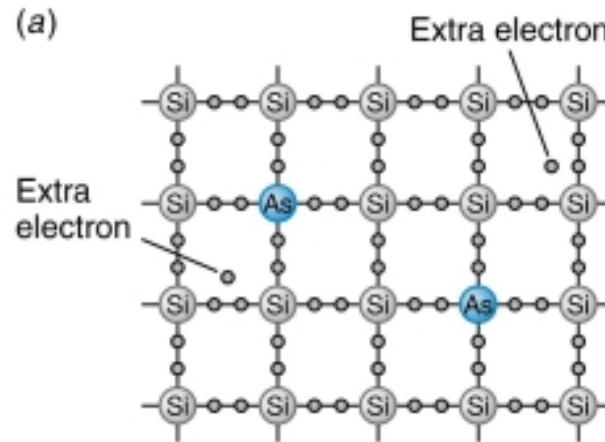
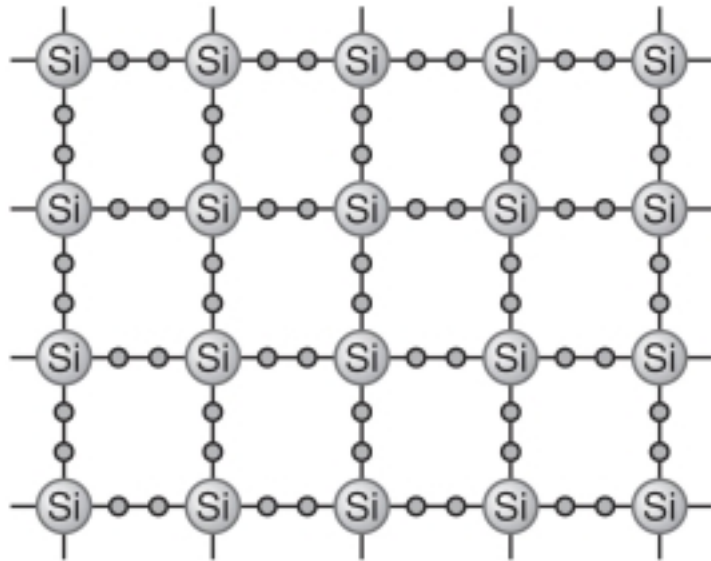


# Impurity Semiconductors

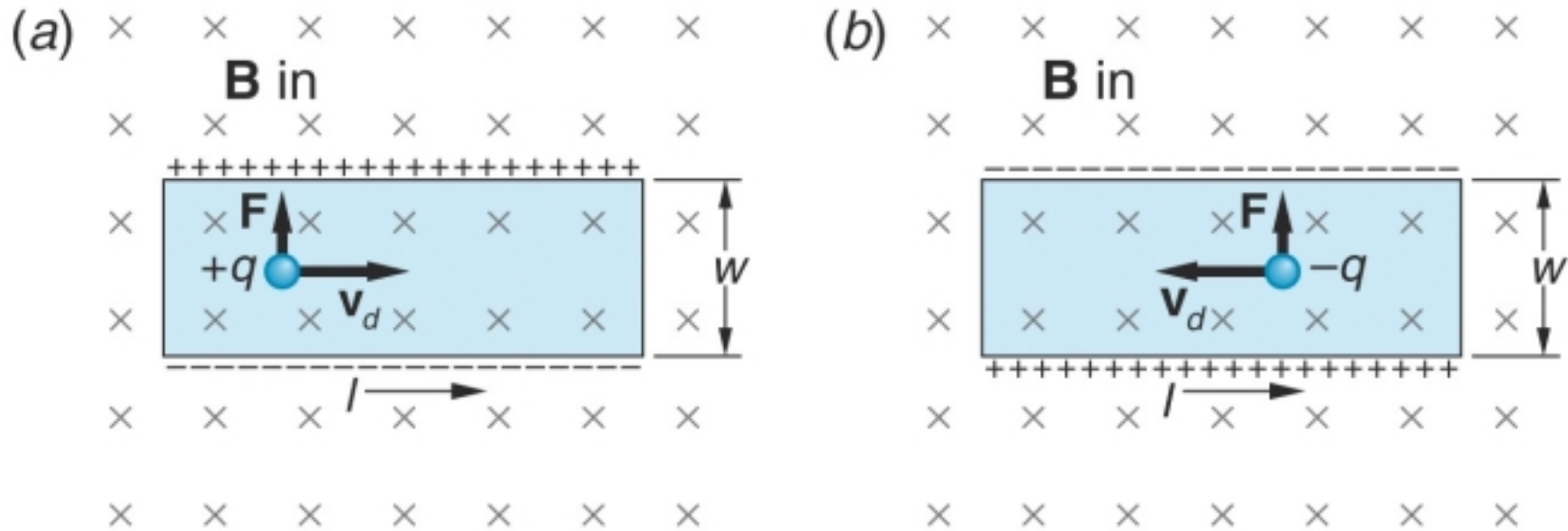
The energy of the donor state relative to the bottom of the conduction band is

$$E_n = -\frac{1}{2} \left( \frac{ke^2}{\hbar} \right)^2 \frac{m^*}{n^2 \kappa^2}$$

$$\langle r_n \rangle = \kappa a_0 n^2 \frac{m_e}{m^*}$$



## Hall Effect



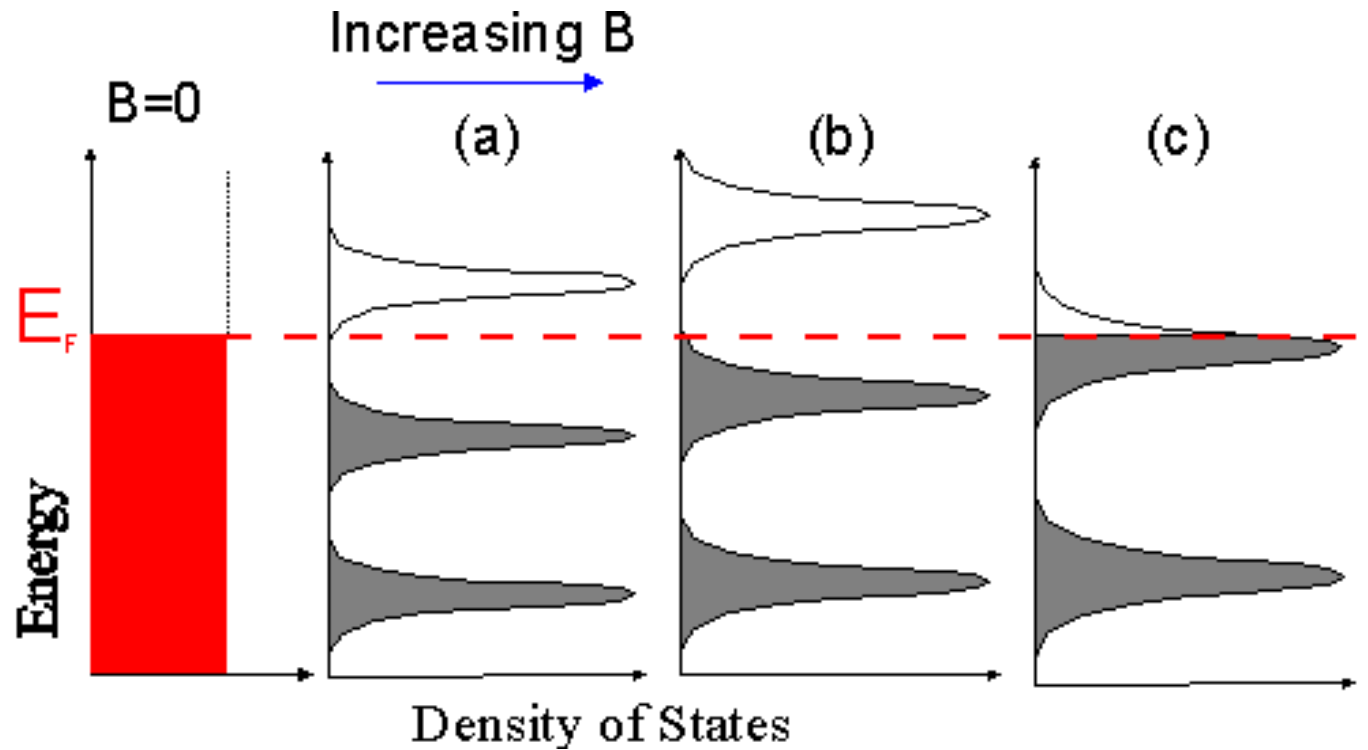
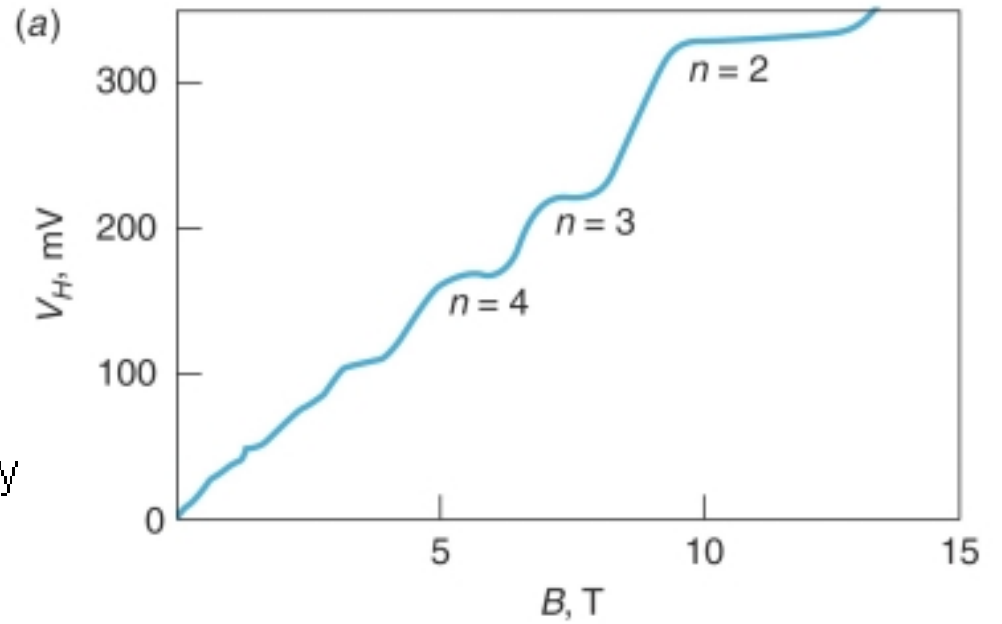
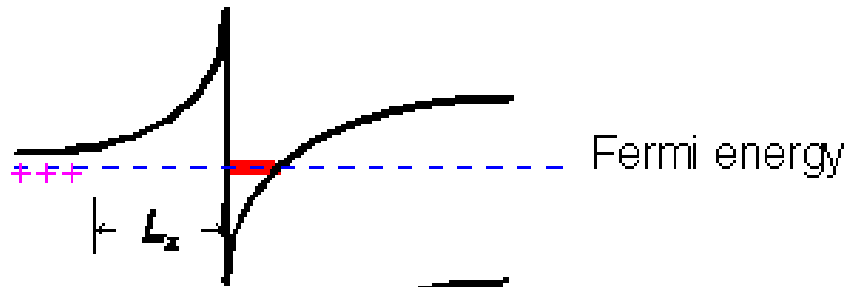
$$q\vec{E} = -q\vec{v}_d \times \vec{B}$$

$$V_H = Ew = v_d Bw$$

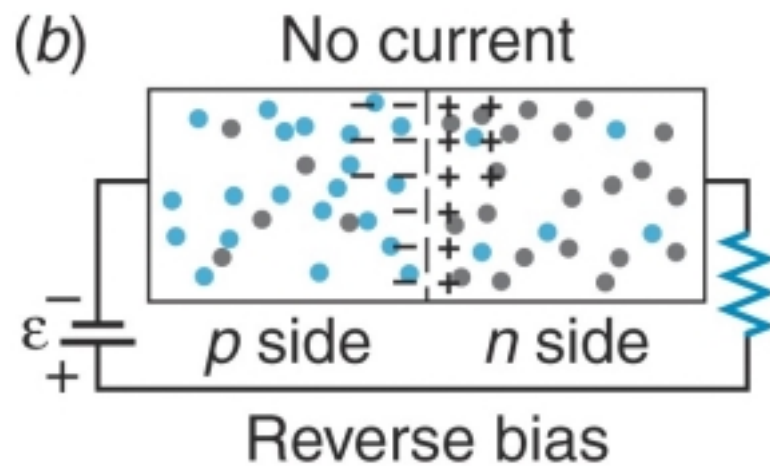
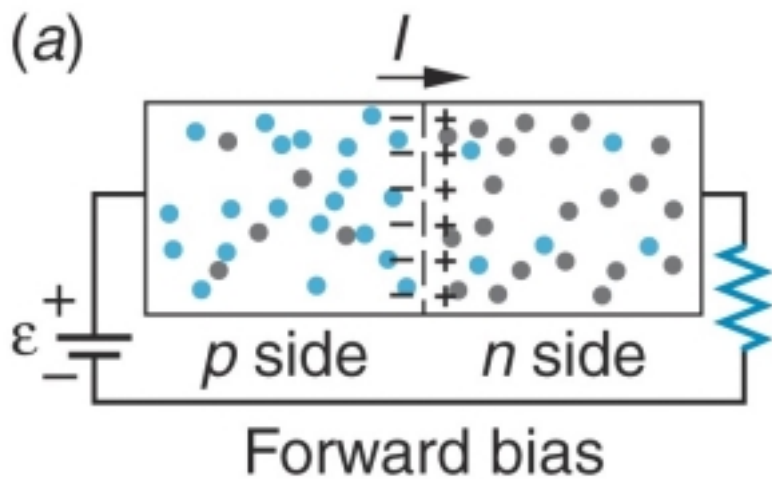
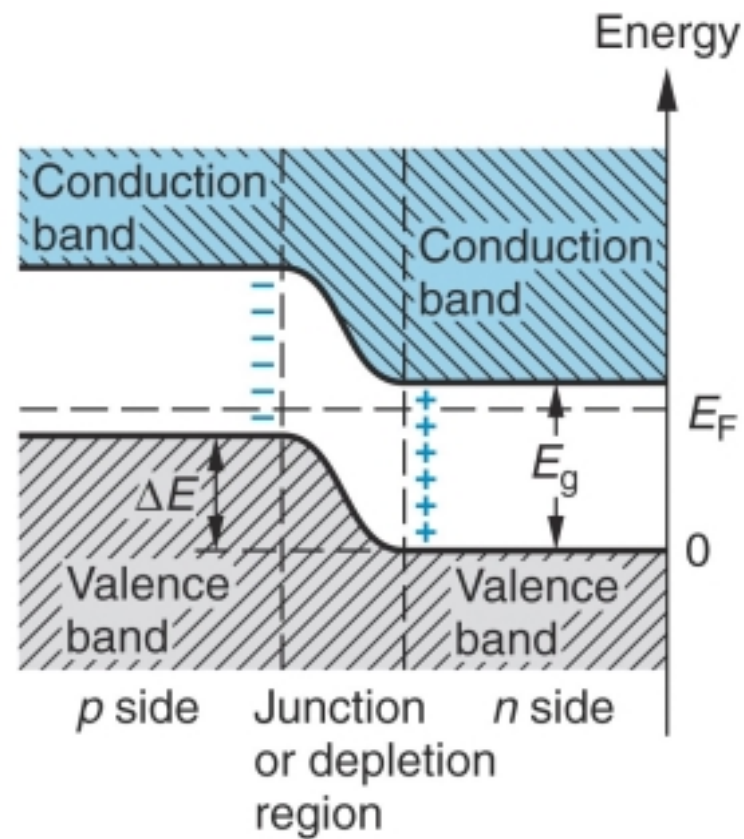
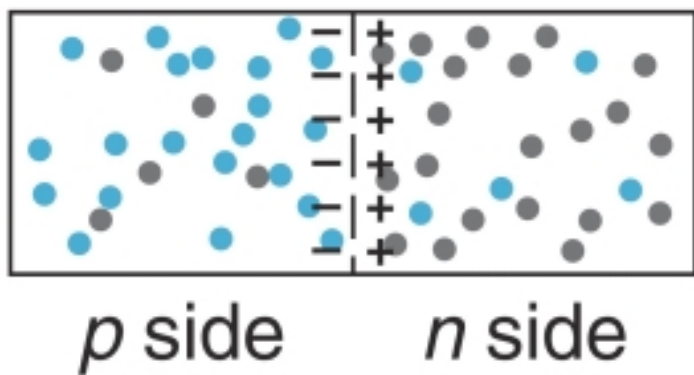
$$V_H = v_d Bw = \left( \frac{j}{ne} \right) Bw = \frac{iB}{ent}$$

# Quantum Hall Effect

$$R_H = \frac{V_H}{i} = \frac{R_K}{n} = \frac{h/e^2}{n} = \frac{25,813\Omega}{n}$$



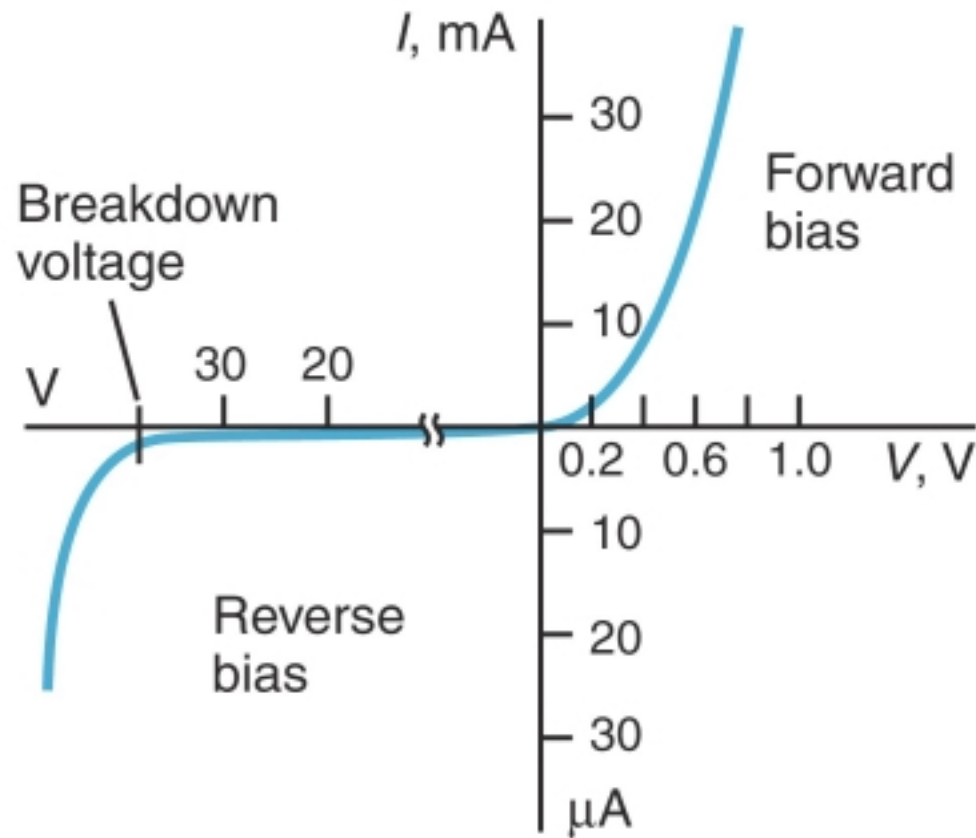
- - electrons
- + holes

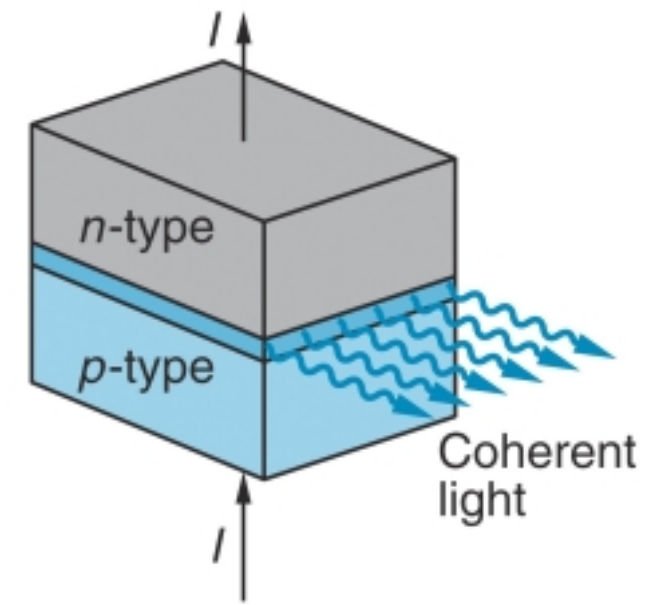
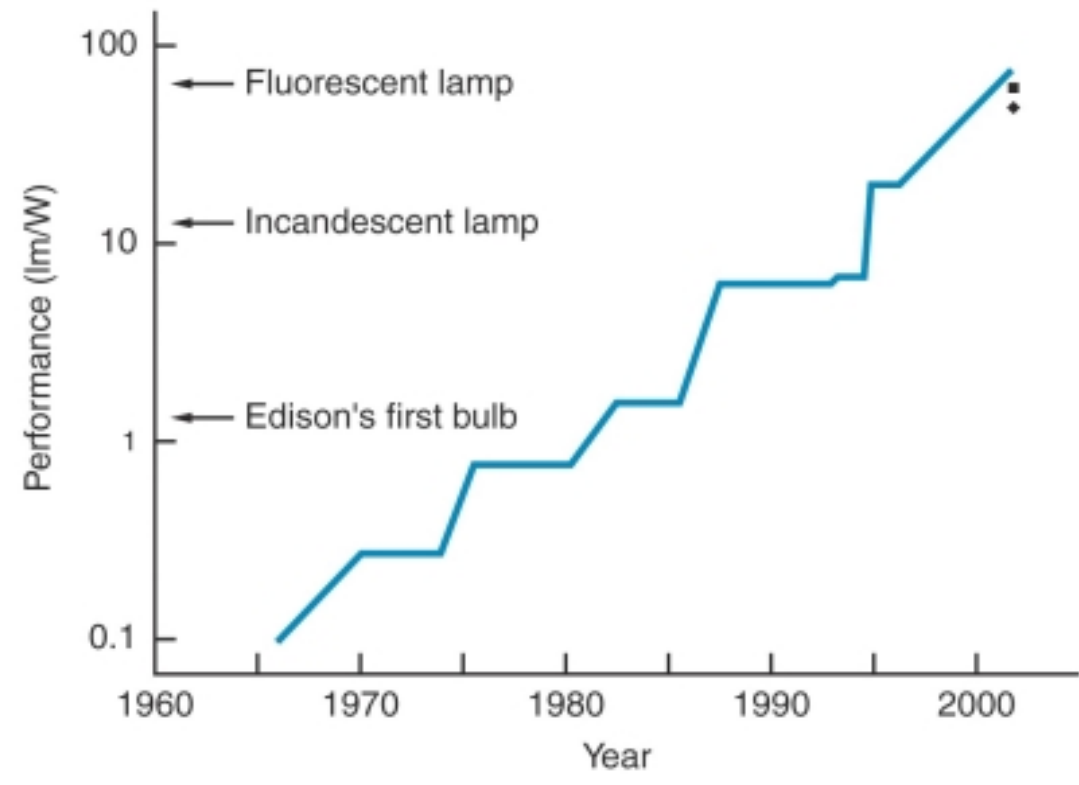
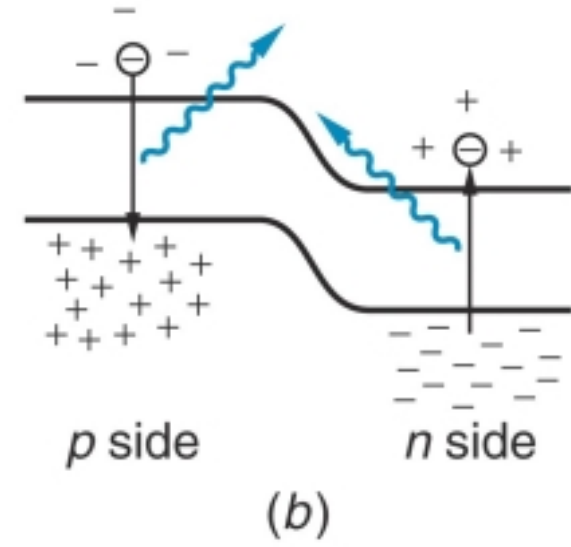
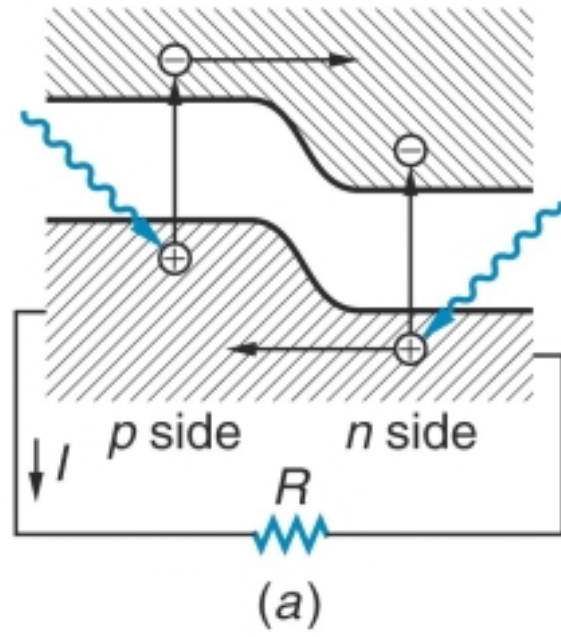


$$N_e e^{-e(V-V_b)/kT} = N_e e^{-eV/kT} e^{eV_b/kT}$$

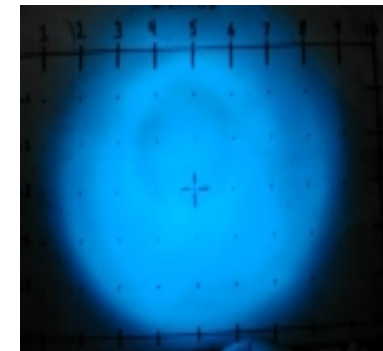
$$I = I_0 e^{eV_b/kT}$$

$$I_{net} = I_0 (e^{eV_b/kT} - 1)$$

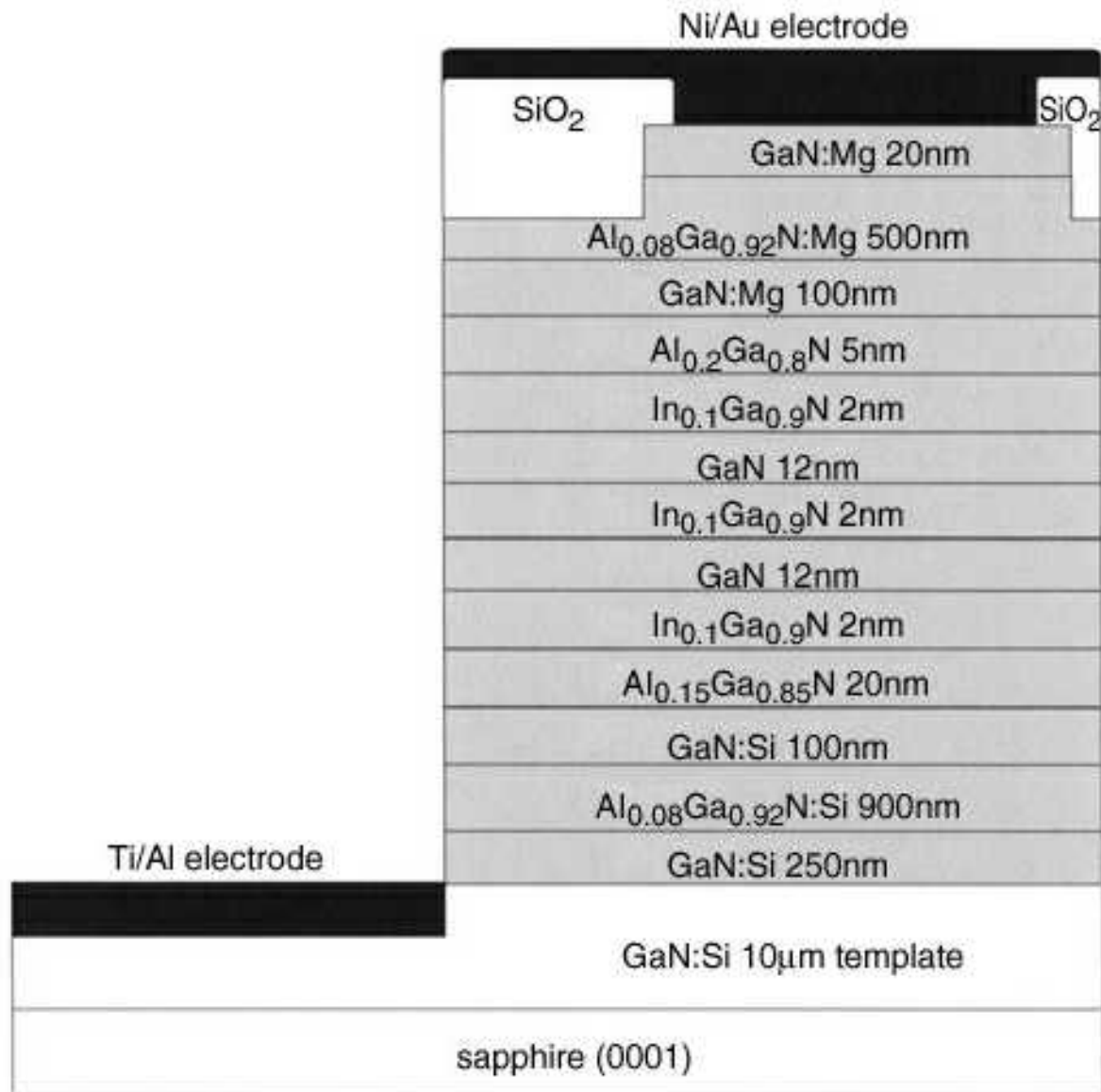




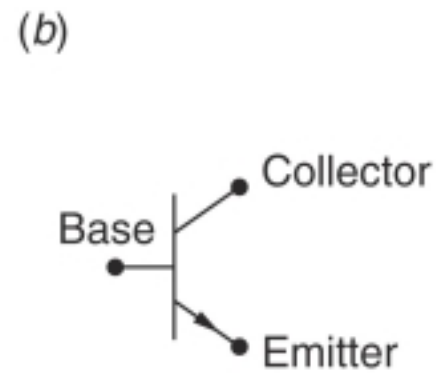
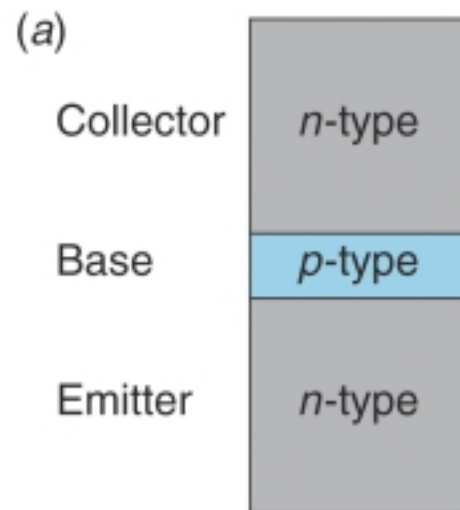
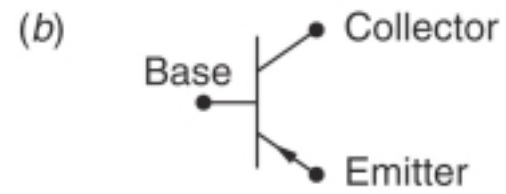
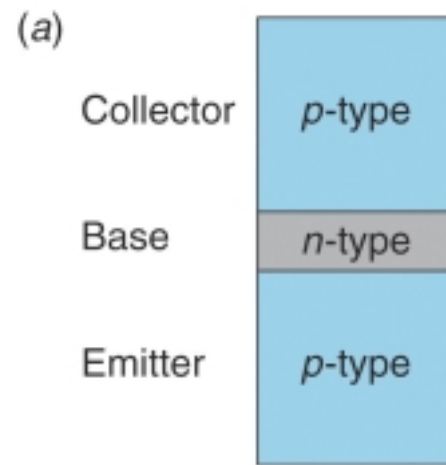
# Solid-State Lighting



- ❖ Small in size,
- ❖ low power consumption
- ❖ low self heating
- ❖ High reliability
- ❖ Resistant to Shock and vibration
- ❖ Cheaper than incandescent lighting system.



**Fig. 1** Schematic cross-section showing structure of InGaN MQW laser diodes



# Superconductivity

Some materials exhibit zero resistivity below a critical temperature,  $T_C$ . The critical temperature is lower in the presence of a magnetic field, and goes to zero for magnetic fields above a critical field,  $B_C$ .

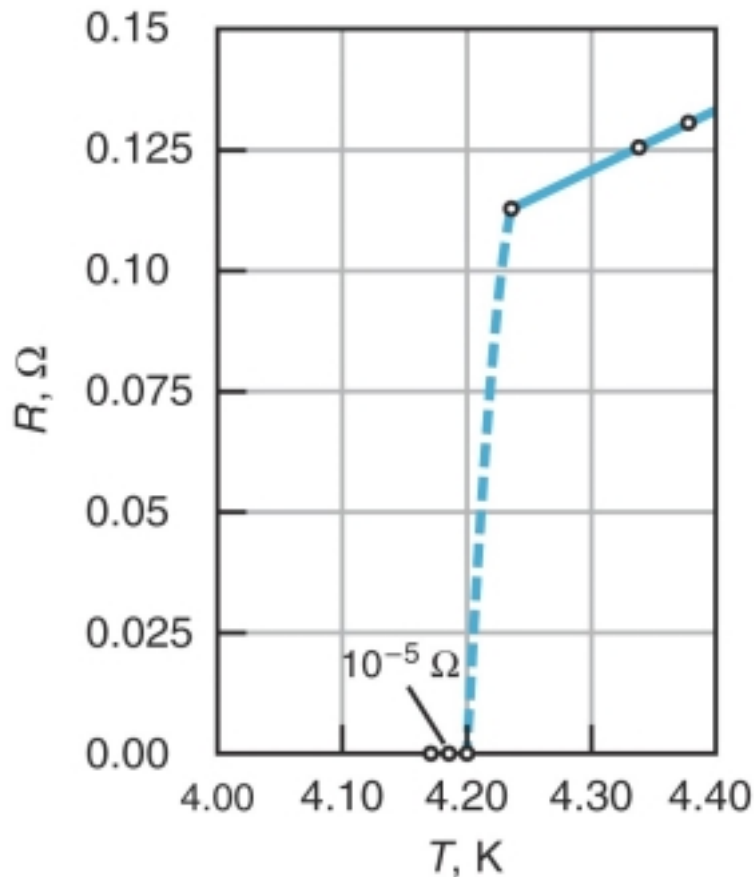


TABLE 10-6  $T_C$  and  $B_C$  values for some type I and type II superconductors

Type I element	$T_C$ (K)	$B_C$ (at 0 K, T)	Type II compound	$T_C$ (K)	$B_{C2}$ (at 0 K, T)
Al	1.175	0.0105	Nb <sub>3</sub> Sn	18.1	24.5
Cd	0.517	0.0028	Nb <sub>3</sub> Ge	23.2	34.0
Hg	4.154	0.0411	NbN	16.0	15.3
In	3.408	0.0282	V <sub>3</sub> Ga	16.5	35.0
Nb	9.25	0.2060	V <sub>3</sub> Si	17.1	15.6
Os	0.66	0.0070	PbMoS	14.4	6.0
Pb	7.196	0.0803	CNb	8.0	1.7
Sn	3.722	0.0305	MgB <sub>2</sub>	39.0	16
Tl	2.38	0.0178	Rb <sub>3</sub> C <sub>60</sub>	29.0	?
Zn	0.85	0.0054	Cs <sub>2</sub> RbC <sub>60</sub>	33.0	?

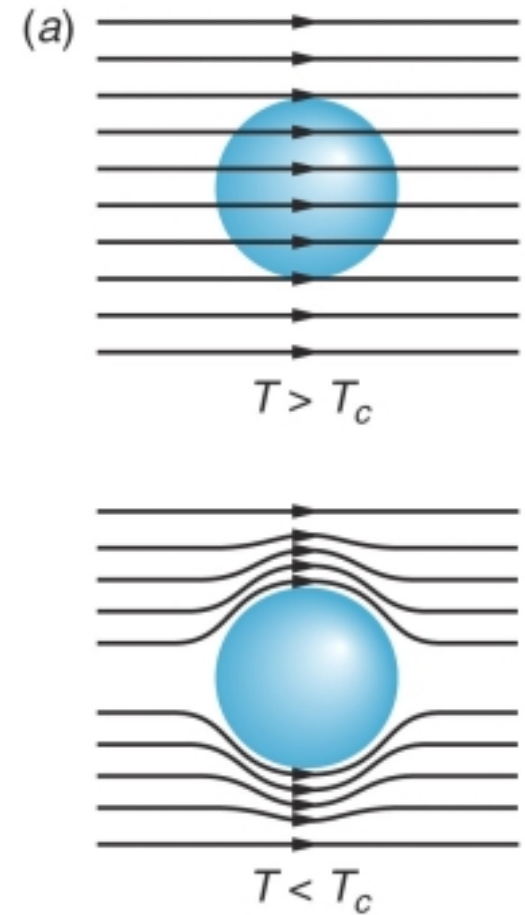
## Meissner Effect

A superconductor has zero resistance, so there can be no electric field or emf since that would produce an infinite current.

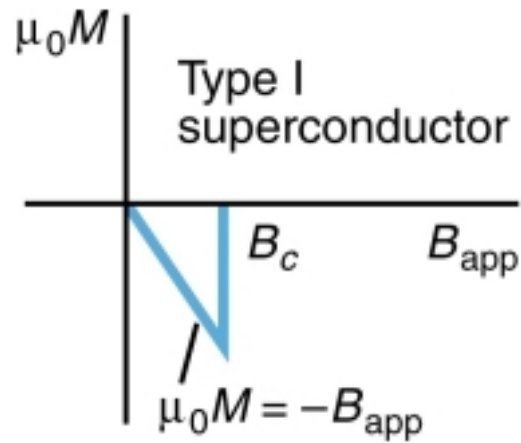
So there can be no changing magnetic fields in a superconductor.

It is observed that the magnetic field is not only constant, the magnetic field is zero in a superconductor.

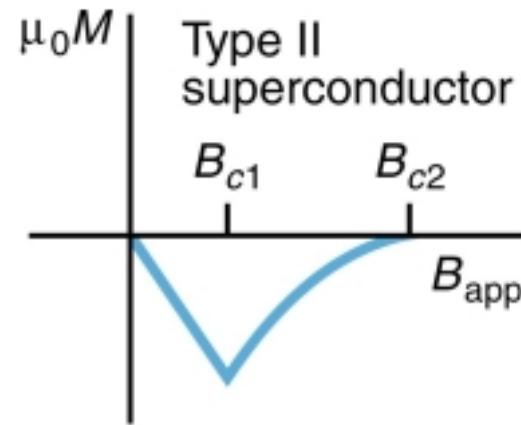
A superconductor in an external magnetic field will have supercurrents which cancel out the magnetic field inside the material, that is, it will be a perfect diamagnet.



There is an energy cost to producing the supercurrents. If the applied field is sufficiently large ( $B > B_c$ ), the energy cost is too high and the superconductivity is destroyed.



(a)

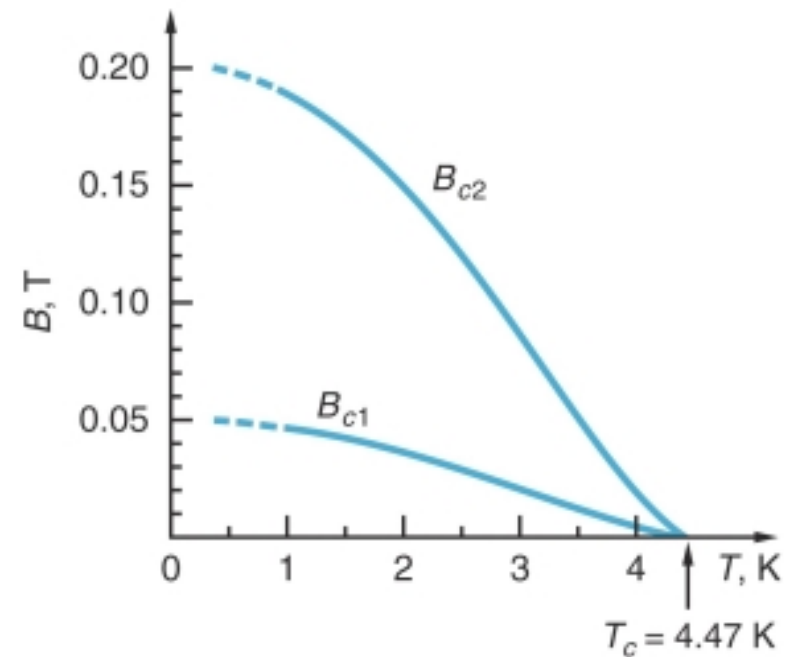


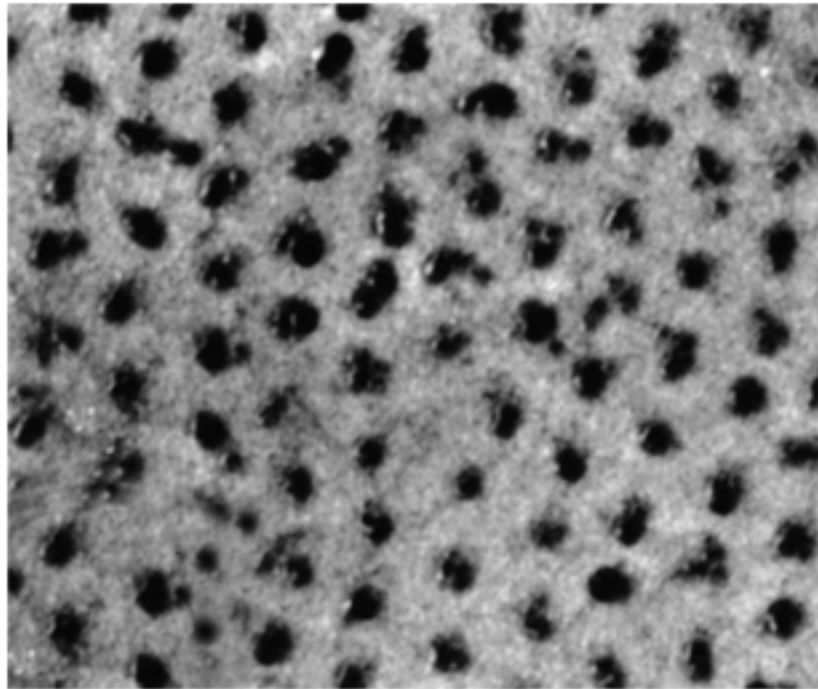
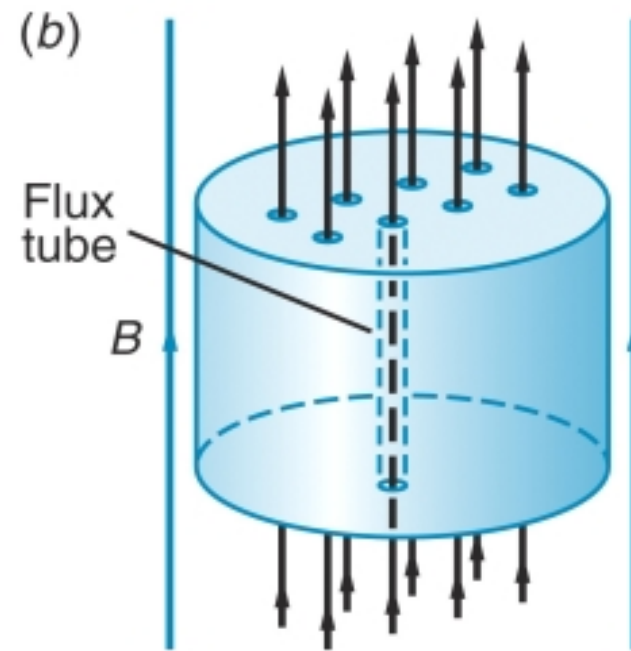
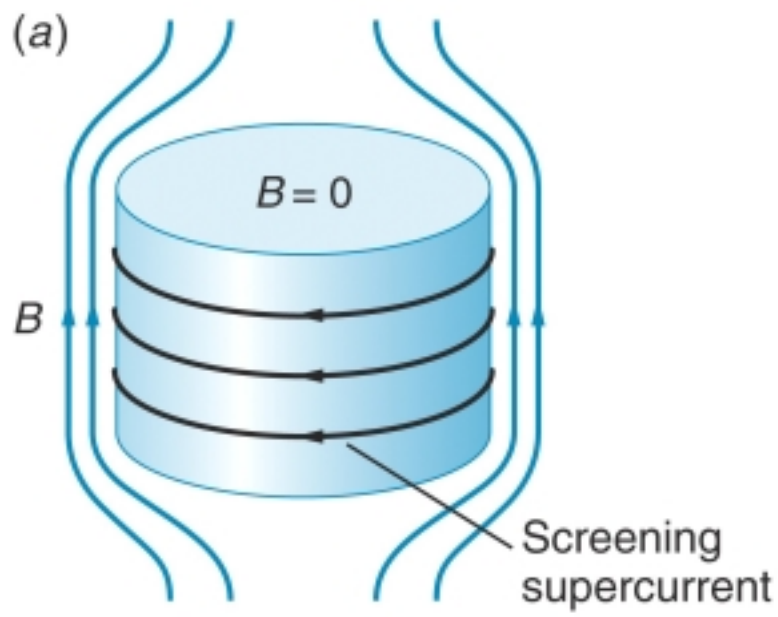
(b)

Superconductors come in two varieties, called Type I and Type II.

Type I superconductors exhibit the Meissner Effect up to their critical field,  $B_c$ , above which the superconductivity and the exclusion of applied magnetic fields abruptly stops.

Type II superconductors exhibit superconductivity and the exclusion of applied magnetic fields up to their lower critical field,  $B_{c1}$ . Above this field, the material still exhibits superconductivity, but the supercurrents can exclude only part of the applied magnetic field. The exclusion of magnetic field decreases with increasing applied field until an applied field  $B_{c2}$ , the upper critical field, above which the superconductivity and the exclusion of applied magnetic fields is gone.





**TABLE 10-7** Experimental values of  $\alpha$  for a few superconductors

Material	$\alpha$	Material	$\alpha$
Cd	0.32	Nb <sub>3</sub> Sn	0.08
Hg	0.50	Os	0.15
Pb	0.49	Zn	0.45

Data from C. Kittel, Introduction to Solid State Physics, 7th ed. (New York: Wiley, 1995).

## BCS Theory (Bardeen, Cooper, Schrieffer)

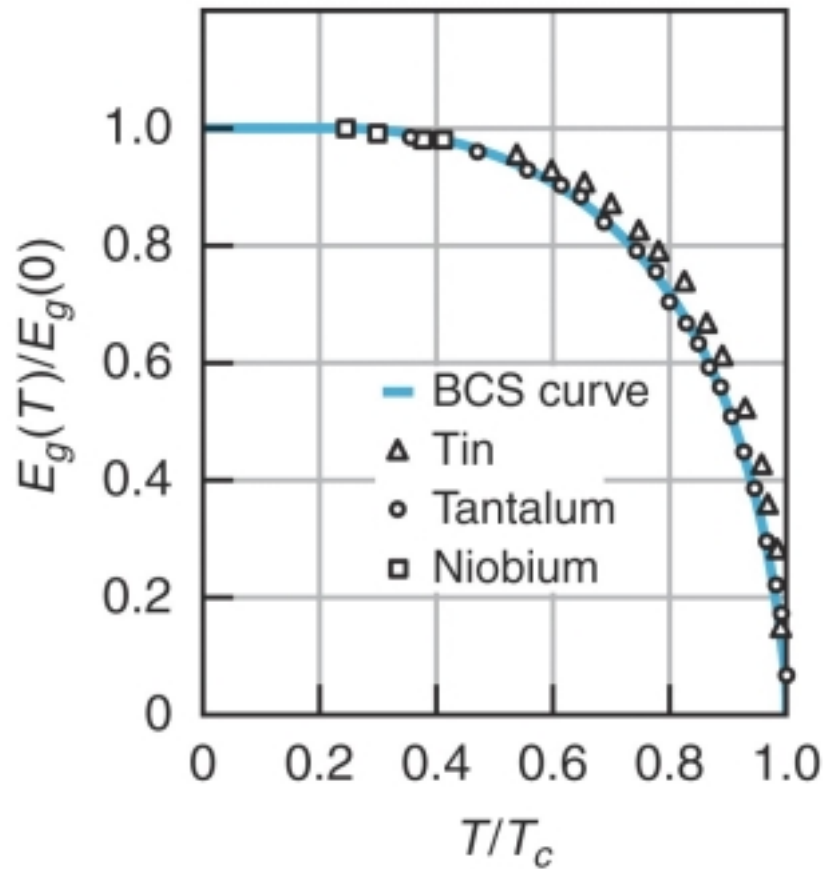
Isotope effect:  $M^\alpha T_C = \text{constant}$

This indicates that lattice vibrations are important to superconductivity.

$$\frac{B_C(T)}{B_C(0)} = 1 - \left( \frac{T}{T_C} \right)^2$$

Theory: At low temperatures electrons pair up. The attractive interaction comes from the fact that an electron moving through the lattice attracts the positive ions and so produces a traveling distortion of the lattice, a phonon. This traveling local increase in the positive charge density is attractive to another electron. So there is an attraction between two electrons mediated by the vibrations of the lattice, phonons. At low enough temperatures, this attractive force is larger than the Coulomb repulsion and a bound state is formed, a Cooper pair.

The electrons that form a pair have opposite spins and opposite linear momenta!  
Together the pair forms a boson and so all pairs can be in the same energy state.



The energy to break up the pair is called the superconducting energy gap,  $E_g$ . As the temperature is increased, more and more pairs get broken up. The unpaired electrons decrease the binding energy of the remaining pairs, i.e. they decrease the energy gap.

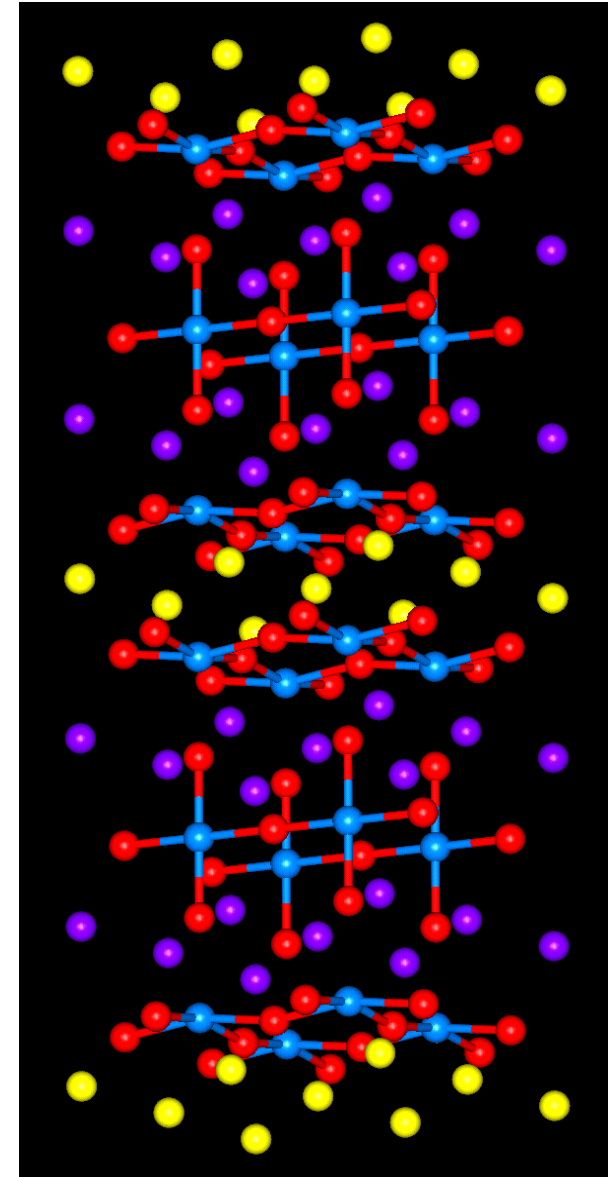
# High $T_c$ Superconductors

Type II superconductors with high critical temperatures and high critical fields.

All have copper and oxygen and are in the perovskite structure.

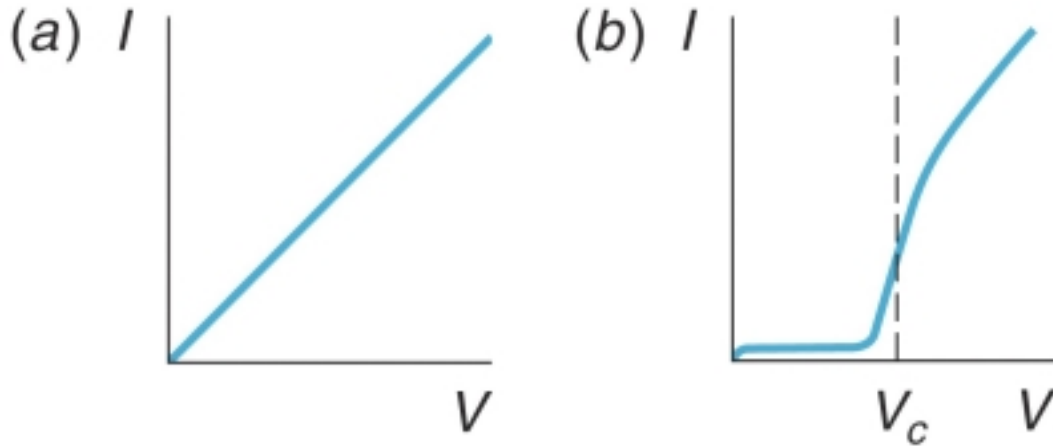
TABLE 10-8 Critical temperatures of some high  $T_c$  superconductors

Material	$T_c$ , K
LaBaCuO	30
La <sub>2</sub> CuO <sub>4</sub>	40
YBa <sub>2</sub> Cu <sub>3</sub> O <sub>7</sub>	92
DyBa <sub>2</sub> Cu <sub>3</sub> O <sub>7</sub>	92.5
C <sub>60</sub> (CHBr <sub>3</sub> )	117
BiSrCaCuO	120
TlBaCaCuO	125



Yttrium atoms are yellow, Barium atoms are purple, Copper atoms are blue and Oxygen atoms are red.

# Josephson Junctions



## dc Josephson effect

Tunneling from one superconductor to another through an insulating barrier.

$$I = I_{\max} \sin(\phi_2 - \phi_1)$$

## ac Josephson effect

If a voltage is applied to the junction, the current oscillates with frequency

$$f = 2eV / h$$

## Superconducting Quantum Interference Device (SQUID)

A small magnetic field produces a phase difference in the two currents and interference effects.

