VE320 – Summer 2021

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
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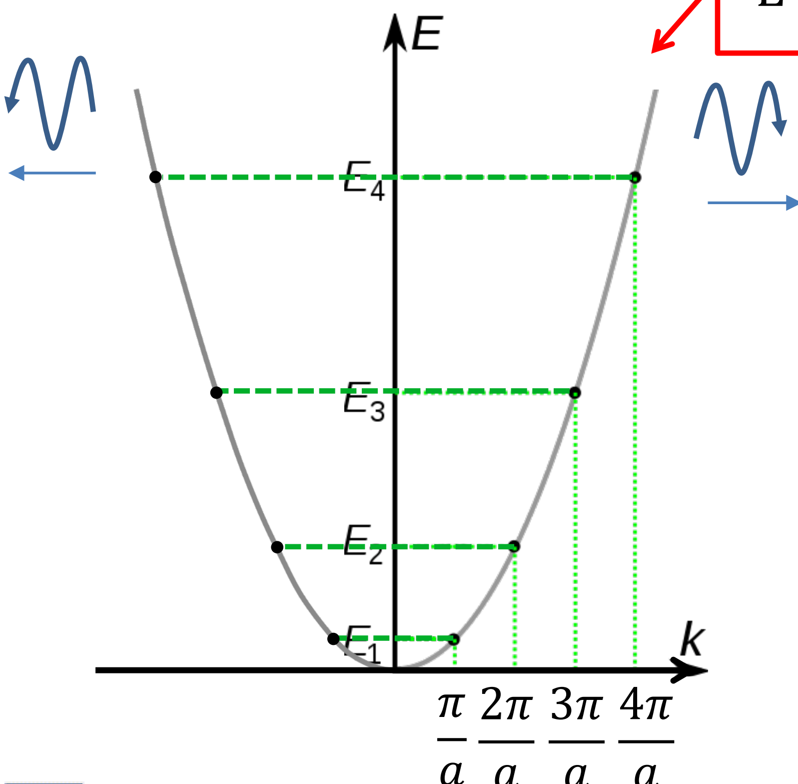
- 3.6 Statistical Mechanics

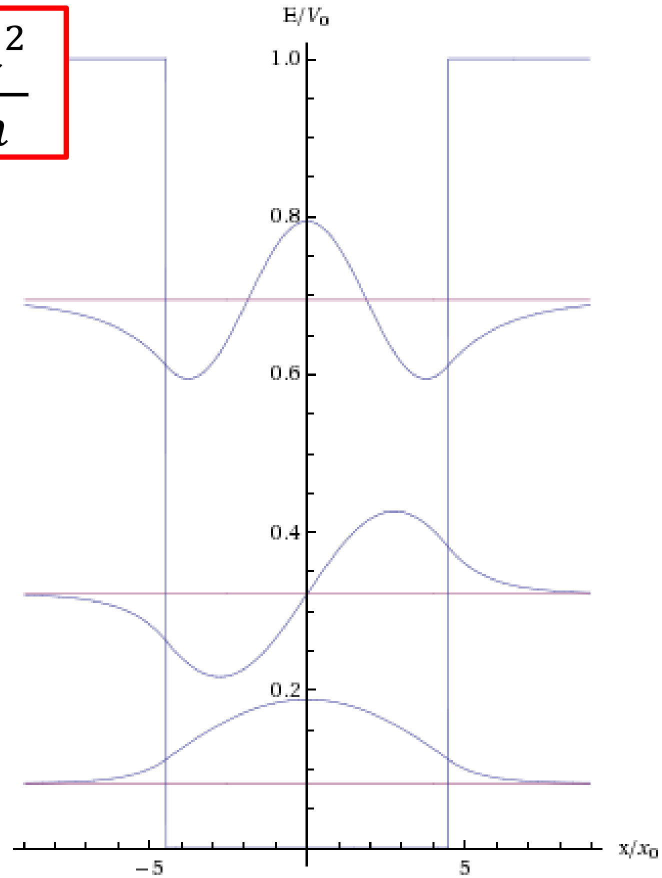
3.1 Allowed and Forbidden Energy Bands

<u>Forming energy bands</u>: analytical

Previously: Electrons in Finite Quantum Well

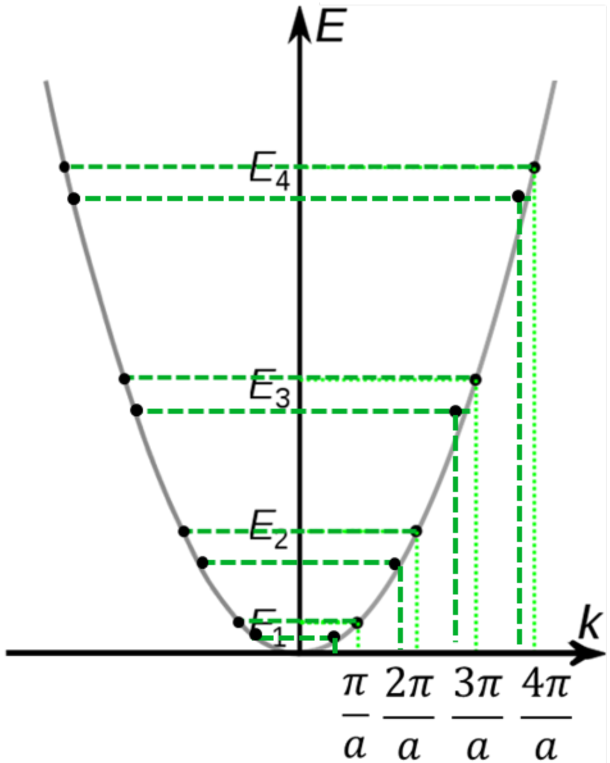
$$\boxed{E = \frac{k^2\hbar^2}{2m}}$$

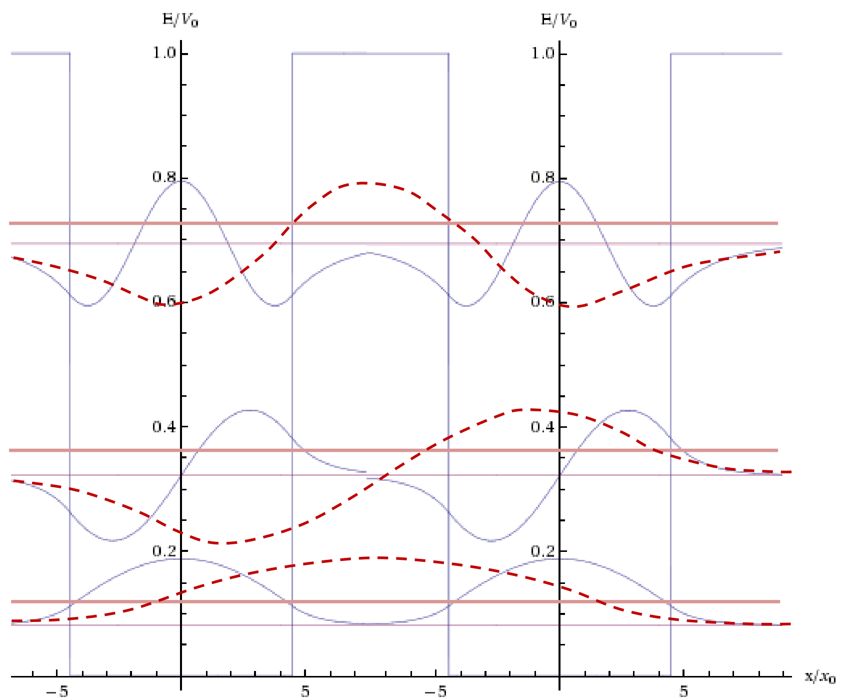




3.1 Allowed and Forbidden Energy Bands

<u>Forming energy bands</u>: analytical

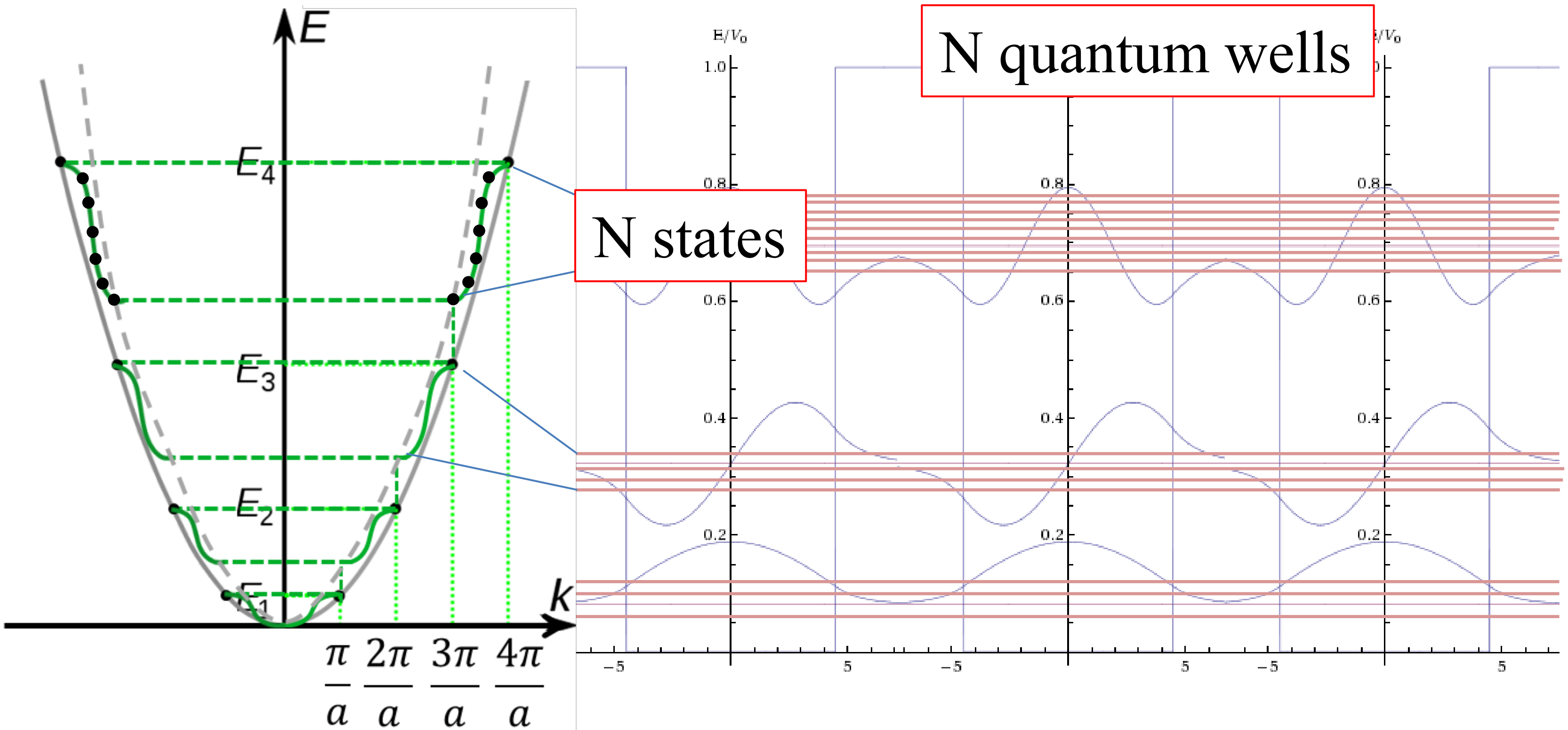




2 quantum wells

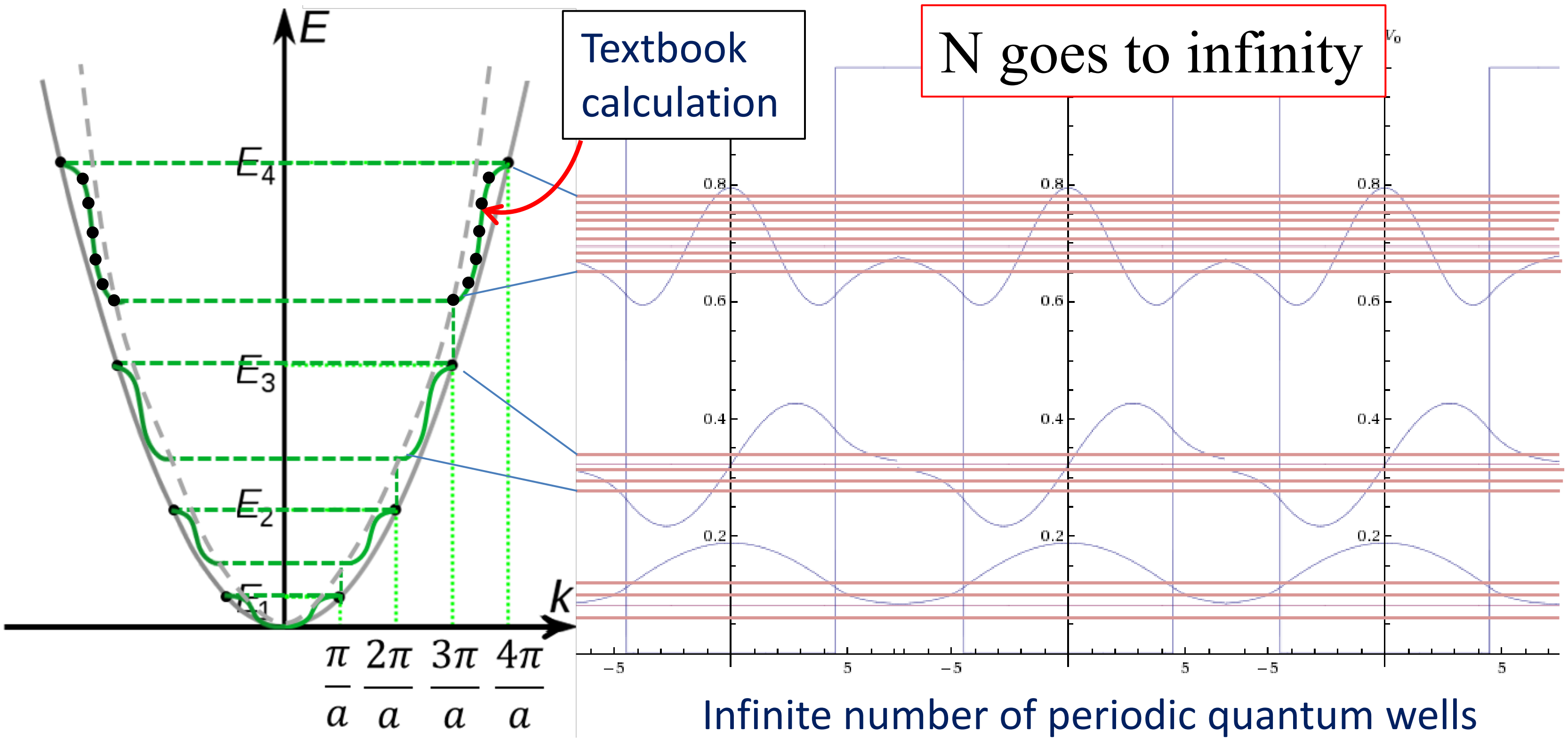
3.1 Allowed and Forbidden Energy Bands

<u>Forming energy bands</u>: analytical



3.1 Allowed and Forbidden Energy Bands

Forming energy bands: analytical



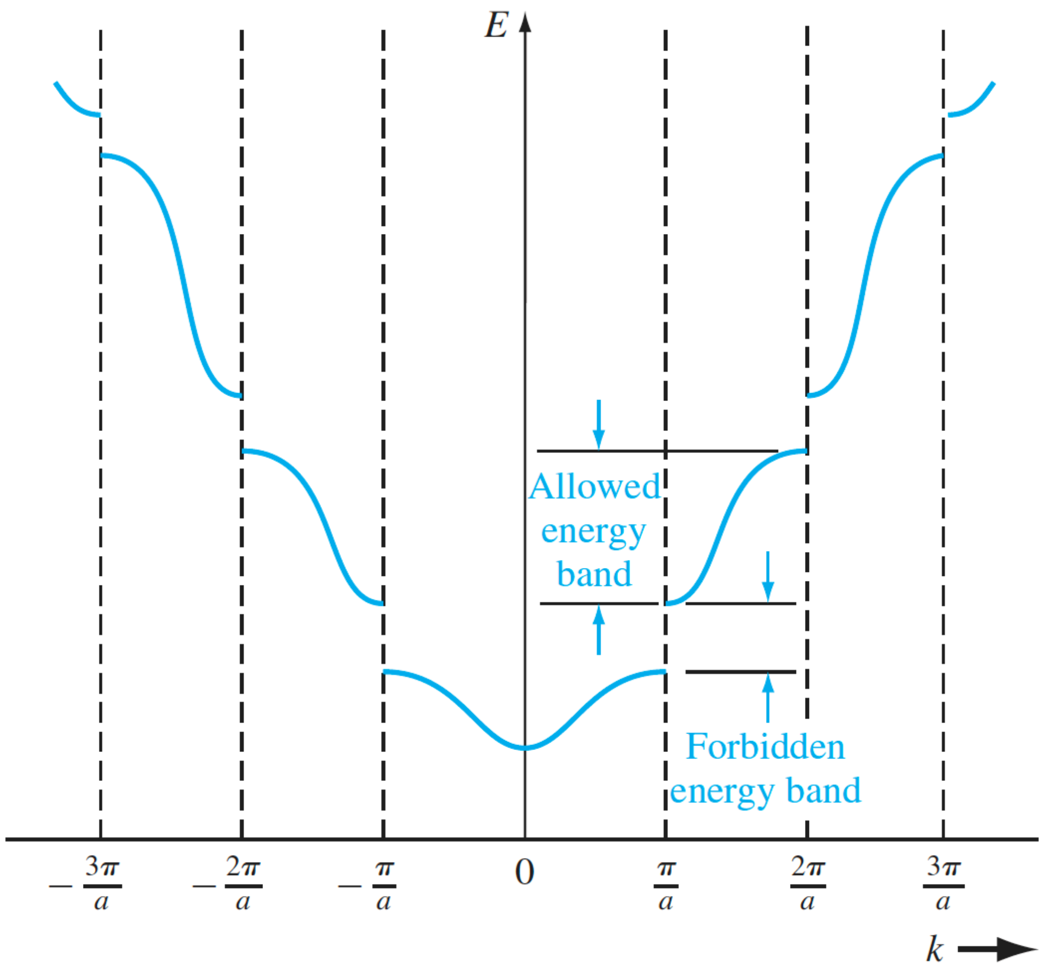
Infinite number of periodic quantum wells

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

On P.67
eq.(3.22)

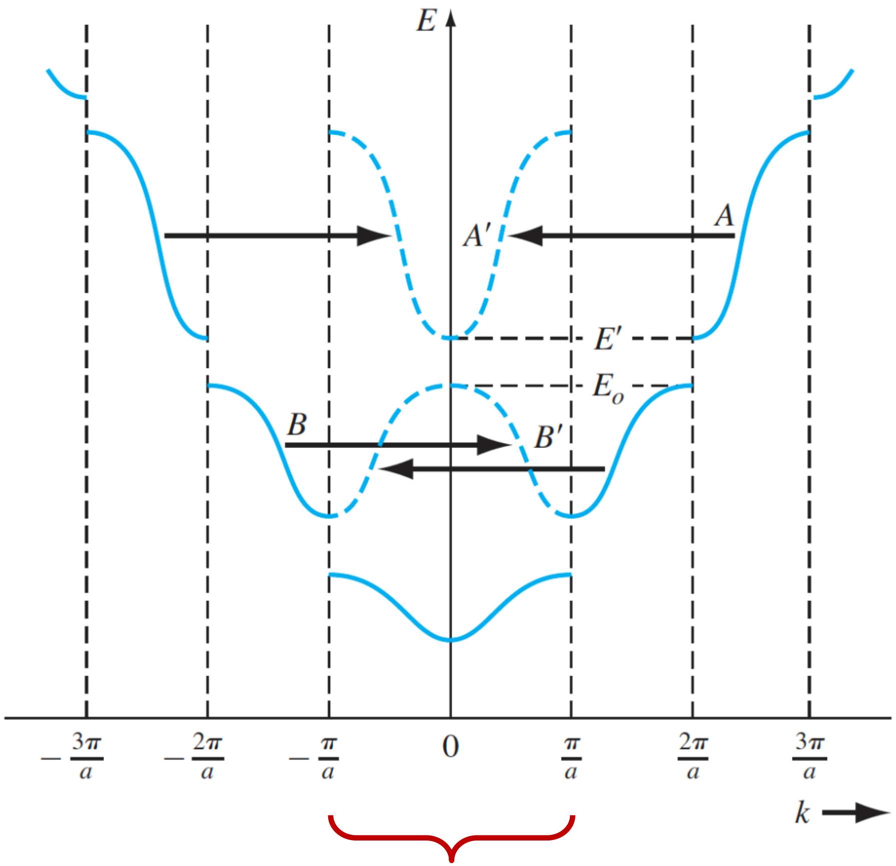
3.1 Allowed and Forbidden Energy Bands

Forming energy bands: analytical

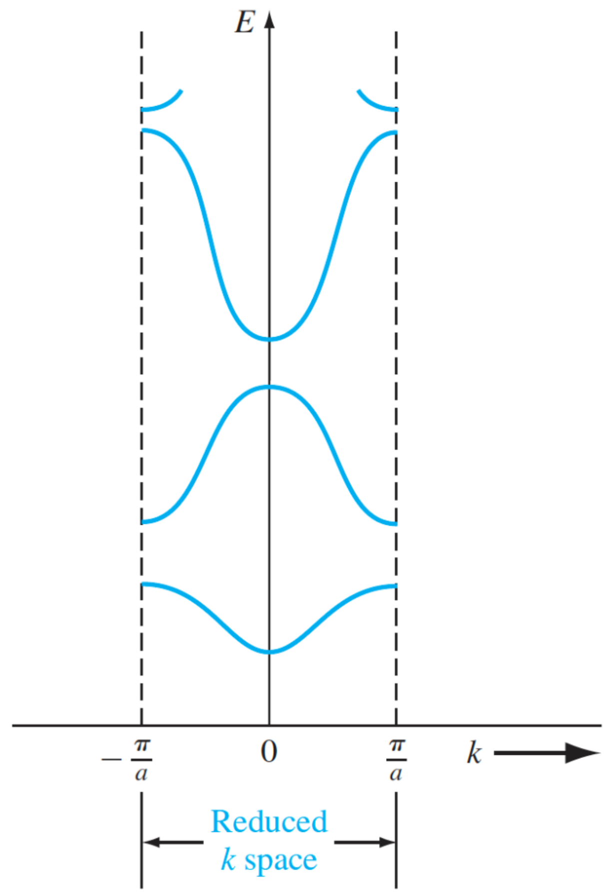


3.1 Allowed and Forbidden Energy Bands

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

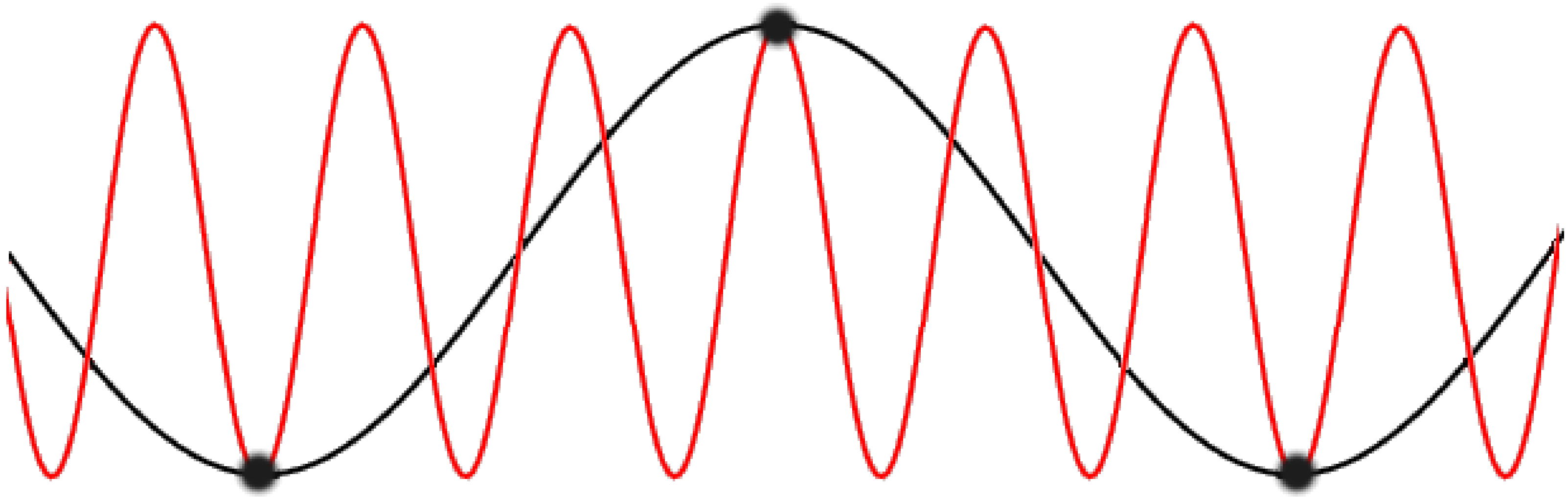


1st Brillouis zone



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**
- 3.3 Extension to Three Dimensions
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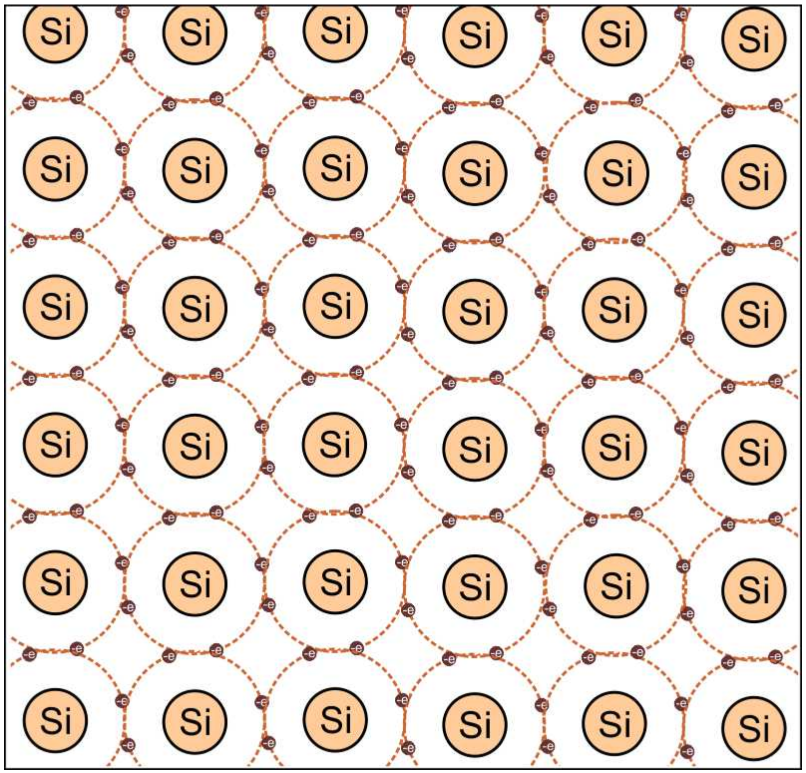
3.2 Electrical Conduction in Solids

The energy band and the bond model

at 0K

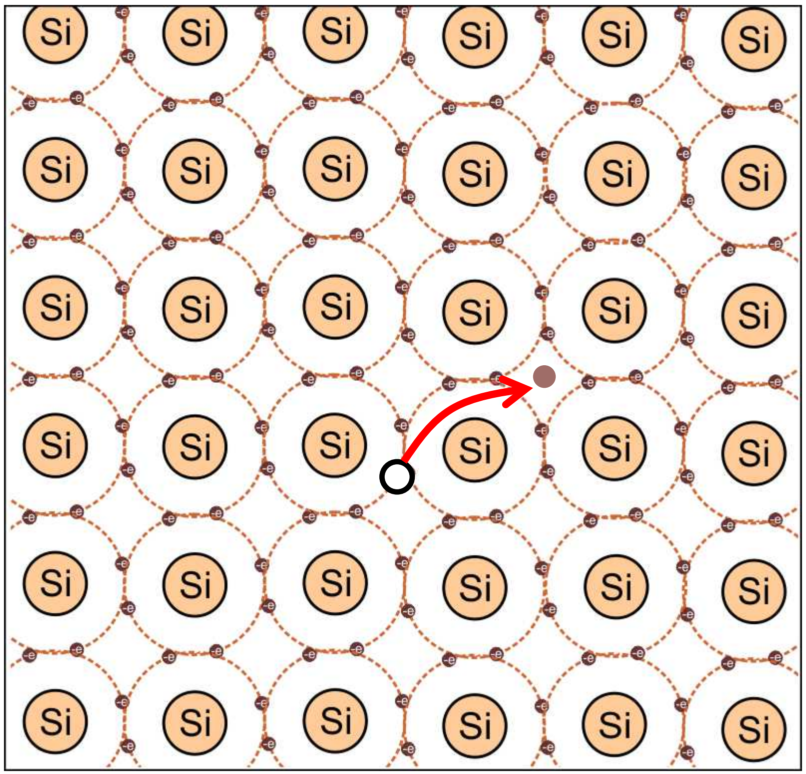


Intrinsic Silicon

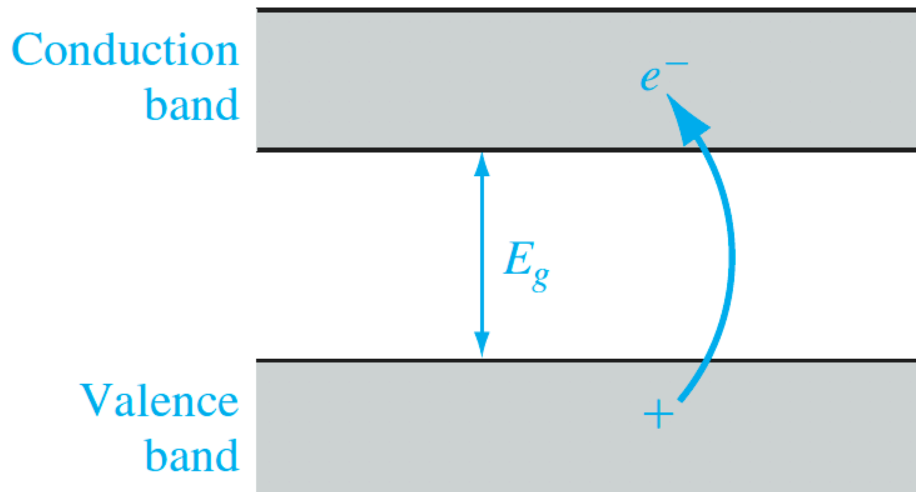
3.2 Electrical Conduction in Solids

<u>The energy band and the bond model</u>

> 0K



Intrinsic Silicon

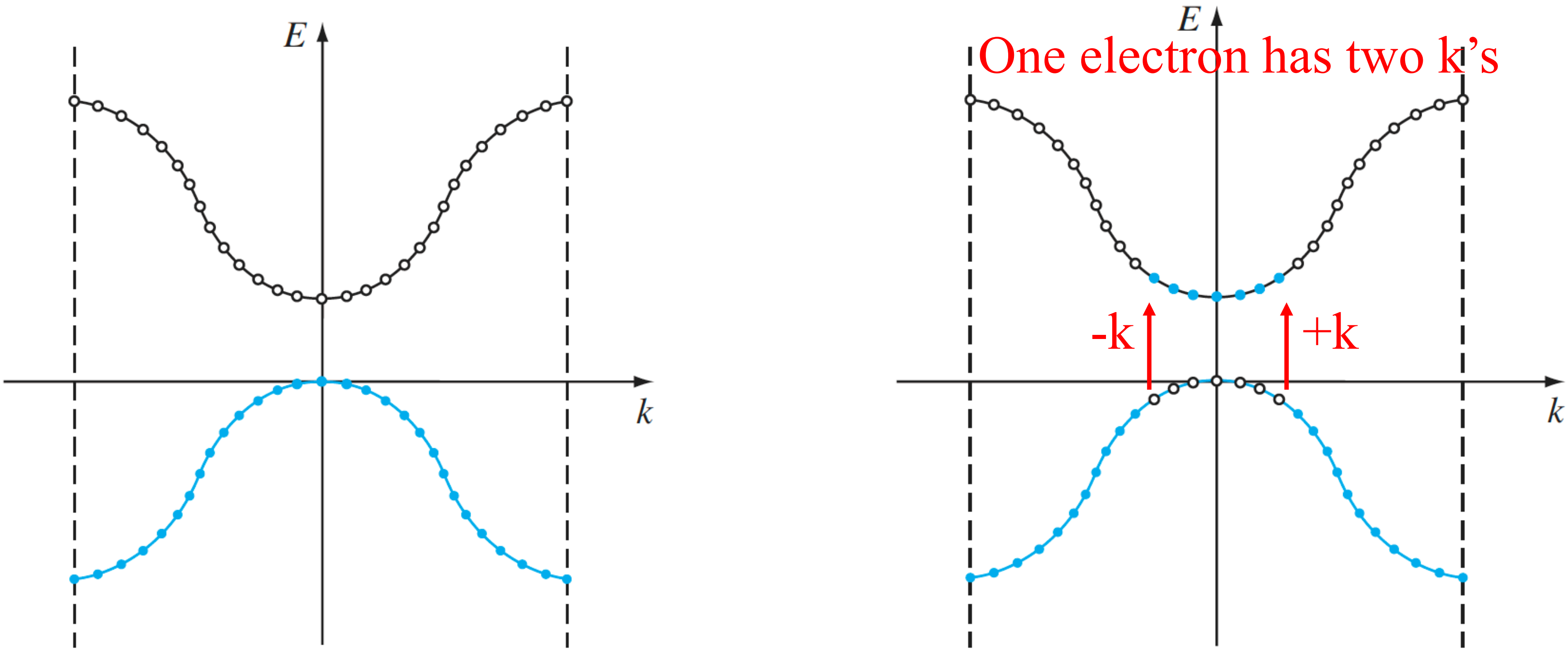


3.2 Electrical Conduction in Solids

The energy band and the bond model

At 0K

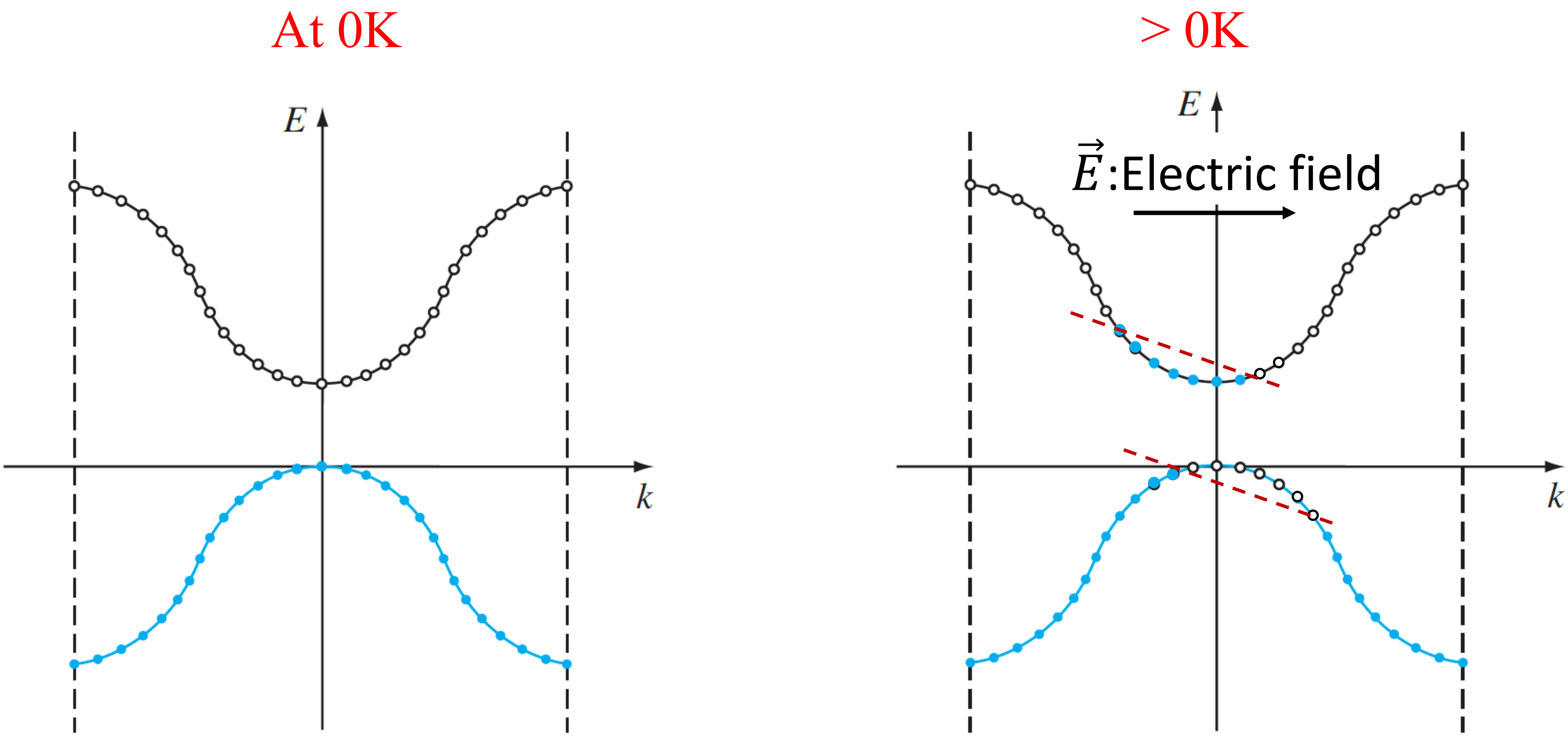
> 0K



(a) (b)

3.2 Electrical Conduction in Solids

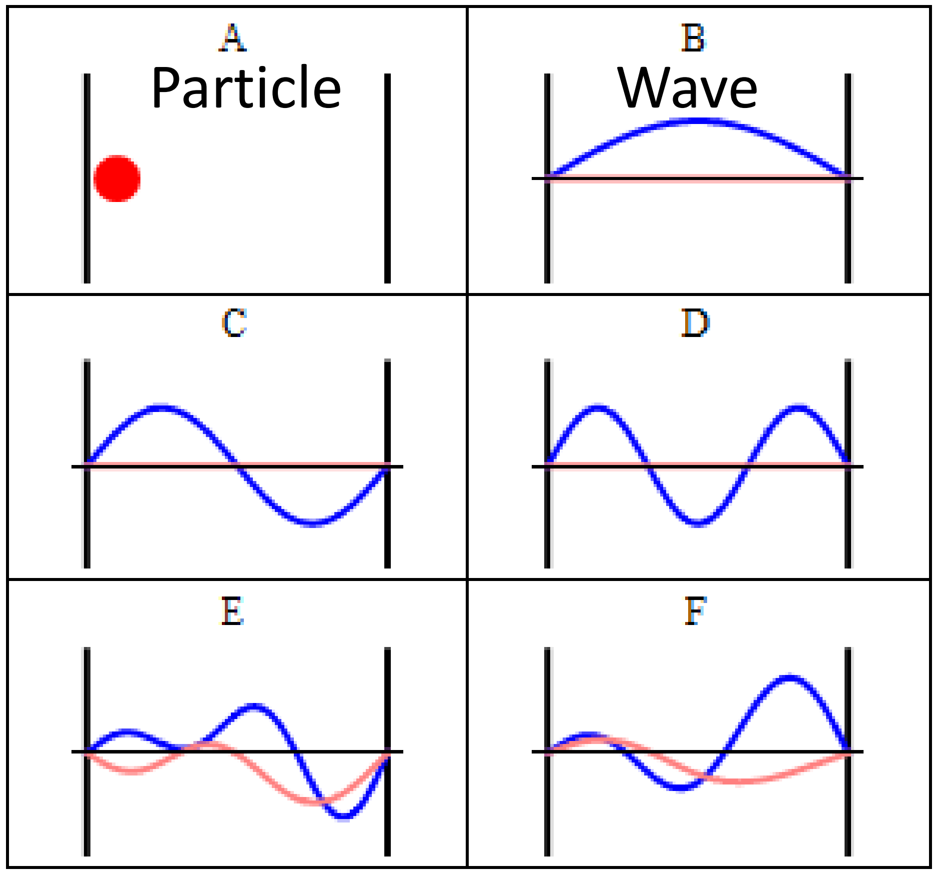
Drift Current



(a) (b)

3.2 Electrical Conduction in Solids

Drift Current



3.2 Electrical Conduction in Solids

Drift Current

$$p = \hbar k = m\upsilon$$

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

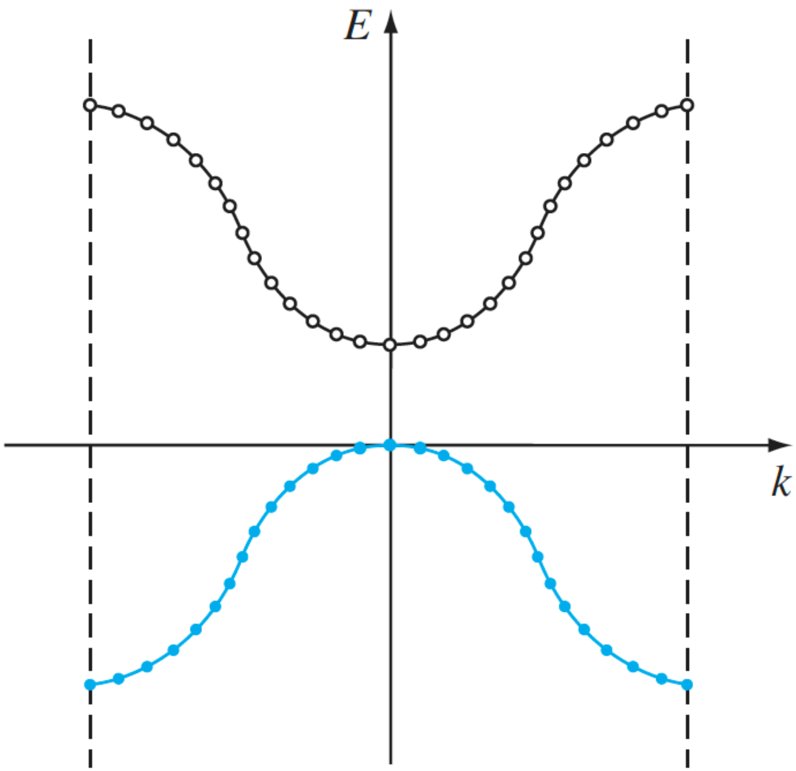
$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

$$\upsilon = \frac{1}{\hbar}\frac{dE}{dk}$$

3.2 Electrical Conduction in Solids

Drift Current

At 0K

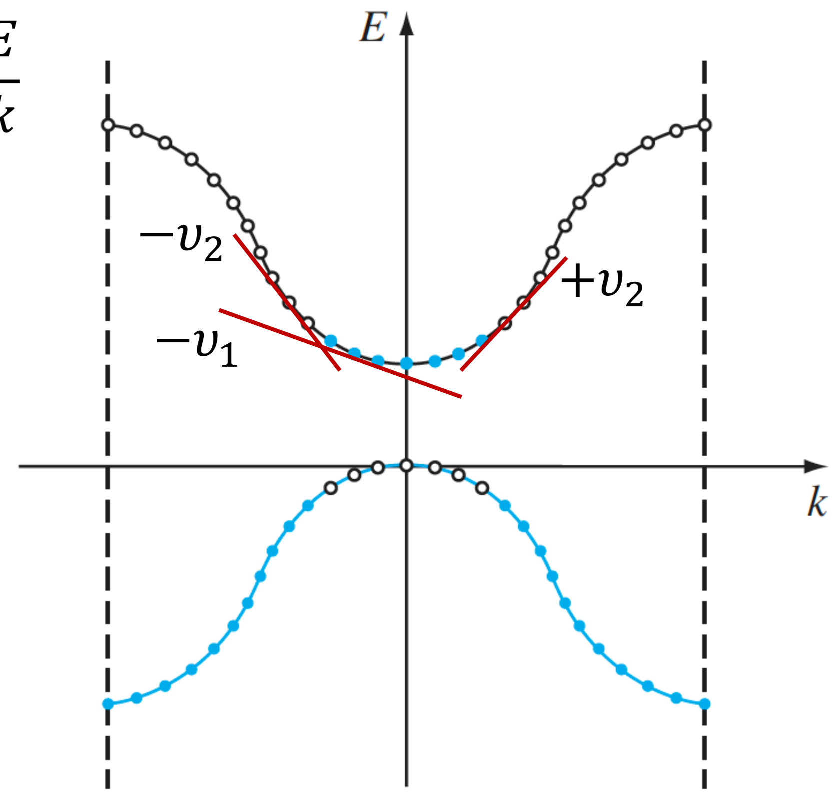


(a)

$$\upsilon = \frac{1}{\hbar}\frac{dE}{dk}$$

$$\upsilon_2 > \upsilon_1$$

> 0K



(b)

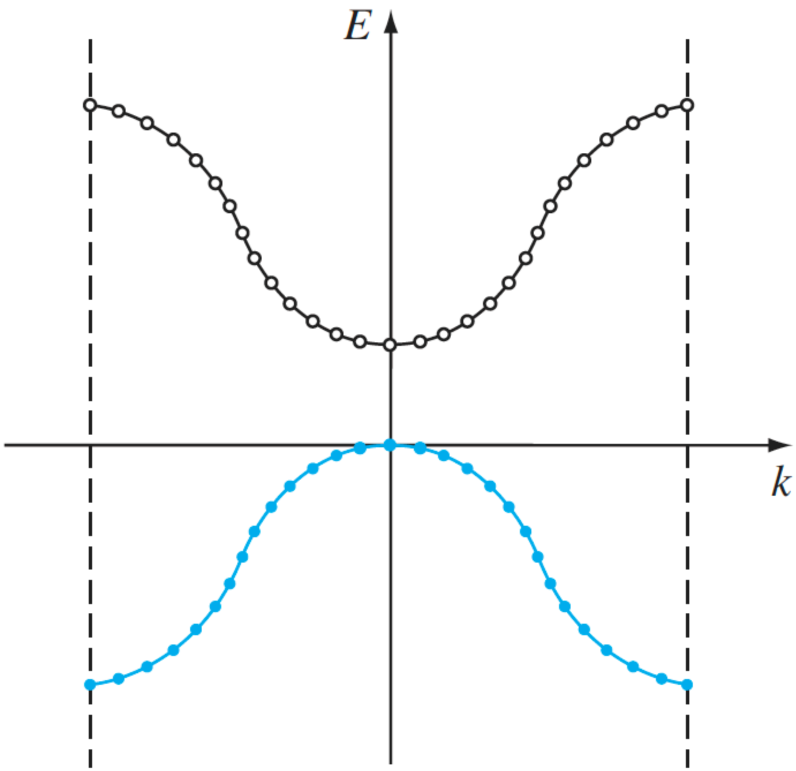
3.2 Electrical Conduction in Solids

Drift Current

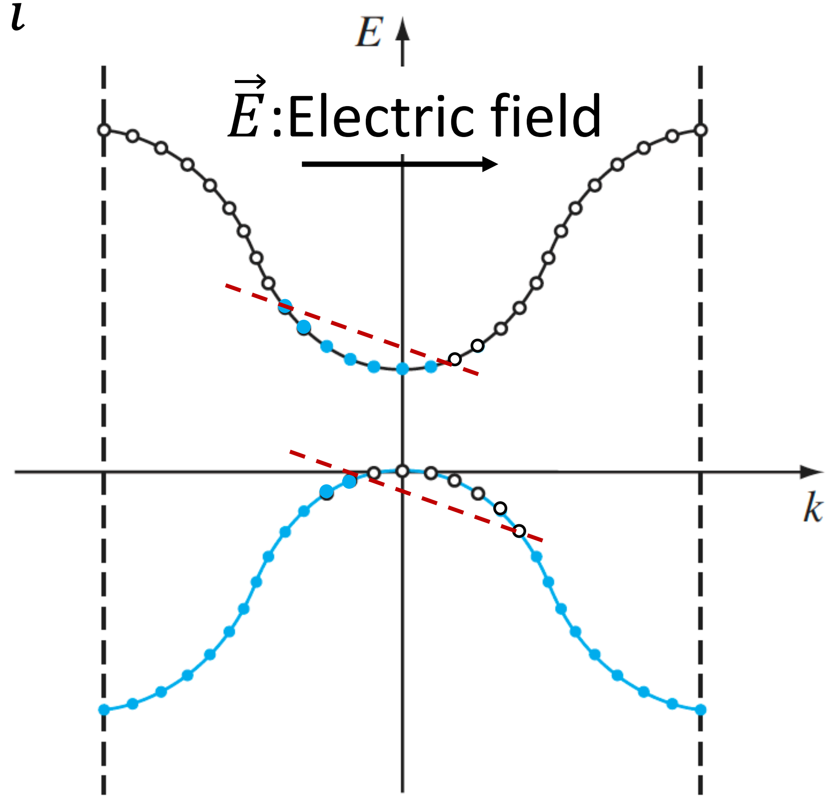
$$J = qNv_d = q\sum_{i}^{N} v_i$$

At 0K

> 0K



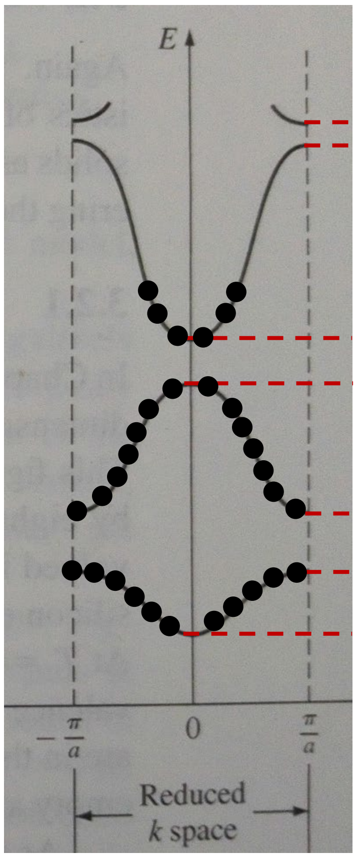
(a)



(b)

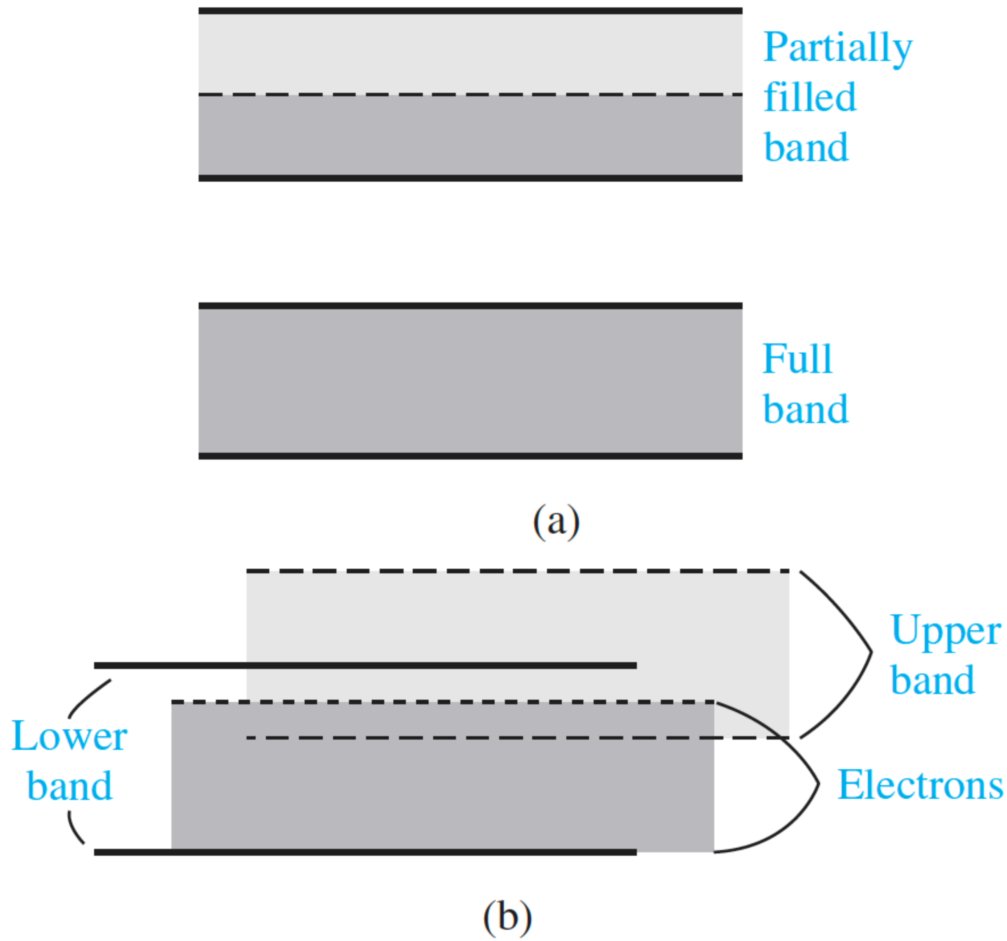
3.2 Electrical Conduction in Solids

<u>Metals, semiconductors and insulators</u>



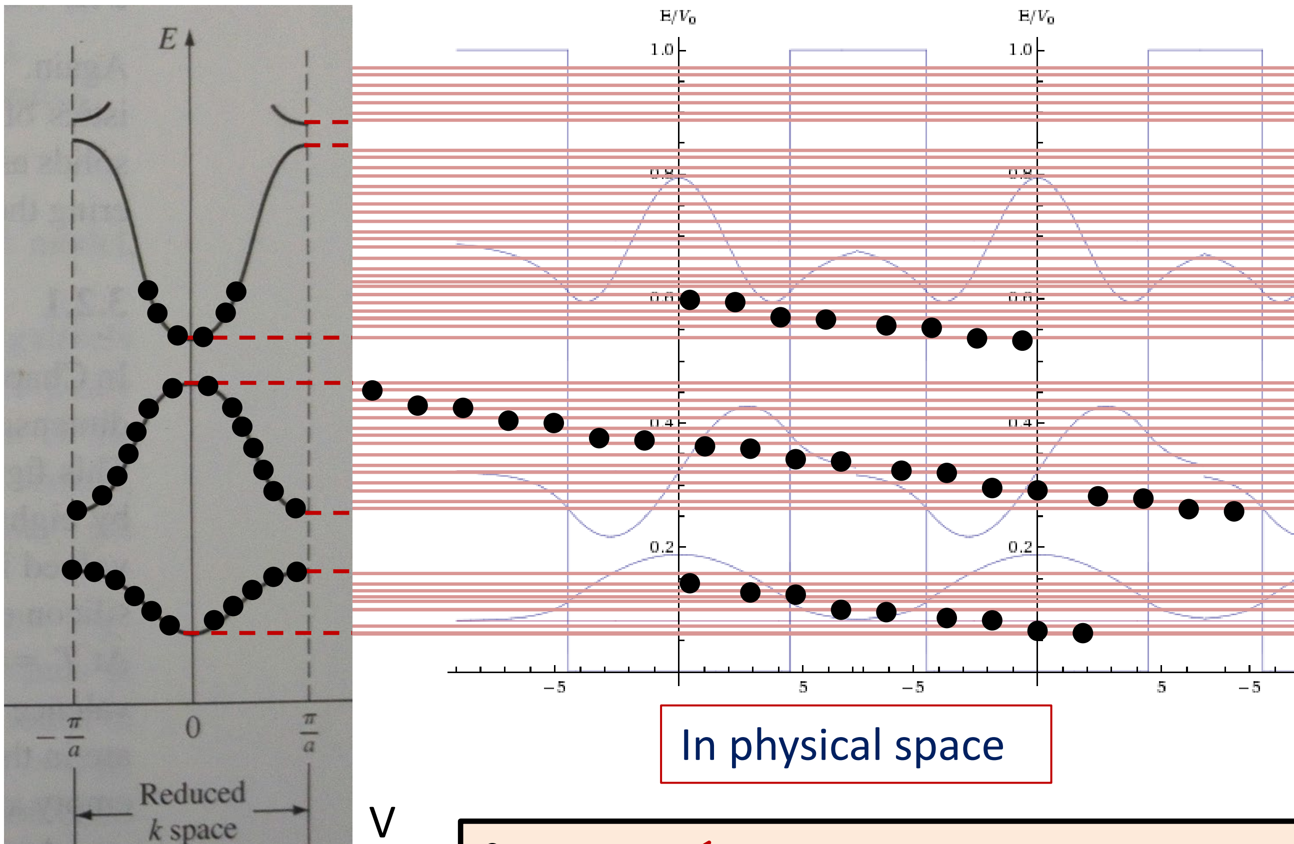
In k space

Forming energy bands is complicated.



3.2 Electrical Conduction in Solids

Metals, semiconductors and insulators



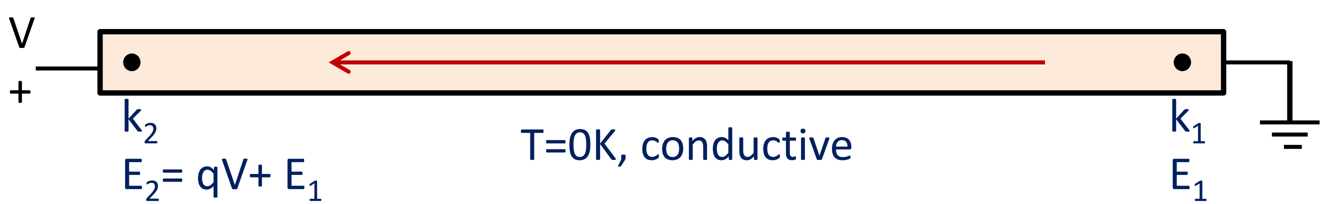
Metals

Partially filled

Completely filled

In physical space

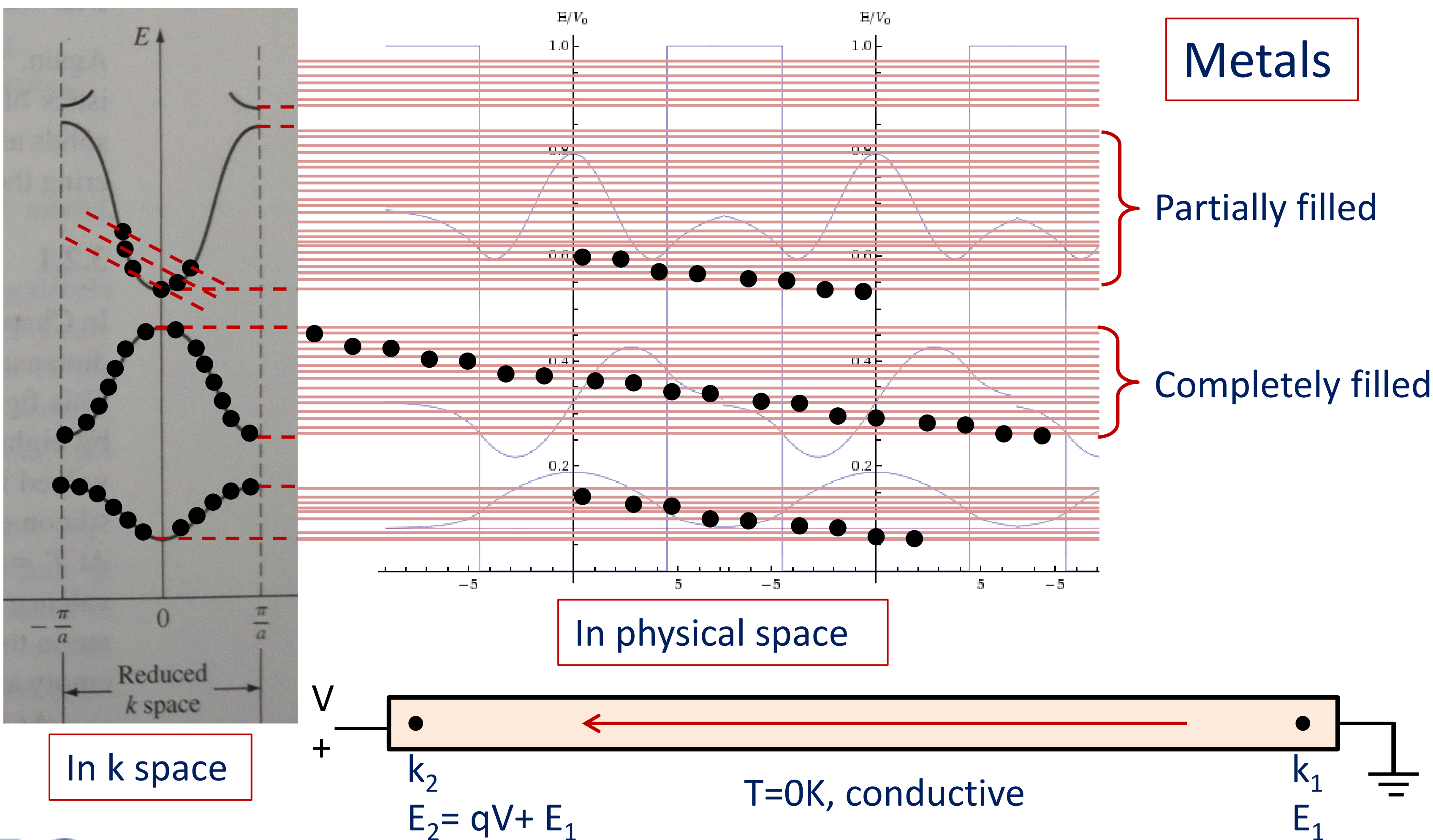
In k space



T=0K, conductive

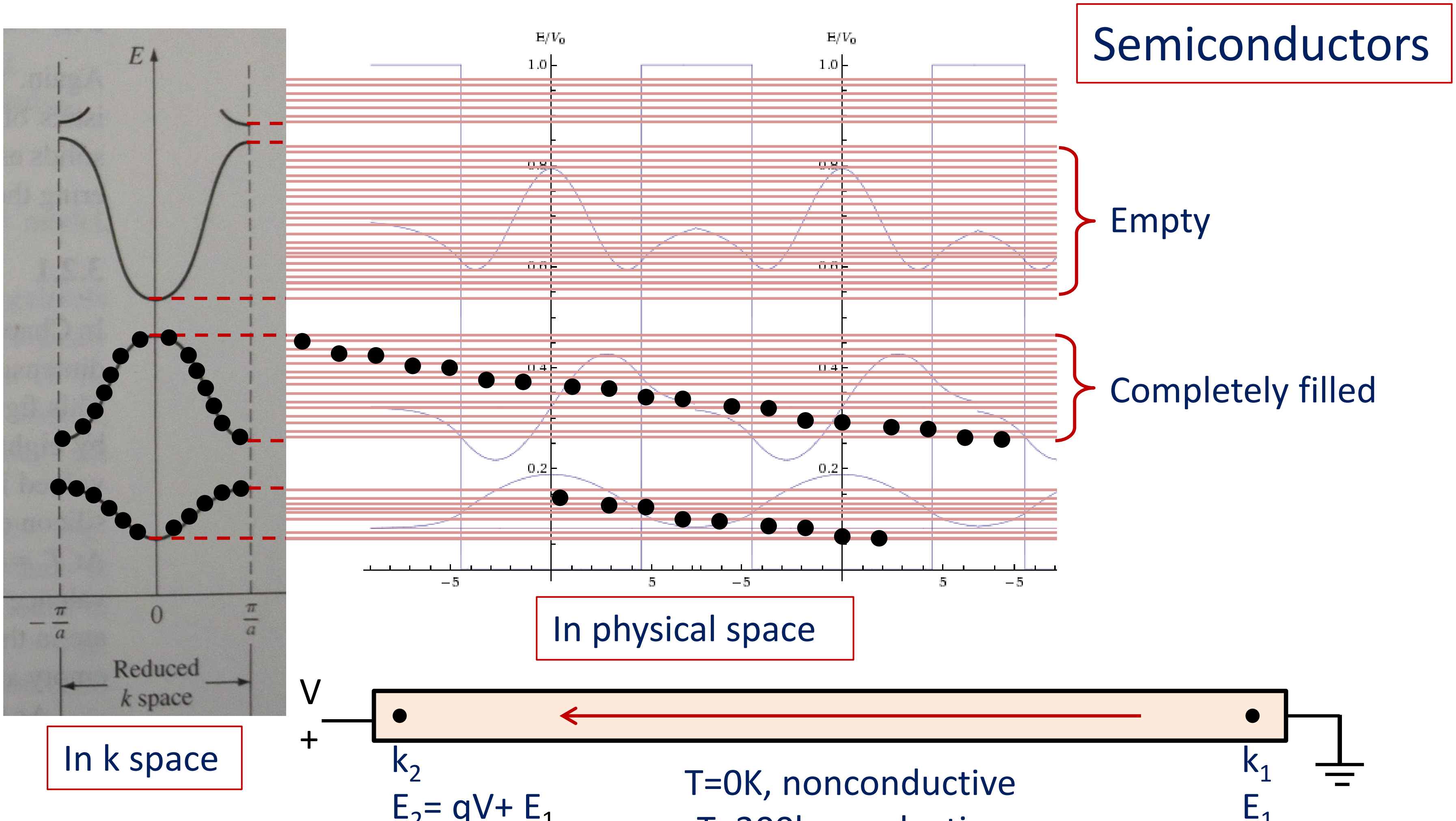
3.2 Electrical Conduction in Solids

Metals, semiconductors and insulators



3.2 Electrical Conduction in Solids

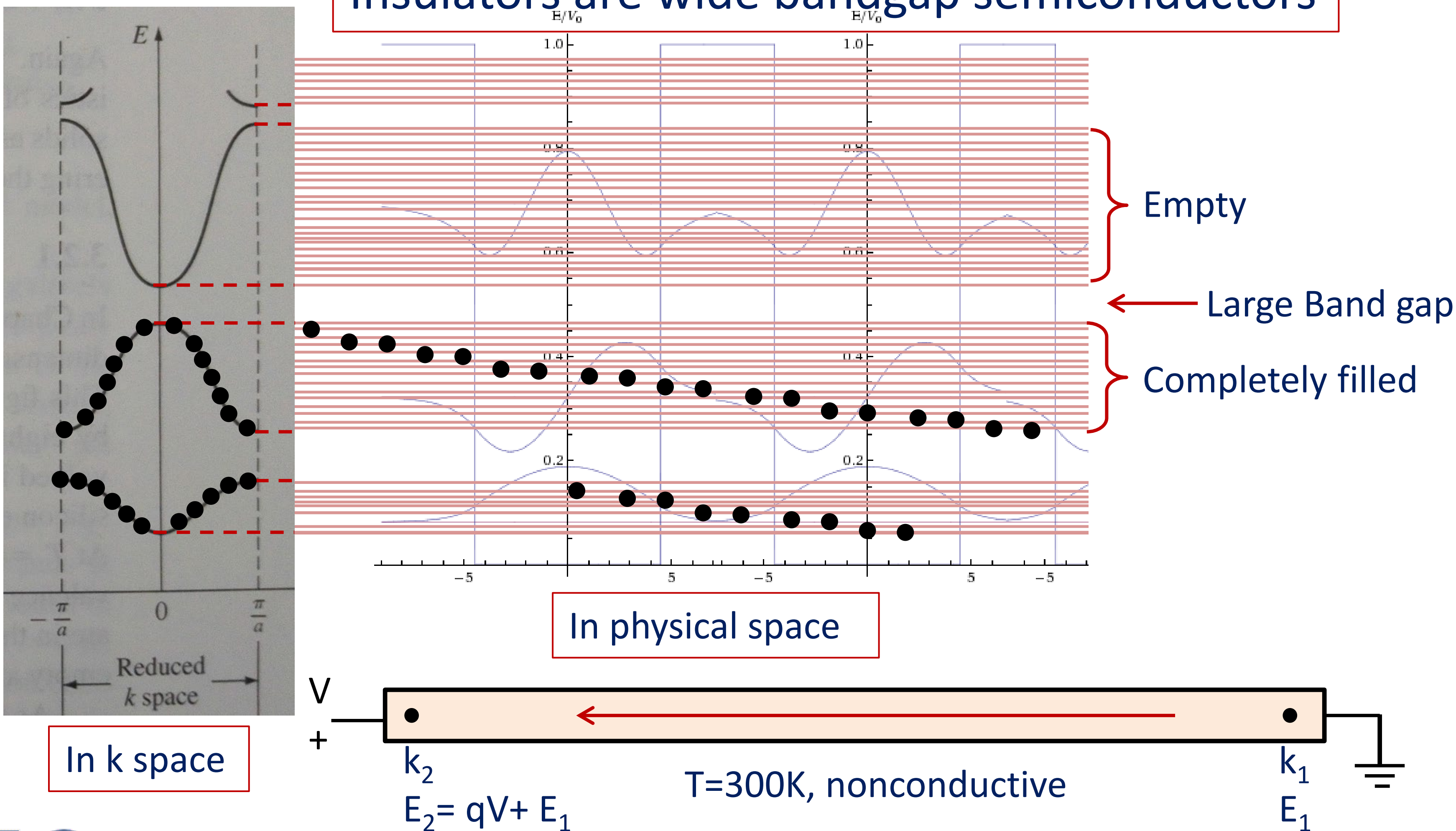
Metals, semiconductors and insulators



3.2 Electrical Conduction in Solids

Metals, semiconductors and insulators

Insulators are wide bandgap semiconductors



3.2 Electrical Conduction in Solids

Doping in semiconductors

Intrinsic semiconductors:
pure semiconductor, no doping, no defects

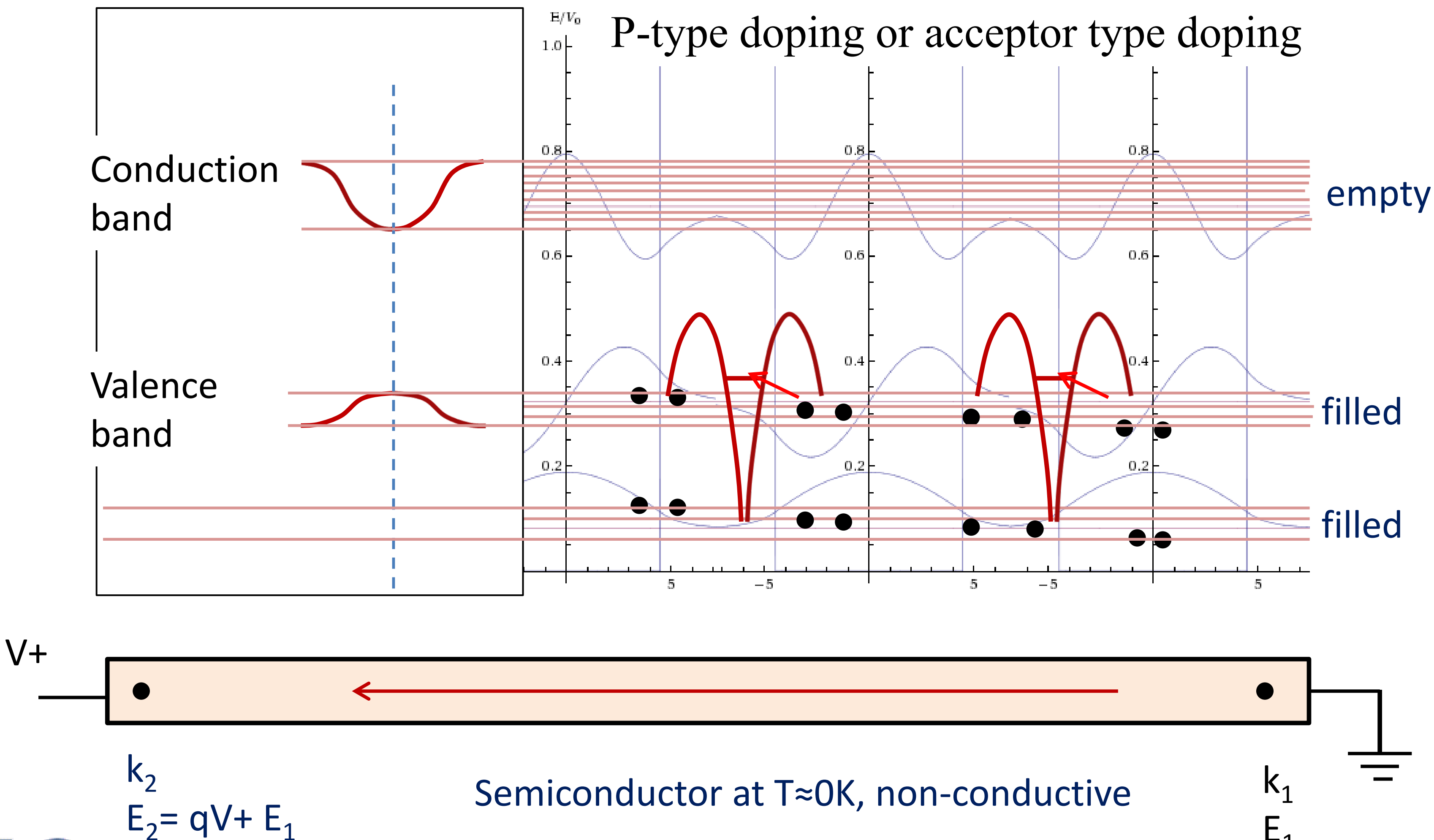
n-type semiconductors :
Charge carriers are negative, i.e. electrons
Doped by donor-type of dopants (impurities)

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

3.2 Electrical Conduction in Solids

Doping in semiconductors

P-type doping or acceptor type doping

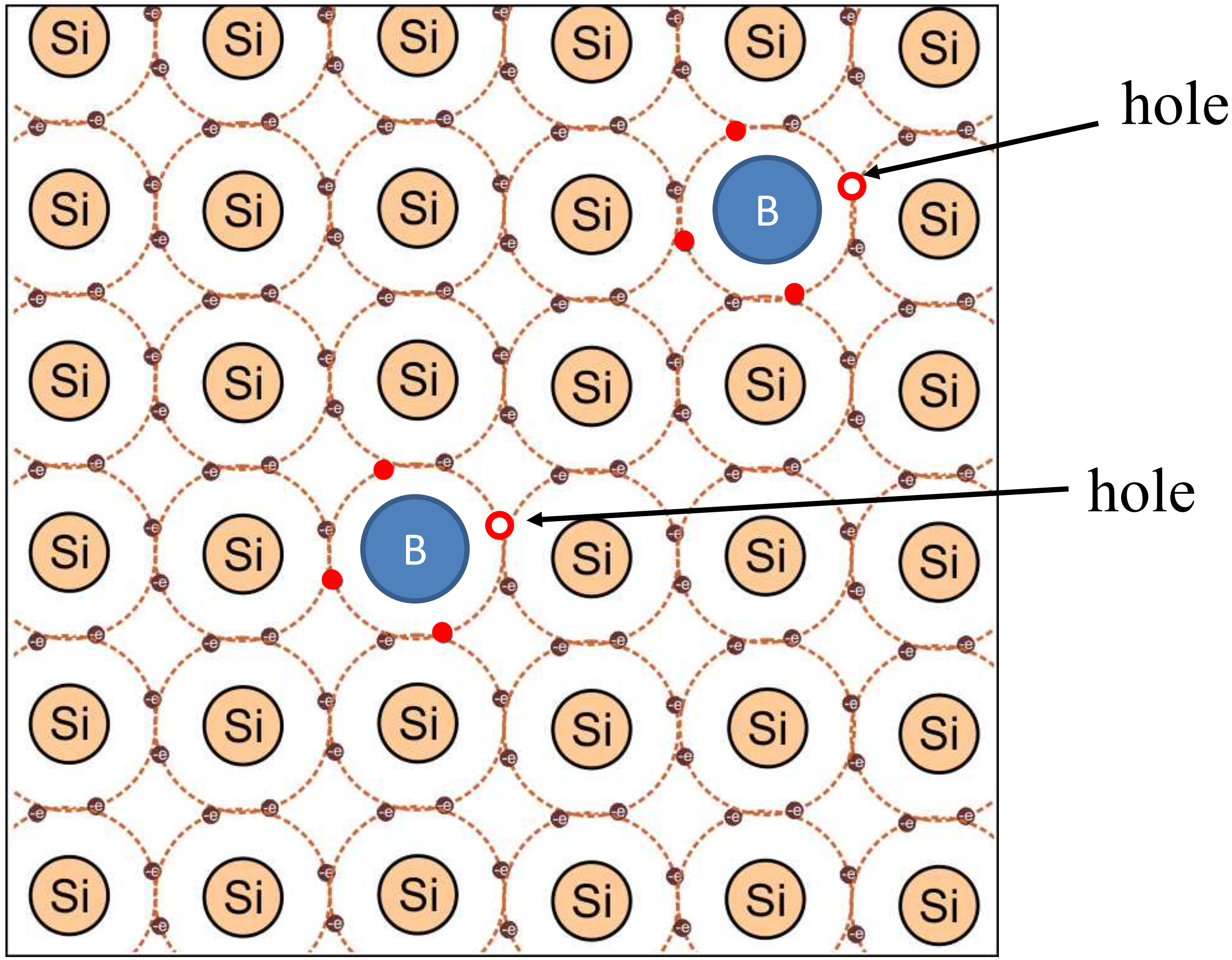


Semiconductor at T≈0K, non-conductive

3.2 Electrical Conduction in Solids

p-type doping

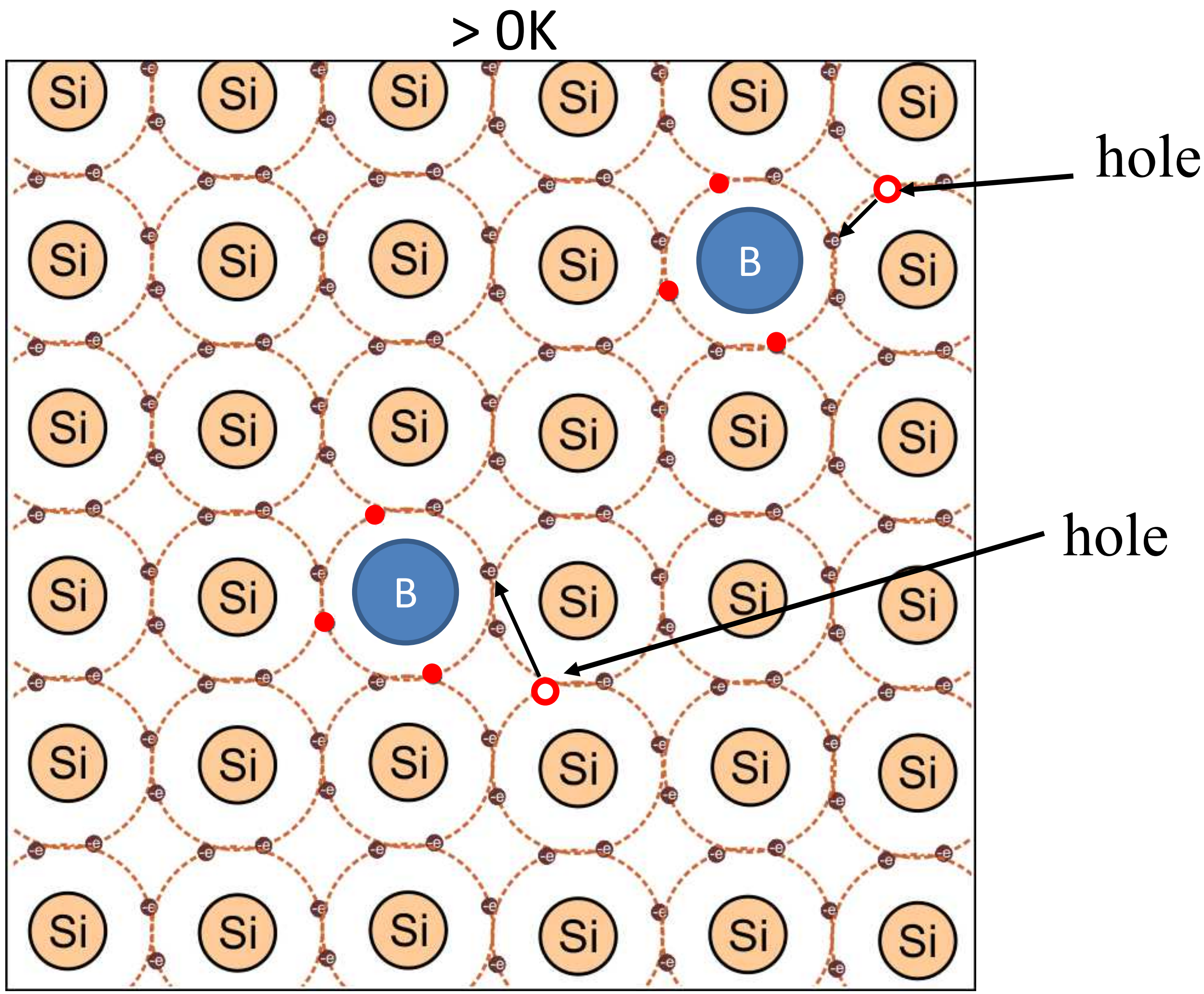
At 0K



Acceptor-type of dopants

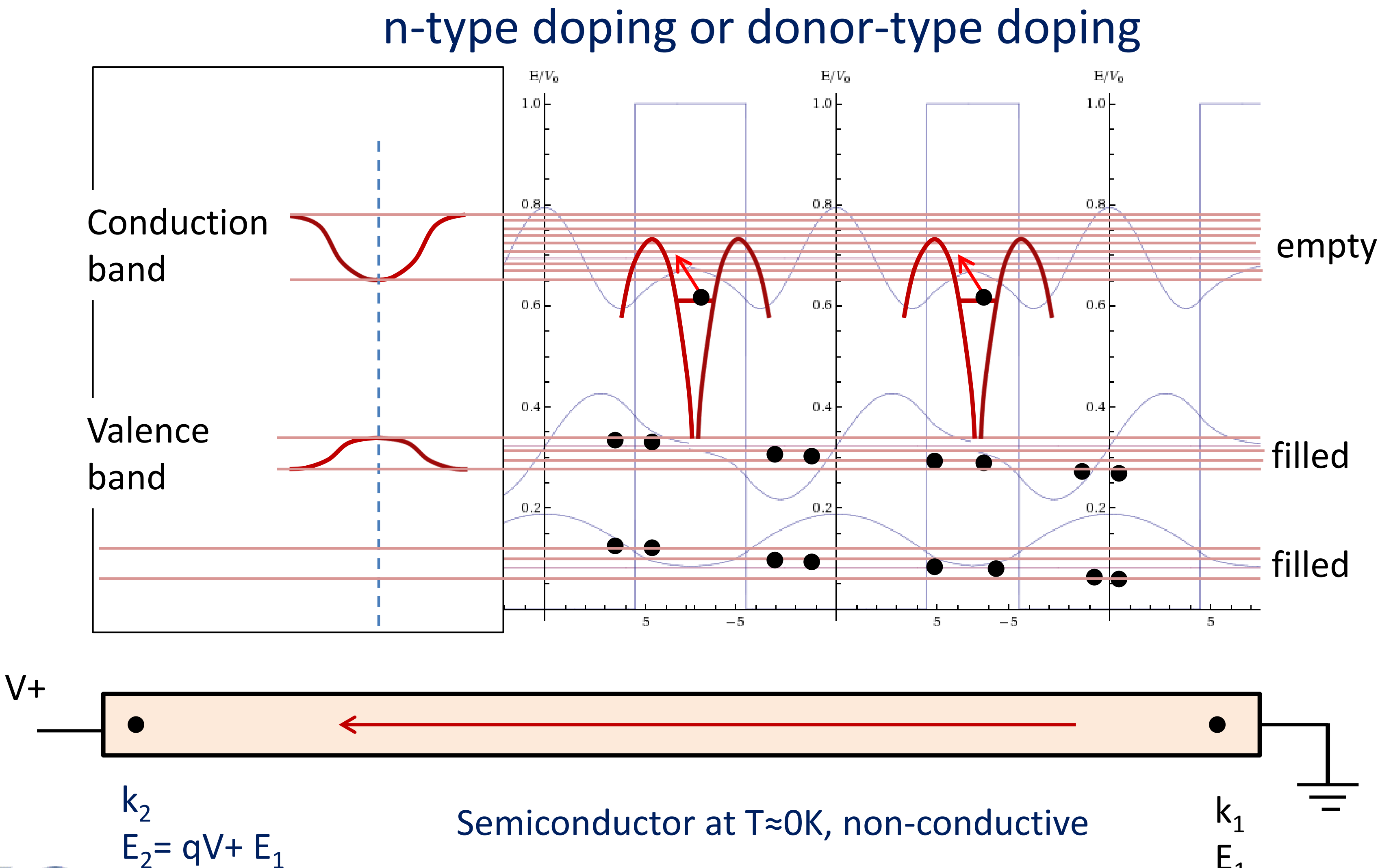
3.2 Electrical Conduction in Solids

p-type doping



Acceptor-type of dopants

3.2 Electrical Conduction in Solids

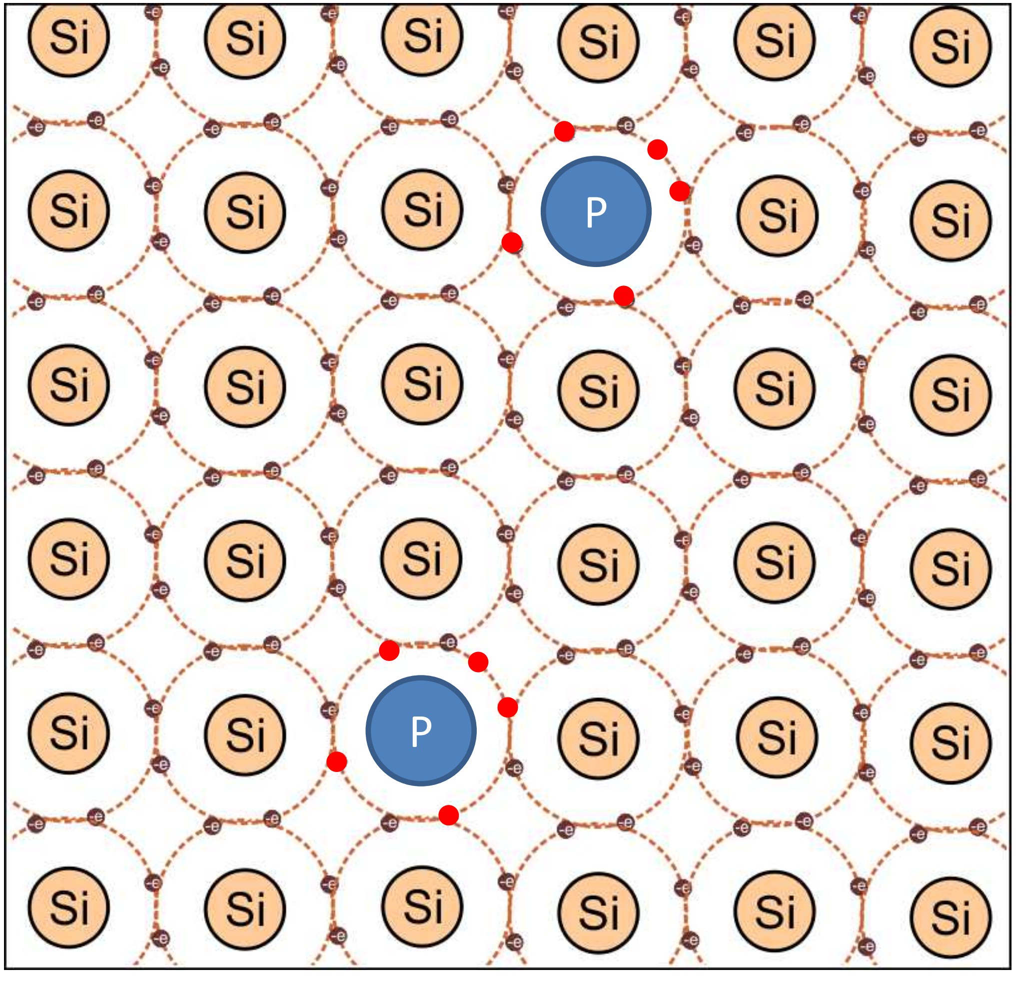


Semiconductor at T≈0K, non-conductive

3.2 Electrical Conduction in Solids

n-type doping

At 0K

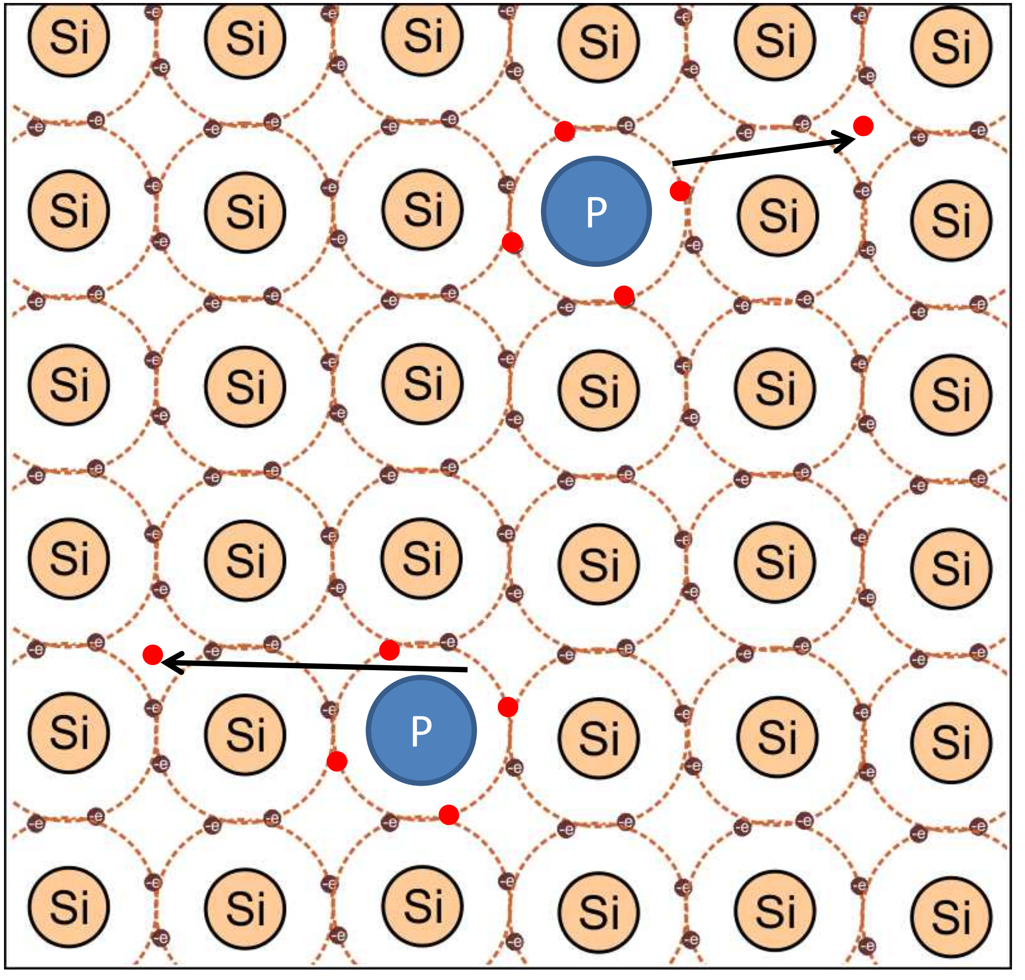


Donor-type of dopants

3.2 Electrical Conduction in Solids

n-type doping

> 0K



Donor-type of dopants

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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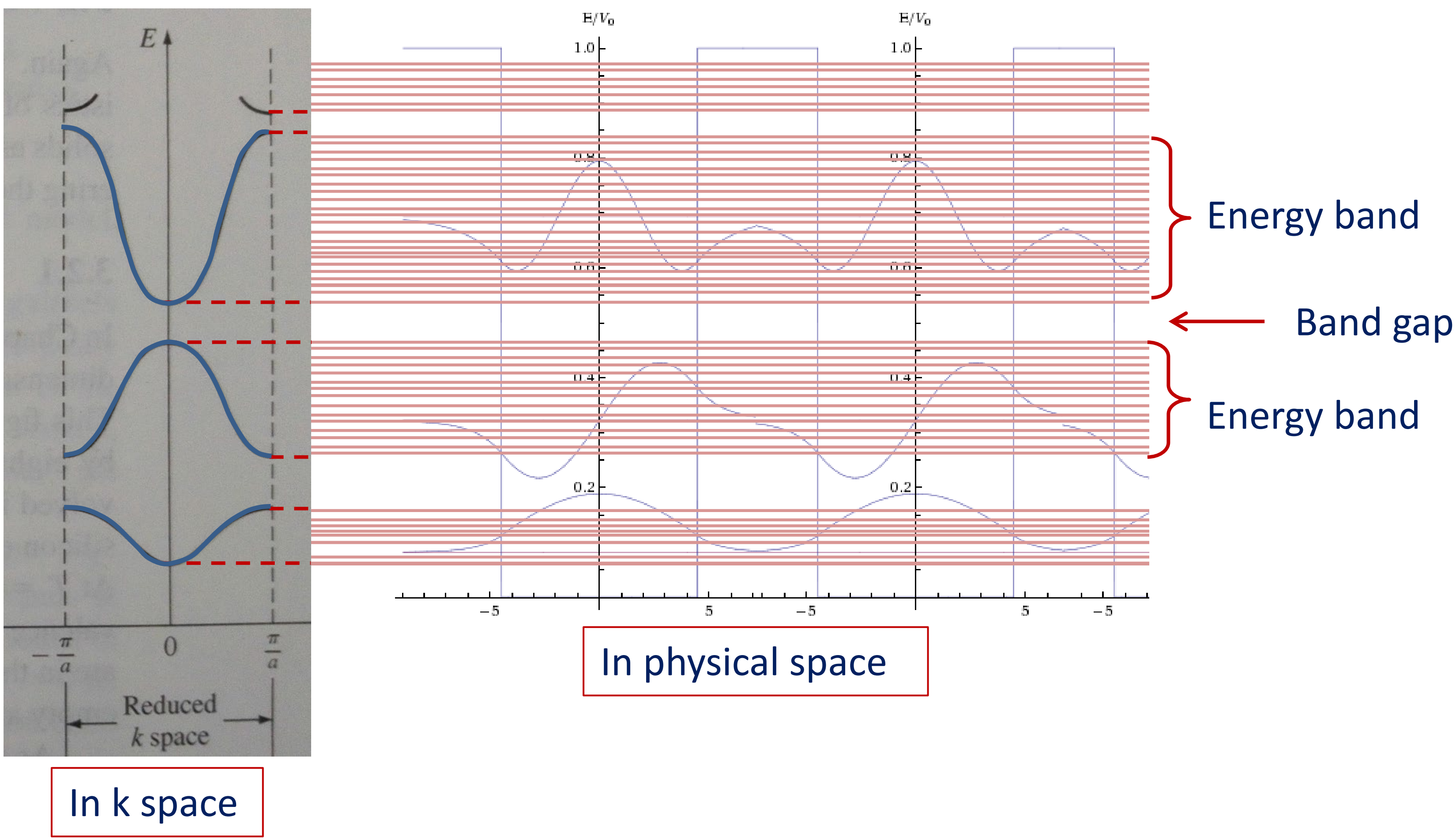
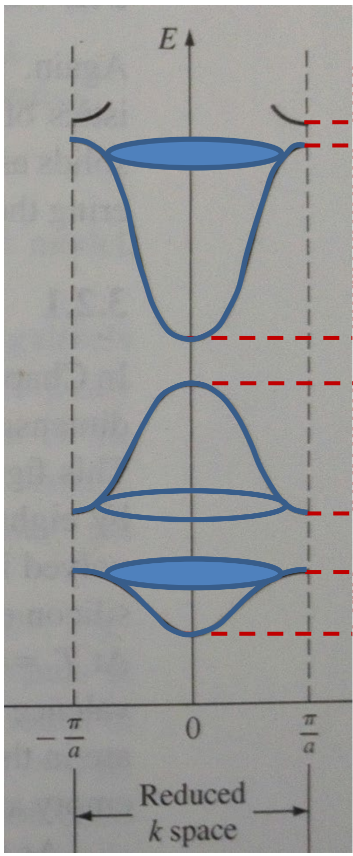
Previously…

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

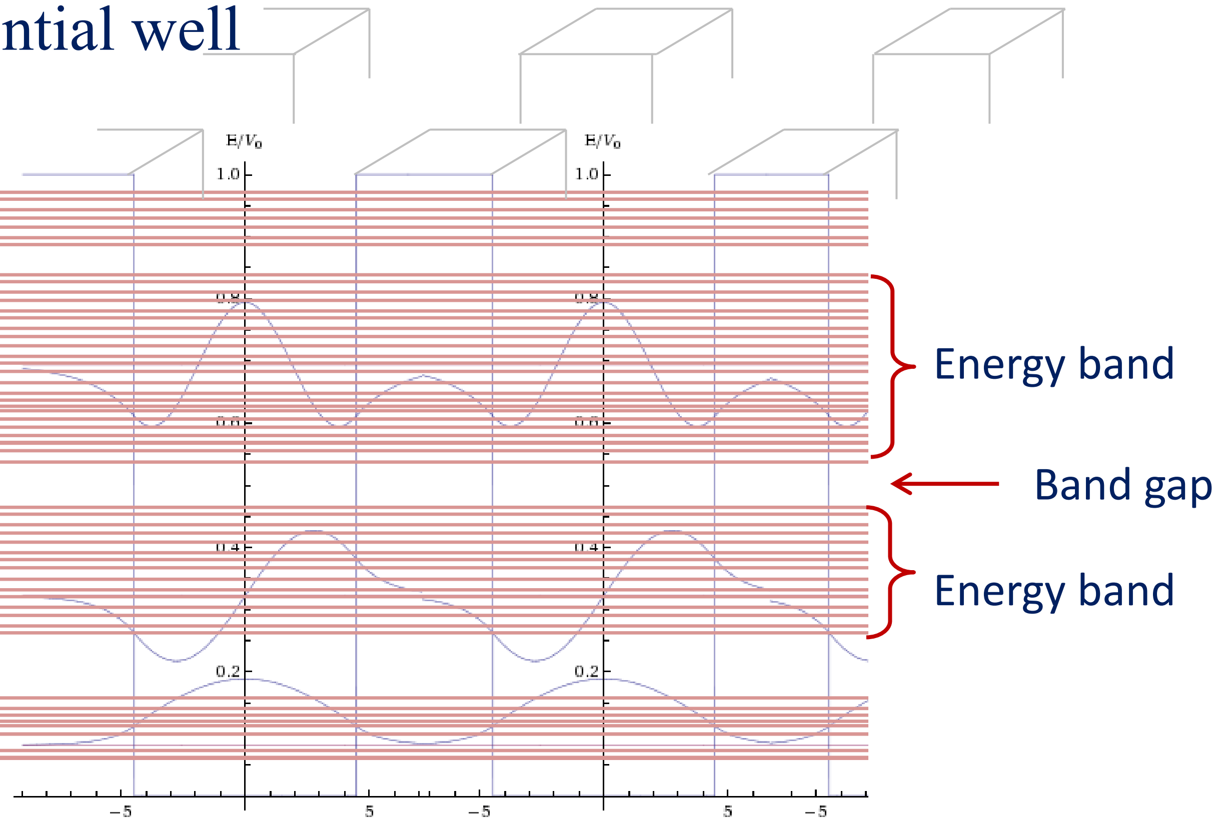


3.3 Extension to Three Dimensions

2D periodic potential well

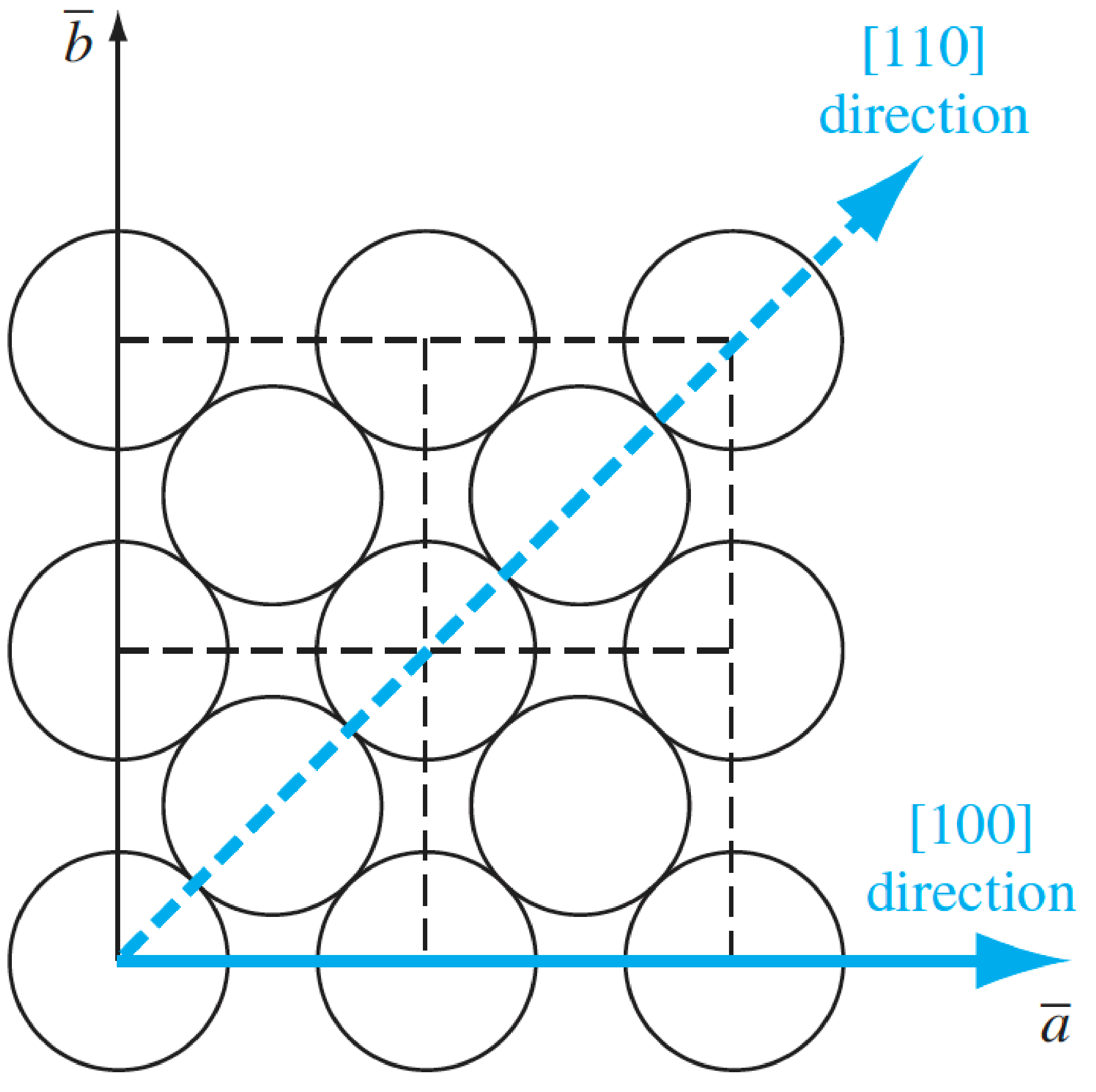


In k space



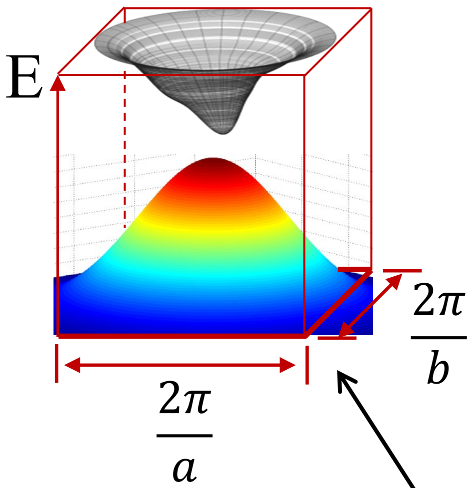
In physical space

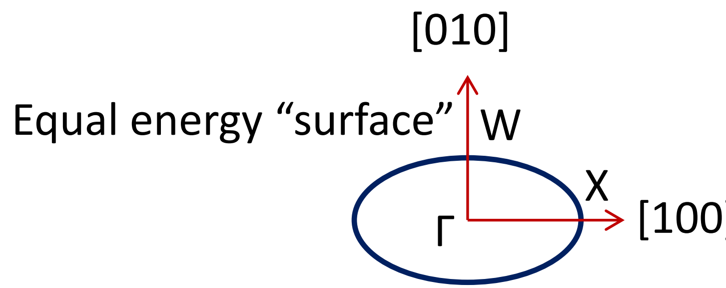
3.3 Extension to Three Dimensions



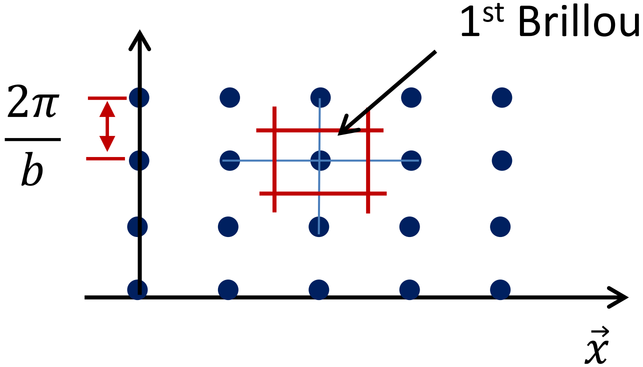
3.3 Extension to Three Dimensions

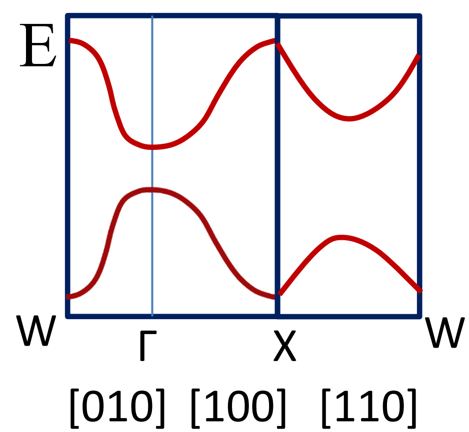
E in 3rd Dimension





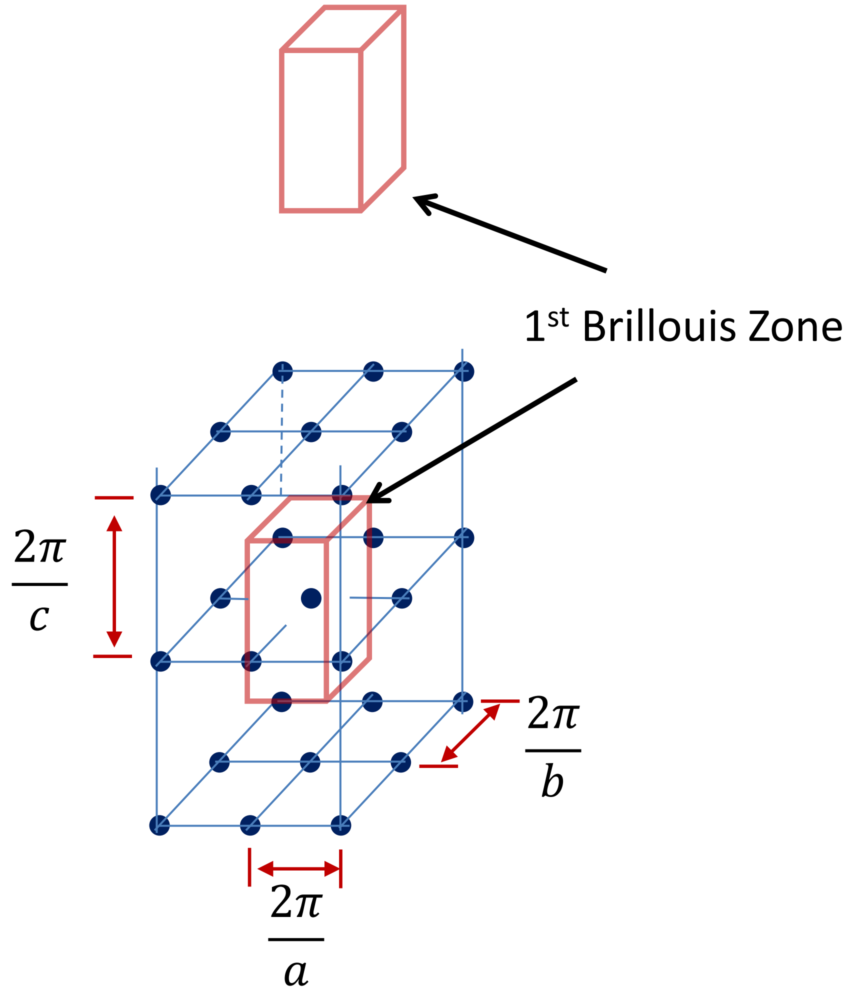
1st Brillouis Zone



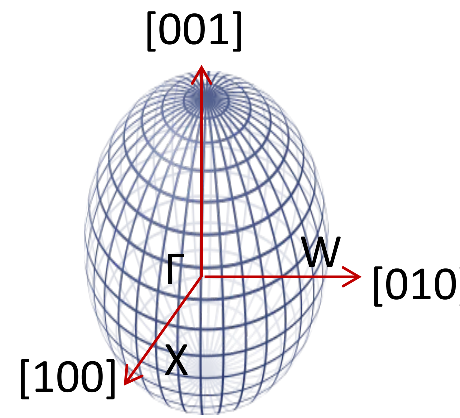


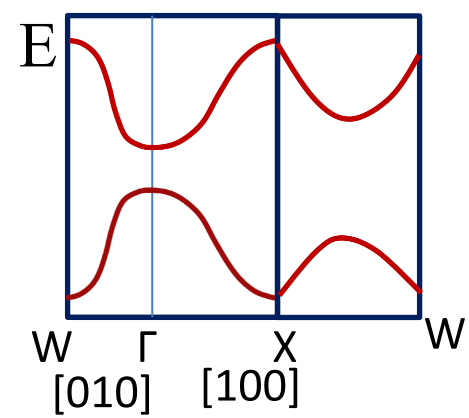
3.3 Extension to Three Dimensions

E in 4th Dimension

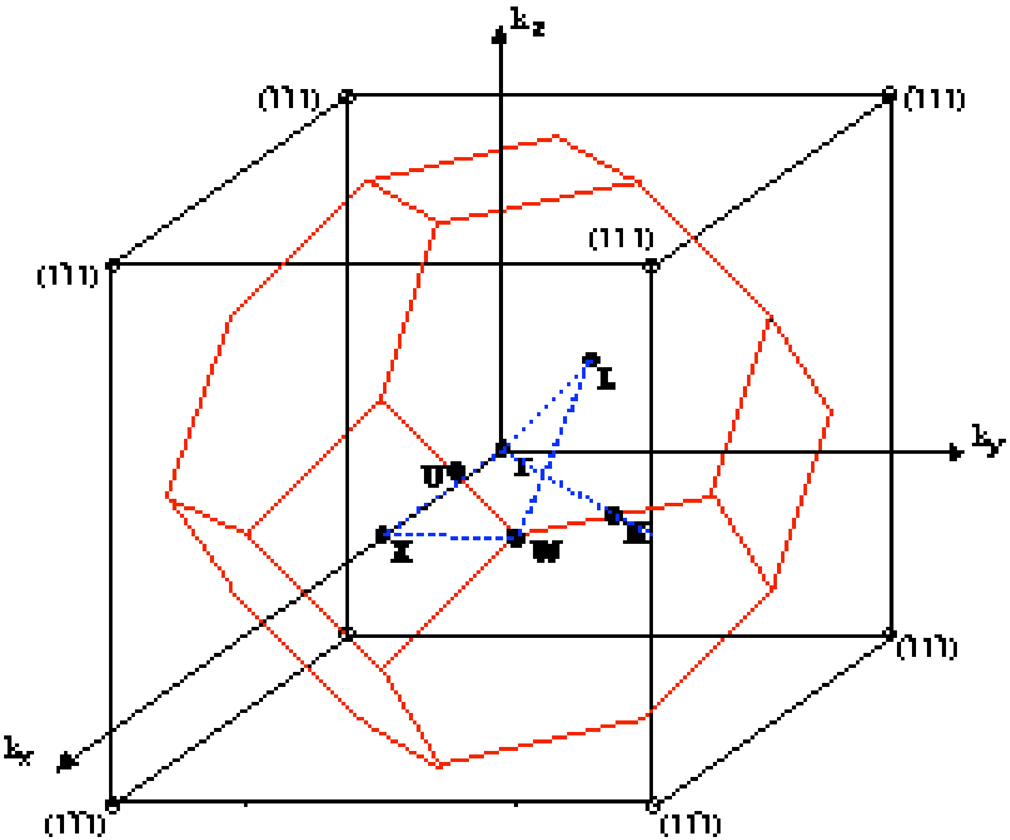


Equal energy "surface"





3.3 Extension to Three Dimensions



Γ - center of the BZ

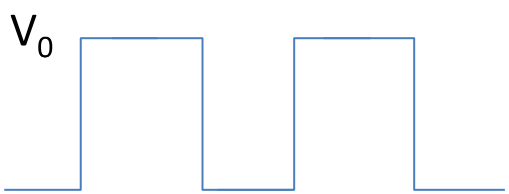
X - [100] intercept; Γ – X path Δ

K - [110] intercept; Γ – K path ∑

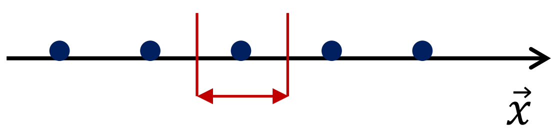
L - [111] intercept; Γ – L path Λ

3.3 Extension to Three Dimensions

Ideal



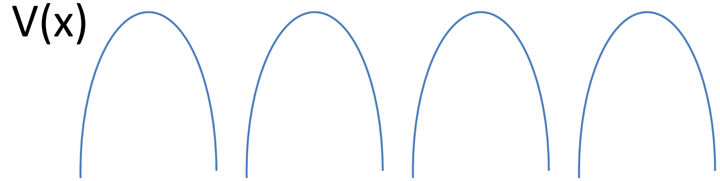
Constant potential



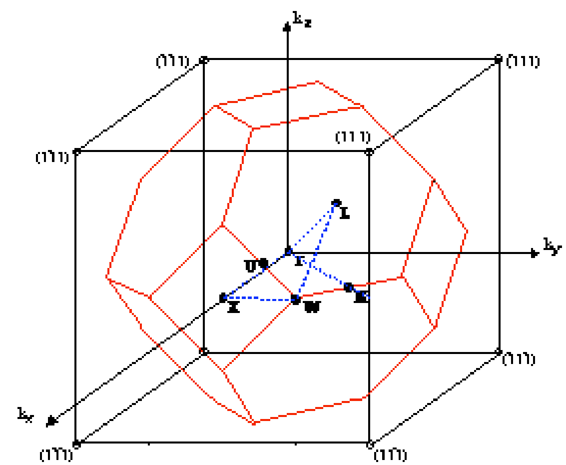
1st Brillouis Zone

Simple 1D structure

Reality



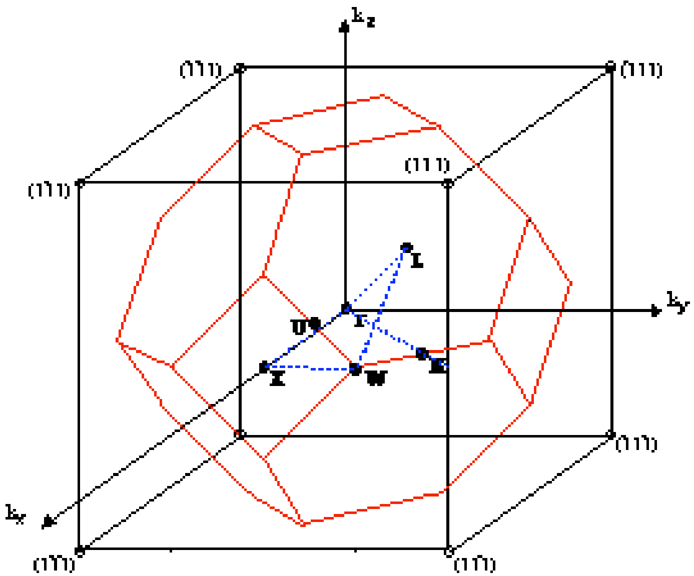
Variable potential

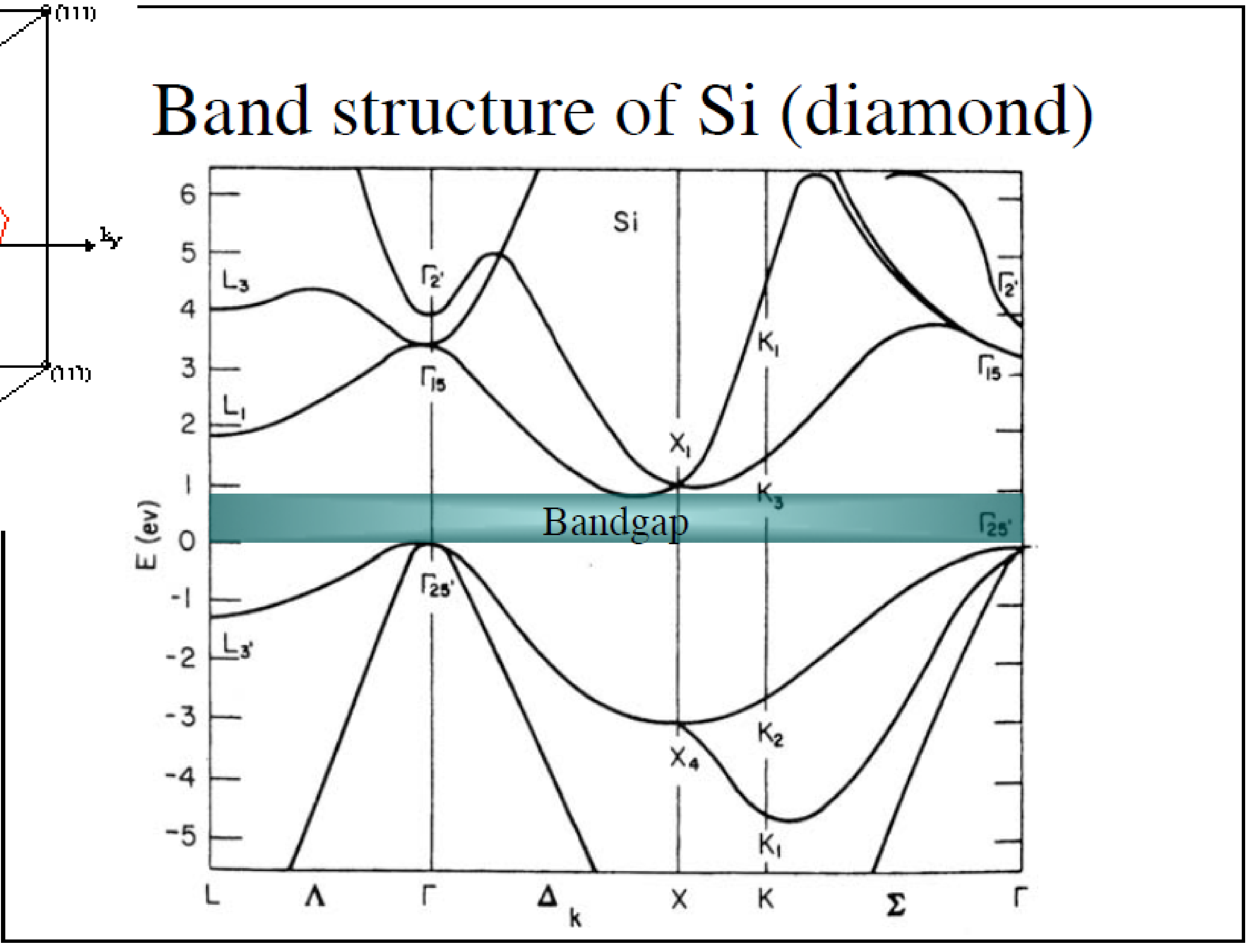


1st Brillouis Zone

Complicated 3D structure

3.3 Extension to Three Dimensions

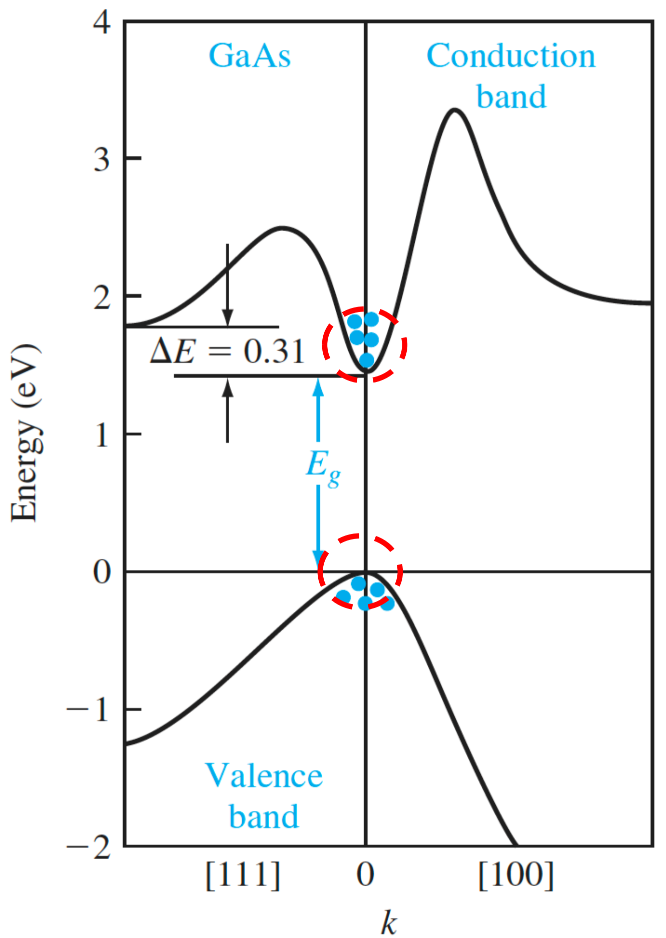




Why is it so complicated?

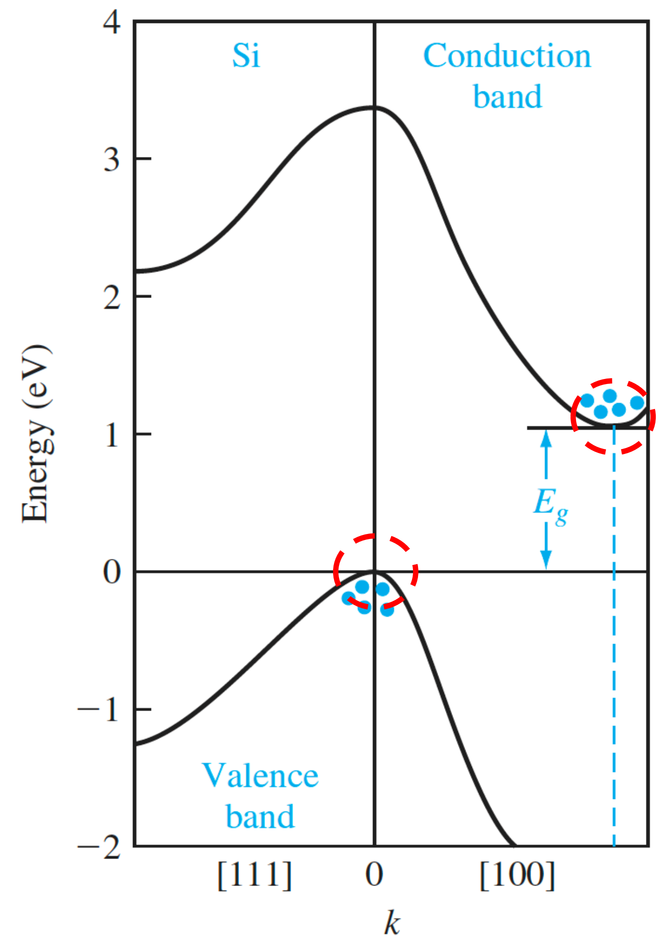
3.3 Extension to Three Dimensions

Direct bandgap



(a)

Indirect bandgap



(b)

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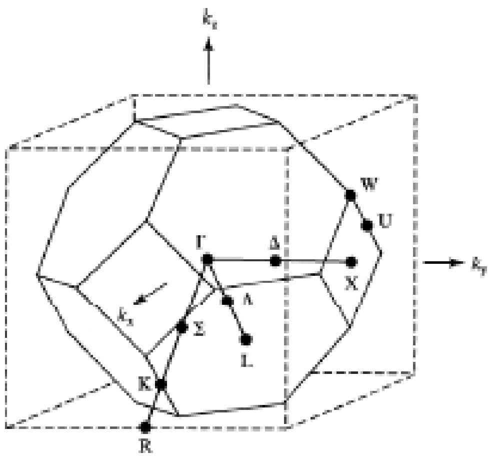
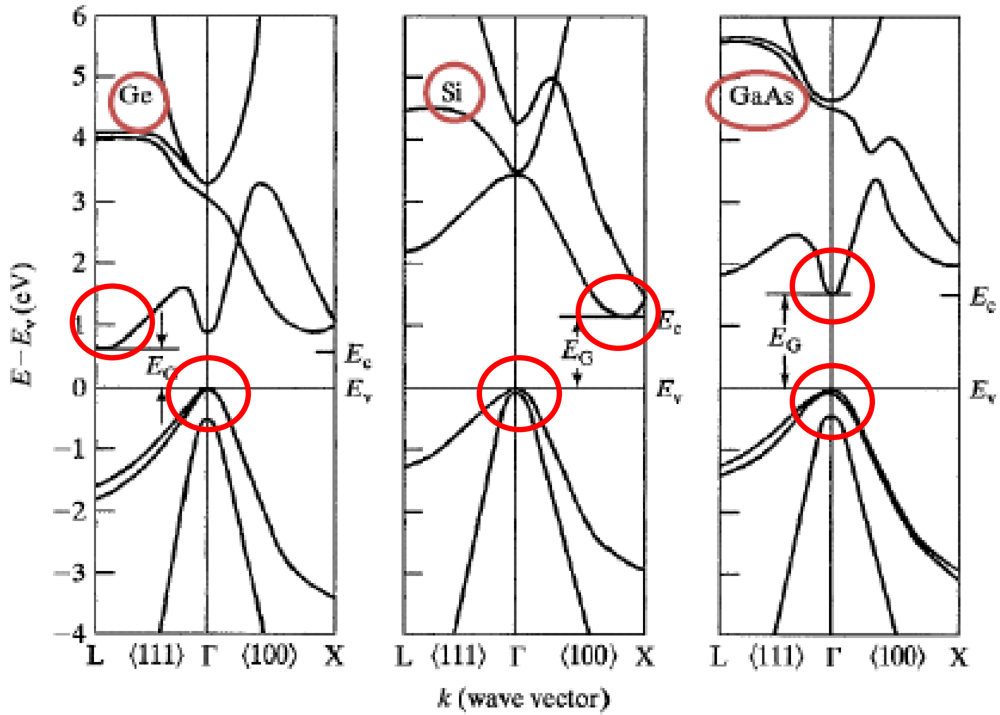
3.4 Effective Mass



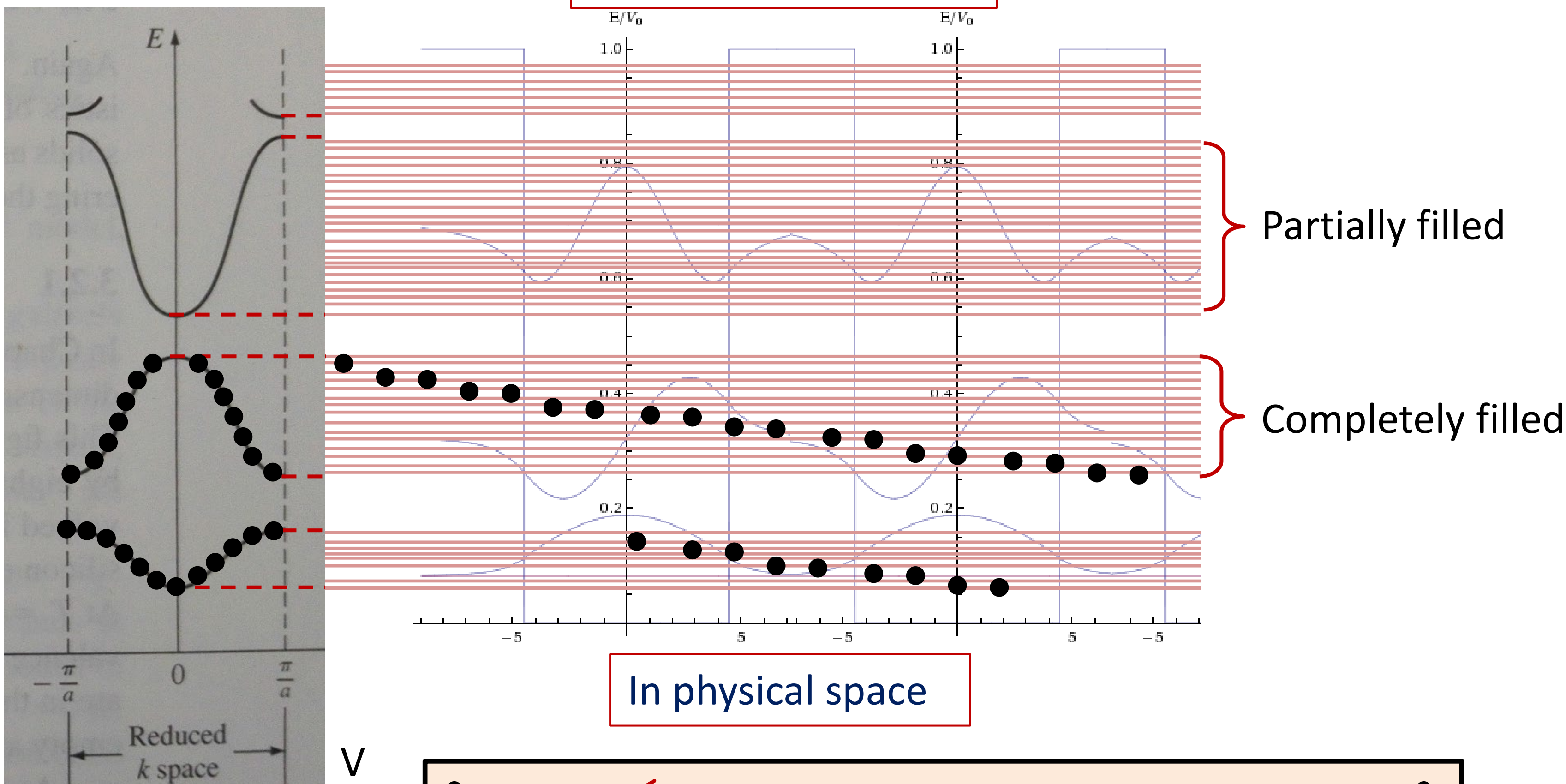


- So far the energy band structure is theoretically calculated.
- How to experimentally find it?

3.4 Effective Mass

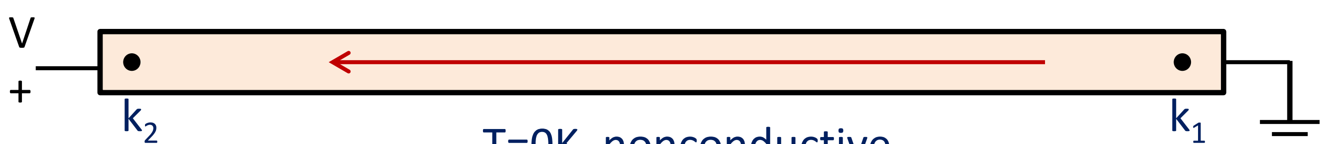
Previously …

Semiconductors



In physical space

In k space

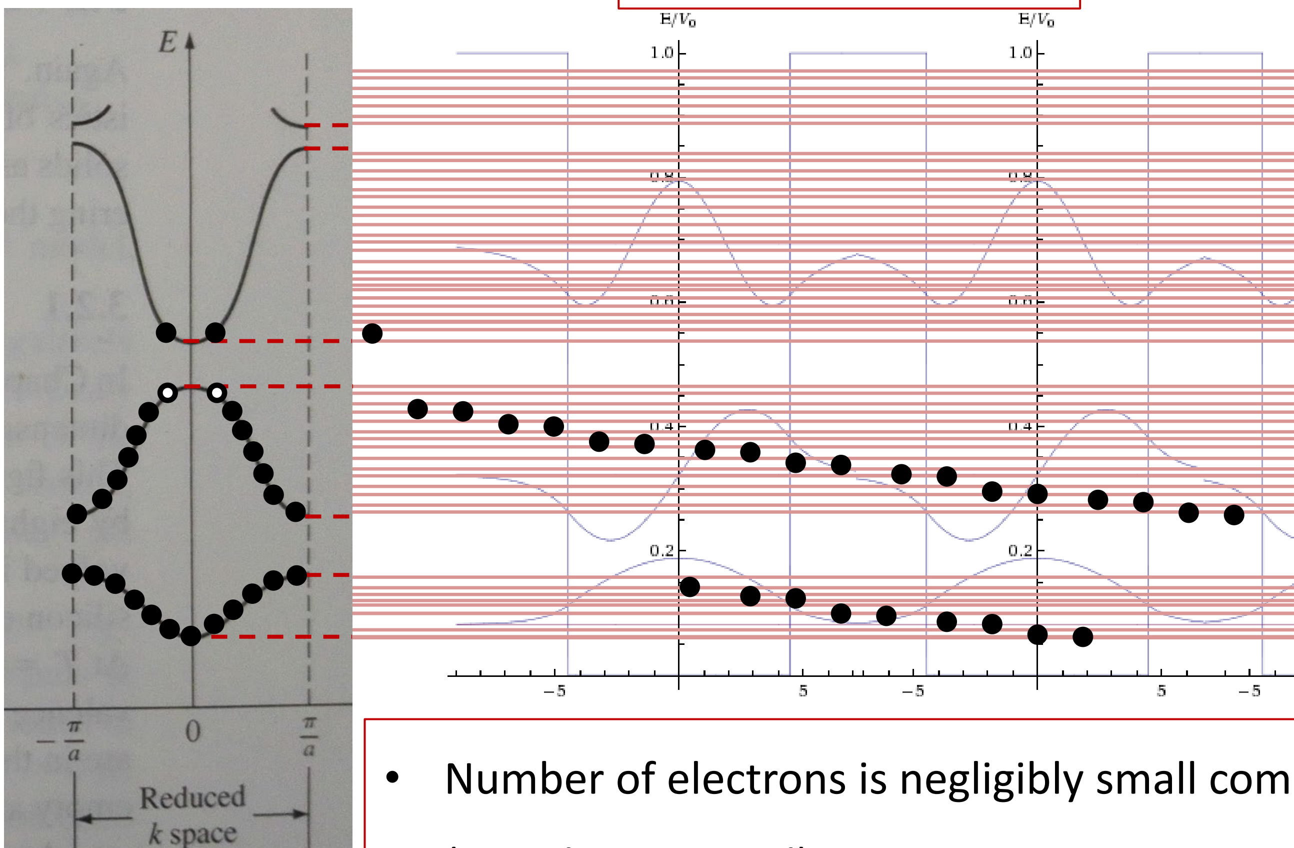


T=0K, nonconductive

T=300k, conductive

3.4 Effective Mass

Semiconductors

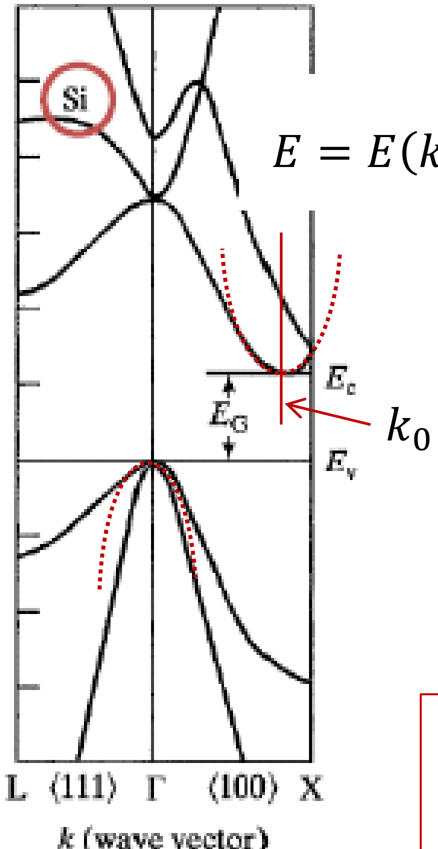


In k space

- Number of electrons is negligibly small compared available states (non-degenerated)
- Electrons mostly located at the bottom of conduction band

3.4 Effective Mass

Semiconductors (1st time approximation)



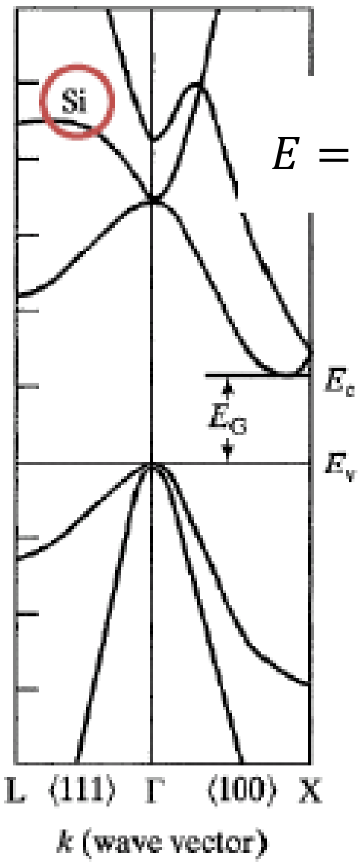
$$E = E(k) = E(k = k_0) + \frac{dE}{dk}|_{k=k_0}(k - k_0) + \frac{d^2E}{2dk^2}|_{k=k_0}(k - k_0)^2 + O((\Delta k)^3)$$

Taylor series

- Number of electrons is negligibly small compared available states (non-degenerated)
- Electrons mostly located at the bottom of conduction band

3.4 Effective Mass

Semiconductors



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

For electrons in free space:

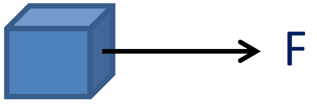
$$E_f = \frac{\hbar^2 k^2}{2m} \Rightarrow \frac{d^2E_f}{dk^2} = \frac{\hbar^2}{m} \qquad \frac{d^2E}{dk^2}|_{k=0} = \frac{\hbar^2}{m^*}$$

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

3.4 Effective Mass

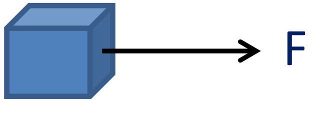
- How to understand effective mass

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



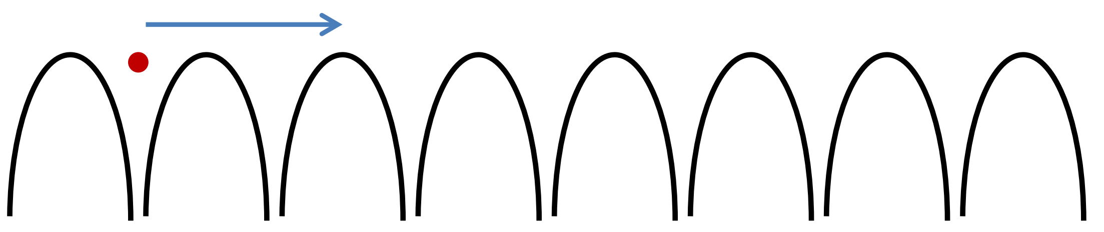
$$m^* = \frac{F}{a} \qquad a = \frac{d^2x}{dt^2}$$

In the water

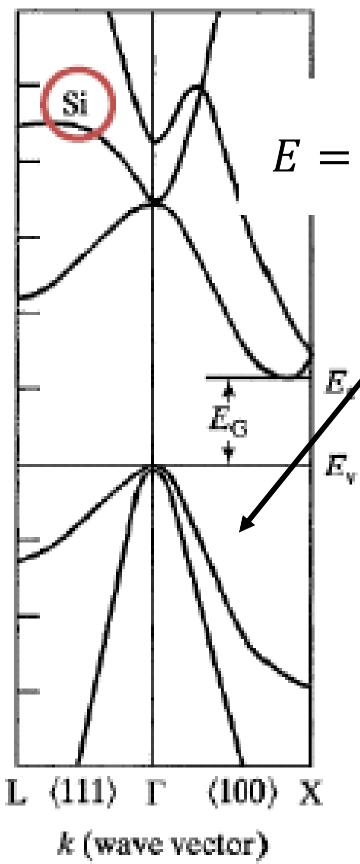
3.4 Effective Mass

- How to understand effective mass

Modulated by Electric potential of ions



3.4 Effective Mass

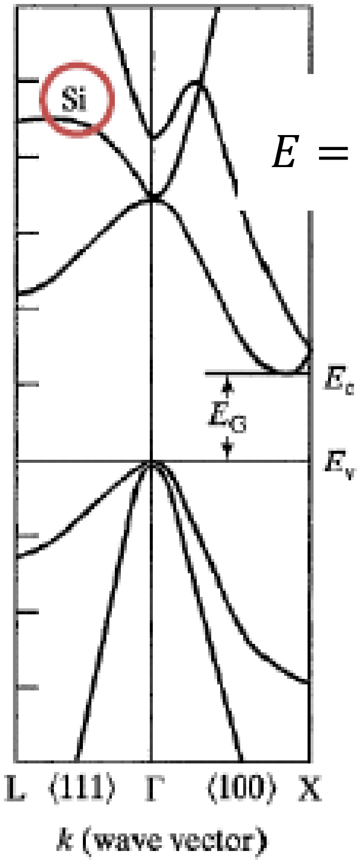


For Electrons in the valence band:

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

3.4 Effective Mass

Semiconductors



For Electrons in the conduction band:

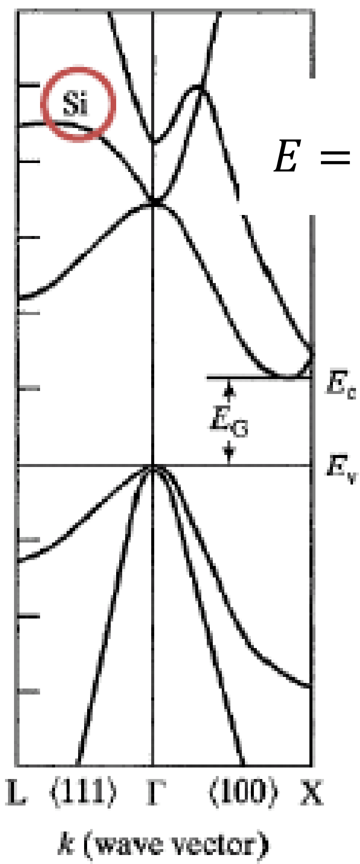
< 0

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

$$\boxed{E = E(k) = E_c - \frac{\hbar^2}{2m_p^*}(k - k_0)^2}$$

3.4 Effective Mass

Semiconductors



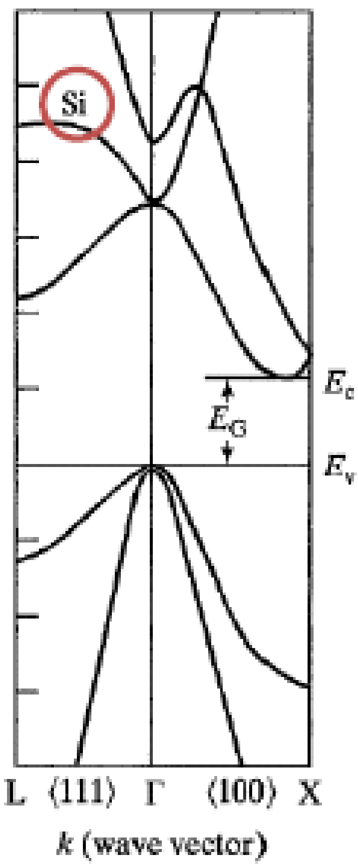
For Electrons in the conduction band:

$$E = E(k) = E(k = k_0) + \frac{dE}{dk}\Big|_{k=k_0}(k - k_0) + \overbrace{\frac{d^2E}{2dk^2}}^{<0}\Big|_{k=k_0}(k - k_0)^2 + O((\Delta k)^3)$$

$$\boxed{E = E(k) = E_c - \frac{\hbar^2}{2m_p^*}(k - k_0)^2}$$

- Equivalent to a positive charge carrier
- Different effective mass (always larger than electrons)
- Electrons and holes can come from dopants separately

3.4 Effective Mass



Conduction Band:

$$\boxed{E = E(k) = E_c + \frac{\hbar^2}{2m_n^*}(k - k_1)^2}$$

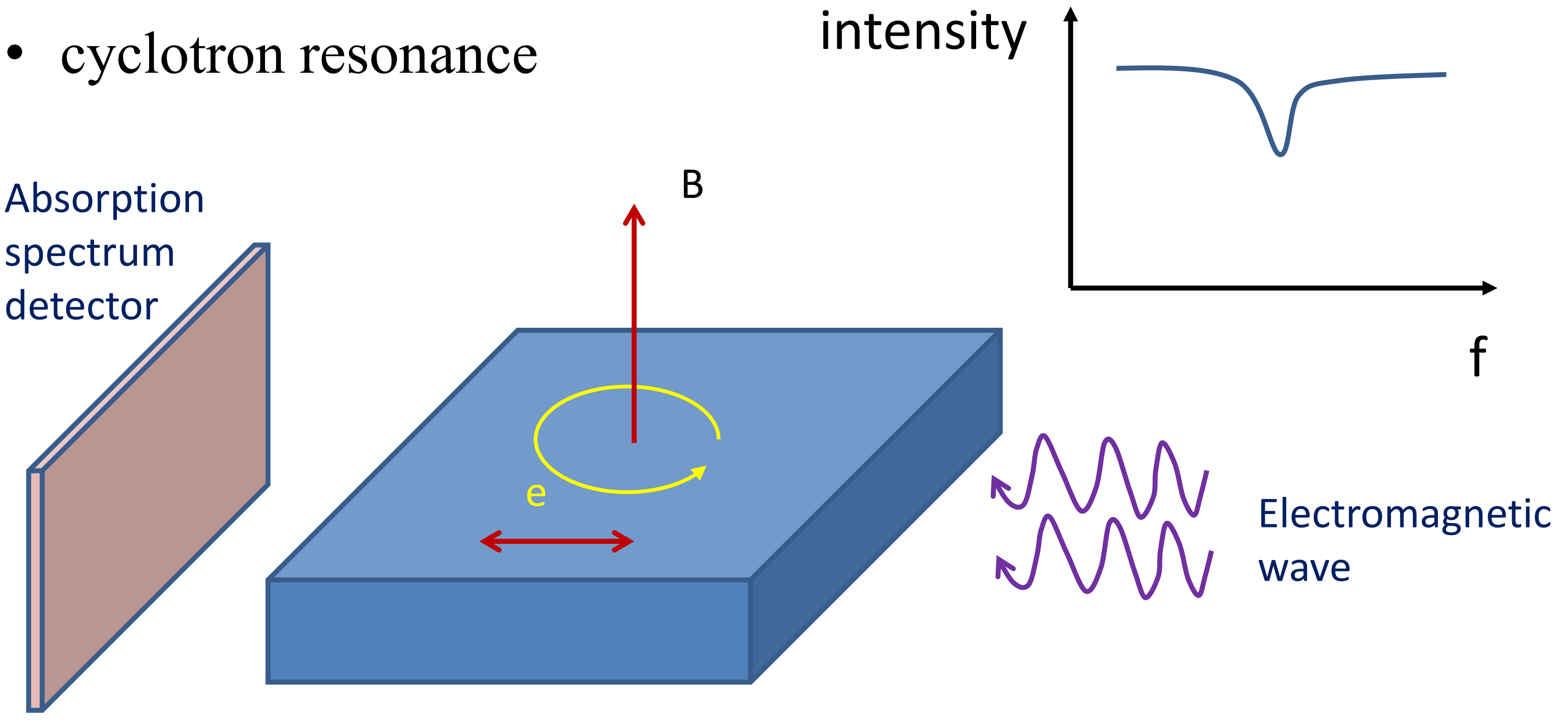
Valence Band:

$$\boxed{E = E(k) = E_c - \frac{\hbar^2}{2m_p^*}(k - k_2)^2}$$

- If we can experimentally measure the effective mass, we will have found the analytical express of energy band structure for semiconductors.
- How?

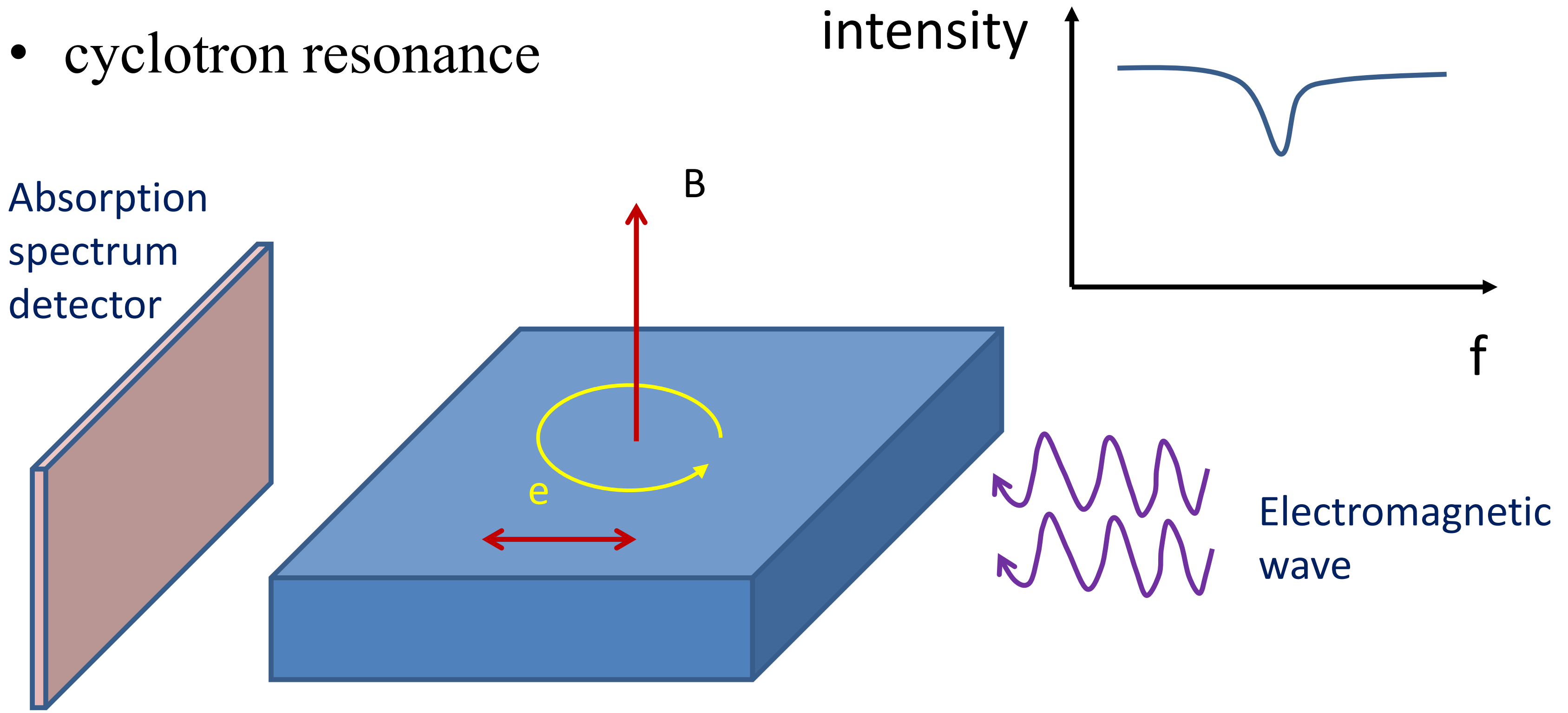
3.4 Effective Mass

- cyclotron resonance



3.4 Effective Mass

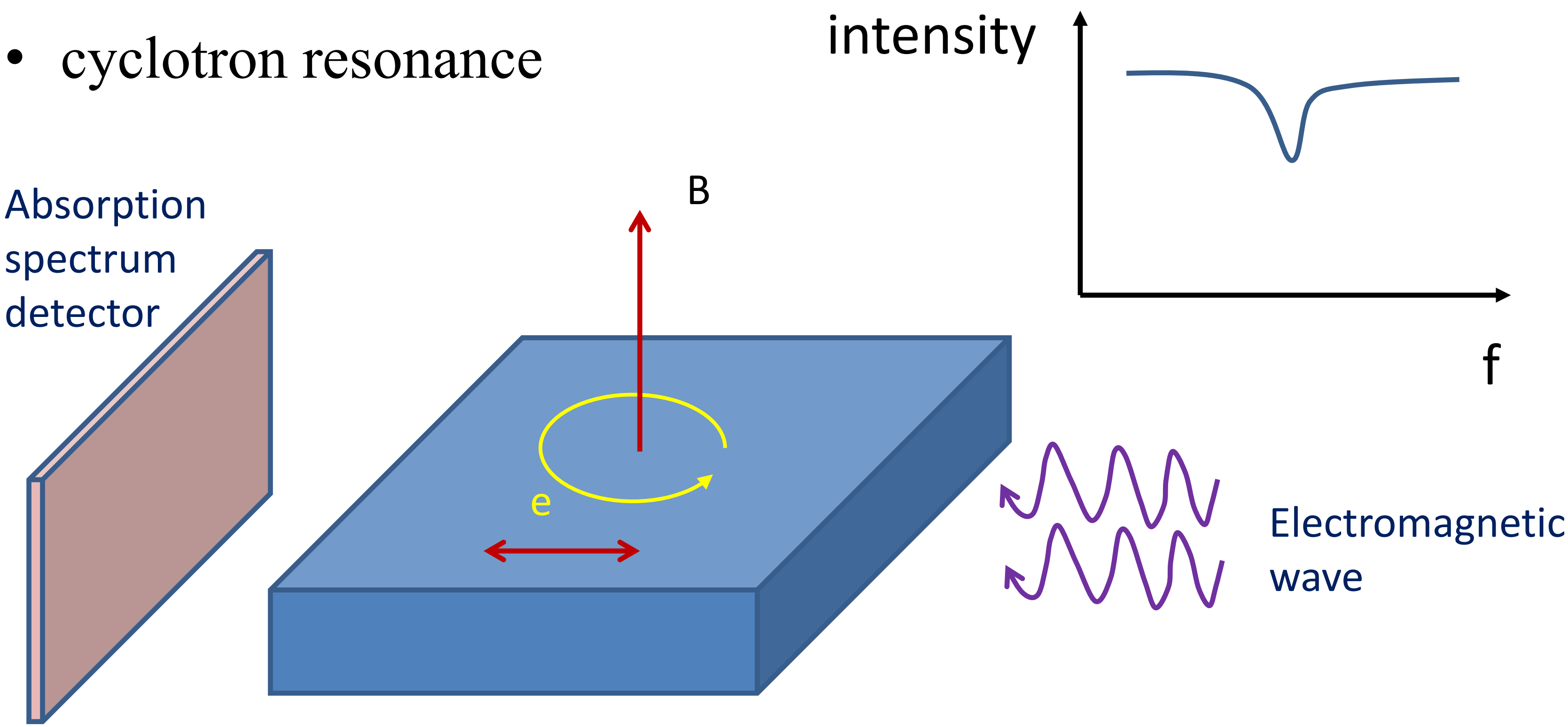
- cyclotron resonance



Suppose a intrinsic silicon wafer is placed in a magnetic field B = 1T. We find a dip at λ=5mm in the absorption spectrum, what is the effective mass of electrons? The mass of electrons in free space m_0 = 9.1e-31kg.

3.4 Effective Mass

- cyclotron resonance



Centrifugal force $F = m^* \omega^2 r$

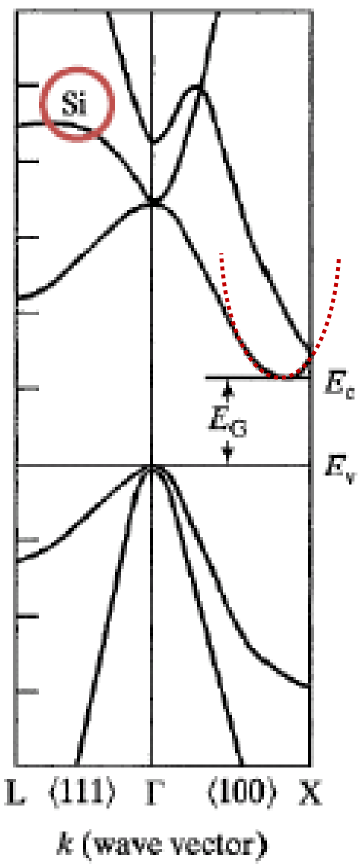
Magnetic force $F_{mag} = e \times v \times B$

$v = \omega r$

$\Rightarrow$ $m^* = eB/\omega$ $\quad \omega = 2\pi f$

$$\Rightarrow m^* = \frac{eB\lambda}{2\pi c} = \frac{1.6 \times 10^{-19} \times 0.005}{2\pi \times 3 \times 10^8} = 0.47 m_0$$

3.4 Effective Mass



- If we can experimentally measure the effective mass, we will have found the analytical express of energy band structure for non-degenerated semiconductors.
- How?

$$\boxed{E = E(k) = E_c + \frac{\hbar^2}{2m_n^*}(k-k_1)^2}$$

For Electrons in the valence band:

$$\boxed{E = E(k) = E_c - \frac{\hbar^2}{2m_p^*}(k-k_2)^2}$$

$$\Rightarrow m^* = \frac{eB\lambda}{2\pi c} = \frac{1.6\times10^{-19}\times0.005}{2\pi\times3\times10^8} = 0.47m_0$$

3.4 Effective Mass

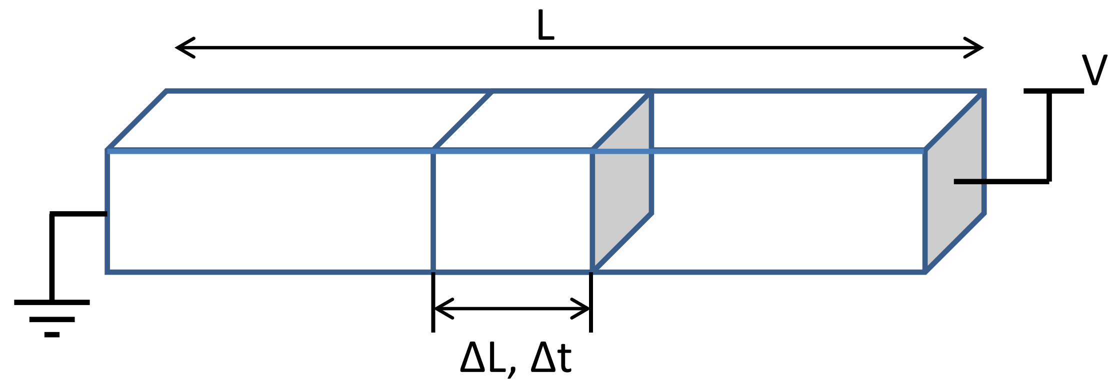
	Symbol	Germanium	Silicon	Gallium Arsenide
Bandgap	E_g (eV)	0.66	1.12	1.424
Electrons	m_e^*/m_0	0.56	1.08	0.067
Holes	m_h^*/m_0	0.29	0.81	0.47

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*



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

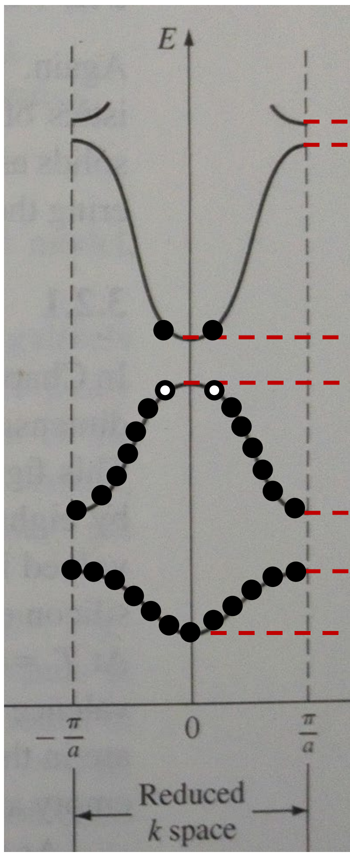
$$v = \mu E = \mu V/L$$

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

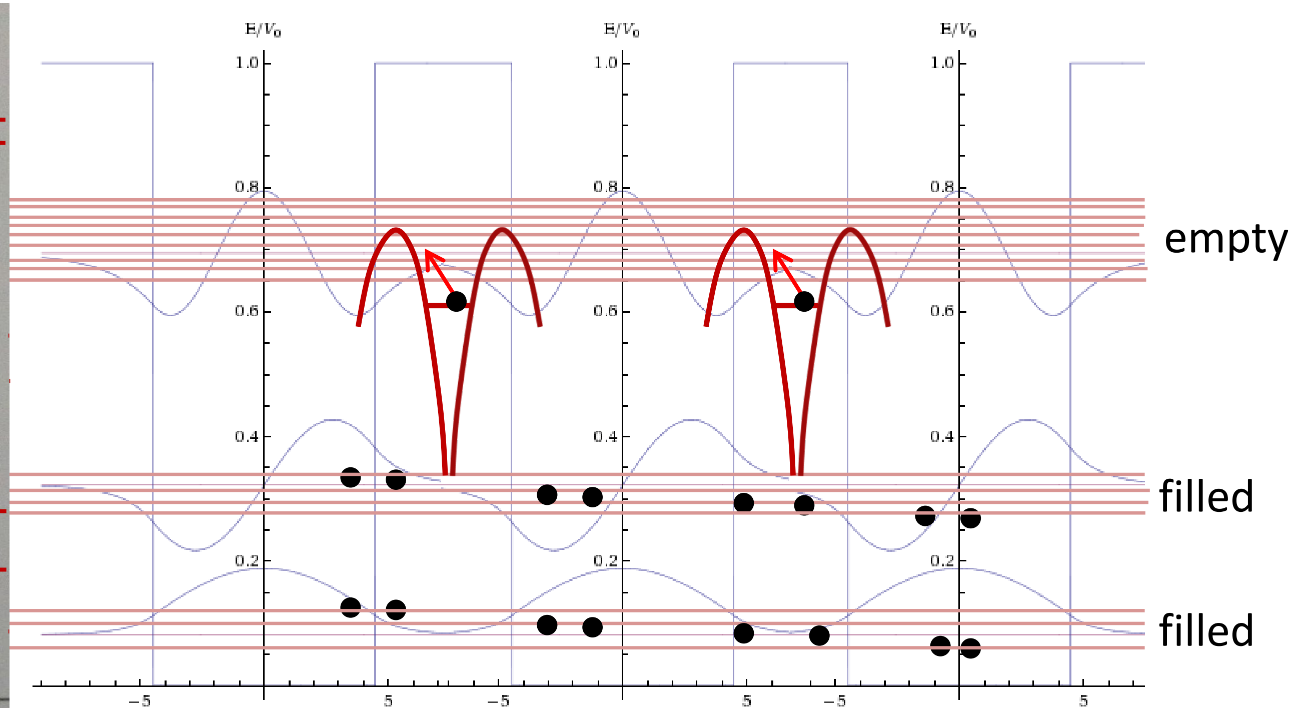
3.5 Density of States Function

Previously…

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

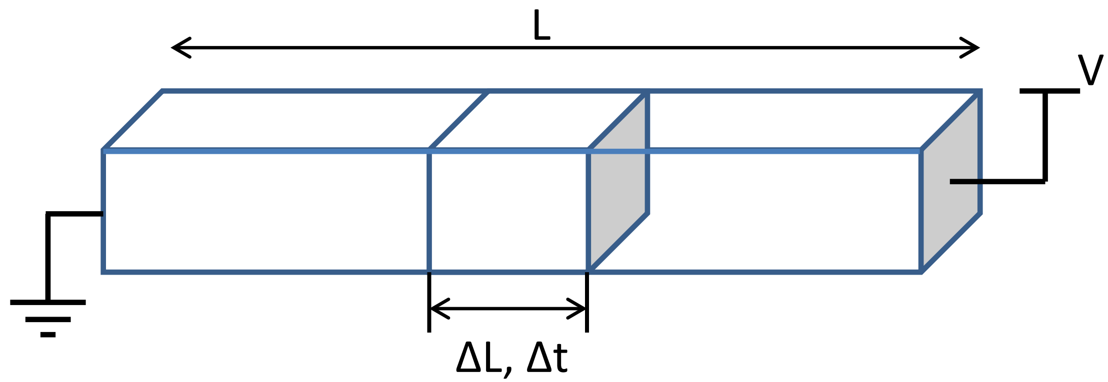


In k space



3.5 Density of States Function

$n\ type\ semiconductor$



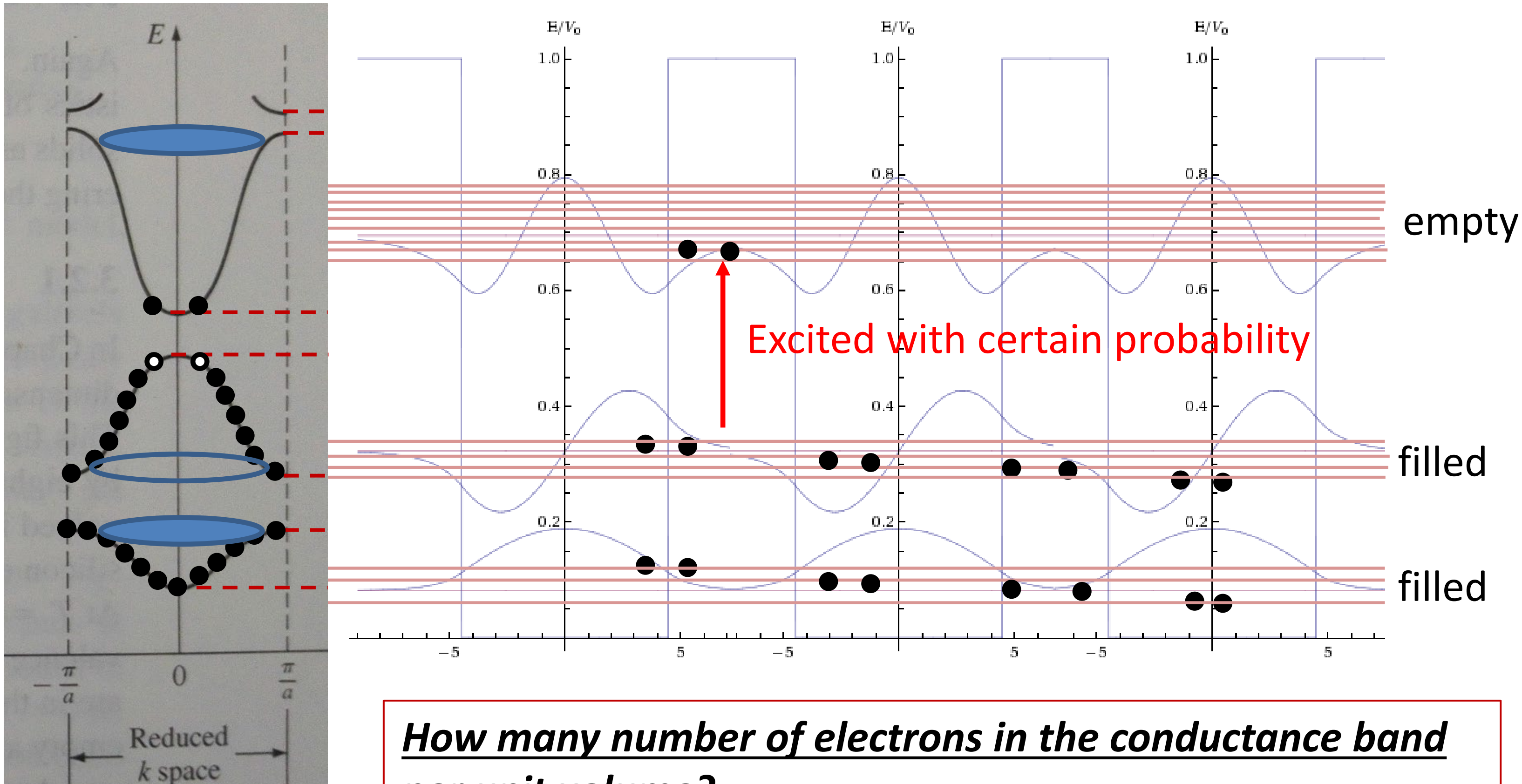
$$I = \frac{\Delta Q}{\Delta t} = \frac{nqA_c\Delta L}{\Delta t} = nqA_c v$$

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

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

3.5 Density of States Function

- If semiconductor is intrinsic



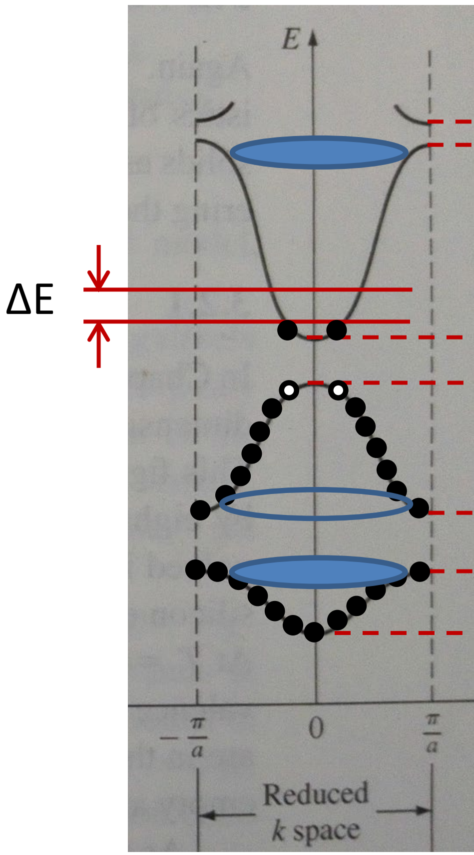
In k space

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

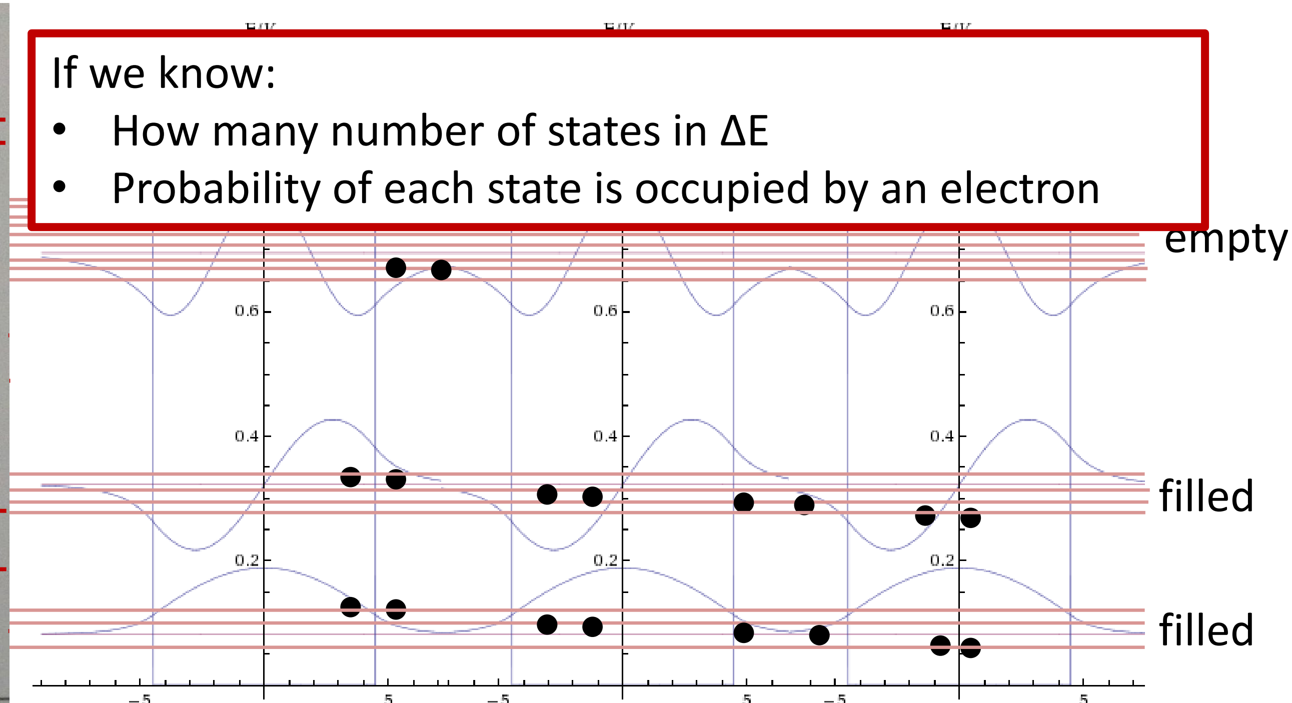
3.5 Density of States Function

- Intrinsic (undoped)
- Electrons are all from the valance

If we know:
- How many number of states in ΔE
- Probability of each state is occupied by an electron



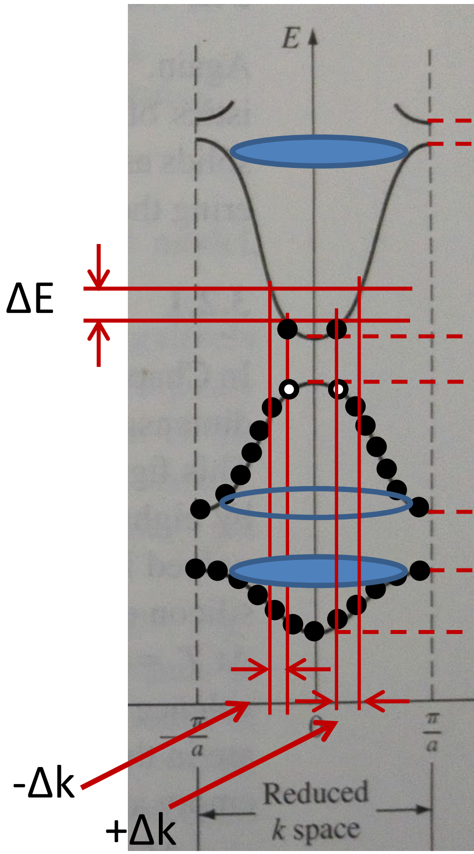
In k space



<u>How many number of electrons in the conductance band per unit volume?</u>

3.5 Density of States Function

- Intrinsic (undoped)
- Electrons are all from the valance



If we know:

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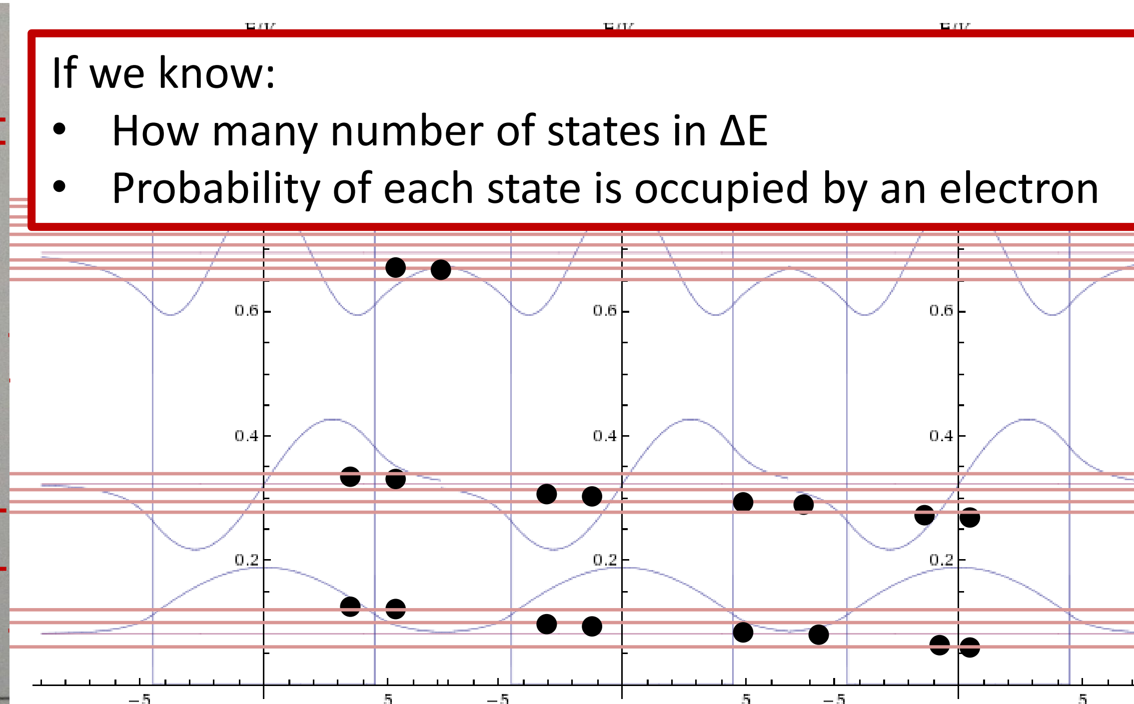
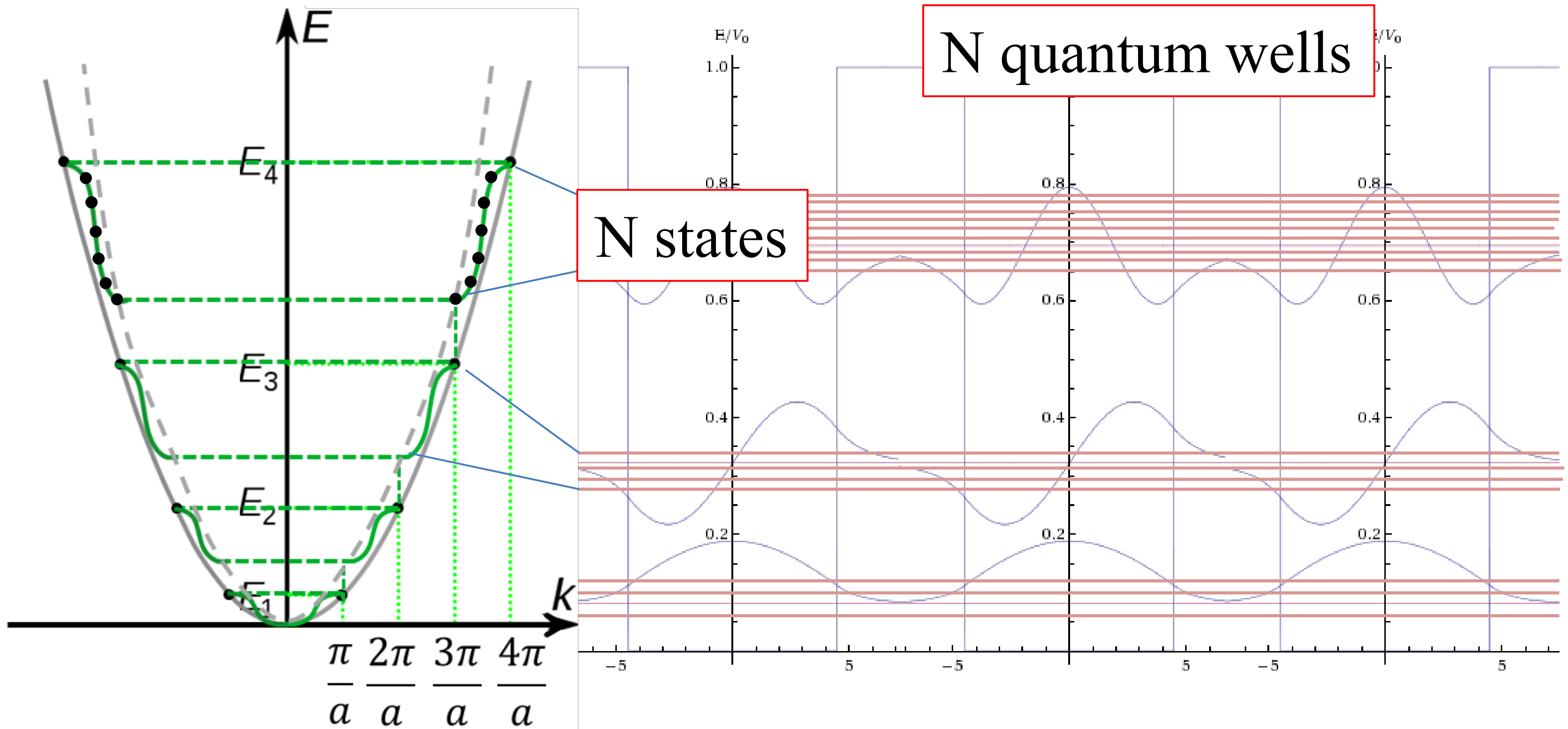


<u>How many number of electrons in the conductance band per unit volume?</u>

In k space

3.1 Allowed and Forbidden Energy Bands

<u>Forming energy bands</u>: analytical



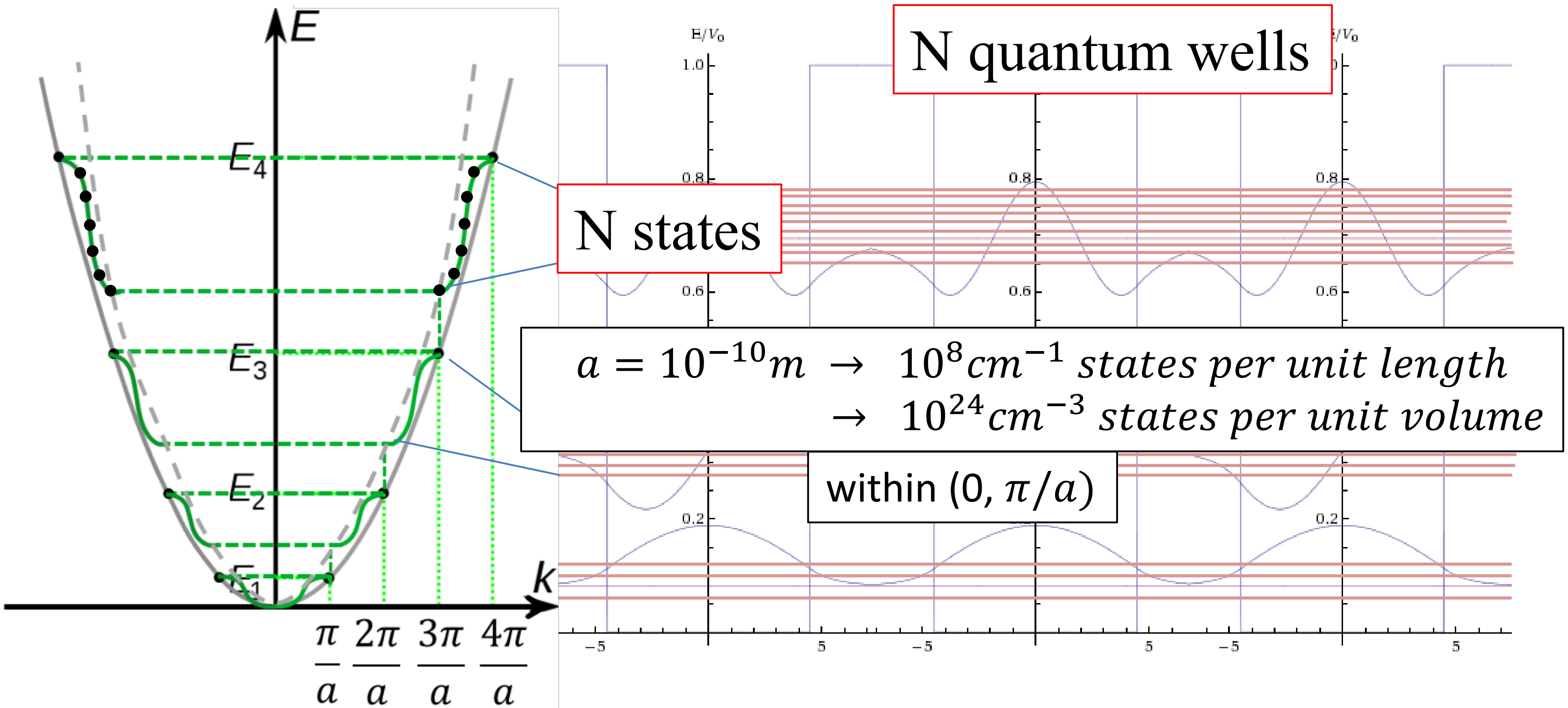
The "density" of states of the whole crystal within $(0, \pi/a)$: $\frac{N}{\pi/a}$

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: $\frac{N}{\pi/a} \times \Delta k \frac{1}{Na} = \frac{\Delta k}{\pi}$

3.1 Allowed and Forbidden Energy Bands

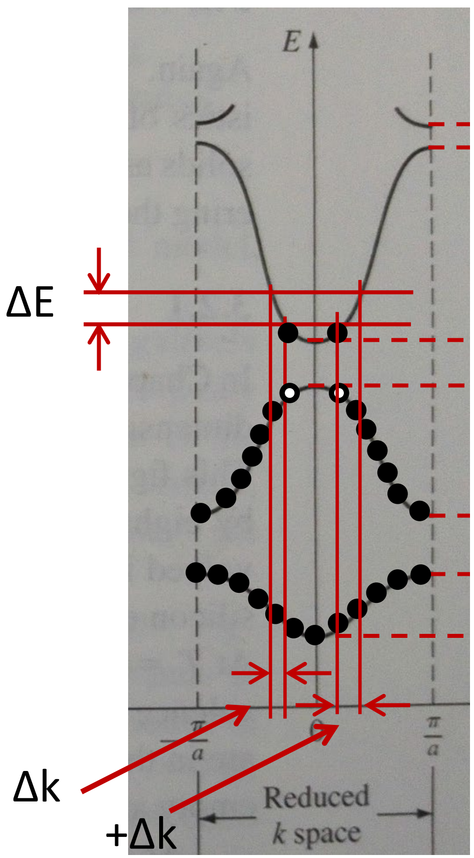
Forming energy bands: analytical



k is wave number. $\frac{k}{\pi}$ *means the number of states per unit volume*

3.5 Density of States Function

- Intrinsic (undoped)
- Electrons are all from the valance



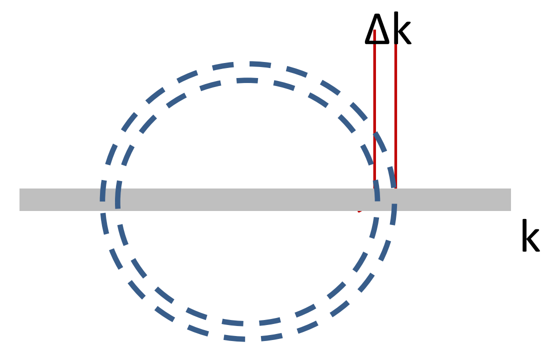
In k space

If we know:

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

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

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

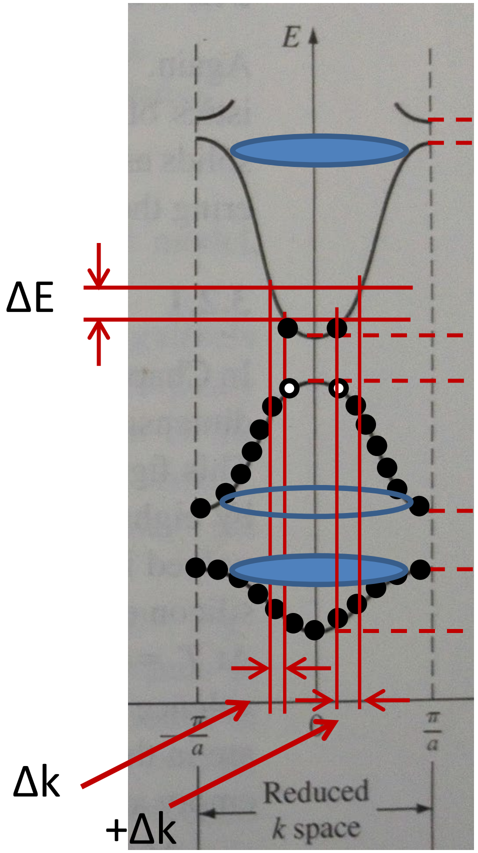


Within ΔE, we have the number of k is $\frac{d(2|k|/\pi)}{dE}\Delta E$

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

3.5 Density of States Function

- Intrinsic (undoped)
- Electrons are all from the valance



In k space

If we know:

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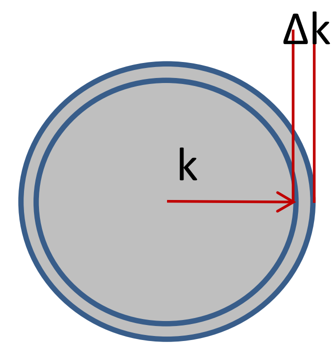


Within ΔE, we have the number of k is $\frac{d(\pi(k/\pi)^2)}{dE}\Delta E$

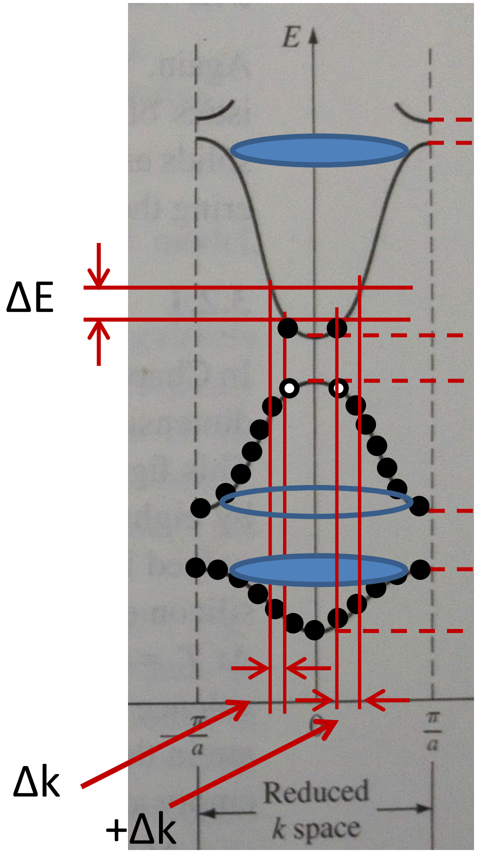
$$g(E) = \frac{1}{4}\frac{d(\pi(k/\pi)^2)}{dE}$$

3.5 Density of States Function

- Intrinsic (undoped)
- Electrons are all from the valance

If we know:

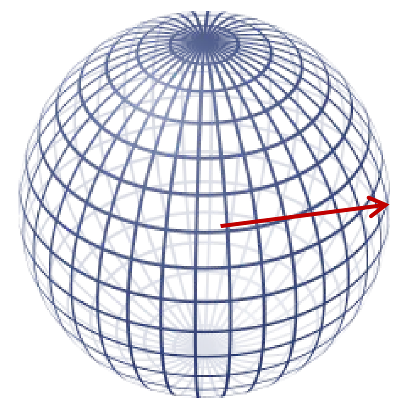
- How many number of states in ΔE
- Probability of each state is occupied by an electron



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

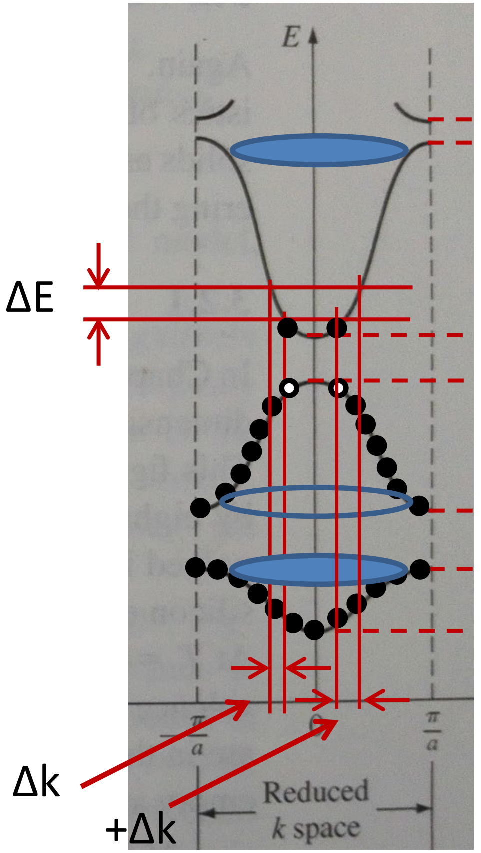
$$g(E) = \frac{1}{8}\frac{d(4\pi\left(\frac{k}{\pi}\right)^3/3)}{dE}$$

3.5 Density of States Function

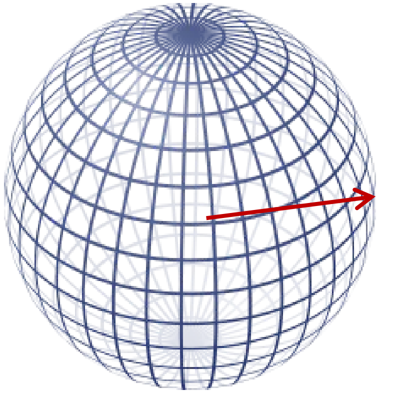
- Intrinsic (undoped)
- Electrons are all from the valance

If we know:

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



In k space



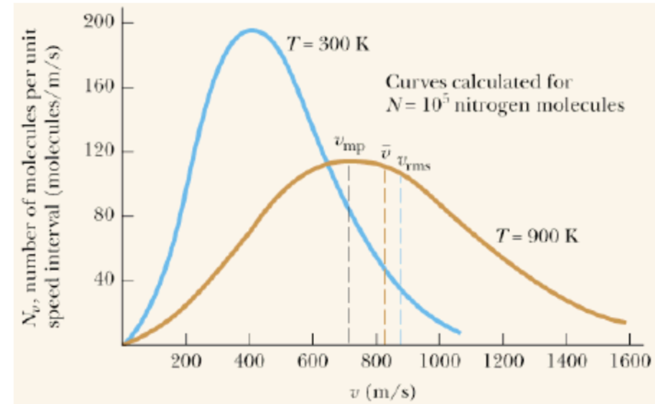
spin

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

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



<u>Maxwell-Boltzmann probability function</u>:

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

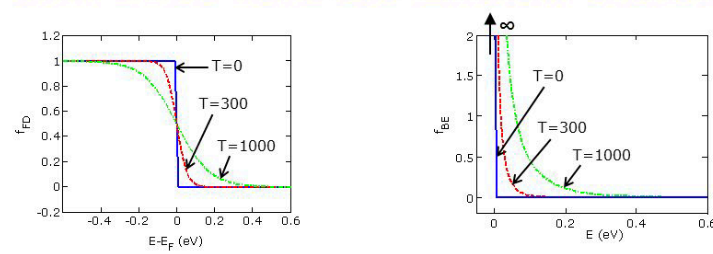
<u>Bose-Einstein probability function</u>:

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

<u>Fermi-Dirac probability function</u>:

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

Fermi-Dirac vs. Bose-Einstein Statistics

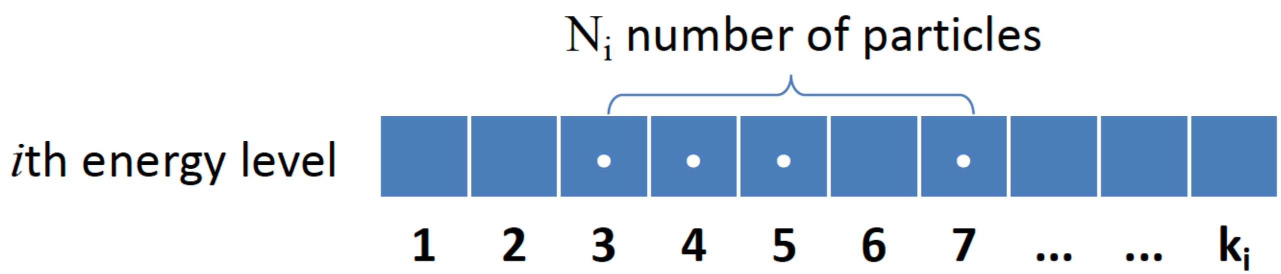


$$f_{FD}(E) = \frac{1}{\exp\left(\frac{E-E_F}{k_B T}\right)+1} \qquad f_{BE}(E) = \frac{1}{\exp\left(\frac{E}{k_B T}\right)-1}$$

3.6 Statistical mechanics

<u>Fermi-Dirac probability function</u>:

- 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

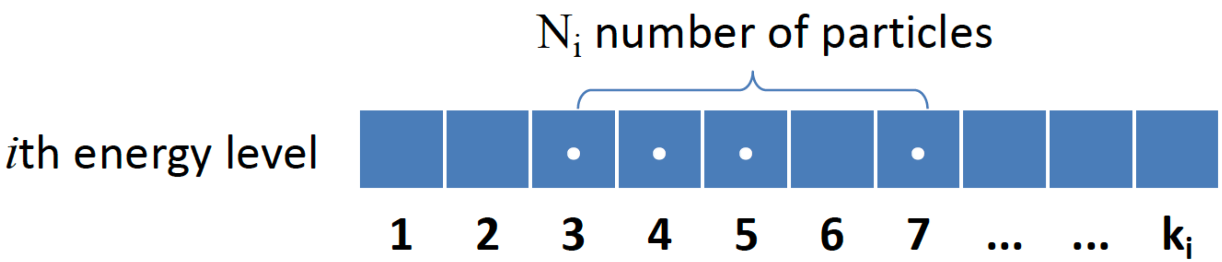
$$k_i(k_i - 1) \cdots (k_i - (N - 1)) = \frac{k_i!}{(k_i - N_i)}$$

(Particles are distinguishable)

3.6 Statistical mechanics

<u>Fermi-Dirac probability function</u>:

- 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

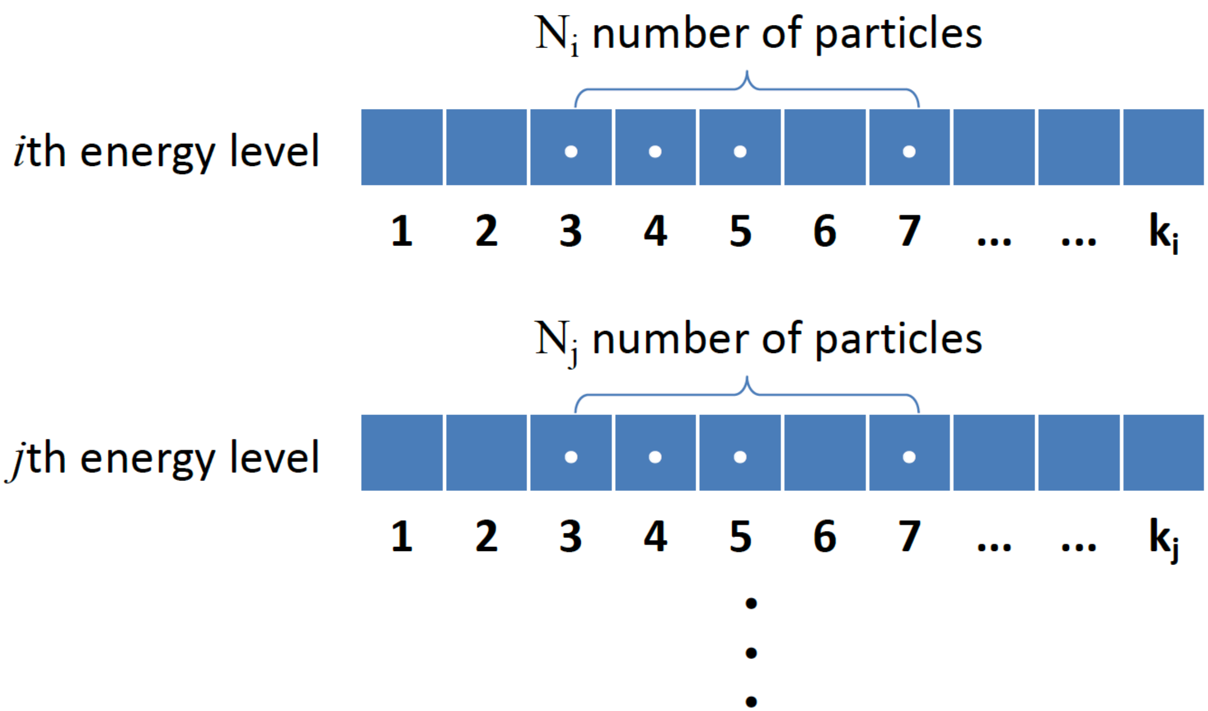
$$W_i = \frac{k_i!}{N_i!(k_i - N_i)!}$$

(Particles are indistinguishable)

3.6 Statistical mechanics

<u>Fermi-Dirac probability function</u>:

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



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

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

$$\vdots$$

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

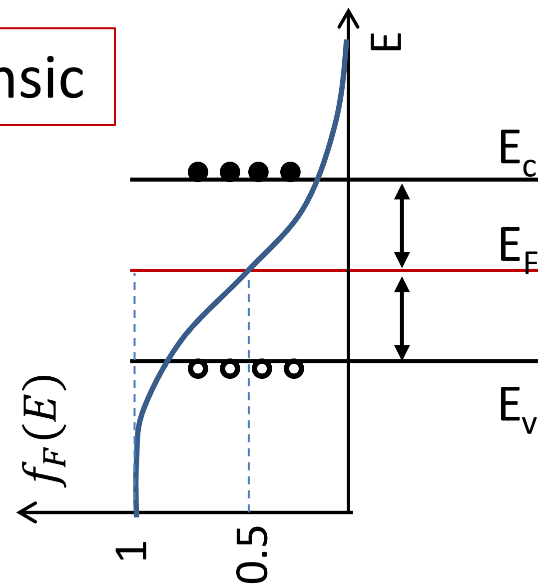
The probability of a state at energy E being occupied by an electron:

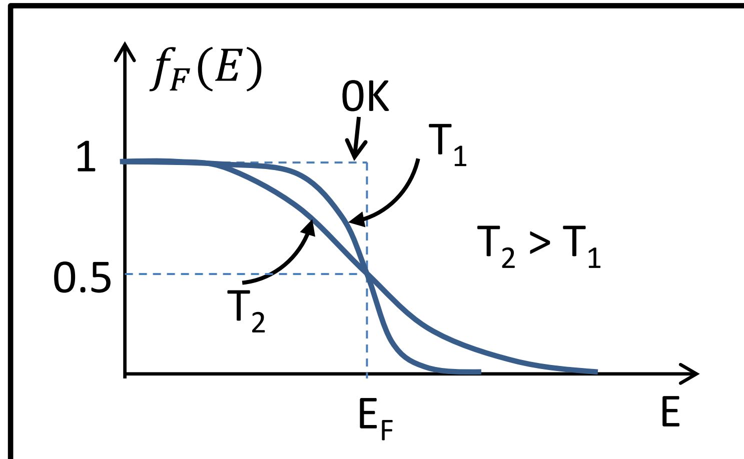
$$f_F(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$

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

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

$\parallel$

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

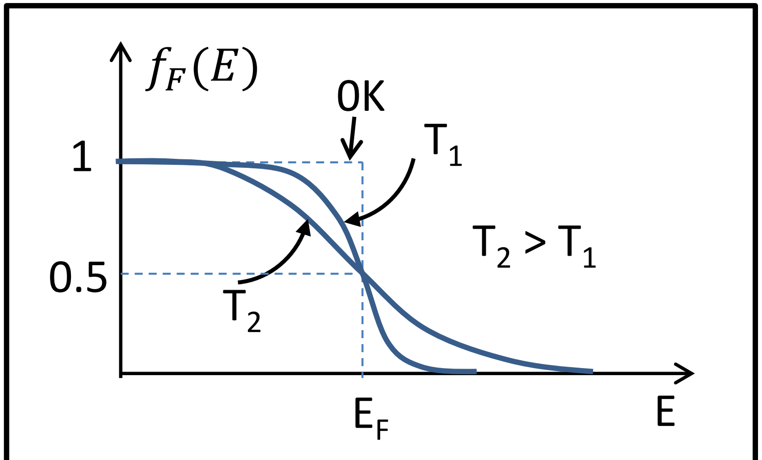
Boltzmann distribution

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

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

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

Boltzmann distribution



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