
VE320 – Summer 2024

Introduction to Semiconductor Devices

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Chapter 3 Introduction to the Quantum Theory of Solids

Outline

- 3.1 Allowed and Forbidden Energy Bands
- 3.2 Electrical Conduction in Solids
- 3.3 Extension to Three Dimensions
- 3.4 Effective Mass
- 3.5 Density of States Function
- 3.6 Statistical Mechanics

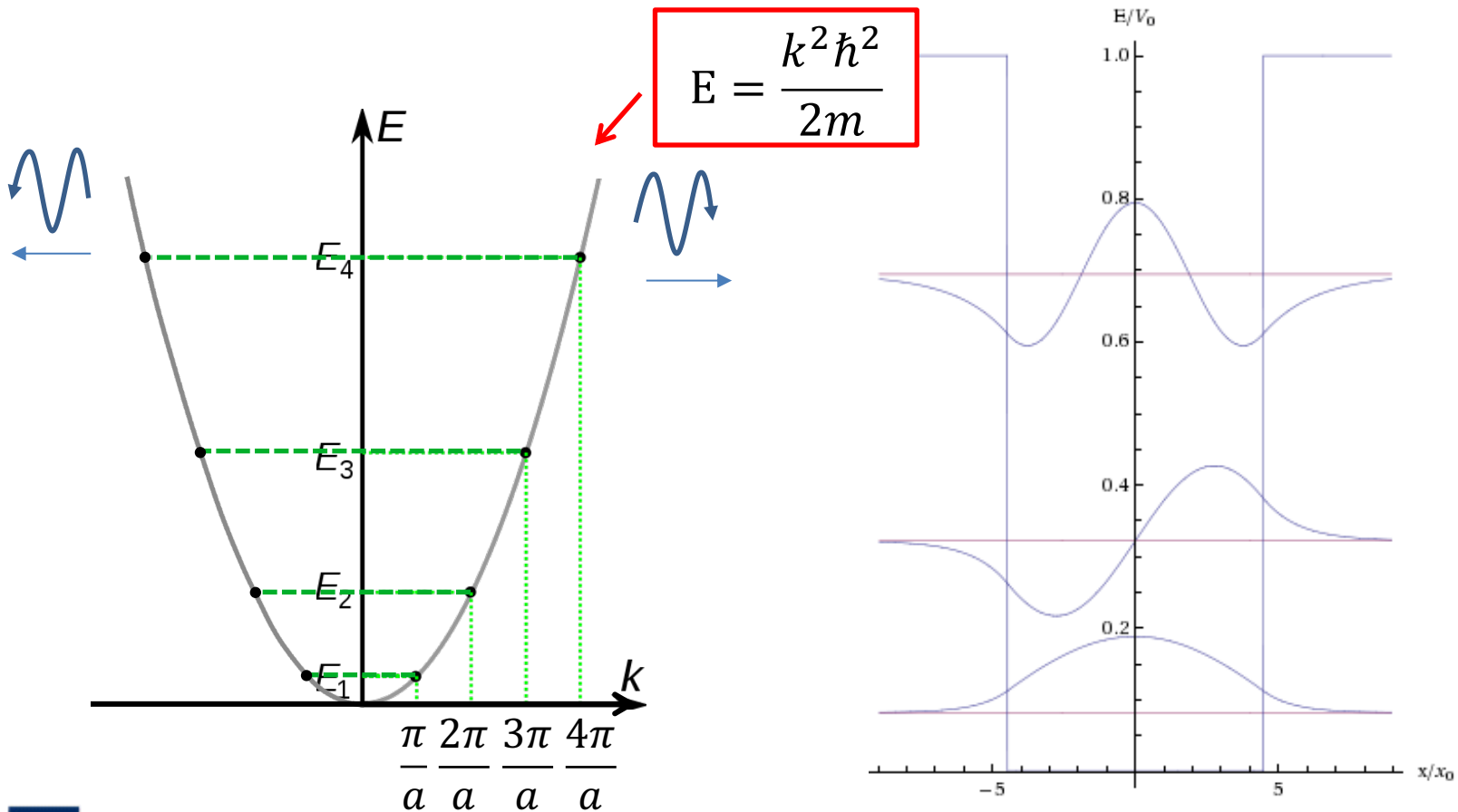
Outline

- **3.1 Allowed and Forbidden Energy Bands**
- 3.2 Electrical Conduction in Solids
- 3.3 Extension to Three Dimensions
- 3.4 Effective Mass
- 3.5 Density of States Function
- 3.6 Statistical Mechanics

3.1 Allowed and Forbidden Energy Bands

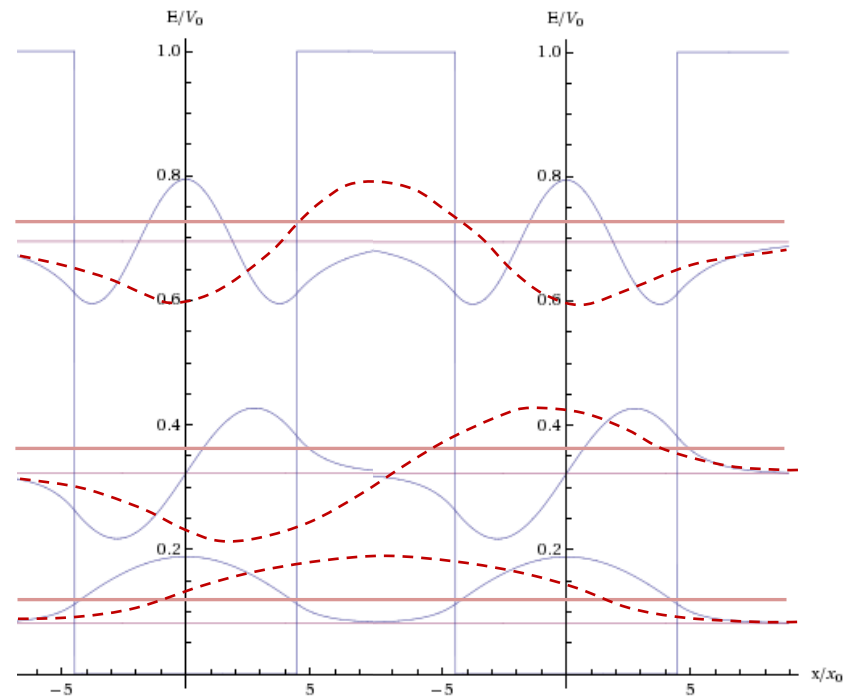
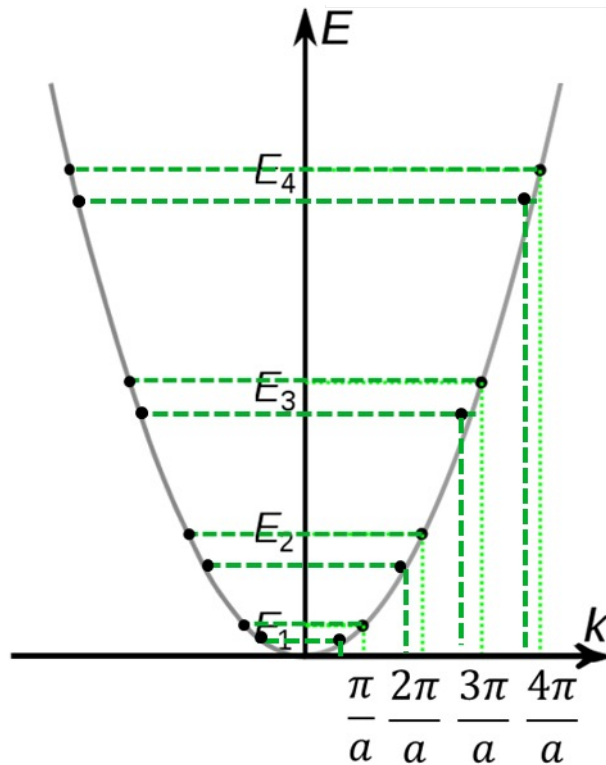
Forming energy bands: analytical

Previously: Electrons in Finite Quantum Well



3.1 Allowed and Forbidden Energy Bands

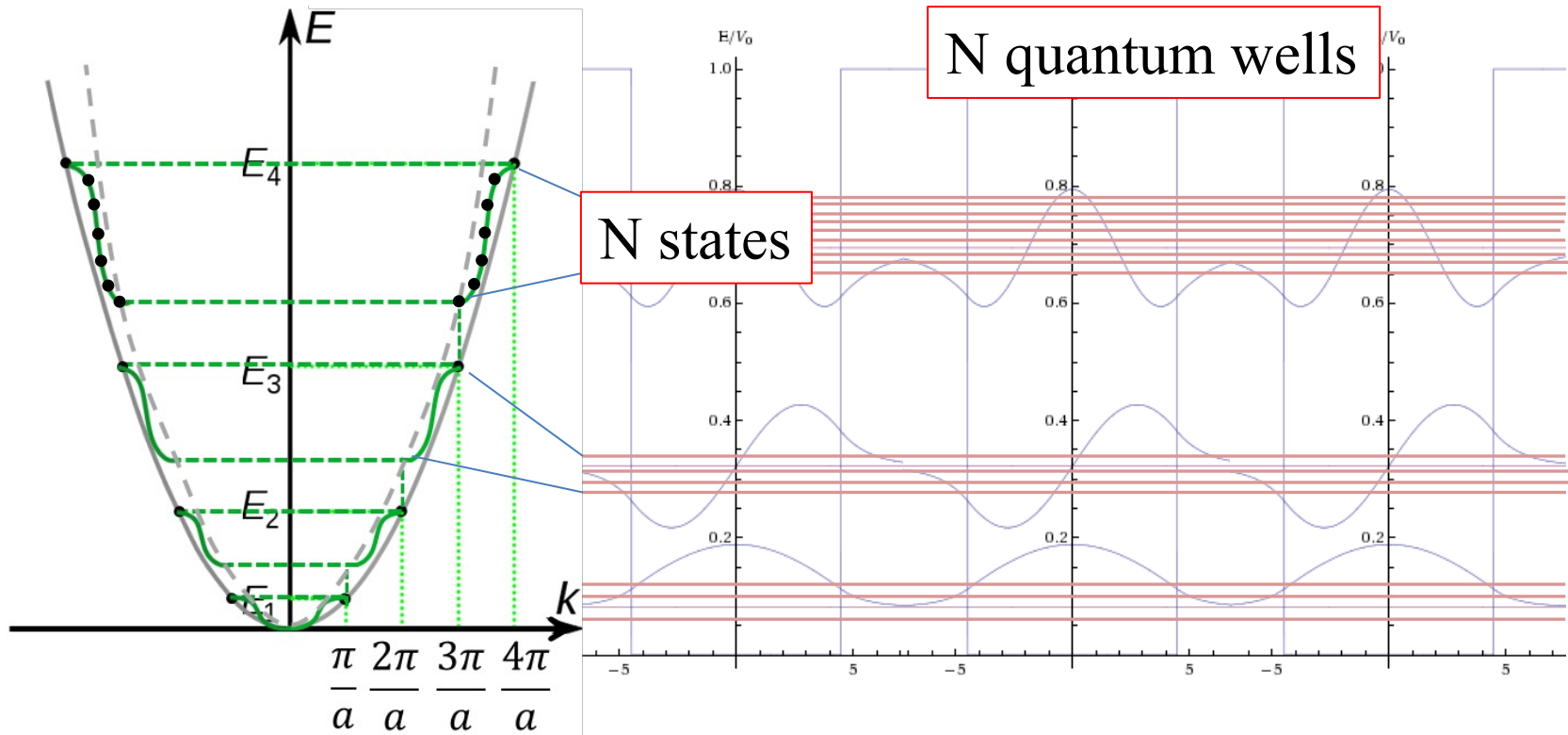
Forming energy bands: analytical



2 quantum wells

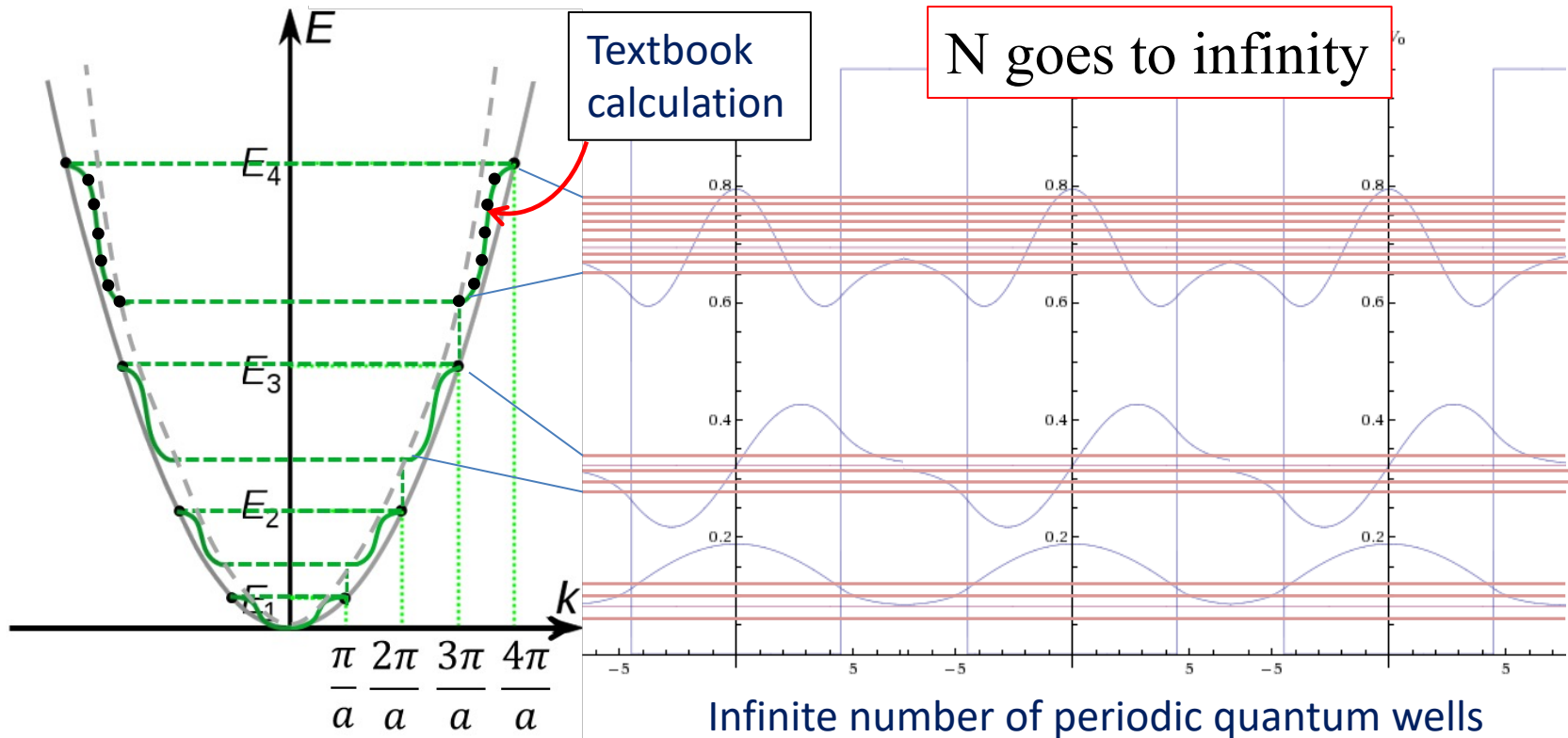
3.1 Allowed and Forbidden Energy Bands

Forming energy bands: analytical



3.1 Allowed and Forbidden Energy Bands

Forming energy bands: analytical

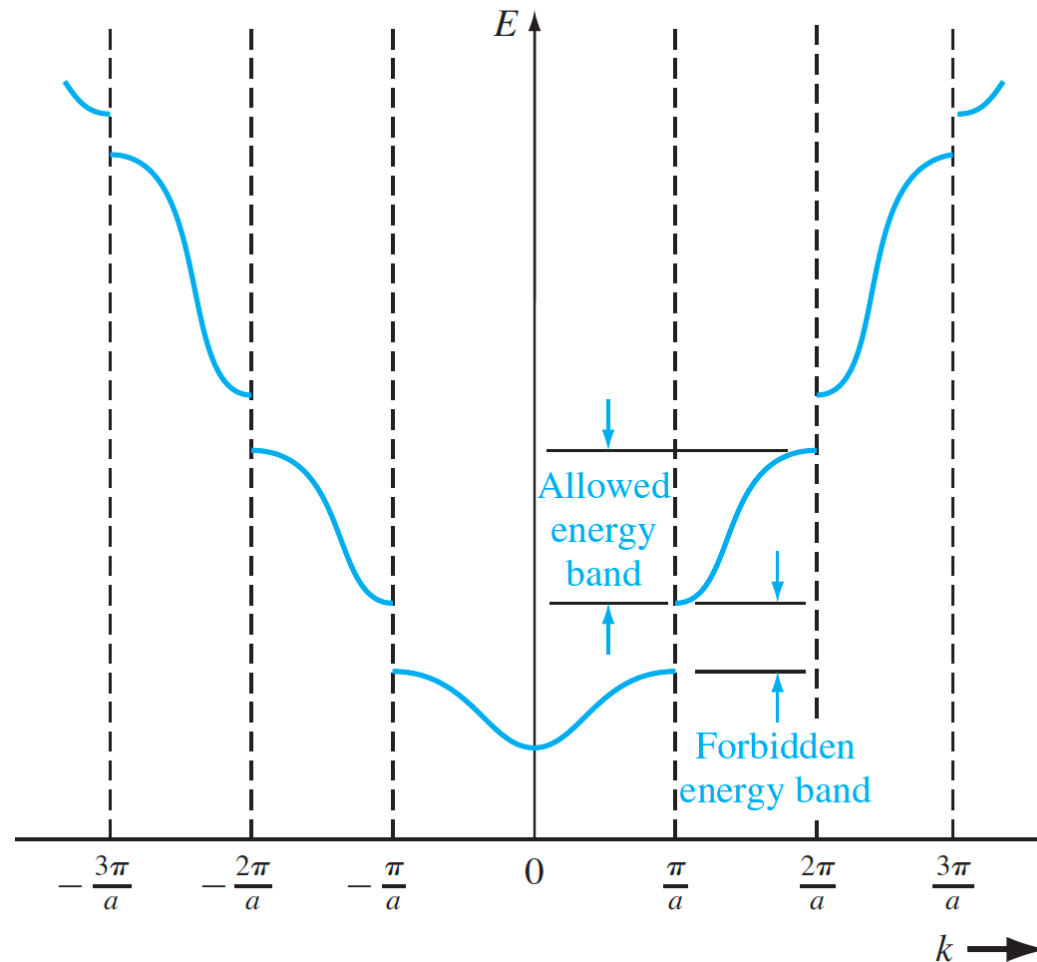


$$\frac{mV_0ba}{\hbar^2} \frac{\sin(\alpha a)}{\alpha a} + \cos(\alpha a) = \cos(ka)$$

On P.67
eq.(3.22)

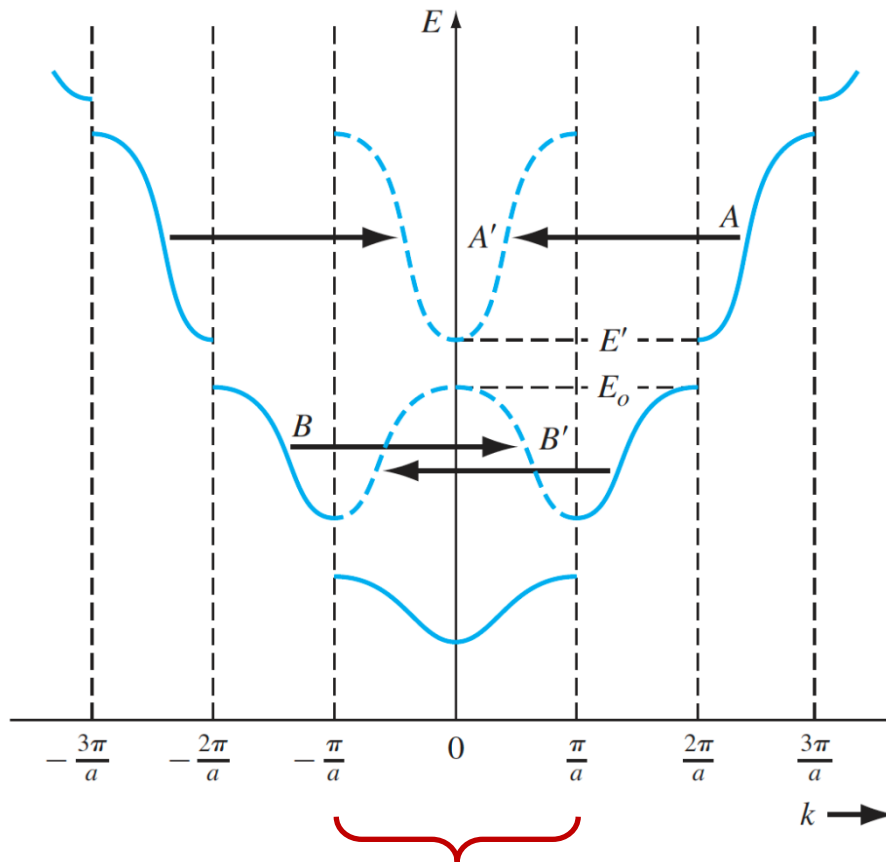
3.1 Allowed and Forbidden Energy Bands

Forming energy bands: analytical

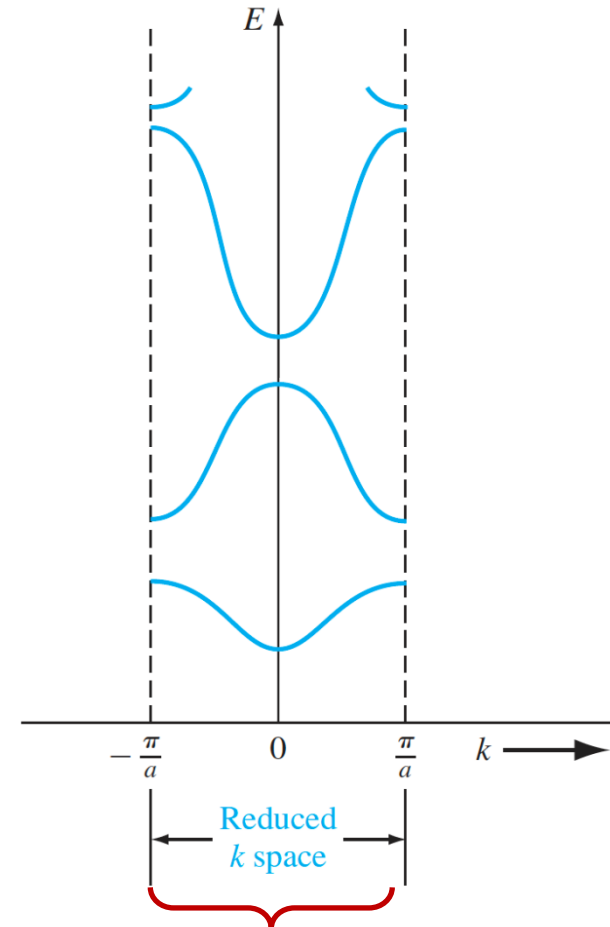


3.1 Allowed and Forbidden Energy Bands

Band structure in physical and k space for 1D periodic quantum wells



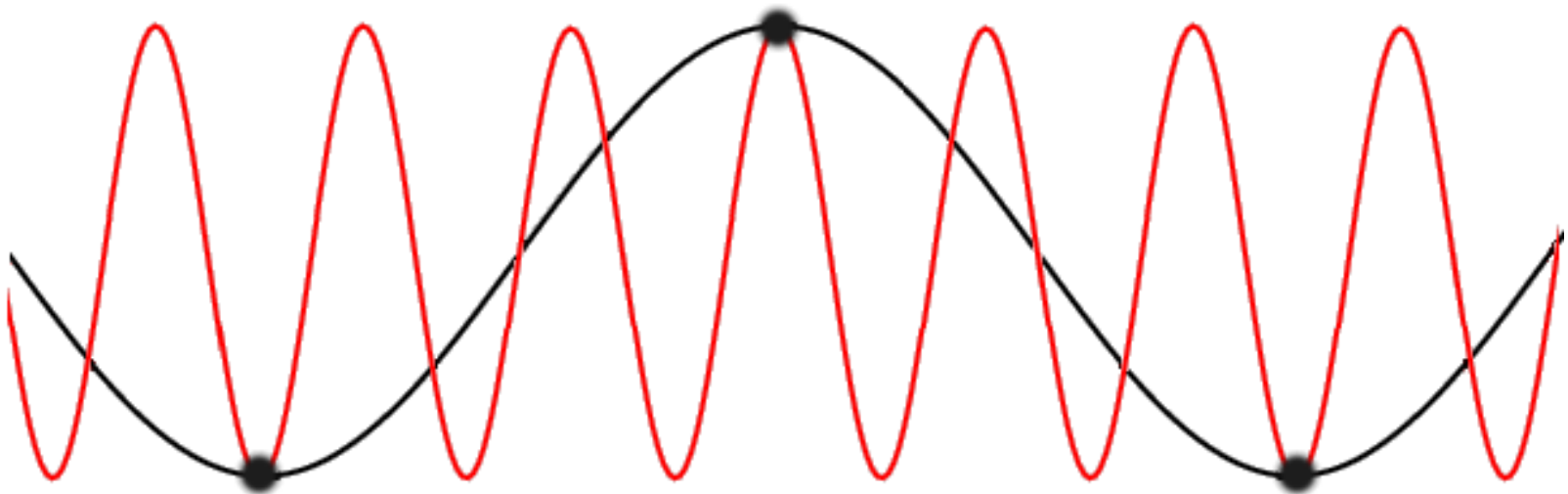
1st Brillouin zone



1st Brillouin zone

3.1 Allowed and Forbidden Energy Bands

- Black wave with a smaller k (longer wavelength) is in the 1st Brillouin zone.
- Red wave with a larger k (short wavelength) is outside of 1st Brillouin zone.
- Both waves have the same frequency (same energy).
- Both waves can describe the exact same information of a particle.



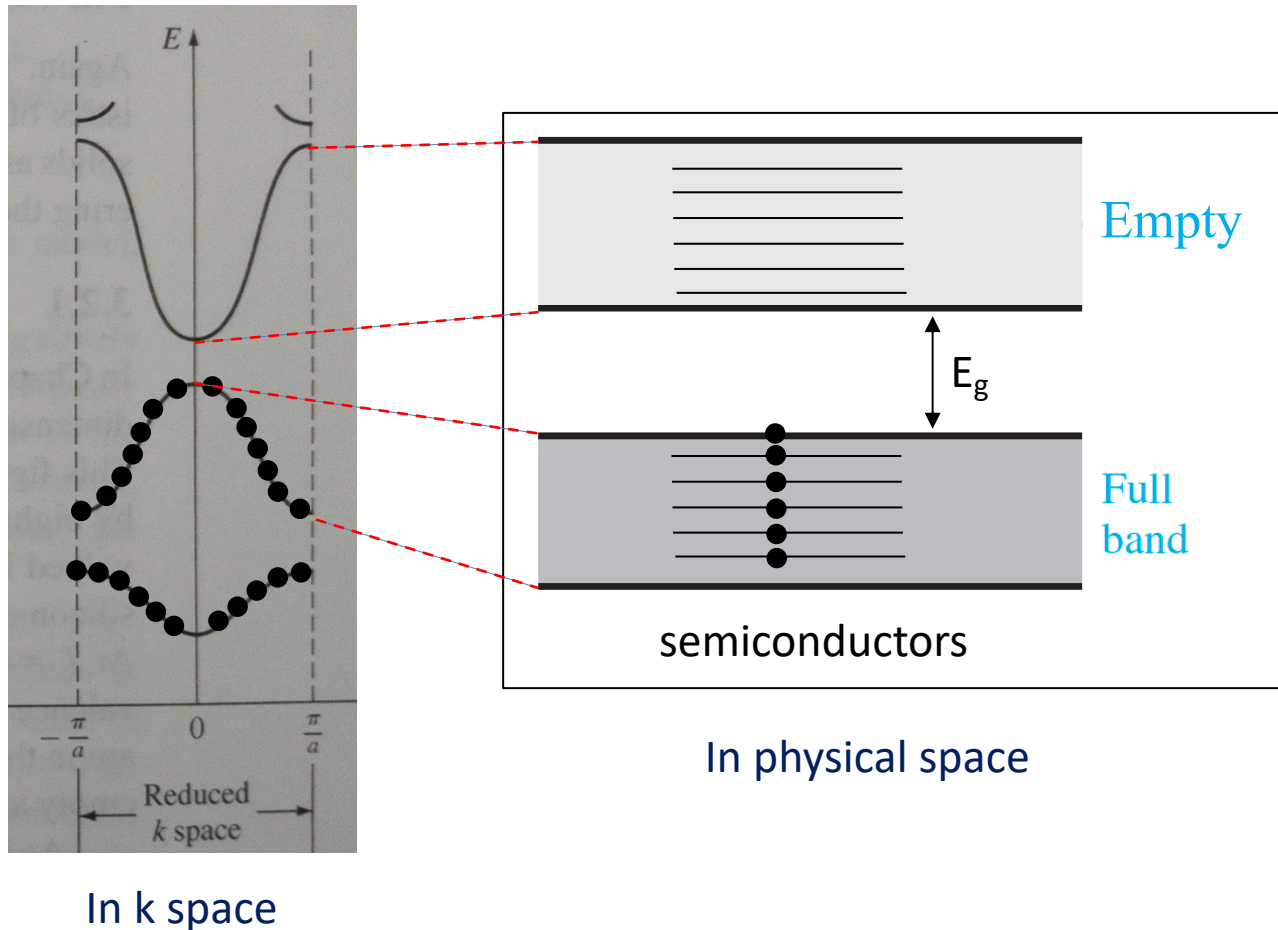
http://en.wikipedia.org/wiki/Phonon#/media/File:Phonon_k_3k.gif

Outline

- 3.1 Allowed and Forbidden Energy Bands
- **3.2 Electrical Conduction in Solids**
- 3.3 Extension to Three Dimensions
- 3.4 Effective Mass
- 3.5 Density of States Function
- 3.6 Statistical Mechanics

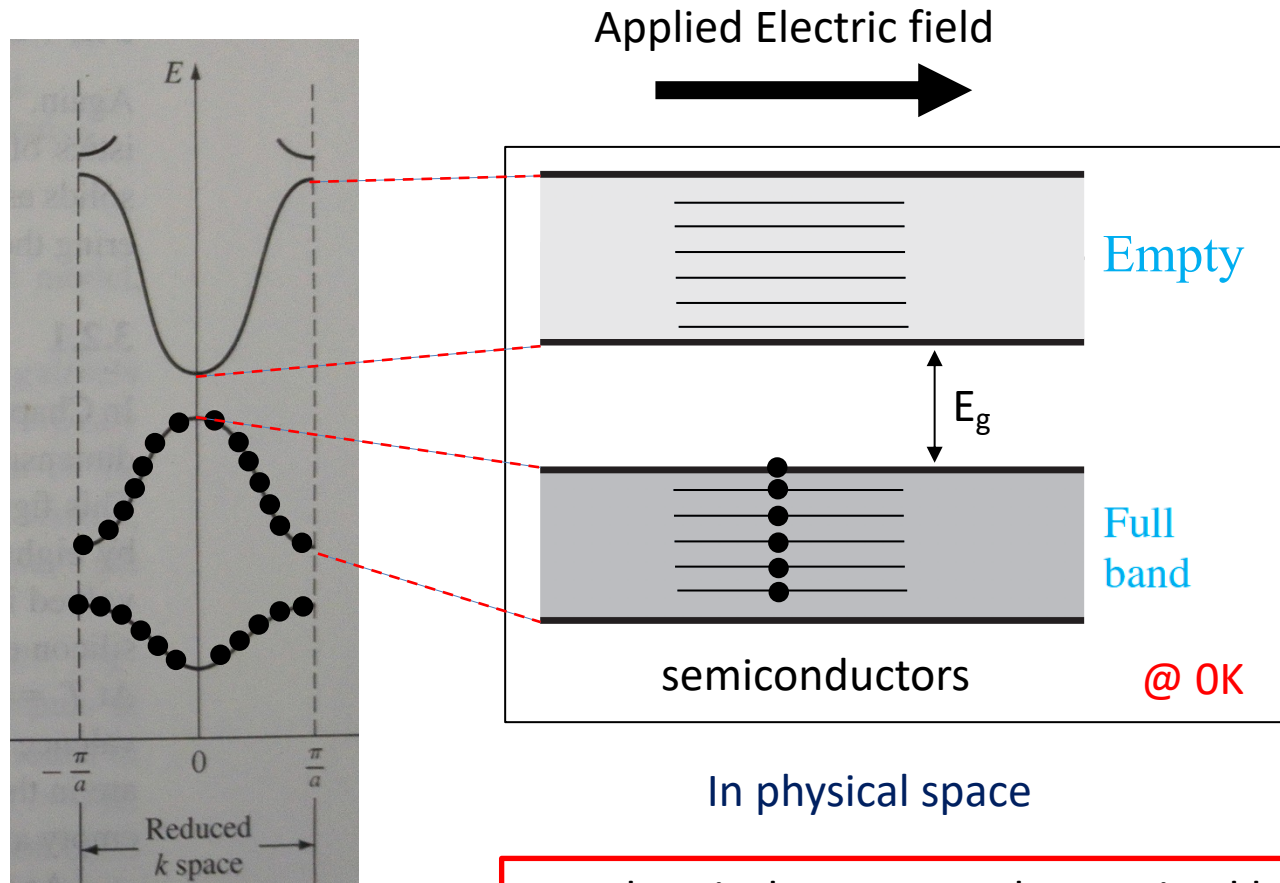
3.2 Electrical Conduction in Solids

Energy band of semiconductors



3.2 Electrical Conduction in Solids

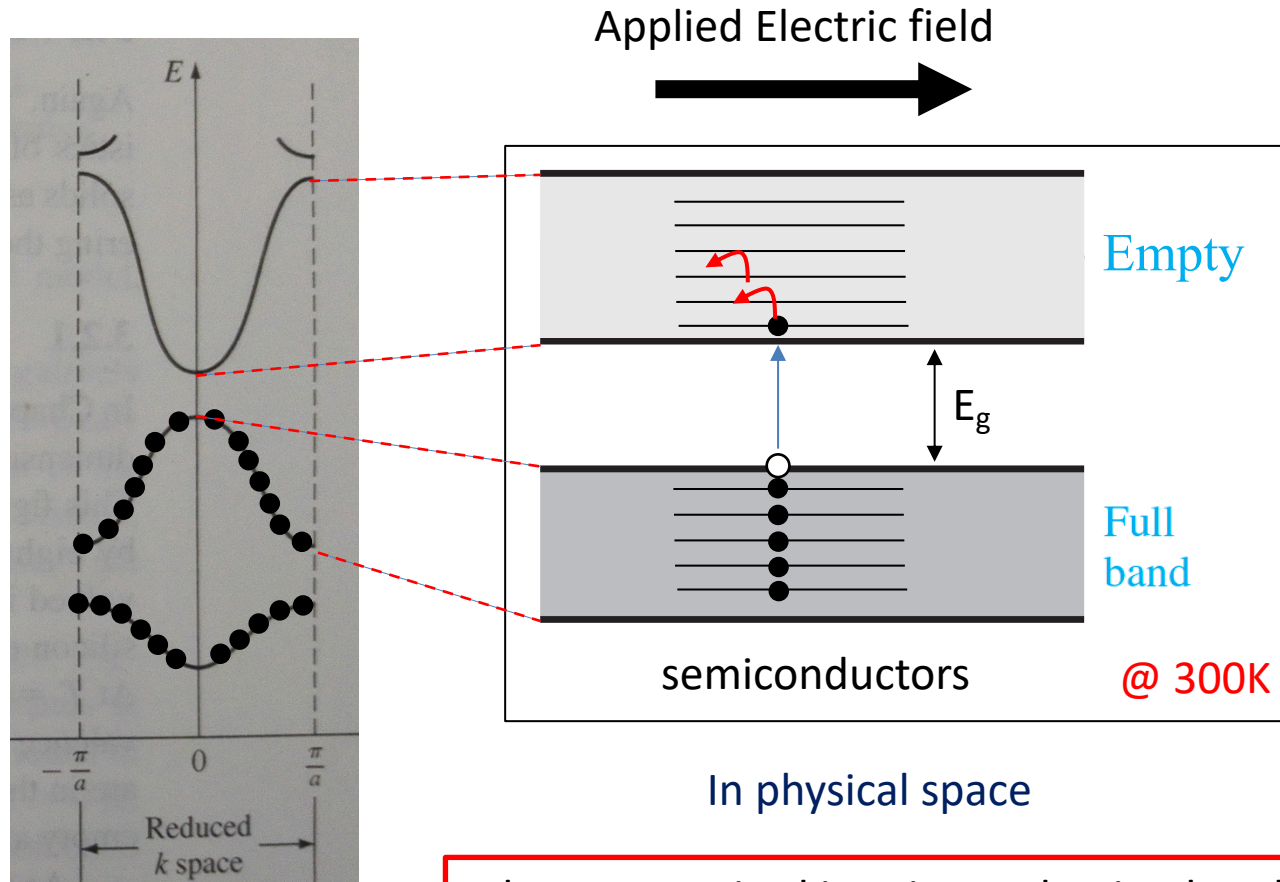
Energy band of semiconductors



No electrical energy can be received by electrons in valence band

3.2 Electrical Conduction in Solids

Energy band of semiconductors



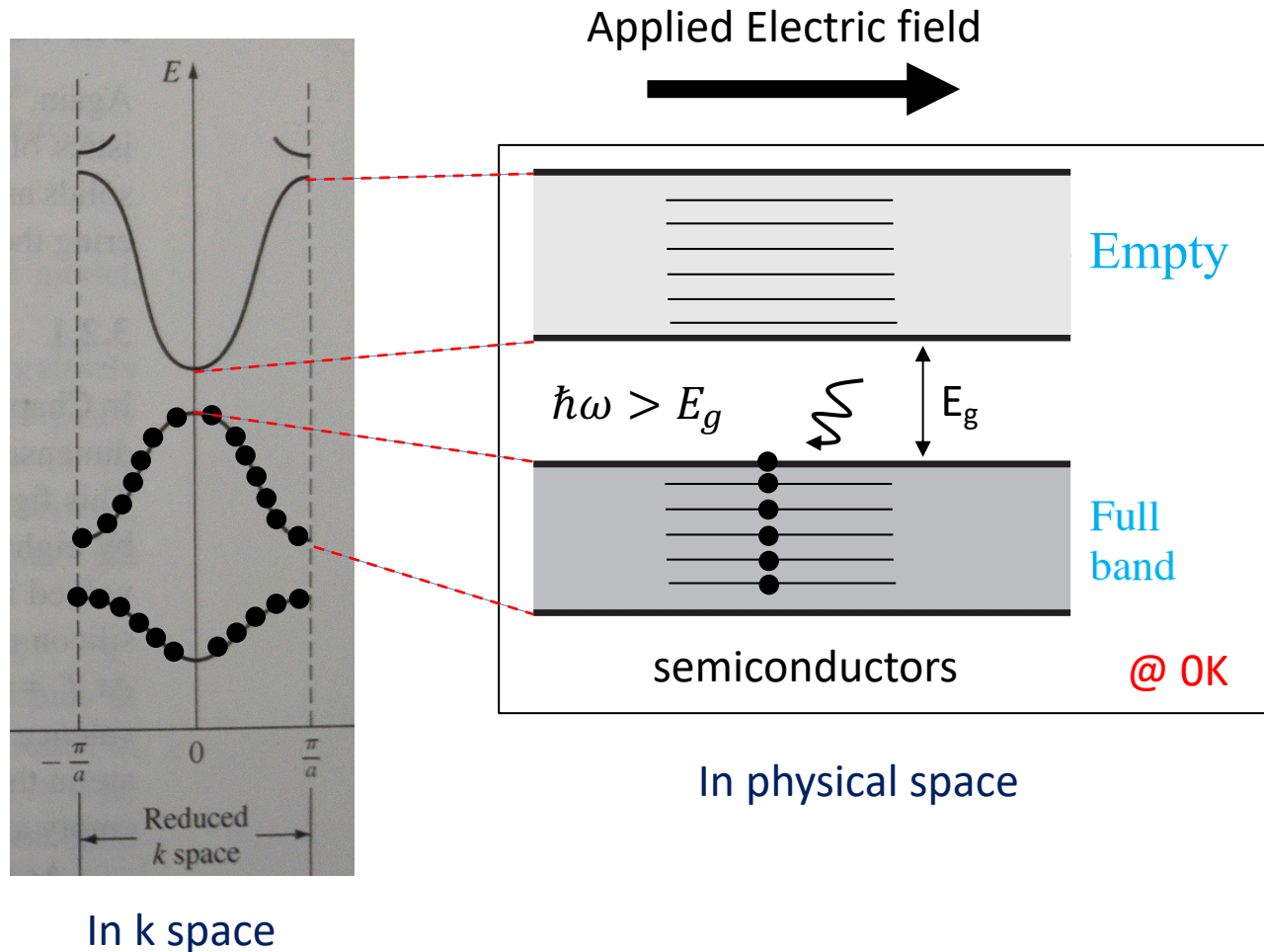
In k space

In physical space

Electrons excited into in conduction band.
Conductive via electrons and holes @RT

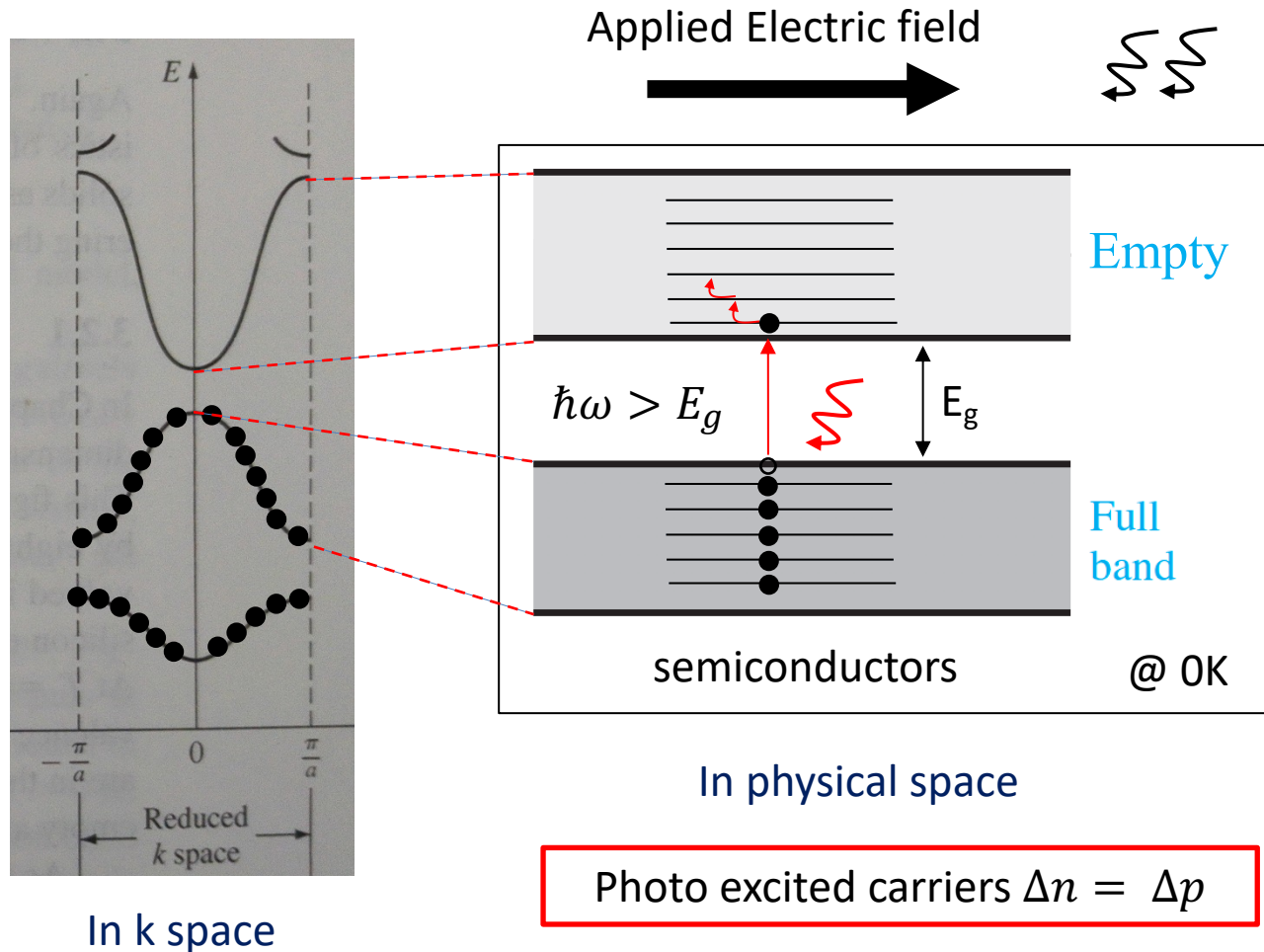
3.2 Electrical Conduction in Solids

Energy band of semiconductors



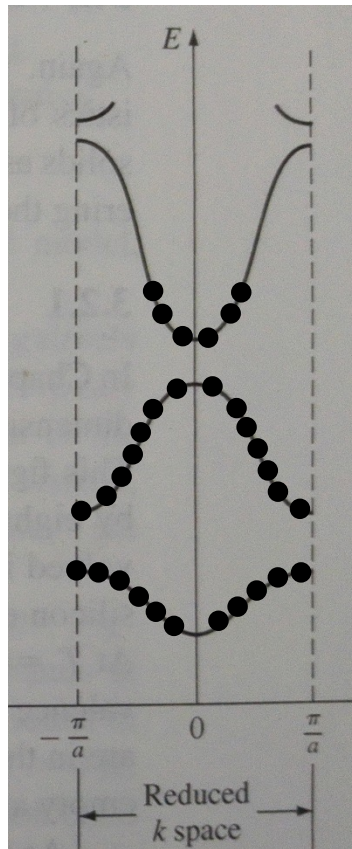
3.2 Electrical Conduction in Solids

Energy band of semiconductors

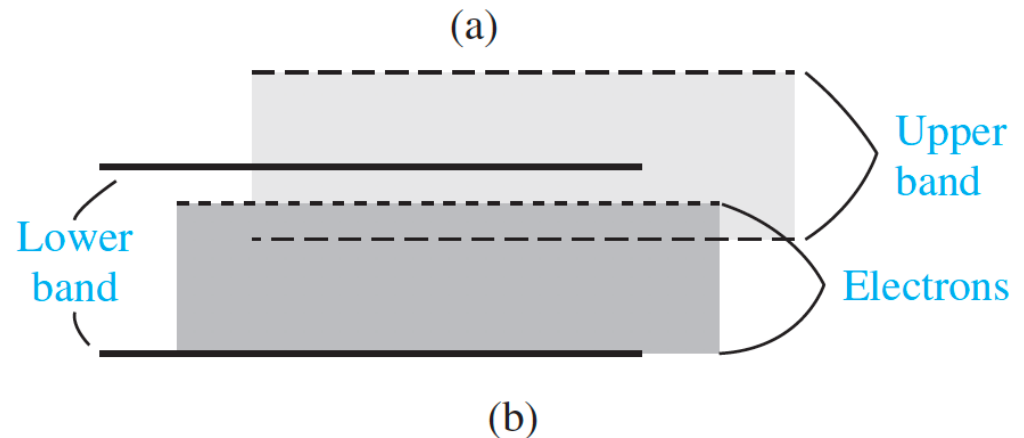


3.2 Electrical Conduction in Solids

Energy band of metals

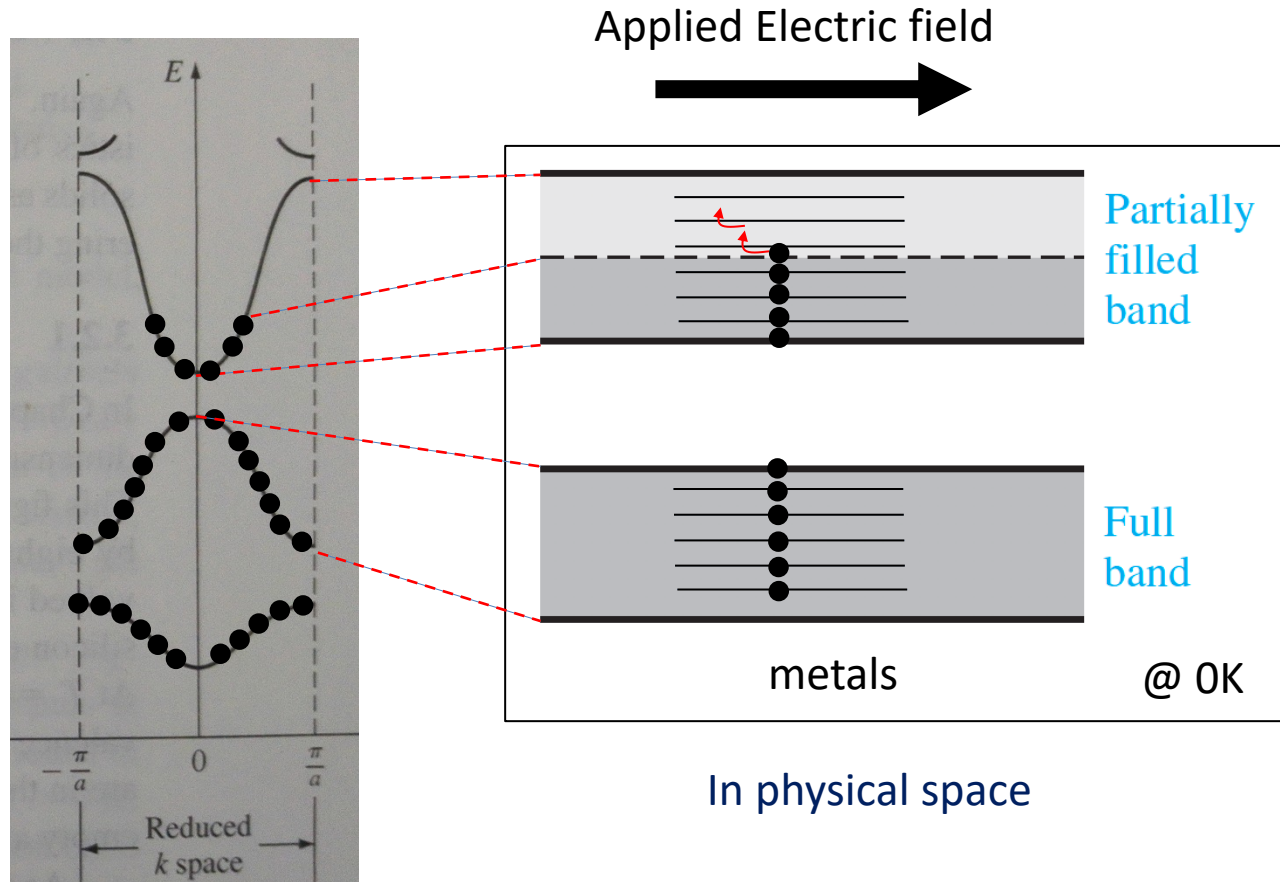


Forming energy bands is complicated.



3.2 Electrical Conduction in Solids

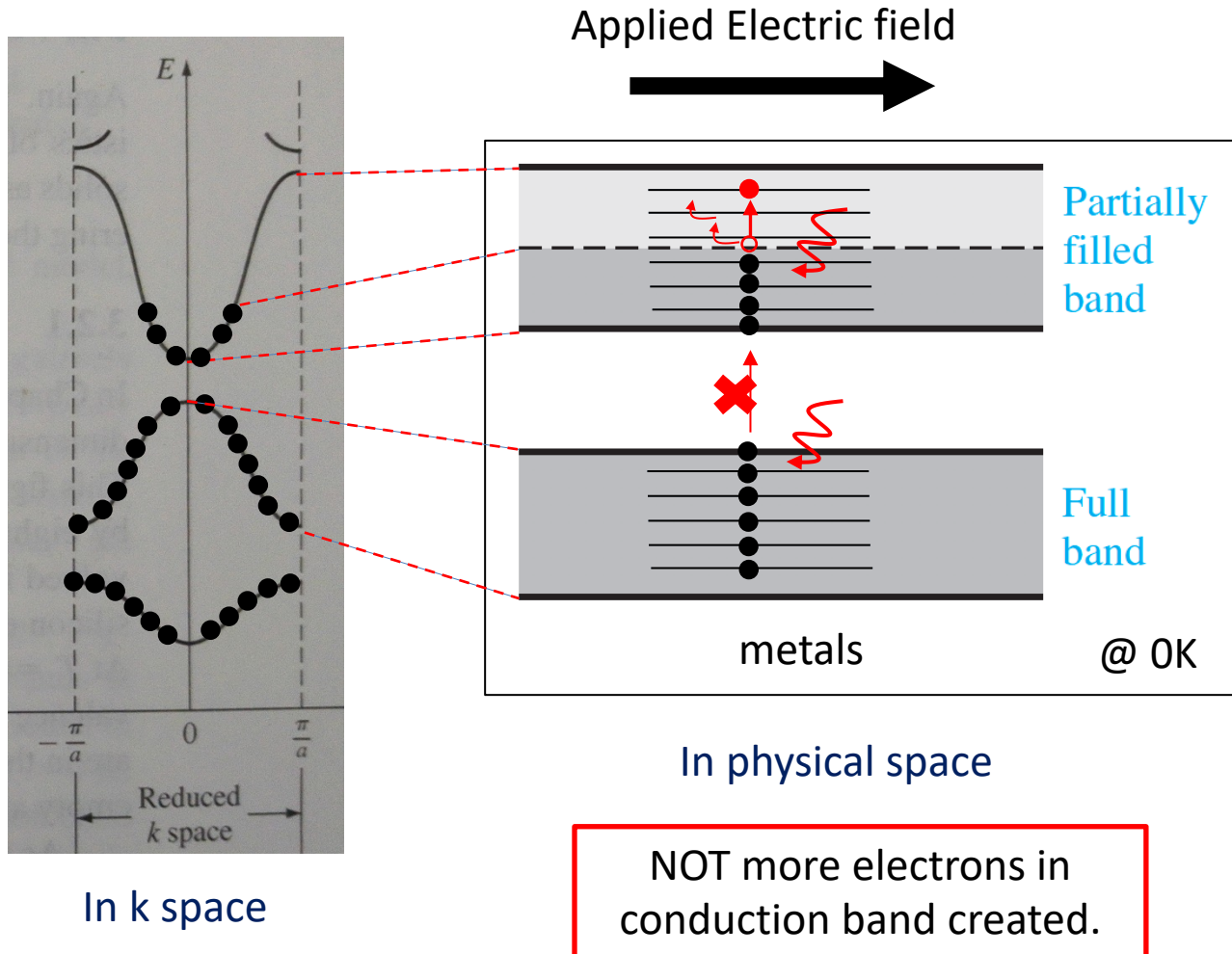
Energy band of metals



In k space

3.2 Electrical Conduction in Solids

Energy band of metals



3.2 Electrical Conduction in Solids

Metals, semiconductors and insulators

Insulators are wide bandgap semiconductors!

Physicists call semiconductors as Insulators.

Check your understanding

When the temperature decreases to 0K, how does the conductivity change for metals and semiconductors?

3.2 Electrical Conduction in Solids

Doping in semiconductors

Intrinsic semiconductors:

pure semiconductor, no doping, no defects

n-type semiconductors :

Charge carriers are **n**egative, i.e. electrons

Doped by donor-type of dopants (impurities)

p-type semiconductors:

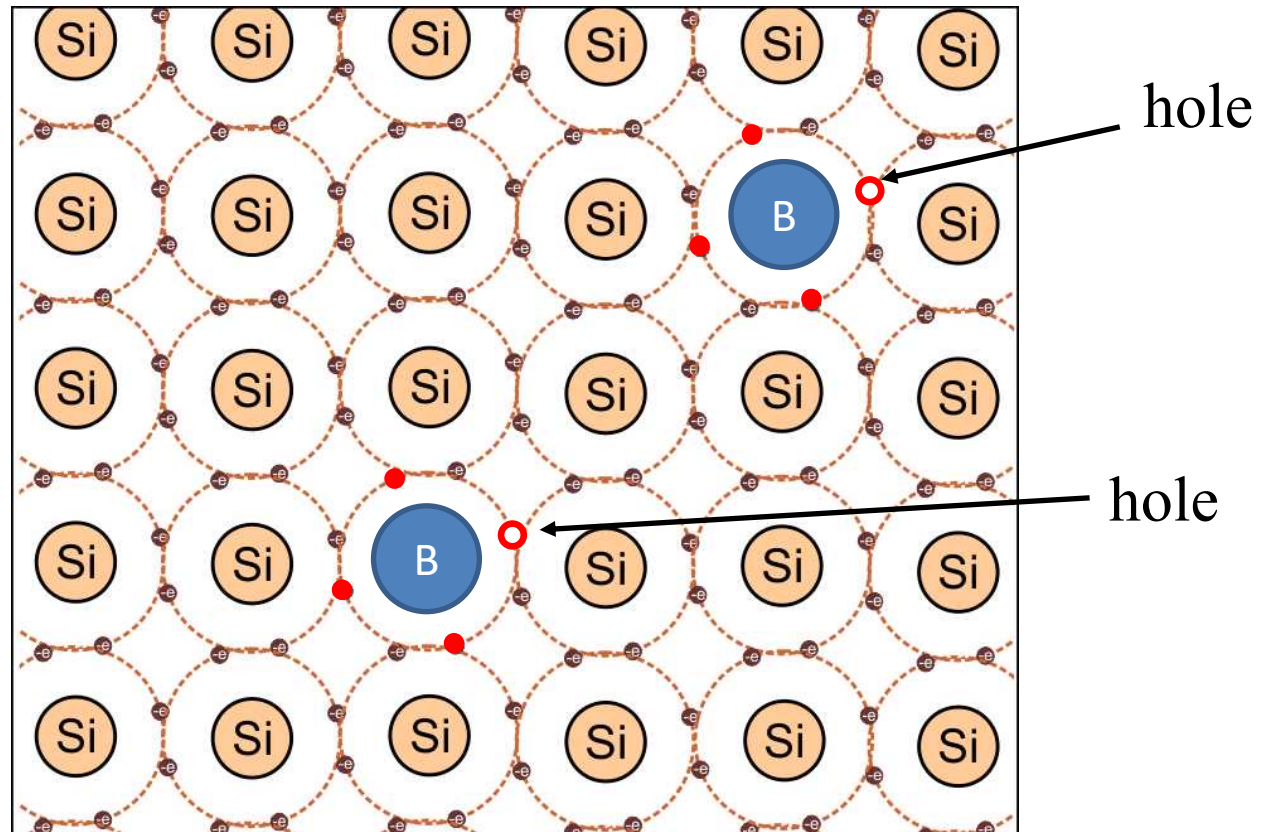
Charge carriers are **p**ositive, i.e. holes

Doped by acceptor-type of dopants (impurities)

3.2 Electrical Conduction in Solids

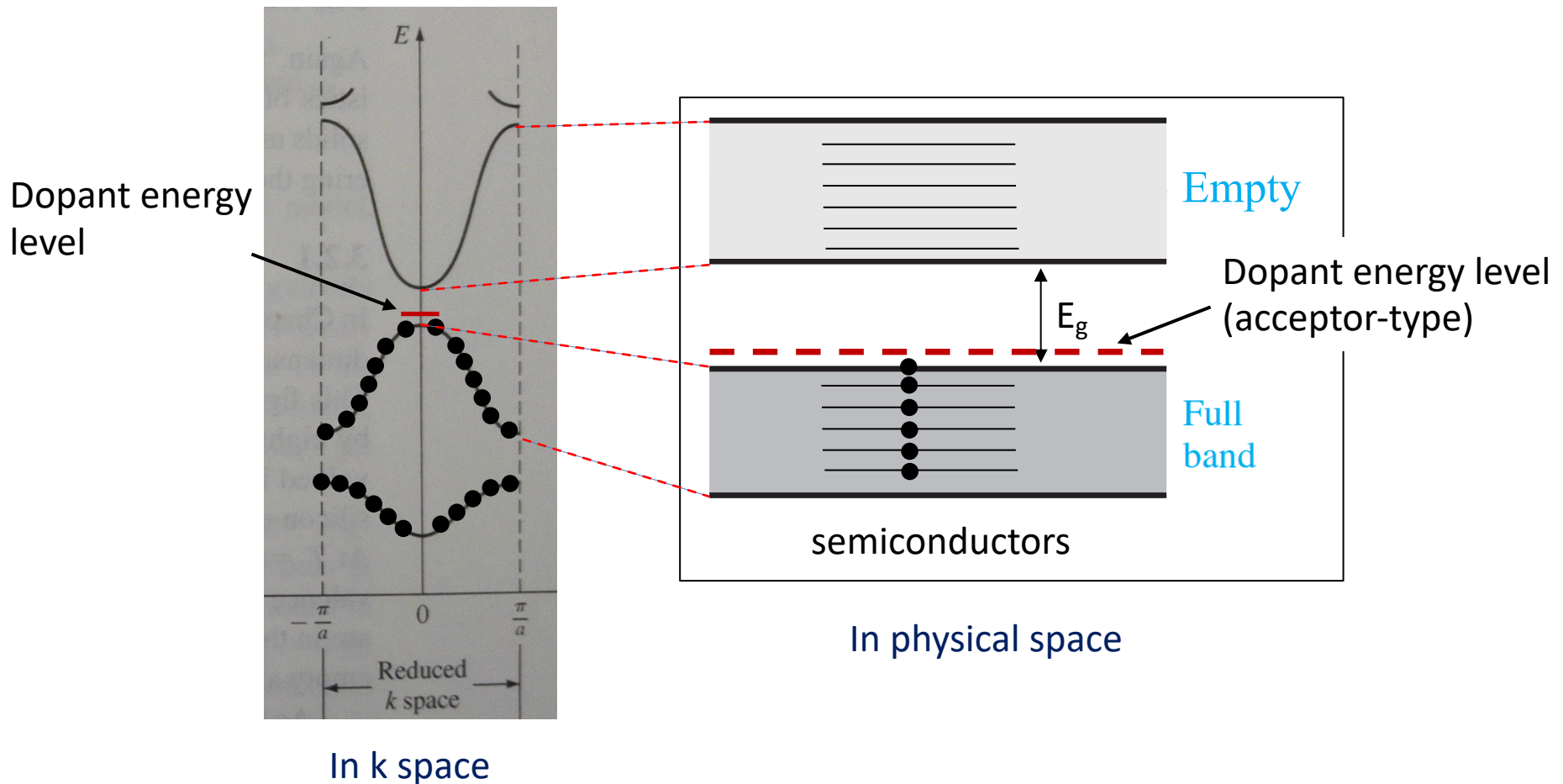
Acceptor-type or **p-type** doping (from the view of physical world)

At 0K



3.2 Electrical Conduction in Solids

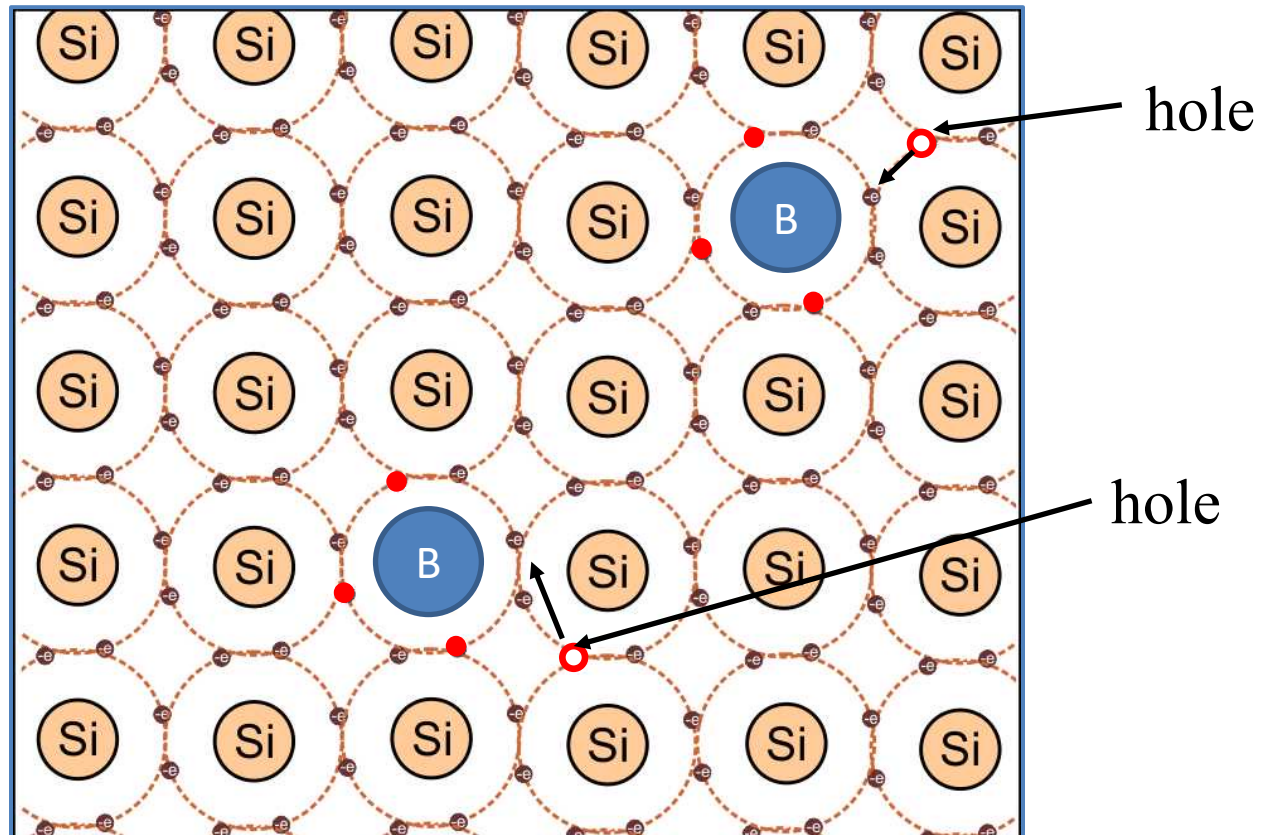
Acceptor-type or **p-type** doping (from the view of energy band)



3.2 Electrical Conduction in Solids

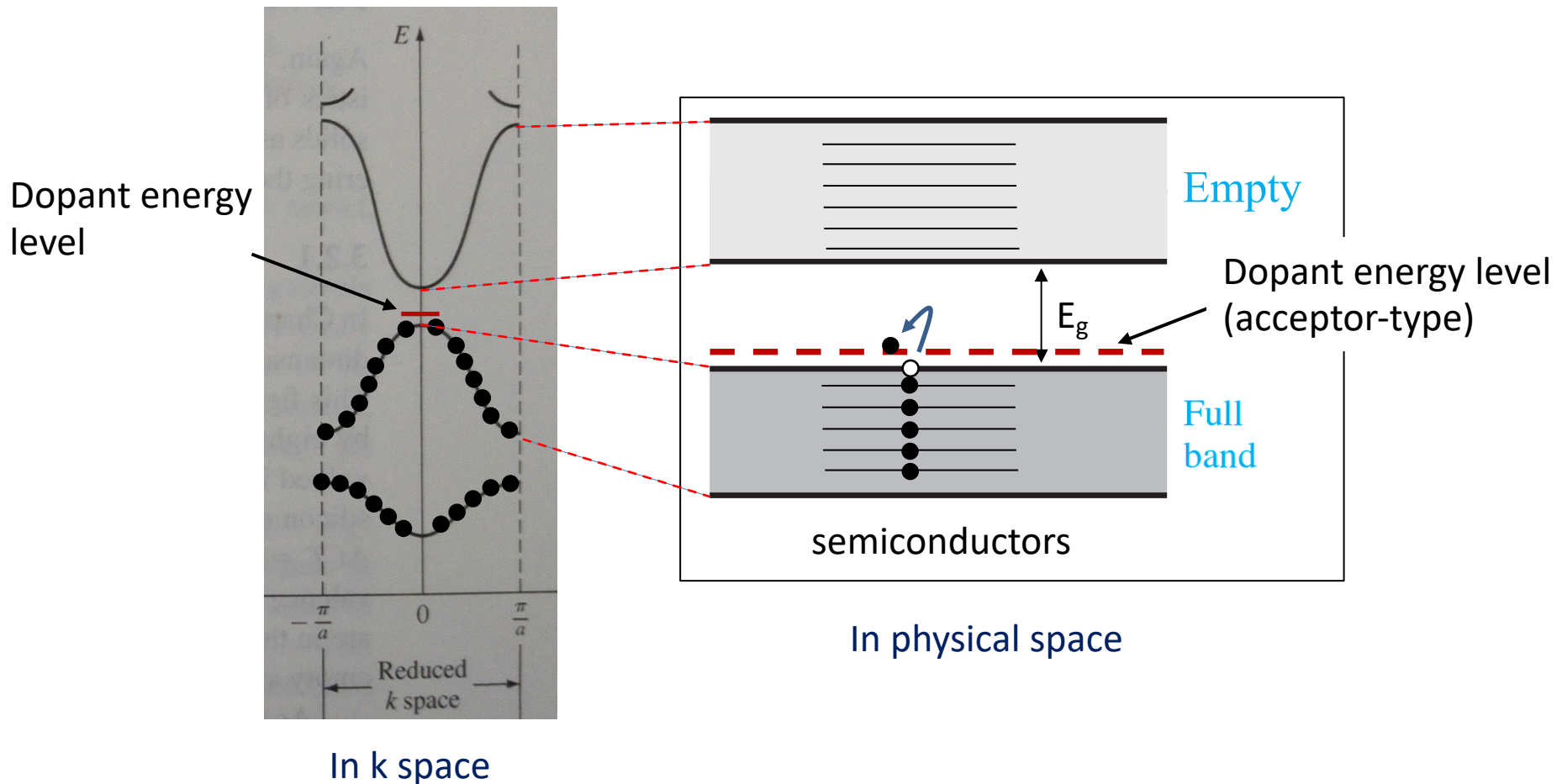
Acceptor-type or **p-type** doping (from the view of physical world)

At 300K



3.2 Electrical Conduction in Solids

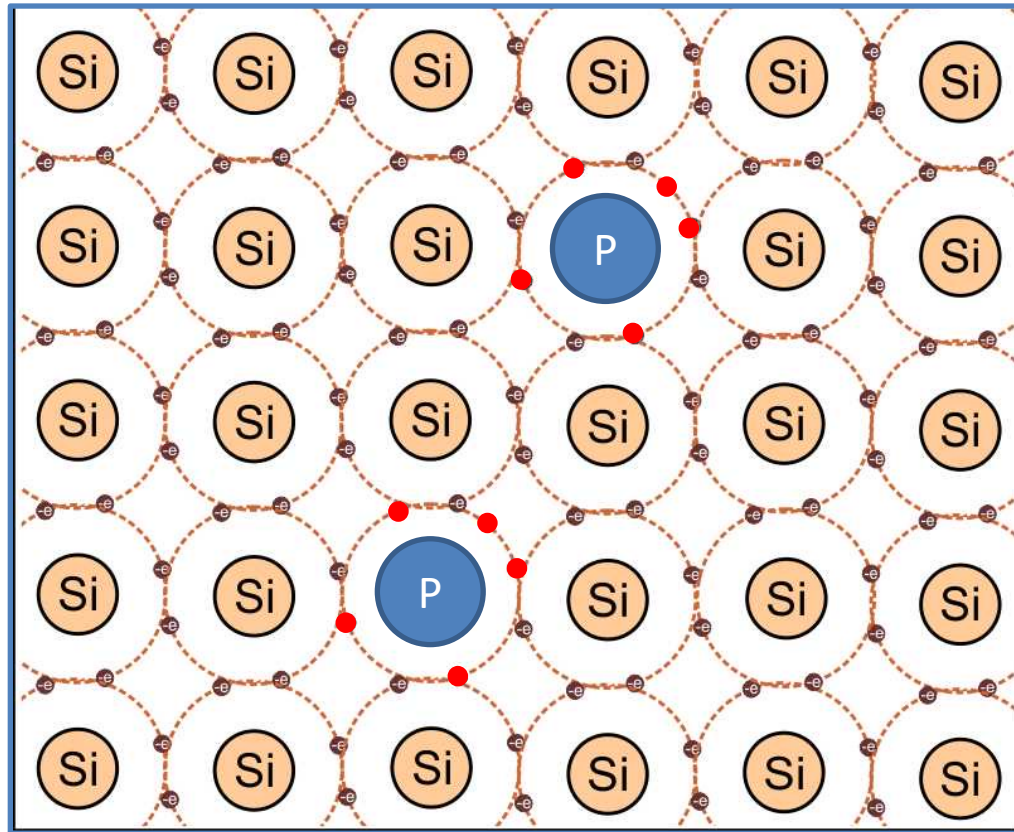
Acceptor-type or **p-type** doping (from the view of energy band)



3.2 Electrical Conduction in Solids

Donor-type or **n-type** doping (from the view of physical world)

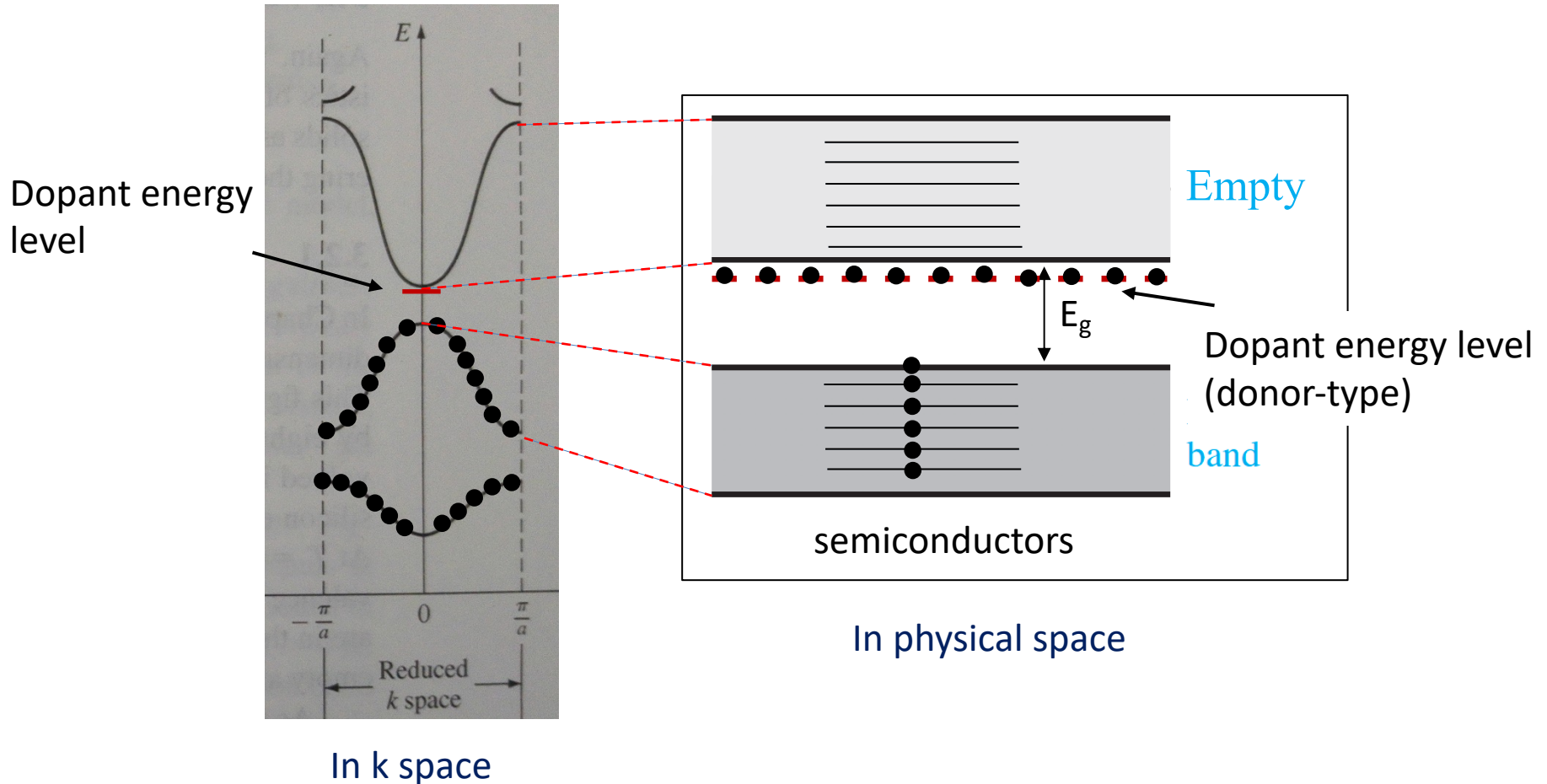
At 0K



Donor-type of dopants

3.2 Electrical Conduction in Solids

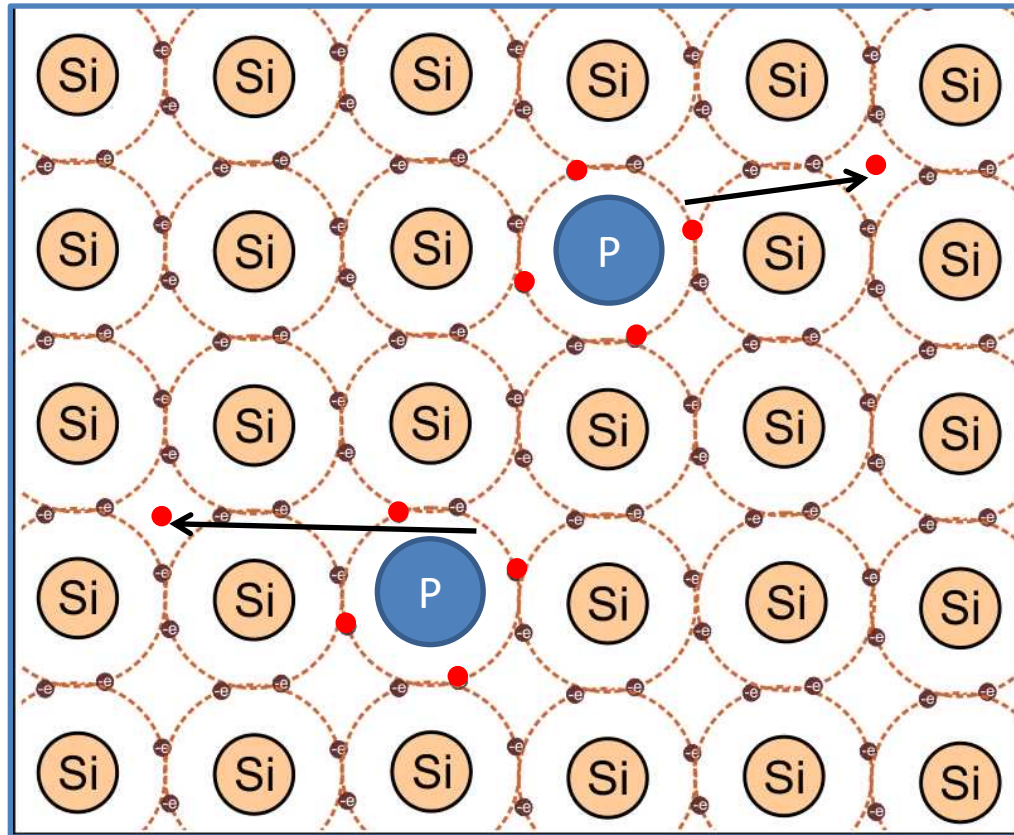
Donor-type or n-type doping (from the view of energy band)



3.2 Electrical Conduction in Solids

Donor-type or **n-type** doping (from the view of physical world)

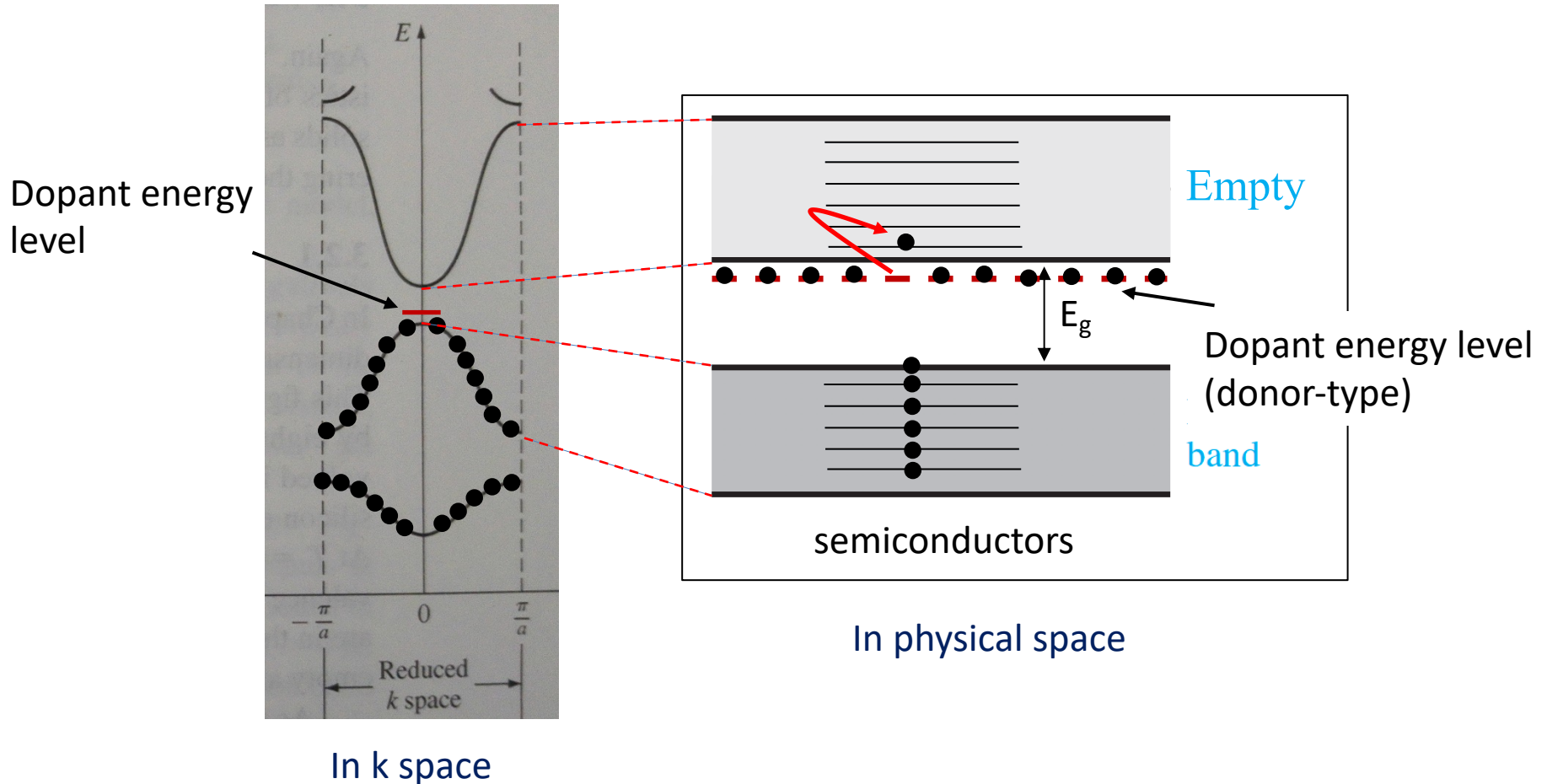
$> 0K$



Donor-type of dopants

3.2 Electrical Conduction in Solids

Donor-type or n-type doping (from the view of energy band)



3.2 Electrical Conduction in Solids

Doping in semiconductors

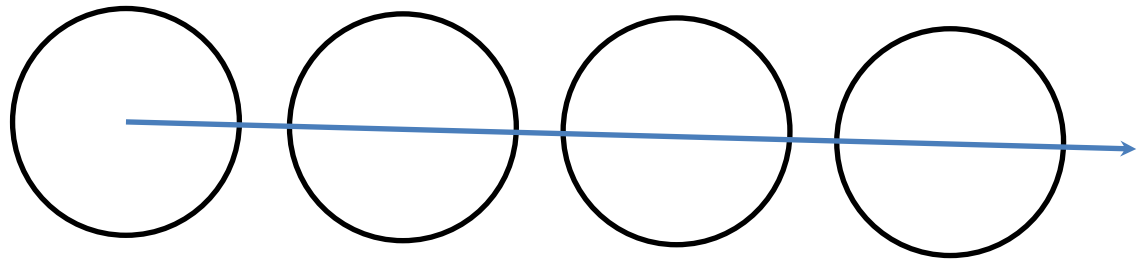
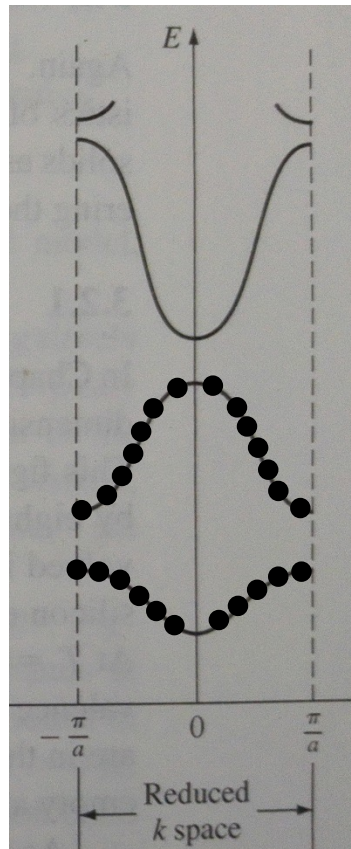
Si atomic concentration: $5 \times 10^{22} \text{ cm}^{-3}$

	Low concentration of doping	Medium concentration doping	High concentration of doping
Concentration (cm^{-3})	$< 10^{16}$	$10^{16} - 10^{18}$	$10^{18} - 10^{20}$
Relative concentration	1ppm	1 -100 ppm	100 ppm – 1%

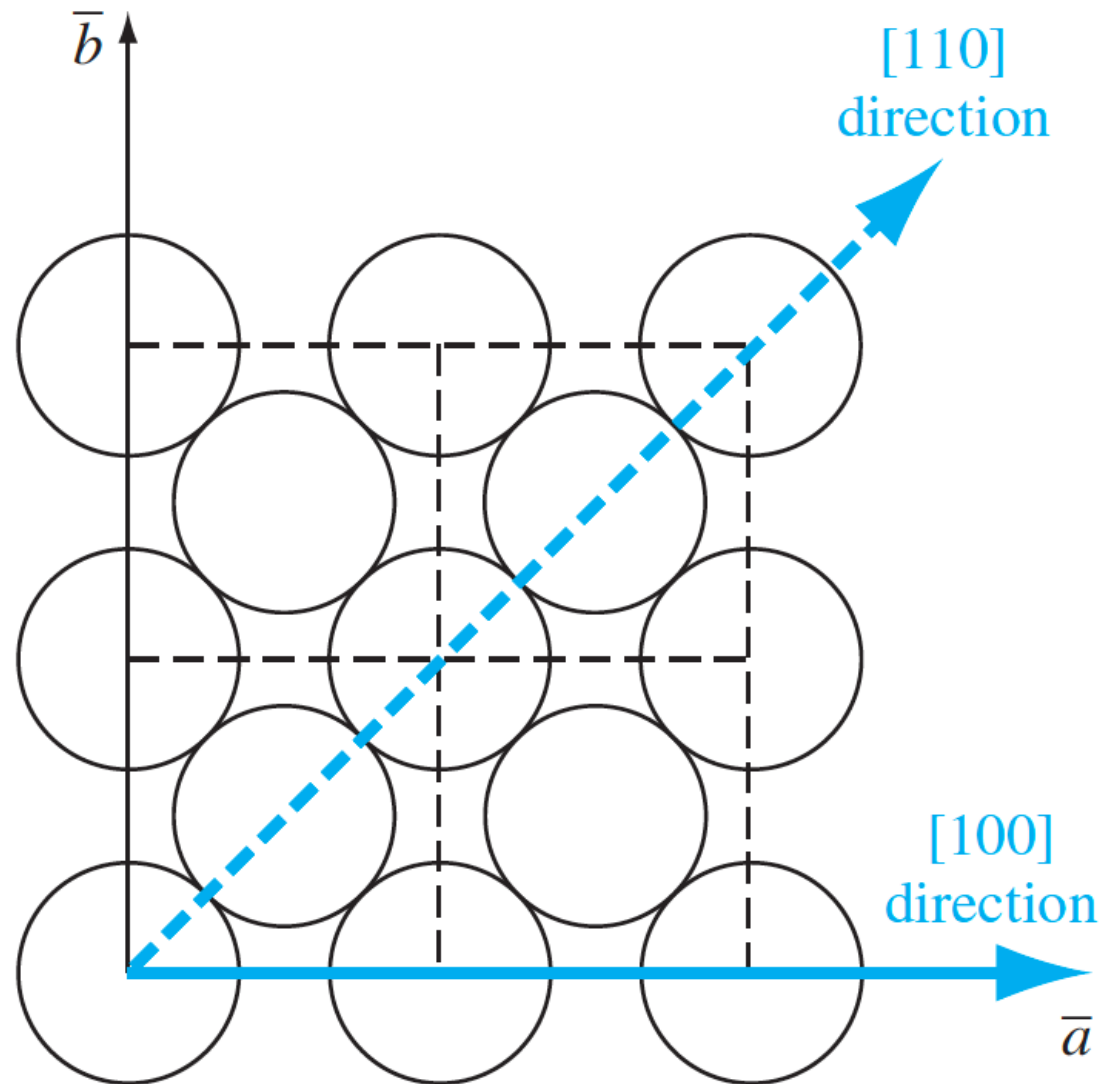
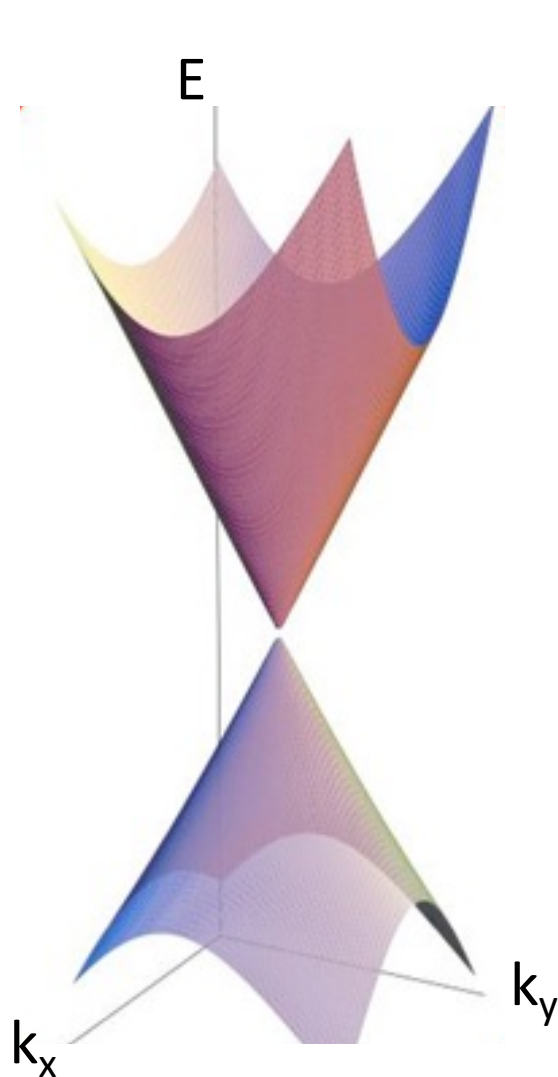
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- 3.5 Density of States Function
- 3.6 Statistical Mechanics

3.3 Extension to Three Dimensions

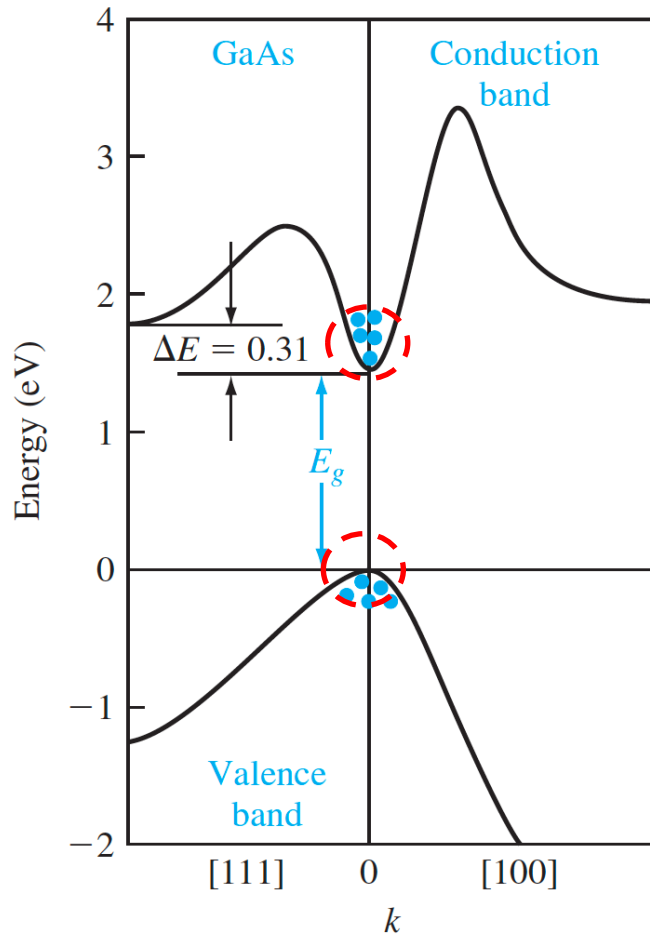


3.3 Extension to Three Dimensions



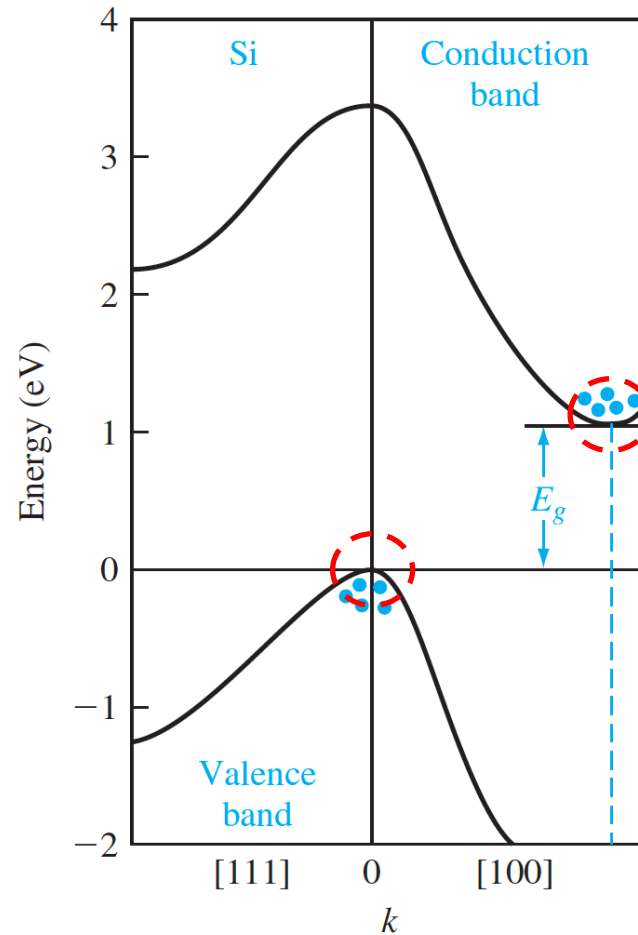
3.3 Extension to Three Dimensions

Direct bandgap



(a)

Indirect bandgap



(b)

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3.4 Effective Mass

- So far the energy band structure is theoretically calculated.
- How to experimentally find it?

3.4 Effective Mass

(1st time approximation)

Taylor series: $E(k) = E(k = k_0) + \frac{dE}{dk} \big|_{k=k_0} (k - k_0) + \frac{d^2E}{2dk^2} \big|_{k=k_0} (k - k_0)^2 + O((\Delta k)^3)$

These conditions are close to reality in most cases.

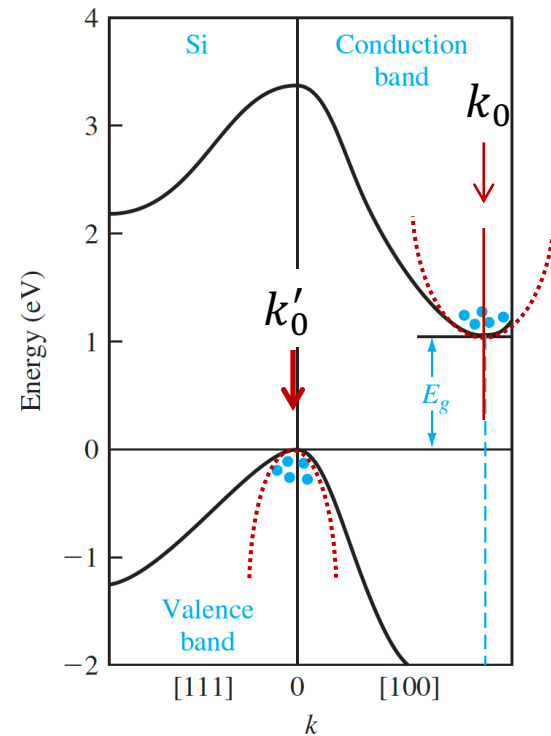
- 1) Number of electrons is negligibly small compared available states.
- 2) Electrons mostly located at the bottom of conduction band.

Conclusions

- a) High order terms $O((\Delta k)^3)$ can be ignored.
- b) $\frac{dE}{dk} \big|_{k=k_0} (k - k_0) = 0$ because the first order differential equals to zero at local minimum or local maximum.

Therefore, we have

$$E(k) = E(k = k_0) + \frac{d^2E}{2dk^2} \big|_{k=k_0} (k - k_0)^2$$



3.4 Effective Mass (For Electrons in the conduction band)

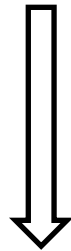
Electrons in free space have:

$$E_f(k) = \frac{\hbar^2 k^2}{2m} \Rightarrow \frac{d^2 E_f(k)}{dk^2} = \frac{\hbar^2}{m}$$

Electrons in crystalline semiconductors have:

$$E(k) = E(k = k_0) + \frac{d^2 E}{2dk^2} \Big|_{k=k_0} (k - k_0)^2$$

$$\frac{d^2 E}{dk^2} \Big|_{k_0} = \frac{\hbar^2}{m^*}$$



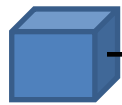
- m^* has a unit of mass
- We call it the effective mass of electrons in the crystal

$$E(k) = E(k = k_0) + \frac{\hbar^2}{2m^*} (k - k_0)^2$$

3.4 Effective Mass

- How to understand effective mass

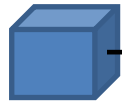
Example: use Newton's law to find mass of an object



$$m = \frac{F}{a}$$

$$a = \frac{d^2x}{dt^2}$$

In the air

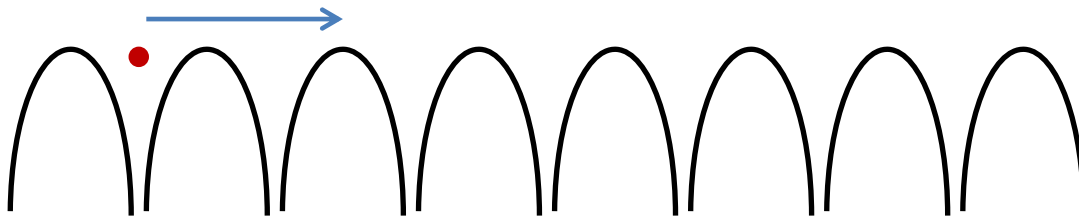


$$m^* = \frac{F}{a}$$

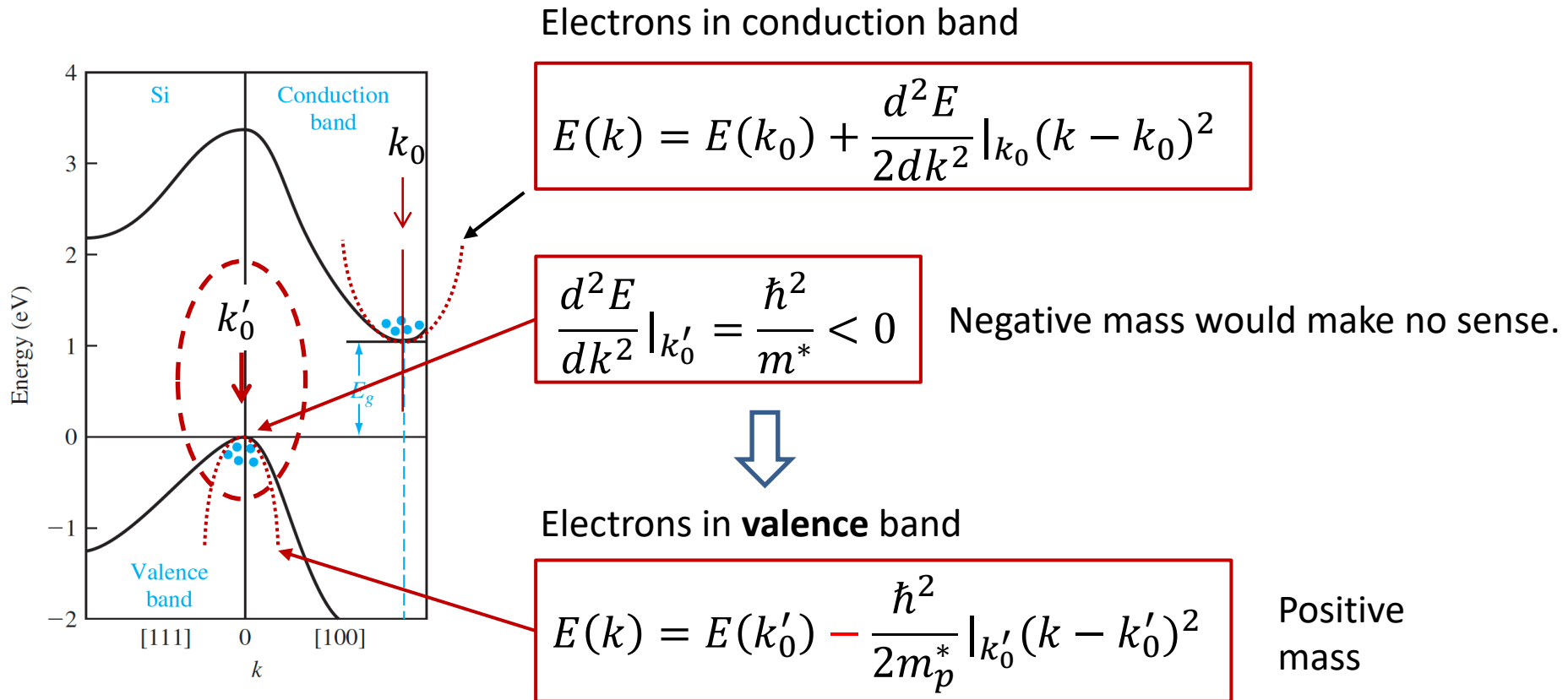
$$a = \frac{d^2x}{dt^2}$$

In the water

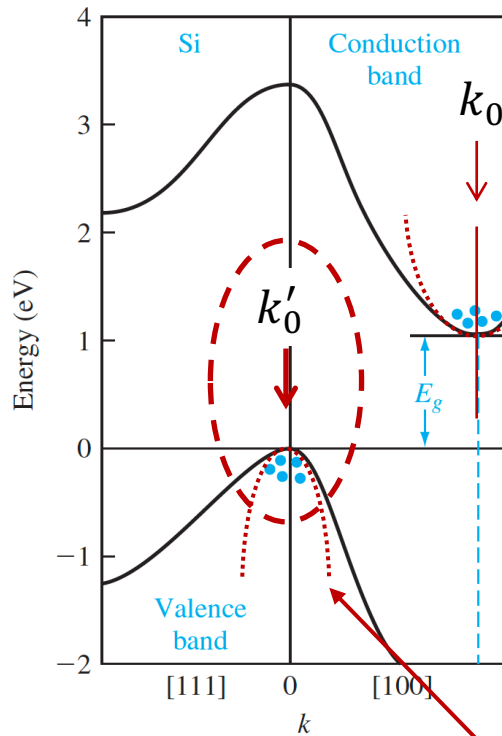
Modulated by Electric potential of ions



3.4 Effective Mass (For Electrons in the valence band)



3.4 Effective Mass (A new particle defined: holes)



Electrons in **conduction** band

$$E(k) = E(k_0) + \frac{\hbar^2}{2m_n^*} |k_0| (k - k_0)^2$$

Positive mass

- Equivalent to a positive charge carrier
- Different effective mass
- Electrons and holes can come from dopants separately

Holes in **valence** band

$$E(k) = E(k'_0) - \frac{\hbar^2}{2m_p^*} |k'_0| (k - k'_0)^2$$

Positive mass

3.4 Effective Mass

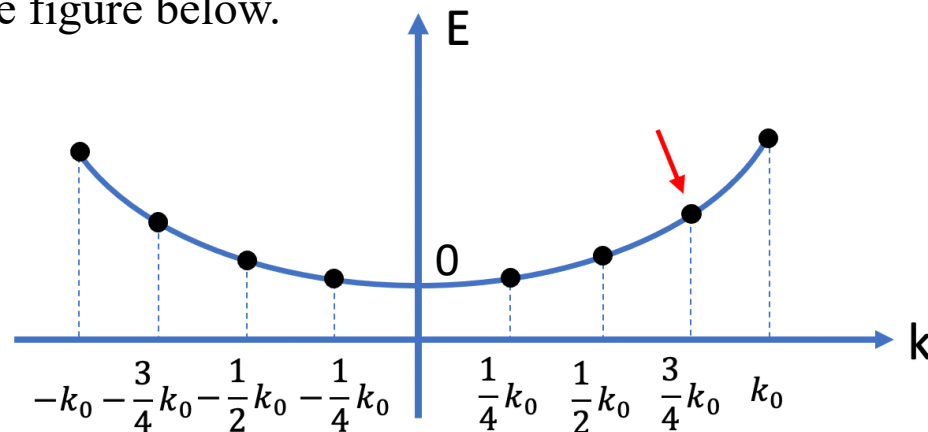
Effective mass can be experimentally measured

	Symbol	Germanium	Silicon	Gallium Arsenide
Bandgap	E_g (eV)	0.66	1.12	1.424
Electrons	m_e^*/m_0	0.55	1.08	0.067
Holes	m_h^*/m_0	0.37	0.56	0.48

It means that energy band structure can be experimentally found.
(at least near conduction band bottom and valence band top)

Problem Example #1

1. In an infinite quantum well, the wavenumber k and energy E is quantized as shown in Figure 1. Please answer the following questions:
 - a) Write the static wavefunction of the dot ($k = \frac{3}{4}k_0$) that the red arrow is pointing to. Find the wavelength of this wavefunction.
 - b) If all the states are filled with electrons, how many electrons can be filled in the figure below? The electron spin is not considered.
 - c) If the effective mass of this quantum system is m_n^* , can this system allow an electron to have a quantized energy of $\frac{\hbar^2 k_0^2}{9m_n^*}$? If yes, mark the state of this electron in the figure below. How about a quantized energy of $\frac{\hbar^2 k_0^2}{8m_n^*}$? If yes, mark the state of this electron in the figure below.



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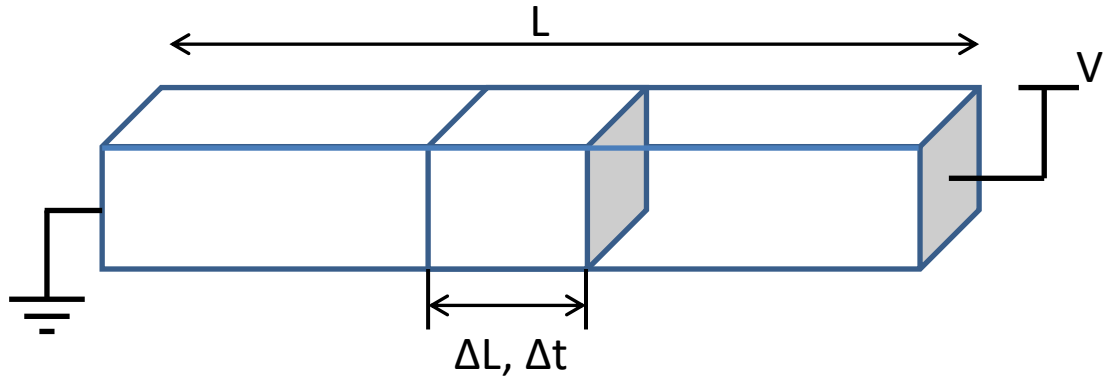
3.5 Density of States Function

n type semiconductor

$$I = \frac{\Delta Q}{\Delta t} = \frac{nqA_c\Delta L}{\Delta t} = nqA_cv$$

$$v = \mu E = \mu V/L$$

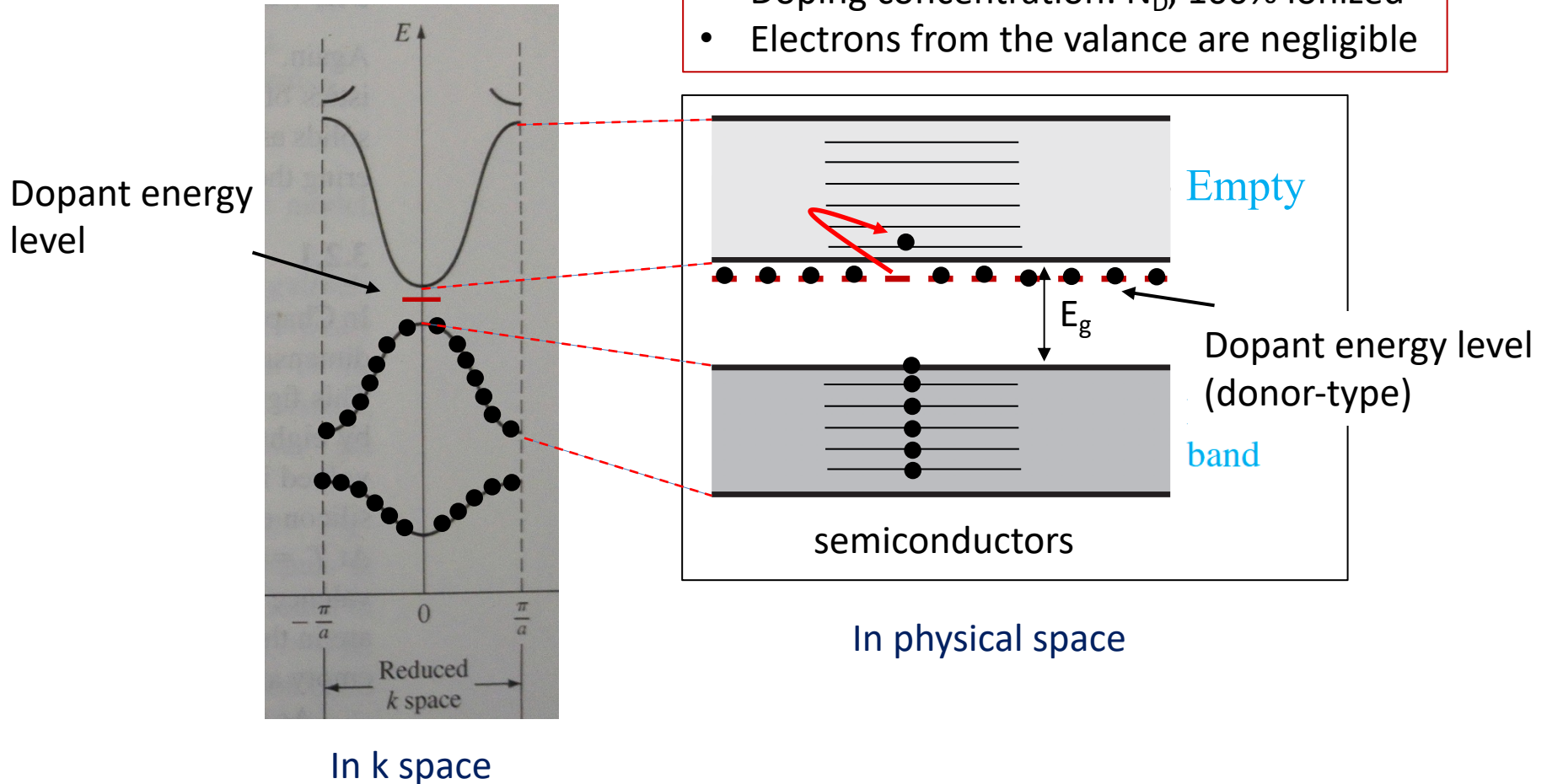
$$I = \frac{\Delta Q}{\Delta t} = \frac{nqA_c\Delta L}{\Delta t} = nqA_c\mu V/L \quad \Rightarrow \quad \sigma = \frac{I}{V} = \frac{nqA_c\mu}{L}$$



3.2 Electrical Conduction in Solids

Donor-type or n-type doping (from the view of energy band)

- Doping concentration: N_D , 100% ionized
- Electrons from the valance are negligible



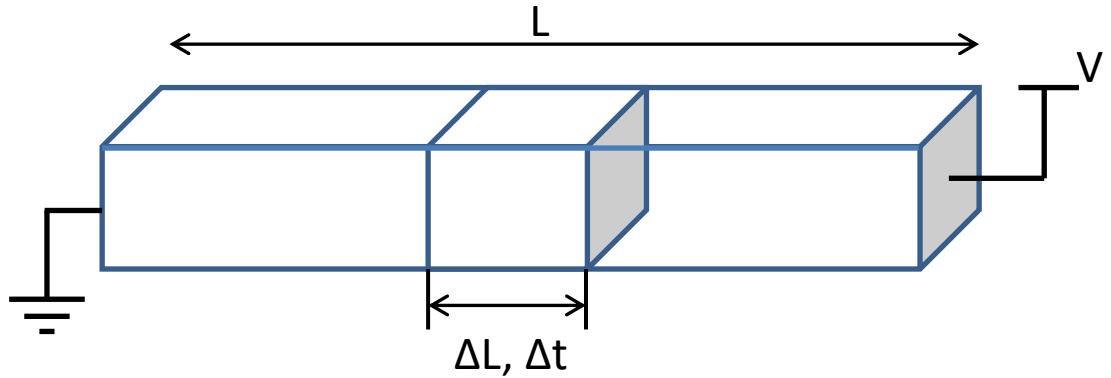
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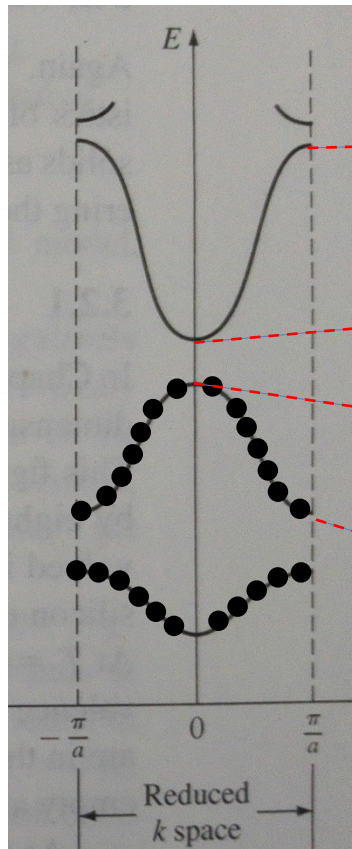
$$v = \mu E = \mu V/L$$

$$I = \frac{\Delta Q}{\Delta t} = \frac{nqA_c\Delta L}{\Delta t} = nqA_c\mu V/L \quad \Rightarrow \quad \sigma = \frac{I}{V} = \frac{N_D q A_c \mu}{L}$$



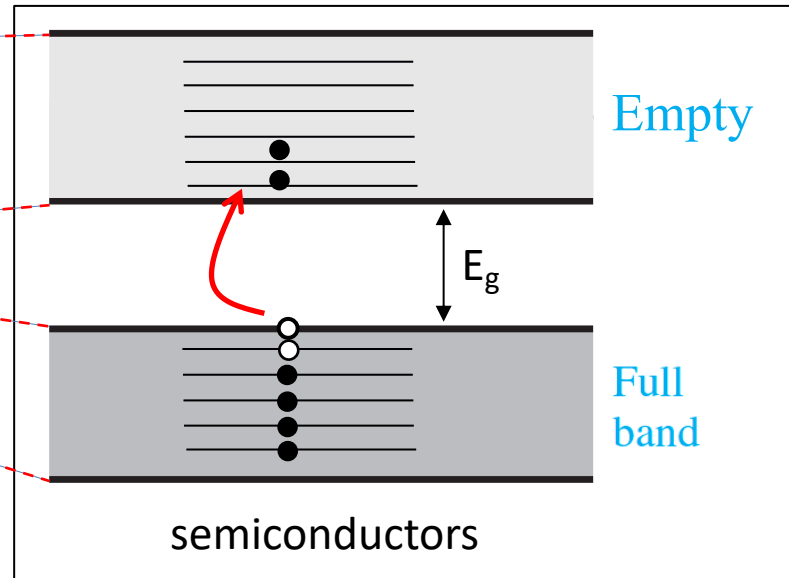
3.2 Electrical Conduction in Solids

If the semiconductor is intrinsic:



In k space

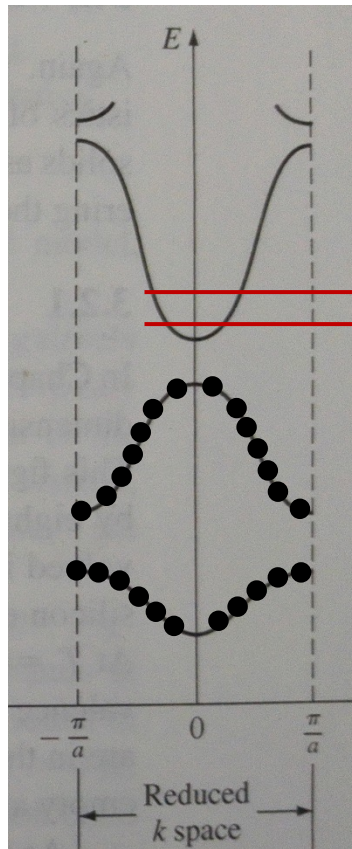
How many number of electrons in the conductance band per unit volume?



In physical space

3.2 Electrical Conduction in Solids

If the semiconductor is intrinsic:



How many number of electrons in the conduction band per unit volume?

Only if we know:

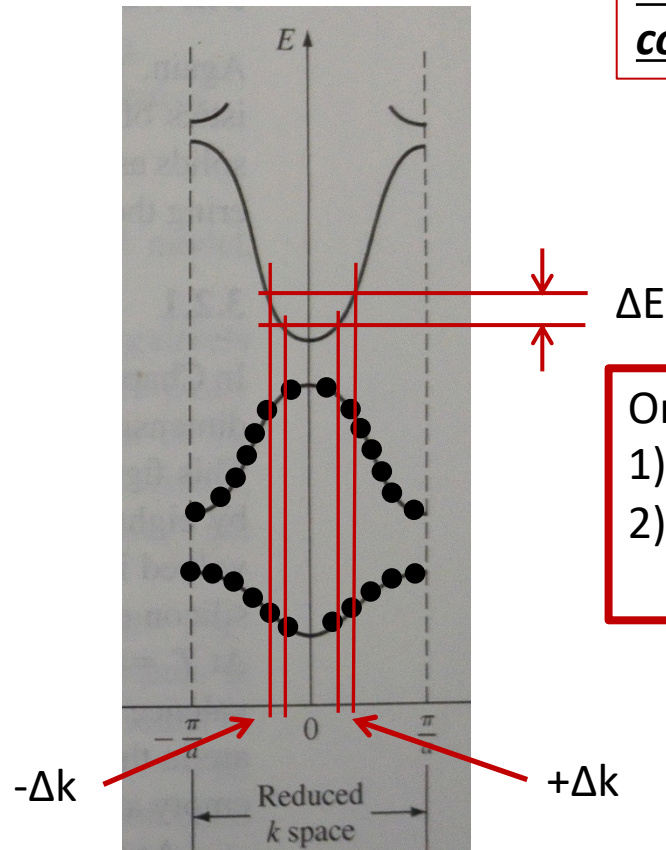
- 1) How many number of states in ΔE
- 2) Probability of each state is occupied by an electron

In k space

3.2 Electrical Conduction in Solids

If the semiconductor is intrinsic:

How many number of electrons in the conduction band per unit volume?



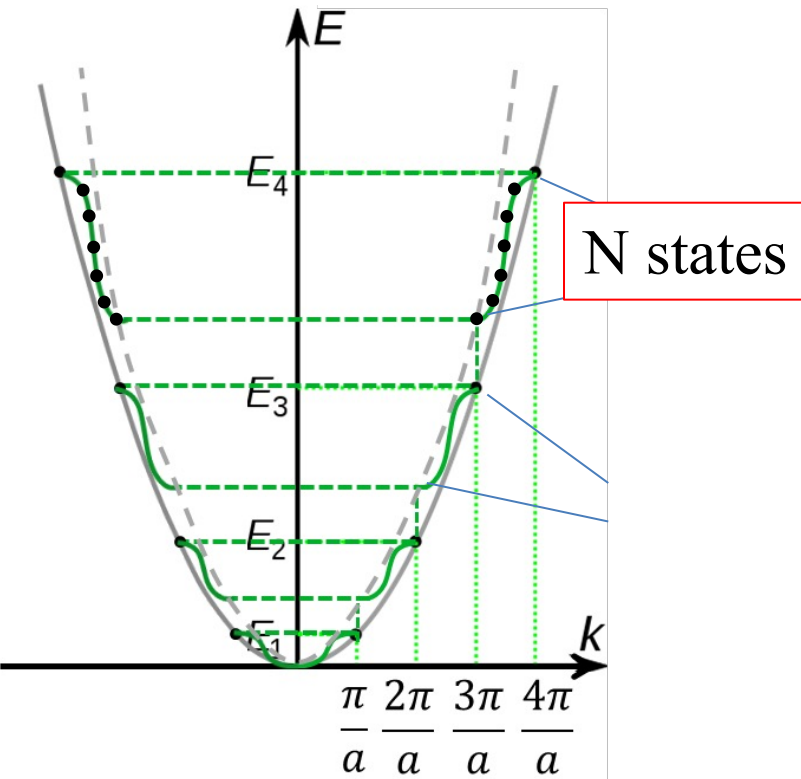
Only if we know:

- 1) How many number of states (k 's) in ΔE
- 2) Probability of each state is occupied by an electron

In k space

3.1 Allowed and Forbidden Energy Bands

Forming energy bands: analytical



The total number of states in the whole crystal within $(0, \pi/a)$: N



The "density" of states in the whole crystal within $(0, \pi/a)$: $\frac{N}{\pi/a}$



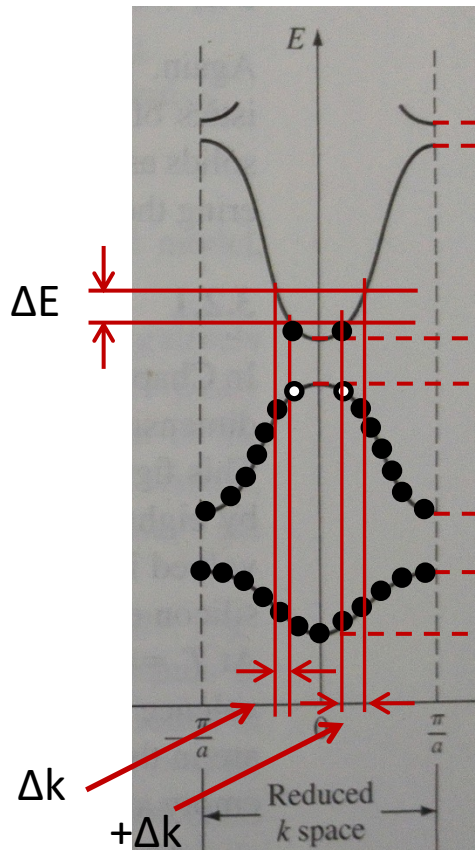
The number of states of the whole crystal within Δk : $\frac{N}{\pi/a} \times \Delta k$



The number of states **per unit volume** within Δk : $\frac{N}{\pi/a} \times \Delta k \frac{1}{Na} = \frac{\Delta k}{\pi}$

3.5 Density of States Function

One-dimensional



In k space

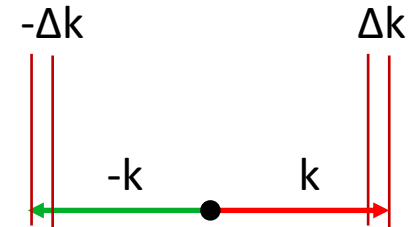
$$E = E(k) = E_c + \frac{\hbar^2}{2m_n^*} k^2$$

$$k = \mp \frac{\sqrt{2m_n^*(E - E_c)}}{\hbar}$$

Within ΔE , we have the number of k 's is $\frac{d(2|k|/\pi)}{dE} \Delta E$

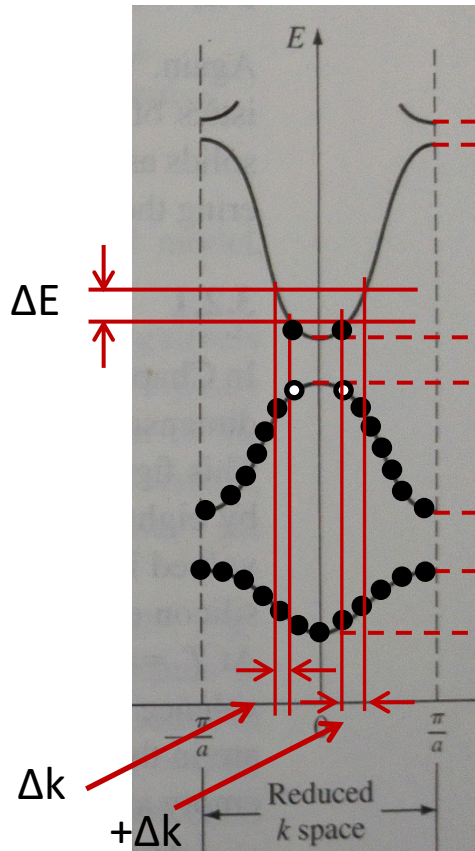
$$g(E) = \frac{1}{2} \frac{d(2|k|/\pi)}{dE}$$

One electron has two k 's, i.e. $+k$ and $-k$.



3.5 Density of States Function

Two-dimensional



In k space

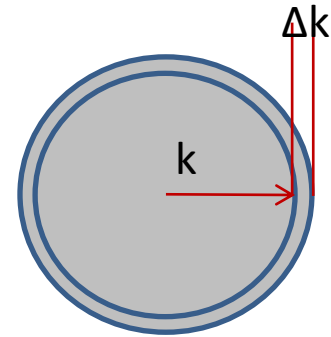
$$E = E(k) = E_c + \frac{\hbar^2}{2m_n^*} k^2$$

$$k = \mp \frac{\sqrt{2m_n^*(E - E_c)}}{\hbar}$$

Within ΔE , we have the number of k is $\frac{d(\pi(k/\pi)^2)}{dE} \Delta E$

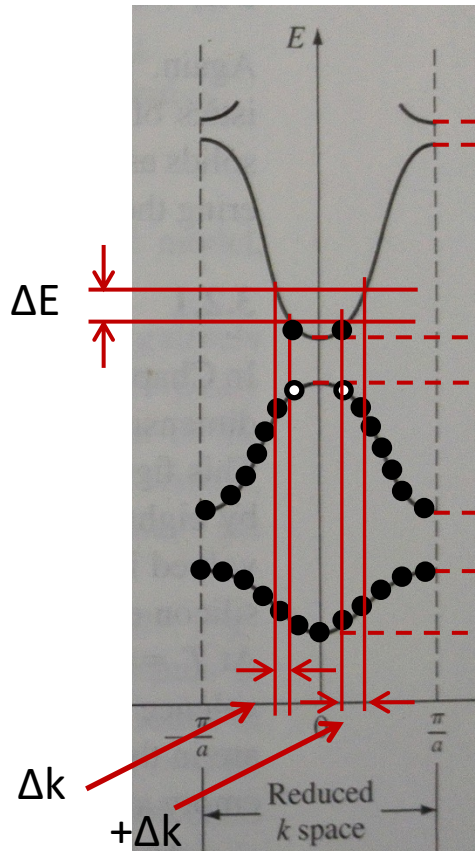
$$g(E) = \frac{1}{4} \frac{d(\pi(k/\pi)^2)}{dE}$$

One electron has four k 's, i.e. $+k_x$ and $-k_x$, $+k_y$ and $-k_y$.



3.5 Density of States Function

Three-dimensional



In k space

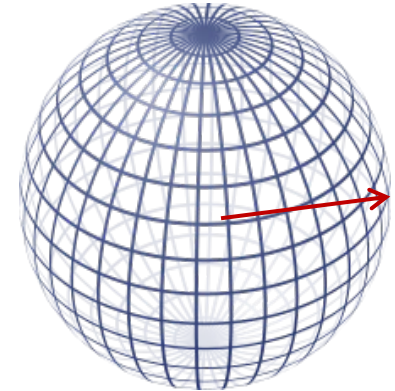
$$E = E(k) = E_c + \frac{\hbar^2}{2m_n^*} k^2$$

$$k = \mp \frac{\sqrt{2m_n^*(E - E_c)}}{\hbar}$$

Within ΔE , we have the number of k is $\frac{d(4\pi(\frac{k}{\pi})^3/3)}{dE} \Delta E$

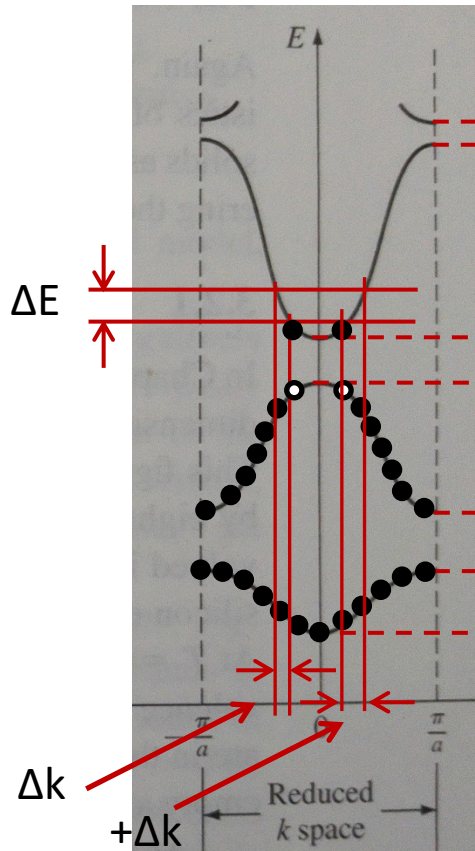
$$g(E) = \frac{1}{8} \frac{d(4\pi(\frac{k}{\pi})^3/3)}{dE}$$

+ k_x and - k_x
One electron has eight k 's, i.e. + k_y and - k_y
+ k_z and - k_z



3.5 Density of States Function

Three-dimensional



$$g(E) = \frac{dV_k}{dE} = \overset{\text{spin}}{\downarrow} \underset{2}{\text{red}} \frac{2\pi(2m^*)^{3/2}}{h^3} \sqrt{E - E_c}$$

The concept of electron spin was developed later, which is out of the scope of Schrodinger Equation.

3.5 Density of States Function

Problem Example #2

Determine the number of quantum states (per unit volume) in silicon between $(E_v - kT)$ and E_v at 300K.

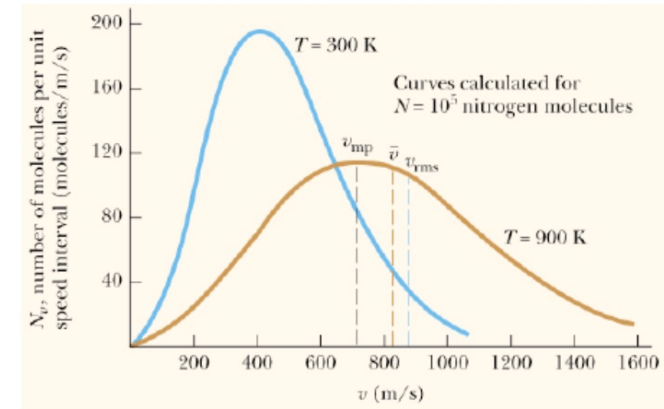
Outline

- 3.1 Allowed and Forbidden Energy Bands
- 3.2 Electrical Conduction in Solids
- 3.3 Extension to Three Dimensions
- 3.4 Effective Mass
- 3.5 Density of States Function
- **3.6 Statistical Mechanics**

3.6 Statistical mechanics

Maxwell-Boltzmann probability function:

- distinguishable
- no limit on the particle number in each state
- Example: gas molecules in a container



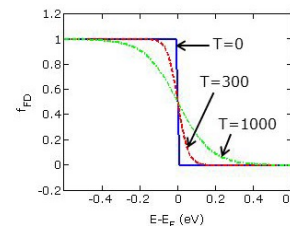
Bose-Einstein probability function:

- indistinguishable,
- no limit on the particle number in each state
- Example: photons

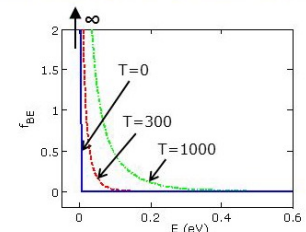
Fermi-Dirac probability function:

- indistinguishable
- one particle limit in each state
- Example: electrons in solids

Fermi-Dirac vs. Bose-Einstein Statistics



$$f_{FD}(E) = \frac{1}{\exp\left(\frac{E - E_F}{k_B T}\right) + 1}$$

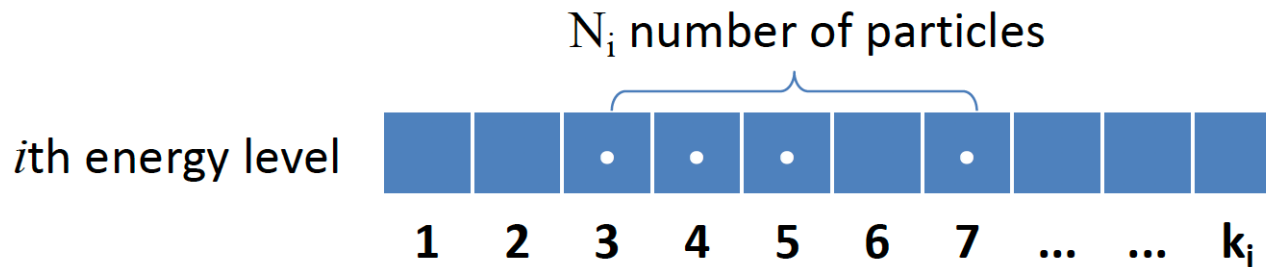


$$f_{BE}(E) = \frac{1}{\exp\left(\frac{E}{k_B T}\right) - 1}$$

3.6 Statistical mechanics

Fermi-Dirac probability function:

- indistinguishable
- one particle limit in each state
- Example: electrons in solids



The total number of ways of arranging N_i particles in each i th energy level

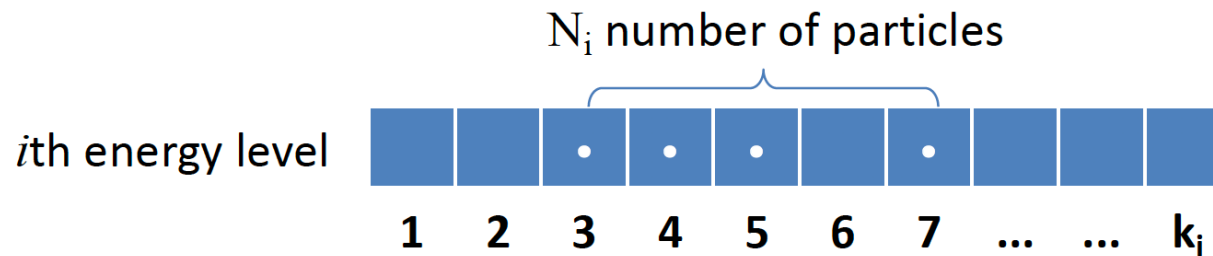
$$k_i(k_i - 1) \cdots (k_i - (N_i - 1)) = \frac{k_i!}{(k_i - N_i)!}$$

(Particles are distinguishable)

3.6 Statistical mechanics

Fermi-Dirac probability function:

- indistinguishable
- one particle limit in each state
- Example: electrons in solids



The total number of ways of arranging N_i indistinguishable particles in each i th energy level

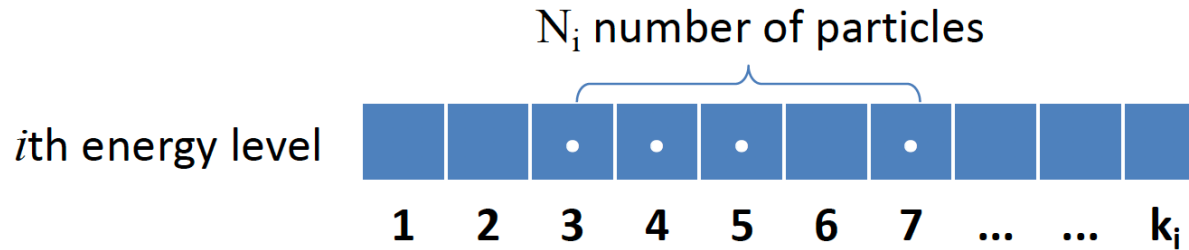
$$W_i = \frac{k_i!}{N_i!(k_i - N_i)!}$$

(Particles are indistinguishable)

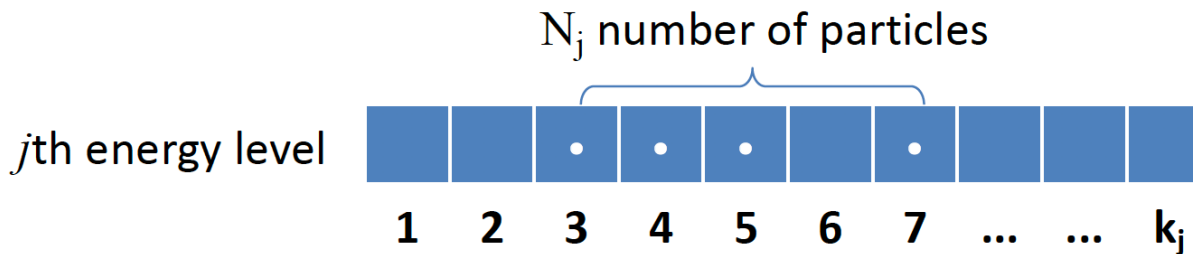
3.6 Statistical mechanics

Fermi-Dirac probability function:

- indistinguishable
- one particle limit in each state
- Example: electrons in solids



$$W_i = \frac{k_i!}{N_i!(k_i - N_i)!}$$



$$W_j = \frac{k_j!}{N_j!(k_j - N_j)!}$$

⋮

⋮

3.6 Statistical mechanics

For a given total number (N) of particles, the total number of ways of arranging indistinguishable particles among n energy levels is

$$W = \prod_{i=1}^n \frac{k_i!}{N_i!(k_i - N_i)!}$$

$f_F(E)$

The highest probable distribution at following given constraints:

$$N = \sum_{i=1}^n N_i \quad \text{constant}$$

$$E_{total} = \sum_{i=1}^n E_i N_i \quad \text{constant}$$

3.6 Statistical mechanics

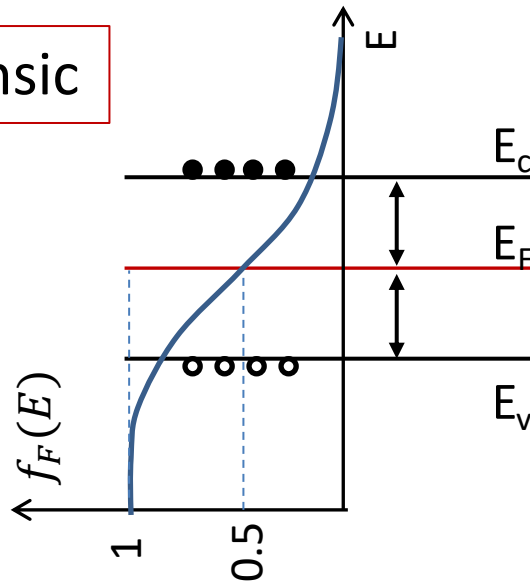
The probability of a state at energy E being occupied by an electron:

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

E is the energy level; E_F is the Fermi energy level; k is the Boltzmann constant; T is the absolute temperature.

3.6 Fermi distribution and Fermi level

Intrinsic



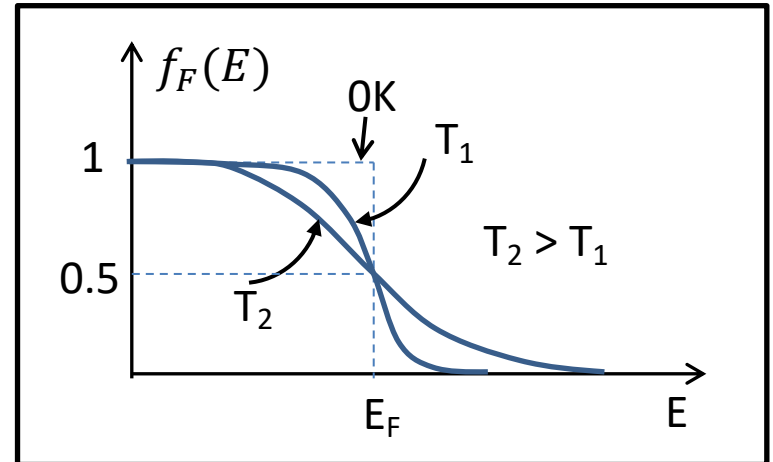
Probability of a state at E_c occupied

||

Probability of a state at E_v unoccupied

Physical meaning of Fermi energy level:

At equilibrium, when an electron is added to the system, the change of the system energy



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

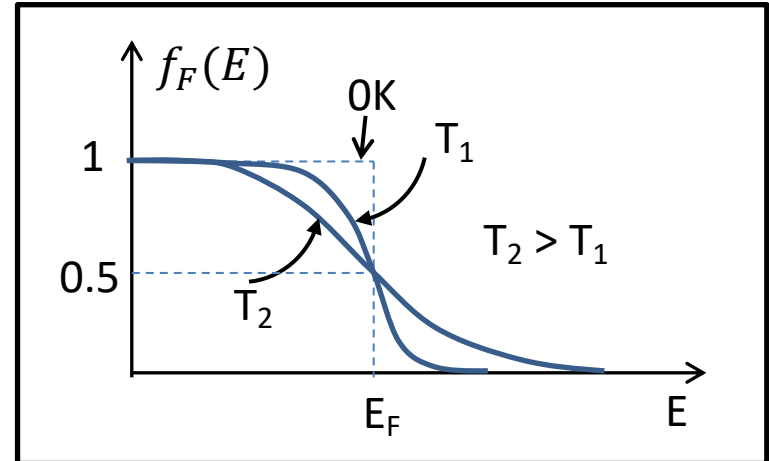
3.6 Boltzmann distribution

when $\exp\left(\frac{E - E_F}{kT}\right) \gg 1 \Rightarrow E - E_F > 3kT$

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

$$f_F(E) \approx \exp\left(-\frac{E - E_F}{kT}\right)$$

Boltzmann distribution



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

3.6 Boltzmann distribution

Problem Example #3

Assume that the Fermi energy level is 0.35eV above the valence band energy. Let $T=300\text{K}$. Determine the probability of a state being empty of an electron at $E = E_v - kT/2$.