Chapter 3

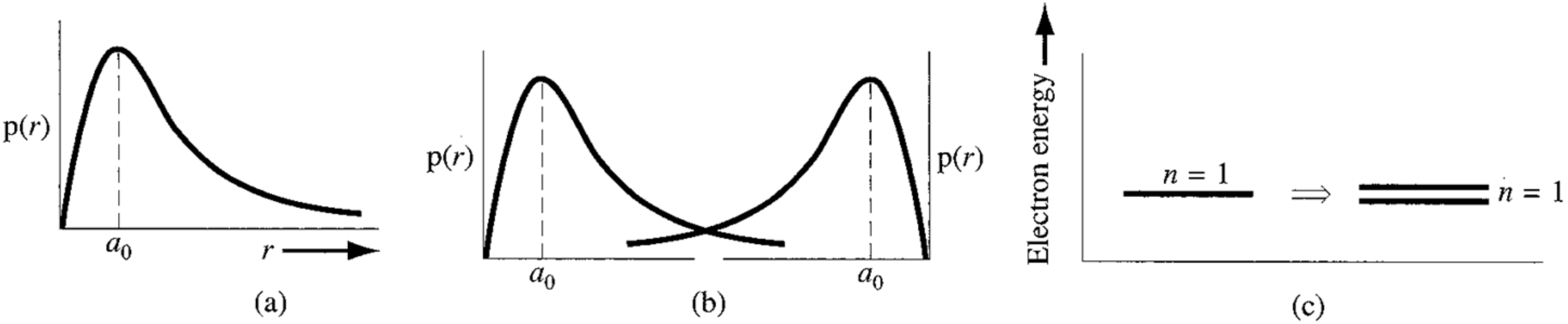
Electron in a finite space → energy is quantized.

Pauli exclusion principle → one quantum state can be occupied by only one electron

Can we extend these concepts to electron in a crystal lattice?

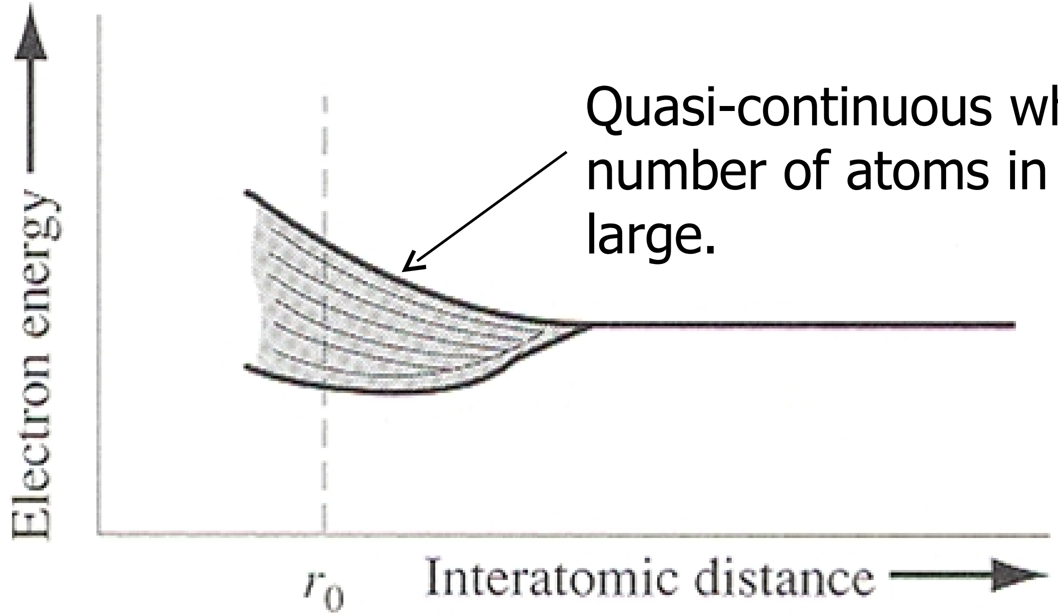
Formation of Energy Bands

When two hydrogen atoms are brought close enough for the wave functions of n=1 electrons to start interacting, the n=1 state splits into two different energies, in accordance with Pauli exclusion principle.



(a) Probability density function of n=1 electron in an isolated hydrogen atom.
(b) Overlapping probability density functions in two adjacent hydrogen atoms.
(c) splitting of n=1 state.

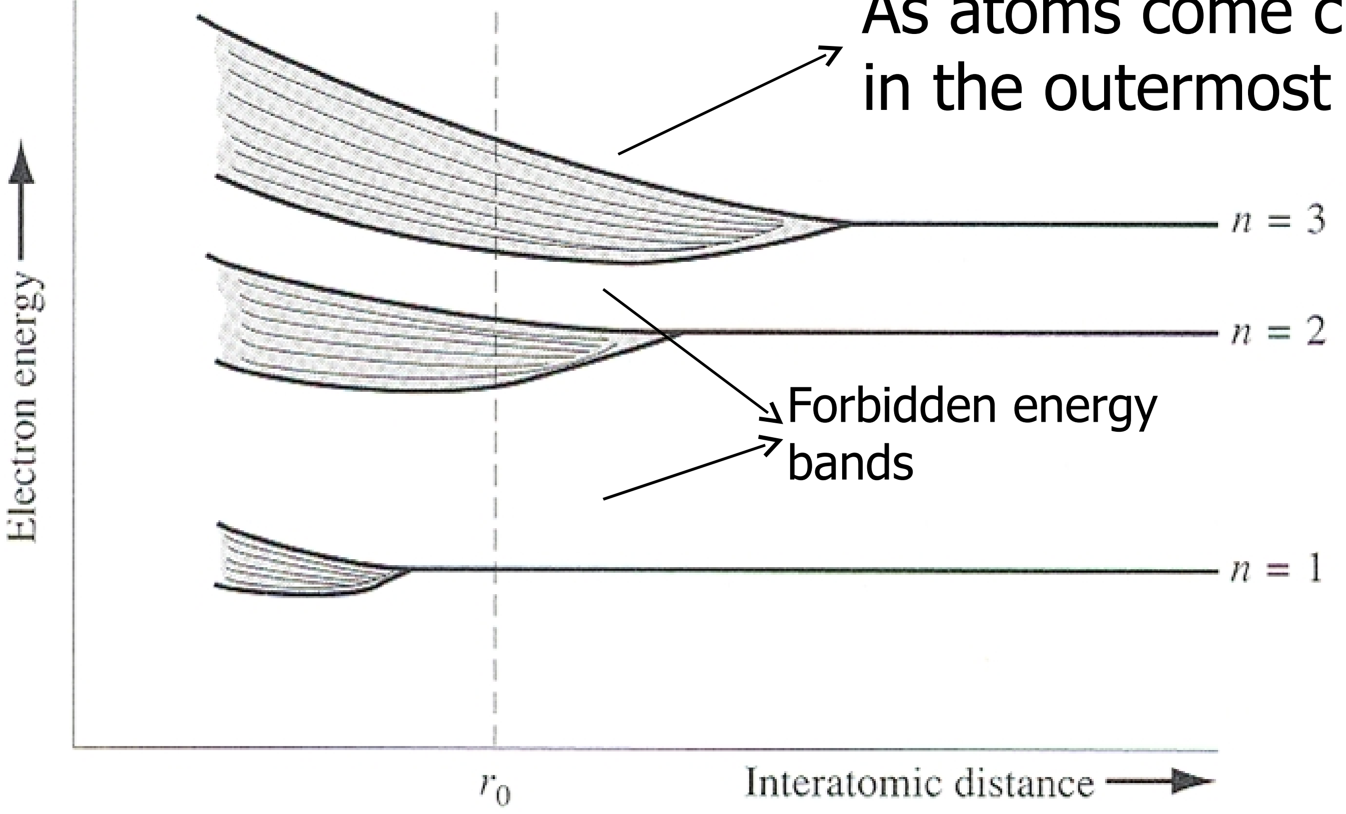
Hypothetically, if we have a periodic arrangement of many hydrogen atoms and they are brought close enough → initial quantized energy level will split into band of discrete levels.



Quasi-continuous when the number of atoms in the system is large.

The splitting of an energy state into a band of allowed energies (r_0 is the equilibrium inter-atomic distance in the crystal)

What happens in an atom containing many more electrons?



As atoms come closer, the states in the outermost shell split first.

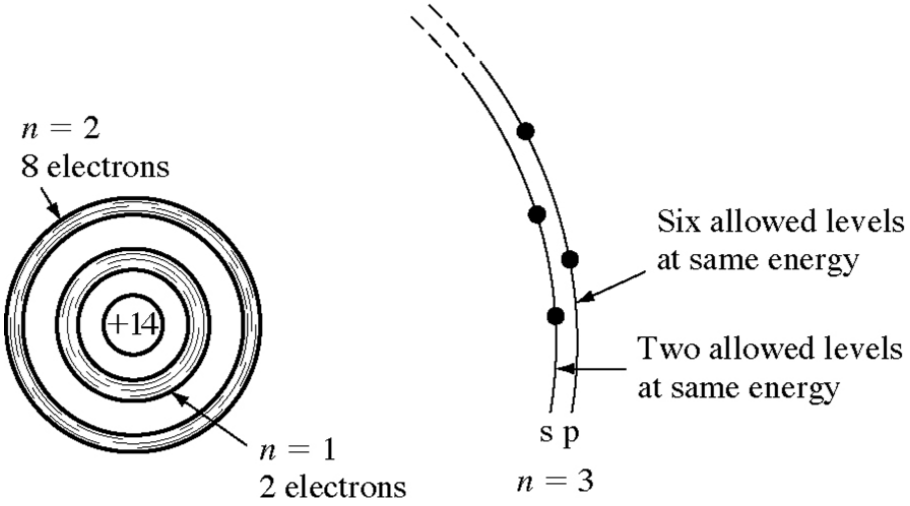
Forbidden energy bands

Based on r_0, other energy states may or may not split

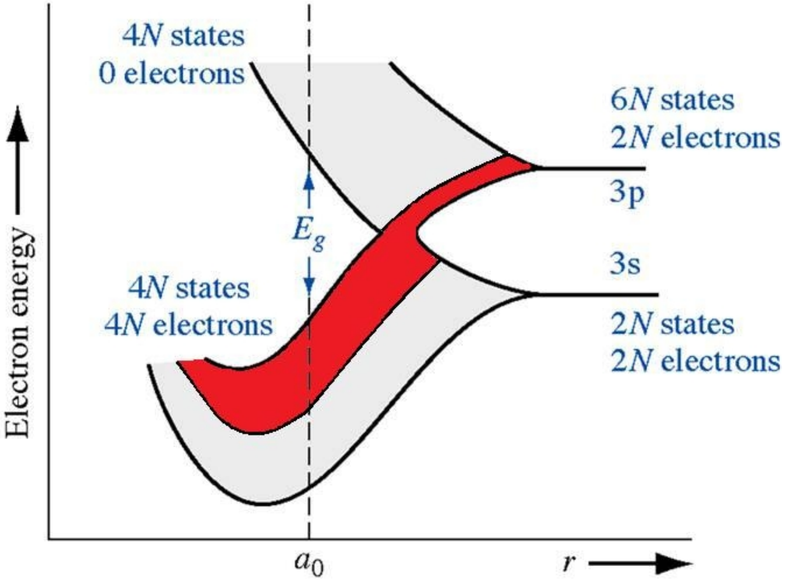
Splitting of energy states into allowed bands of energies in an atom containing electrons up to n=3.

Actual splitting can be more complex as indicated for n=3 shell in silicon.

T=0K lower (valence) band full, upper (conduction) band empty



(a)



(b)

Isolated silicon atom.

2N 3s and 6N 3p states merge and form 8N new states, in which lower 4N states are occupied and upper 4N states are empty.

KRONIG-PENNEY MODEL

To develop the concept of allowed and forbidden energy levels using Schrodinger’s wave equation → we consider Kronig-Penny model.

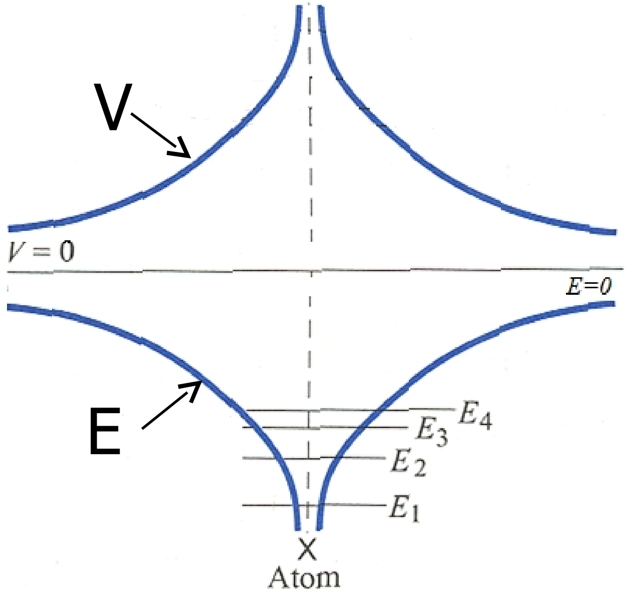
First we need to understand how potential and electron energy vary inside an atom

KRONIG-PENNEY MODEL

- potential (V) is inversely proportional to distance from positively charged nucleus.

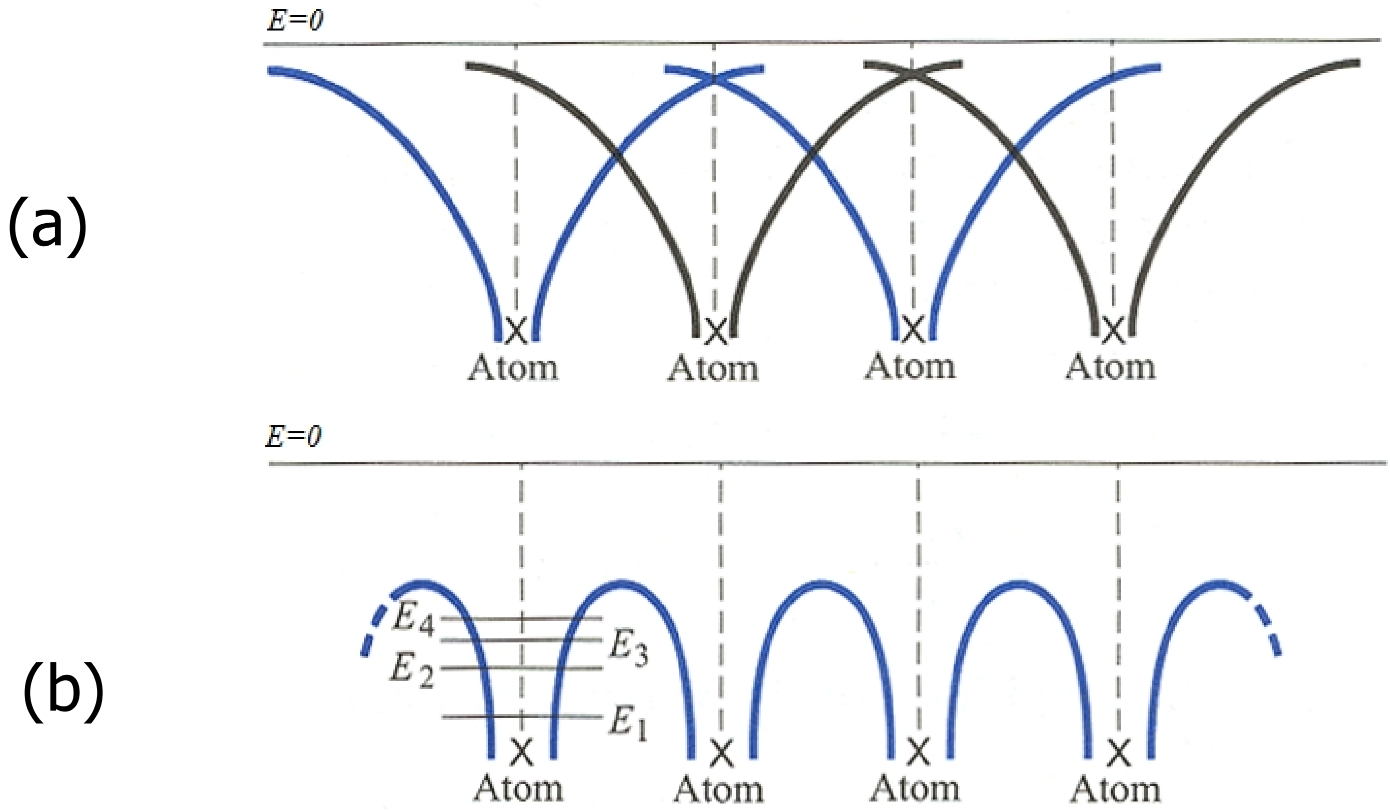
- electron is negatively charged. E=-eV → energy is negative (which means the electron is attracted to the nucleus)

- At infinite distance from nucleus both V and E are zero (free electron)



Potential and electron energy functions of a single, non-interacting, one-electron atom

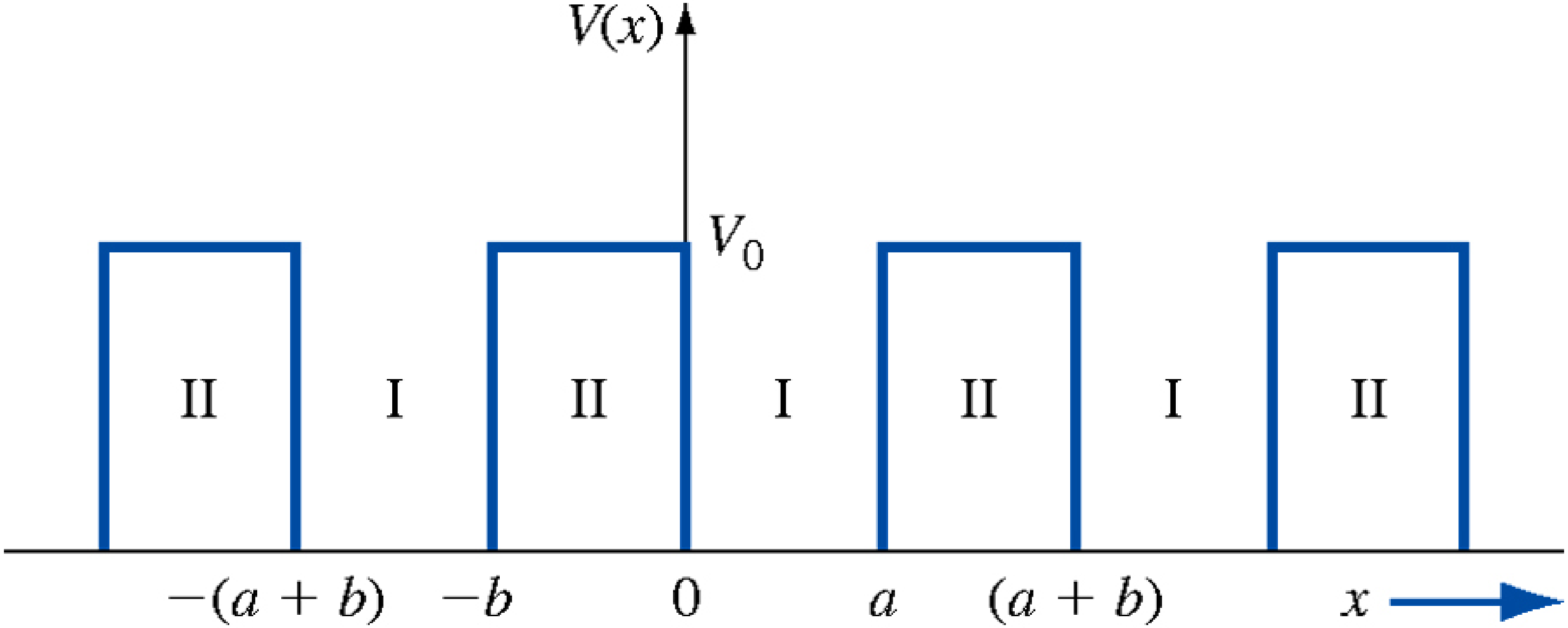
KRONIG-PENNEY MODEL



(a) Overlapping Energy functions of adjacent atoms (b) Net Energy function of a one-dimensional single crystal.

KRONIG-PENNEY MODEL

Simplified potential function → Kronig-Penny model



One-dimensional periodic potential function of the Kronig-Penny model

Two regions:

I. $V = \mathbf{0}$ → **a** ***"free"*** particle in a potential well.

II. $V=V_{\mathbf{0}}$ → ∞ **an** ***infinite number of potential barriers.***

- Electron is bound in the crystal when $E<V_0$

- Electrons are contained in the potential wells.

- There is possibility of tunneling between potential wells.

KRONIG-PENNEY MODEL

Bloch Theorem – All one-electron wave functions for problems involving periodically varying potential functions, must be of the form –

$$\psi(x) = u(x)e^{jkx} \longrightarrow \text{Bloch function}$$

k → constant of motion (explained later)

u(x) → periodic function with period (a+b)

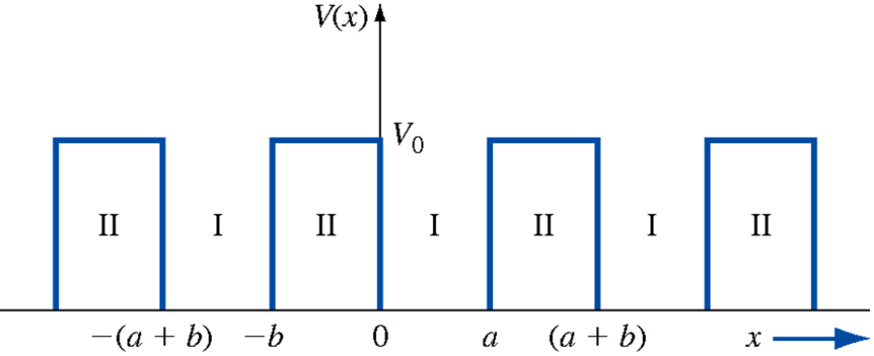
Referring to chapter 2, total solution to Schrodinger’s equation =
Time-independent solution x Time-dependent solution

$$\Psi(x,t) = \boxed{\psi(x)}\varphi(t) = \boxed{u(x)e^{jkx}}.e^{-j\left(E/\hbar\right)t}$$

$$\Psi(x,t) = u(x)e^{j\left(kx - \frac{E}{\hbar}t\right)}$$

This travelling wave solution represents the motion of an electron in a single-crystal material.

k → also referred to as wave number.



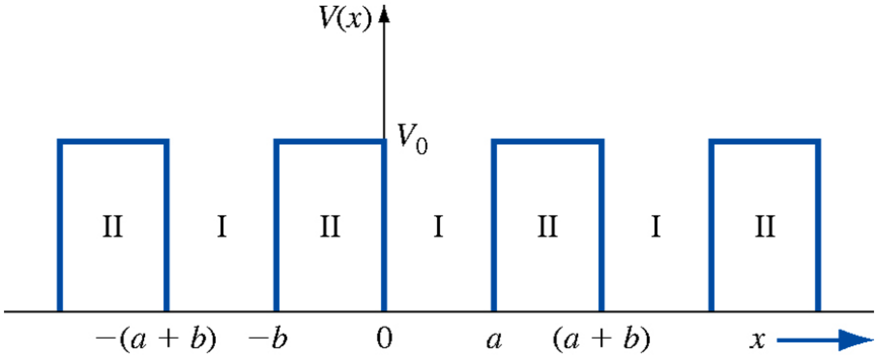
Time-independent Schrodinger wave equation -

$$\boxed{\frac{\partial^2\psi(x)}{\partial x^2}+\frac{2m}{\hbar^2}(E-V(x))\psi(x)=0}$$

Region I : V(x)=0. Substituting $\psi(x) = u_1(x)e^{jkx}$

$$\frac{d^2u_1(x)}{dx^2}+2jk\frac{du_1(x)}{dx}-(k^2-\alpha^2)u_1(x)=0$$

Where $\alpha^2 = \frac{2mE}{\hbar^2}$



$$\boxed{\frac{\partial^2\psi(x)}{\partial x^2}+\frac{2m}{\hbar^2}(E-V(x))\psi(x)=0}$$

region II, $-b < x < 0$, in which $V(x) = V_o$

$$\psi(x) = u_2(x)e^{jkx}$$

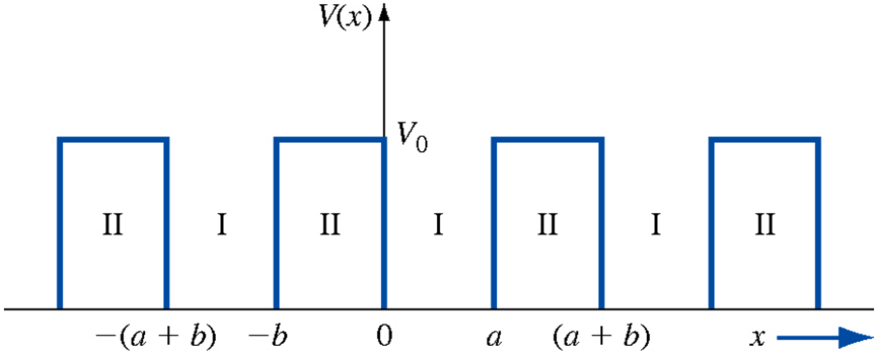
$$\frac{d^2u_2(x)}{dx^2} + 2jk\,\frac{du_2(x)}{dx} - \left(k^2 - \alpha^2 + \frac{2mV_o}{\hbar^2}\right)u_2(x) = 0$$

$$\frac{d^2u_2(x)}{dx^2} + 2jk\frac{du_2(x)}{dx} - \left(k^2 - \alpha^2 + \frac{2mV_o}{\hbar^2}\right)u_2(x) = 0$$

Now, $\alpha^2 = \frac{2mE}{\square^2}$

Let $$\frac{2m}{\hbar^2}(E - V_o) = \alpha^2 - \frac{2mV_o}{\hbar^2} = \beta^2$$

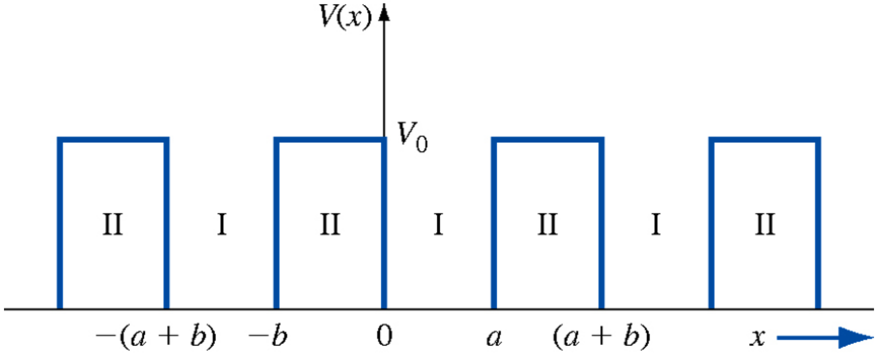
$$\frac{d^2u_2(x)}{dx^2} + 2jk\frac{du_2(x)}{dx} - (k^2 - \beta^2)u_2(x) = 0$$



There are two differential equations for regions I and II

$$\frac{d^2u_1(x)}{dx^2} + 2jk\frac{du_1(x)}{dx} - (k^2 - \alpha^2)u_1(x) = 0 \qquad \alpha^2 = \frac{2mE}{\hbar^2}$$

$$\frac{d^2u_2(x)}{dx^2} + 2jk\frac{du_2(x)}{dx} - (k^2 - \beta^2)u_2(x) = 0 \qquad \frac{2m}{\hbar^2}(E - V_o) = \alpha^2 - \frac{2mV_o}{\hbar^2} = \beta^2$$



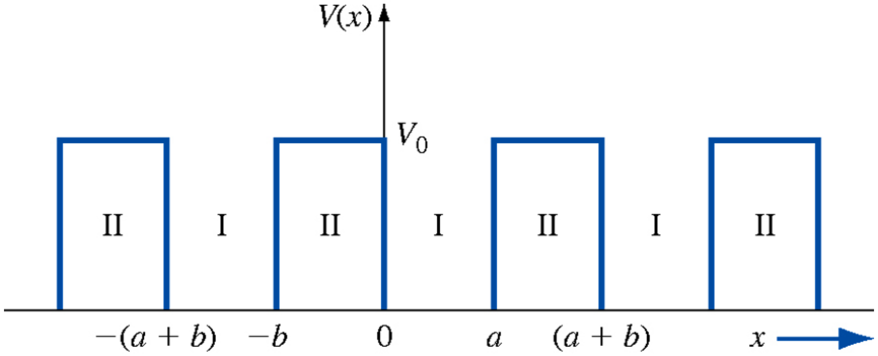
There are two differential equations which give for region I and II the following solutions:

for region I

$$u_1(x) = Ae^{j(\alpha-k)x} + Be^{-j(\alpha+k)x} \text{ for } (0 < x < a)$$

for region II

$$u_2(x) = Ce^{j(\beta-k)x} + De^{-j(\beta+k)x} \text{ for } (-b < x < 0)$$



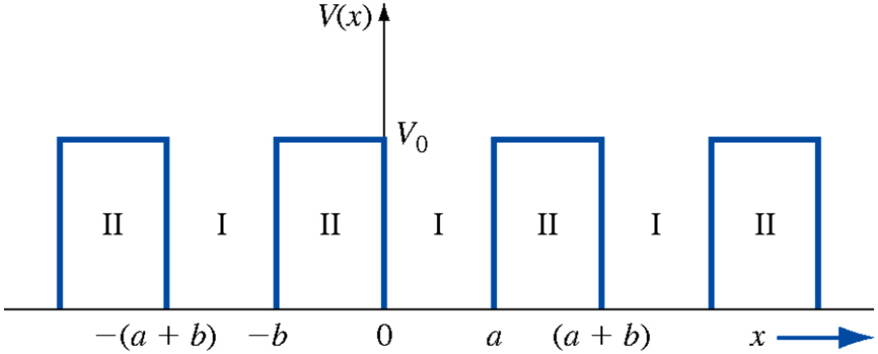
The wave function must be finite everywhere. Also the wave function and its first derivative must be continuous everywhere.

boundary at $x = 0$ $\quad u_1(0) = u_2(0)$

$$\Longrightarrow \quad A + B - C - D = 0$$

boundary at $x = 0$ $\quad \left.\frac{du_1}{dx}\right|_{x=0} = \left.\frac{du_2}{dx}\right|_{x=0}$

$$\Longrightarrow \quad (\alpha - k)A - (\alpha + k)B - (\beta - k)C + (\beta + k)D = 0$$



Due to periodicity,

$$\psi(a) = \psi(-b)$$

Therefore $u_1(a) = u_2(-b)$

$$\Longrightarrow Ae^{j(\alpha-k)a} + Be^{-j(\alpha+k)a} - Ce^{-j(\beta-k)b} - De^{j(\beta+k)b} = 0$$

Also $\left.\frac{du_1}{dx}\right|_{x=a} = \left.\frac{du_2}{dx}\right|_{x=-b}$

$$\Longrightarrow (\alpha - k)Ae^{j(\alpha-k)a} - (\alpha + k)Be^{-j(\alpha+k)a} - (\beta - k)Ce^{-j(\beta-k)b} + (\beta + k)De^{j(\beta+k)b} = 0$$

ur homogeneous equations in the unknowns A,B,C and D.

$$\boxed{A} + \boxed{B} - \boxed{C} - \boxed{D} = 0$$

$$(\alpha - k)\boxed{A} - (\alpha + k)\boxed{B} - (\beta - k)\boxed{C} + (\beta + k)\boxed{D} = 0$$

$$\boxed{A}e^{j(\alpha-k)a} + \boxed{B}e^{-j(\alpha+k)a} - \boxed{C}e^{-j(\beta-k)b} - \boxed{D}e^{j(\beta+k)b} = 0$$

$$(\alpha - k)\boxed{A}e^{j(\alpha-k)a} - (\alpha + k)\boxed{B}e^{-j(\alpha+k)a} -$$

$$(\beta - k)\boxed{C}e^{-j(\beta-k)b} + (\beta + k)\boxed{D}e^{j(\beta+k)b} = 0$$

Only a solution if: determinant (coefficients of A,B,C & D) = 0

Only a solution if: $\det = 0$

For $\det=0$,

$$\frac{-(\alpha^2+\beta^2)}{2\alpha\beta}(\sin \alpha a)(\sin \beta b) + (\cos \alpha a)(\cos \beta b) = \cos k(a+b)$$

Now $\frac{2m}{\hbar^2}(E - V_o) = \alpha^2 - \frac{2mV_o}{\hbar^2} = \beta^2$

for $E < V_o$: β is an imaginary quantity. So $\beta = j\gamma$ $\gamma = real$

Substituting for β,

$$\frac{\gamma^2-\alpha^2}{2\alpha\gamma}(\sin \alpha a)(\sinh \gamma b) + (\cos \alpha a)(\cosh \gamma b) = \cos k(a+b)$$

To simplify further let barrier width b → 0 and V_0 → ∞, such that bV_0 remains constant. Then -

$$\left(\frac{mV_o ba}{\hbar^2}\right)\frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

Let $$P' = \frac{mV_o ba}{\hbar^2}$$

$$\boxed{P'\frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka}$$

$$\boxed{P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka}$$

$$P' = \frac{mV_o ba}{\hbar^2}$$

- This is a relation between parameter k, total Energy E (through parameter α) and potential barrier bV_o.

- This is not a solution to Schrodinger’s equation but a condition for a solution to exist.

- Crystal infinitely large → k can assume a continuum of values and must be real

$$\boxed{P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka}$$

1st case, free electron:

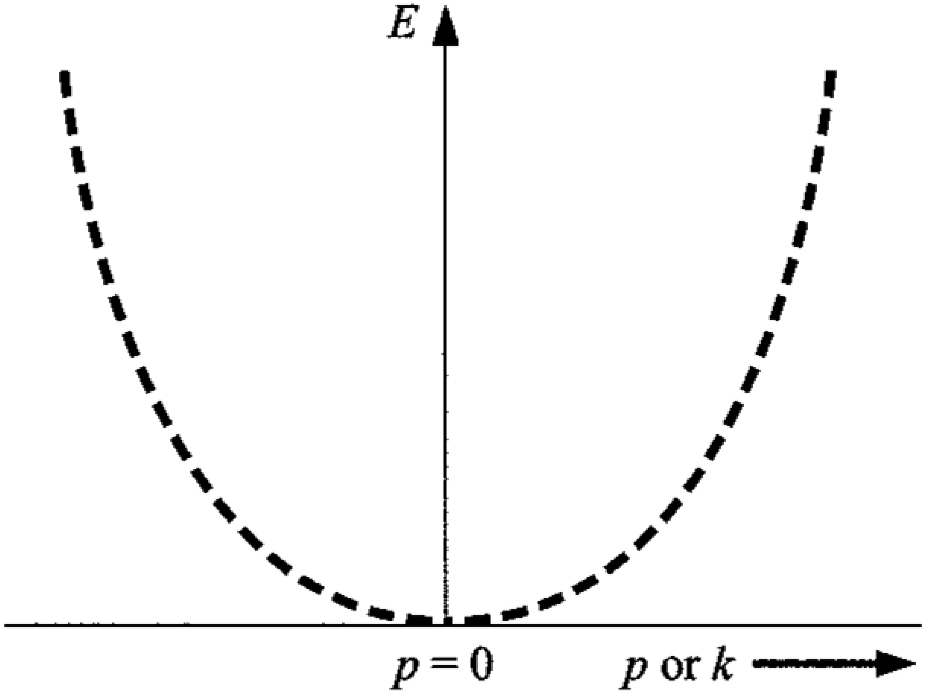
$V_0=0$ hence: $\boxed{\cos \alpha a = \cos ka}$ $\Longrightarrow$ $\alpha = k$

$$\alpha^2 = \frac{2mE}{\hbar^2} \quad \text{and} \quad E = \frac{p^2}{2m} = \frac{k^2\hbar^2}{2m}$$

$k = \frac{p}{\hbar}$ $\Longrightarrow$ Constant of motion parameter k is related to the particle momentum for the free electron

(A result which we already know. This validates Kronig-Penny model)

$$E = \frac{p^2}{2m} = \frac{k^2\hbar^2}{2m}$$



Parabolic E versus k curve for free electron

Coming back to Crystal-lattice →

$$\boxed{P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka}$$

Let $f(\alpha a) = P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$

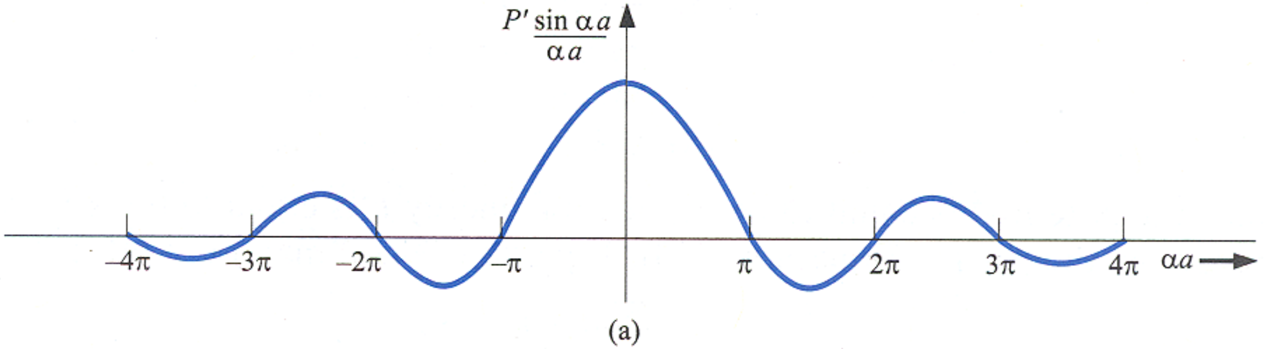
This function can only have values between -1 and +1, because it is equal to cos(ka)

Hence αa can only have certain allowed values

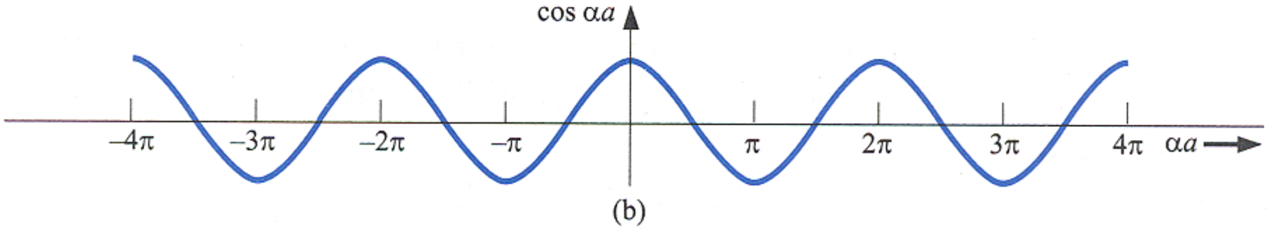
Hence also the energy can have certain allowed values.

$$\alpha^2 = \frac{2mE}{\hbar^2}$$

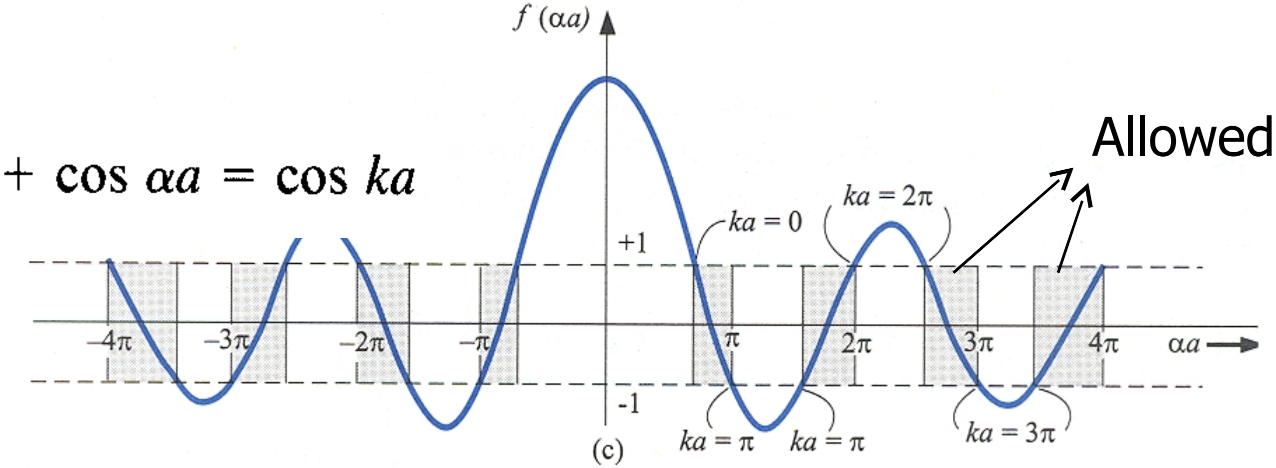
$$P' \frac{\sin \alpha a}{\alpha a}$$



$$\cos \alpha a$$

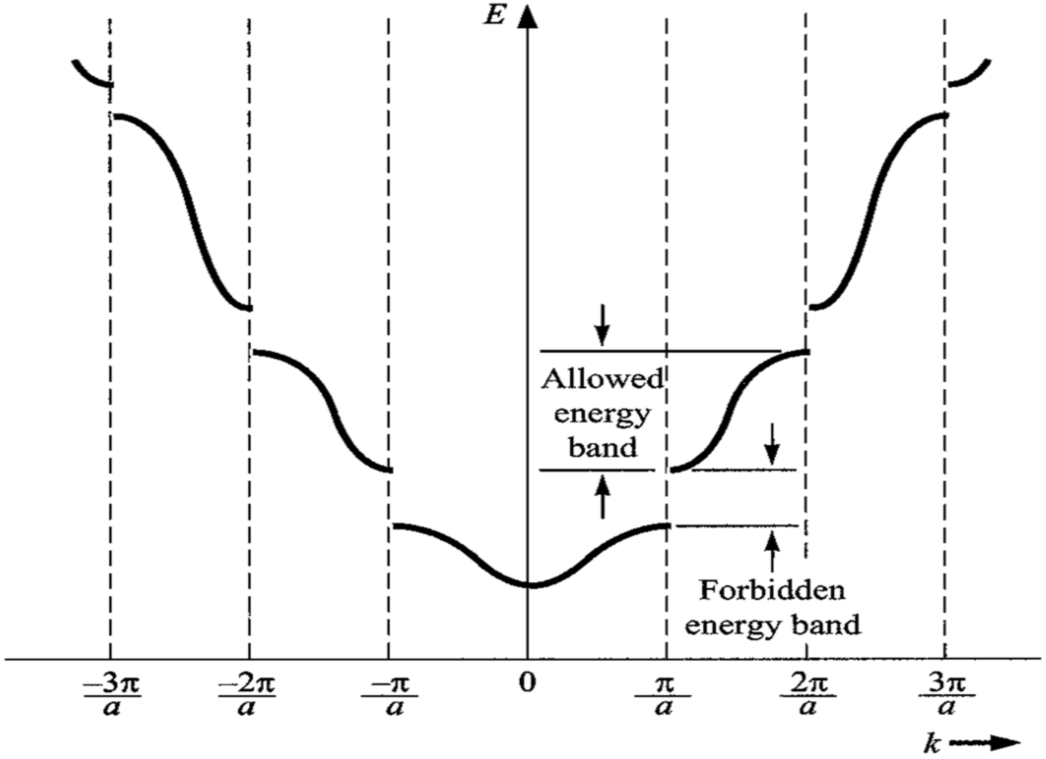


$$P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$



Allowed values of αa

Since E is related to k, we can make a plot of E vs. k.



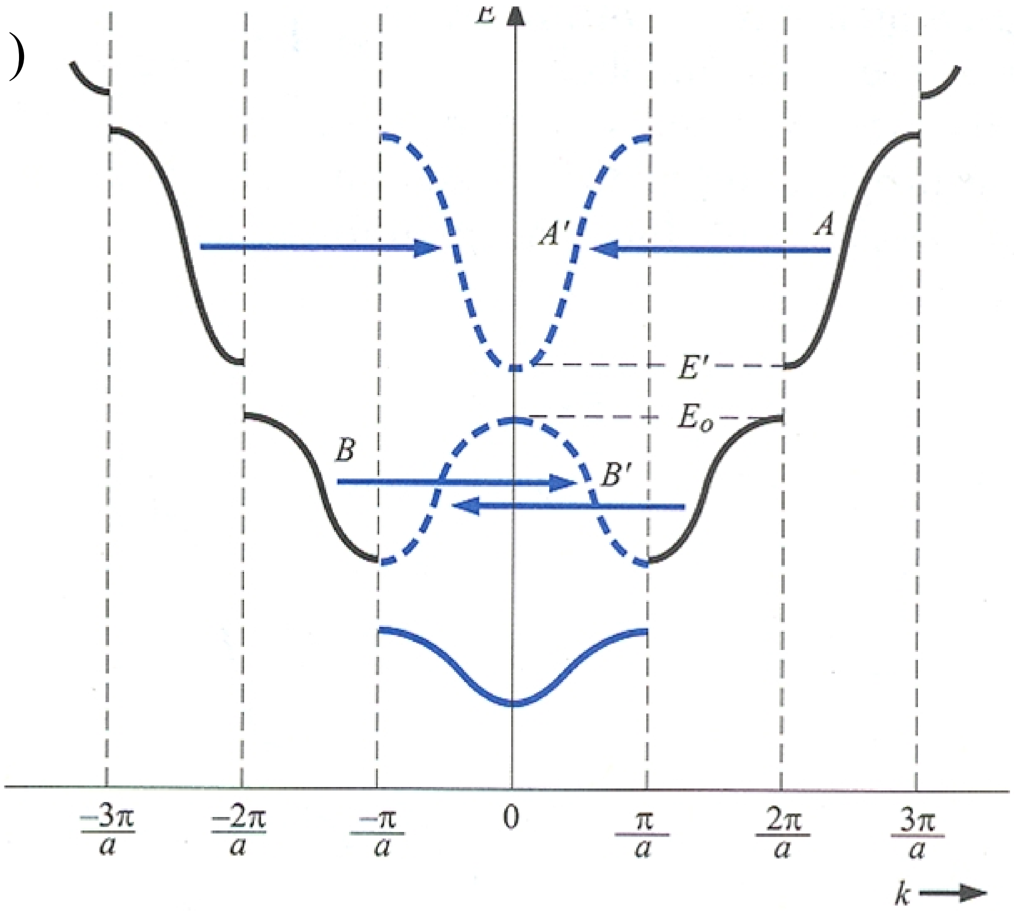
E versus k diagram generated from the figure in the previous slide.

Note that E is discontinuous → there are allowed and forbidden energy bands.

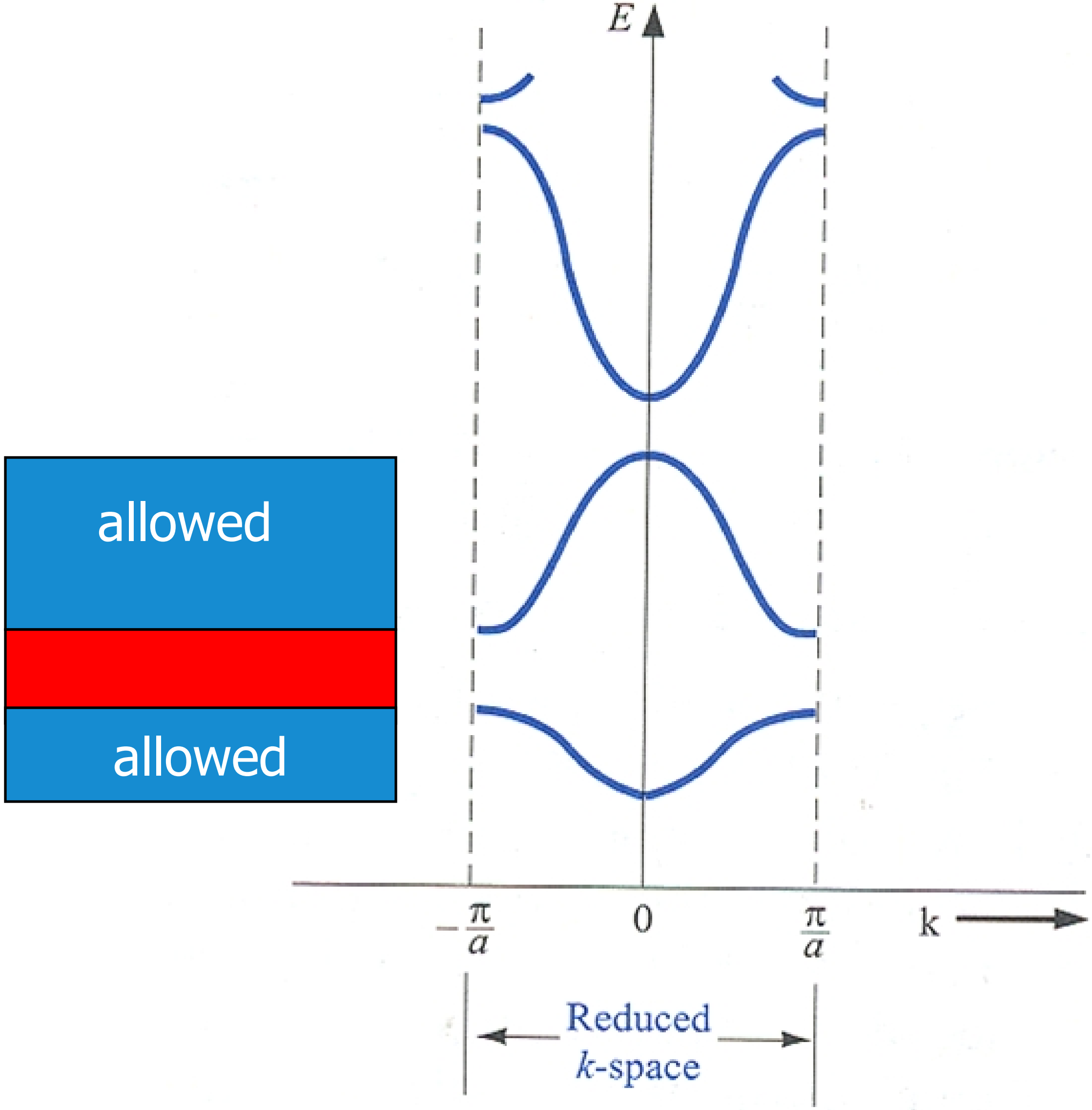
$$\cos ka = \cos(ka + 2\pi) = \cos(ka - 2\pi)$$

$$\Downarrow$$

Various sections of the E versus k diagram can be shifted by $n\frac{2\pi}{a}$

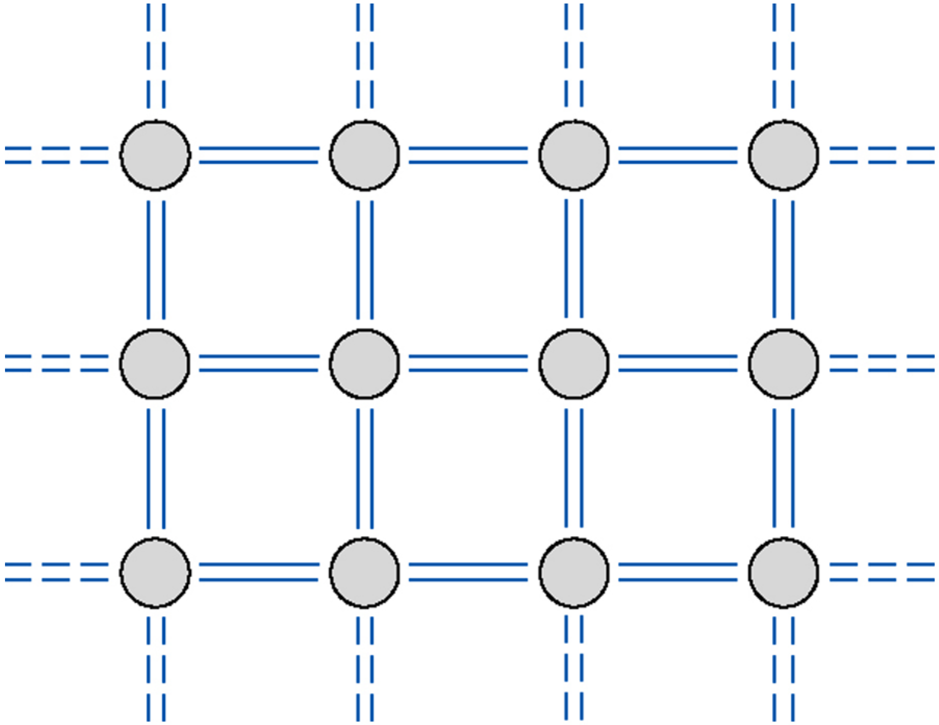


E versus k diagram showing displacements by $n\frac{2\pi}{a}$ of several sections of the allowed energy bands.

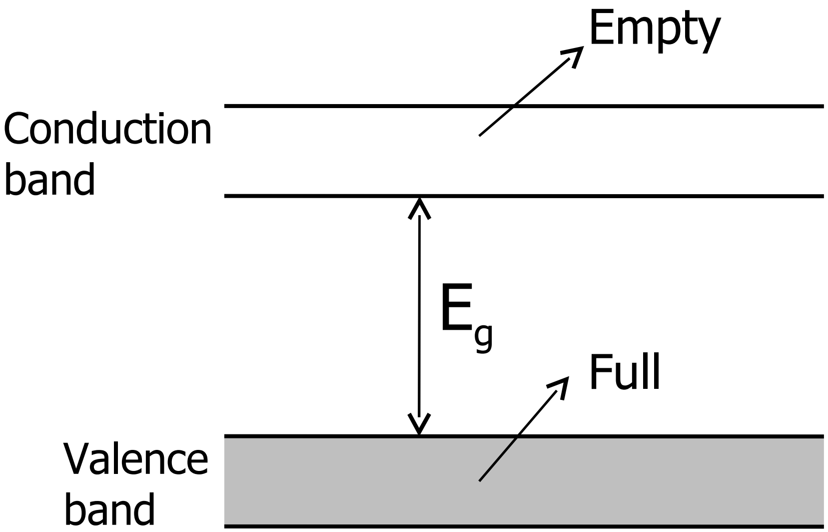


E versus k diagram in the reduced k-space representation

T=0K



(a) Covalent bonding in Si

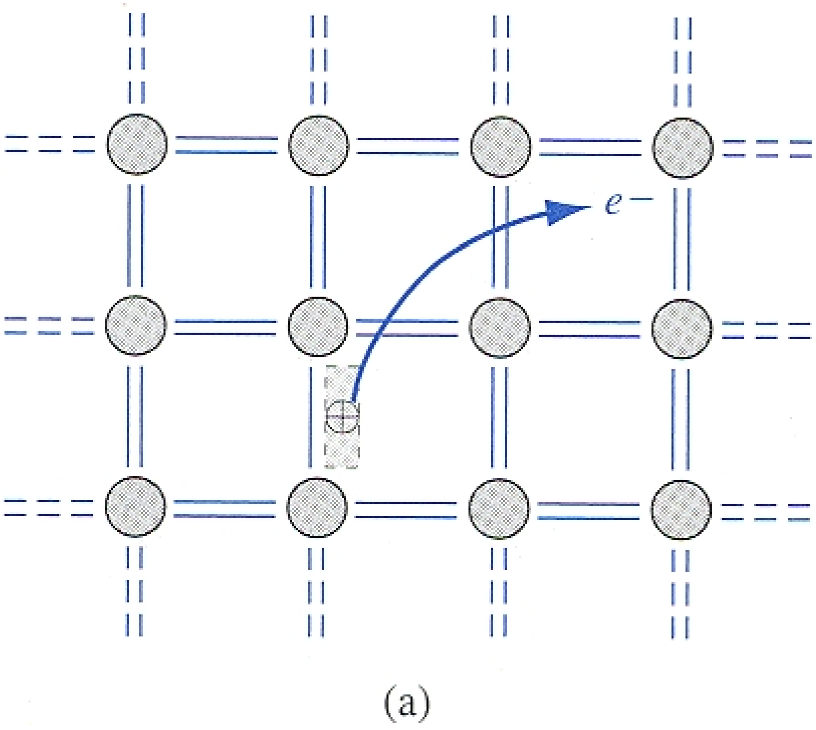


(b) line representation of energy band diagram

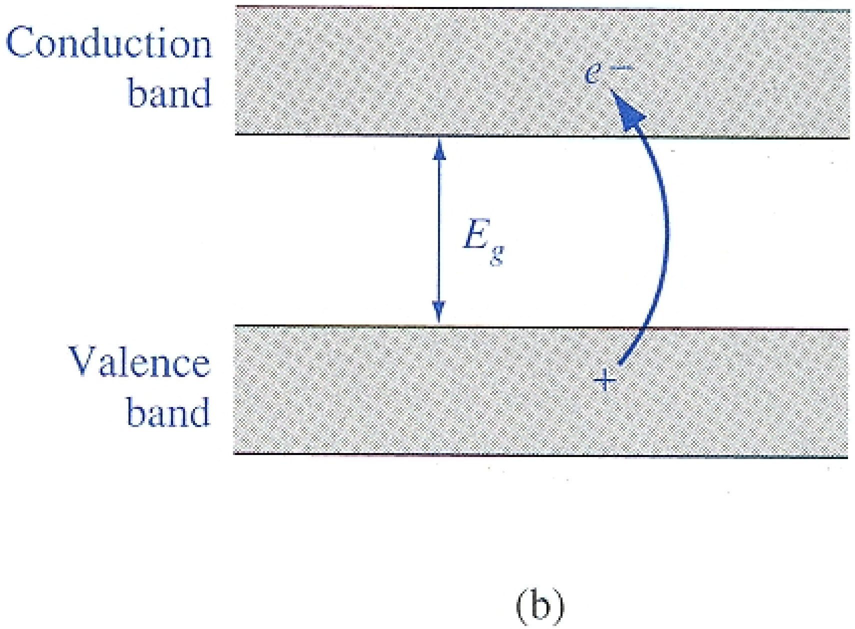
Band-gap energy in some covalent elements

Element	**E_g (eV)**
C (diamond)	5.48
Si	1.1
Ge	0.7
Sn (gray)	0.08

T>0K



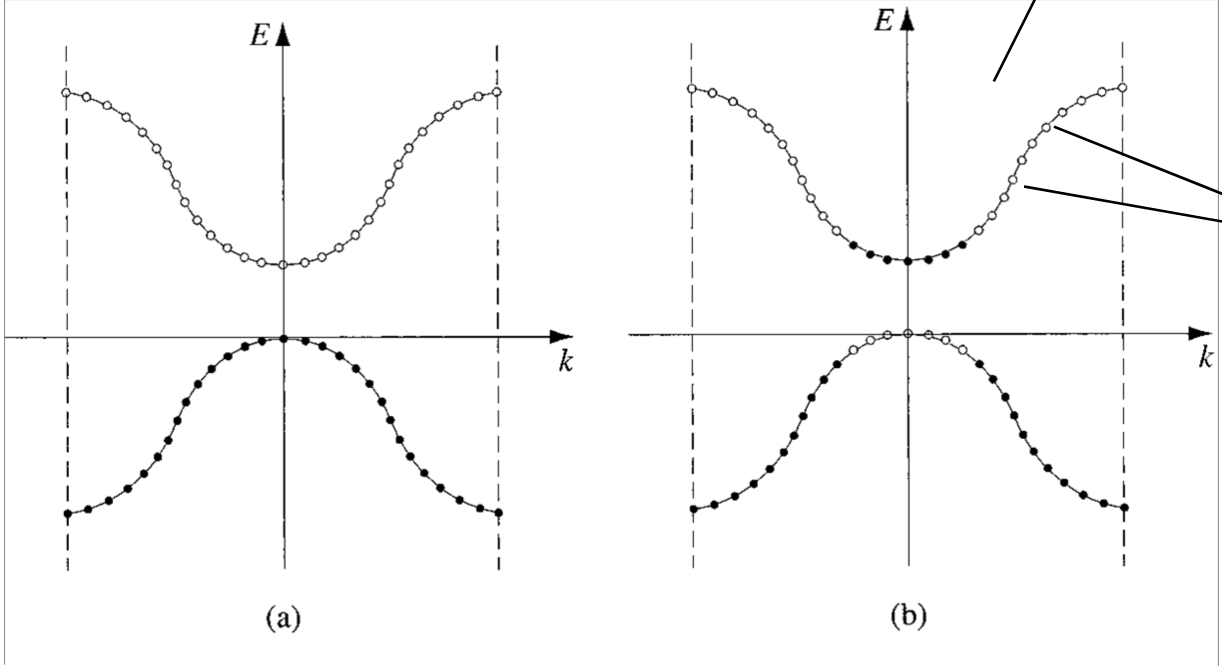
Two dimensional representation of breaking of a covalent bond.



At T>0K, some covalent bonds break giving rise to positively charged empty states and electrons

E vs. K diagrams at T=0K and T>0K in the absence of external electric field.

Electron and empty states are symmetric with respect to k.



(a)

(b)

Even within a band allowed energies are still quantized. This is because electrons are still confined to potential wells.

The *E* versus *k* diagram of the conduction and valence bands of a semiconductor at (a) $T = 0°\mathrm{K}$ and (b) $T > 0°\mathrm{K}$

Drift current

$$J = qNv_d(\mathrm{A/cm^2})$$

q → electron charge
N → charge density (C/cm^3)
V_d → drift velocity of electron

Considering individual electron velocities →

$$J = q\sum_{i=1}^{N} v_i$$

(summation taken over unit volume)

Drift current


V_d in +x direction

K +ve

V_d in -x direction

K -ve

No external force

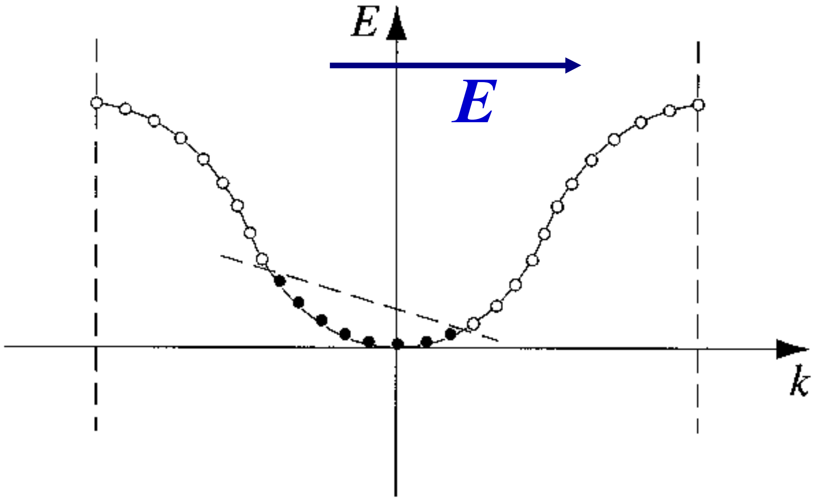
→

No of electrons with +|k| value = No of electrons with -|k| value.

→

k related to momentum. So drift current J = 0

When ext force (electric field) applied → Electrons move into empty energy states in conduction band, gain net energy and a net momentum.



Drift current density due to motion of electrons -

$$J = -e \sum_{i=1}^{n} v_i$$

(summation taken over unit volume)

Asymmetric distribution of electrons in E vs. k diagram when ext force is applied.

Electron effective mass

Total force acting on electrons in crystal –

$$F_{Total} = F_{ext} + F_{int} = ma$$

F_{int} → internal forces in the crystal due to +vely charged ions and –vely charged electrons

F_{ext} → externally applied electric field

m → rest mass of electron

a → acceleration.

Electron effective mass

It is difficult to account for all of the internal force. So we define –

$$F_{ext} = m^{*}a$$

m* → effective mass of the electron (which takes into account internal forces)

Acceleration a → directly related only to ext applied force.

Free electron:

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}, \text{since } p = \frac{h}{\lambda} = \hbar k$$

$$\Longrightarrow$$

Taking derivative of E w.r.t k,

$$\frac{dE}{dk} = \frac{\hbar^2 k}{m} = \frac{\hbar p}{m}$$

$$\frac{1}{\hbar}\frac{dE}{dk} = \frac{p}{m} = \boxed{v}$$

This implies that from E vs. k diagram we can get the velocity of the electron in real space.

$$\frac{1}{\hbar}\frac{dE}{dk} = \frac{p}{m} = v$$

Again taking derivative of E w.r.t k,

$$\frac{d^2E}{dk^2} = \frac{\hbar^2}{m} \quad \Longrightarrow \quad \frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{1}{m}$$

This implies that from E vs. k diagram we can also get the effective mass of the electron in real space. For a free electron, the second derivative and hence mass is constant.

(why do we need to extract the electron mass, when we already know it ??? - read further)

Free electron

$$F = ma = -e\mathrm{E} \quad \Longrightarrow \quad a = \frac{-e\mathrm{E}}{m}$$

Motion of electron is in opposite direction of the applied electric field due to the negative charge.

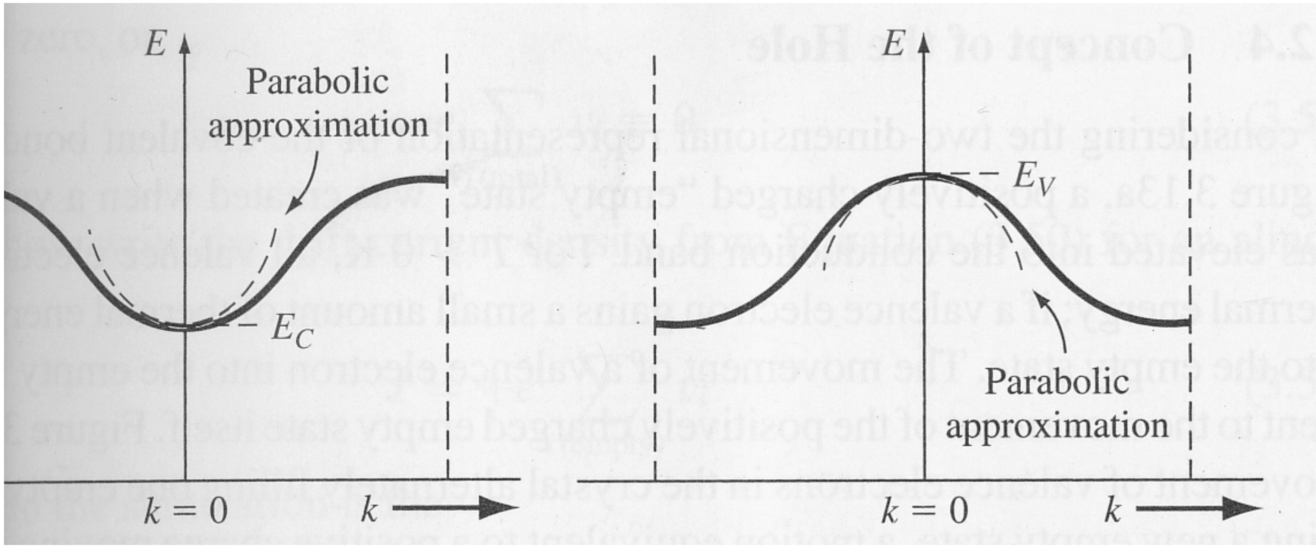
We now apply these concepts to the electrons in the crystal

Electron in conduction band

The energy of electrons at the bottom of the conduction band can be approximated as -

$$E - E_c = C_1(k)^2$$

C_1 → +ve



Conduction and valence bands in reduced k space with their parabolic approximations to compare with free electron

Electrons in conduction band

$$\frac{d^2E}{dk^2} = 2C_1$$

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{2C_1}{\hbar^2}$$

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{2C_1}{\hbar^2} = \frac{1}{m^*}$$

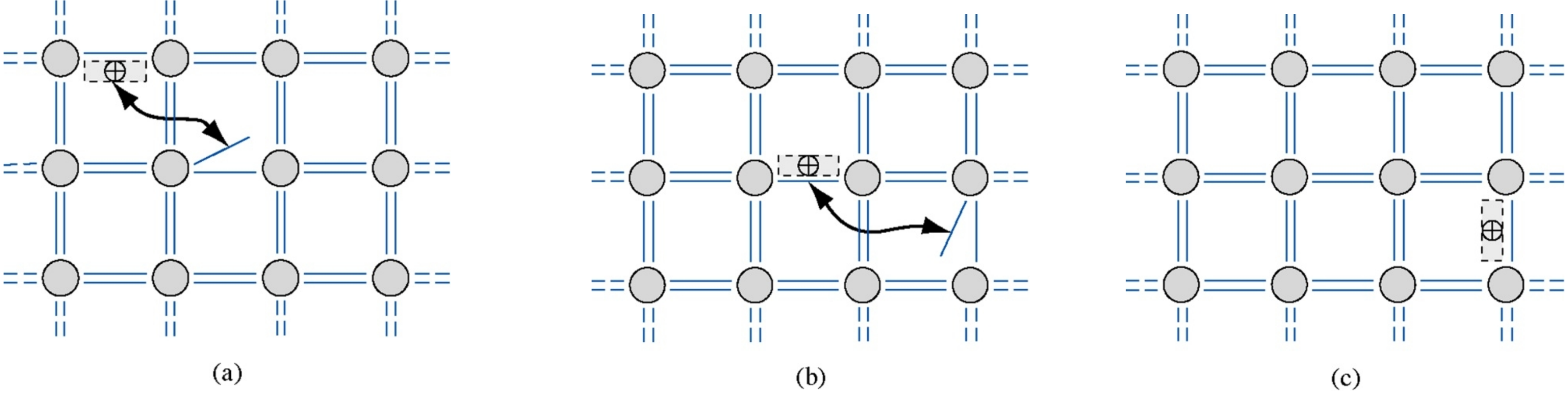
$$a = \frac{-e\mathrm{E}}{m_n^*}$$

Effective mass:

- connects quantum mechanics and classical mechanics
- effective mass varies with k, but almost constant at the bottom of the conduction band.
- positive value since C_1 is +ve

Concept of the hole

- When valence electron goes to conduction band positively charged empty state is created.
- If a valence electron gets a small amount of energy, it can occupy this empty state.
- Movement of valence electron ⟺ movement of +vely charged empty state in opposite direction.
- The charge carrier in the form of +vely charged empty state is called the hole.



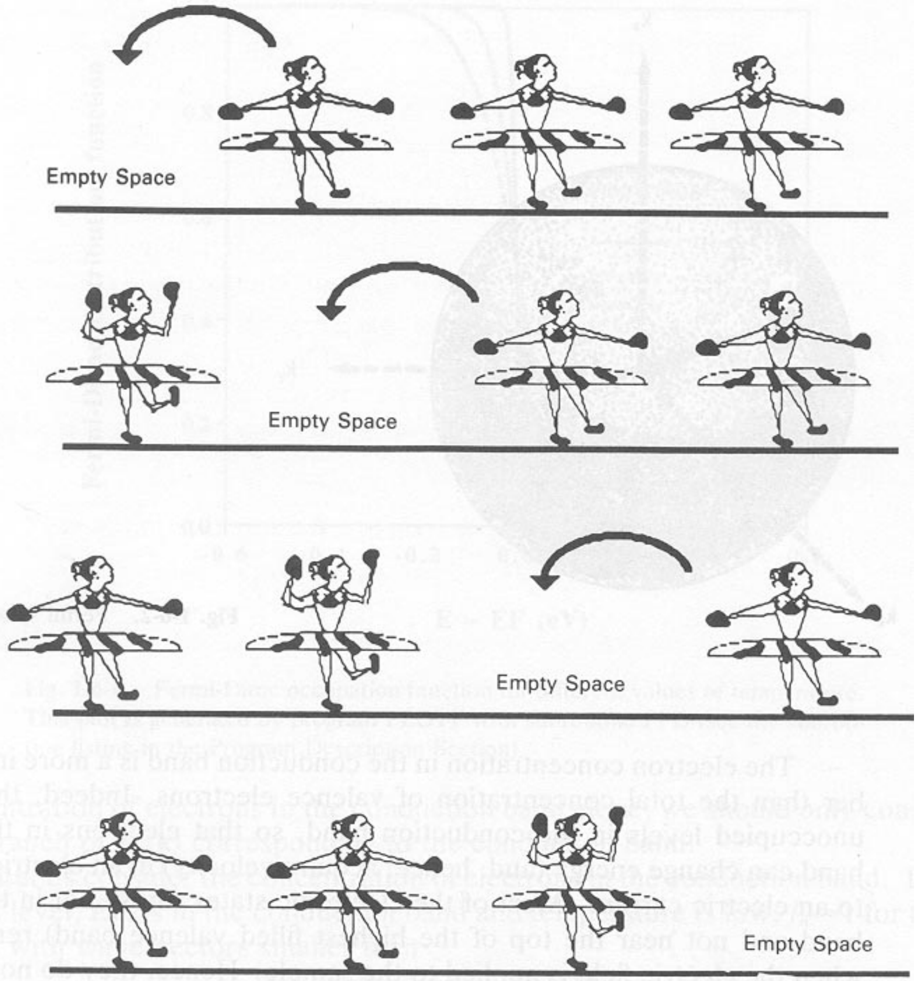


Fig. 1-6-3. Concept of a *hole*.

Drift current density due to electrons in valence band is -

$$\sum_{i(filled)} v_i = \sum_{i(total)} v_i - \sum_{i(empty)} v_i$$

$$J = -e \sum_{i\,(\text{filled})} v_i \longrightarrow J = -e \sum_{i\,(\text{total})} v_i + e \sum_{i\,(\text{empty})} v_i$$

Now, $v(E) = \left(\frac{1}{\hbar}\right)\left(\frac{dE}{dk}\right)$

Also in a band that is completely full, electron distribution is symmetric with respect to k. The net drift current density generated from a completely full band is then 0.

$$\longrightarrow -e \sum_{i\,(\text{total})} v_i \equiv 0$$

$$J = -e \sum_{i\,(\text{total})} v_i + e \sum_{i\,(\text{empty})} v_i$$

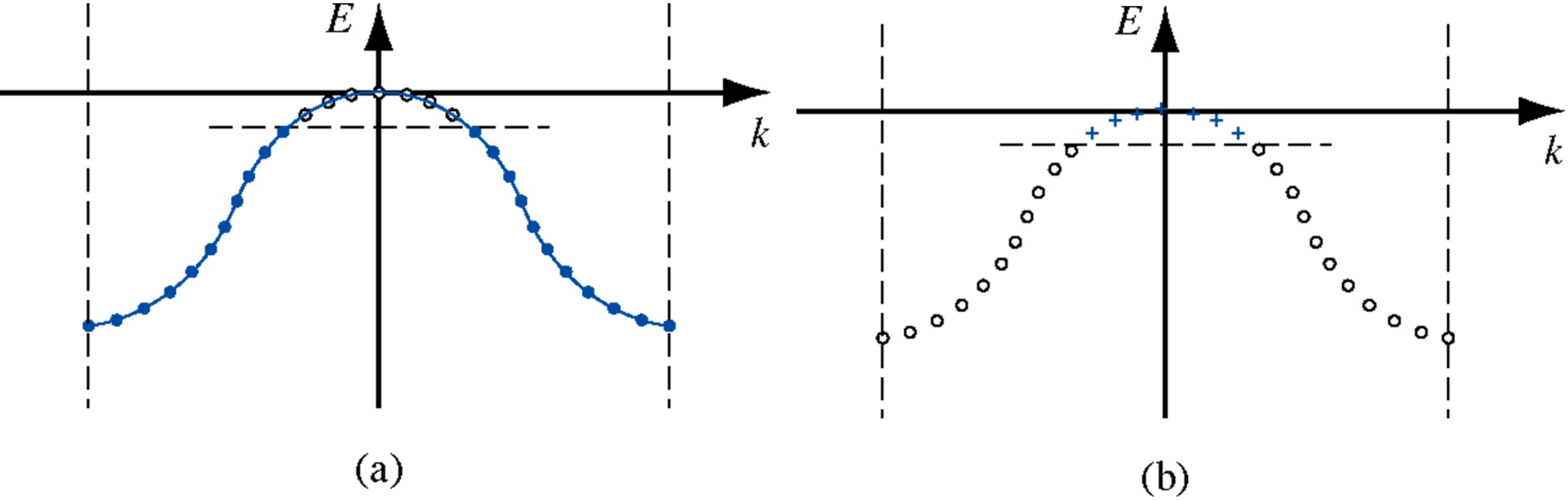
and

$$-e \sum_{i\,(\text{total})} v_i \equiv 0$$

Therefore

$$J = +e \sum_{i\,(\text{empty})} v_i$$

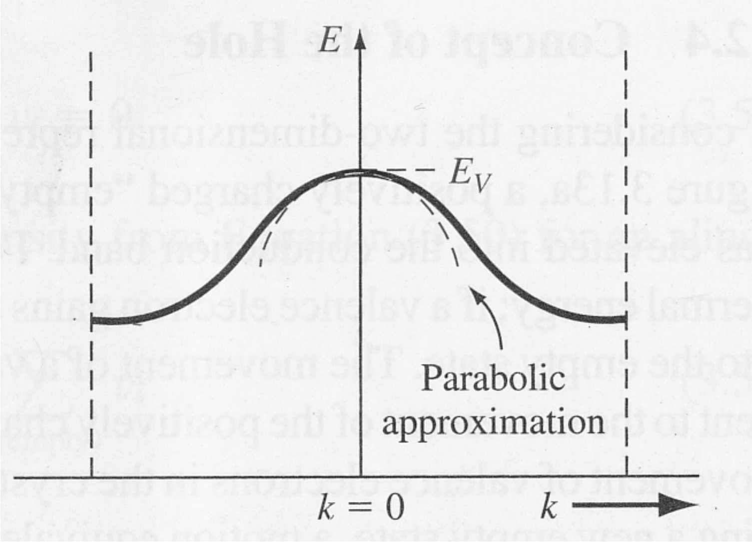
Drift current due to electrons in the filled state can also be looked at as that due to placing positively charged particles in the empty states.



Valence band with conventional electron filled states and empty states

Concept of positive charges occupying the original empty states.

Energy at the top of allowed energy band can be written as -



$$(E - E_v) = -C_2(k)^2$$

C_2 → +ve

$$\frac{d^2E}{dk^2} = -2C_2$$

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{-2C_2}{\hbar^2}$$

Compare with free electron:

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{1}{m}$$

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{-2C_2}{\hbar^2} = \frac{1}{m^*}$$

Negative effective mass

Bit strange!

$$F = m^* a = -e\text{E}$$

$$a = \frac{-e\text{E}}{-|m^*|} = \frac{+e\text{E}}{|m^*|}$$

- negative mass is a result of our attempt to relate quantum and classical mechanics. It is due to the inclusion of the effect of internal forces due to ions and other electrons.

- The net motion of electrons in the nearly full valence band can also be described by considering the empty states, provided +ve electronic charge and +ve effective mass is associated with them

- This new particle with +ve electronic charge and +ve effective mass denoted by m_p^* is called the hole

Electrons:

- in almost empty band
- negative charge
- positive effective mass

Holes:

- in almost full band
- positive charge
- positive effective mass

Both:

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{1}{m^*}$$

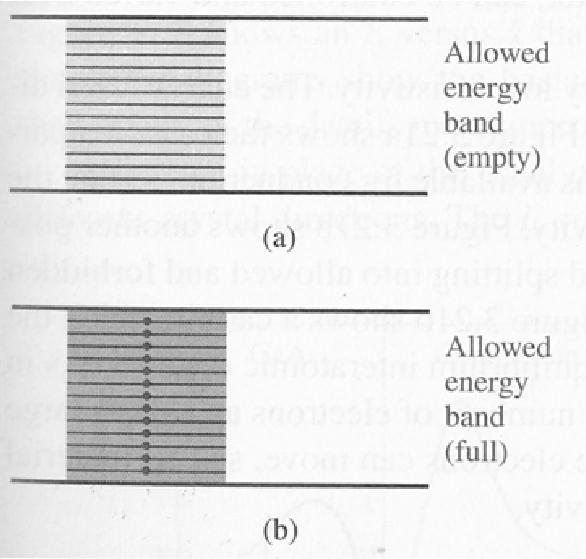
$$F = m^* a = qE$$

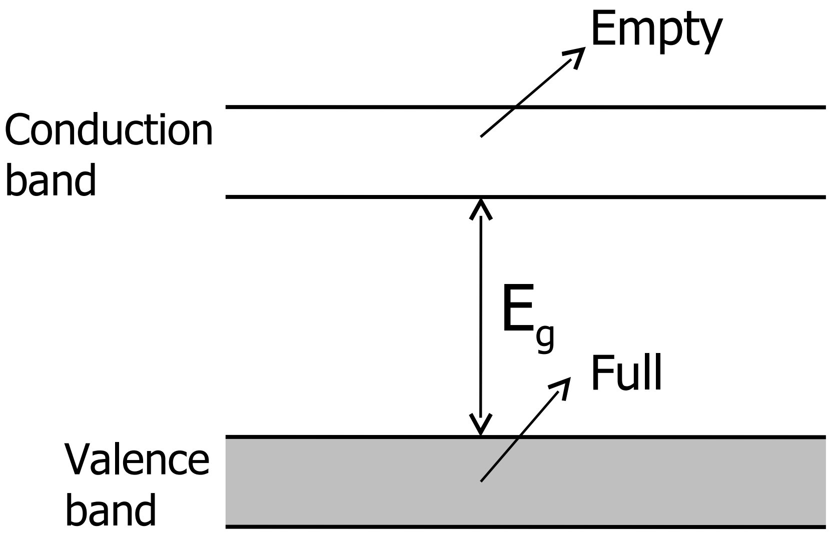
Electron and Hole effective mass in different semiconductors.

	m_n^*/m_0	m_p^*/m_0
Silicon	1.08	0.56
Gallium Arsenide	0.067	0.48
Germanium	0.55	0.37

Metals, semiconductors and insulators

Insulators:





Empty

Conduction band

E_g

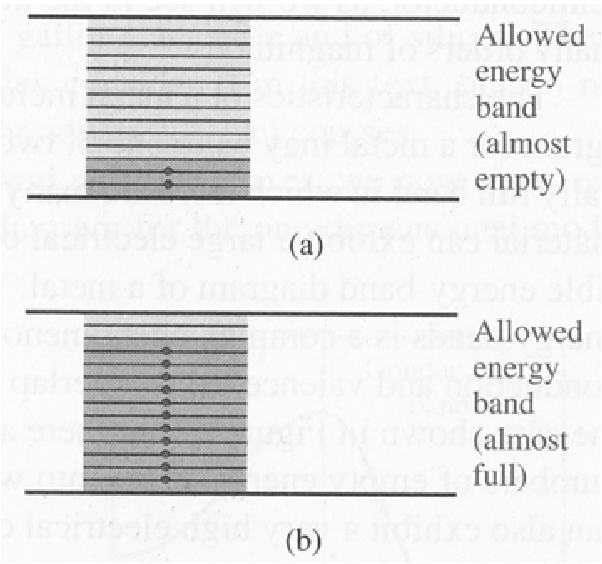
Full

Valence band

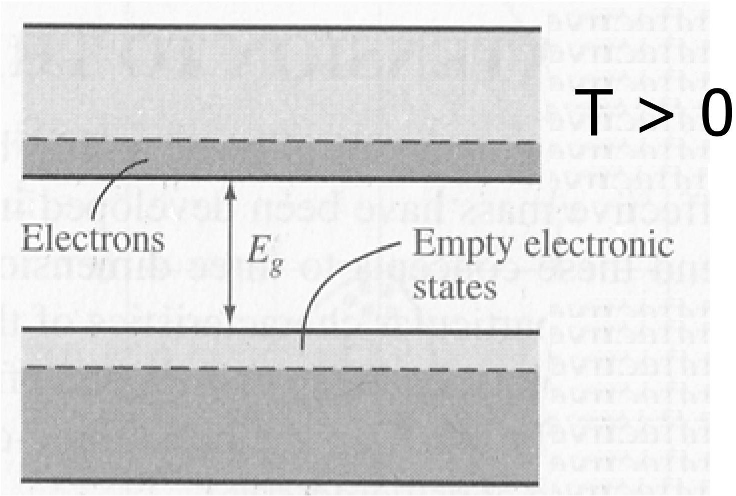
- E_g 3.5 to 6 eV or higher
- valence band full, conduction band empty
- no charged particles that contribute to drift current.

Semiconductors:

- E_g in semiconductors is small. E_g ~ 1eV
- At T>0K, there will be some electrons in conduction band and holes in valence band, which can contribute to current.

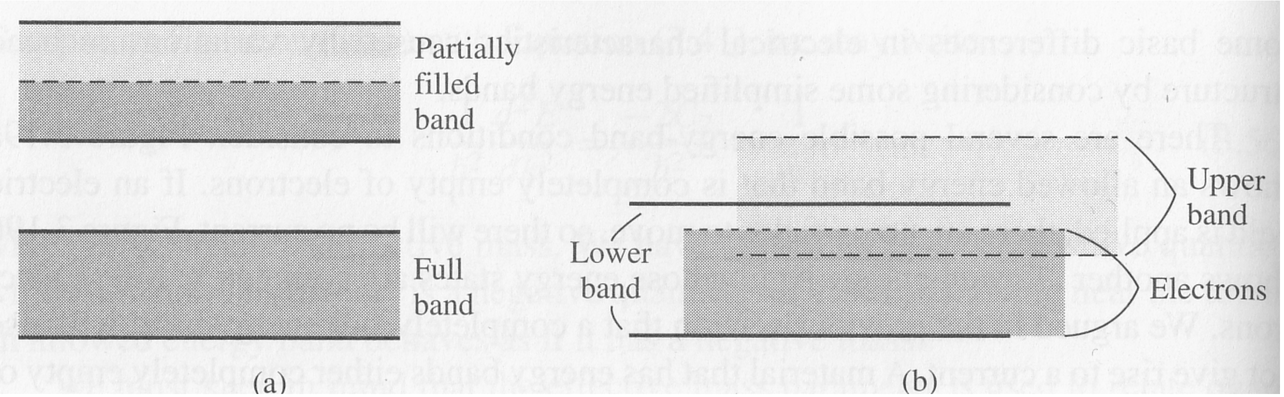


- resistivity can be varied over many orders of magnitude by doping



T > 0K

Metals:



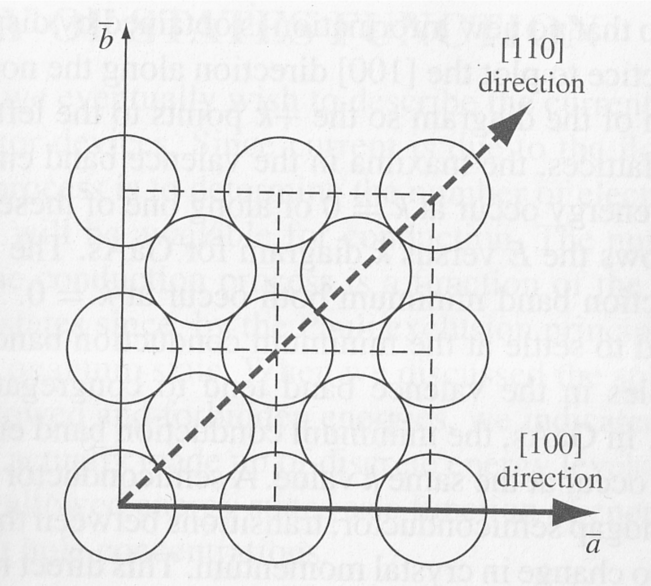
- Two possibilities - half filled conduction band or conduction and valence bands overlap.

- plenty of electrons and empty energy states that these electrons can move into.

- Very high electrical conductivity.

Extending energy band theory to three dimensions

- Extend concepts of energy band and effective mass to 3-dimensions

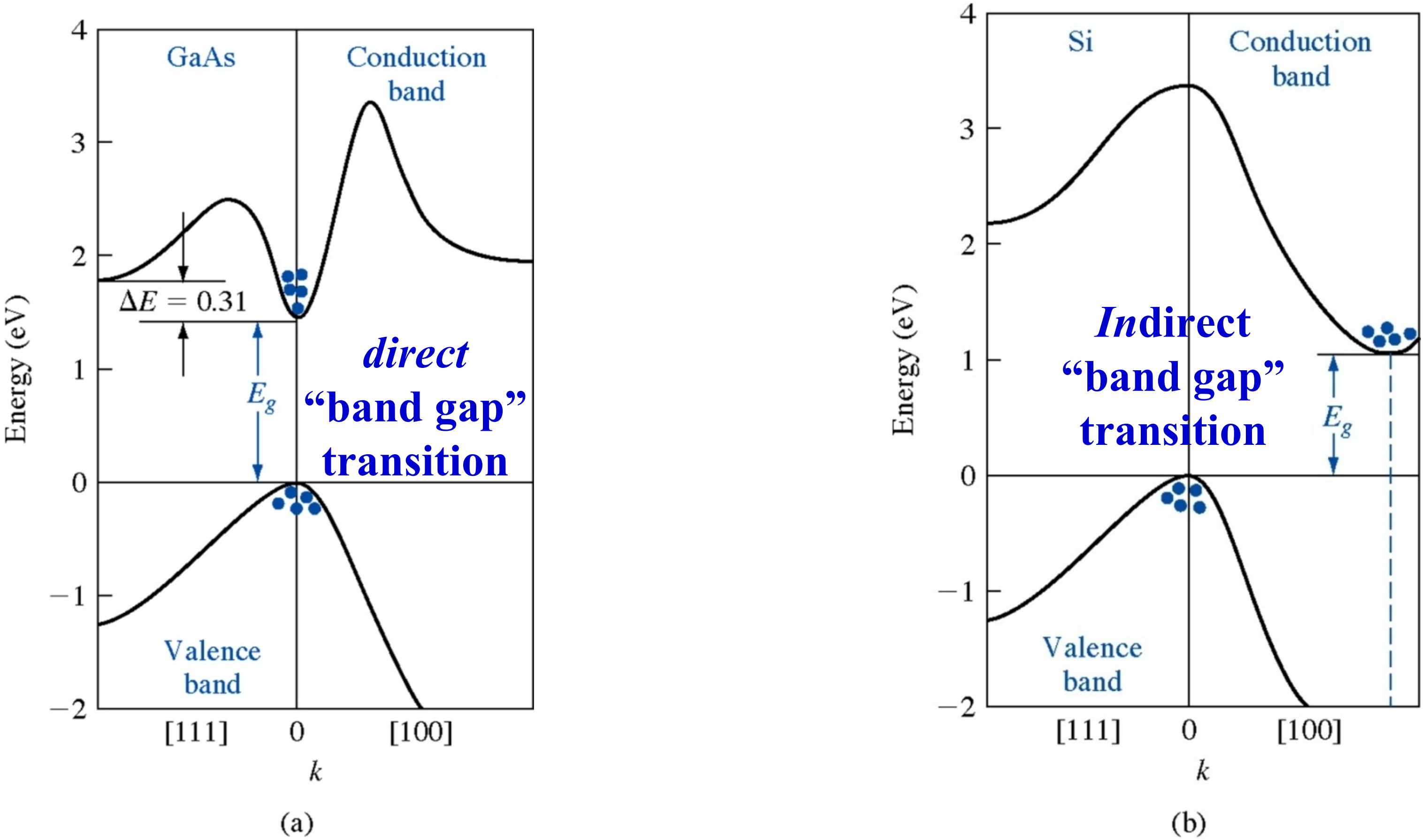


- distance between atoms not the same in different directions

•E vs. k diagram → as seen before depends on 'a' and 'a' varies with direction.

Different potentials in different directions

E vs. k diagrams of Si and GaAs



- [100] and [111] directions plotted along +k and –k axes.

E vs. k space diagrams of Si and GaAs

- In GaAs the minimum conduction band energy and maximum valence band energy occur at same k value. Such semiconductors are called *direct* band-gap semiconductors. Others are called *indirect* band-gap semiconductors. Eg. Si, Ge.

- Direct bandgap semiconductors are used for making optical devices. In indirect bandgap semiconductors there is loss of momentum during transition from conduction band to valence band, making them unsuitable for optical devices.

E vs. k space diagrams of Si and GaAs

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{1}{m*} \longrightarrow$$

$\frac{d^2E}{dk^2}$ is larger in GaAs than in silicon

So m* in GaAs < m* in silicon

- effective mass can be different along 3 different k-vectors. We consider average effective mass hence forth.

Density of states function

- we want to know the number of charge carriers and their temperature dependence

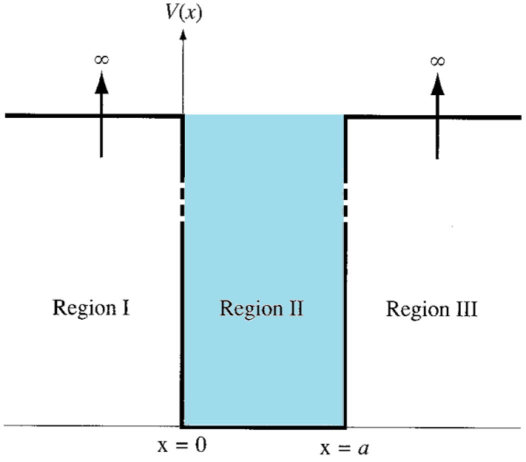
- hence the question is: how many energy levels do we have and what is the chance that they are populated in dependence of the temperature.

Mathematical model for density of states

- we consider a free electron confined to an 3-dimensional cubical infinite potential well of side 'a'.

$$V(x,y,z) = 0 \quad \text{for} \quad \begin{array}{l} 0 < x < a \\ 0 < y < a \\ 0 < z < a \end{array}$$

$$V(x,y,z) = \infty \quad elsewhere$$

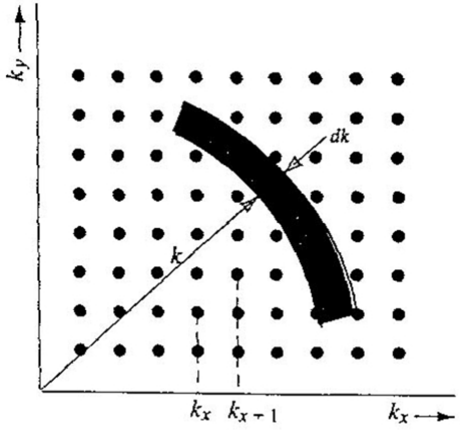


One dimensional potential well $\longrightarrow$ $K = \dfrac{n\pi}{a}$ and $K = \sqrt{\dfrac{2mE}{\hbar^2}}$

Extending to 3-dimensions,

$$\frac{2mE}{\hbar^2} = k^2 = k_x^2 + k_y^2 + k_z^2 = (n_x^2 + n_y^2 + n_z^2)(\frac{\pi^2}{a^2})$$

Where n_x, n_y and n_z are positive integers (negative values lead to the same orbitals and hence do not represent a different quantum state)

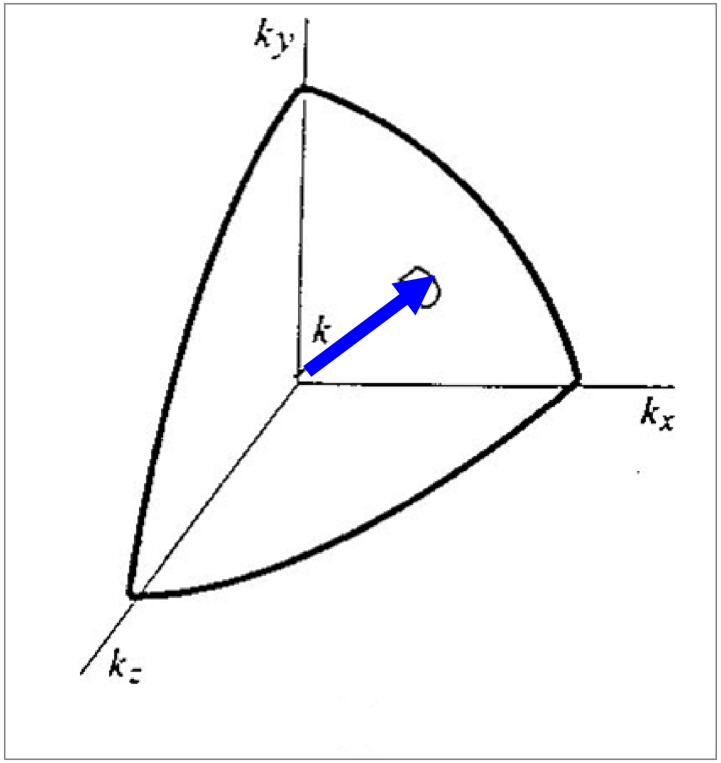


Two-dimensional array of allowed quantum states in k-space

In 3-dimensional k-space, only 1/8th of the spherical k-space needs to considered for determining the density of states

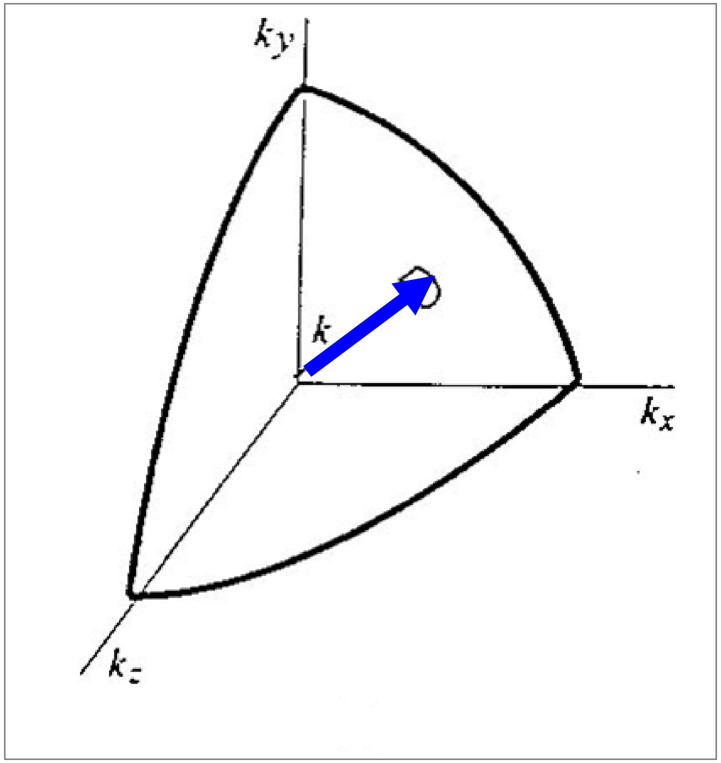
-ve value of (k_x,k_y,k_z) result in same $k^2 = k_x^2 + k_y^2 + k_z^2$ and hence same energy. Since these do not result in separate energy state, they are not considered.

Spherical surface is considered because value of k^2 and hence energy is same along this surface.



Positive 1/8th of spherical k-space.

Distance between quantum states in any one axial direction is -



$$k_{x+1} - k_x = (n_x + 1)\left(\frac{\pi}{a}\right) - n_x\left(\frac{\pi}{a}\right) = \frac{\pi}{a}$$

Positive 1/8th of spherical k-space.

Therefore Volume of a *k*-point: $V_k = \left(\frac{\pi}{a}\right)^3$

Number of energy states between *k*, *k+Δk* ⟶ $g_T(k)dk = 2\left(\frac{1}{8}\right)\frac{4\pi k^2 dk}{\left(\frac{\pi}{a}\right)^3}$

Where:

2→ two spin states allowed for each quantum number

$4\pi k^2 dk$ → differential volume in k-space between shells of radius k and K+ Δk

Simplifying, $g_T(k)dk = \frac{\pi k^2 dk}{\pi^3}\cdot a^3$

Use relationship between k & E → to move from k-space to real space.

$$k^2 = \frac{2mE}{\hbar^2} \longrightarrow k = \frac{1}{\hbar}\sqrt{2mE} \longrightarrow dk = \frac{1}{\hbar}\sqrt{\frac{m}{2E}}\,dE$$

Substituting for *dk* in previous equation,

$$g_T(E)dE = \frac{\pi\, a^3}{\pi^3}\left(\frac{2mE}{\hbar^2}\right)\cdot\frac{1}{\hbar}\sqrt{\frac{m}{2E}}\,dE$$

$$g_T(E)dE = \frac{\pi a^3}{\pi^3}\left(\frac{2mE}{\hbar^2}\right)\cdot\frac{1}{\hbar}\sqrt{\frac{m}{2E}}\,dE$$

$$\Big\downarrow \quad \hbar = \frac{h}{2\pi}$$

$$g_T(E)dE = \frac{4\pi a^3}{h^3}\cdot(2m)^{3/2}\cdot\sqrt{E}\cdot dE$$

$g_T(E)dE$ is the density of states in volume a^3. Dividing by a^3 we can get the volume density of states as

$$\boxed{g(E) = \frac{4\pi(2m)^{3/2}}{h^3}\sqrt{E}}$$

Extension to semiconductors.

We have derived expression for density of allowed electron quantum states using model of free electron in an infinite potential well.

Electrons and holes are also confined within a semiconductor crystal

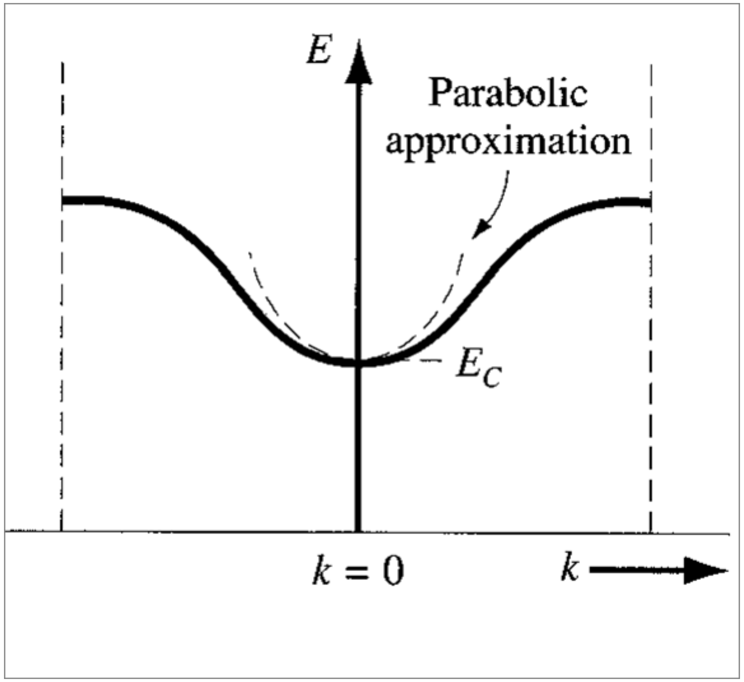
So we can extend this model to derive density of quantum states in conduction and valence bands.

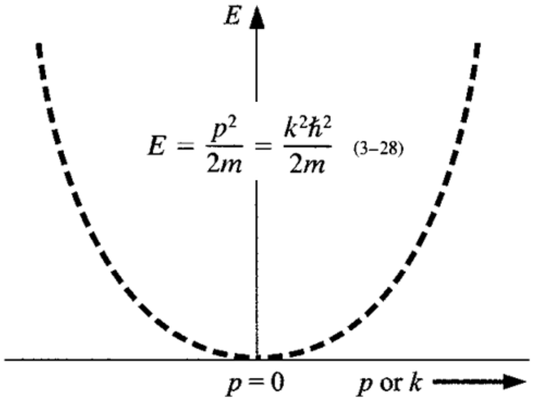
Extension to semiconductors.

Conduction band:

$$E = E_c + \frac{\hbar^2 k^2}{2m_n^*}$$

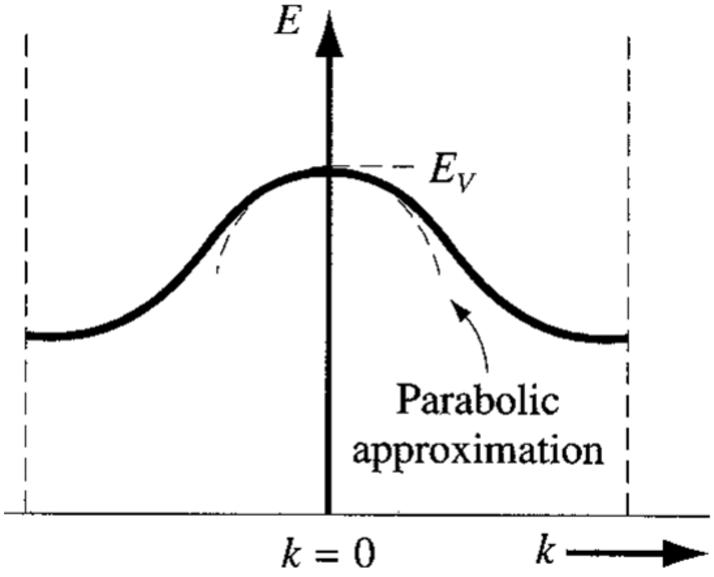
$$E - E_c = \frac{\hbar^2 k^2}{2m_n^*}$$





Parabolic E vs. k for free electron

Valence band:



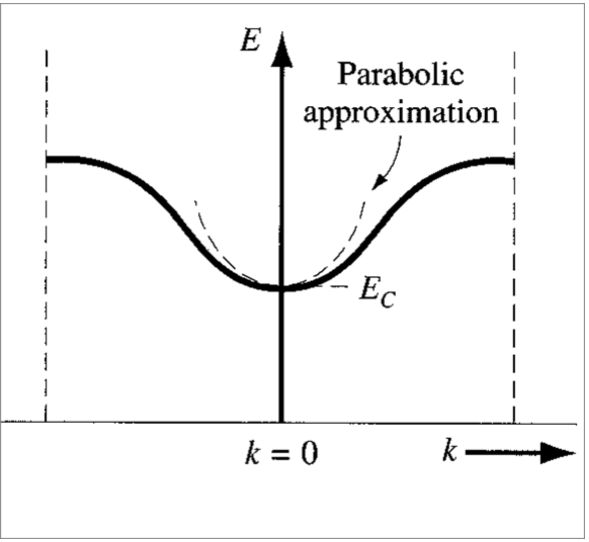
$$E = E_v - \frac{\hbar^2 k^2}{2m_p^*}$$

$$E_v - E = \frac{\hbar^2 k^2}{2m_p^*}$$

Density of states in the conduction band

For free electron, $E = \dfrac{\hbar^2 k^2}{2m}$ and $g(E) = \dfrac{4\pi(2m)^{3/2}}{h^3}\sqrt{E}$

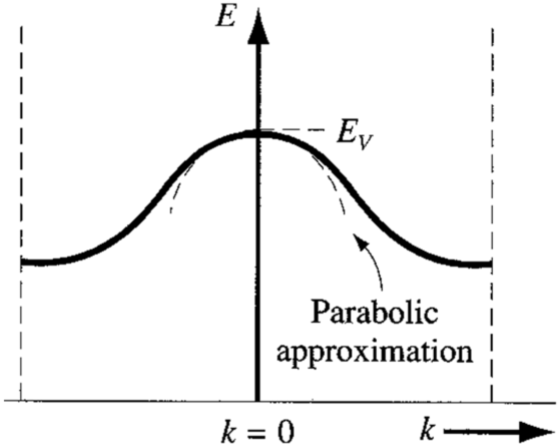
For conduction band, $E - E_c = \dfrac{\hbar^2 k^2}{2m_n^*}$



$$\boxed{g_c(E) = \frac{4\pi(2m_n^*)^{3/2}}{h^3}\sqrt{E - E_c}}$$

Density of states in the valence band

for $E \leq E_v$



$$E_v - E = \frac{\hbar^2 k^2}{2m_p^*}$$

$$\boxed{g_v(E) = \frac{4\pi (2m_p^*)^{3/2}}{h^3}\sqrt{E_v - E}}$$

Density of states function

In general: $$g(E) = \frac{4\pi(2m)^{3/2}}{h^3}\sqrt{E}$$

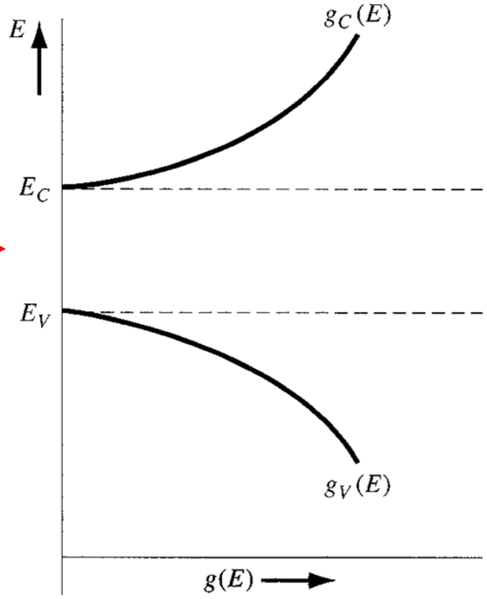
for $E \geq E_c$

$$\boxed{g_c(E) = \frac{4\pi(2m_n^*)^{3/2}}{h^3}\sqrt{E - E_c}}$$

$$g(E) = 0 \text{ for } E_v < E < E_c$$

for $E \leq E_v$

$$\boxed{g_v(E) = \frac{4\pi(2m_p^*)^{3/2}}{h^3}\sqrt{E_v - E}}$$



Statistical Mechanics.

- While studying, large number of particles, we are interested only in statistical behavior of the group as a whole.

- In a semiconductor crystal, we are not interested in the behavior of each individual electron.

- The electrical characteristics will be determined by statistical behavior of large number of electrons.

- While studying statistical behavior, we must consider the laws that the particles obey.

Distribution Laws:

Distribution of particles among energy states → 3 laws.

	Particles distinguishable	Particles Identical
Unlimited number of particles allowed in each energy state	Maxwell-Boltzmann probability function. E.g. Behavior of gas at low pressure.	Bose-Einstein function. E.g. Behavior of photons or black body radiation.
Limited number of particles allowed in each energy state		Fermi-Dirac probability function E.g. Electrons is a semiconductor crystal.

Fermi-Dirac distribution function:

$$\frac{N(E)}{g(E)} = f_F(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$

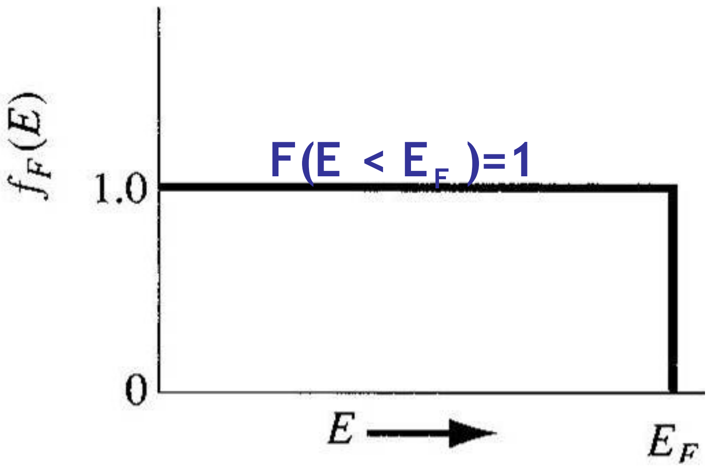
N(E) → number of electrons per unit volume per unit energy.

g(E) → number of quantum states per unit vol per unit energy.

E_F → Fermi energy (explained in more detail later)

At T = 0 K

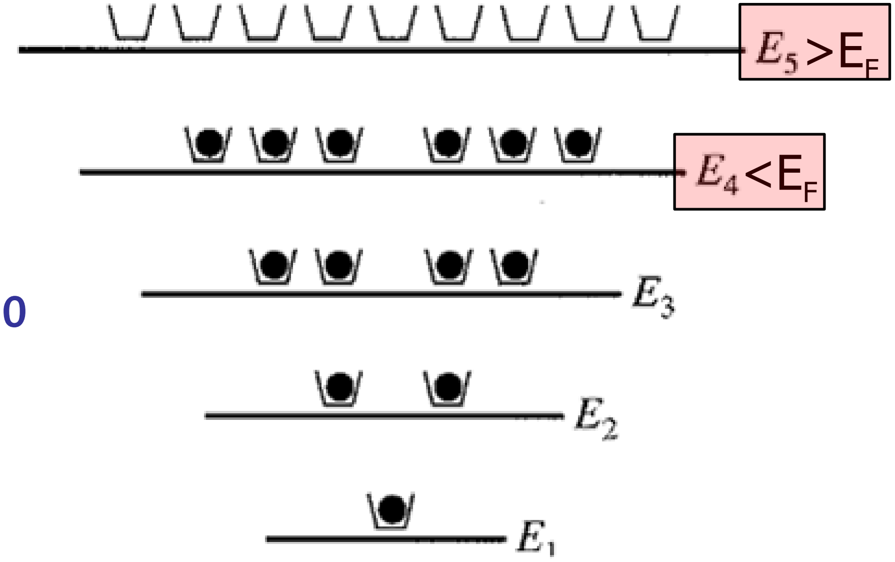
$$f_F(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$



$F(E < E_F) = 1$

$F(E > E_F) = 0$

The Fermi probability function versus energy for T=0K



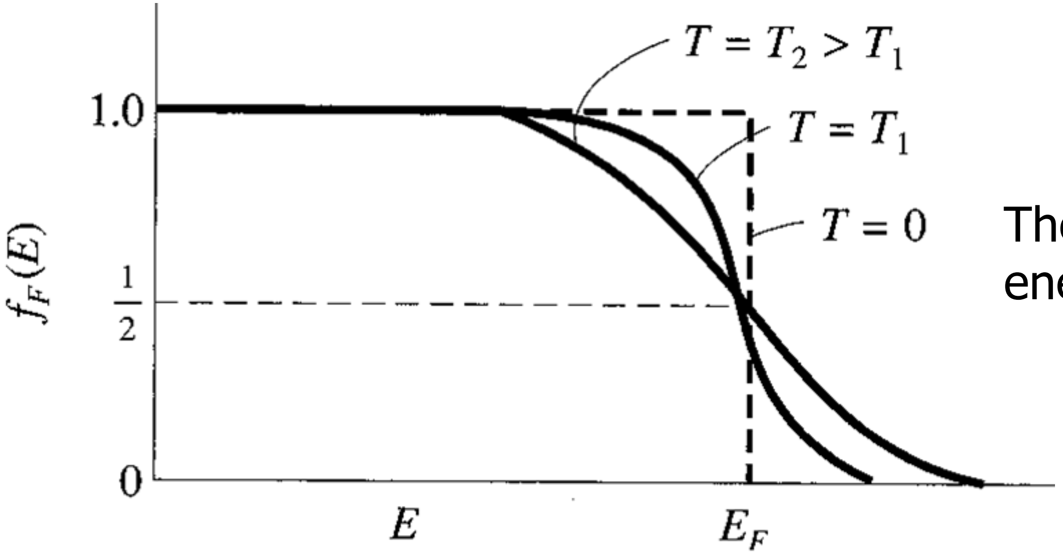
Discrete energy states and quantum states for a particular system.

At $E=E_F$

$$f_F(E=E_F)=\frac{1}{1+\exp(0)}=\frac{1}{1+1}=\frac{1}{2}$$

So Fermi Energy is the energy level where probability is ½.

At T>0

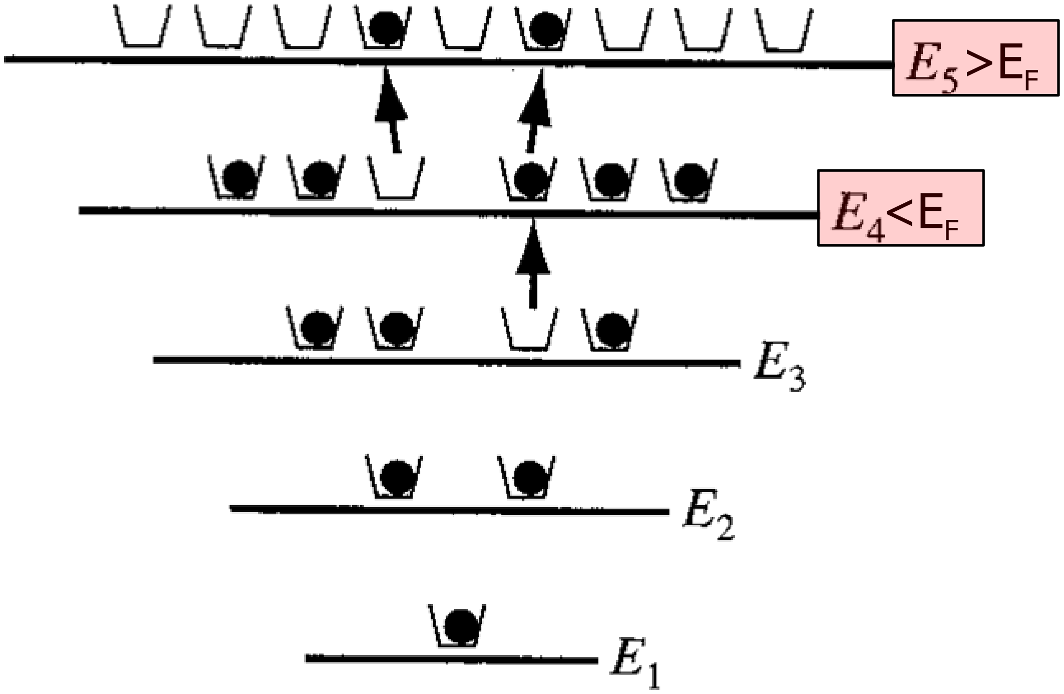


The fermi probability function versus energy for different temperatures.

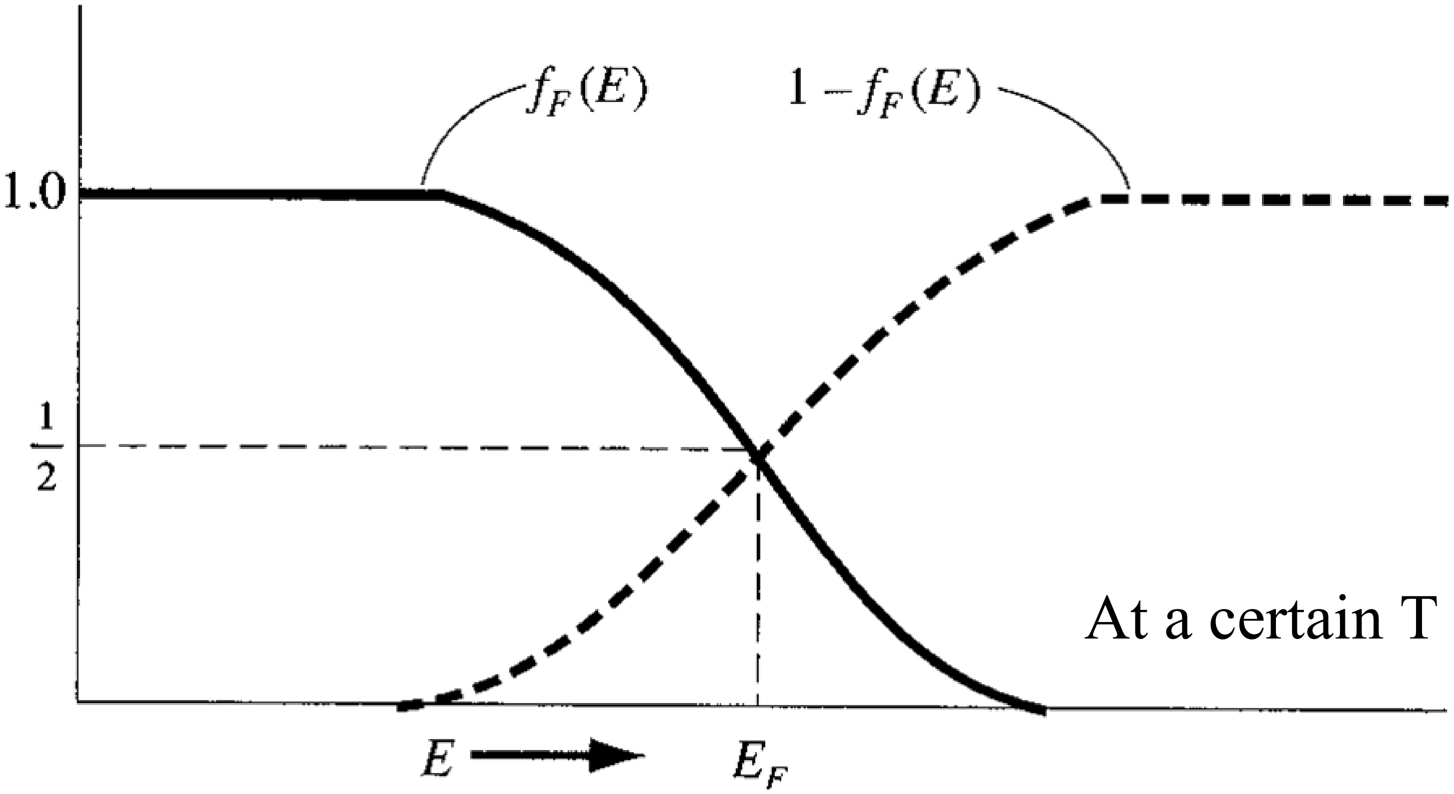
Applet

At T>0K, there is non-zero probability that some states above EF are occupied and some states below are empty → some electrons have jumped to higher energy levels with increasing thermal energy.

At T > 0 K



Discrete energy states and quantum states for the same system at T>0K



The function $f_F(E)$ is symmetrical with the function $1-f_F(E)$ about the Fermi energy E_F