VE320 – Summer 2022

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
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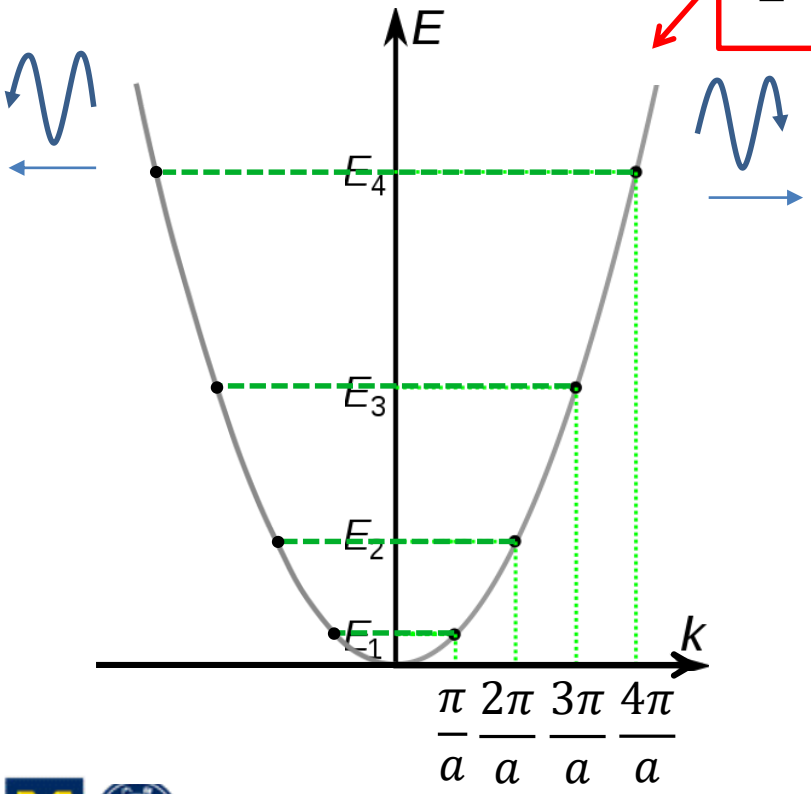
- 3.5 Density of States Function
- 3.6 Statistical Mechanics

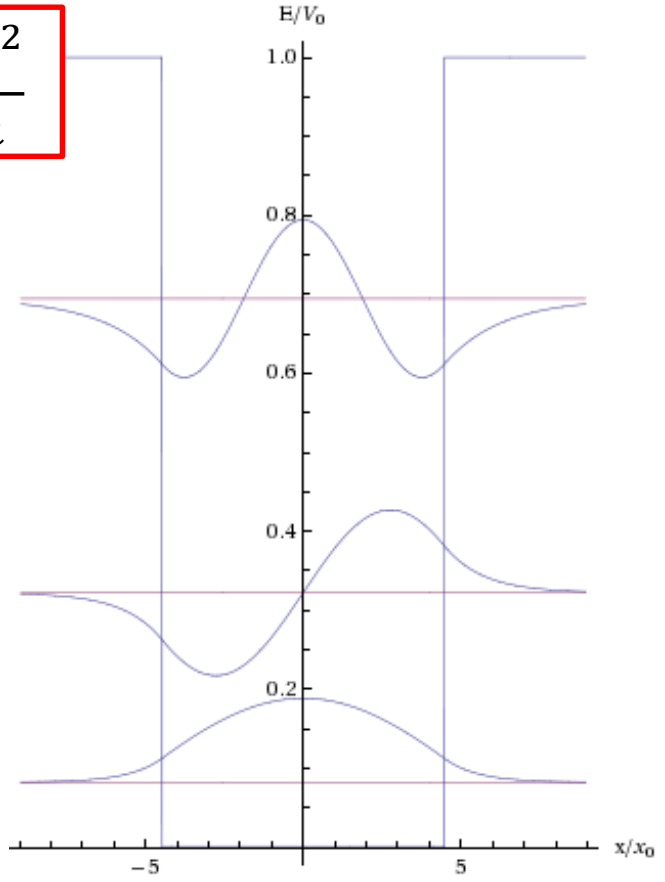
3.1 Allowed and Forbidden Energy Bands

Forming energy bands: analytical

Previously: Electrons in Finite Quantum Well

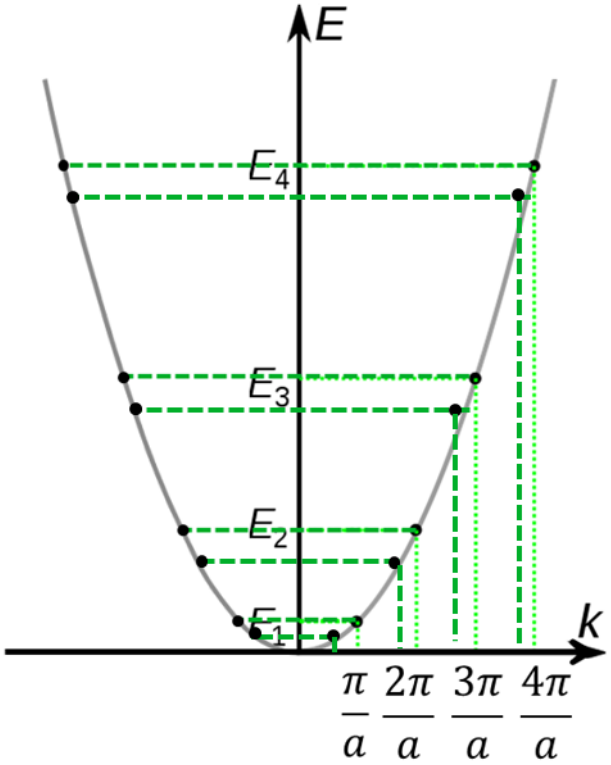
$$E = \frac{k^2\hbar^2}{2m}$$

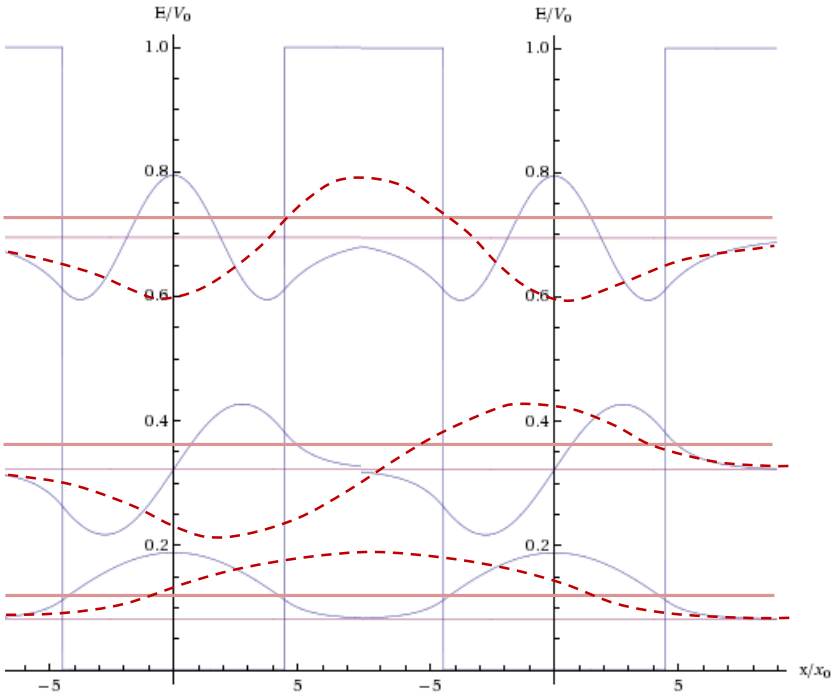




3.1 Allowed and Forbidden Energy Bands

Forming energy bands: analytical

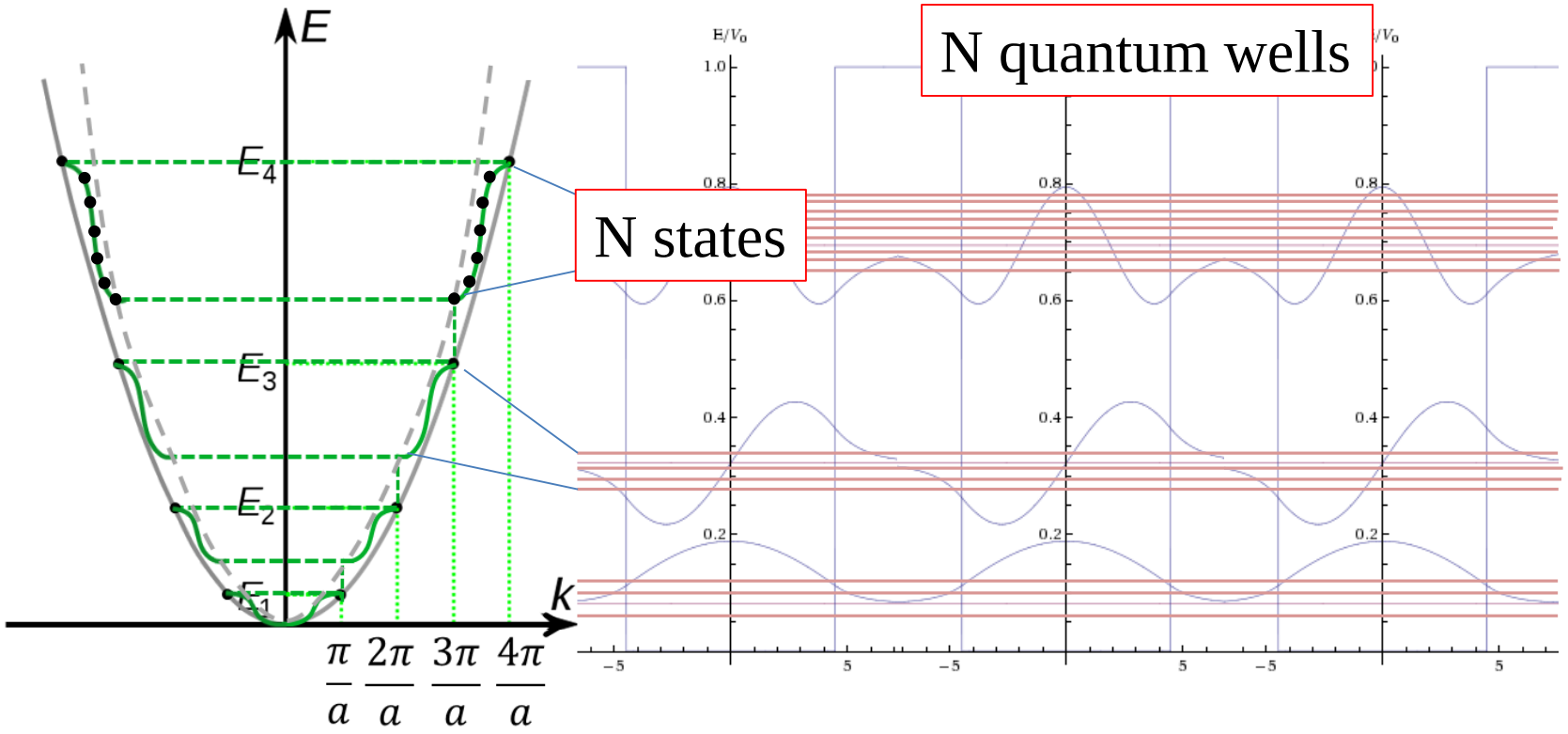




2 quantum wells

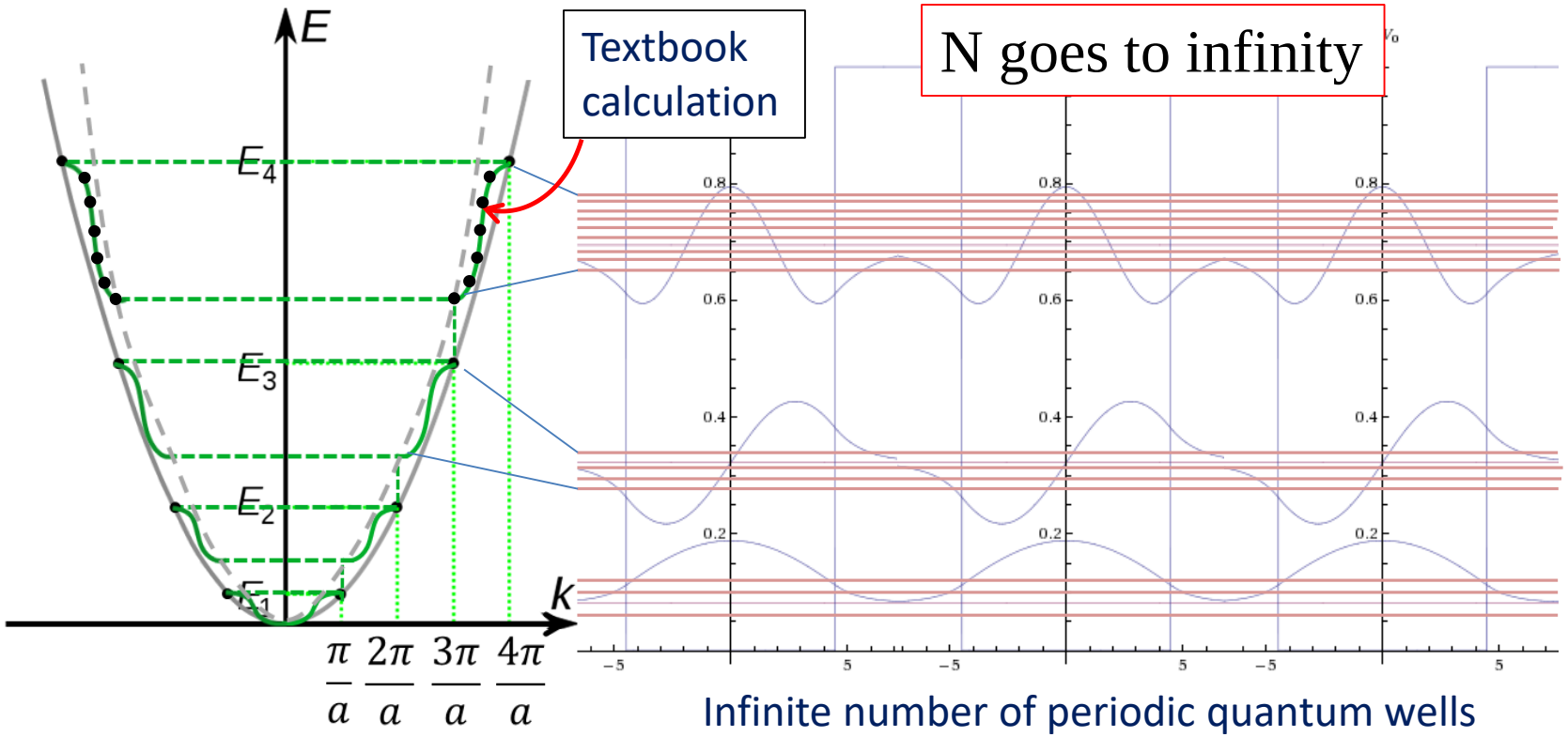
3.1 Allowed and Forbidden Energy Bands

Forming energy bands: analytical



3.1 Allowed and Forbidden Energy Bands

Forming energy bands: analytical

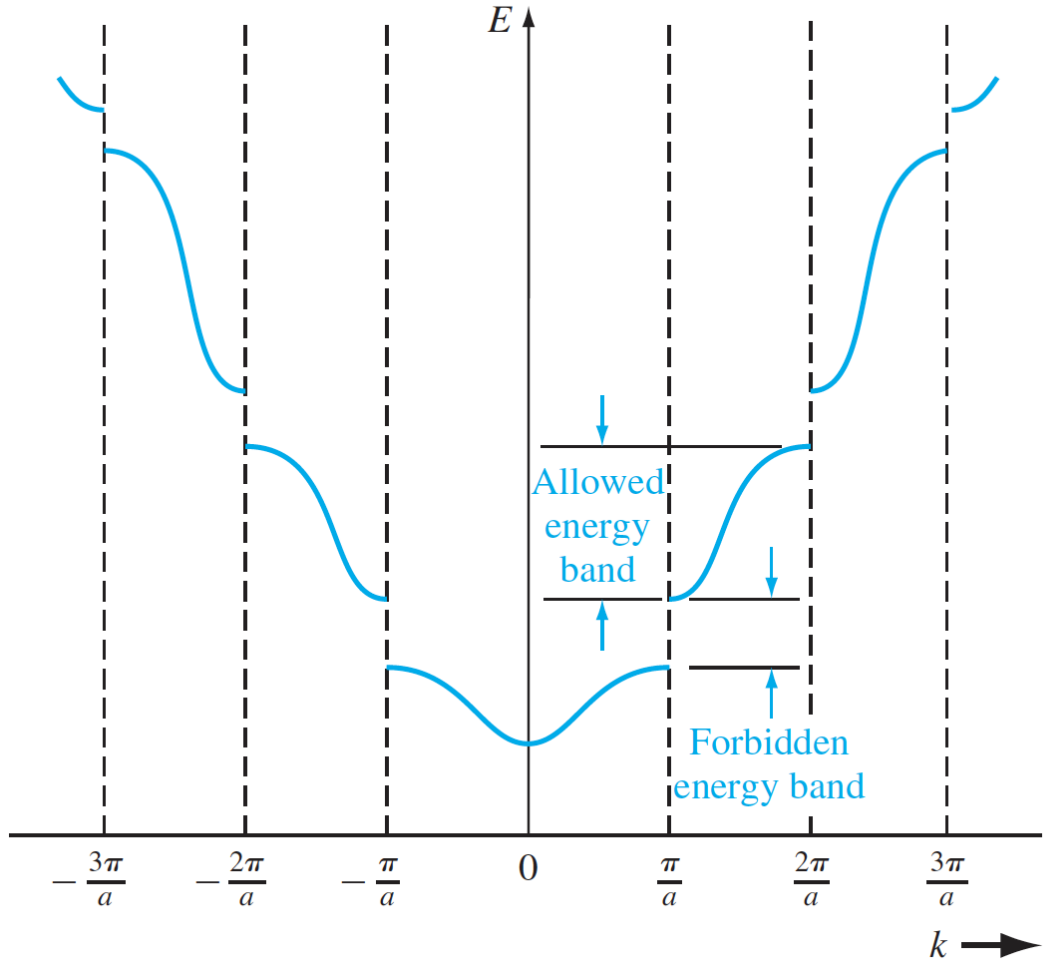


$$\frac{mV_0ba}{\hbar^2}\frac{sin(\alpha a)}{\alpha a} + \cos(\alpha a) = \cos(ka)$$

On P.67
eq.(3.22)

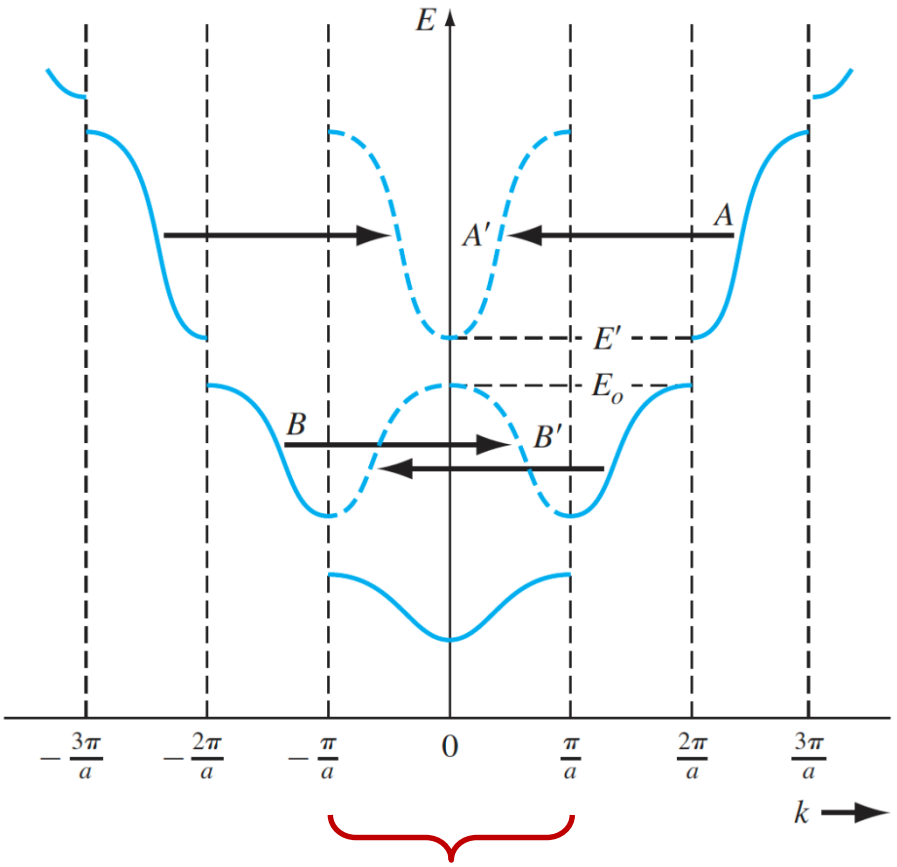
3.1 Allowed and Forbidden Energy Bands

Forming energy bands: analytical

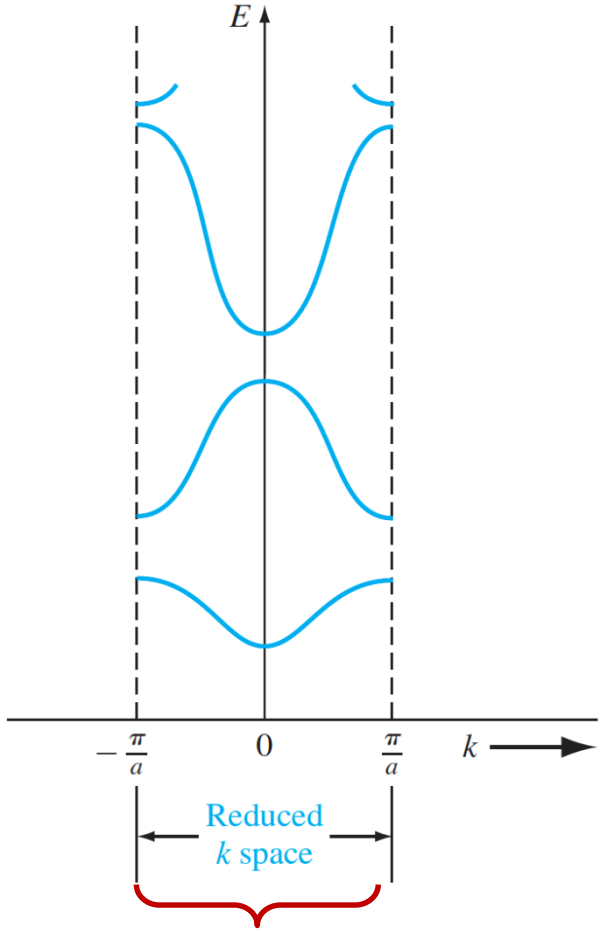


3.1 Allowed and Forbidden Energy Bands

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



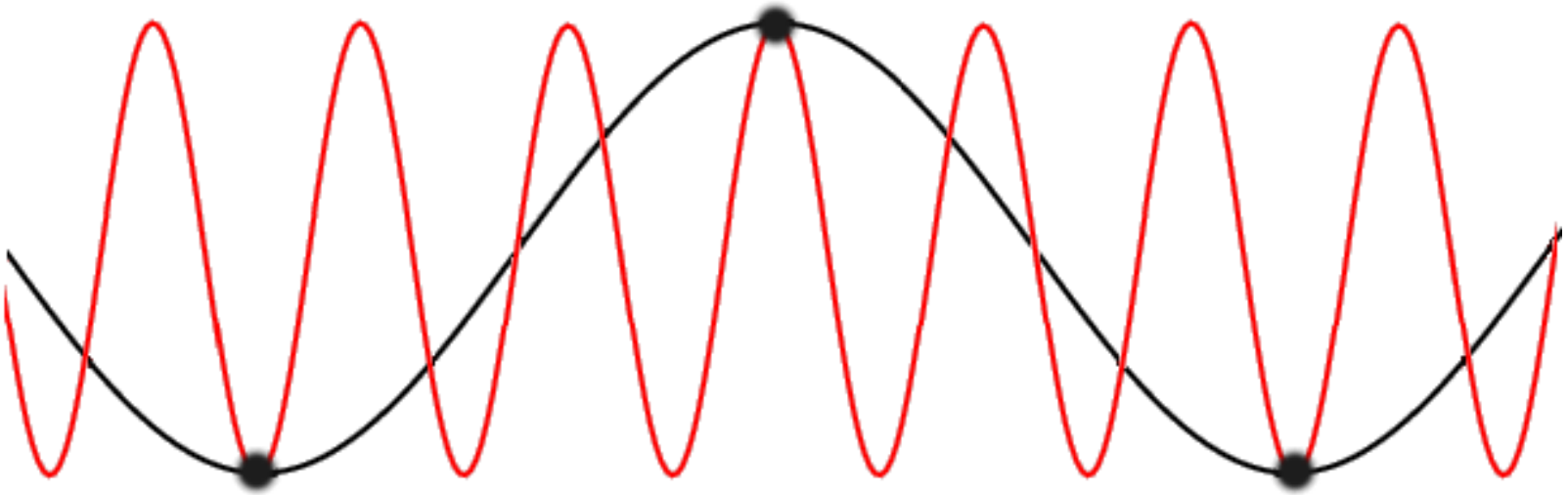
1st Brillouis zone



1st Brillouis zone

3.1 Allowed and Forbidden Energy Bands

- Black wave with a smaller k (longer wavelength) is in the 1st Brillouis zone.
- Red wave with a larger k (short wavelength) is outside of 1st Brillouis zene.
- 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

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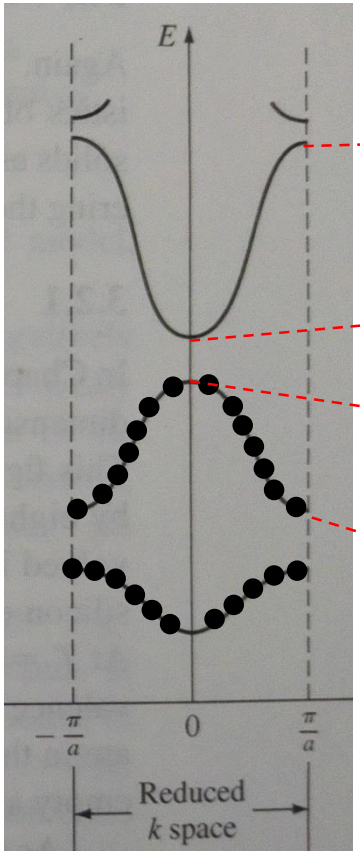
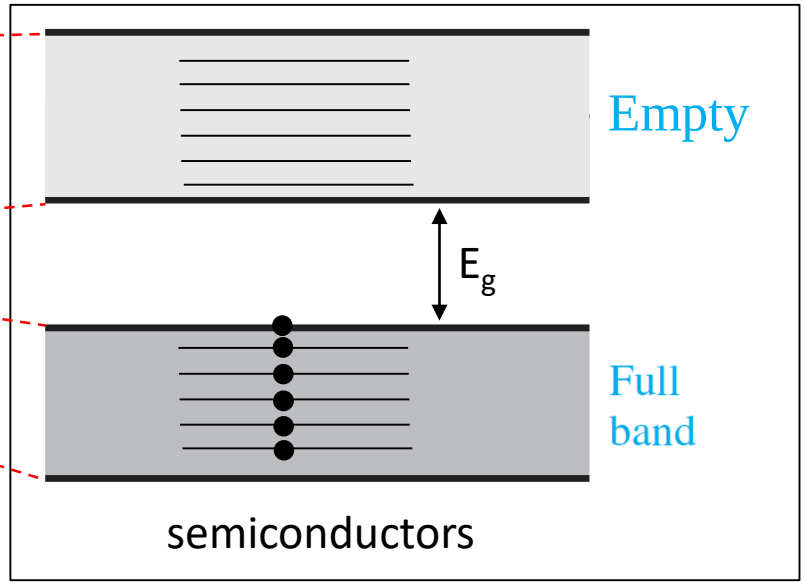
3.2 Electrical Conduction in Solids

Energy band of semiconductors



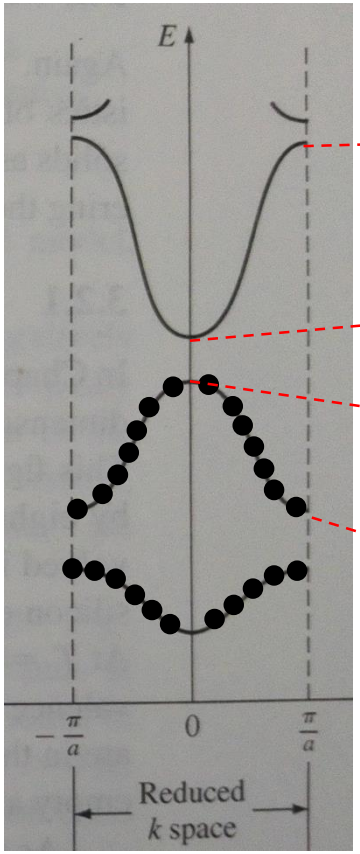
In k space



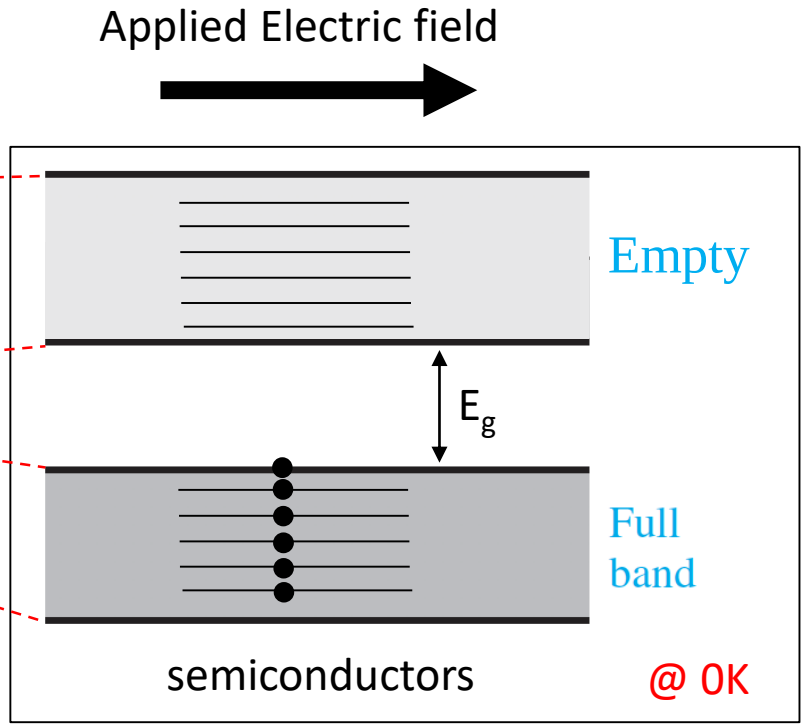
In physical space

3.2 Electrical Conduction in Solids

Energy band of semiconductors



In k space

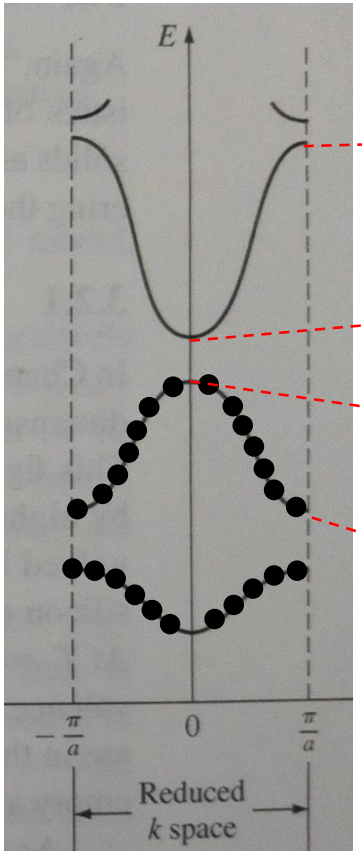


In physical space

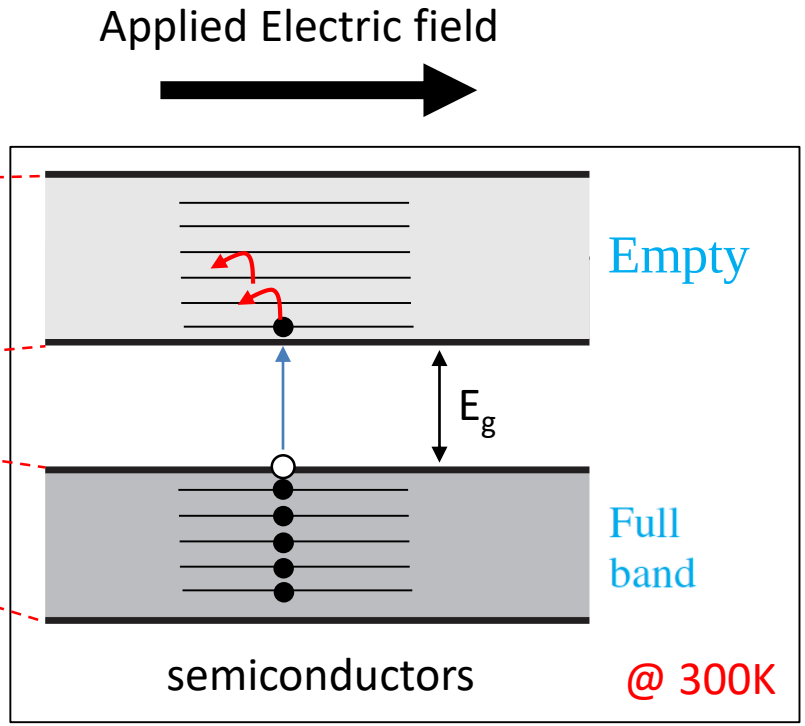
No electrical energy can be received by electrons in valence band

3.2 Electrical Conduction in Solids

Energy band of semiconductors



In k space

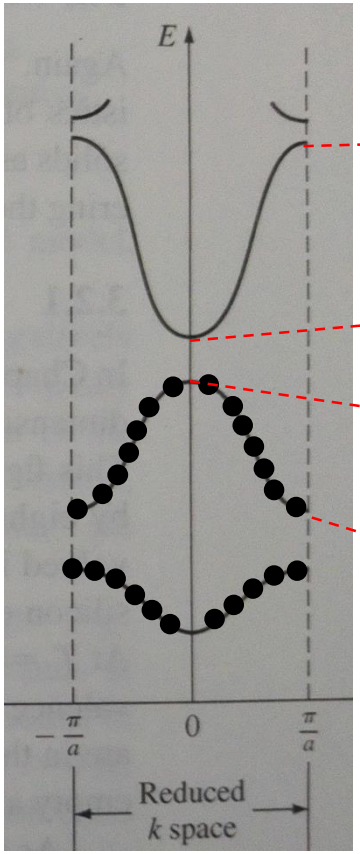


In physical space

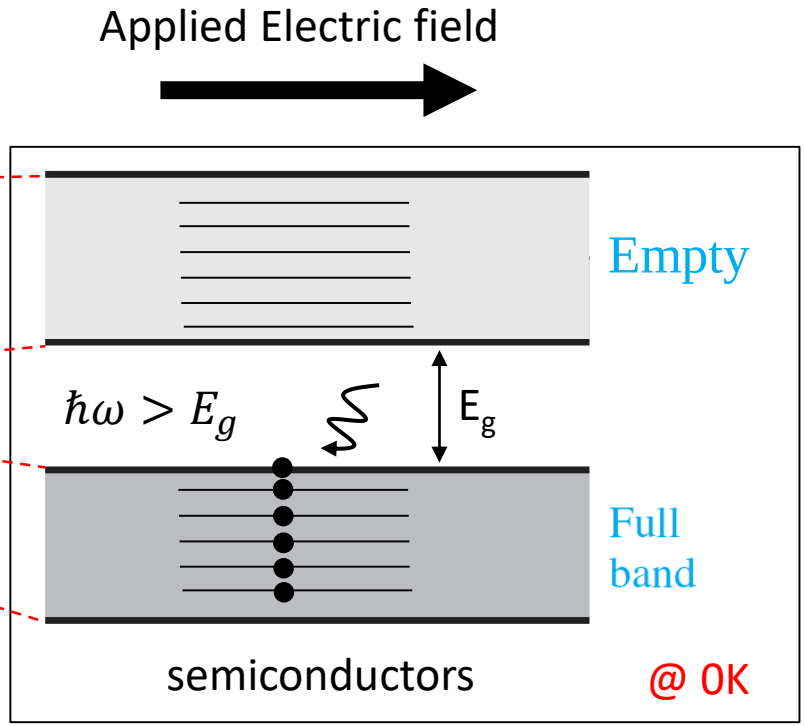
Electrons excited into in conduction band.
Conductive via electrons and holes @RT

3.2 Electrical Conduction in Solids

Energy band of semiconductors



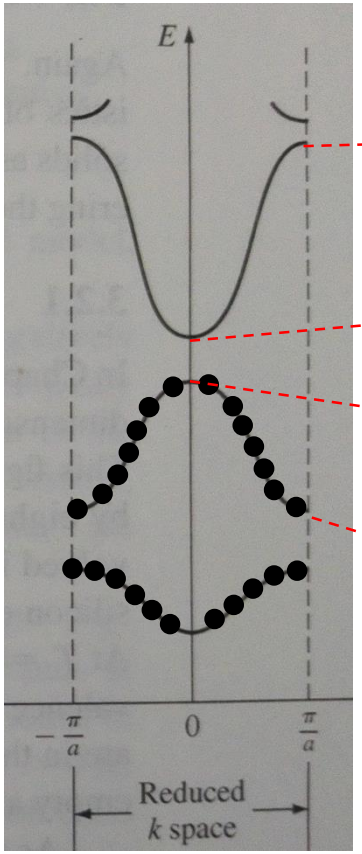
In k space



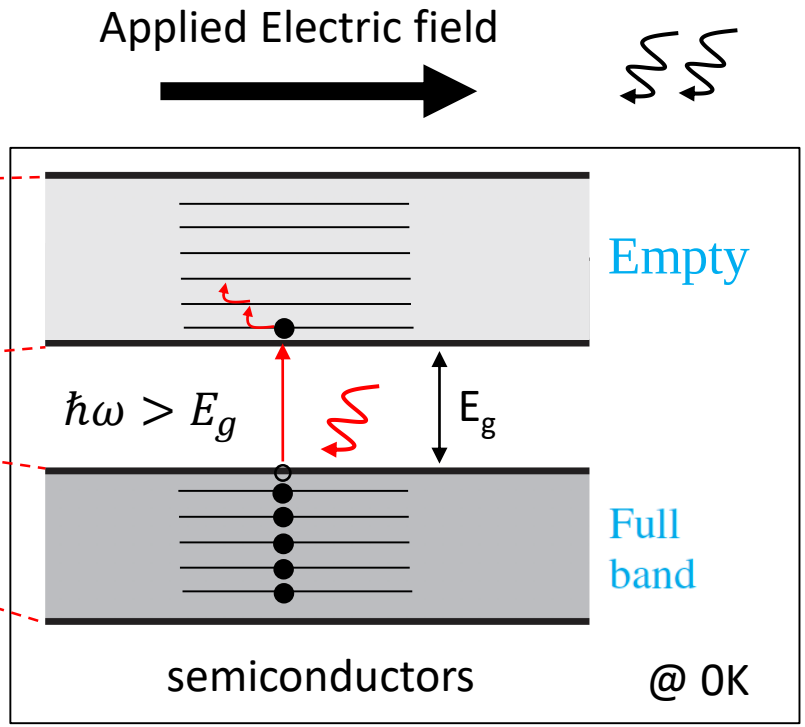
In physical space

3.2 Electrical Conduction in Solids

Energy band of semiconductors



In k space

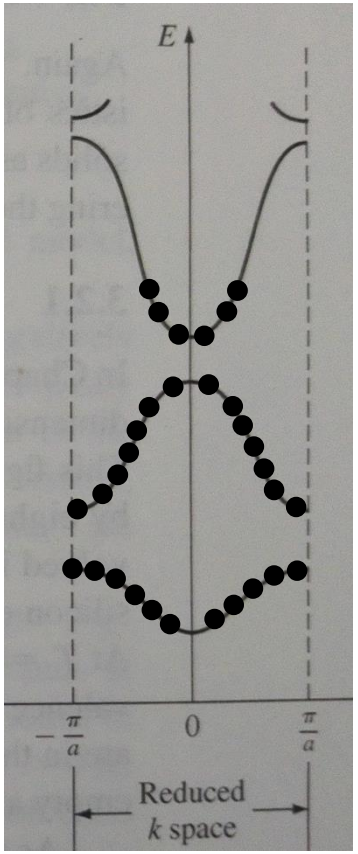


In physical space

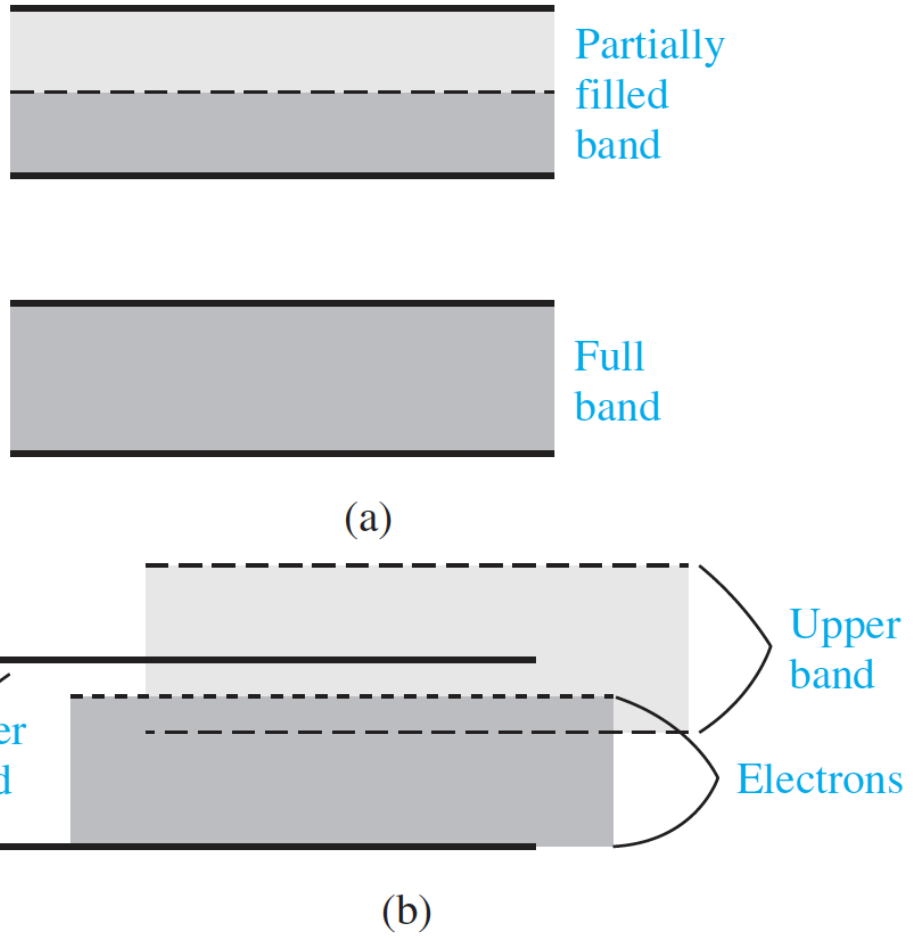
Photo excited carriers $\Delta n = \Delta p$

3.2 Electrical Conduction in Solids

Energy band of metals

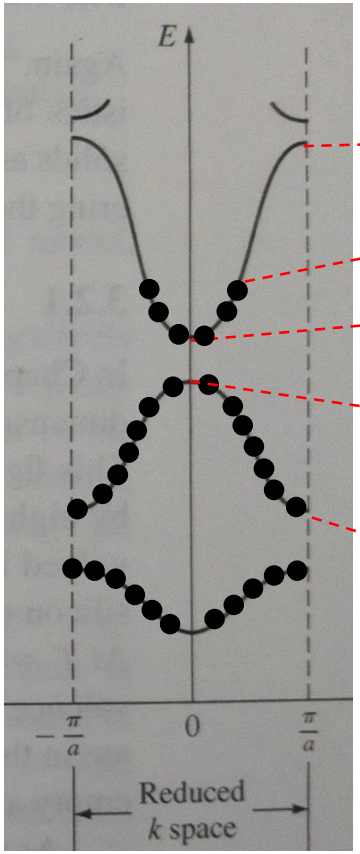


Forming energy bands is complicated.

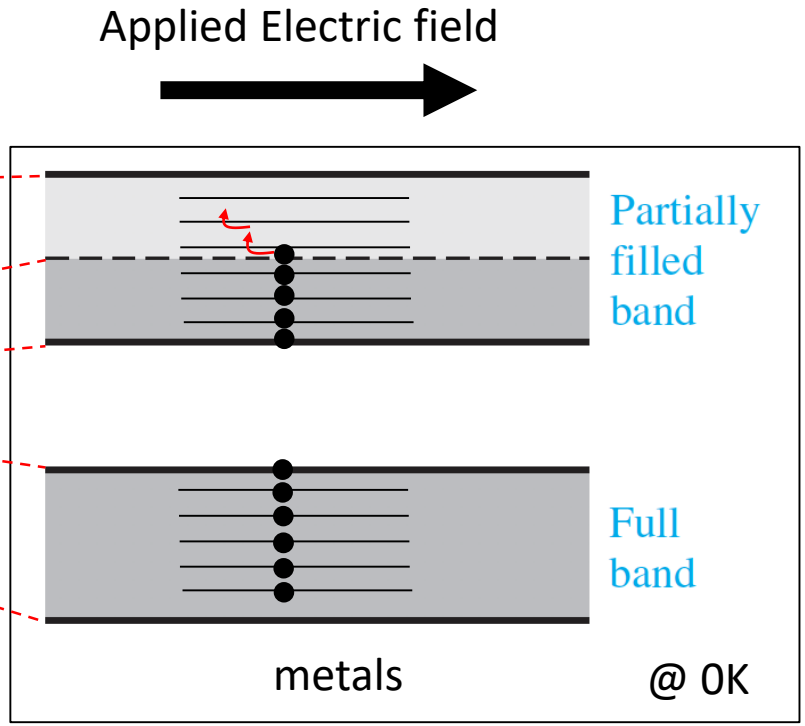


3.2 Electrical Conduction in Solids

Energy band of metals



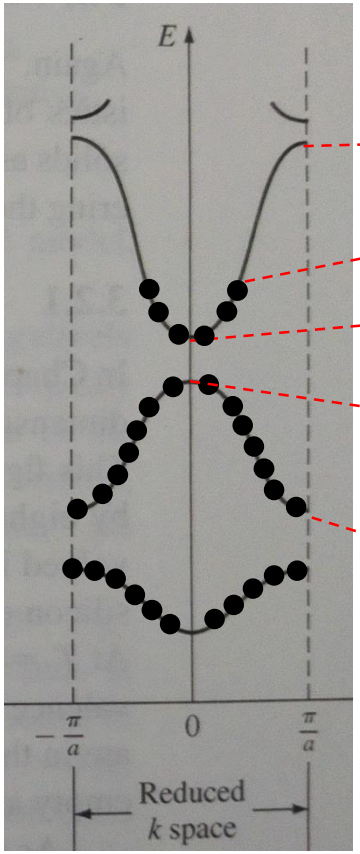
In k space



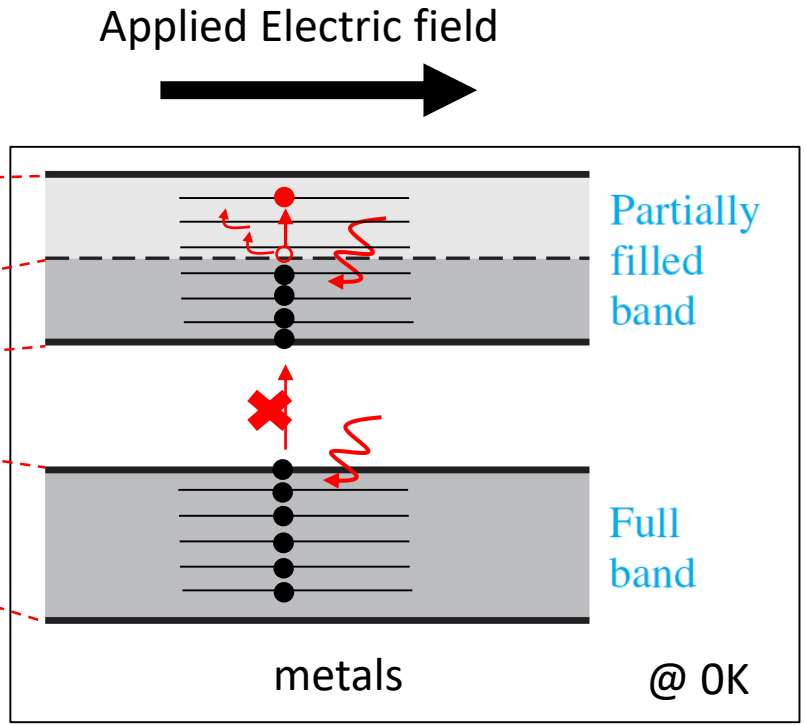
In physical space

3.2 Electrical Conduction in Solids

Energy band of metals



In k space



In physical space

NOT more electrons in conduction band created.

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

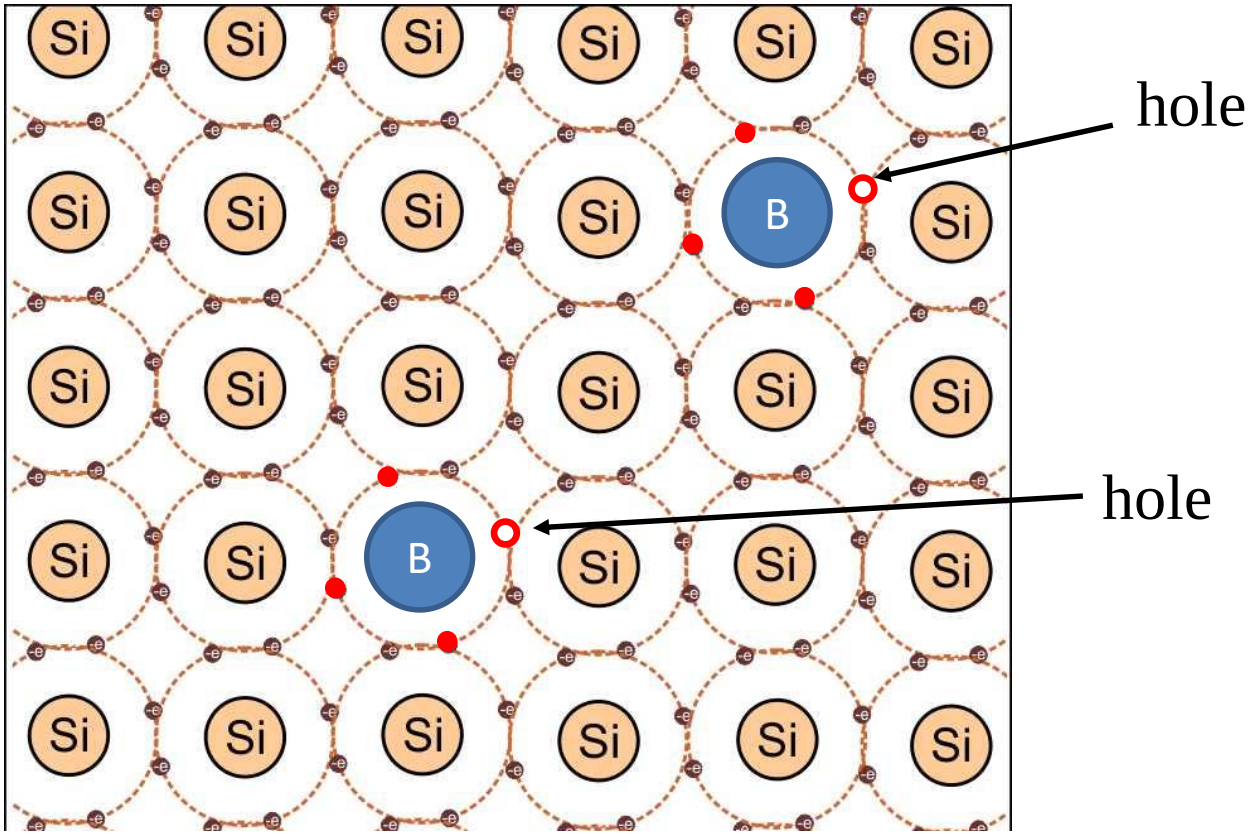
n-type semiconductors :
Charge carriers are negative, i.e. electrons
Doped by donor-type of dopants (impurities)

p-type semiconductors:
Charge carriers are positive, i.e. holes
Doped by acceptor-type of dopants (impurities)

3.2 Electrical Conduction in Solids

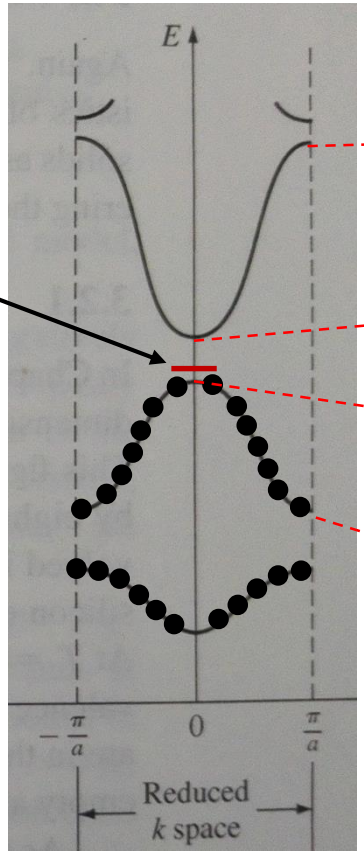
Acceptor-type or **p-type** doping (from the view of physical world)

At 0K



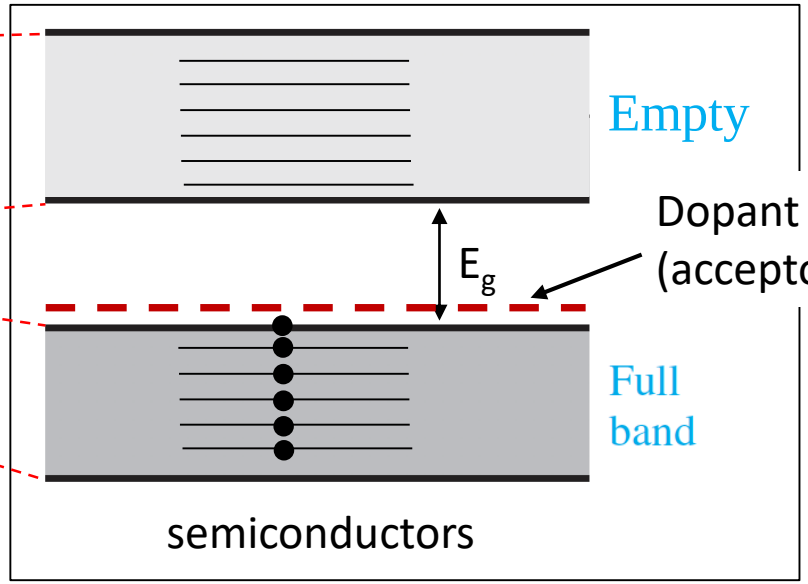
3.2 Electrical Conduction in Solids

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



In k space

Dopant energy level

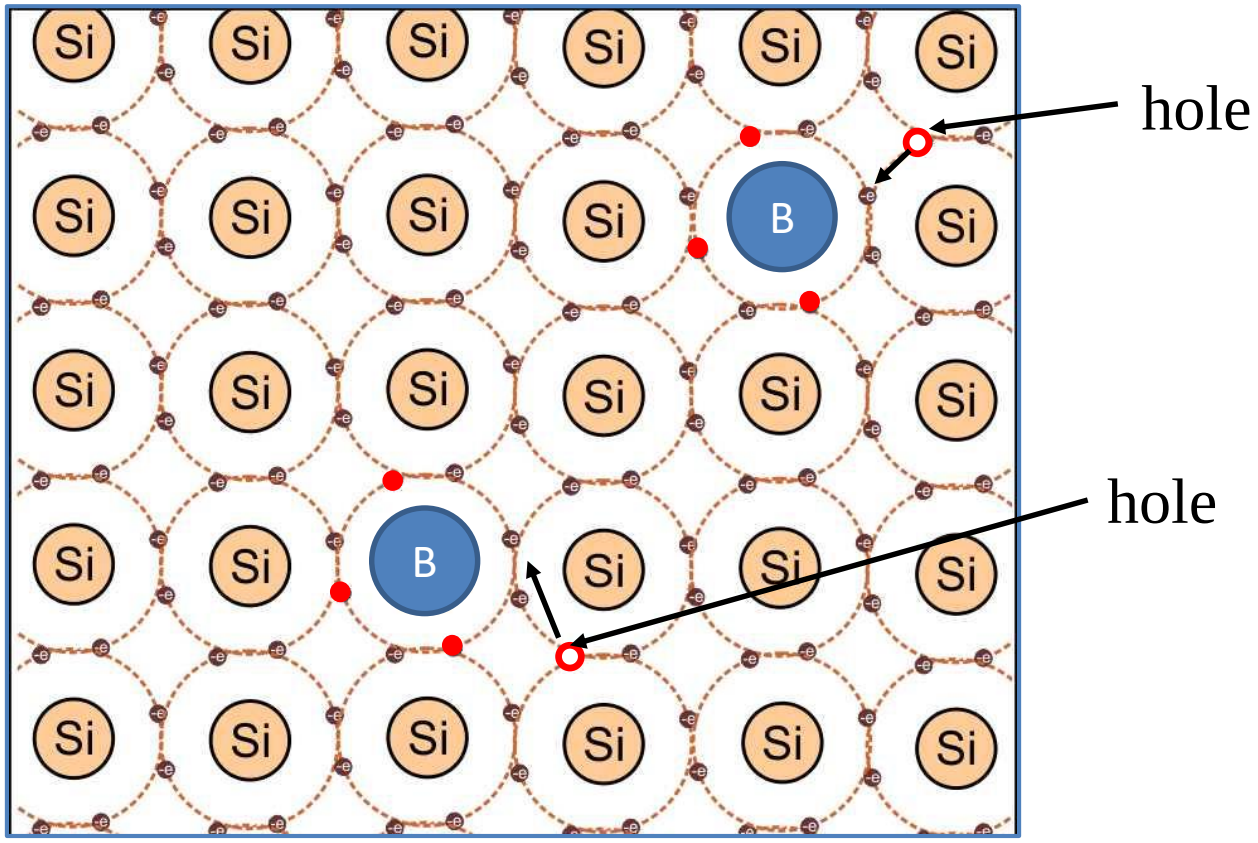


In physical space

3.2 Electrical Conduction in Solids

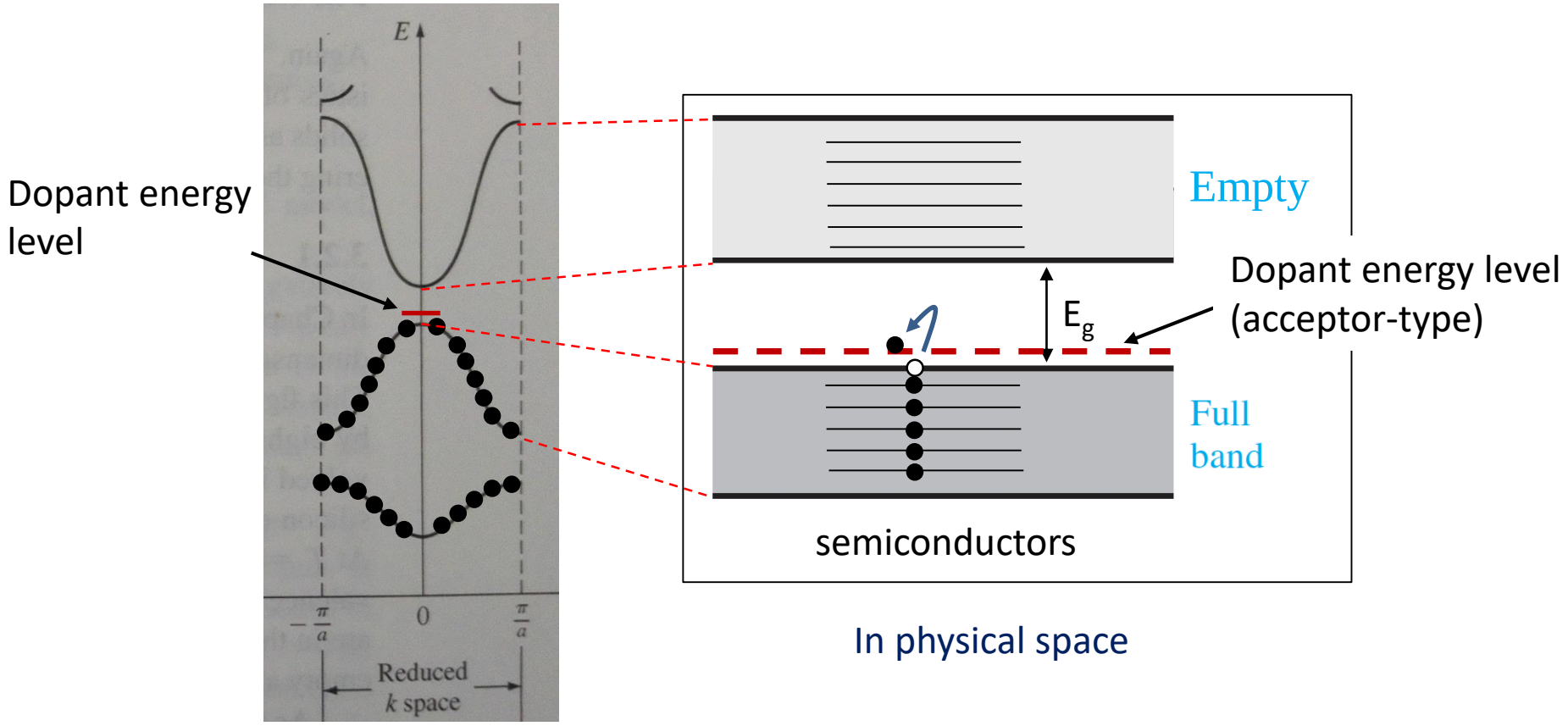
Acceptor-type or **p-type** doping (from the view of physical world)

At 300K



3.2 Electrical Conduction in Solids

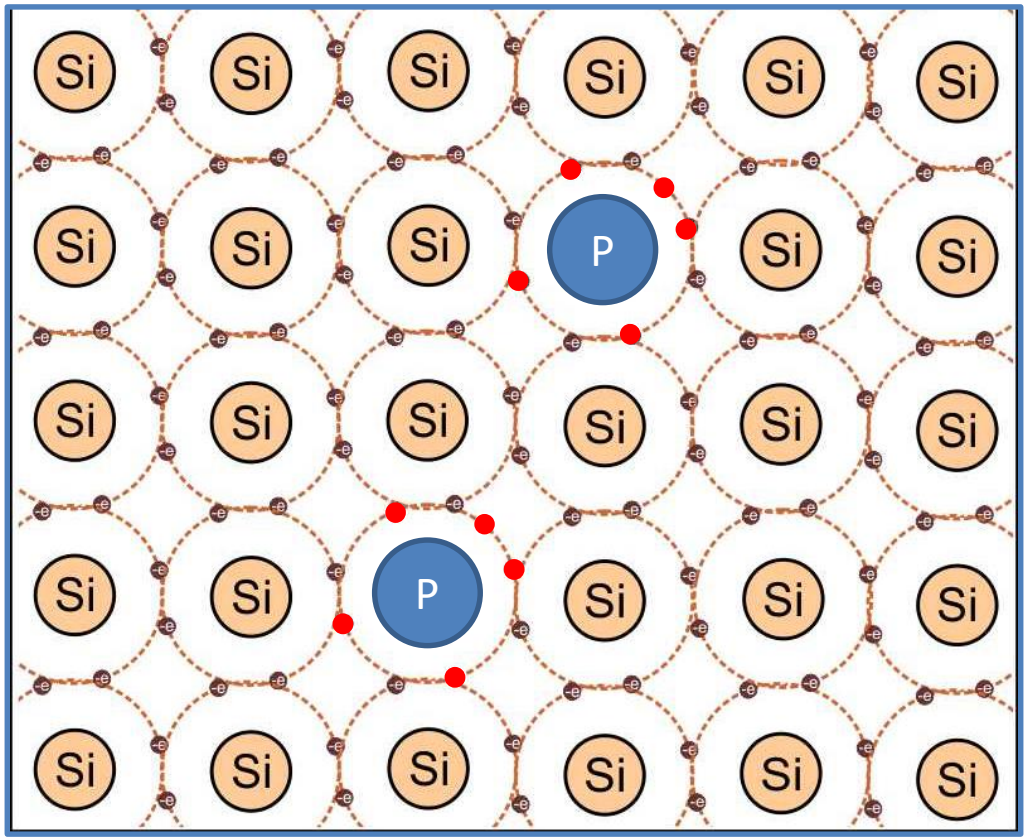
Acceptor-type or **p-type** doping (from the view of energy band)



3.2 Electrical Conduction in Solids

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

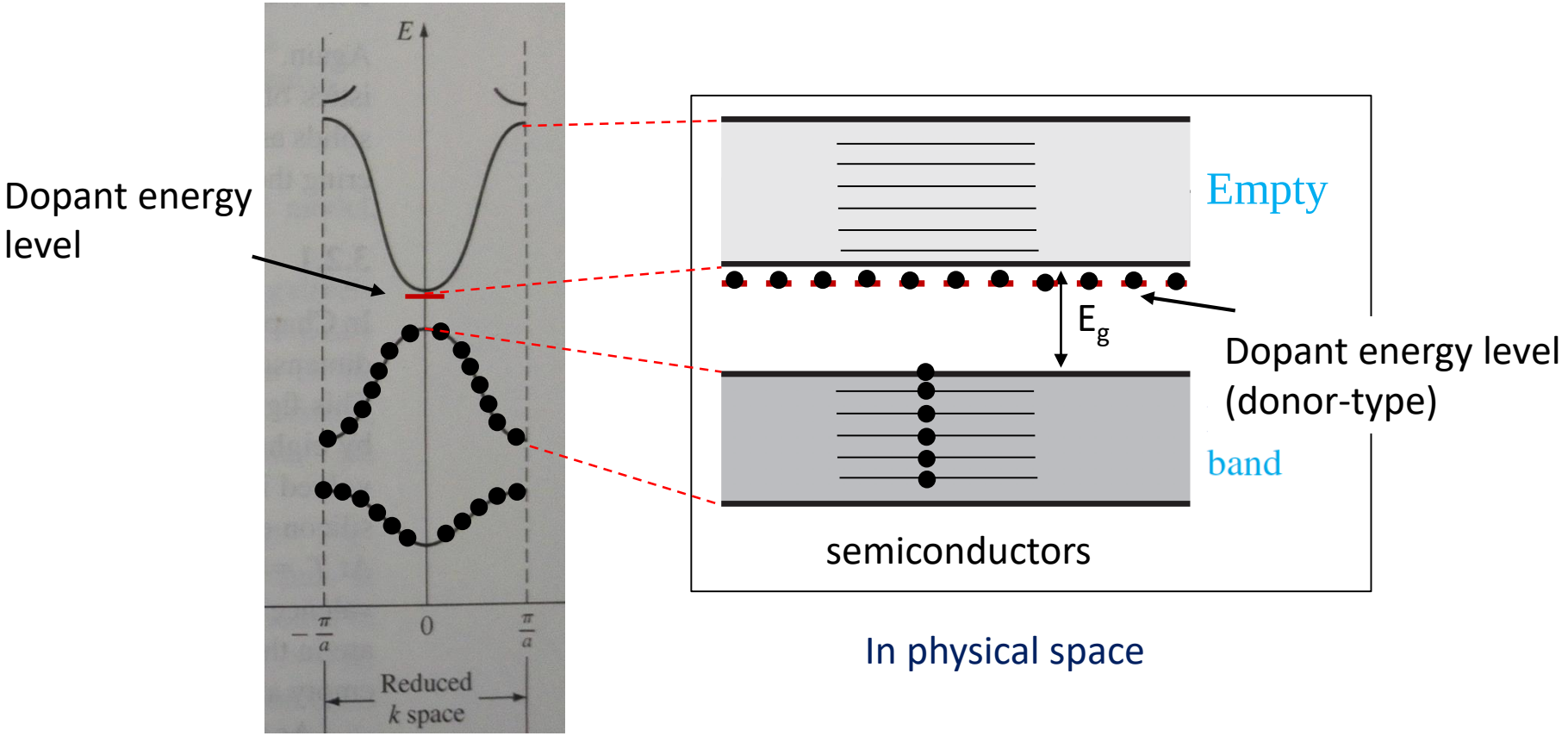
At 0K



Donor-type of dopants

3.2 Electrical Conduction in Solids

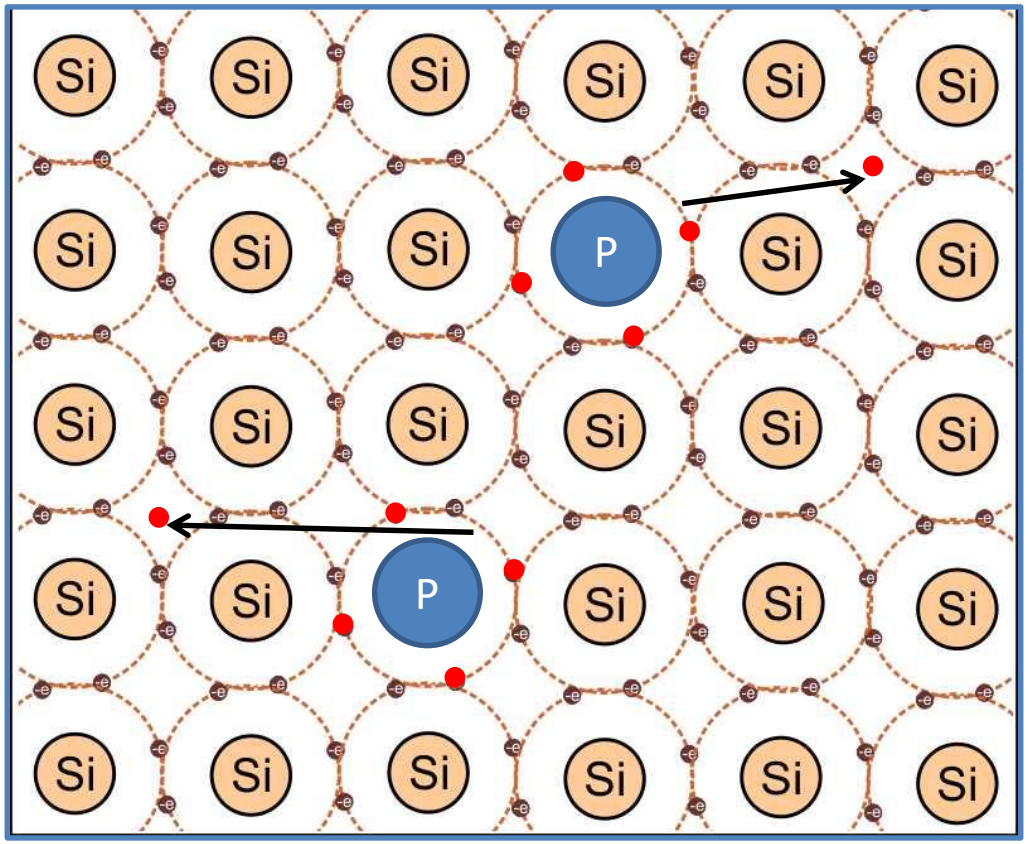
Donor-type or **n-type** doping (from the view of energy band)



3.2 Electrical Conduction in Solids

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

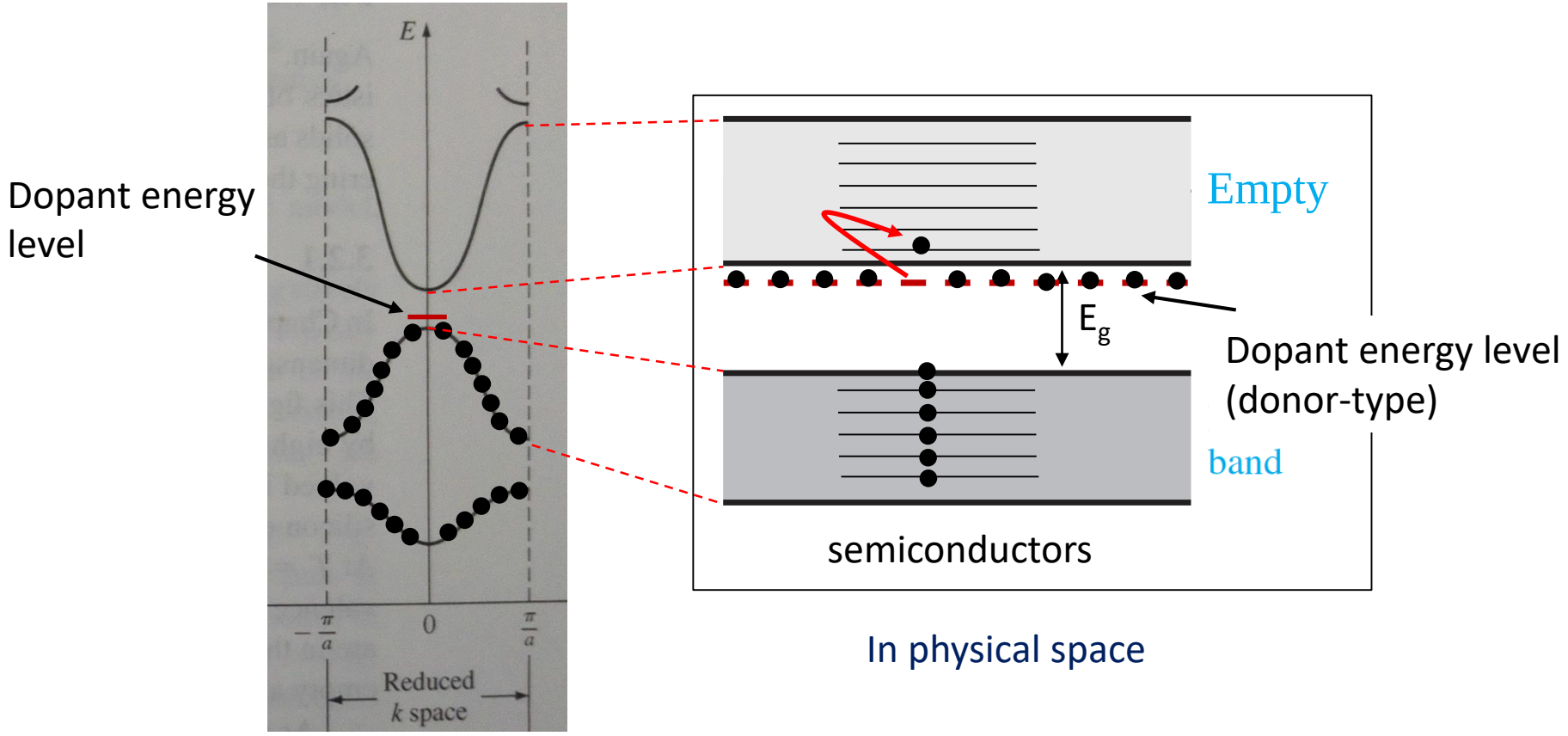
> 0K



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: 5×10^{22} 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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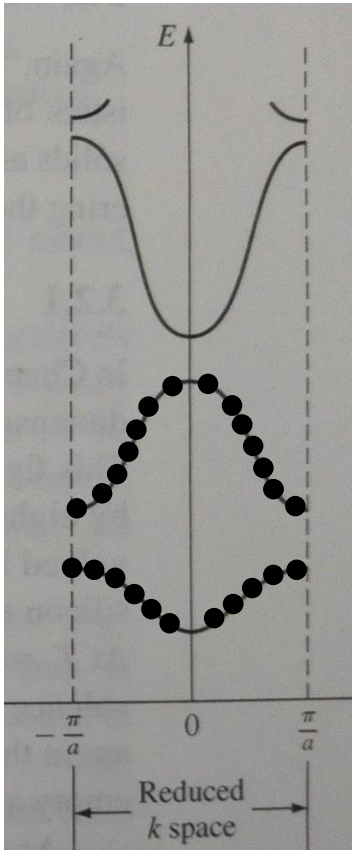
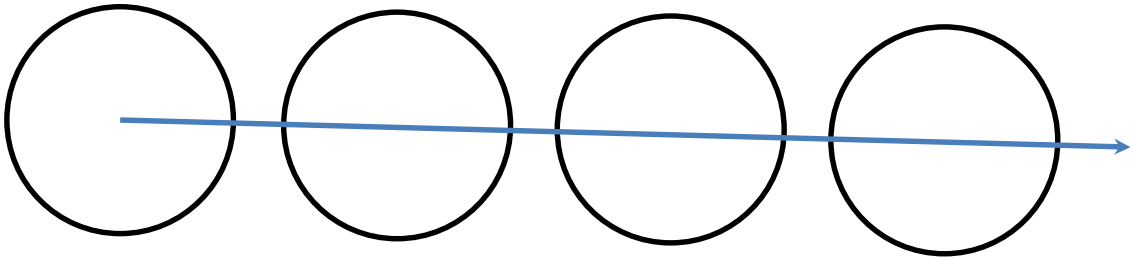
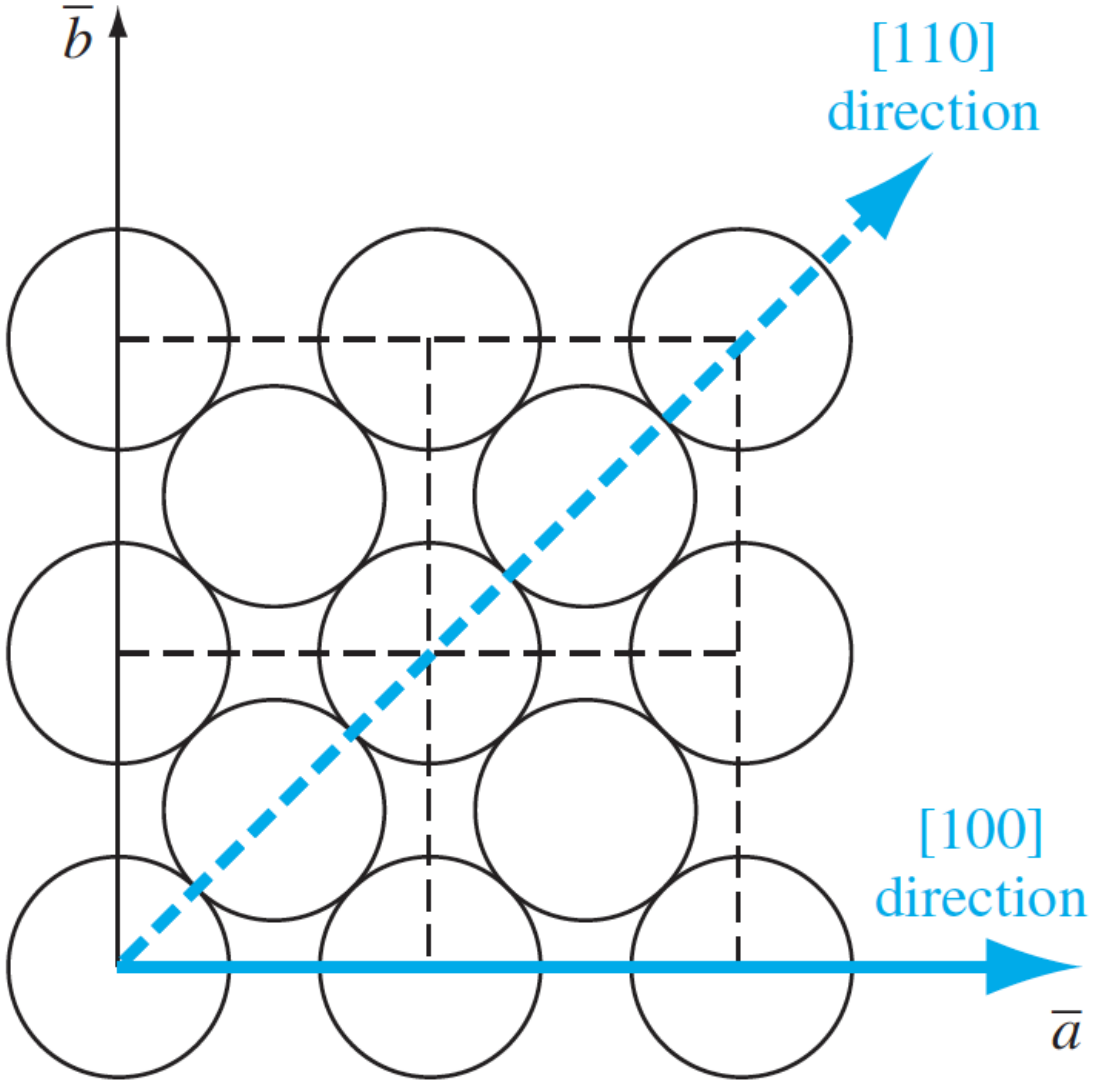
3.3 Extension to Three Dimensions



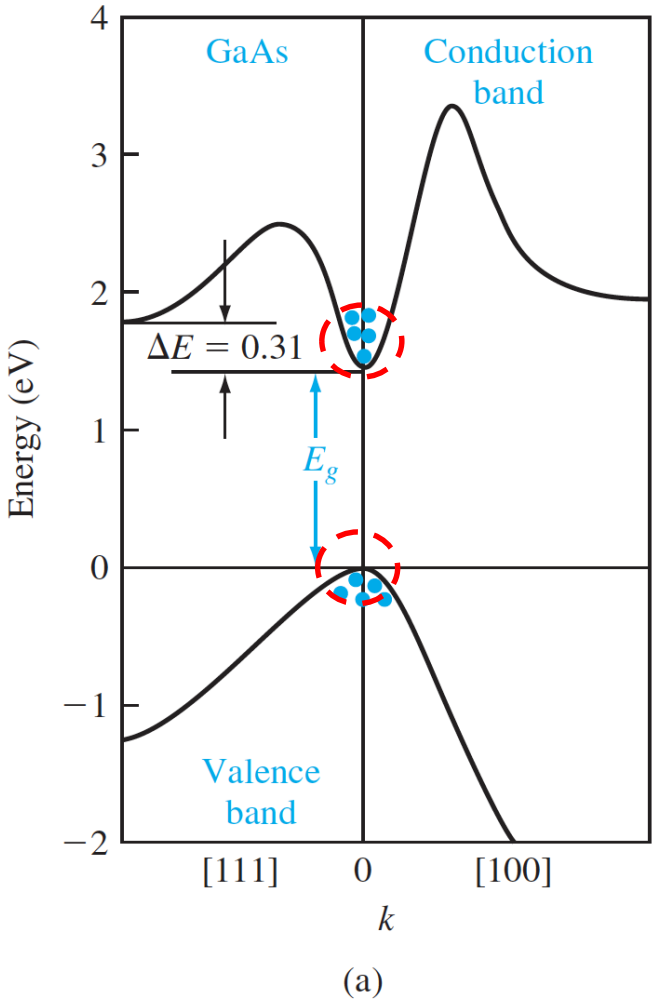


3.3 Extension to Three Dimensions



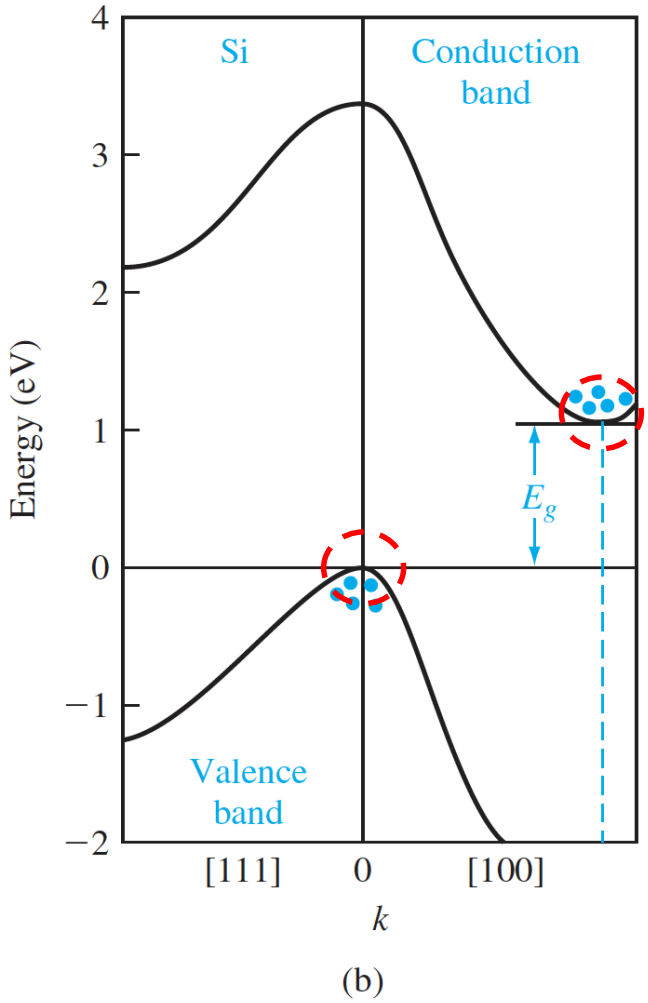
3.3 Extension to Three Dimensions

Direct bandgap



(a)

Indirect bandgap



(b)

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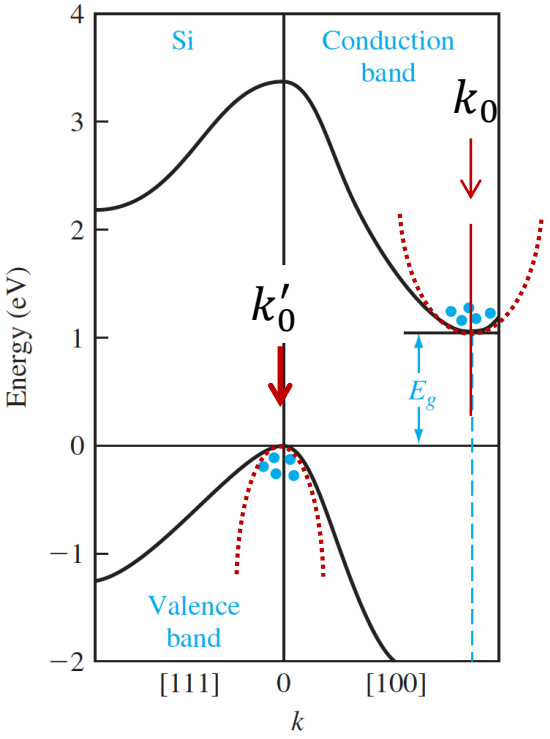
3.4 Effective Mass

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

3.4 Effective Mass (1st time approximation)

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



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) $\frac{dE}{dk}|_{k=k_0}(k - k_0) = 0$ because the first order differential equals to zero at local minimum or local maximum.

⇩

Therefore, we have

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

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:

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

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

- 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

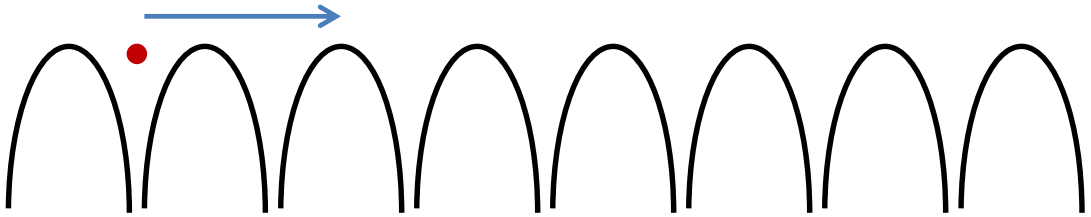
$$m = \frac{F}{a} \qquad a = \frac{d^2x}{dt^2}$$

In the air

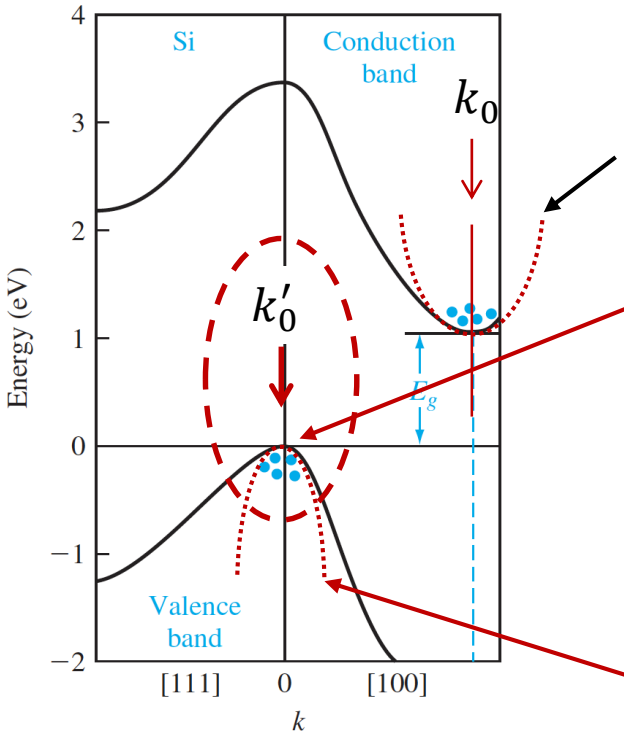
$$m^* = \frac{F}{a} \qquad a = \frac{d^2x}{dt^2}$$

In the water

Modulated by Electric potential of ions



3.4 Effective Mass (For Electrons in the valence band)



Electrons in conduction band

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

$$\frac{d^2E}{dk^2}\Big|_{k_0'} = \frac{\hbar^2}{m^*} < 0$$

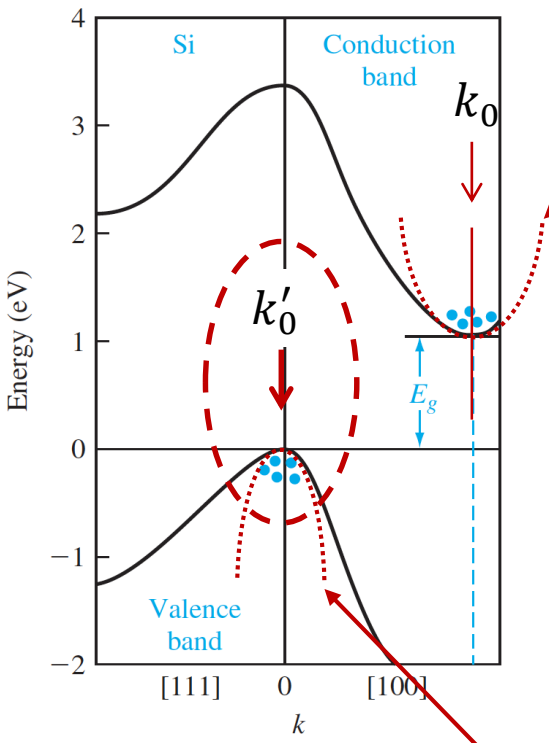
Negative mass would make no sense.

Electrons in **valence** band

$$E(k) = E(k_0') - \frac{\hbar^2}{2m_p^*}\Big|_{k_0'}(k-k_0')^2$$

Positive mass

3.4 Effective Mass (A new particle defined: holes)



Electrons in **conduction** band

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

Positive mass

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

Holes in **valence** band

$$E(k) = E(k_0') - \frac{\hbar^2}{2m_p^*}\Big|_{k_0'}(k-k_0')^2$$

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	0.067	1.08	0.55
Holes	m_h^*/m_0	0.48	0.56	0.37

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

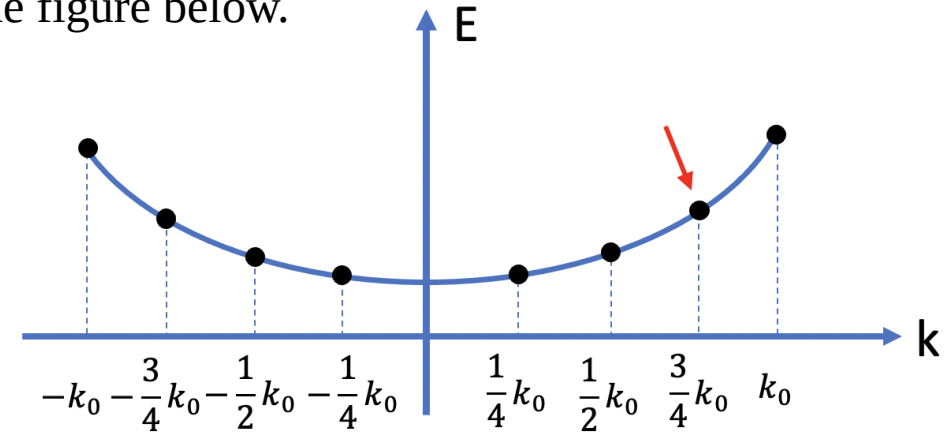
Problem Example #1

1. In a quantum system, 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.

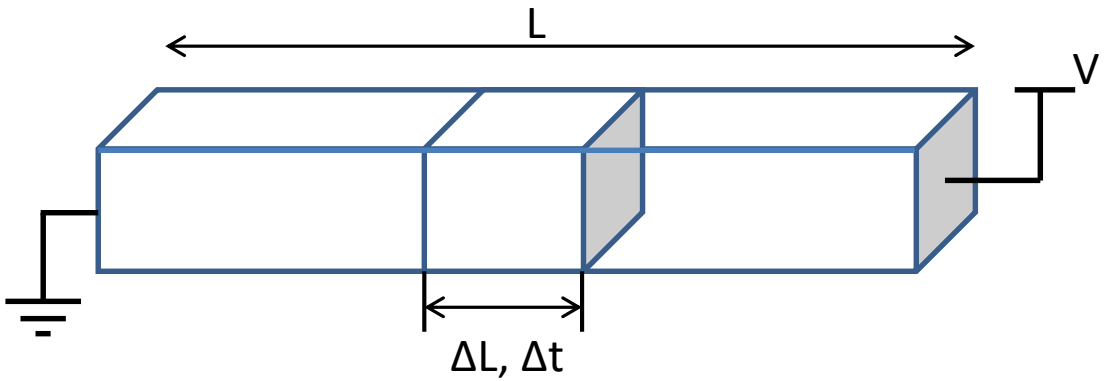


Outline

- 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

3.5 Density of States Function

n type semiconductor



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

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

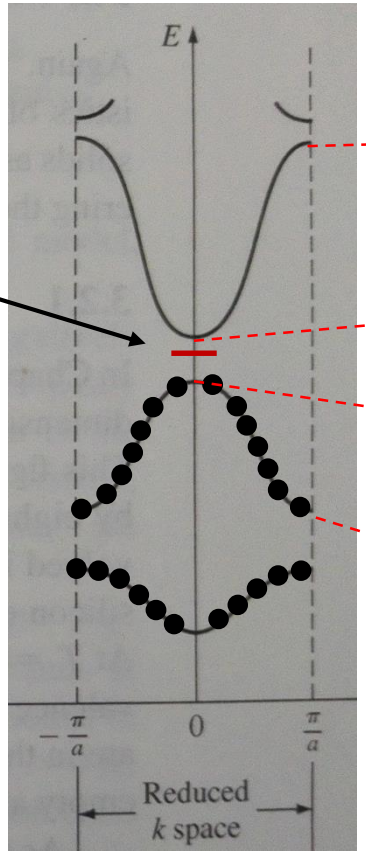
$$I = \frac{\Delta Q}{\Delta t} = \frac{nqA_c\Delta L}{\Delta t} = nqA_c\mu V/L \quad \Rightarrow \quad \sigma = \frac{I}{V} = \frac{nqA_c\mu}{L}$$

3.2 Electrical Conduction in Solids

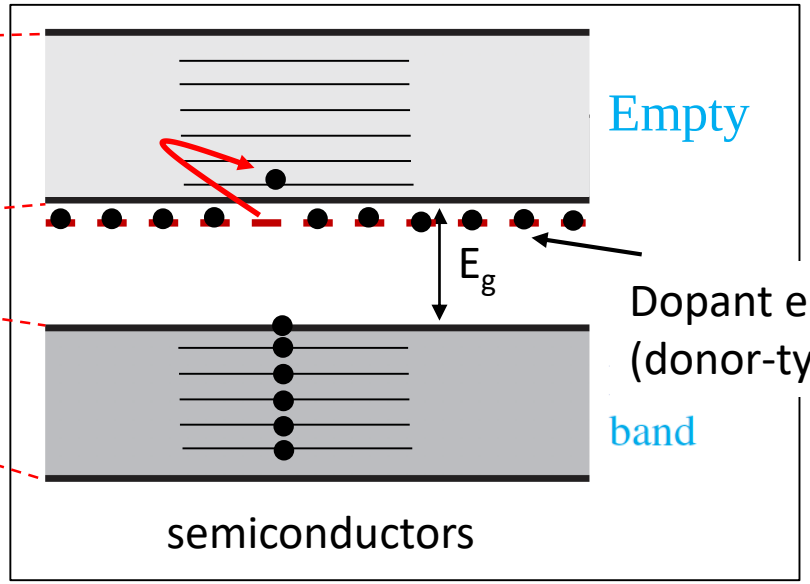
Donor-type or **n-type** doping (from the view of energy band)

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

Dopant energy level



In k space

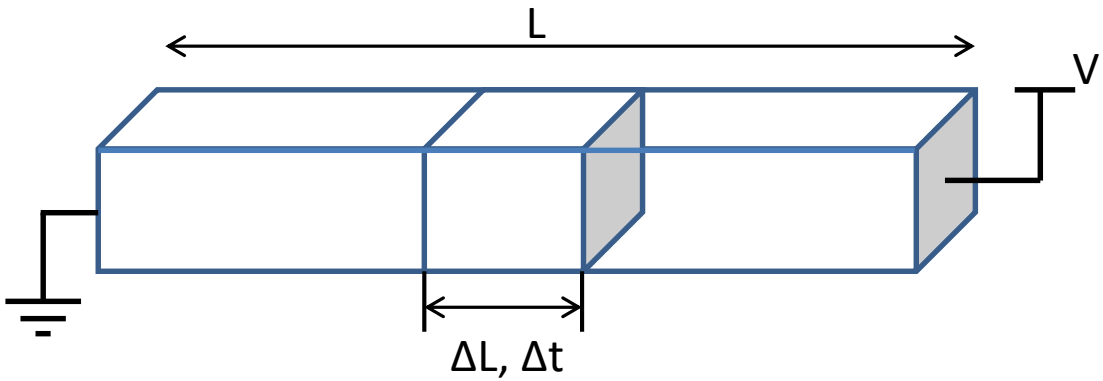


Dopant energy level (donor-type)

In physical space

3.5 Density of States Function

n type semiconductor



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

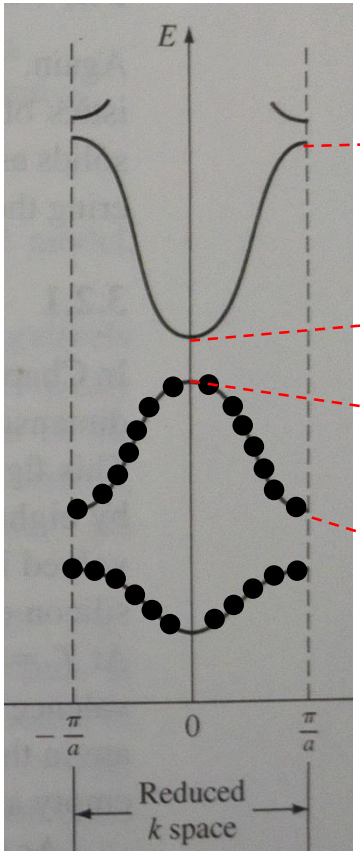
$$v = \mu E = \mu V/L$$

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

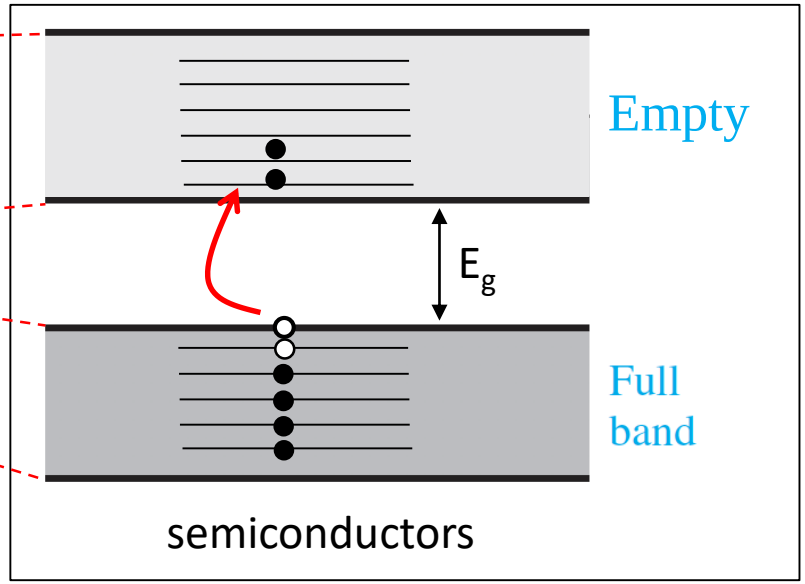
3.2 Electrical Conduction in Solids

If the semiconductor is intrinsic:

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



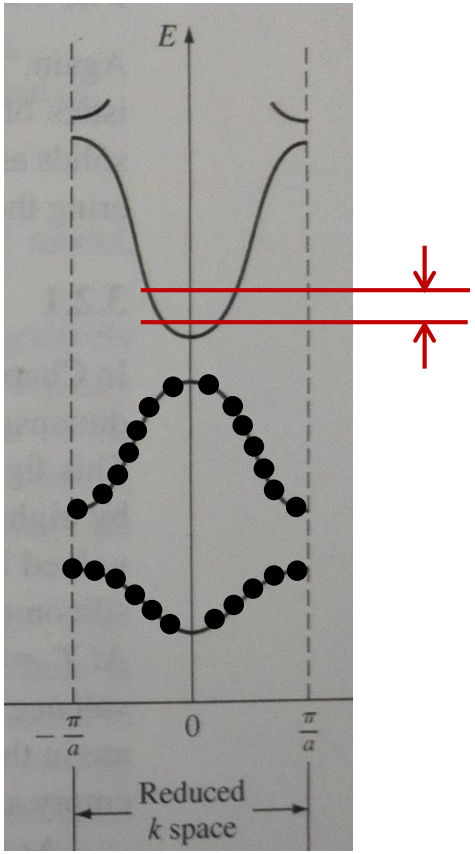
In k space



In physical space

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?

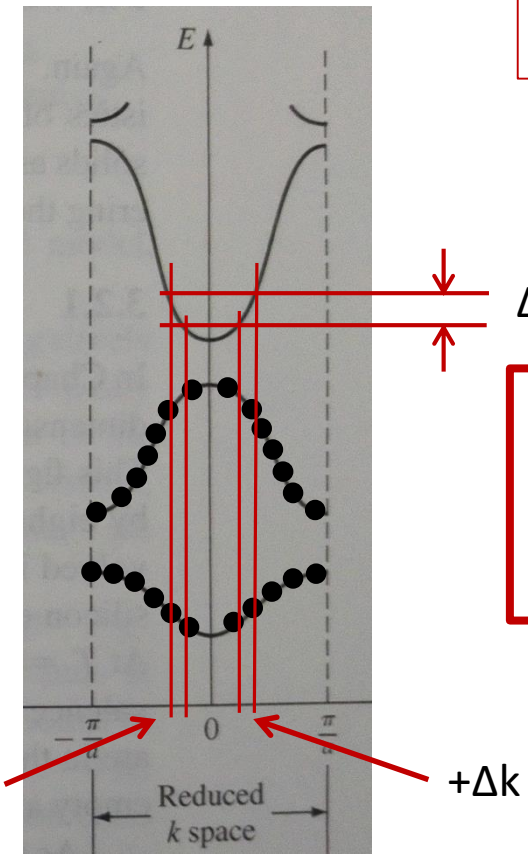
Only if we know:

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

3.2 Electrical Conduction in Solids

If the semiconductor is intrinsic:

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



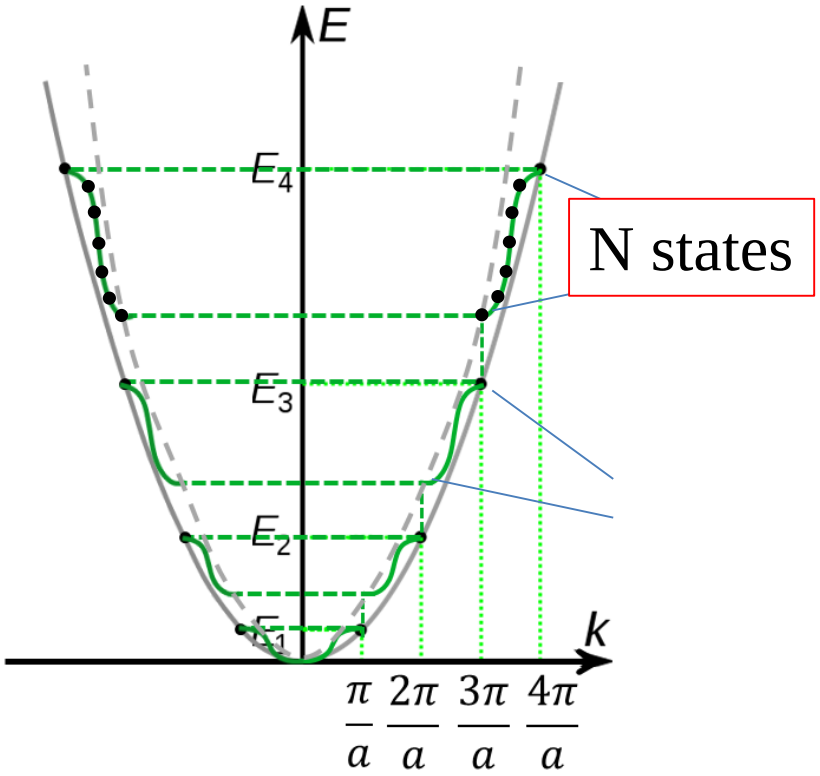
In k space

Only if we know:

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

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 $(0, \pi/a)$: $\frac{N}{\pi/a}$

⇩

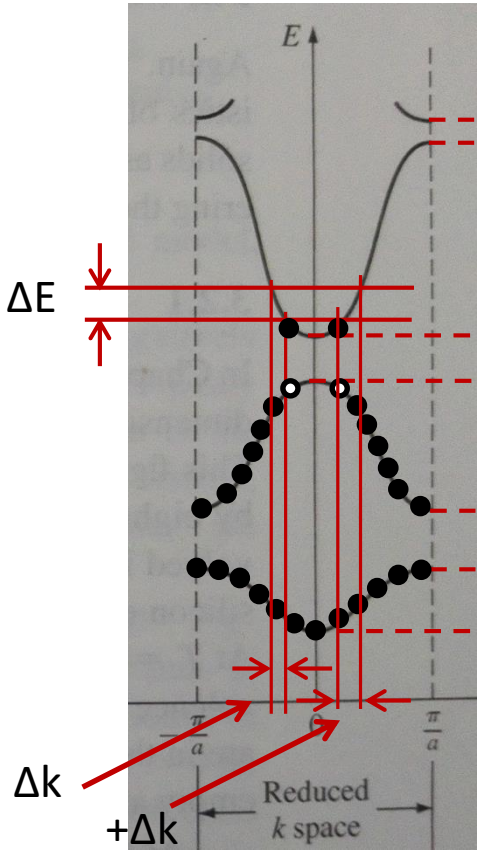
The number of states of the whole crystal within Δk: $\frac{N}{\pi/a} \times \Delta k$

⇩

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

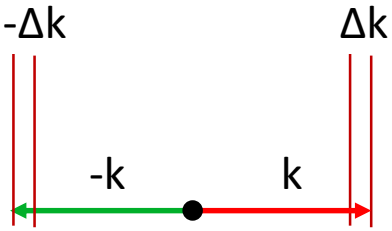
One-dimensional



In k space

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

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



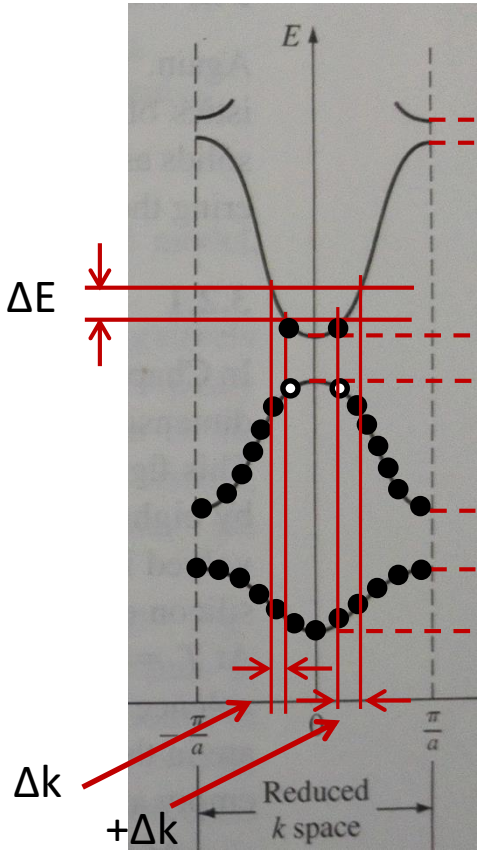
Within ΔE, we have the number of k's is $\frac{d(2|k|/\pi)}{dE}\Delta E$

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

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

3.5 Density of States Function

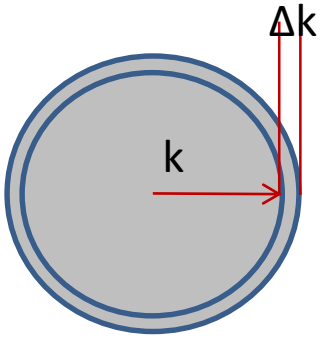
Two-dimensional



In k space

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

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



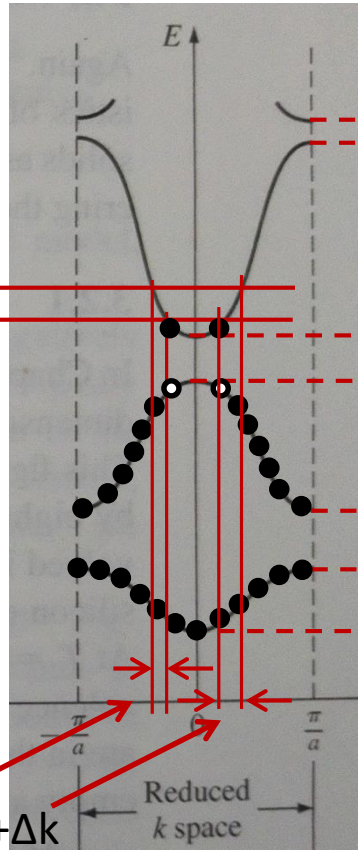
Within ΔE, we have the number of k is $\frac{d(\pi(k/\pi)^2)}{dE}\Delta E$

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

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

3.5 Density of States Function

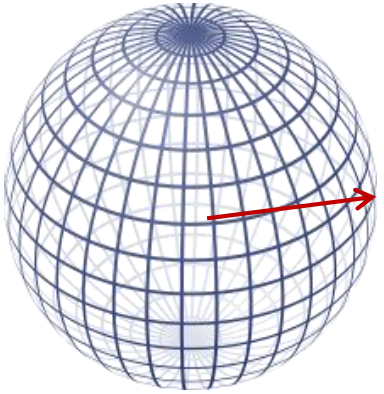
Three-dimensional



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 $\frac{d(4\pi\left(\frac{k}{\pi}\right)^3/3)}{dE}\Delta E$

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

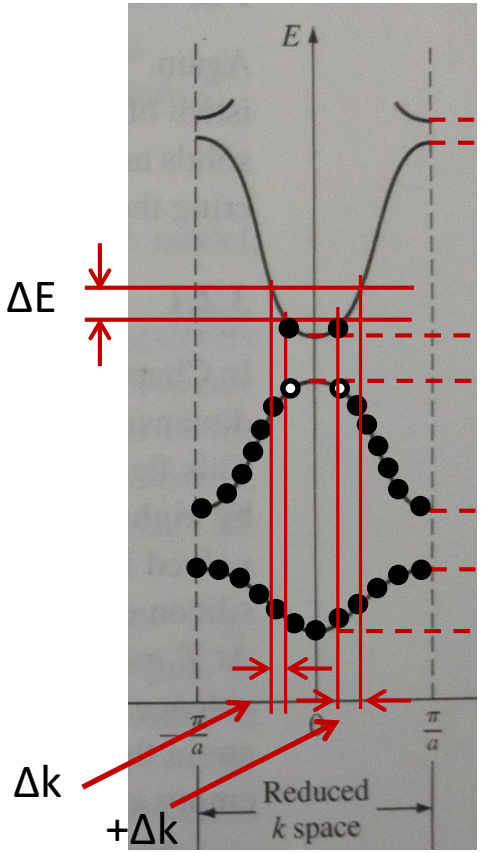
$+k_x$ and $-k_x$

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



In k space

spin

$$g(E) = \frac{dV_k}{dE} = 2\frac{2\pi(2m^*)^{3/2}}{h^3}\sqrt{E - E_c}$$

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

3.5 Density of States Function

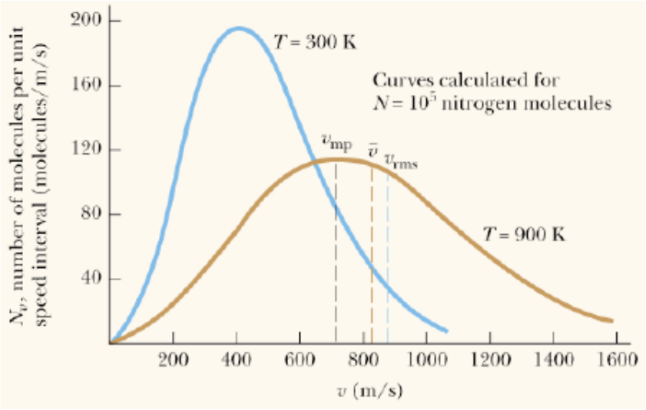
Problem Example #2

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

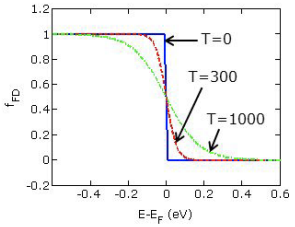
Bose-Einstein probability function:

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

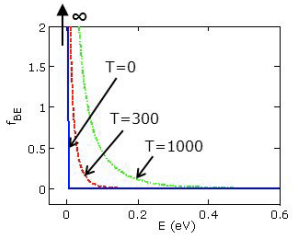
Fermi-Dirac probability function:

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

Fermi-Dirac vs. Bose-Einstein Statistics



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

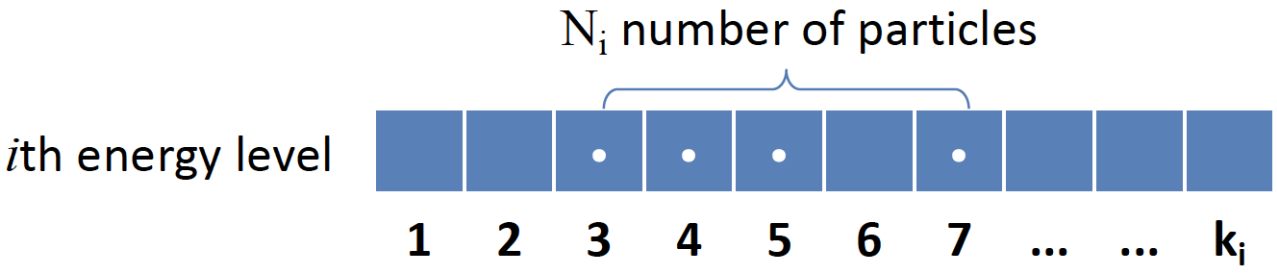


$$f_{BE}(E) = \frac{1}{\exp\left(\frac{E}{k_B T}\right) - 1}$$

3.6 Statistical mechanics

Fermi-Dirac probability function:

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



The totoal number of ways of arranging N_i particles in each ith energy level

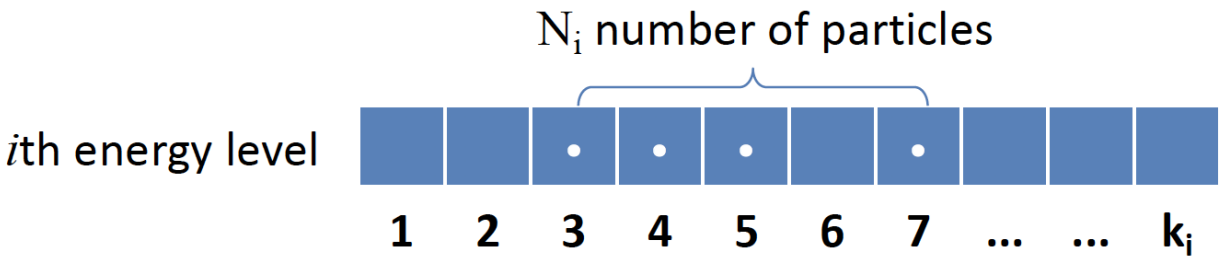
$$k_i(k_i-1)\cdots(k_i-(N-1)) = \frac{k_i!}{(k_i-N_i)}$$

(Particles are distinguishable)

3.6 Statistical mechanics

Fermi-Dirac probability function:

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



The totoal number of ways of arranging N_i indistinguishable particles in each ith energy level

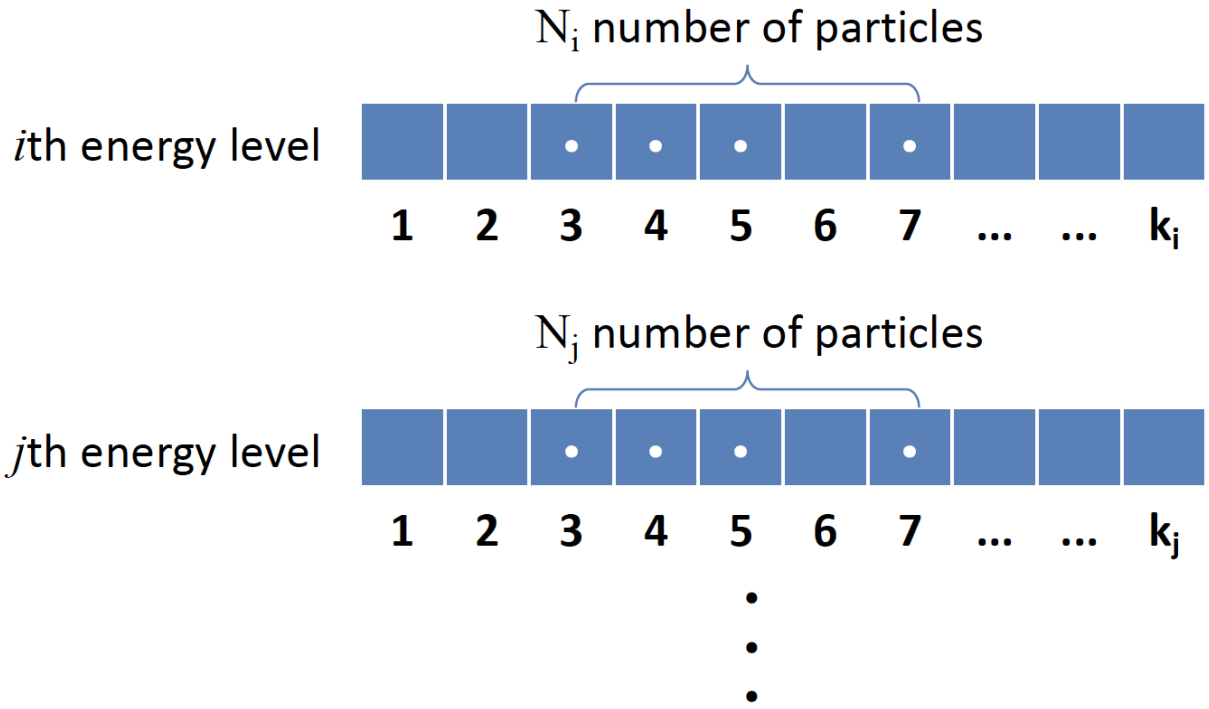
$$W_i = \frac{k_i!}{N_i!(k_i - N_i)!}$$

(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 totoal number (N) of particles, the total number of ways of arranging indistiguishable 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:

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

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

3.6 Statistical mechanics

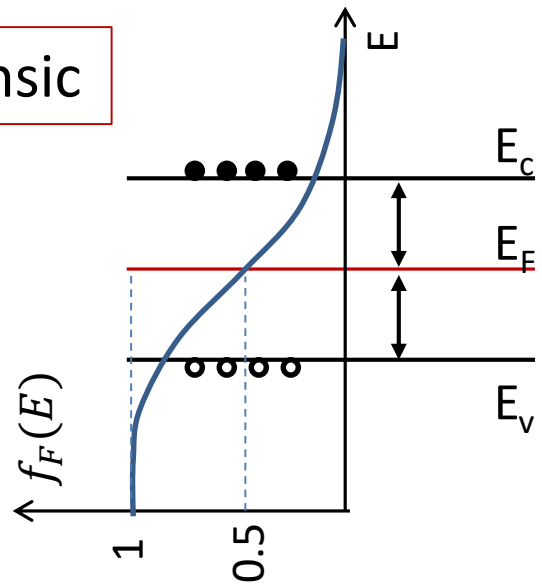
The probability of a state at energy E being occupied by an electron:

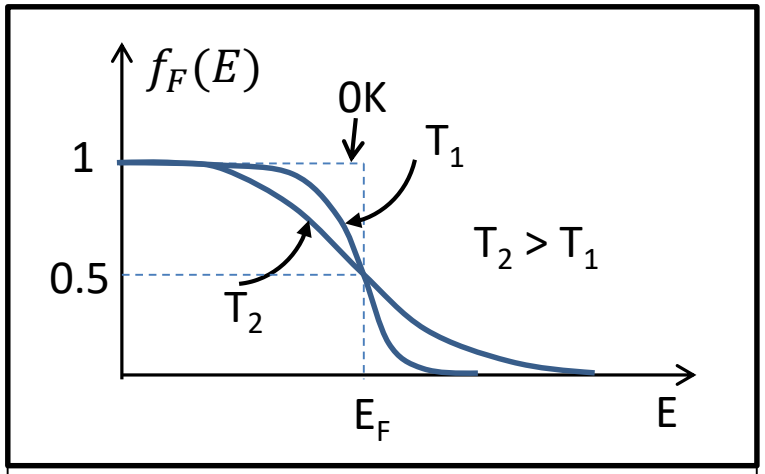
$$f_F(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$

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





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

Probability of a state at E_c occupied

II

Probability of a state at E_v unoccupied

Physical meaning of Fermi energy level:

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

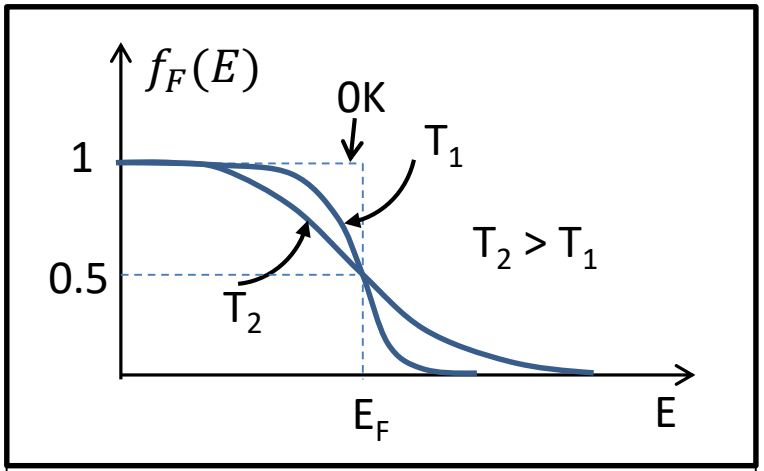
3.6 Boltzmann distribution

$$when \exp\left(\frac{E-E_F}{kT}\right) \gg 1 \Rightarrow E - E_F > 2kT$$

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

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

Boltzmann distribution



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

3.6 Boltzmann distribution

Problem Example #3

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