

# Primer on Semiconductors

## Unit 1: Material Properties

### Lecture 1.1: Energy levels to energy bands

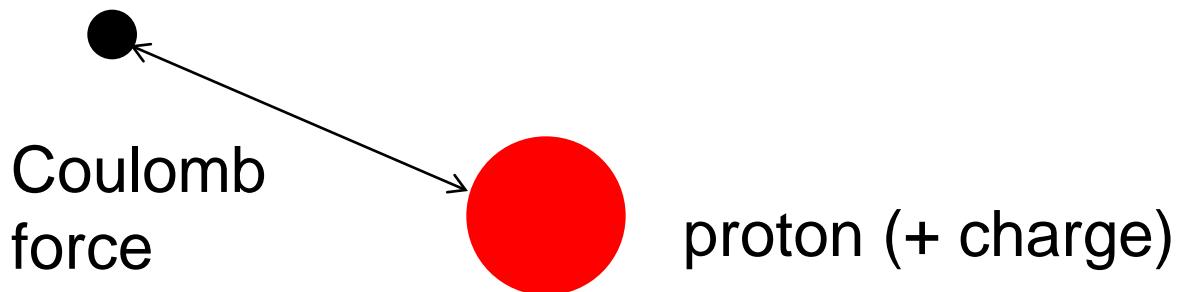
Mark Lundstrom

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# The hydrogen atom

---

electron (- charge)



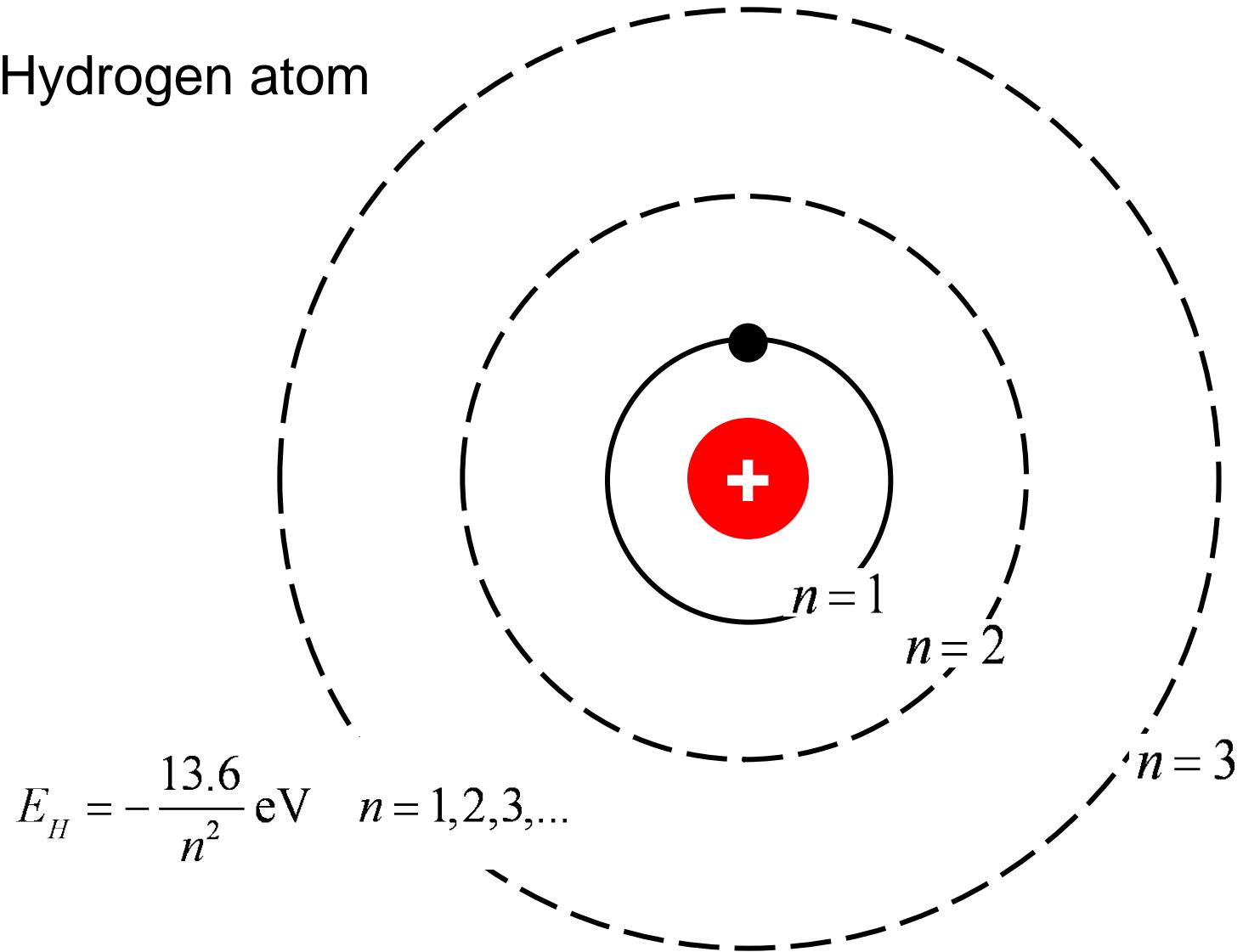
Electrons reside in “orbitals” (s, p, d, f, ...)

[https://en.wikipedia.org/wiki/Hydrogen\\_atom](https://en.wikipedia.org/wiki/Hydrogen_atom)

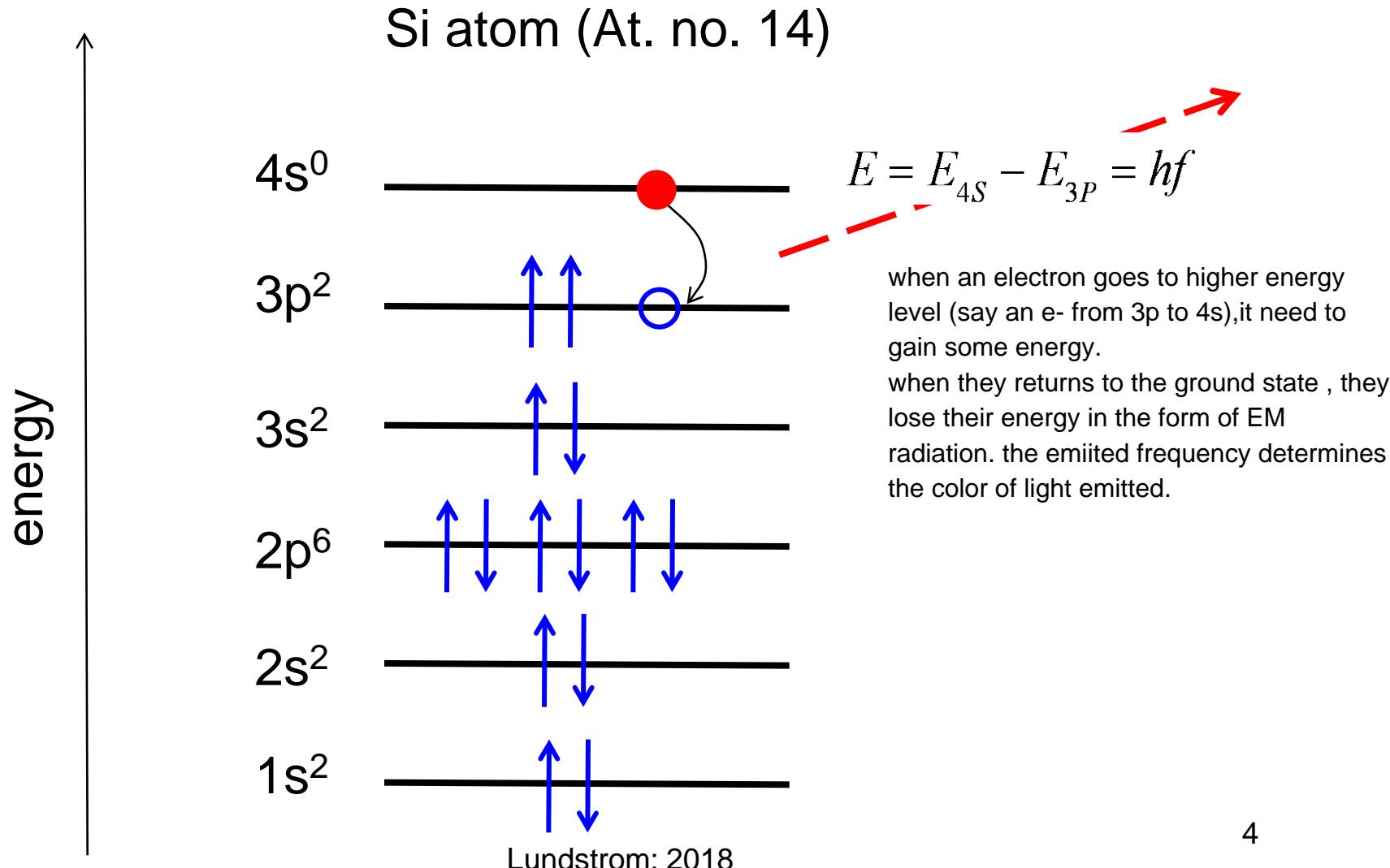
# Quantization of energy levels

---

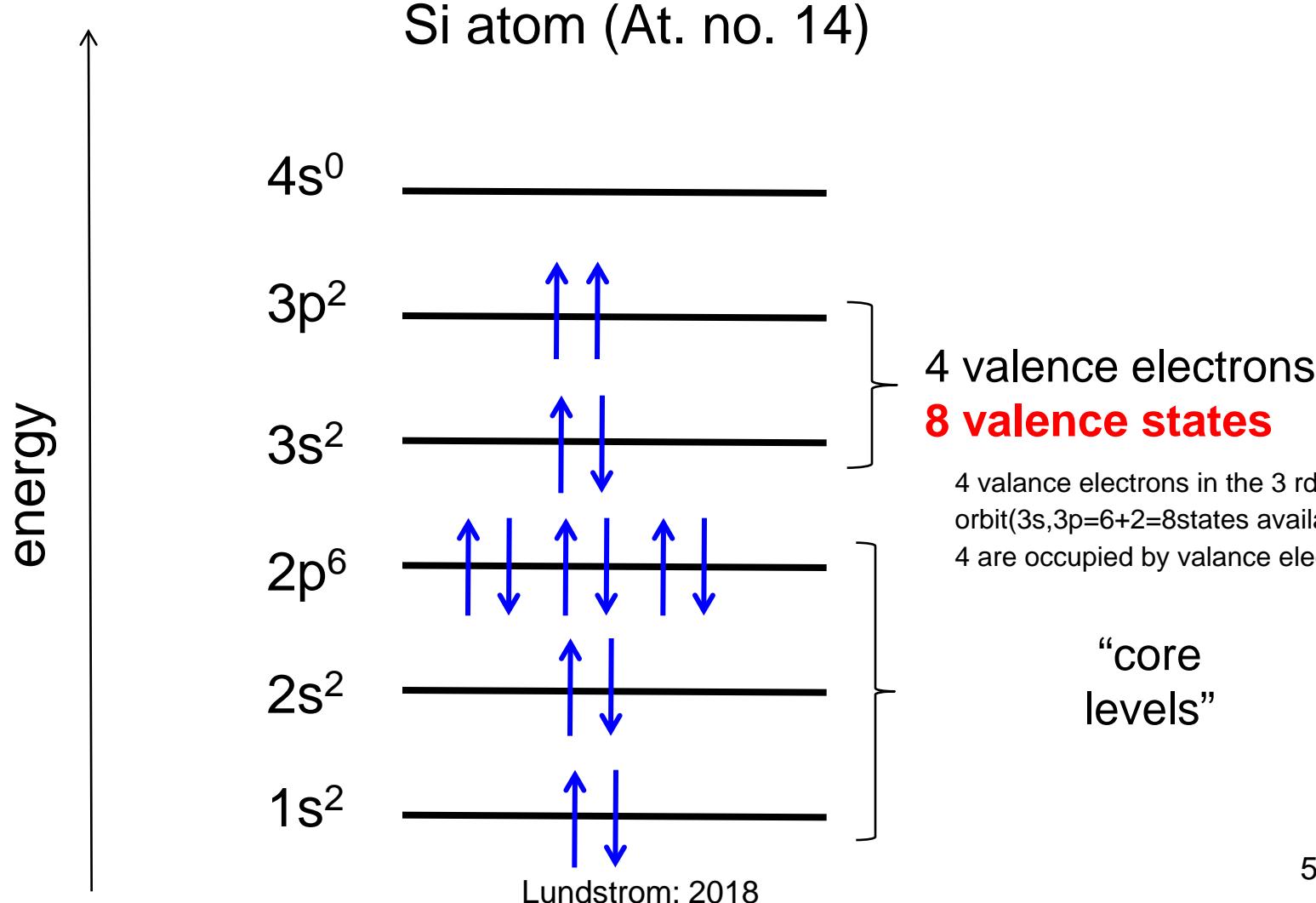
Hydrogen atom



# Silicon atom energy levels

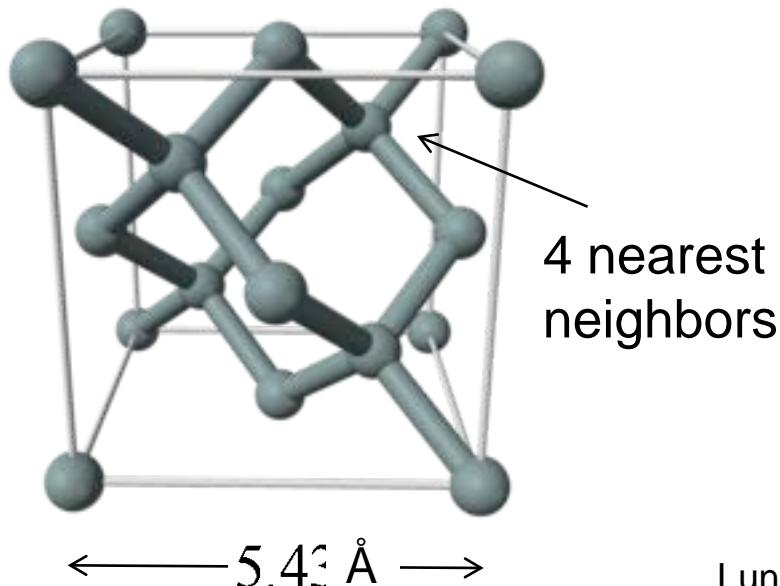
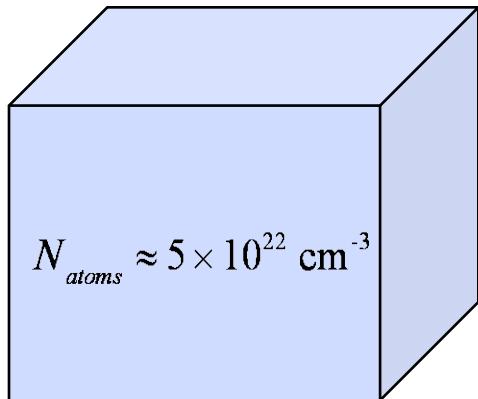


# Valence vs. core levels



# Silicon energy levels / energy bands

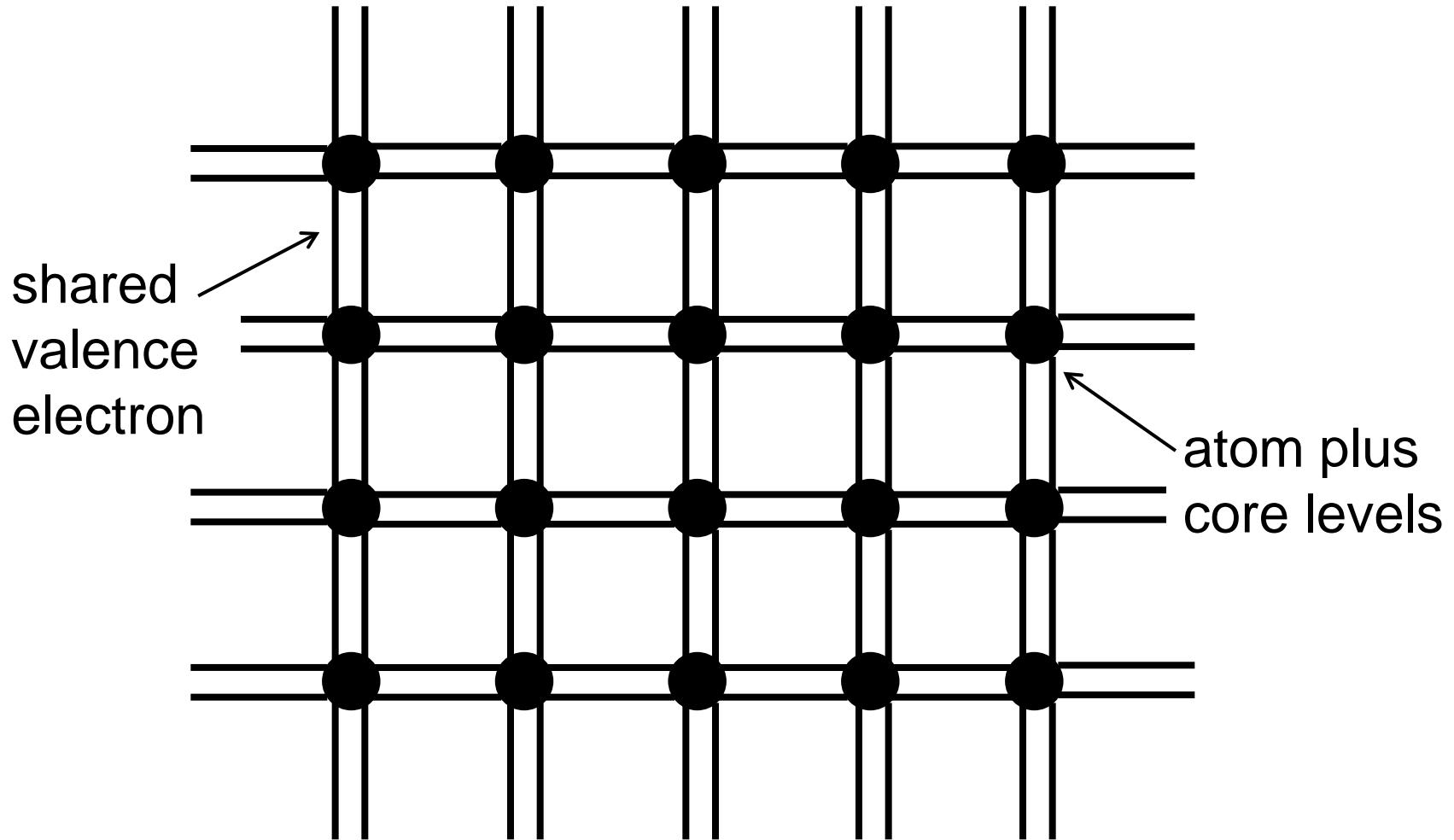
---



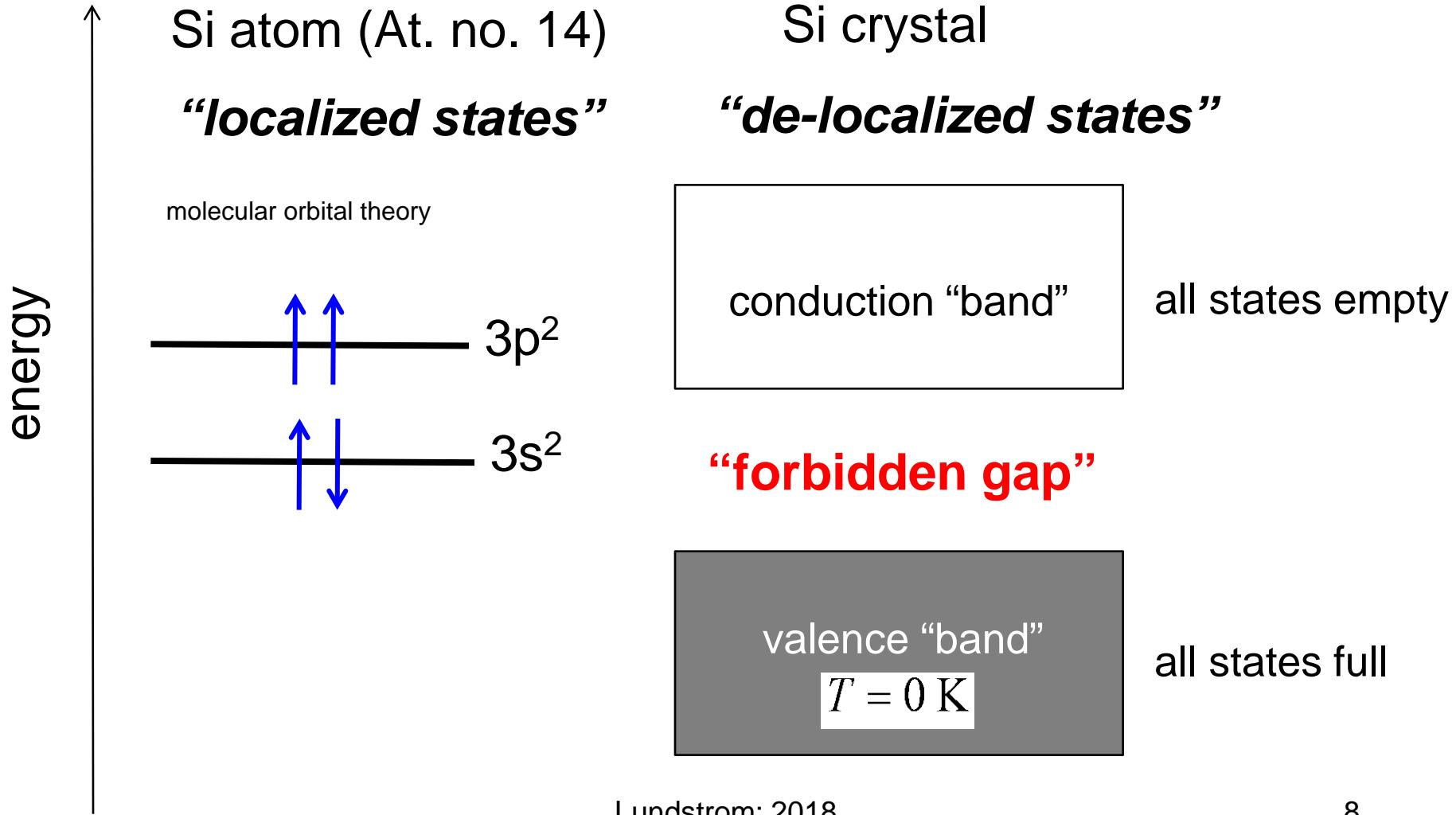
- Only the valence states are of interest to us.
- Each Si atom has 4 valence electrons and 4 nearest neighbors.
- The 8 valence states give rise to  $8N_{atoms}$  states per  $\text{cm}^3$  in the solid.
- But the **interaction** of the electron wavefunctions alters the discrete energy levels of the isolated Si atoms.

# Bonding (cartoon)

---



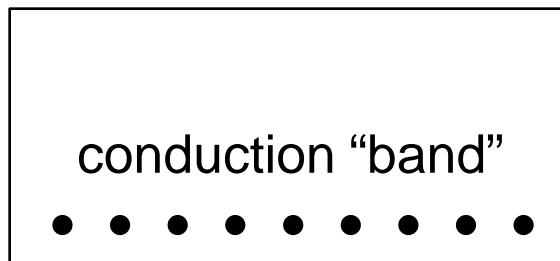
# Silicon energy levels → energy bands



# Above T = 0 K

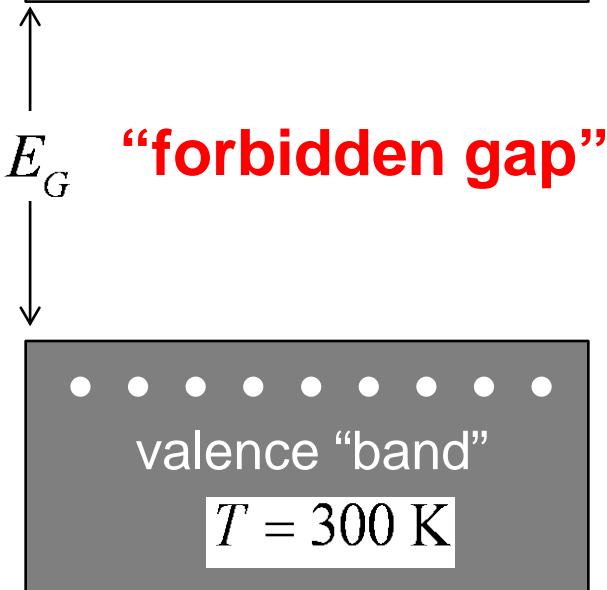
---

Si crystal



$$\langle E \rangle = \frac{3}{2} k_B T = 0.039 \text{ eV}$$

$n = p = n_i$  in an  
***intrinsic***  
semiconductor



A few states full

A few states empty

# Joules and electron volts

---

$$\langle E \rangle = \frac{3}{2} k_B T = 0.039 \text{ eV}$$

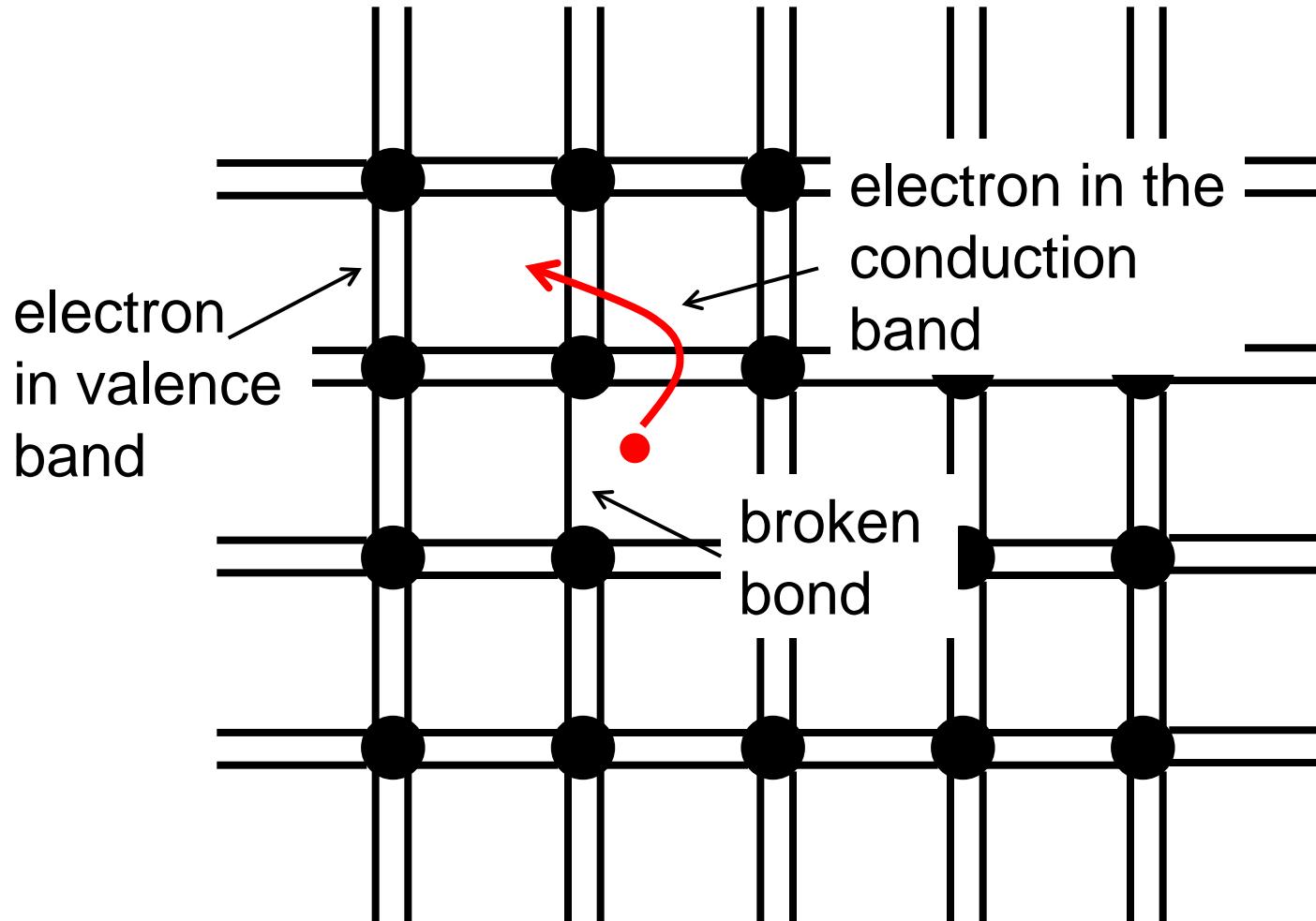
We should do our calculations in SI (MKS) units, but it is convenient to express energies in electron volts, which is not a proper SI unit. Electron volts should be converted to Joules before using them in calculations.

$$\langle E \rangle = \frac{3}{2} (1.38 \times 10^{-23} \text{ J/K}) \times 300 \text{ K} = 6.21 \times 10^{-21} \text{ J}$$

$$E(\text{eV}) = \frac{E(\text{J})}{q} = \frac{6.21 \times 10^{-21} \text{ J}}{1.6 \times 10^{-19} \text{ C}} = 0.039 \text{ eV}$$

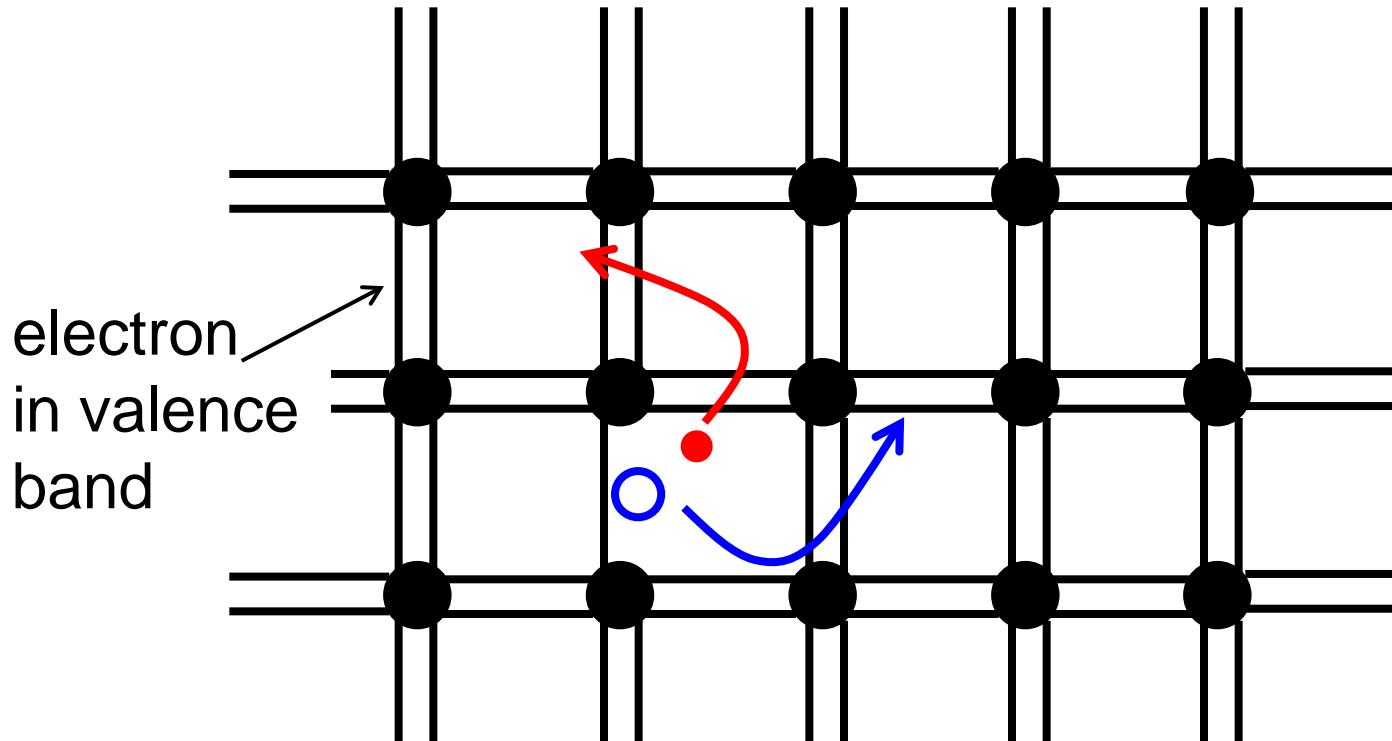
# Another view

---



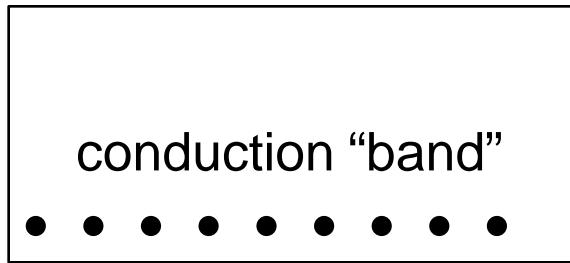
# Electrons and holes in semiconductors

---

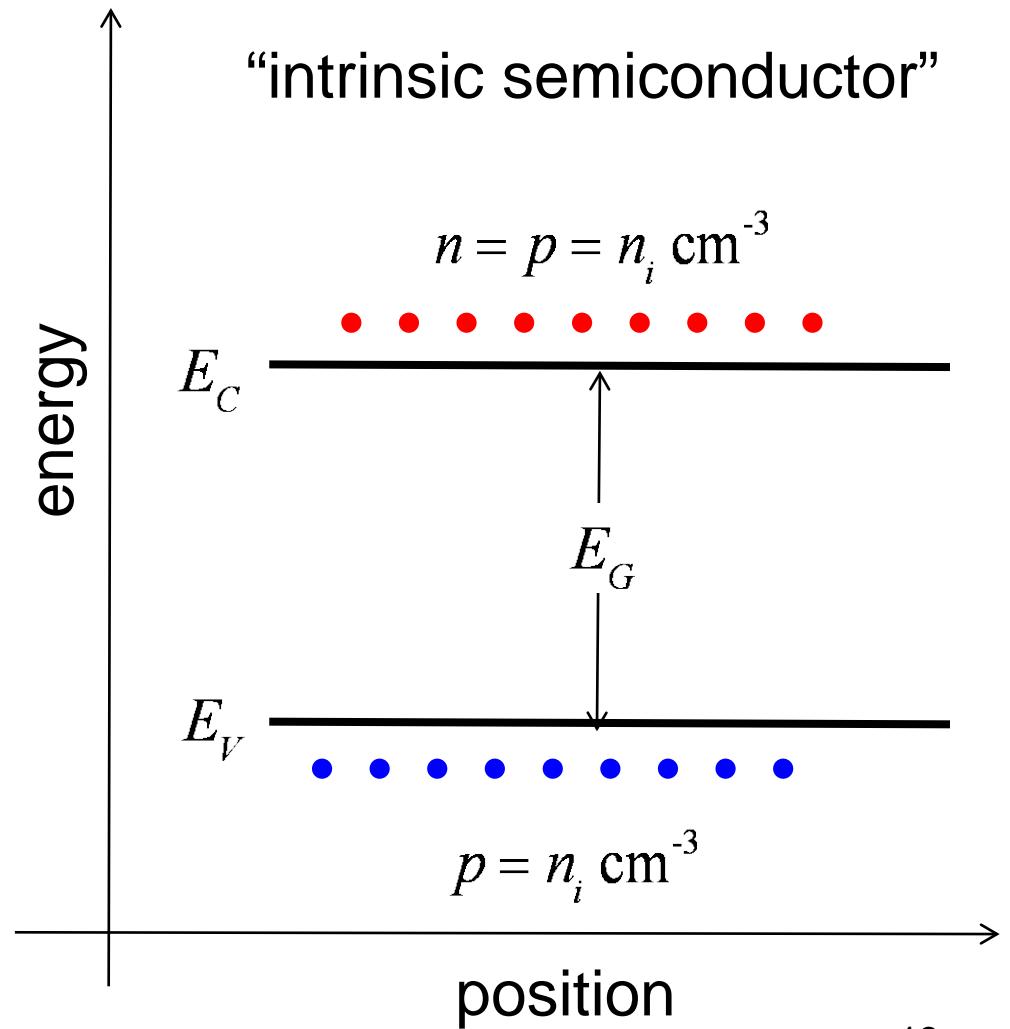
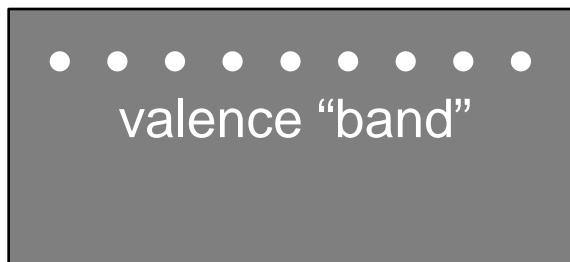


- 1) Electrons in the conduction can move
- 2) Holes in the valence band can also move
- 3) Electrons and holes can recombine

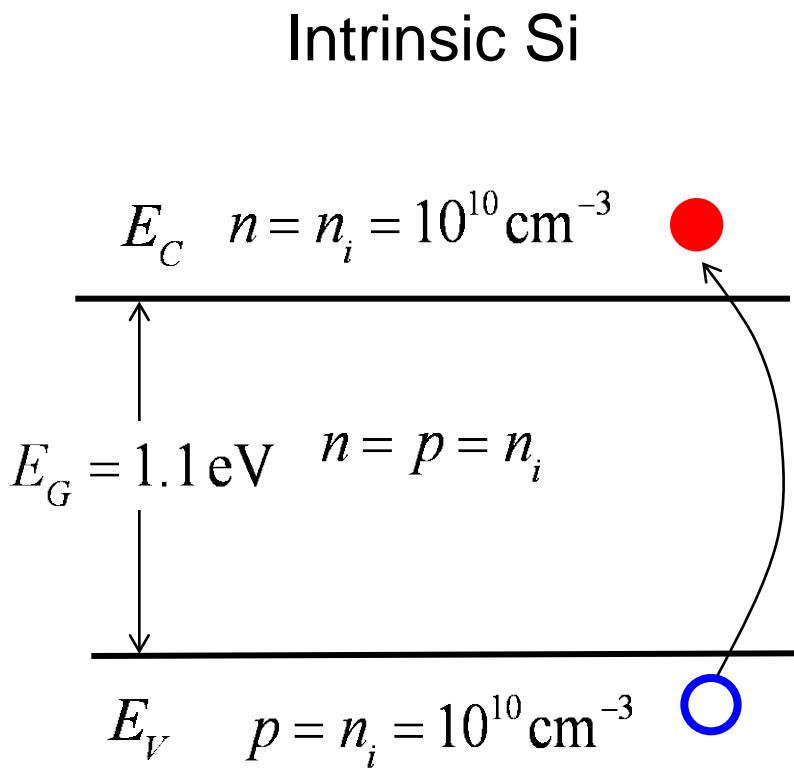
# “Energy band diagrams”



**“forbidden gap”**



# Two key parameters



$$E_G(\text{Si}) = 1.1 \text{ eV}$$

$$E_G(\text{GaAs}) = 1.4 \text{ eV}$$

$$k_B T = 0.026 \text{ eV} \quad (T = 300 \text{ K})$$

$P \sim e^{-E_G/k_B T}$  the probability of breaking one of these bonds grows exponentially harder to break with increase in band gap.

$$n_i(\text{Si}) = 1 \times 10^{10} \text{ cm}^{-3} \quad (T = 300 \text{ K})$$

$$n_i(\text{GaAs}) = 2 \times 10^6 \text{ cm}^{-3} \quad (T = 300 \text{ K})$$

remember  
that there  
are 5 times  
ten to  
the power  
of atoms  
per cubic  
cm in a  
silicon

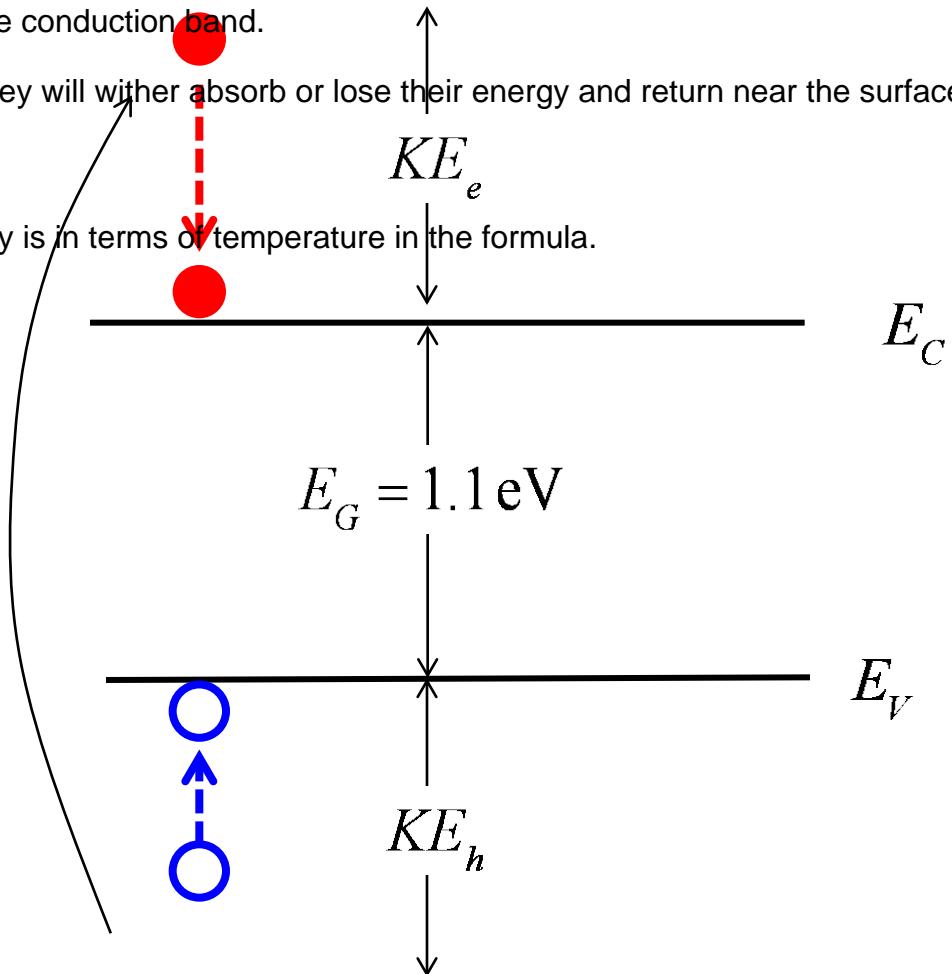
# “Hot electrons” and “hot holes”

deep in the valance band far up in the conduction band.  
very quickly with in few femto seconds they will either absorb or lose their energy and return near the surface of VB and CB.  
why hot electrons or holes : since energy is in terms of temperature in the formula.

$$E_{ph} = hf \gg E_G$$

Why “hot”?

$$E = \frac{3}{2} k_B T$$



# Metals insulators and semiconductors

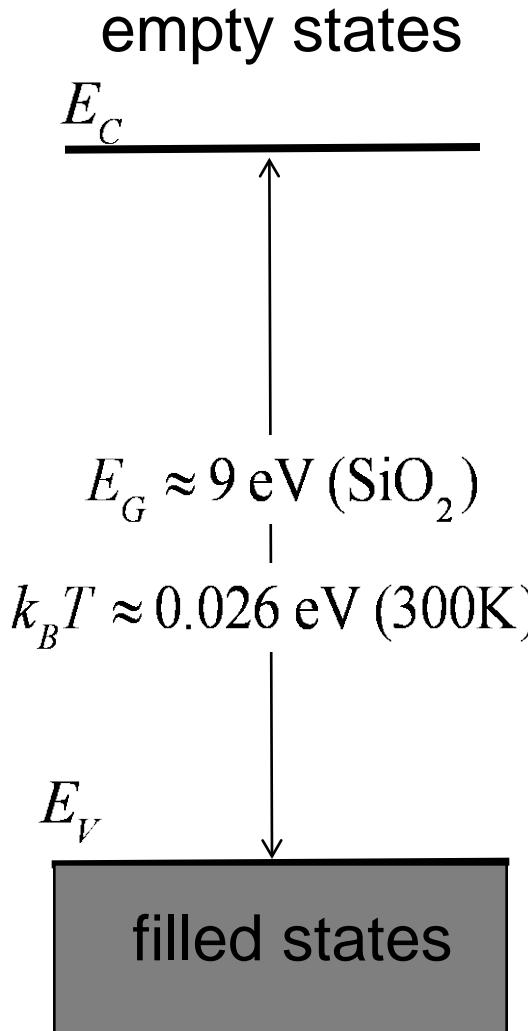
---

**Metals:** conduct electricity (and heat) well.

**Insulators:** don't conduct electricity well  
usually don't conduct heat well

**Semiconductors:** in-between, **but**  
their properties can be controlled

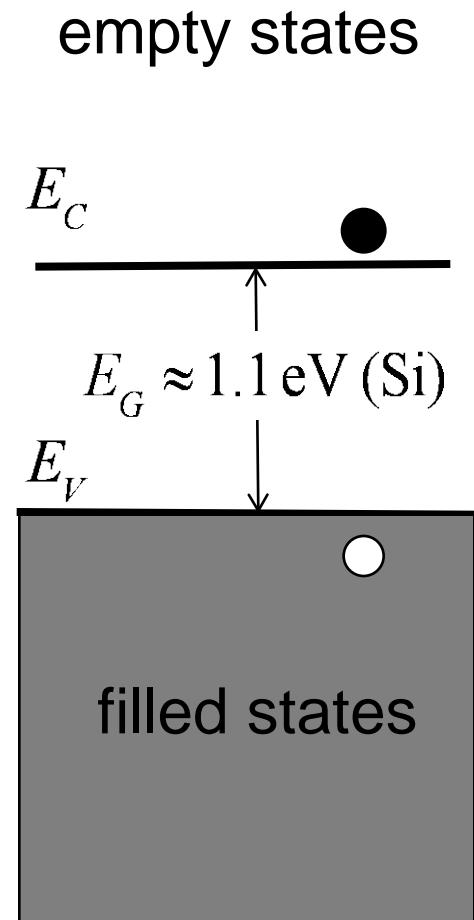
# Insulators



# Metals



# Semiconductors



# Summary

---

The localized **energy levels** in isolated atoms become delocalized **energy bands** in a solid.

Everything happens very near the top of the valence band and very near the bottom of the conduction band.

The electrical current in a semiconductor is carried by electrons in the conduction band and by holes in the valence band.

The band gap and intrinsic carrier concentration are key parameters for semiconductors.

# Primer on Semiconductors

## Unit 1: Material Properties

### Lecture 1.2: **Crystalline, polycrystalline, and amorphous semiconductors**

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

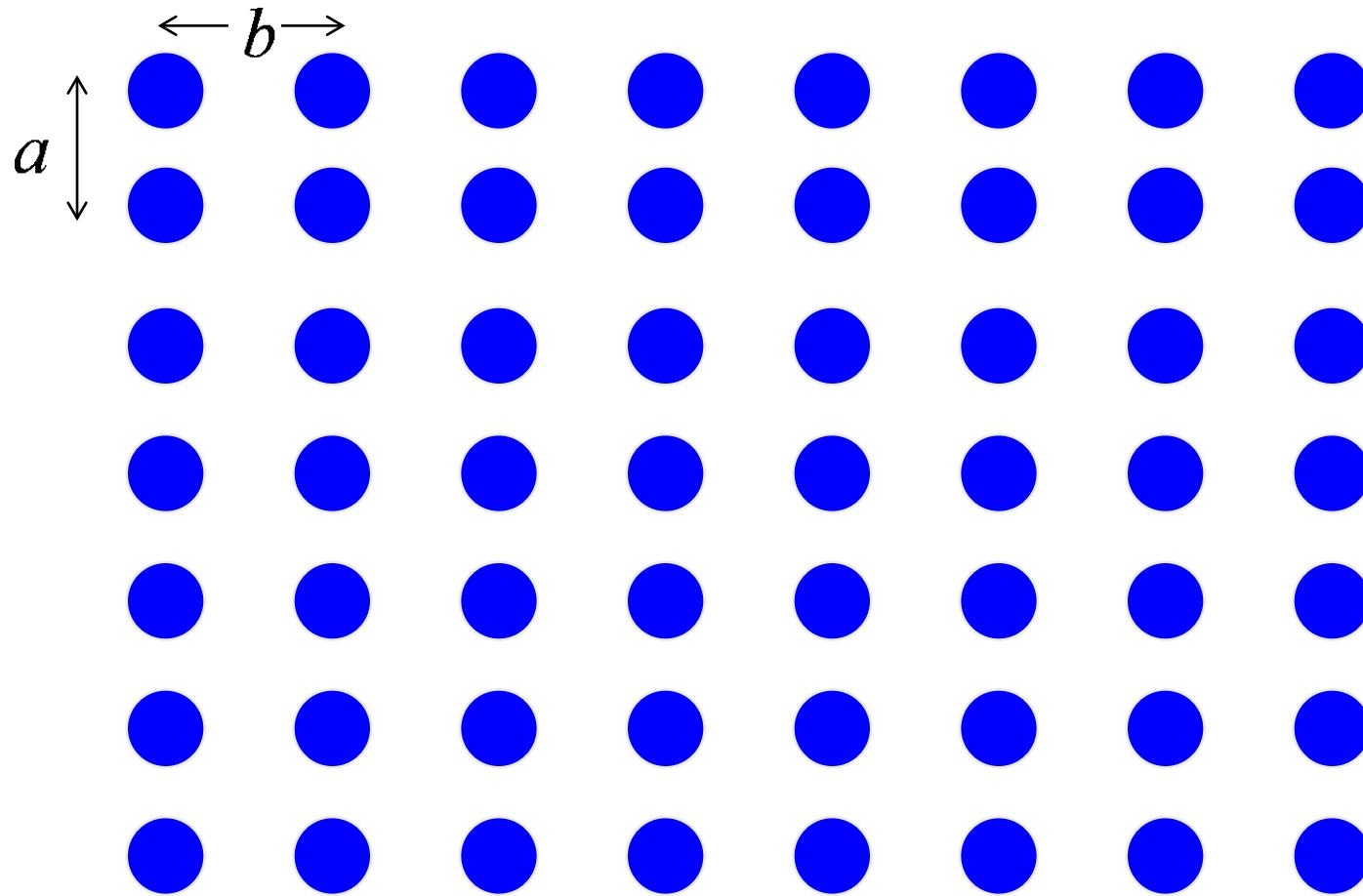
# Semiconductor materials

---

- 1) In a semiconductor **crystal**, each atom occupies a specific location in a “crystal lattice”.
- 2) **Polycrystalline** semiconductors consist of many crystalline “grains” with different orientations.
- 3) In **amorphous** semiconductors, the atoms are more or less randomly distributed throughout the solid.

# A 2D crystal

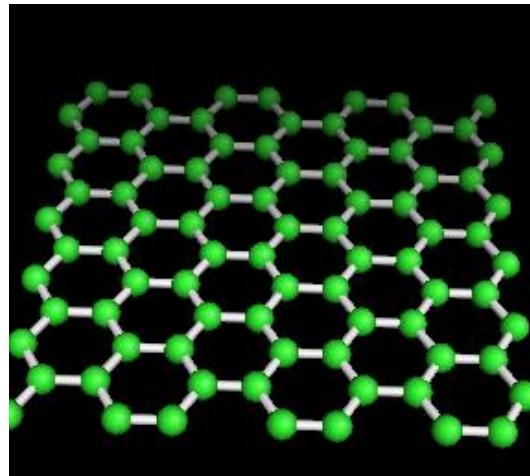
---



# Graphene: 2011 Nobel Prize in Physics

---

**Graphene** is a one-atom-thick planar carbon sheet with a honeycomb lattice.

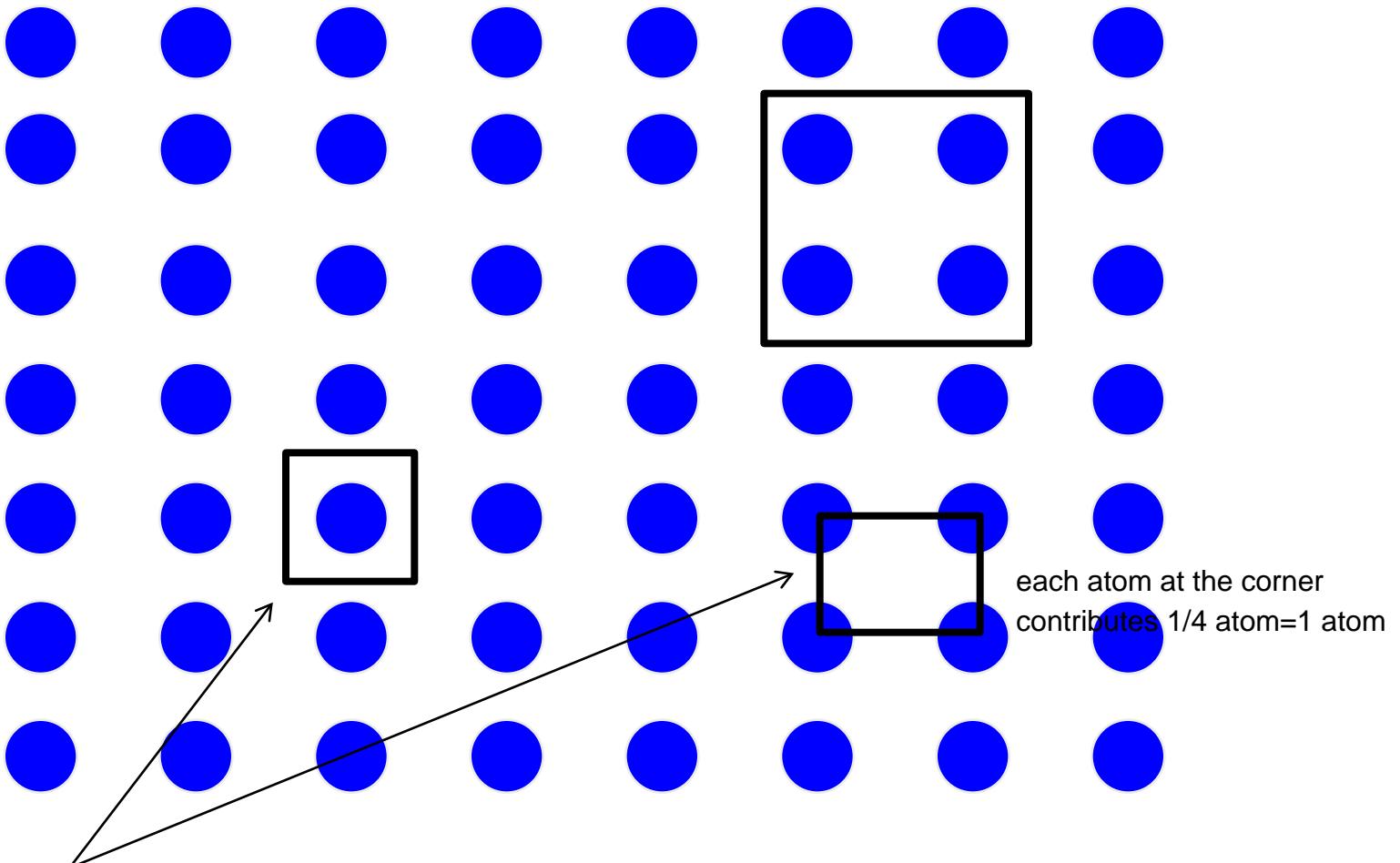


nobel prize won innovation.

source: CNTBands 2.0 on nanoHUB.org

# Unit cells

---

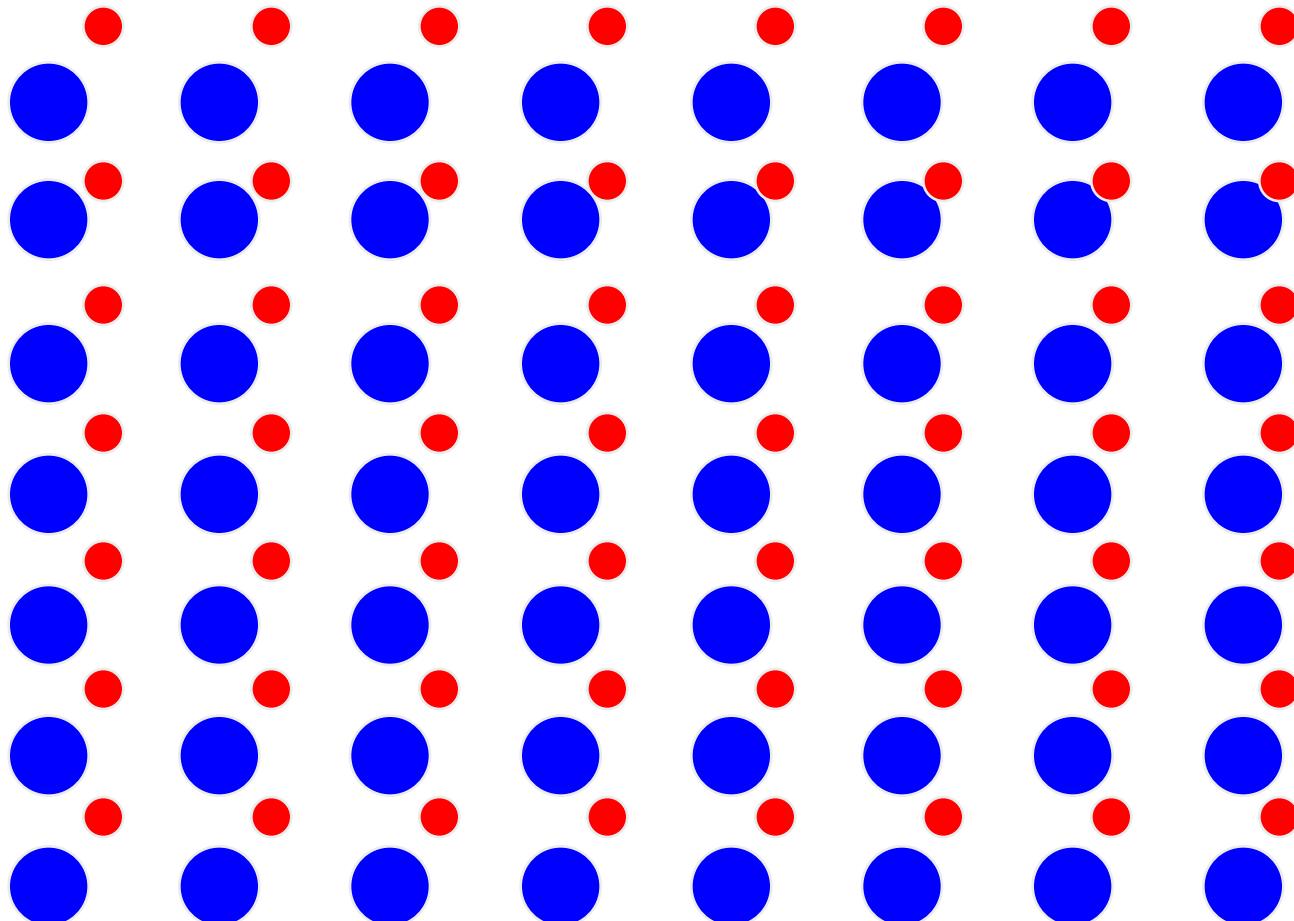


primitive unit cells

Lundstrom: 2018

# Lattice plus basis

---

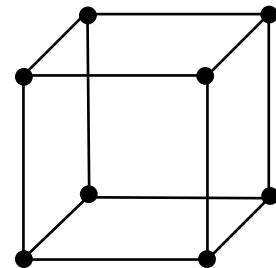


# 3D crystal structures

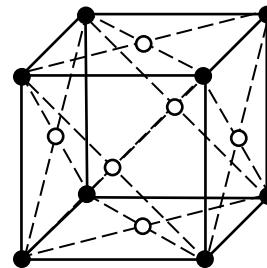
---

In 3D, there are 14 different ways to arrange lattice points such that at any point, the view is the same as at any other point. same from seeing at any side and at any point. only 14 ways to do it.

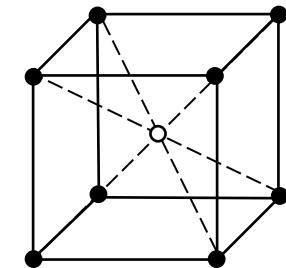
14 Bravais lattices; 3 are cubic:



simple cubic



face centered cubic



body centered cubic

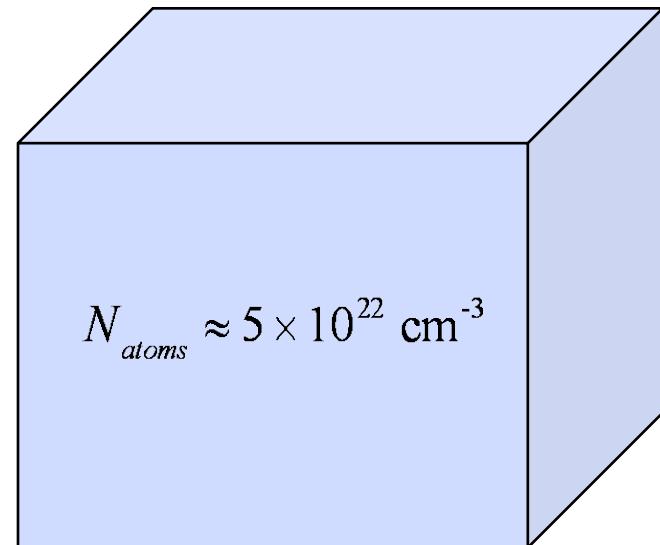
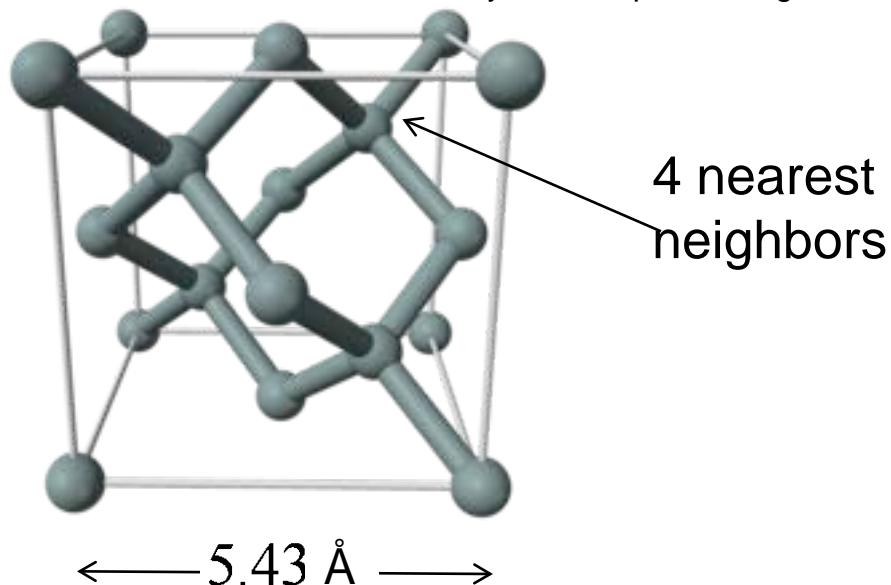
[http://en.wikipedia.org/wiki/Bravais\\_lattice](http://en.wikipedia.org/wiki/Bravais_lattice)

# Si crystal structure (diamond lattice)

each atom has 4 neighbour atoms.

(this is not a primitive unit cell)

this is actually two interpenetrating fcc lattices.

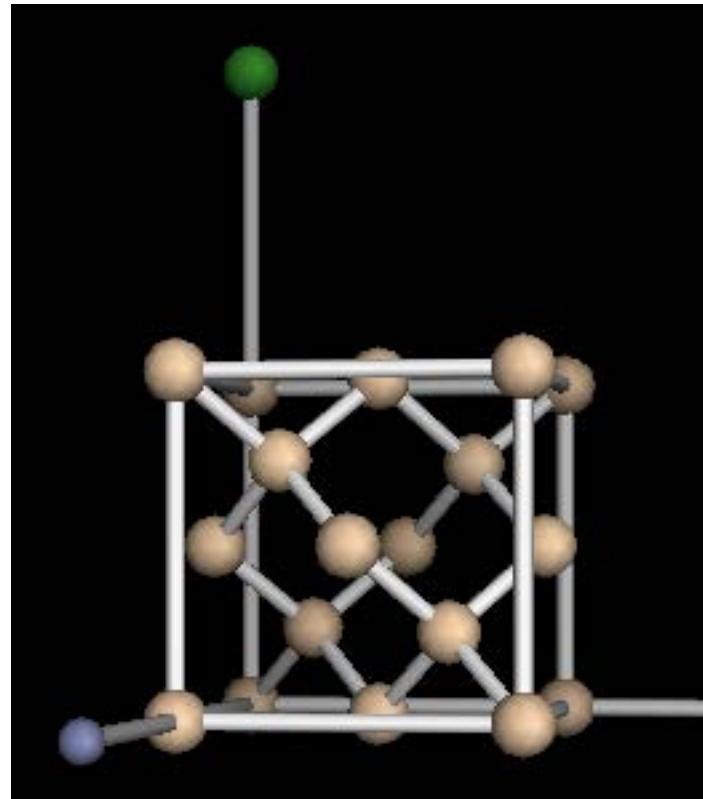


Two interpenetrating fcc lattices offset by  $\frac{1}{4}$  of the body diagonal.

that are offset by one quarter of the diagonal from the body of this cube.

# Diamond lattice

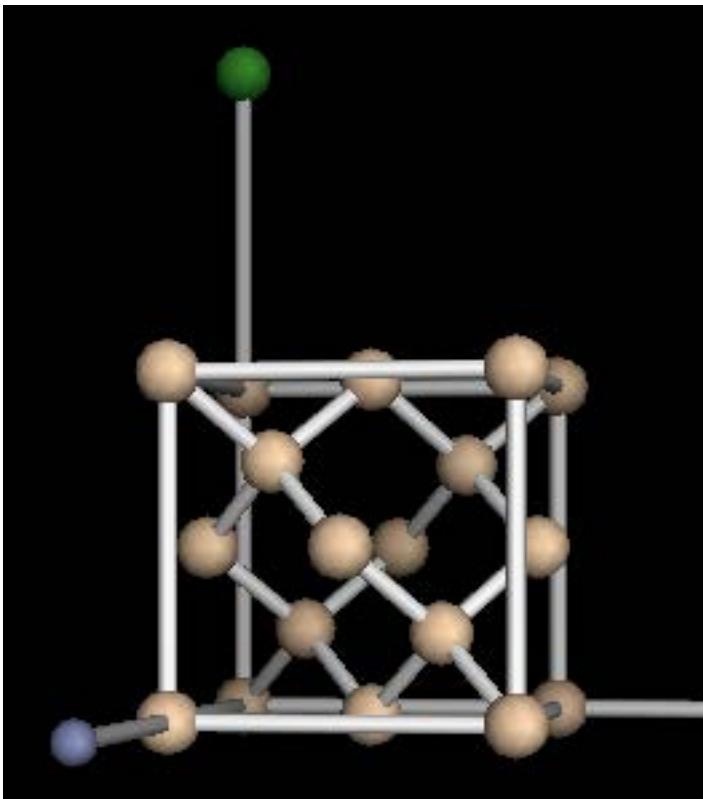
---



[https://nanohub.org/tools/crystal\\_viewer](https://nanohub.org/tools/crystal_viewer)

# Diamond lattice: atoms per unit cell

---



The 8 atoms on the corners are each shared with 8 neighboring cubes.

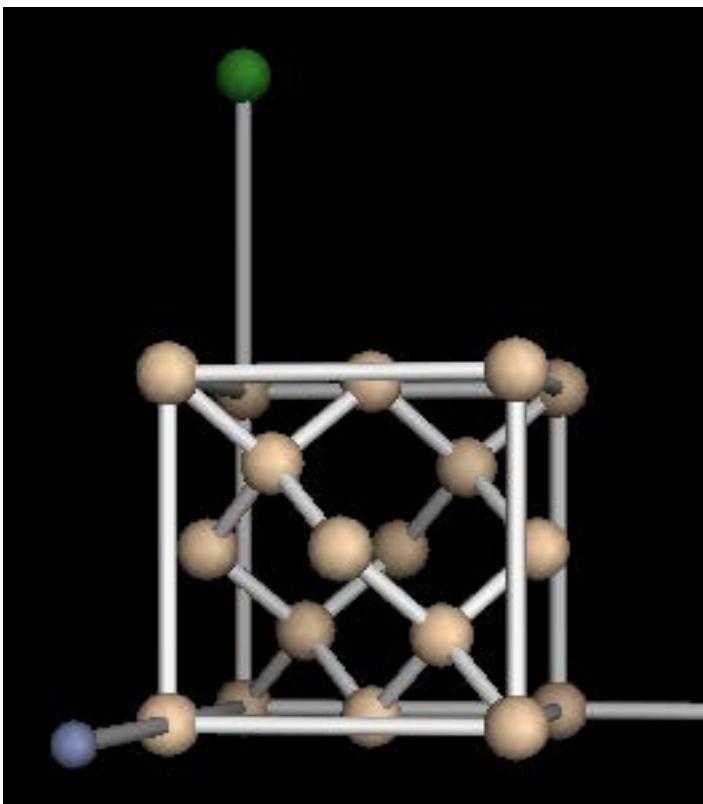
The 6 atoms on the faces are each shared with the face of an adjacent cube.

$$(8 \text{ times } \frac{1}{8}) + (6 \text{ times } \frac{1}{2}) + 4 = \\ 8 \text{ atoms per unit cell}$$

[https://nanohub.org/tools/crystal\\_viewer](https://nanohub.org/tools/crystal_viewer)

# Silicon: # atoms / cc

---



Lattice constant:  $a = 5.4307 \text{ \AA}$

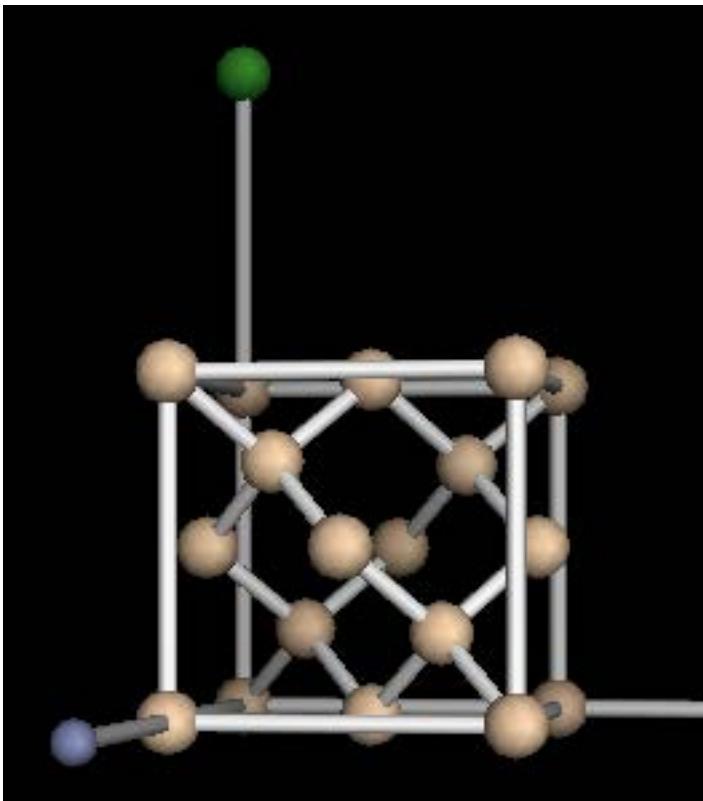
8 atoms per unit cell.

$$\begin{aligned}N_{atoms} &= \frac{8}{(5.4307 \times 10^{-10})^3} \text{ /m}^3 \\&= 4.99 \times 10^{28} \text{ /m}^3 \\&= 4.99 \times 10^{22} \text{ /cm}^3\end{aligned}$$

[https://nanohub.org/tools/crystal\\_viewer](https://nanohub.org/tools/crystal_viewer)

# Silicon: density

---



Lattice constant:  $a = 5.4307 \text{ \AA}$

Density = total mass/vol. of unit cell.

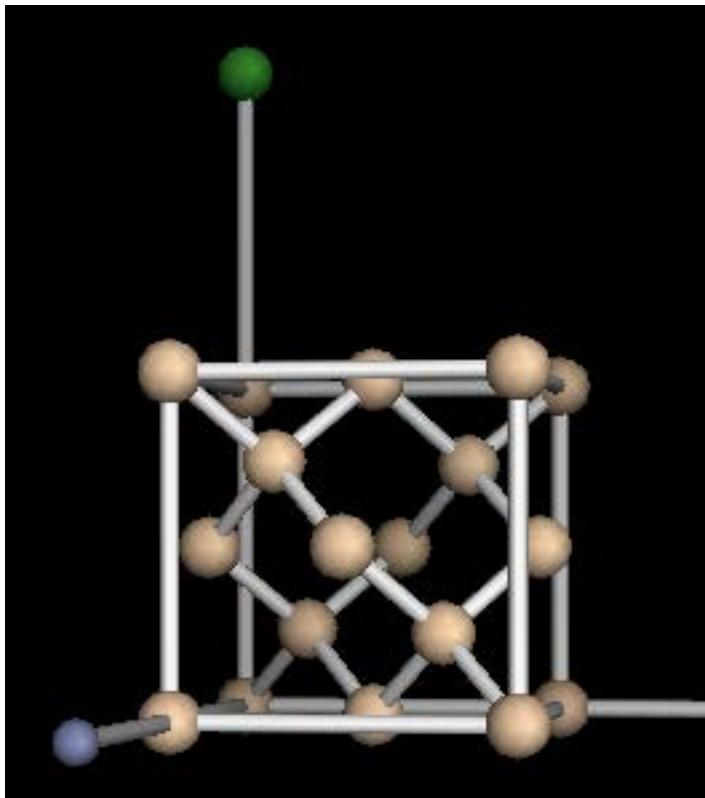
Atomic mass of Si: 28.0855 amu

$$1 \text{ amu} = 1.6605 \times 10^{-27} \text{ kg}$$

$$\rho = \frac{8 \times 28.0855 \times 1.6605 \times 10^{-27}}{(5.4307 \times 10^{-10})^3} \text{ kg/m}^3$$

$$\rho = 2.3296 \text{ g/cm}^3$$

# Silicon: NN spacing



Lattice constant:  $a = 5.4307 \text{ \AA}$

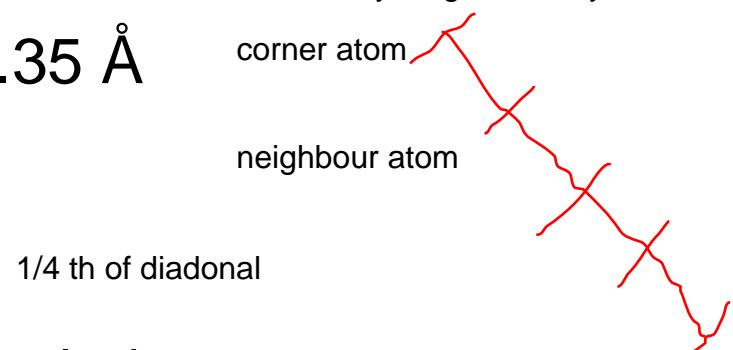
Body diagonal =  $\sqrt{3} a$ .

square root of 3 \*  
edge of the cube

NN spacing =  $\sqrt{3}a/4$

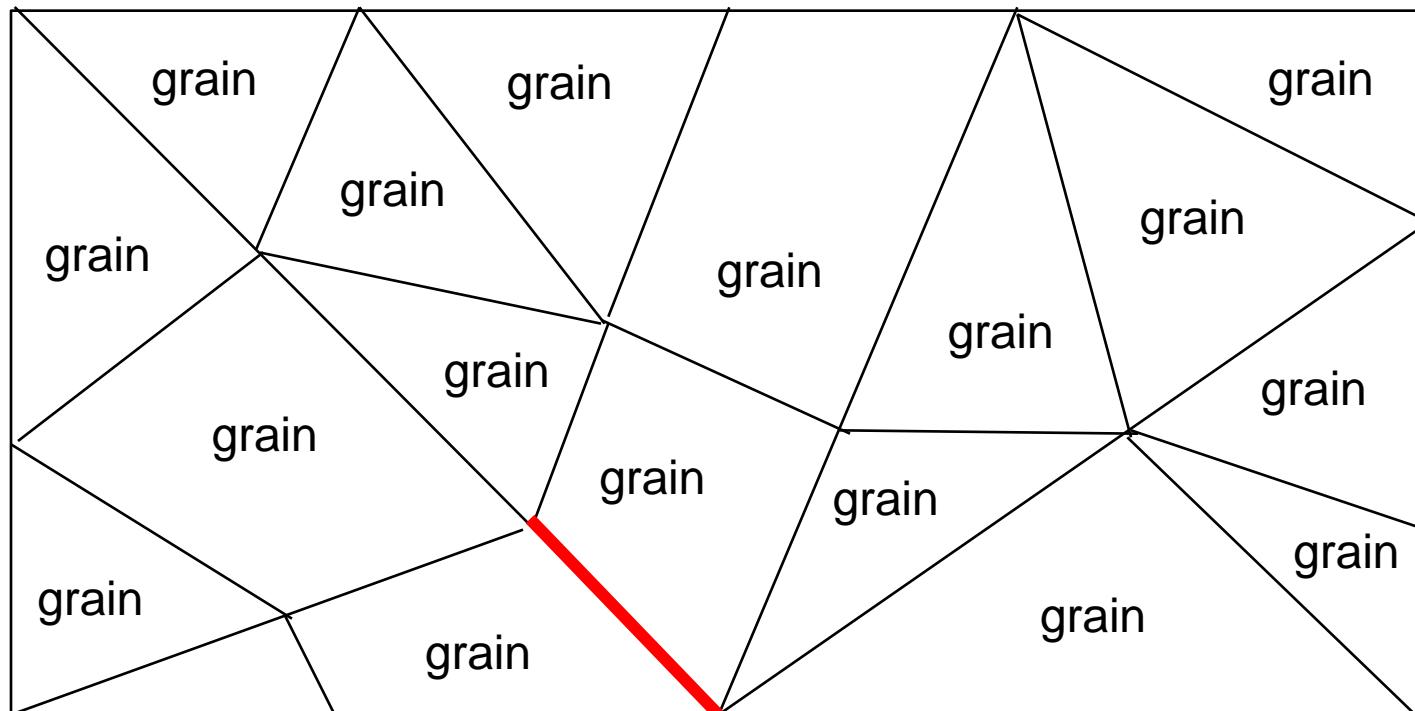
if we see the corner atom it is 1/4 of the body diagonal away from it.

NN =  $2.35 \text{ \AA}$



[https://nanohub.org/tools/crystal\\_viewer](https://nanohub.org/tools/crystal_viewer)

# Polycrystalline materials



Each grain is  
crystalline, but the  
grains are oriented  
differently.

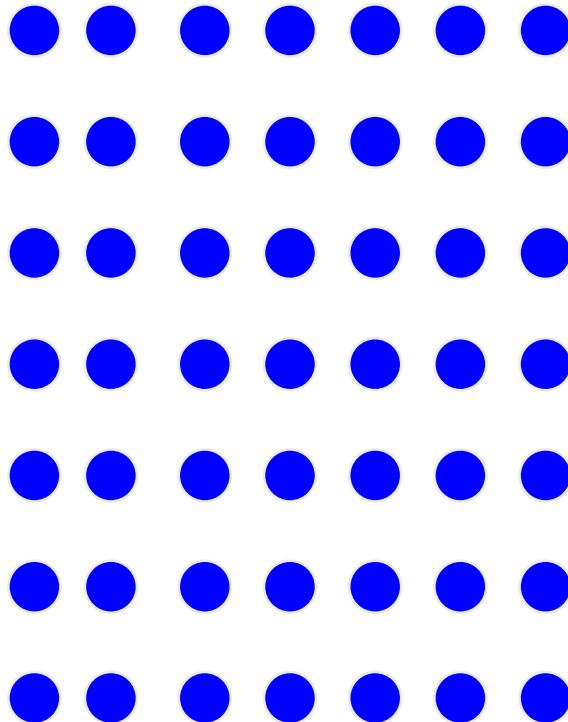
grain  
boundary

Lundstrom: 2018

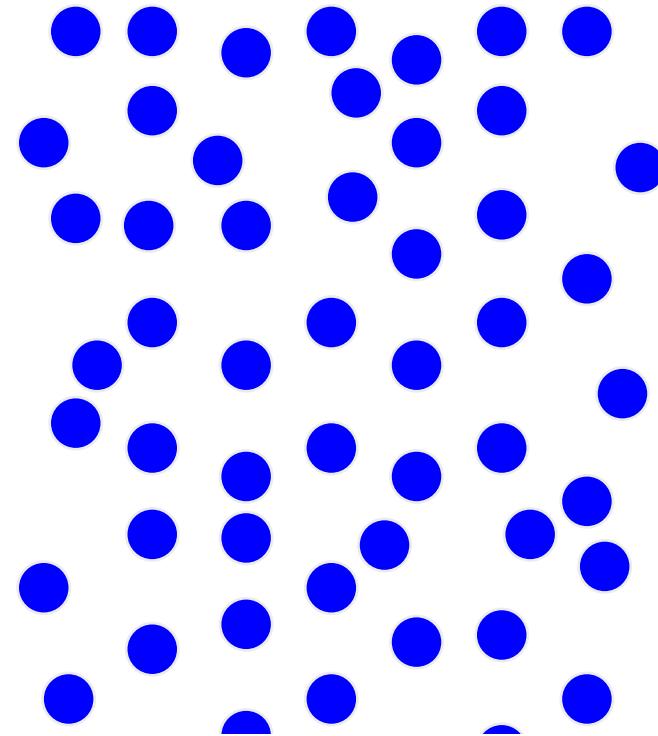
grain boundary is the source of defects which degrades device's performance. the atoms at the grain boundary doesn't match well with grains.

# Crystalline vs. amorphous

---



**Crystal:** long range order.



**Amorphous:** no long range order, but often short range order.

by average the si atom is surrounded by four neighbour atoms.

# Crystalline, polycrystalline, and amorphous

---

**Crystalline semiconductors** are the most expensive, but they are the highest quality because they have the fewest defects.

**Polycrystalline semiconductors** are less expensive, but grain boundaries can impede current flow. They are used when the highest quality is not needed, but cost is important (e.g. solar cells).

**Amorphous semiconductors** are the least expensive, but their electrical properties are the poorest. They are used when cost is a critical consideration (e.g. flat panel displays).

# Summary

---

Semiconductors crystalize in specific structures (e.g. the diamond lattice for Si and Ge).

Crystalline, polycrystalline, and amorphous semiconductors are all used – depending on cost and performance considerations.

We will focus on crystalline semiconductors, but the general concepts apply to polycrystalline and amorphous semiconductors as well.

# Primer on Semiconductors

## Unit 1: Material Properties

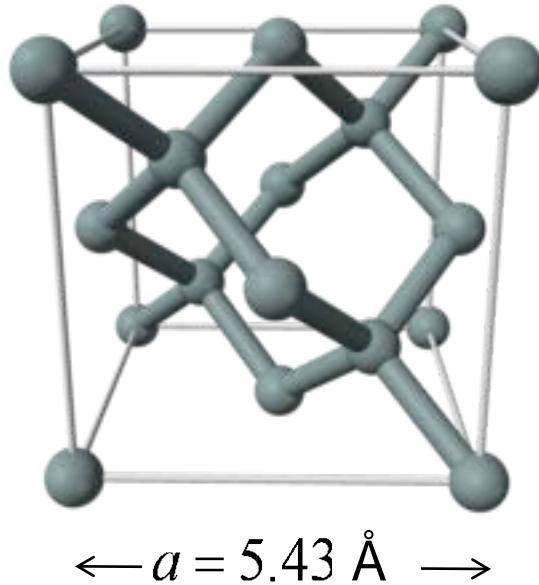
### Lecture 1.3: Miller indices

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Si crystal structure (diamond lattice)

---

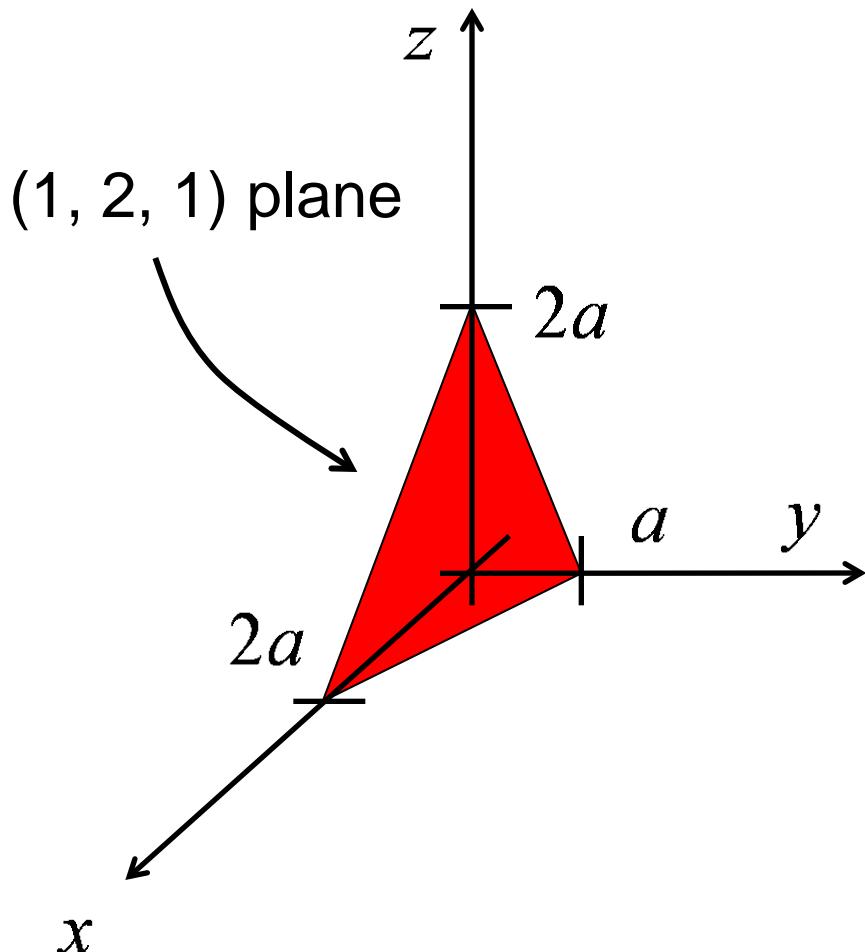


How do we specify planes and directions in a crystal?

For cubic crystals, there is a simple prescription.

# Miller index prescription for describing planes

---



1) x, y, and z-axis intercepts:

$$\begin{matrix} 2a, 1a, 2a \\ 2, 1, 2 \end{matrix}$$

2) invert:

$$\begin{matrix} \frac{1}{2}, 1, \frac{1}{2} \end{matrix}$$

3) Rationalize:

$$1, 2, 1$$

# Question

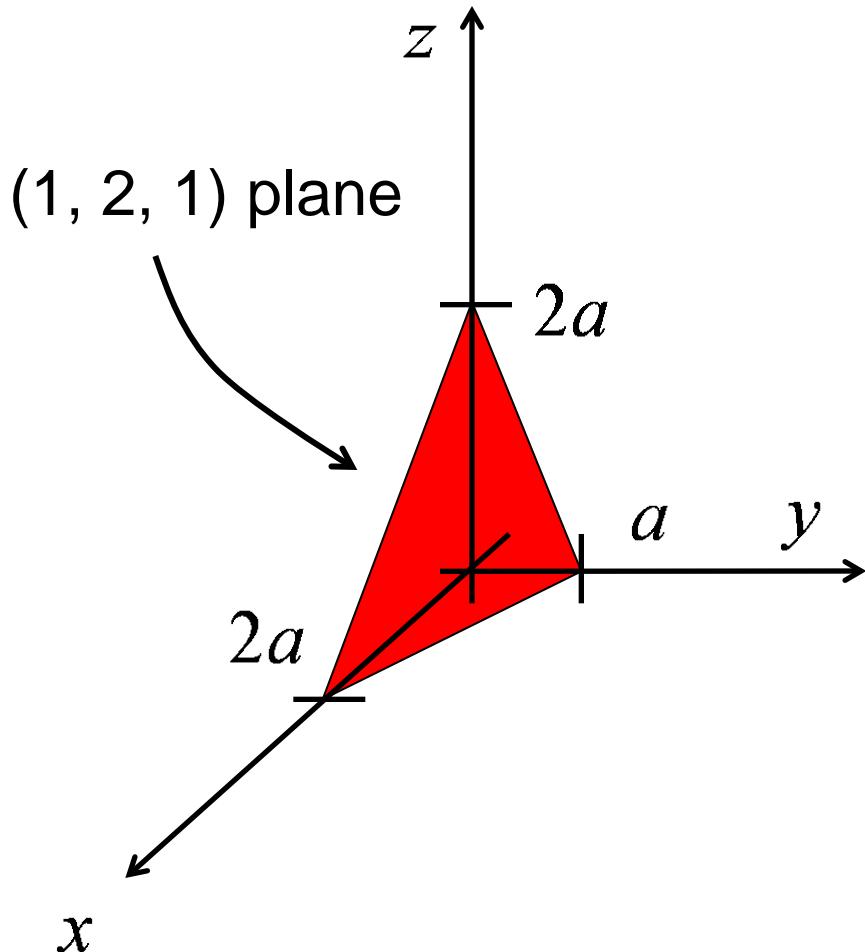
---

Where does this prescription come from?

Answer: If we remember the equation for a plane, we can figure it out.

# Where it comes from?

---



equation of a plane:

$$\frac{x}{x_{\text{int}}} + \frac{y}{y_{\text{int}}} + \frac{z}{z_{\text{int}}} = 1$$

describe with the numbers:

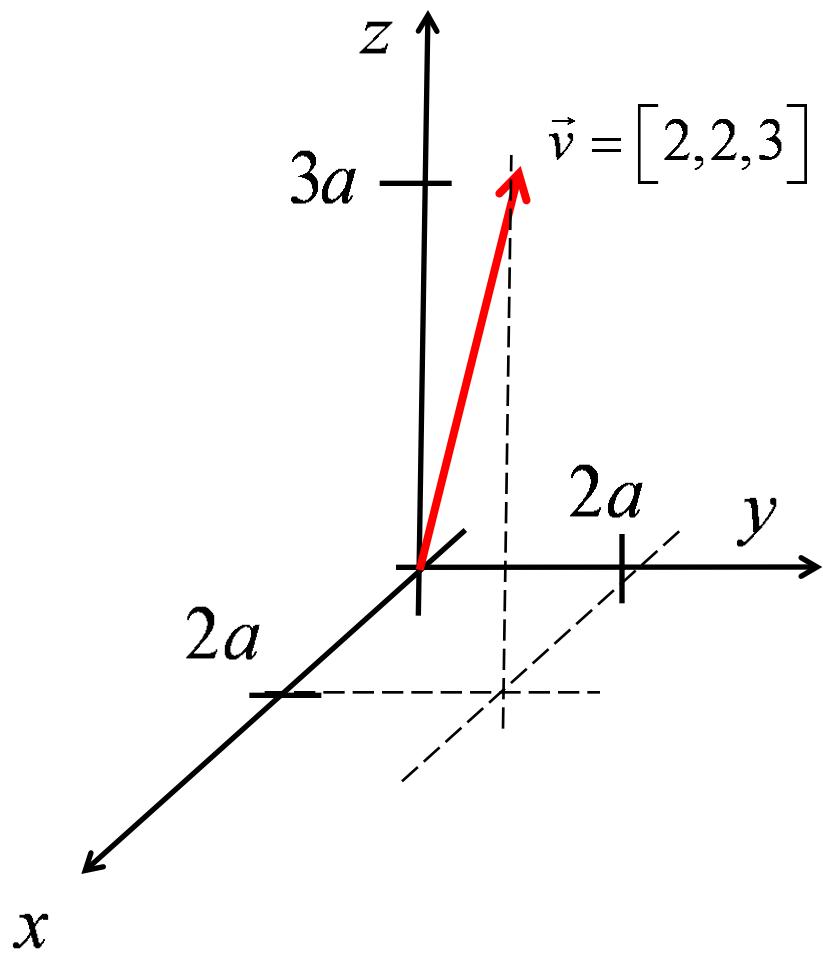
$$\frac{1}{x_{\text{int}}}, \frac{1}{y_{\text{int}}}, \frac{1}{z_{\text{int}}}$$

equivalent to:

$$\frac{1}{x_{\text{int}}/a}, \frac{1}{y_{\text{int}}/a}, \frac{1}{z_{\text{int}}/a}$$

# Prescription for describing directions

---



1) equation of a vector:

$$\vec{v} = 2a\hat{x} + 2a\hat{y} + 3a\hat{z}$$

2) describe with components:

$$2a, 2a, 3a$$

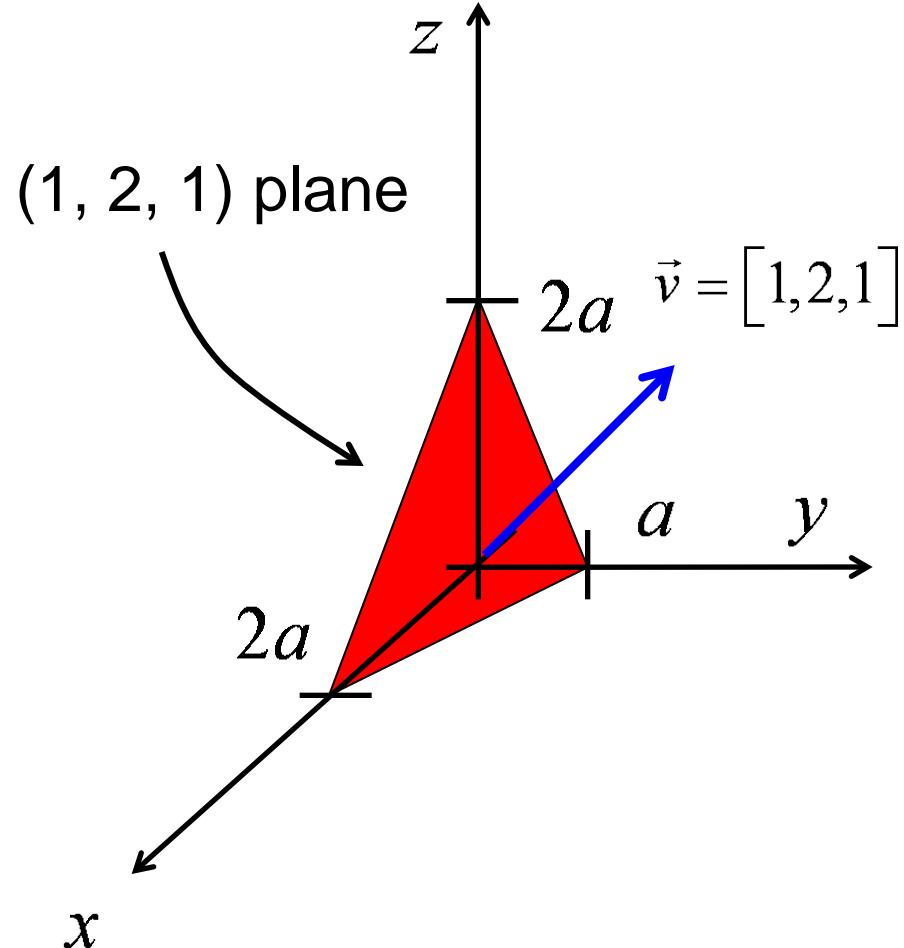
3) equivalent to:

$$2, 2, 3$$

(smallest set of  
whole numbers)

# Direction normal to a plane

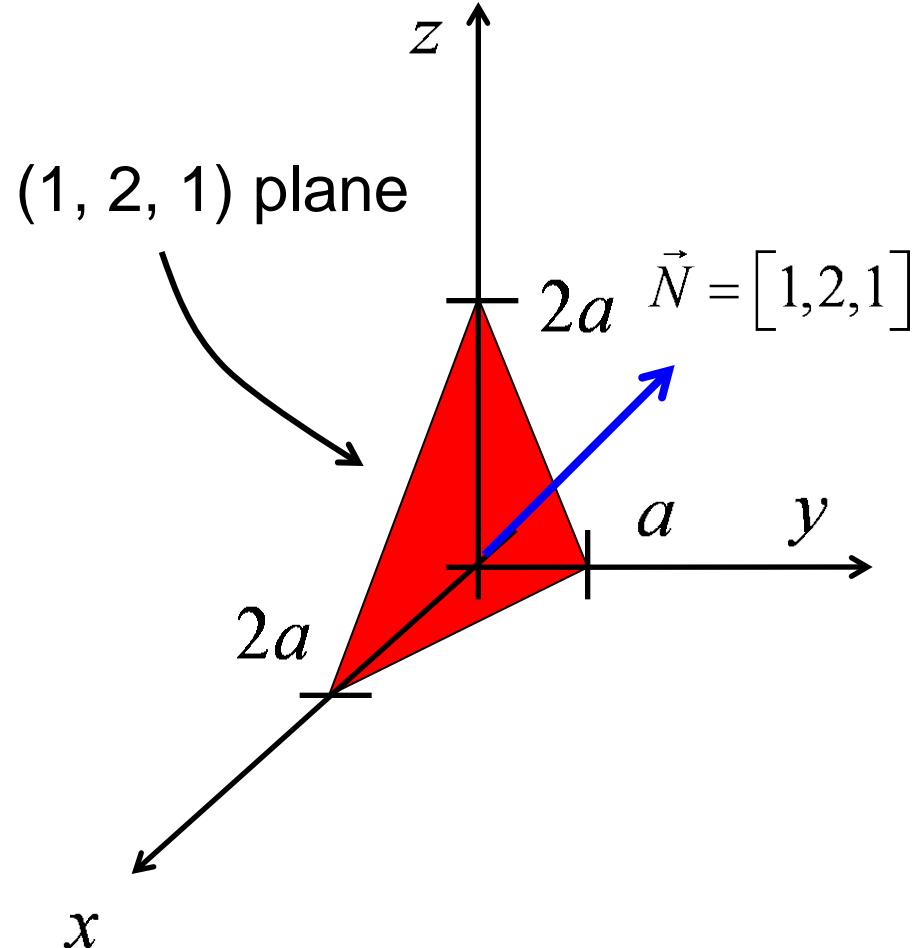
---



The vector  $[1, 2, 1]$  is normal to the plane  $(1, 2, 1)$ .

Why?

# Why is $[h k l]$ normal to $(h k l)$ ?



equation of a plane:

$$f(x, y, z) = \frac{x}{x_{\text{int}}} + \frac{y}{y_{\text{int}}} + \frac{z}{z_{\text{int}}} = 1$$

normal to a plane:

$$\vec{N} = \nabla f(x, y, z) = \frac{\partial f}{\partial x} \hat{x} + \frac{\partial f}{\partial y} \hat{y} + \frac{\partial f}{\partial z} \hat{z}$$

(gradient)

$$\vec{N} = \frac{1}{x_{\text{int}}} \hat{x} + \frac{1}{y_{\text{int}}} \hat{y} + \frac{1}{z_{\text{int}}} \hat{z}$$

# Angle between planes

depends upon etching

normal of 1,0,0 plane

$$\vec{N}_1 = [1, 0, 0]$$

(1, 0, 0) plane

(KOH etching)

$$\vec{N}_2 = [1, 1, 1]$$

$$\vec{N}_1 \bullet \vec{N}_2 = N_1 N_2 \cos \theta \quad (\text{dot product formula})$$

$$\cos \theta = \frac{\vec{N}_1 \bullet \vec{N}_2}{N_1 N_2}$$

# Angle between planes

$$\cos \theta = \frac{\vec{N}_1 \bullet \vec{N}_2}{N_1 N_2}$$

$$\vec{N}_1 = [h_1, k_1, l_1]$$

$$\vec{N}_2 = [h_2, k_2, l_2]$$

$$\cos \theta = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2} \sqrt{h_2^2 + k_2^2 + l_2^2}}$$

$$\vec{N}_1 = [1, 0, 0]$$

$$\vec{N}_2 = [1, 1, 1]$$

$$\cos \theta = \frac{1+0+0}{\sqrt{1^2 + 0^2 + 0^2} \sqrt{1_2^2 + 1_2^2 + 1_2^2}}$$

$$\cos \theta = \frac{1}{\sqrt{3}}$$

$$\theta = 54.7^\circ$$

# Notation for planes and directions

---

$(h \ k \ l)$  A specific plane.

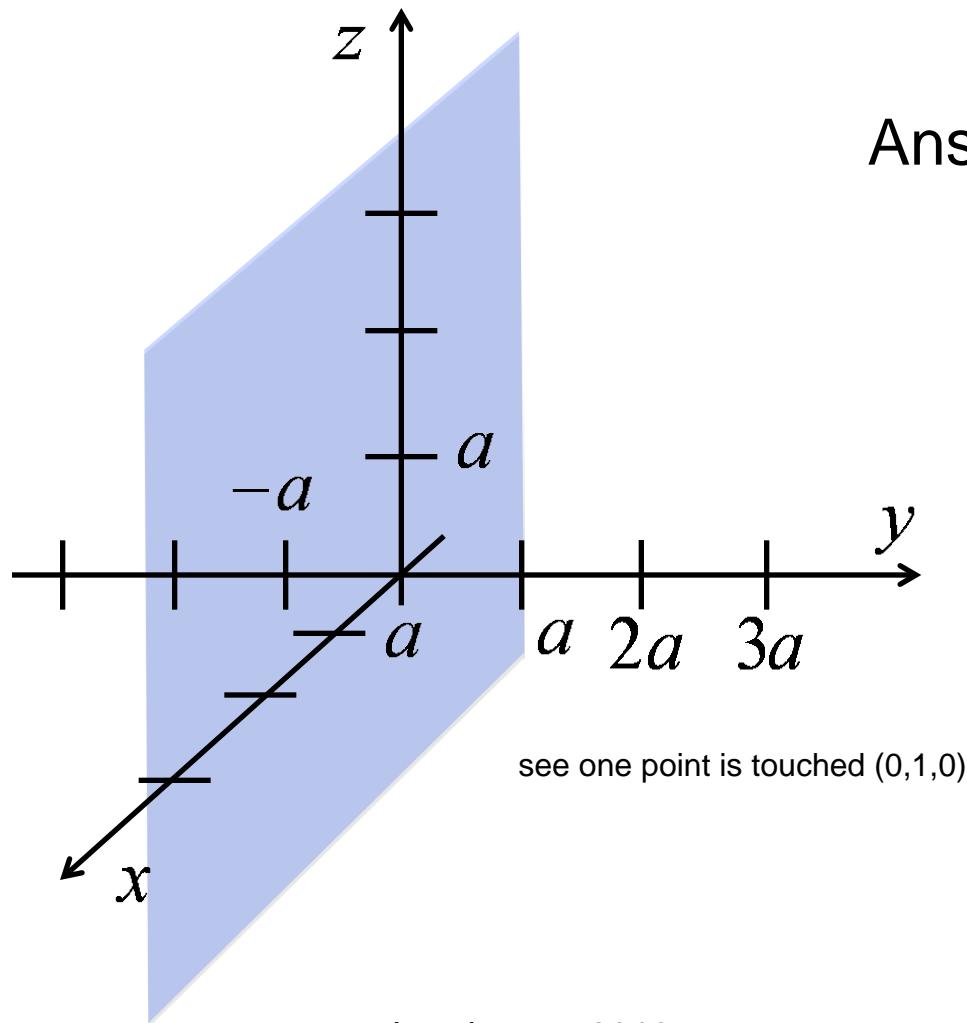
$[h \ k \ l]$  A direction normal  
to the plane above.  $\vec{N} = h\hat{x} + k\hat{y} + l\hat{z}$

$\{h \ k \ l\}$  A set of equivalent planes.

$\langle h \ k \ l \rangle$  A set of equivalent directions.

# What plane is this?

---

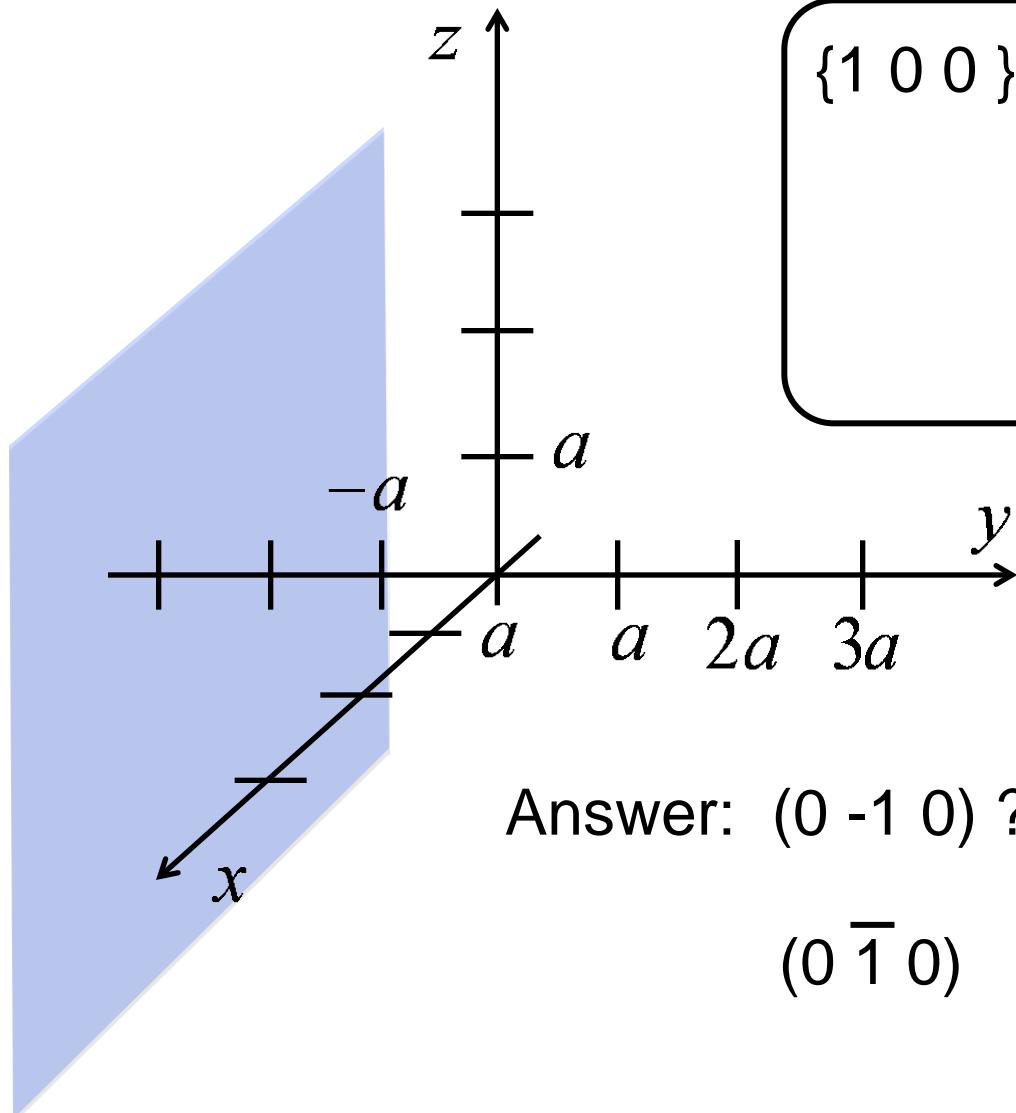


Answer:  $(0 \ 1 \ 0)$

$(0 \ 2 \ 0)$  ?

see one point is touched  $(0,1,0)$

# What plane is this?



$\{1\ 0\ 0\}$  set of equivalent planes

$(100)\ (010)\ (001)$

$(\bar{1}00)\ (0\bar{1}0)\ (00\bar{1})$

if the plane intersects the origin, simply translate the origin to an equivalent location.

intercepts:  $1/0, -1, 1/0$

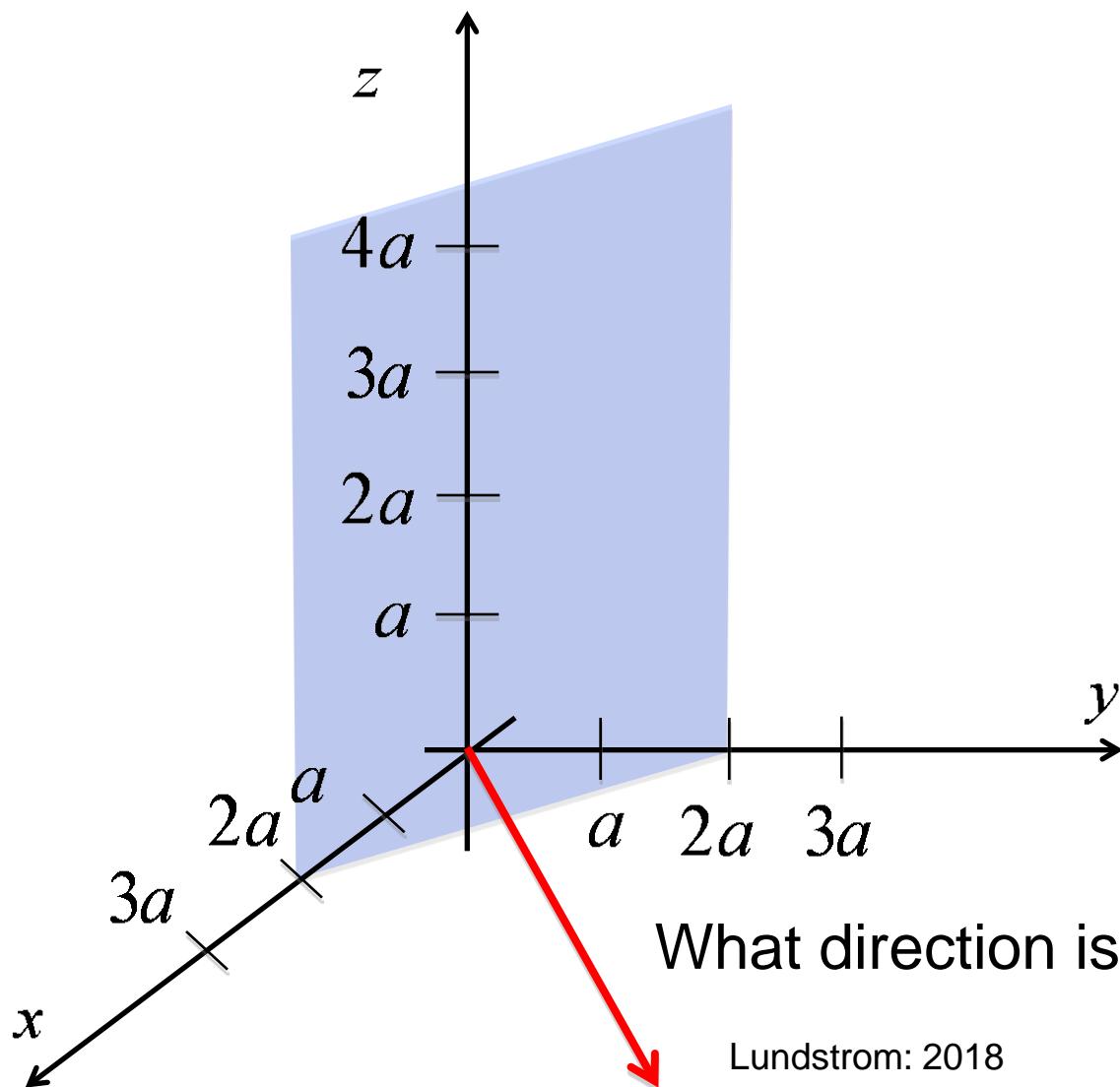
planes :  $0 -1 0$

Answer:  $(0 -1 0)$  ?

$(0 \bar{1} 0)$

note: parallel planes are equal if we do miller indices method.

# What plane is this?



Answer: (1 1 0)

intercepts : 2 2 infinity

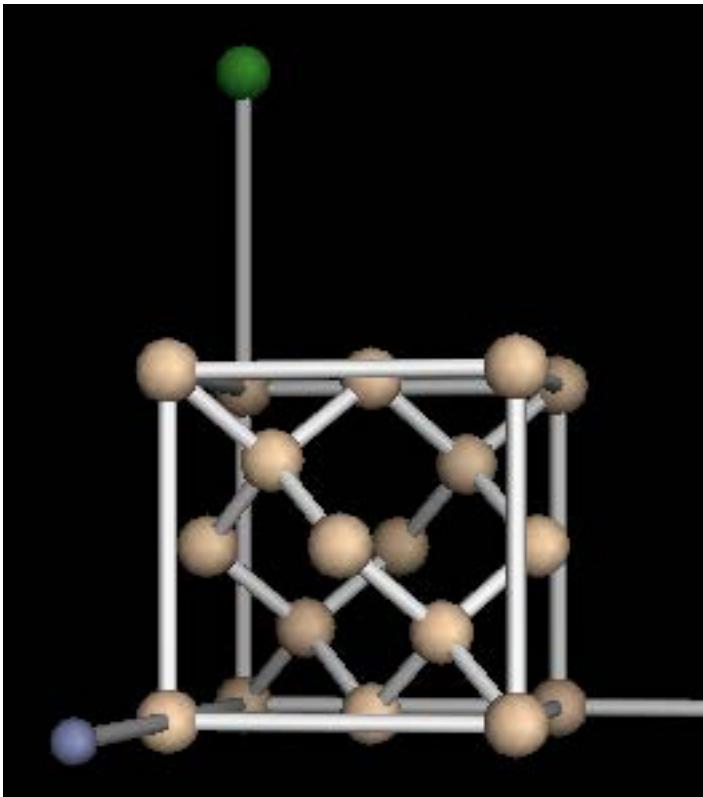
inverse : 1/2 1/2 0

planes: 2 2 0

What direction is this?

# Silicon: atoms / cm<sup>2</sup> on a {100} plane

---



Lattice constant: 5.4307 Å

Atoms on face = (4 times  $\frac{1}{4}$ ) + 1 = 2

$$N_S = 2/a^2 \quad (\text{density of atoms per square cm})$$

$$N_S = 6.81 \times 10^{14} / \text{cm}^2$$

[https://nanohub.org/tools/crystal\\_viewer](https://nanohub.org/tools/crystal_viewer)

# Summary

---

Miller indices provide a simple way to describe planes and directions in crystals.

For cubic systems, the prescription is simple.

# Summary of Miller index notation

---

$(h k l)$  A specific plane.

$[h k l]$  A direction normal  
to the plane above.

$\{h k l\}$  A set of equivalent planes.

since in a cube if we rotate x=y=z directions.

$\langle h k l \rangle$  A set of equivalent directions.

# Primer on Semiconductors

## Unit 1: Material Properties

### Lecture 1.4: Properties of common semiconductors

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Semiconductors

**column IV**

Period	1	2	3	4	5	6	7	8	9	10	
1	1 H									2 He	
2	3 Li	4 Be									
3	11 Na	12 Mg									
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	
6	55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	
7	87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	
* Lanthanoids		57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy
** Actinoids		89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf

[http://en.wikipedia.org/wiki/Periodic\\_table](http://en.wikipedia.org/wiki/Periodic_table)

# III-V semiconductors

Period															Col. III	Col. V			
1		1 H														2 He			
2		3 Li	4 Be														10 Ne		
3		11 Na	12 Mg														18 Ar		
4		19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5		37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6		55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7		87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Uuo	115 Uup	116 Uuh	117 Uus	118 Uuo
* Lanthanoids		57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu			
** Actinoids		89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr			

[http://en.wikipedia.org/wiki/Periodic\\_table](http://en.wikipedia.org/wiki/Periodic_table)

# II-VI semiconductors

Period	Col. II										Col. VI									
1	1 H																	2 He		
2	3 Li	4 Be																10 Ne		
3	11 Na	12 Mg																		
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr		
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe		
6	55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn		
7	87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo		
* Lanthanoids		57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu				
** Actinoids		89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr				

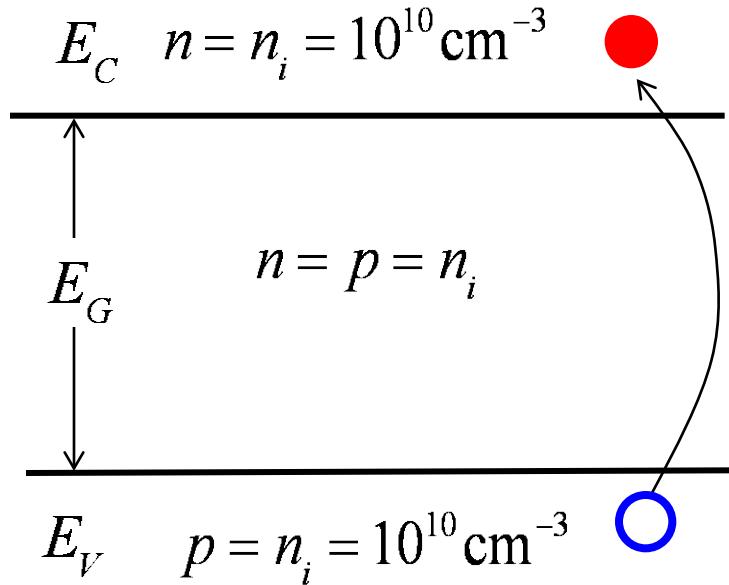
[http://en.wikipedia.org/wiki/Periodic\\_table](http://en.wikipedia.org/wiki/Periodic_table)

Lundstrom: 2018

# Two key numbers

---

## Intrinsic Si



$$E_G(\text{Si}) = 1.1 \text{ eV}$$

$$n_i(\text{Si}) = 1 \times 10^{10} \text{ cm}^{-3} \quad (T = 300 \text{ K})$$

$$n_i \propto e^{-E_G/2k_B T}$$

# A few common semiconductors

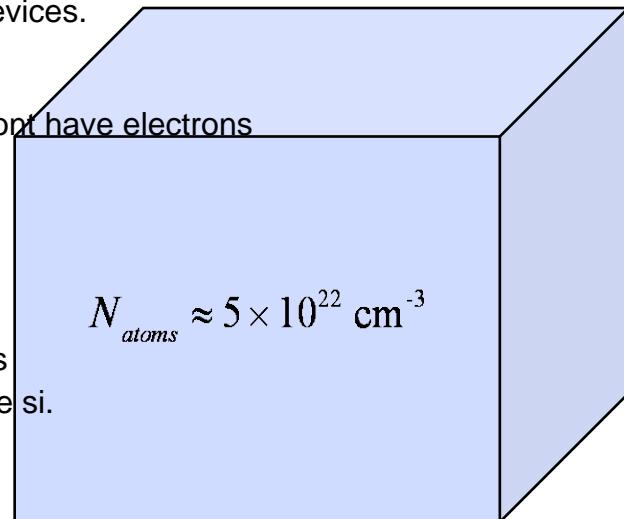
---

Semiconductor	Band gap (eV)	intrinsic density
Ge	0.663	$2.0 \times 10^{13} \text{ cm}^{-3}$
Si	1.125	$1.0 \times 10^{10} \text{ cm}^{-3}$
InP	1.344	
GaAs	1.422	$2.3 \times 10^6 \text{ cm}^{-3}$
CdTe	1.5	
6H SiC	2.99	
4H SiC	3.26	
GaN	3.4	

Later, we will learn how to calculate  $n_i$ .

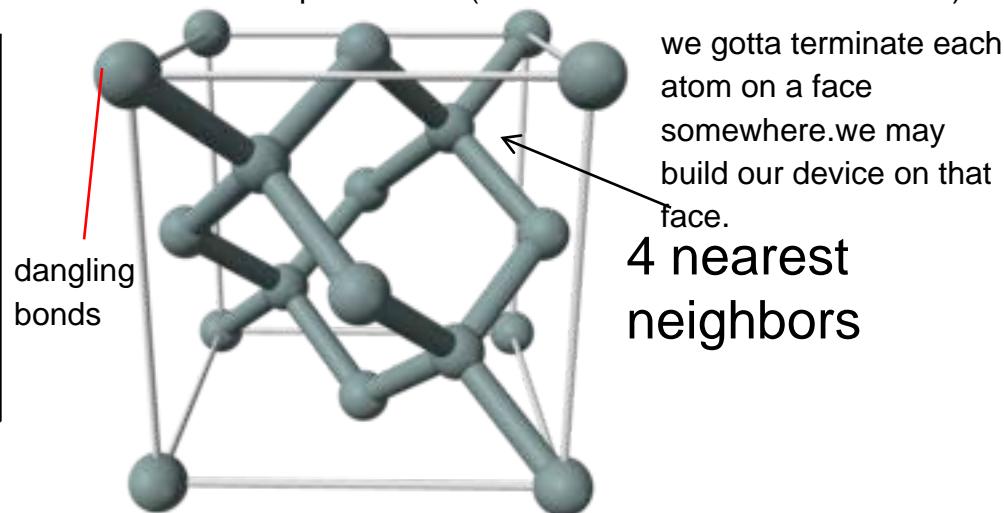
# Why is Si so common in electronics?

remarkable property that makes it use to manufacture high performance devices.



other scs don't have these kinds of property unlike si.

because of its important use.(not because of electronic devices)



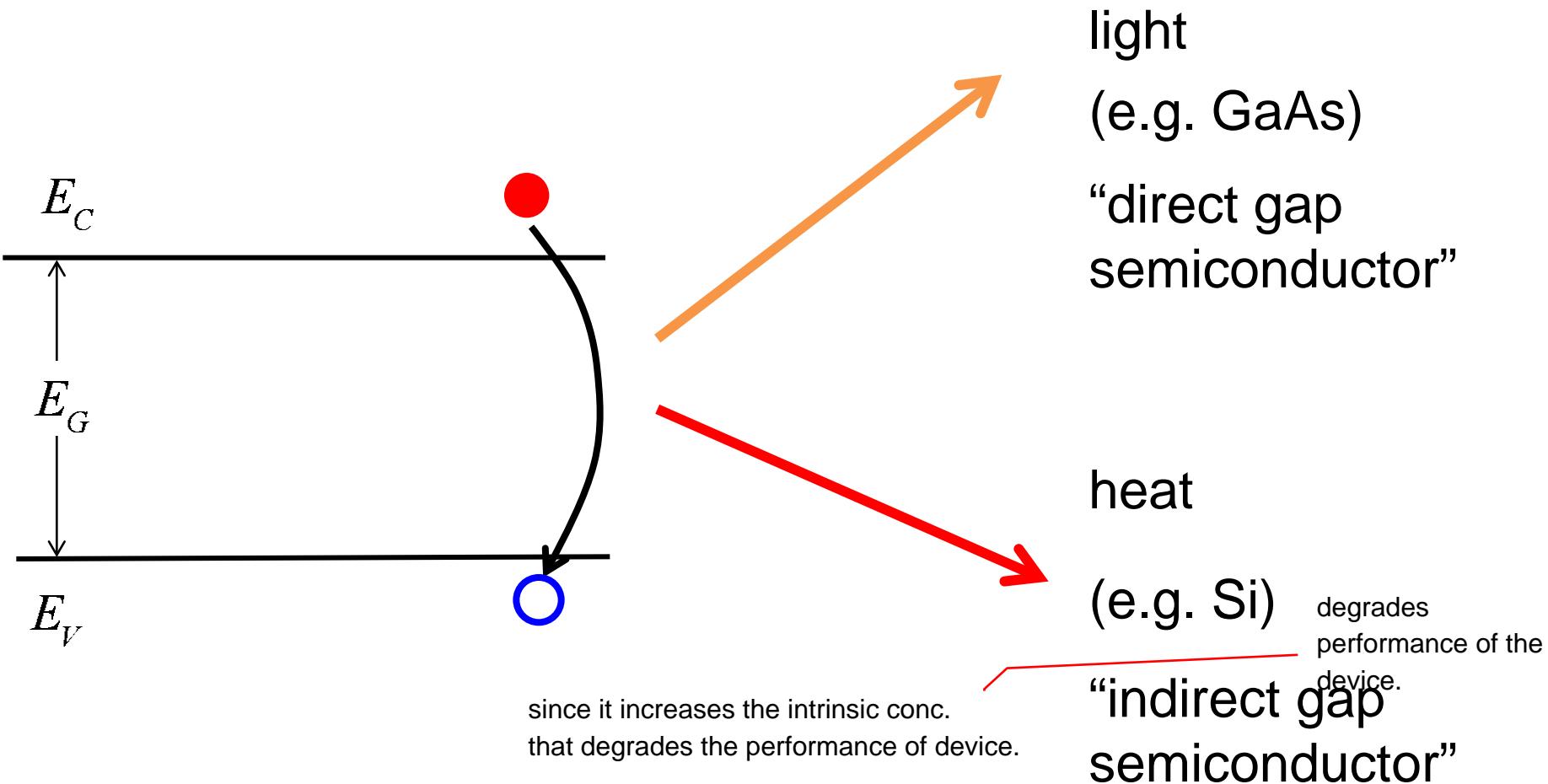
Inside the crystal, each atom has four nearest neighbors and all bonds are satisfied.

Surfaces are defects with many “dangling bonds”.

Silicon has a “native oxide” ( $\text{SiO}_2$ ) that ties up dangling bonds and “passivates” the surface.

si has a significant property.( $\text{SiO}_2$ - hard high quality insulator)  
sio<sub>2</sub> s crystalline property is quartz.sio<sub>2</sub> will tie up with these dangling bonds.hence nullify the effect of defects on electronic devices.

# Recombination



# Other properties

---

How fast do charge carriers move (mobility)?

What is the thermal conductivity?

At what electric field does the semiconductor “break down”?

Effective mass?

etc.

# Summary

---

Silicon is the most commonly used semiconductor because it has a native oxide that passivates the surface.

Other semiconductors are used when Si isn't suitable (e.g. to make light-emitting devices).

The **bandgap and intrinsic carrier concentration** are two key (related) parameters for a semiconductor. We will encounter several other important parameters later.

## Primer on Semiconductors

# Unit 1: Material Properties

## Lecture 1.5: Free carriers in semiconductors

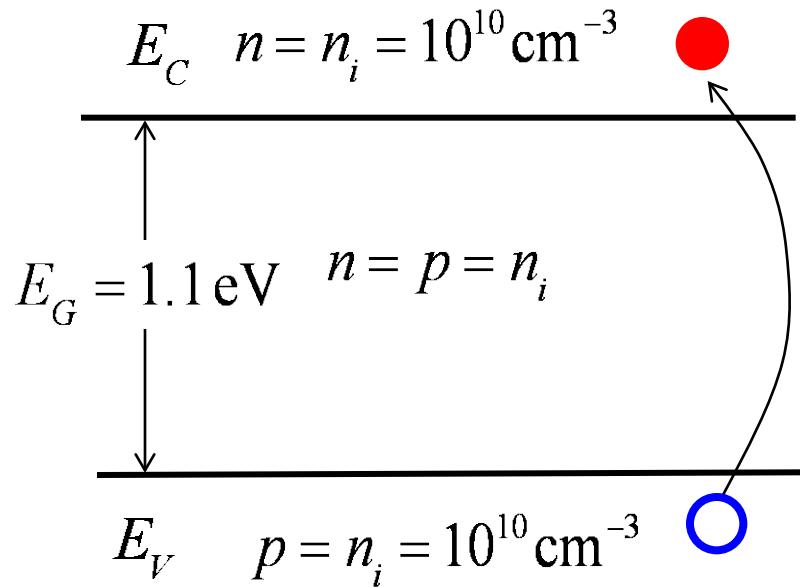
**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Electrons and holes in semiconductors

---

Intrinsic Si

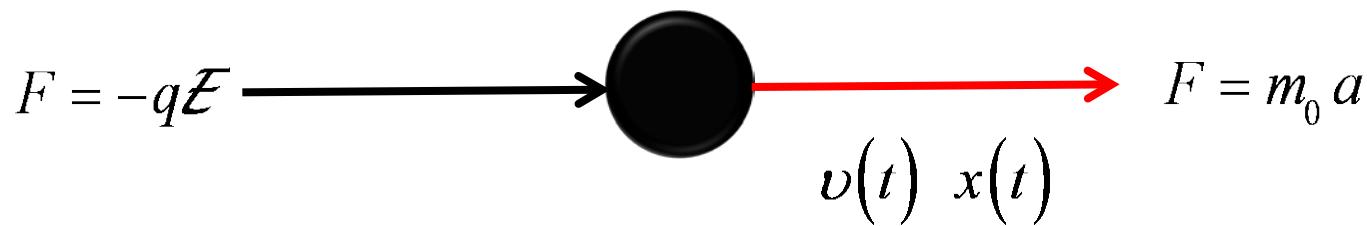


What are the properties of  
**electrons** in the conduction  
band?

What are the properties of  
**holes** in the valence band?

# Free electron mass

---



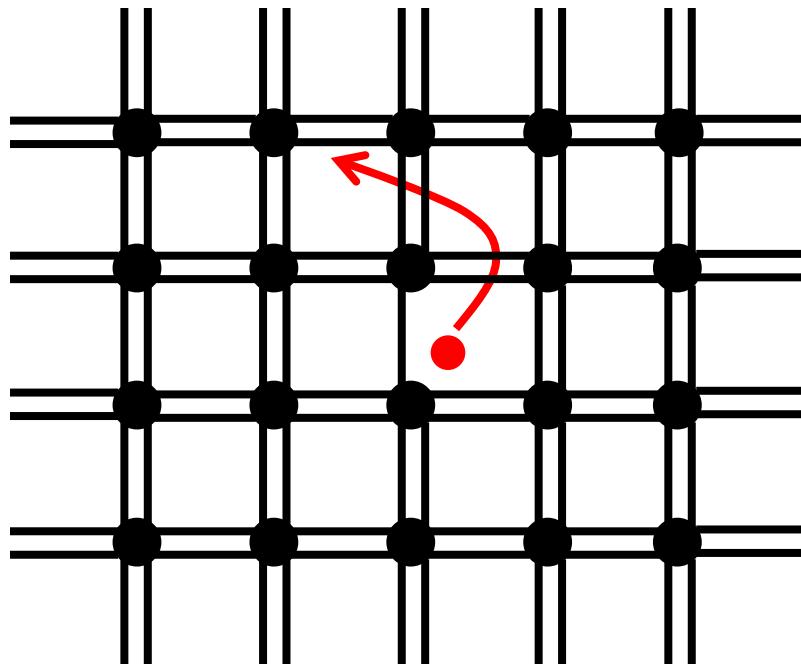
$$m_0 = 9.11 \times 10^{-31} \text{ kg}$$

$$q = 1.6 \times 10^{-19} \text{ C}$$

charge =  $-q$

# “Effective mass” of electrons

---



“crystal potential”

classical

semi-classical

$$F = m_0 a \rightarrow m_n^* a$$

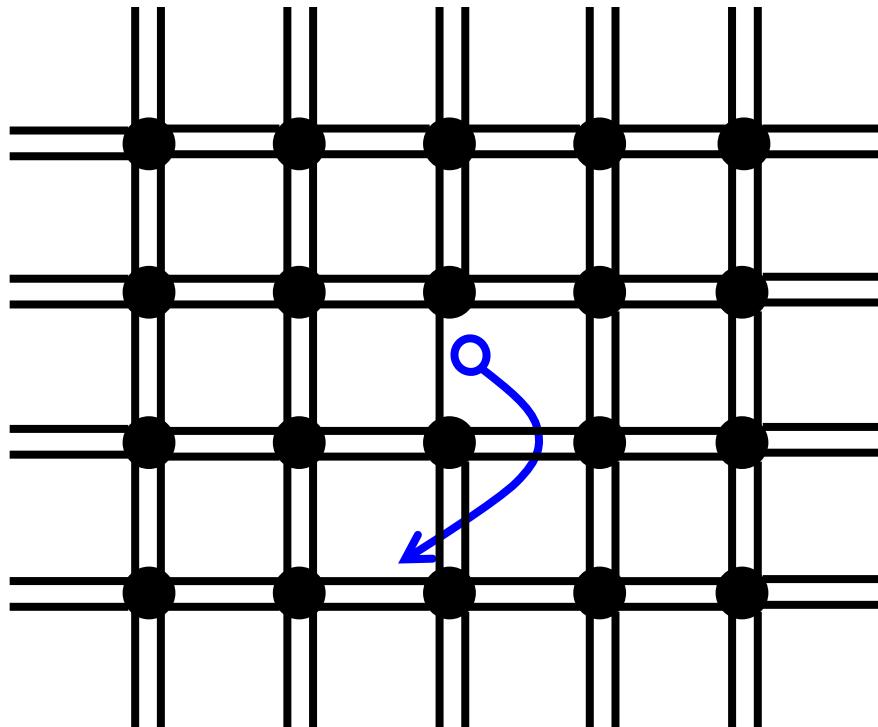
“effective mass” for electrons

Si:  $m_n^* = 1.18m_0$

GaAs:  $m_n^* = 0.066 m_0$

# Effective mass of holes

---



“crystal potential”

$$F = m_0 a \rightarrow m_p^* a$$

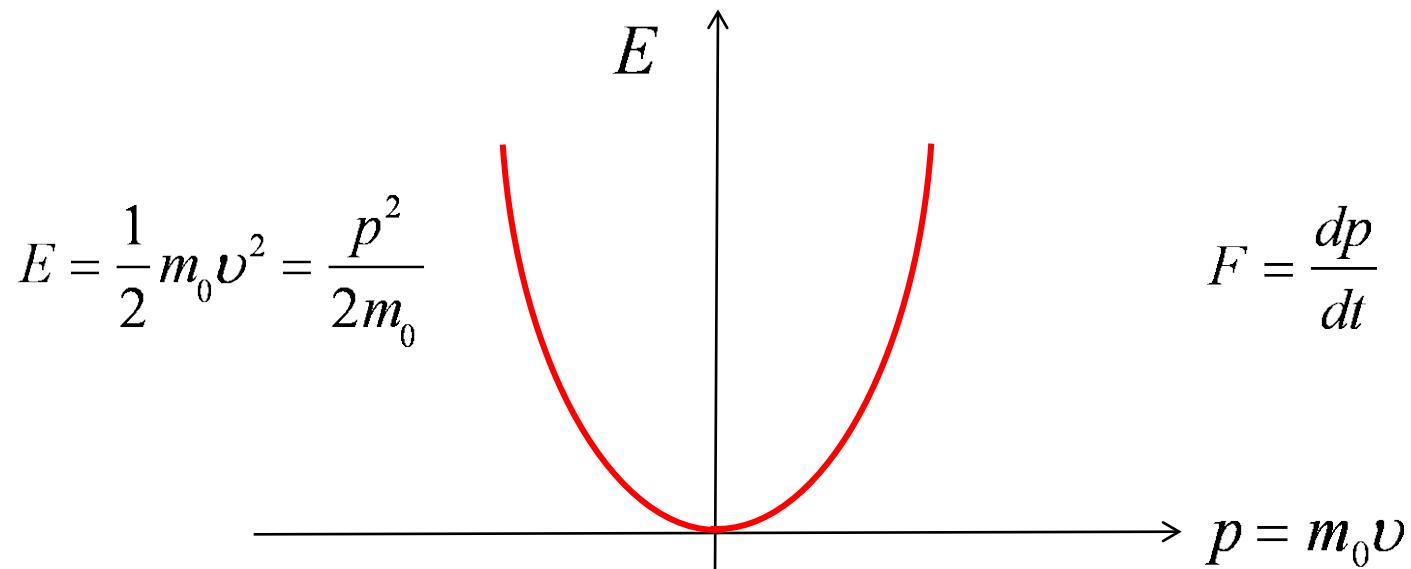
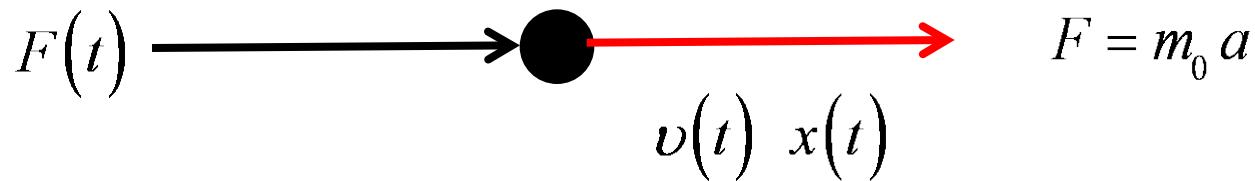
effective mass for holes

Si:  $m_p^* = 0.81m_0$   
 $(m_n^* = 1.18m_0)$

GaAs:  $m_p^* = 0.52m_0$   
 $(m_n^* = 0.066m_0)$

# Energy and momentum (free electron)

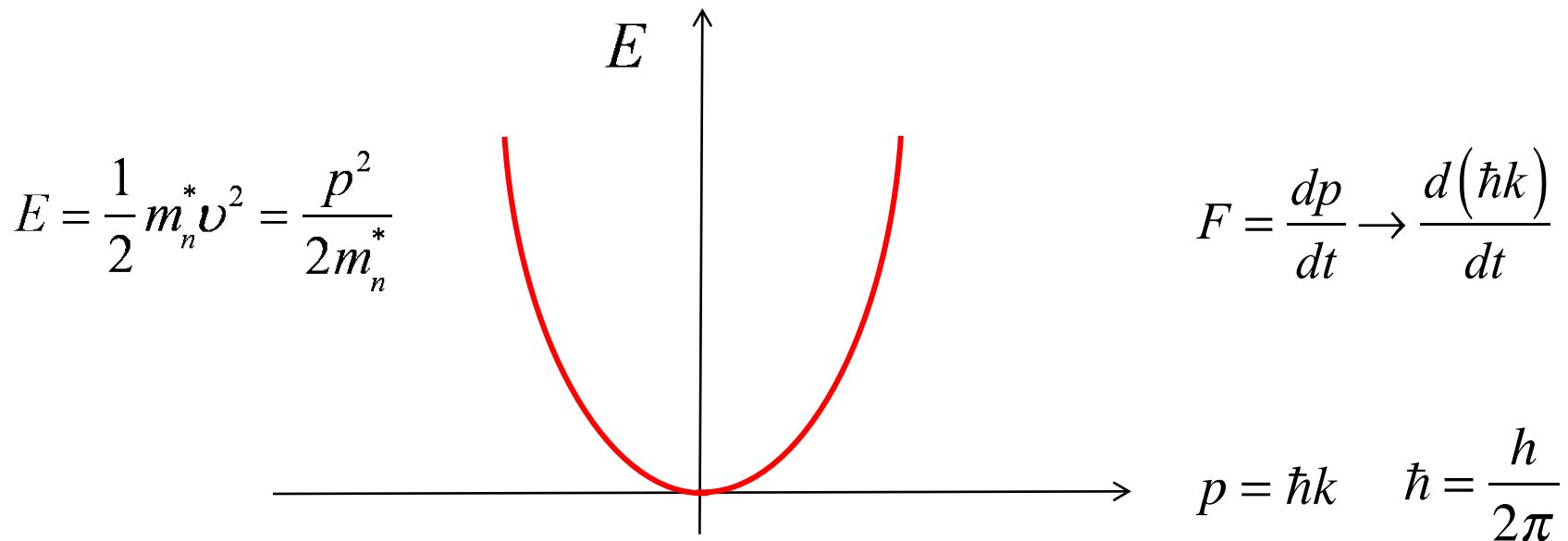
---



# Energy and “crystal momentum” (electron in cb)

$$F(t) \longrightarrow \bullet \longrightarrow F = m_n^* a$$

$v(t) \ x(t)$



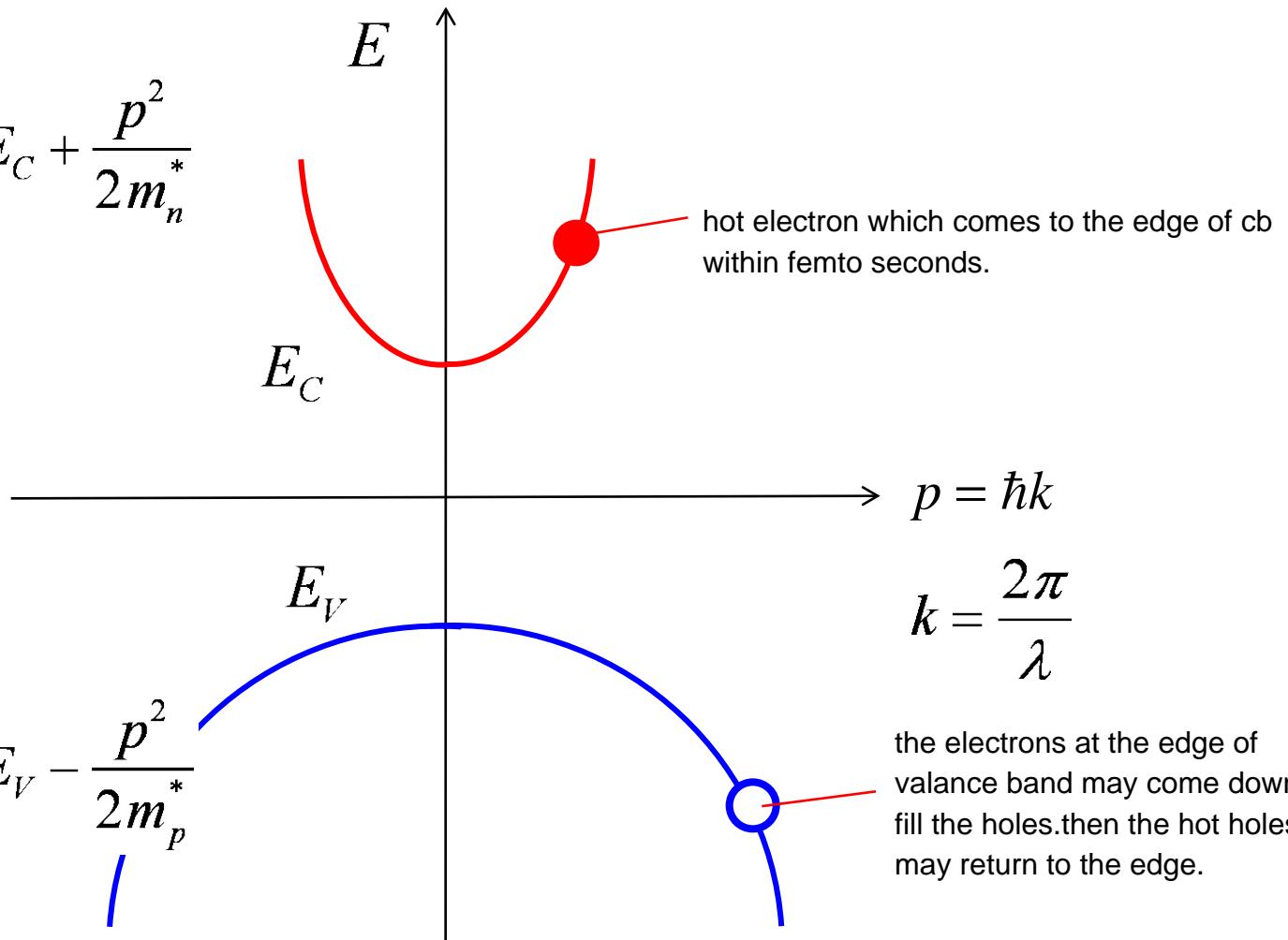
Electrons are particles **and** waves!  $k = \frac{2\pi}{\lambda}$

Lundstrom: 2018 they have a wavelength or wave number.<sup>7</sup>

# Conduction and valence band

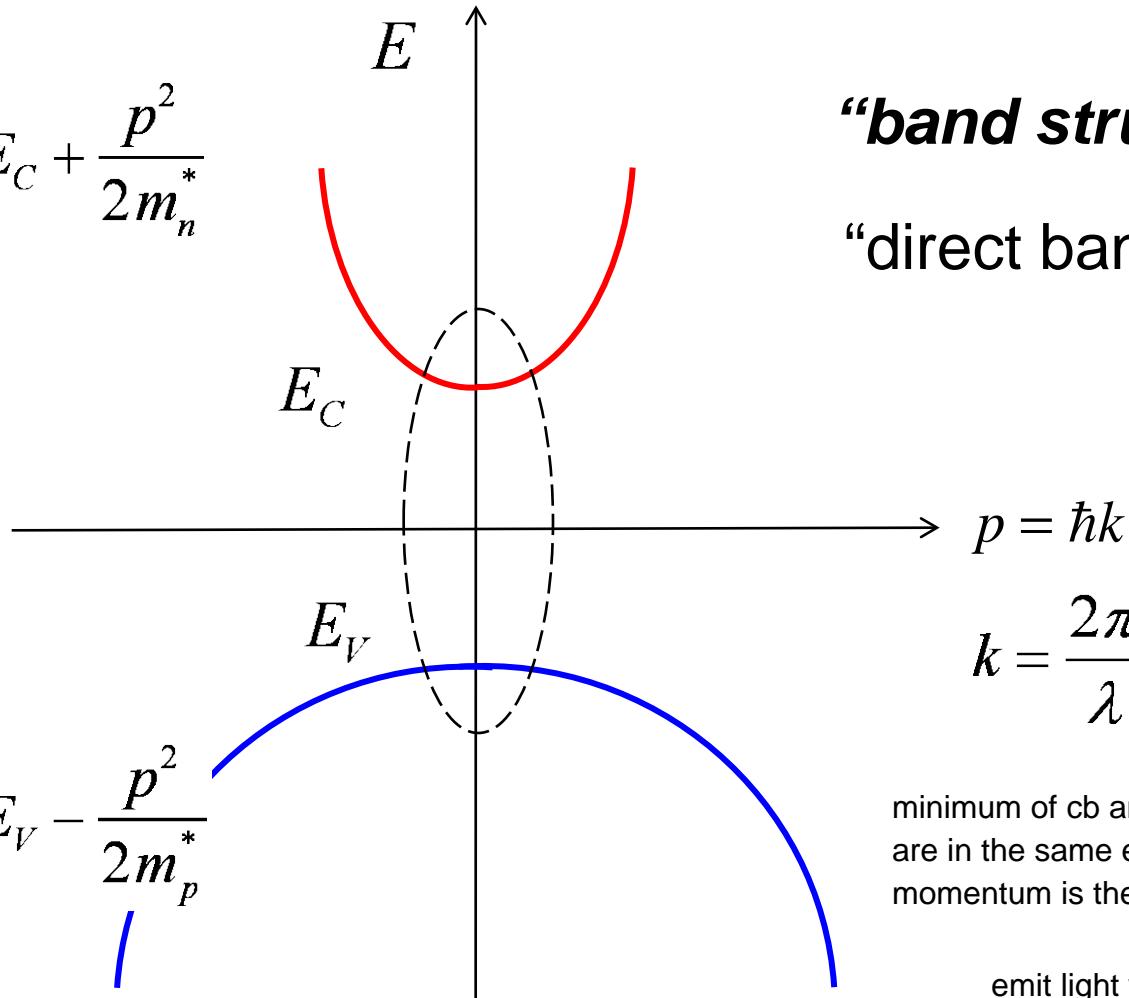
$$E = \frac{p^2}{2m_0} \rightarrow E = E_C + \frac{p^2}{2m_n^*}$$

electrons



# “Direct gap semiconductors”

$$E = \frac{p^2}{2m_0} \rightarrow E = E_C + \frac{p^2}{2m_n}$$



$$E = \frac{p^2}{2m_0} \rightarrow E = E_V - \frac{p^2}{2m_p}$$

Lundstrom: 2018

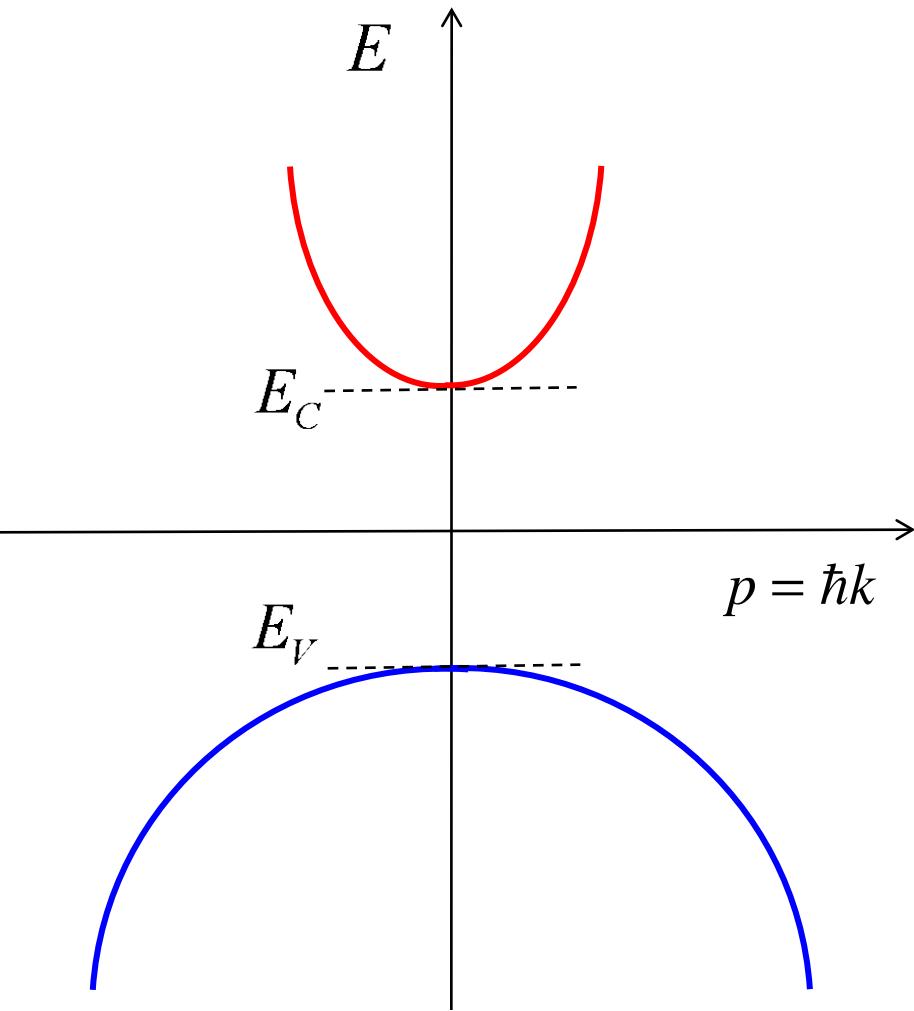
“**band structure**”  
“direct bandgap”

$$k = \frac{2\pi}{\lambda}$$

minimum of cb and maximum of vb  
are in the same energy point.hence  
momentum is the same.

emit light while recombination.

# Band structure vs. energy band diagram



Band structure is a plot of energy **vs. crystal momentum** (or  $k$ ).

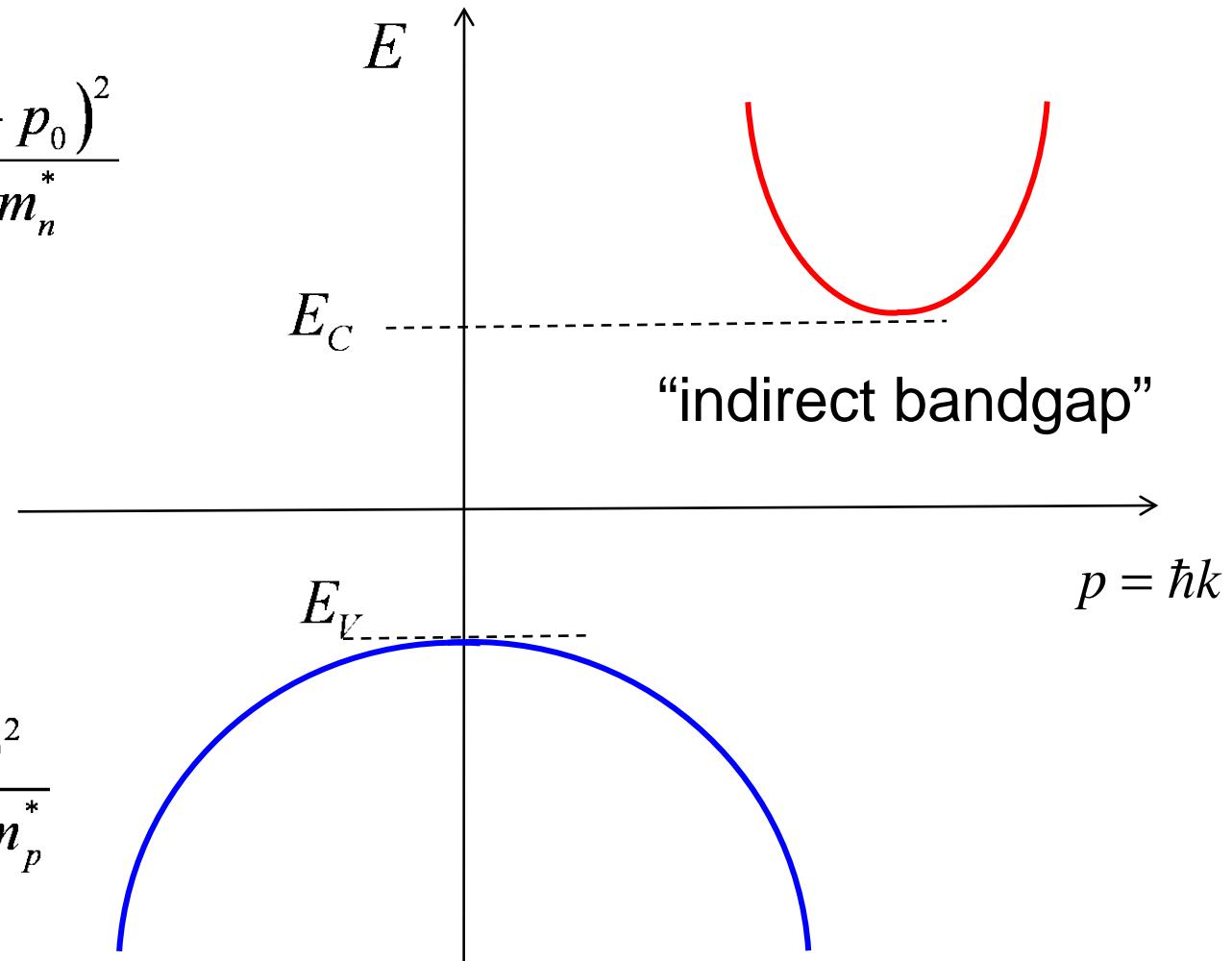
An energy band diagram is a plot of the bottom of the cb and top of the vb **vs. position**.

# “Indirect gap semiconductors”

---

$$E = E_C + \frac{(p - p_0)^2}{2m_n^*}$$

$$E = E_V - \frac{p^2}{2m_p^*}$$



# Summary

---

## **1) Electrons in the conduction band (“electrons”):**

Free to move about within the crystal.

Can often be treated as Newtonian particles with an effective mass.

## **2) Holes in the conduction band (“holes”):**

Free to move about within the crystal.

Can often be treated as Newtonian particles with a different effective mass.

# Primer on Semiconductors

## Unit 1: Material Properties

### Lecture 1.6: Doping

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Doping makes semiconductors useful

---

metal



semiconductor



insulator



gold (Au)

silicon (Si)

glass ( $\text{SiO}_2$ )

# Things have changed

---

“One shouldn’t work on semiconductors, that is a filthy mess; who knows whether any semiconductors exist.”

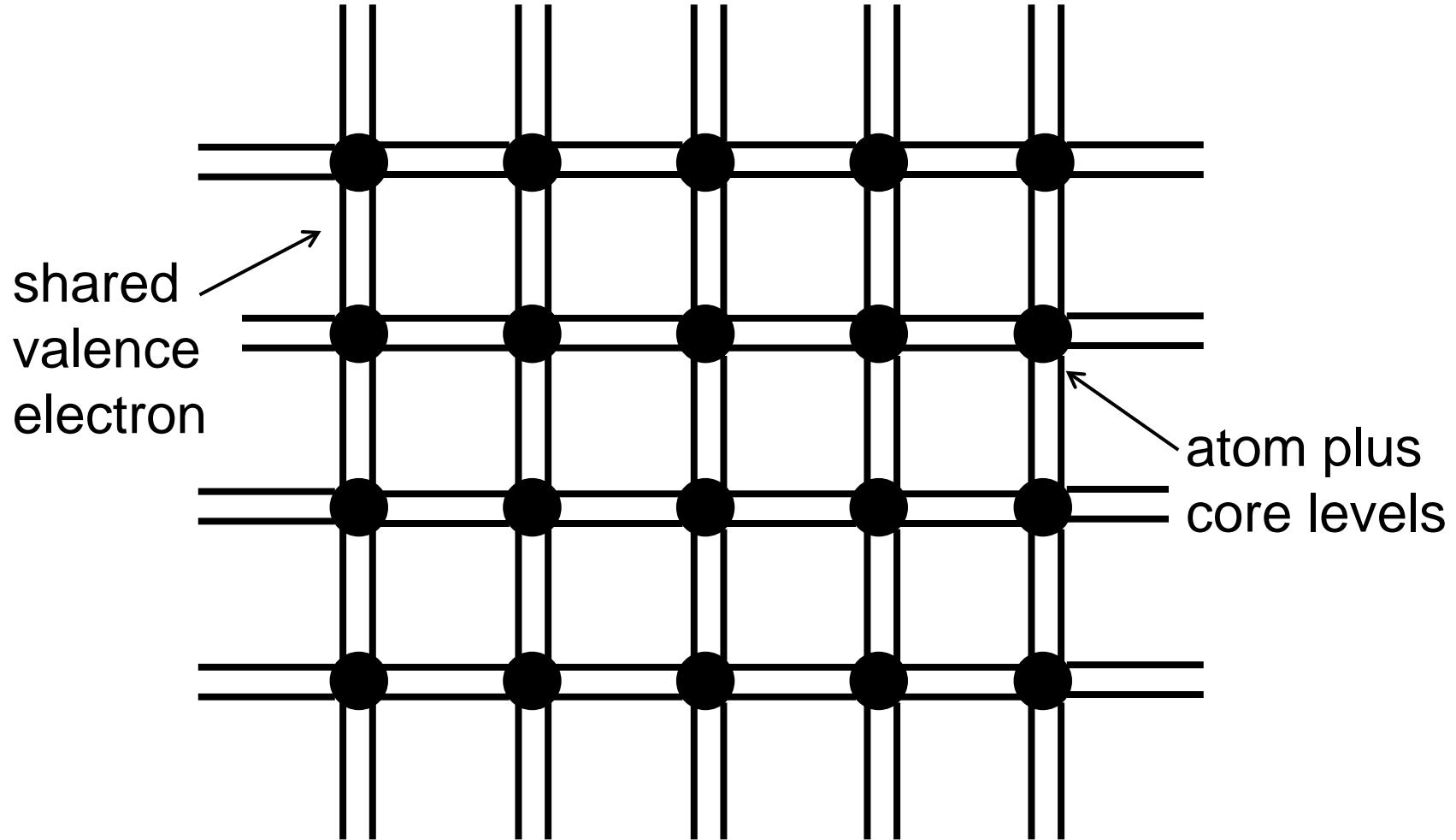
Wolfgang Pauli, 1931

in earlier times peoples avoided sc because there is an unknown concentrations of defects,producing large kinds of effects which are so difficult to observe.so we dont know whats going on in an experiment . so it a difficult jobin reproducing them.s

but now we are able to produce high quality silicon.

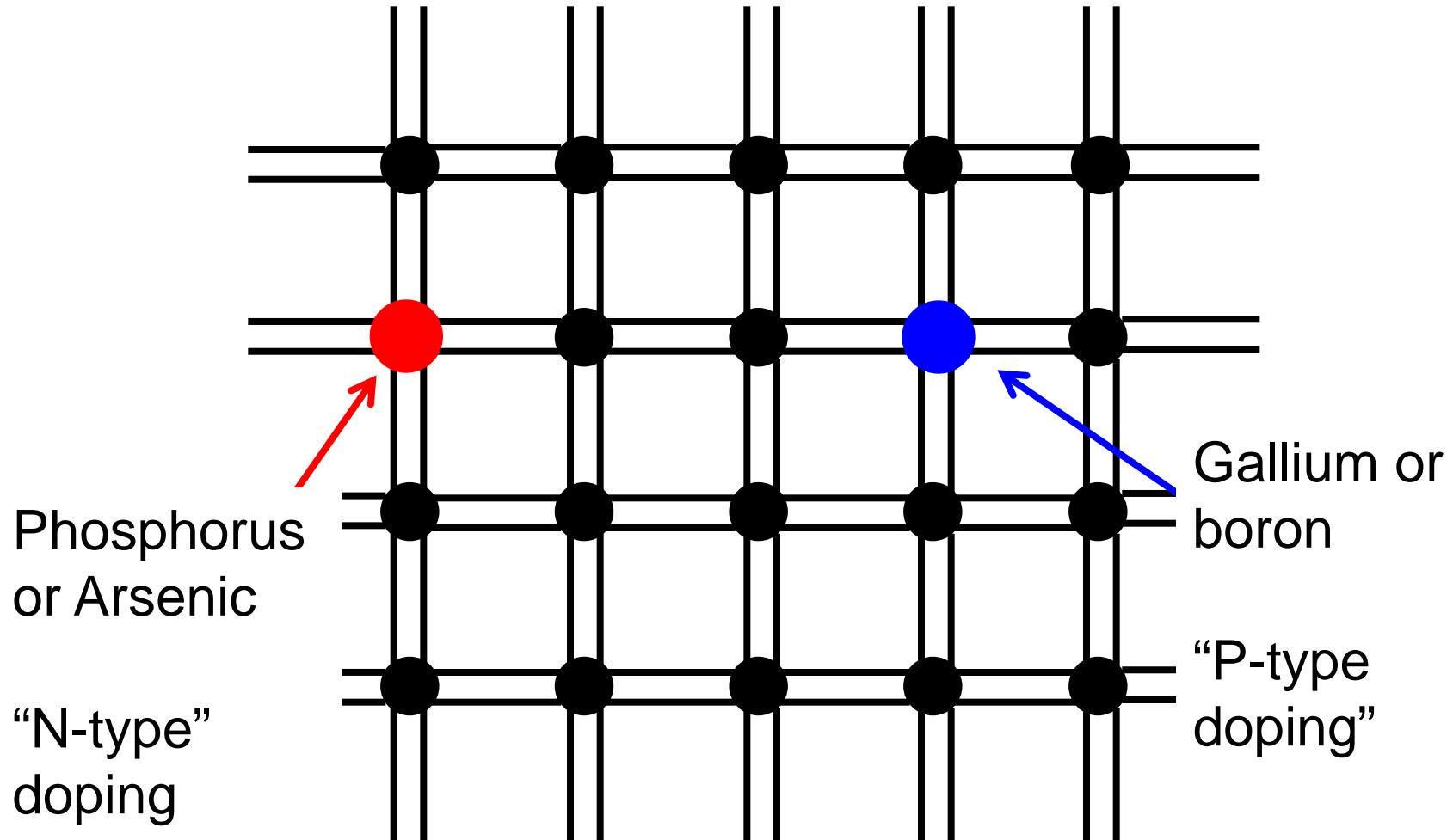
# Recall: Bonding cartoon of Si lattice

---



# Doping a semiconductor

---



# Dopants in Si

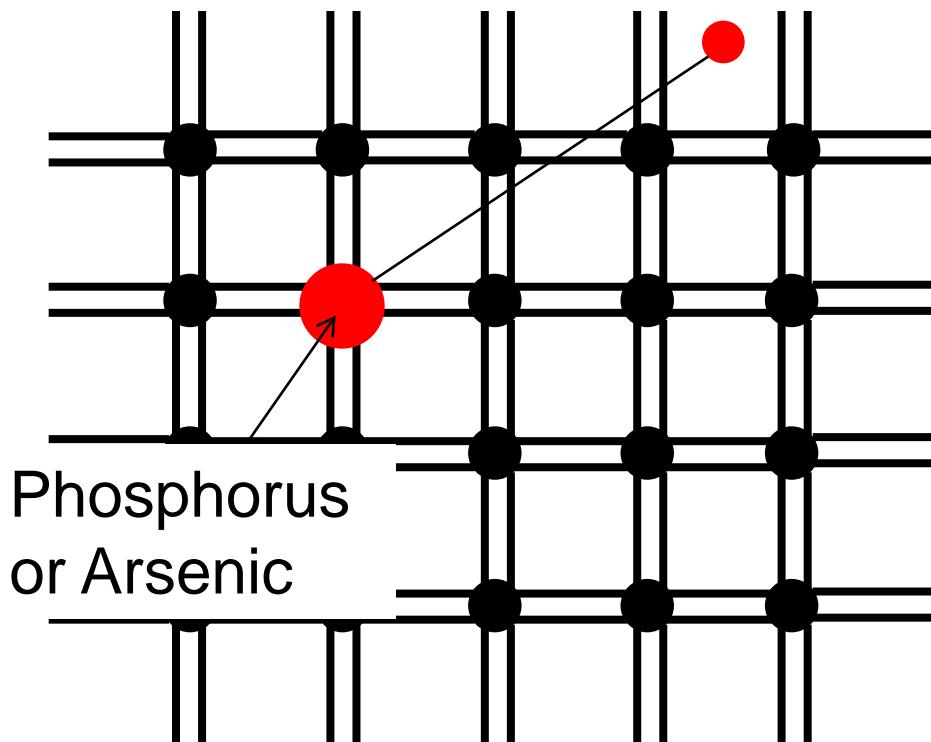
Group #	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18		
Period																				
1	1 H																2 He			
2	3 Li	4 Be															10 Ne			
3	11 Na	12 Mg															18 Ar			
4	19 K												28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	34 As	36 Kr	
5	37 Rb												46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	53 Te	54 Xe
6	55 Cs												78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	85 Po	86 At
7	87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uu	114 ...	115 ...	116 ...	117 ...	118 ...		
* Lanthanoids																				
** Actinoids																				

column IV

P-type dopants come from column III

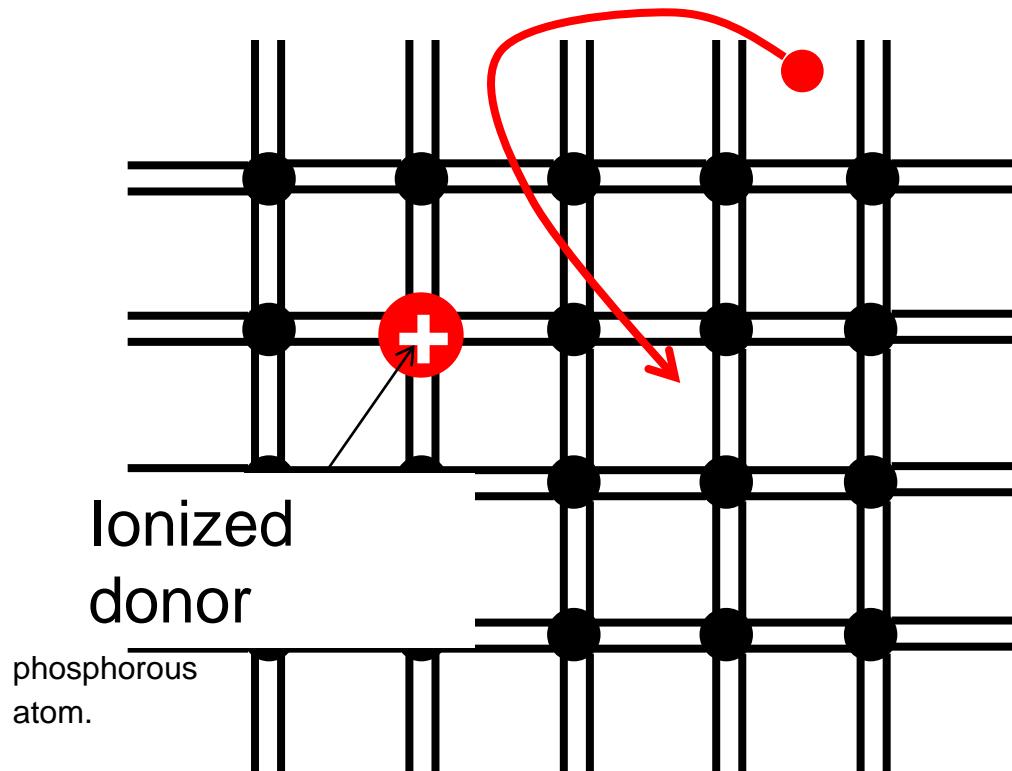
N-type dopants come from column V

# N-type doping



Weakly bound  
Easily broken at room temperature  
Produces an electron in the conduction band.

# Ionized donor



Concentration of dopants:

$$N_D \text{ cm}^{-3}$$

Concentration of ionized donors:

$$N_D^+ \text{ cm}^{-3}$$

Concentration of electrons in the conduction band:

$$n \approx N_D^+ \text{ cm}^{-3}$$

# Be careful about units!

---

$$n \approx N_D^+ \text{ cm}^{-3}$$

We will be working in SI (MKS) units. The carrier concentration should be given per cubic **meter**, but semiconductor people like to mix their units.

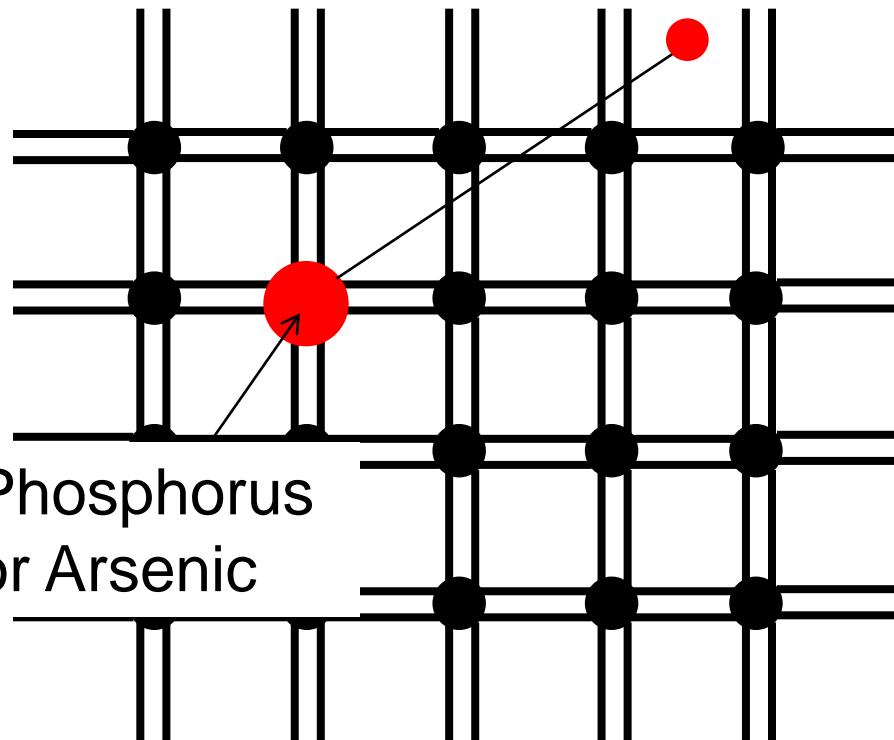
It is safest to do the calculations in SI units, and then convert to cubic cm.

$$n = 10^{26} \text{ m}^{-3} \rightarrow n = 10^{26} \frac{1}{\text{m}^3} \times \left( \frac{10^{-2} \text{ m}}{\text{cm}} \right)^3 \rightarrow n = 10^{20} \text{ cm}^{-3}$$

looks like a hydrogen atom which has one e- and 1 proton.

## Binding energy of the donor

$$E_B \approx ?$$



Phosphorus  
or Arsenic

since among 5 valence e- of a phosphorous, 4 e- s forms a covalent bond with si. balance 1 e- of p and 1 hole at p are available.

Hydrogen atom:

$$E_B = -\frac{m_0 q^4}{2(4\pi\epsilon_0 \hbar)^2} \text{ eV}$$

$$E_B = -13.6 \text{ eV}$$

Donor in Si:

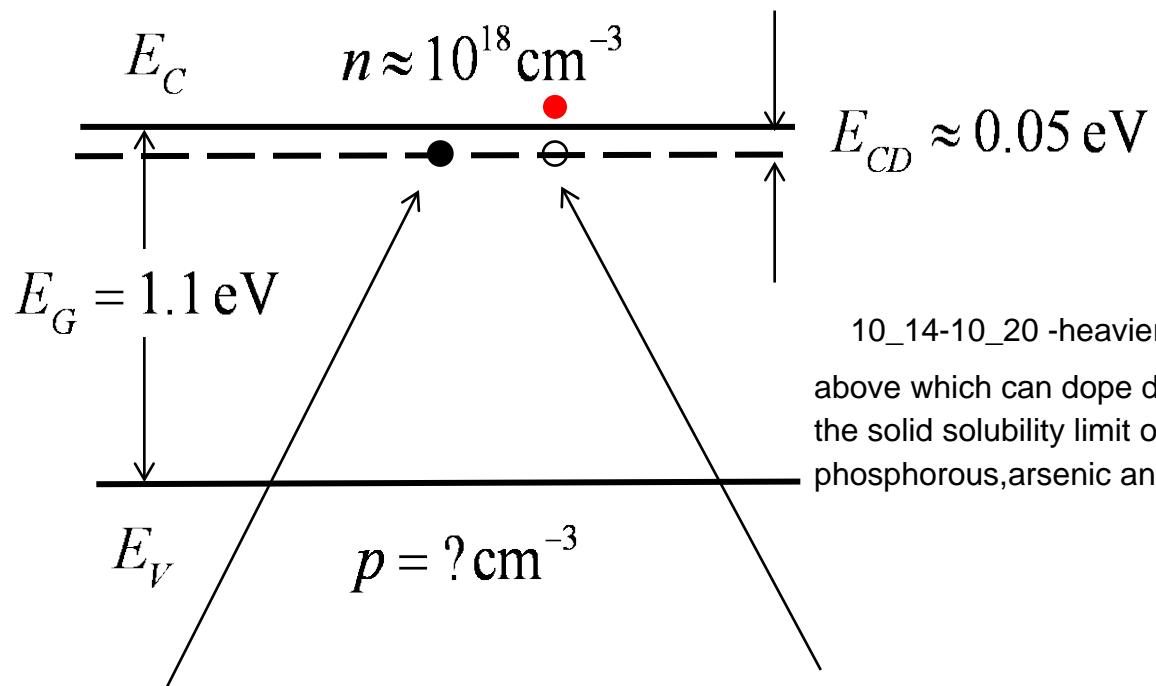
$$\begin{aligned} \epsilon &= K_s \epsilon_0 && \text{dielectric constant of si} \\ &= 11.8 \times (8.854 \times 10^{-12} \text{ F/m}) && k_s \text{ is much greater than } \epsilon_{\text{on}} \end{aligned}$$

$$m_n^* = 0.26 m_0 \quad \text{cond. eff mass}$$

$$E_B \approx -0.025 \text{ eV}$$

# Energy band view (n-type)

n-doped Si



neutral donor

ionized donor

Lundstrom: 2018

$$N_D = 10^{18} \text{ cm}^{-3}$$

$$N_D^+ = 10^{18} \text{ cm}^{-3}$$

$$n \approx N_D^+ = 10^{18} \text{ cm}^{-3}$$

$$p \approx ? \text{ cm}^{-3} \quad \begin{matrix} \text{new} \\ \text{minority carrier conc} \end{matrix}$$

$$(T = 300 \text{ K})$$

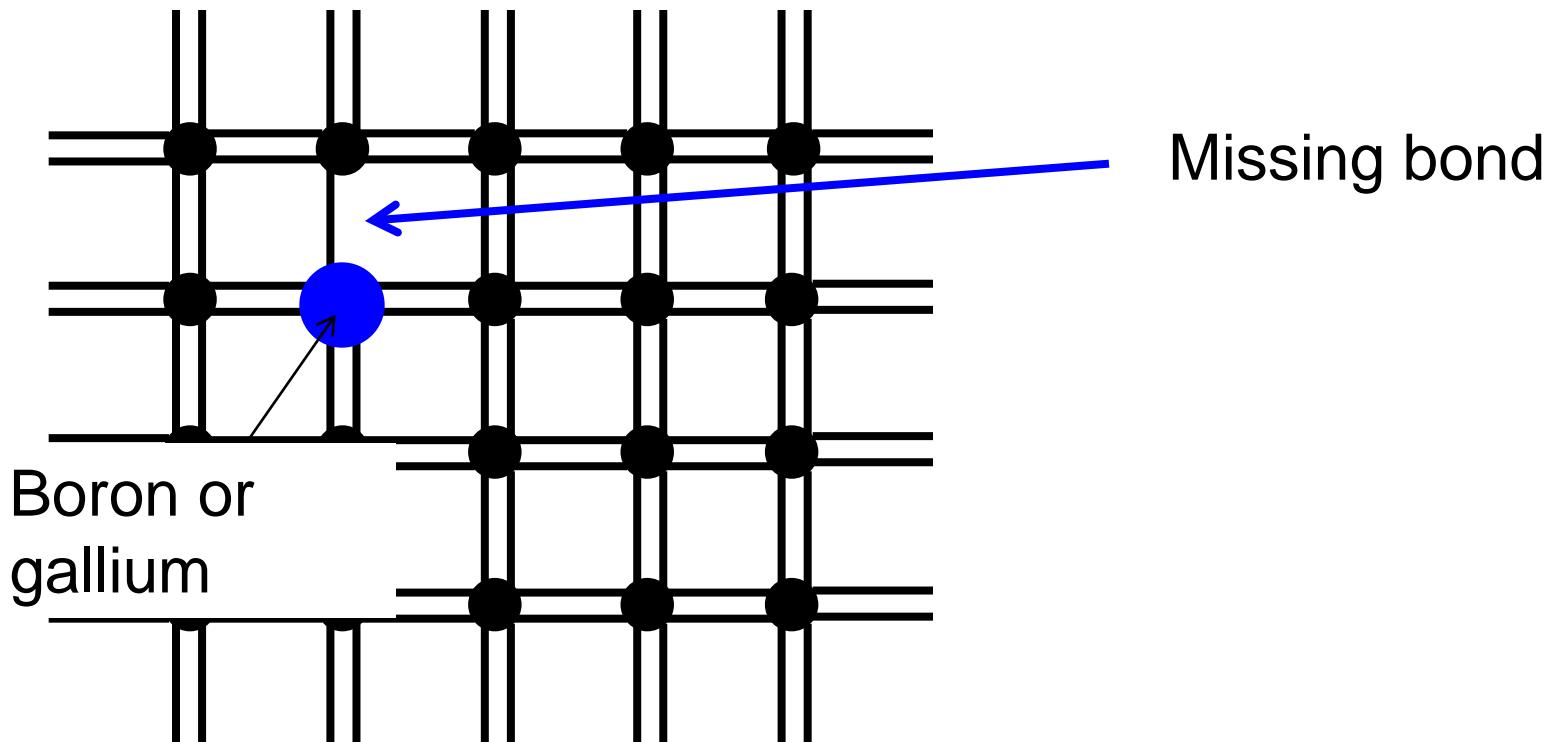
10\_10 to 10\_14 - lighter doping

$$10^{14} \leq N_D \leq 10^{20} \text{ cm}^{-3}$$

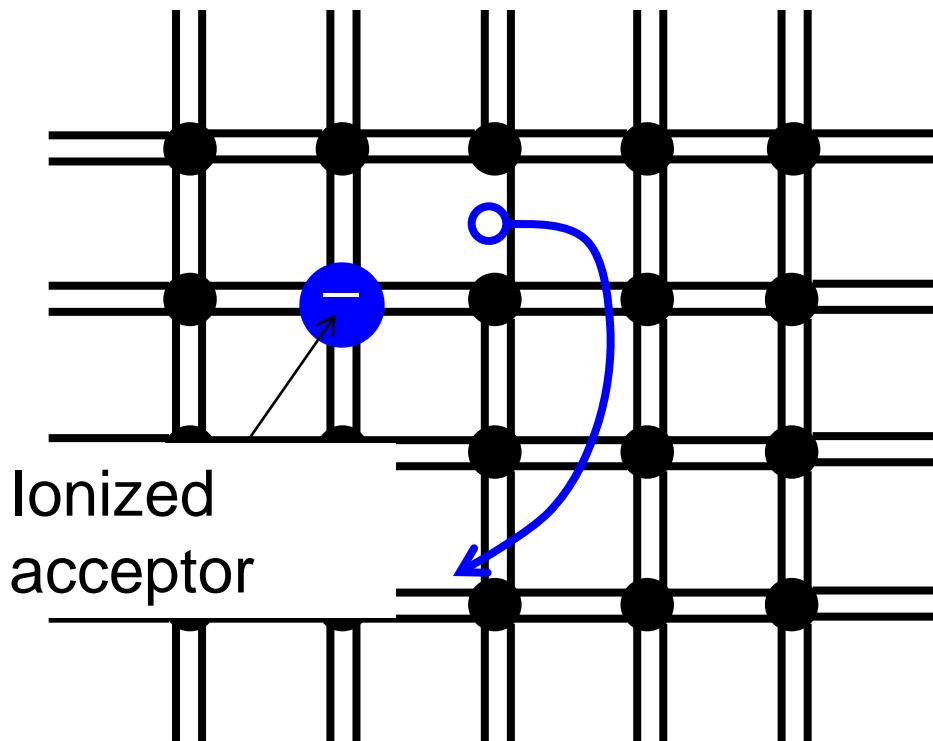
$$N_{atoms} \approx 5 \times 10^{22} \text{ cm}^{-3}$$

# P-type doping

---



# Ionized acceptor



Concentration of dopants:

$$N_A \text{ cm}^{-3}$$

Concentration of ionized acceptors:

$$N_A^- \text{ cm}^{-3}$$

Concentration of “holes” in the valence band:

$$p \approx N_A^- \text{ cm}^{-3}$$

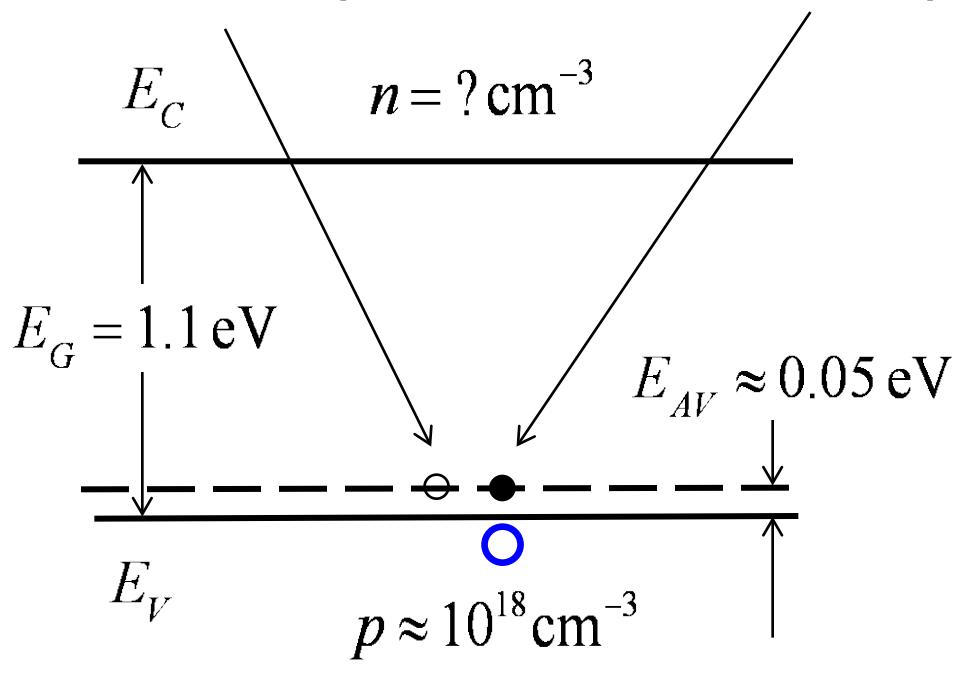
good thing about si is its dopants are fully ionized at room temperature.

## Energy band view (p-type)

a deep dopant is the one having high binding energy. so the dopant is not able to ionize fully due to high need of energy for ionizing. so they remain as not fully ionized. many semiconductors other than si has deep dopants. hence they dont fully ionize.

p-doped Si

neutral acceptor      ionized acceptor



$$N_A = 10^{18} \text{ cm}^{-3}$$

$$N_A^- = 10^{18} \text{ cm}^{-3}$$

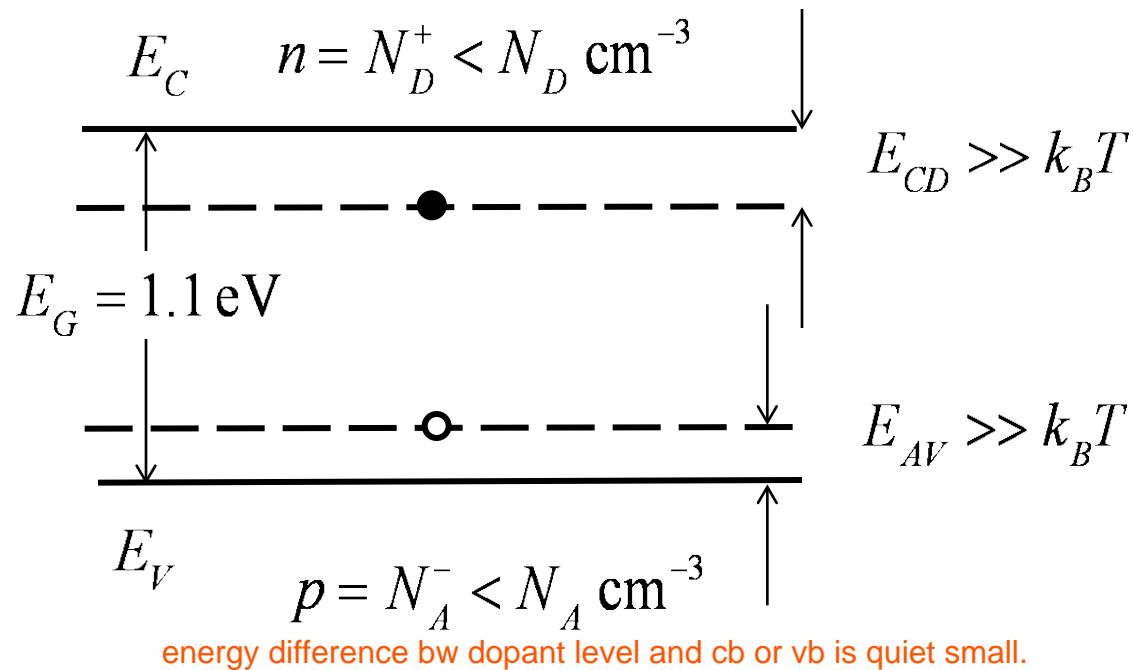
$$p \approx N_A^- = 10^{18} \text{ cm}^{-3}$$

$$n \approx ?$$

$$(T = 300 \text{ K})$$

$$10^{14} \leq N_A \leq 10^{20} \text{ cm}^{-3}$$

# “Deep donors” and “deep acceptors”



“Shallow” donors and acceptors are fully ionized at room temperature.

If the donor or acceptor level is much larger than  $kT$  (at room temperature), we say that the level is “deep”).

Donors and acceptors will be partially ionized at room temperature.

# Question

---

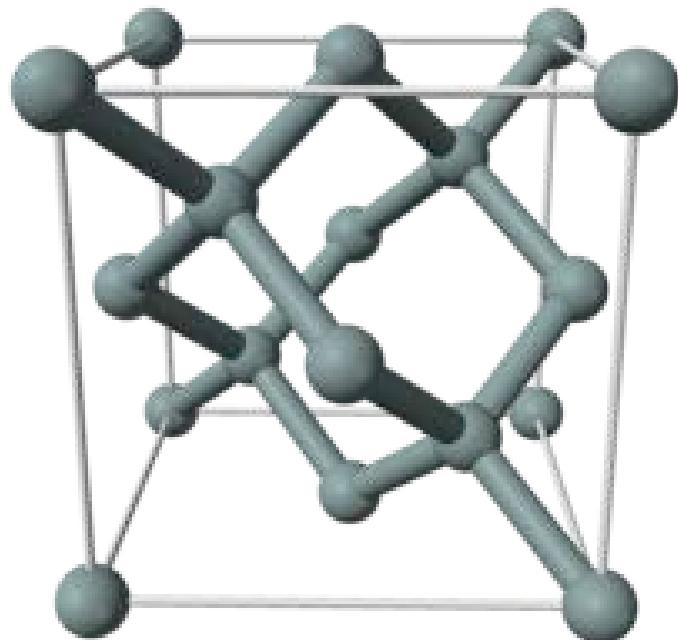
1) What type of dopant is Si in GaAs?

- a) n-type
- b) p-type
- c) either n-type or p-type
- d) neither n-type nor p-type
- e) don't know

# Si vs. GaAs crystals

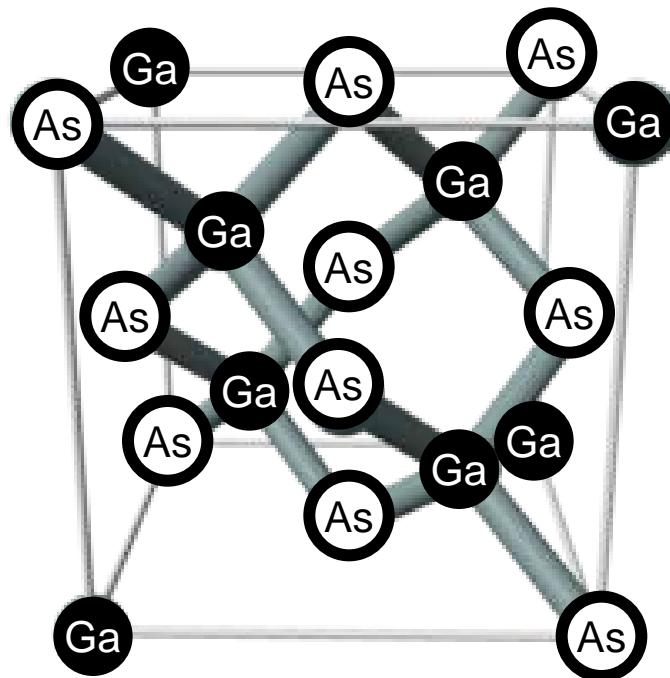
both structure is same except in GaAs every Ga is surrounded by four As and every As is surrounded by four Ga

Si



diamond lattice

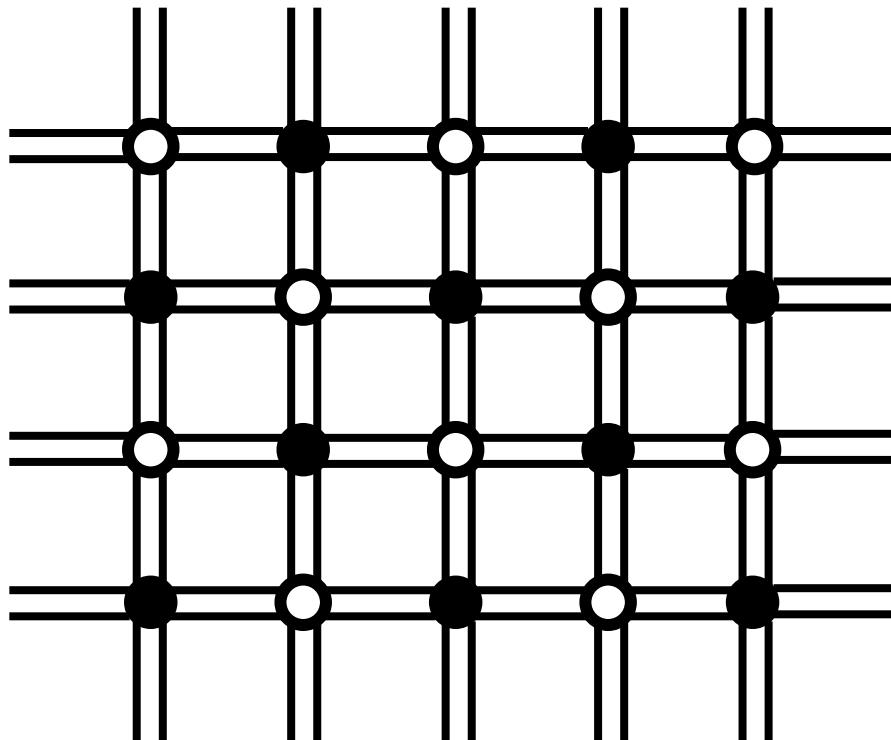
GaAs



zinc blende lattice

# GaAs bonding cartoon

---



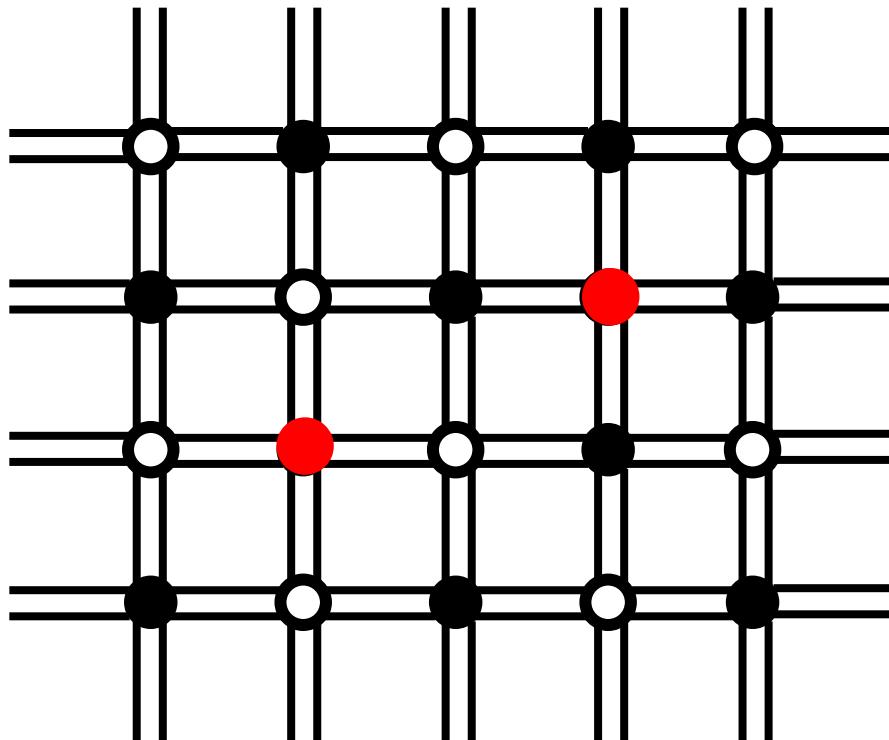
●      Ga  
○      As

Every Ga atom has  
4 NN As atoms.

Every As atom has  
4 NN Ga atoms.

# Si in GaAs: Two possibilities

amphoteric means it can go either n or p type depending on which atom it replaces in the lattice and depending how we introduce these dopants.



Si on a Ga site is a donor.

- Ga (III)
- As (V)
- Si (IV)

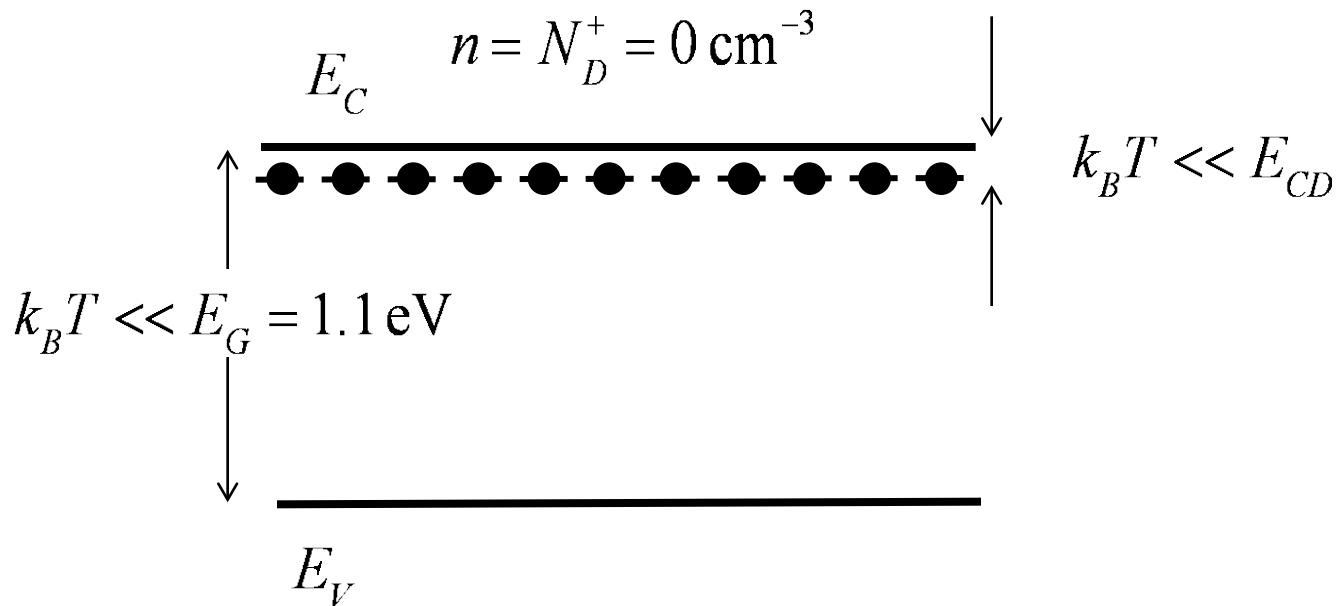
Si on a As site is an acceptor.

Si is an “amphoteric” dopant in GaAs.

# How does the carrier concentration vary with T?

---

T = 0 K

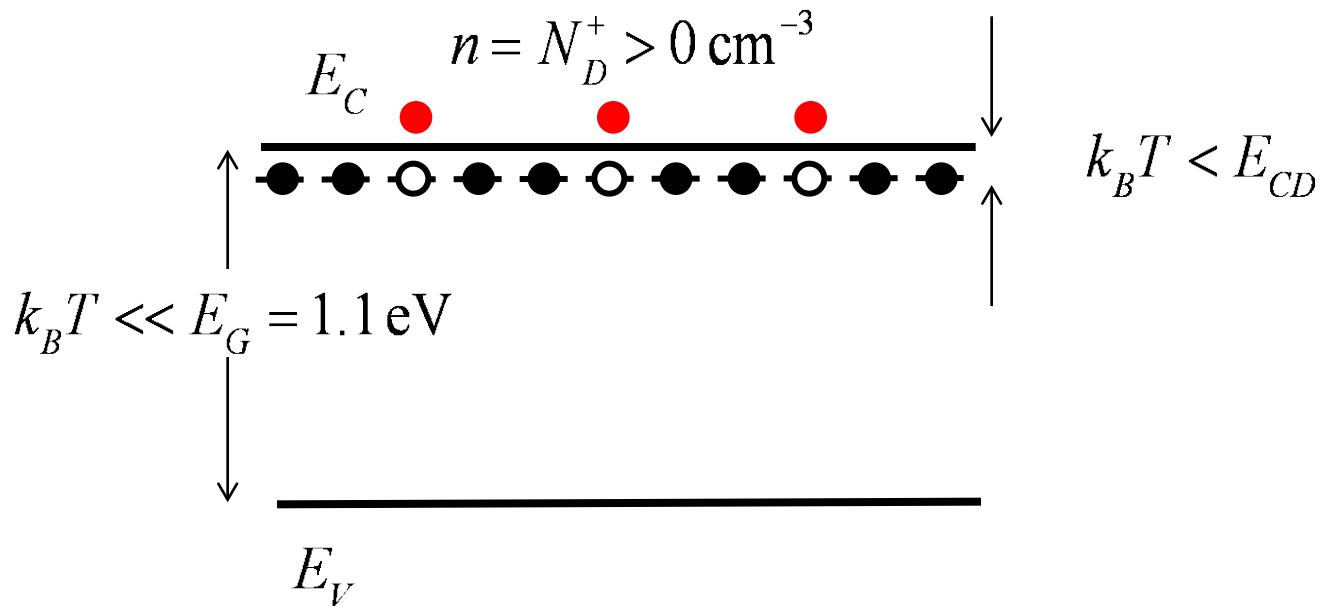


No extrinsic carriers due to doping, and no intrinsic carriers due to thermal excitation across the band gap.

# Low temperature

---

$T > 0 \text{ K}$

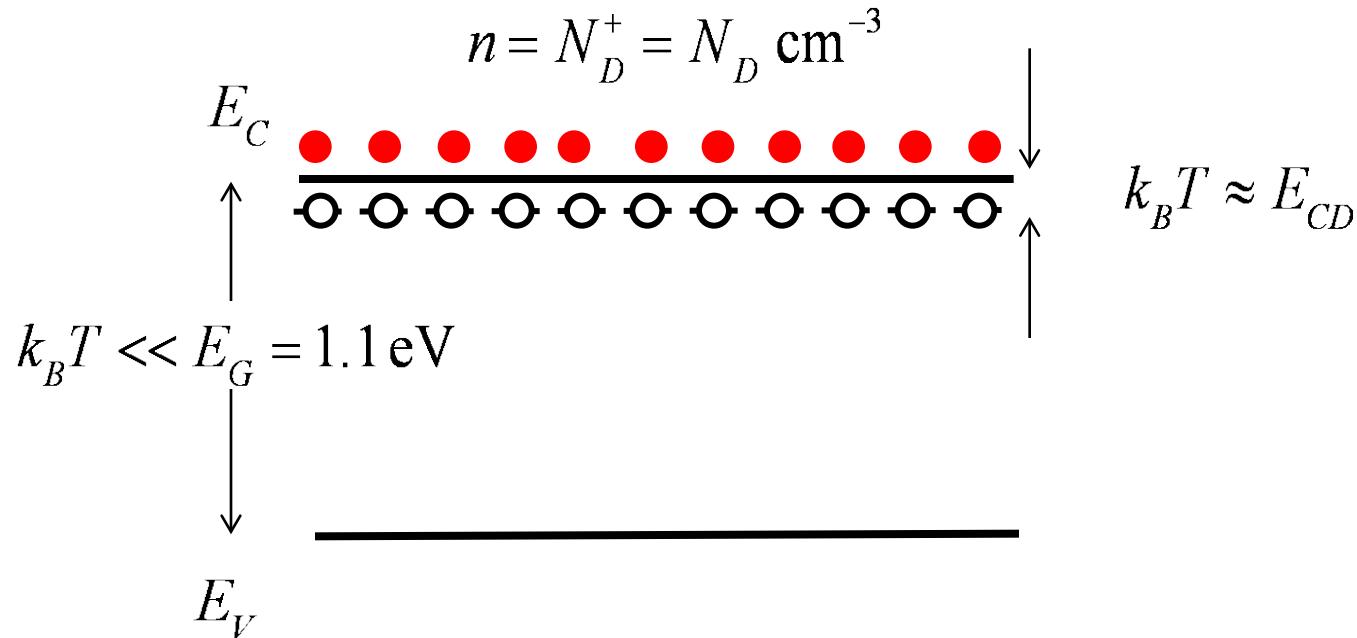


A few extrinsic carriers due to doping, but no intrinsic carriers due to thermal excitation across the band gap.

# Room temperature (shallow dopants)

---

$T = 300 \text{ K}$

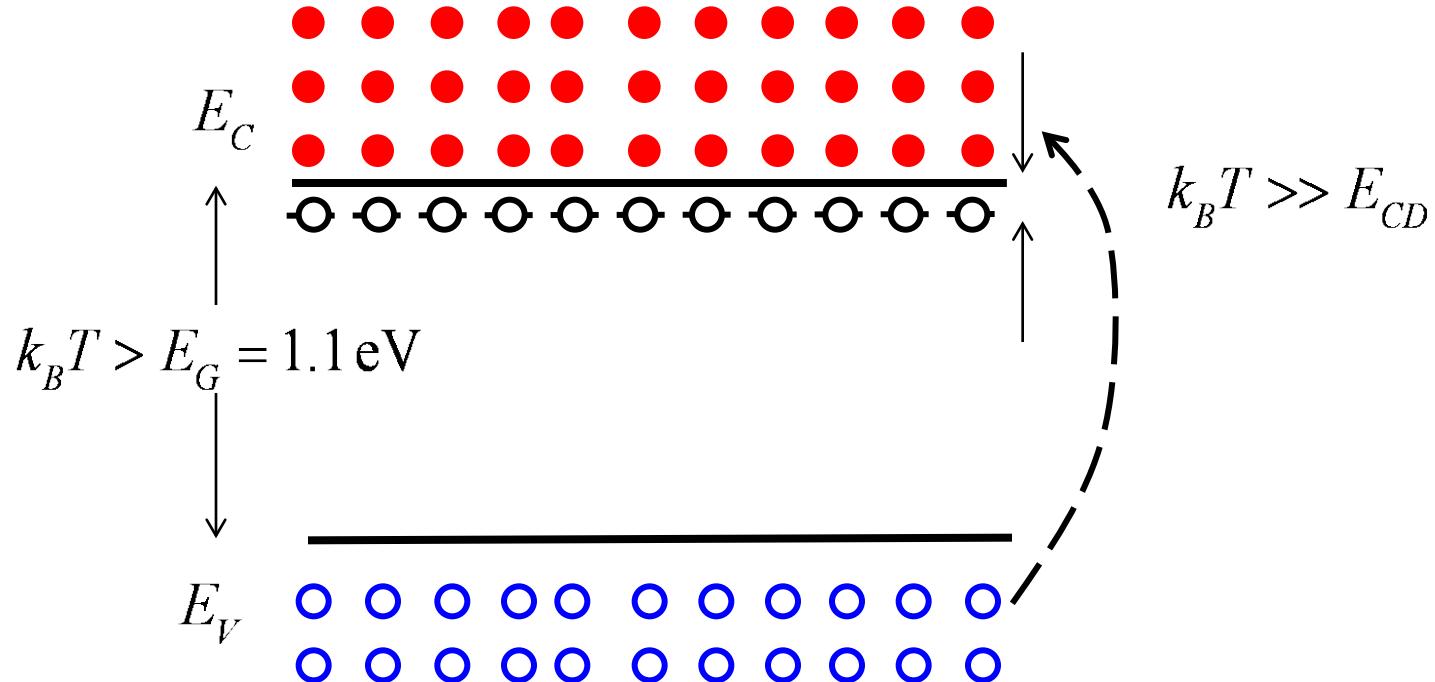


Many extrinsic carriers due to doping, but very few intrinsic carriers due to thermal excitation across the band gap.

# High temperature

$T \gg 300 \text{ K}$

$$n = N_D^+ = N_D \text{ cm}^{-3}$$



Extrinsic carriers due to doping, but also many intrinsic carriers due to thermal excitation across the band gap. Also many holes in the valence band now.

## Comment

---

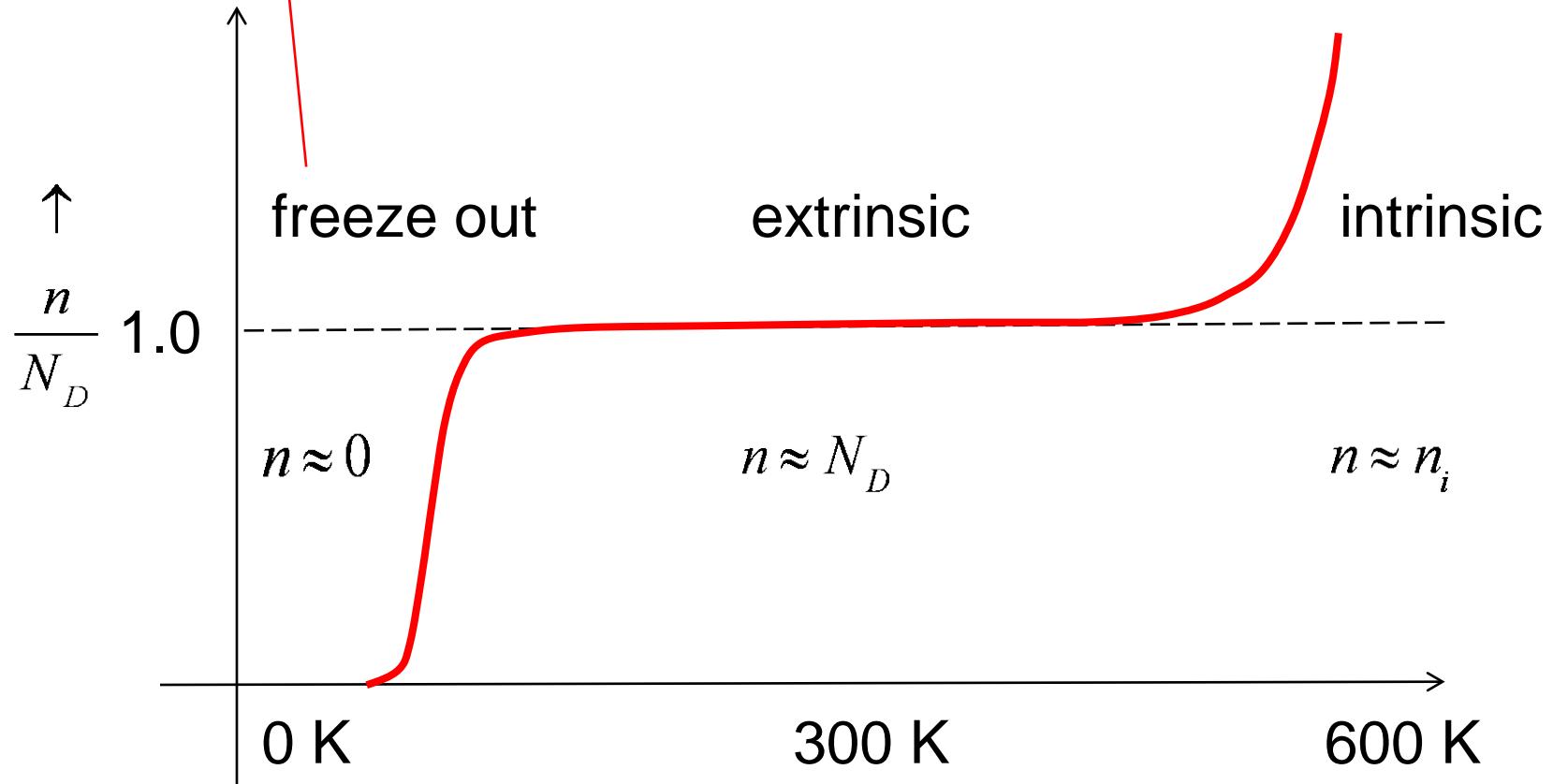
At high temperatures, the intrinsic carriers produced by thermal excitation across the bandgap overwhelm the extrinsic carriers produced by doping.

Because semiconductor devices are produced by selective doping, the device ceases to operate.

Semiconductor devices for operation at high temperature should be made with materials with large band gaps, such as SiC and GaN.

carriers are freezing out to their dopants and they are localized on their specific dopants there are no electrons.

## Carrier concentration vs. temperature



shallow dopants are easy to ionize and deep dopants are hard to ionize fully.

## Summary

---

To dope a semiconductor, we replace a few atoms with atoms from a different column of the periodic table.

Ionized dopants produce electrons in the conduction band or holes in the valence band.

Dopants can be energetically shallow or deep.

The carrier concentration vs. temperature characteristic has freeze out, extrinsic, and intrinsic regions.

A low temperatures, semiconductors become insulators.

# Primer on Semiconductors

## Unit 1: Material Properties

### Lecture 1.7: Unit 1 Recap

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Semiconductors

---

metal



semiconductor



insulator



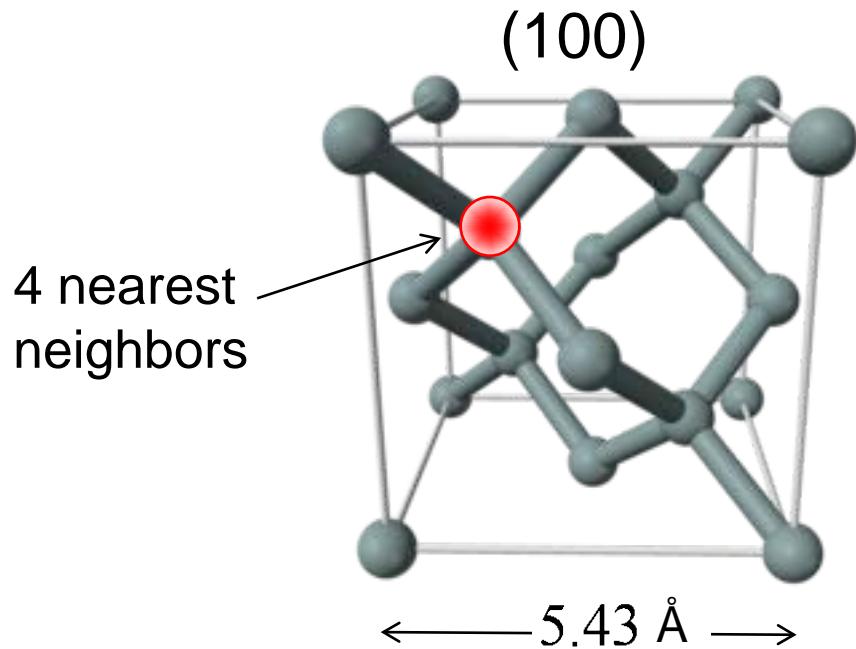
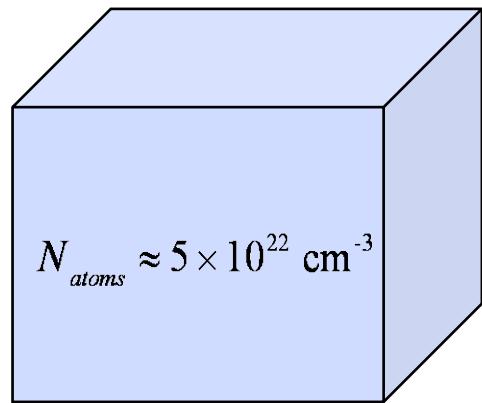
gold (Au)

silicon (Si)

glass ( $\text{SiO}_2$ )

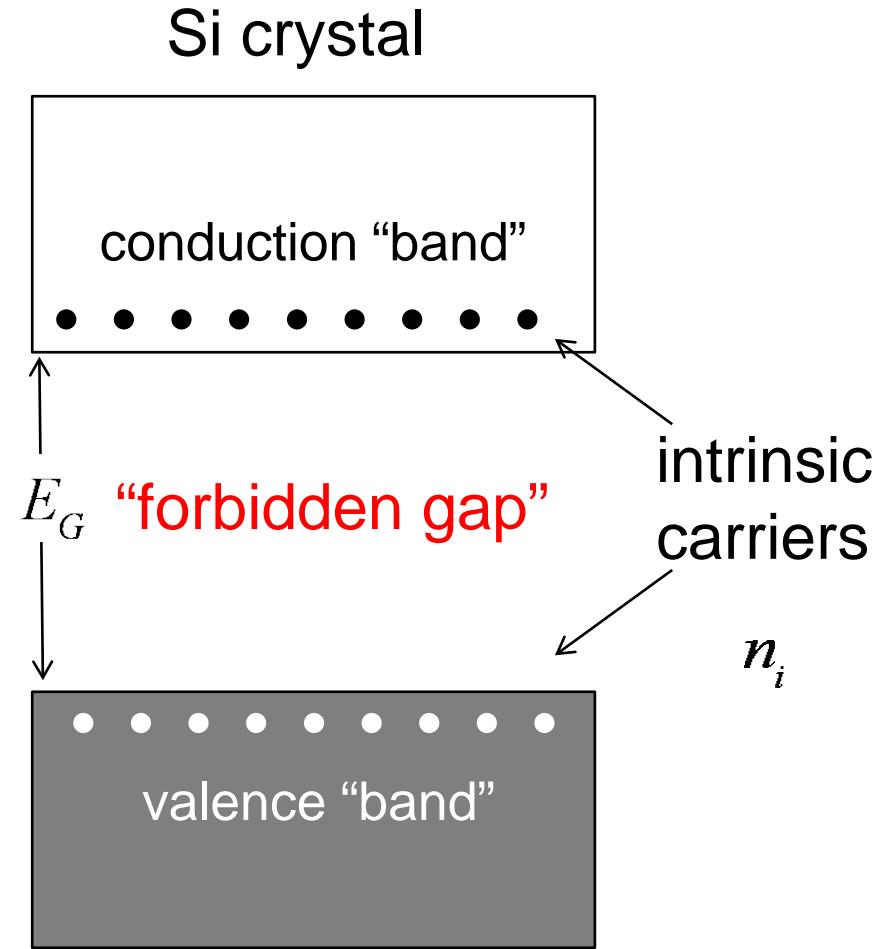
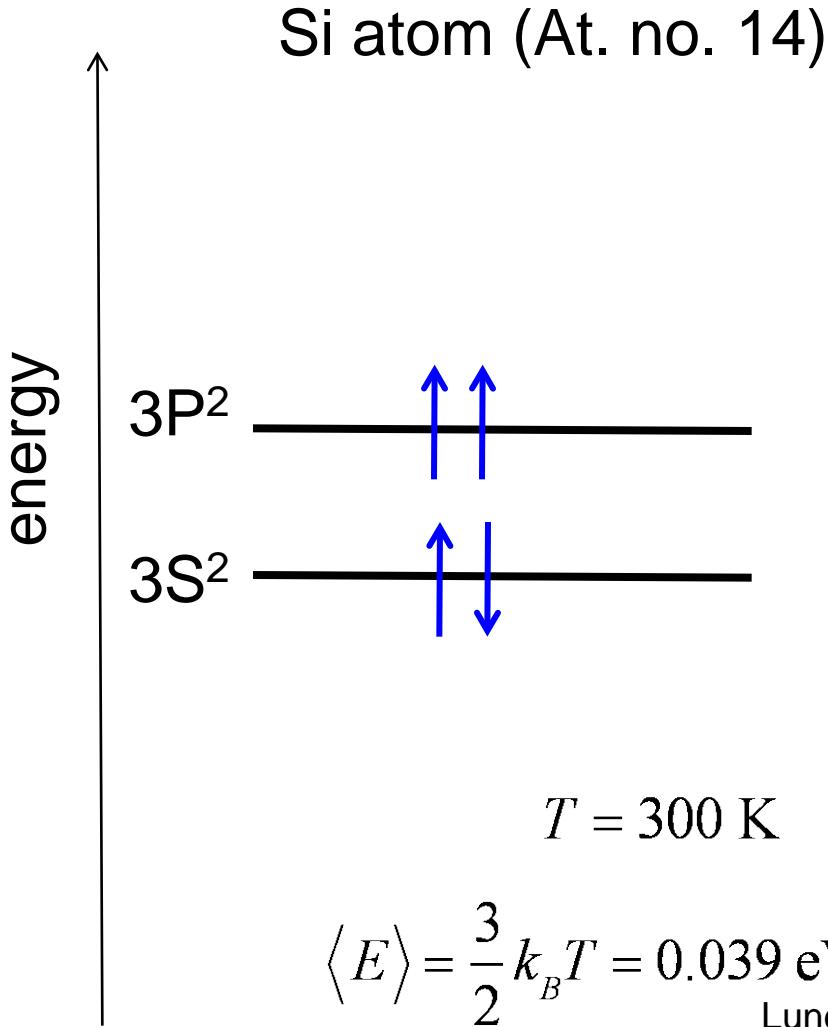
# Example semiconductor: Si

---

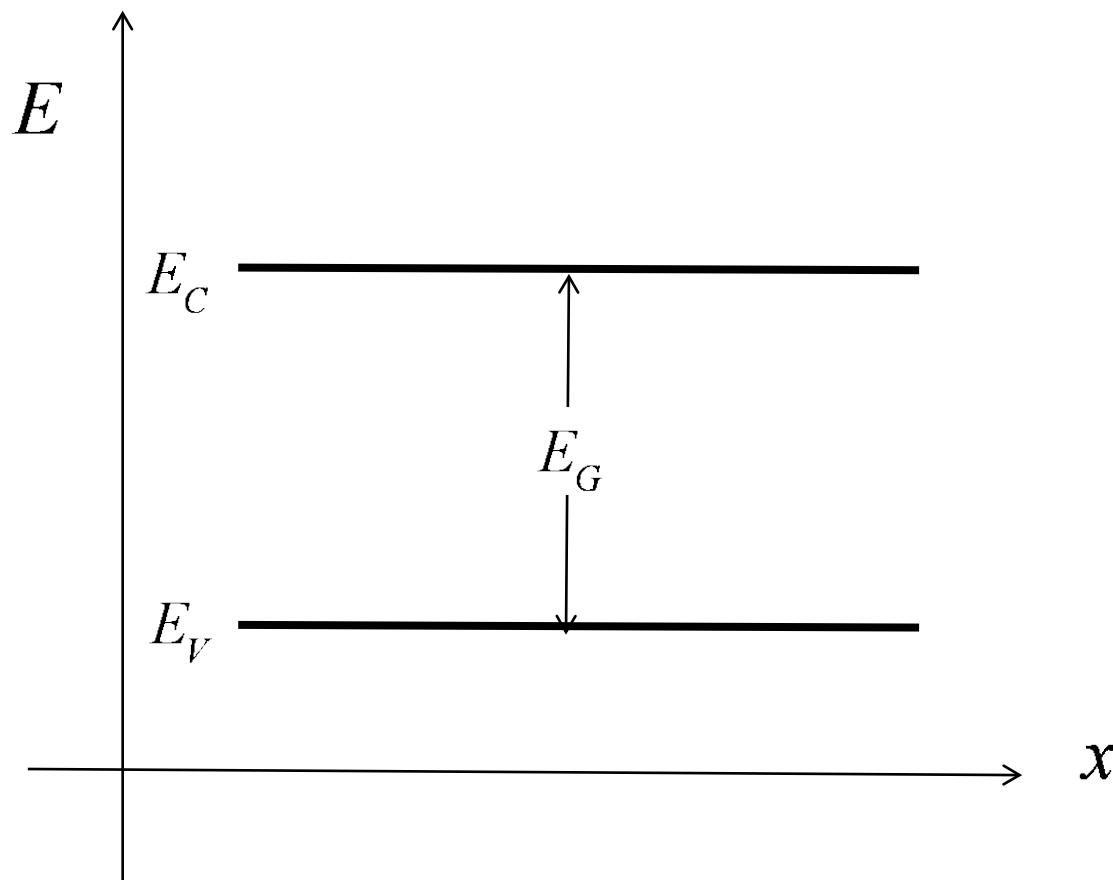


- Si crystallizes in the diamond lattice.
- We specify planes and directions with Miller indices.
- In a solid, energy **levels** become energy **bands**.

# Silicon energy levels → energy bands

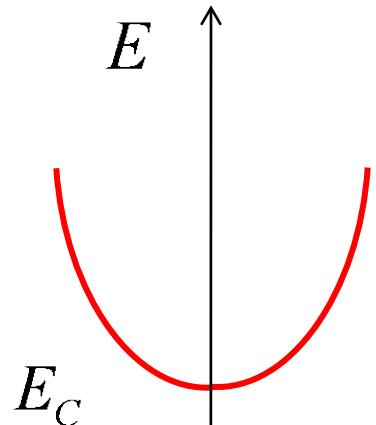


# Energy band diagram



# Energy vs. momentum: E(k)

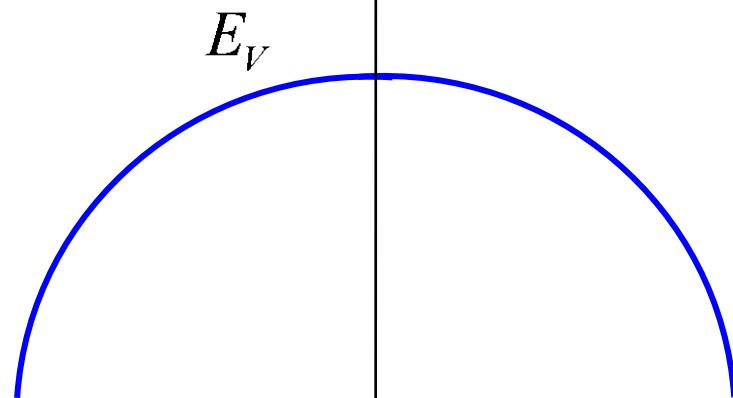
$$E = E_C + \frac{p^2}{2m_n^*}$$



**“band structure”**

“direct bandgap”

$$E = E_V - \frac{p^2}{2m_p^*}$$



$$k = \frac{2\pi}{\lambda}$$

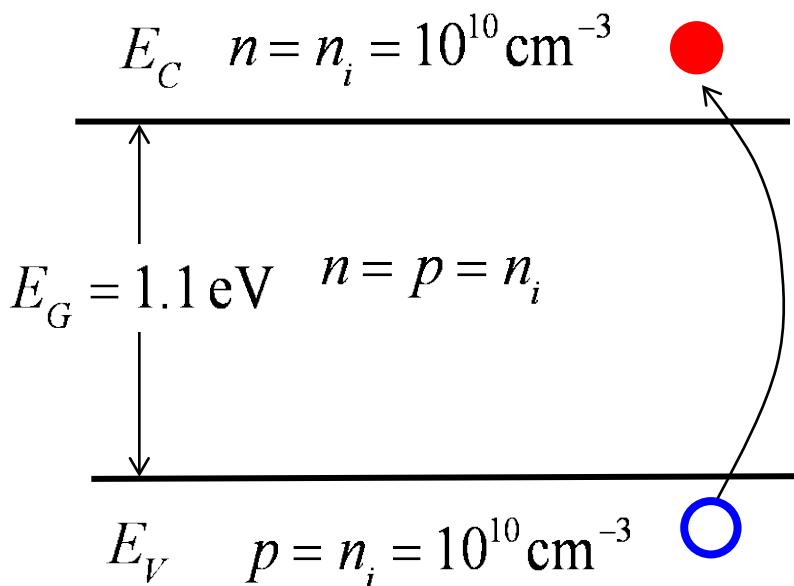
# Energy band structure vs. energy band diagram

---

Band structure is a plot of energy **vs. crystal momentum** (or  $k$ ).

An energy band diagram is a plot of the bottom of the conduction band and top of the valence band **vs. position**.

# Bandgap and intrinsic carrier concentration



$$E_G(\text{Si}) = 1.1 \text{ eV}$$

$$E_G(\text{GaAs}) = 1.4 \text{ eV}$$

$$E_G(\text{Ge}) = 0.66 \text{ eV}$$

$$n_i(\text{Si}) = 1 \times 10^{10} \text{ cm}^{-3} \quad (T = 300 \text{ K})$$

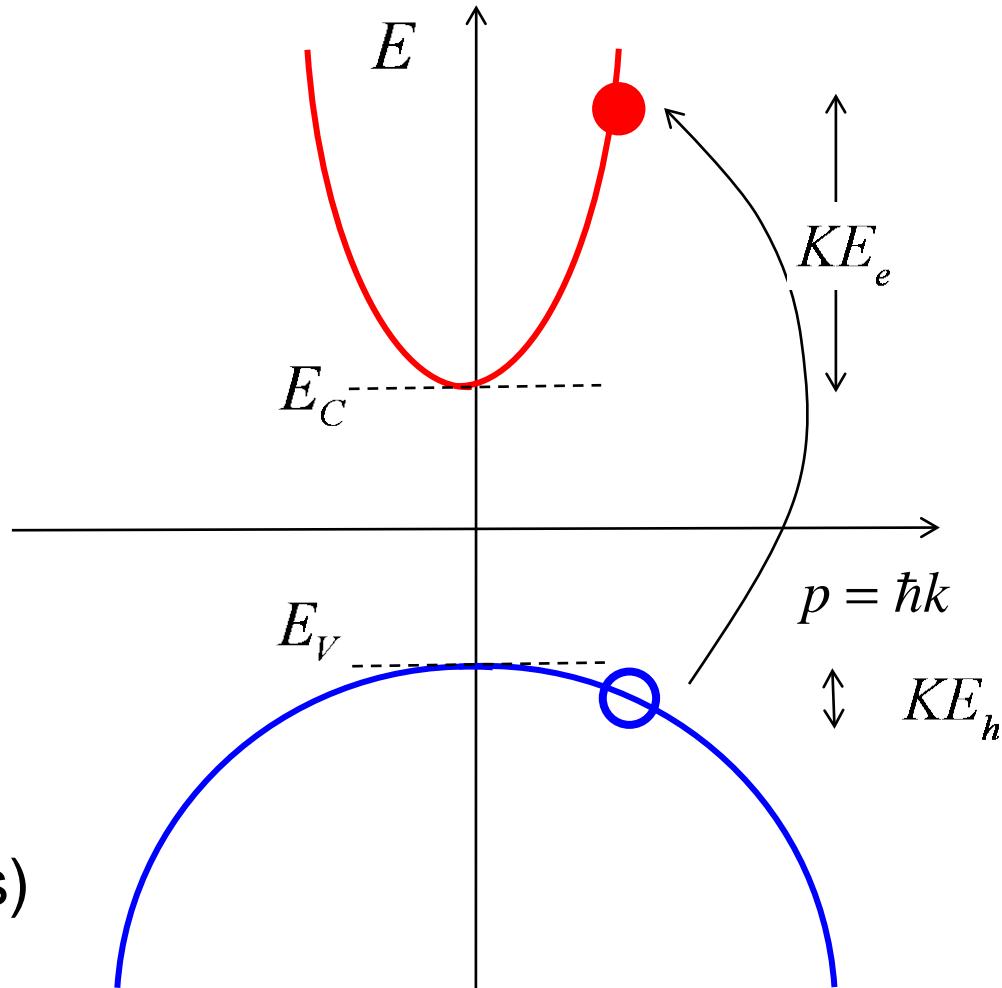
$$n_i(\text{GaAs}) = 2 \times 10^6 \text{ cm}^{-3} \quad (T = 300 \text{ K})$$

$$n_i(\text{Ge}) = 2 \times 10^{13} \text{ cm}^{-3} \quad (T = 300 \text{ K})$$

# Optical generation: $E(k)$

---

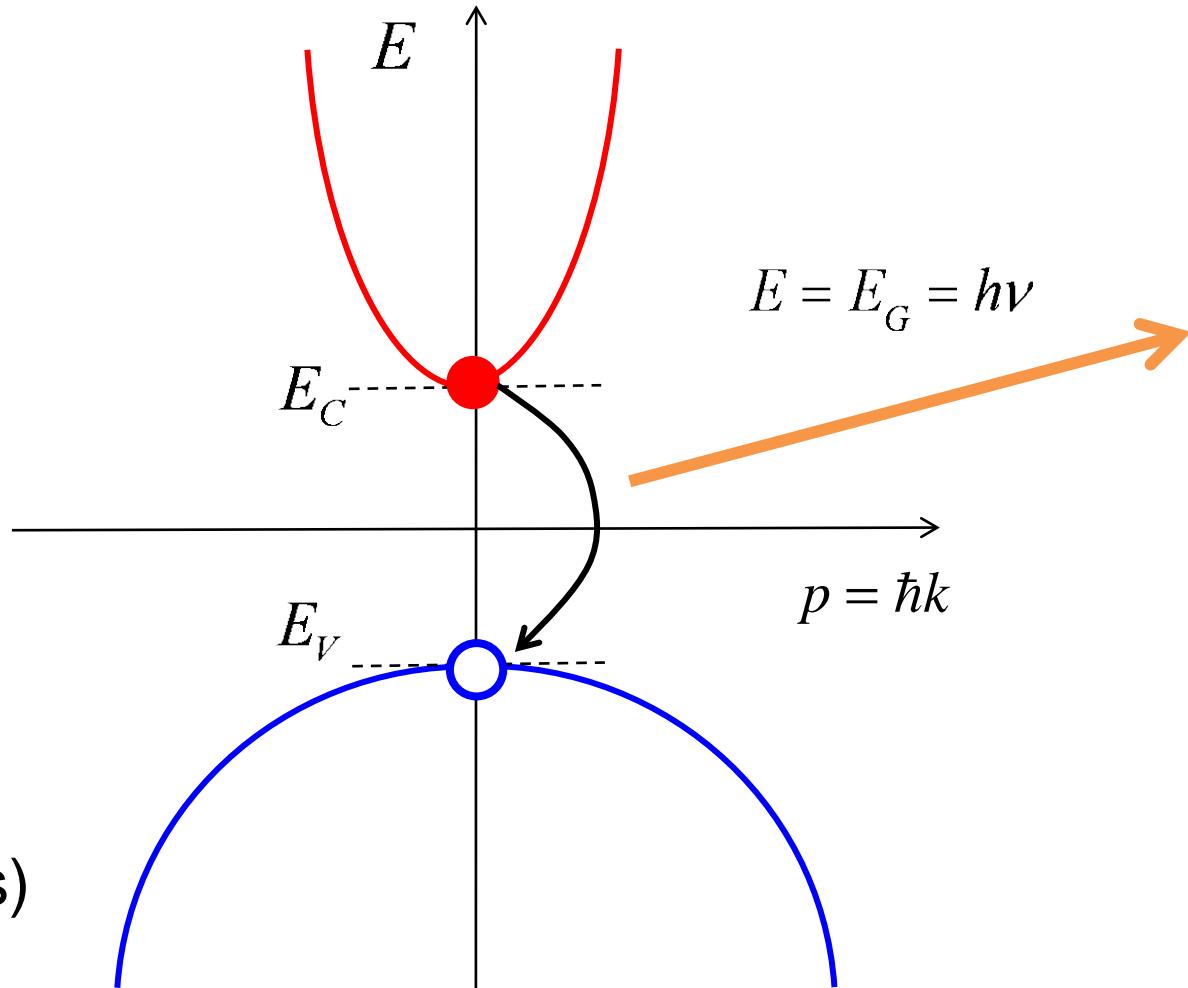
(more  
complicated for  
indirect gap  
semiconductors)



# Direct recombination: $E(k)$

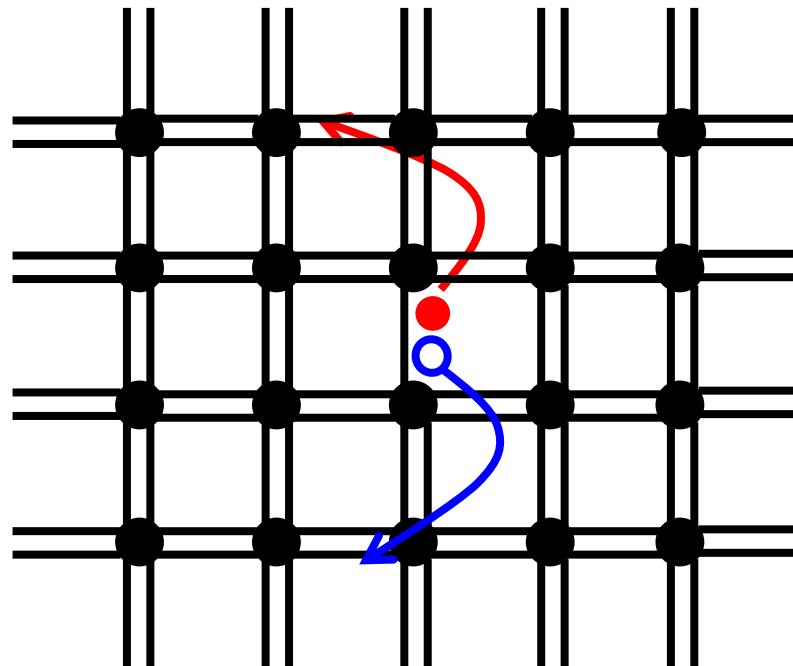
---

(more  
complicated for  
indirect gap  
semiconductors)



# Bonding model view: intrinsic semiconductor

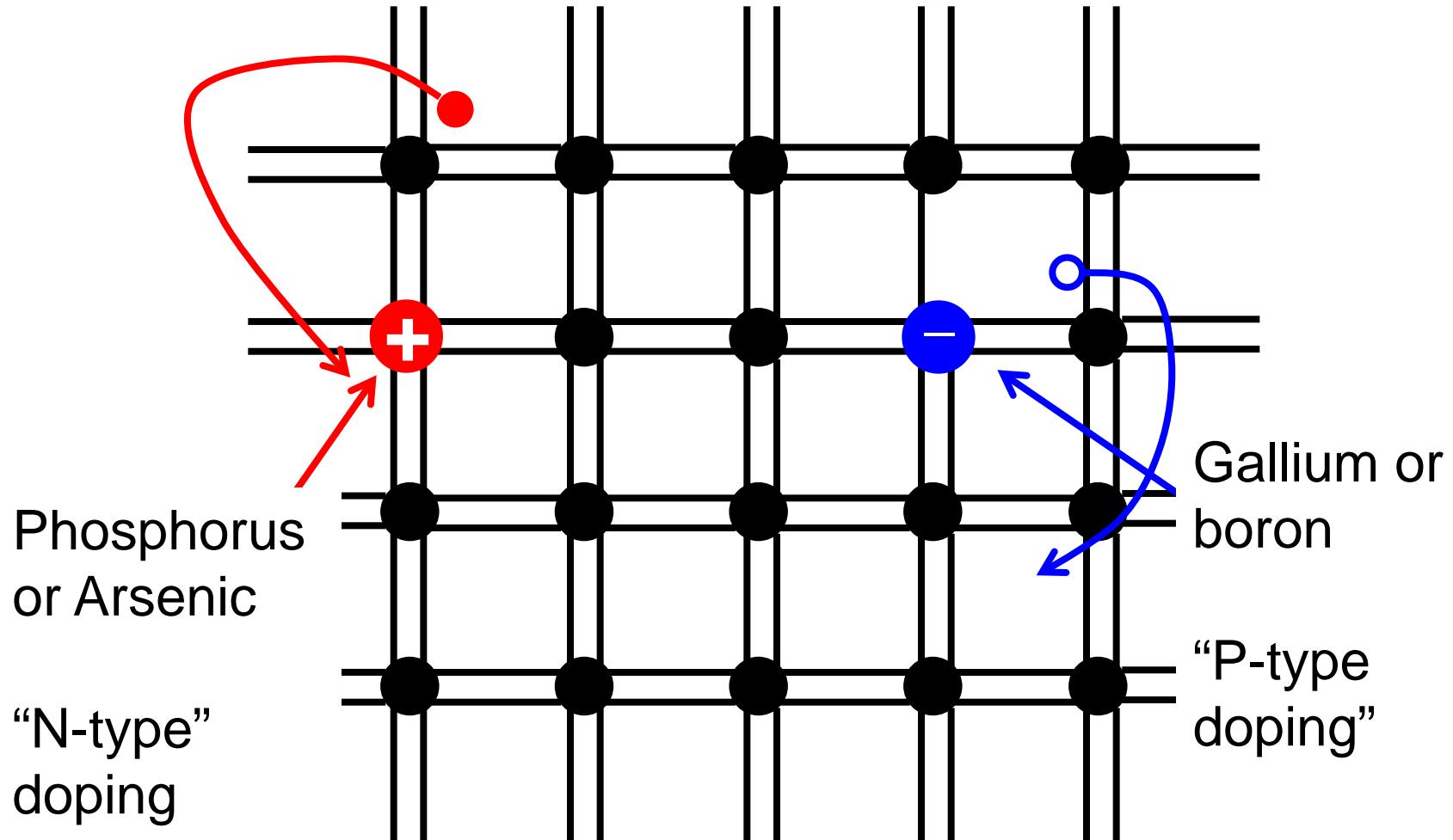
---



- 1) Electrons in the conduction band can move
- 2) Holes in the valence band can move
- 3) Electrons and holes can recombine

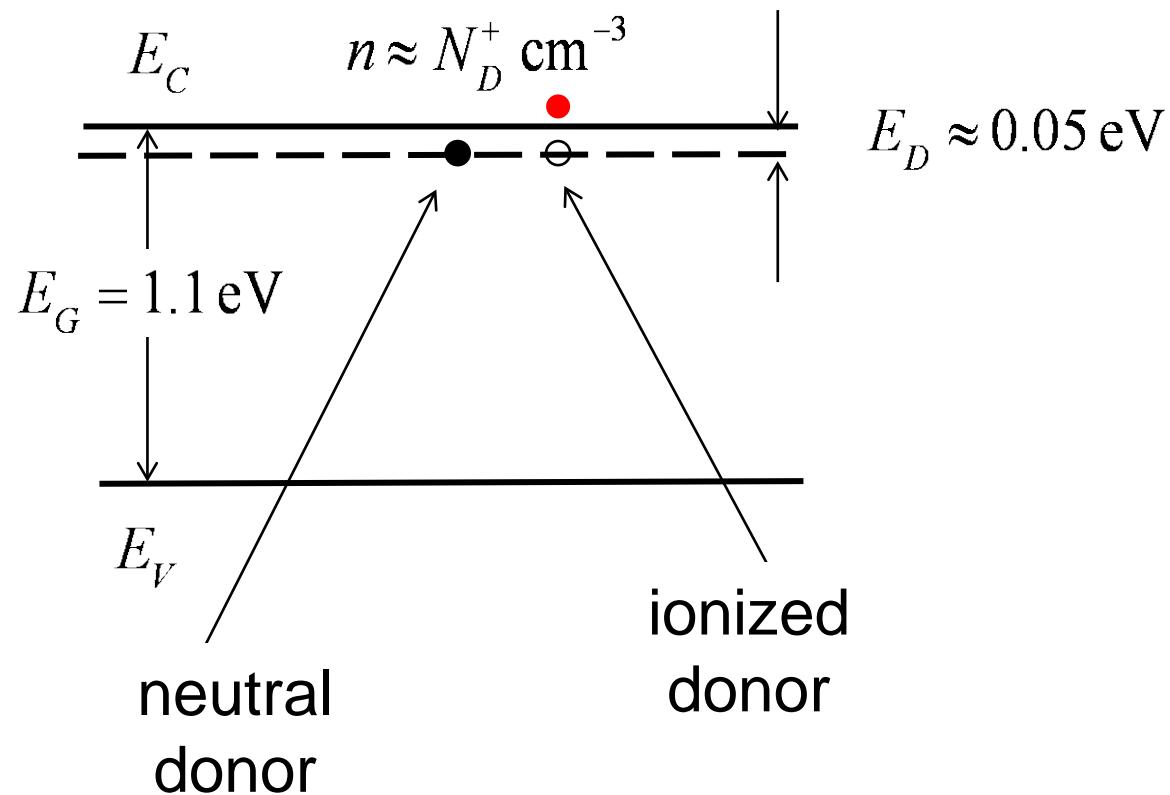
# Doping

---



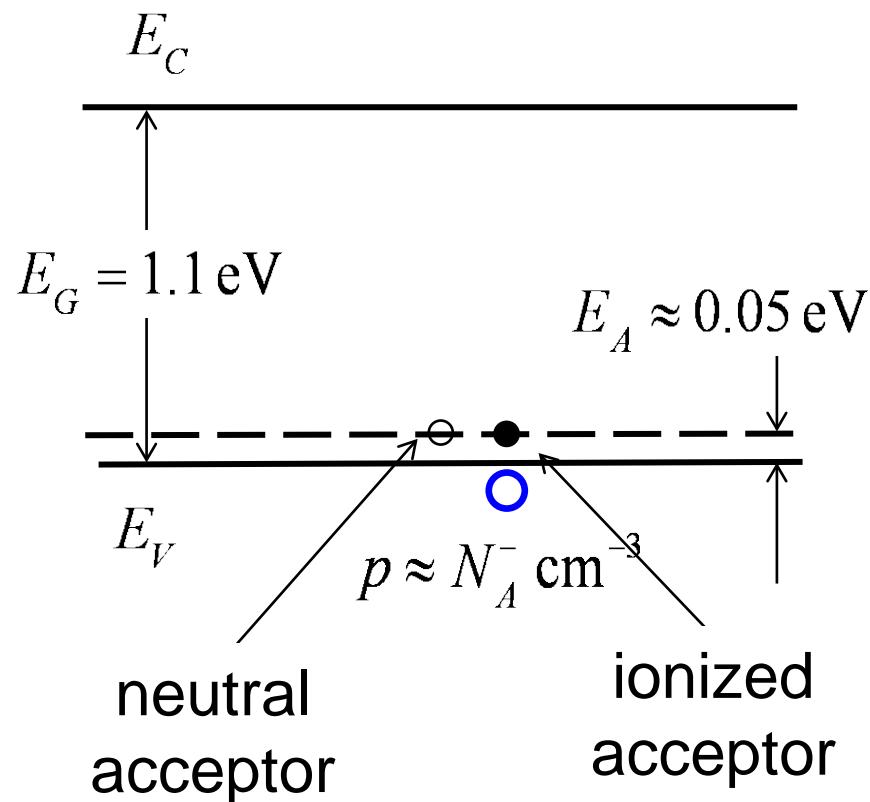
# N-type doping: Energy band view

---

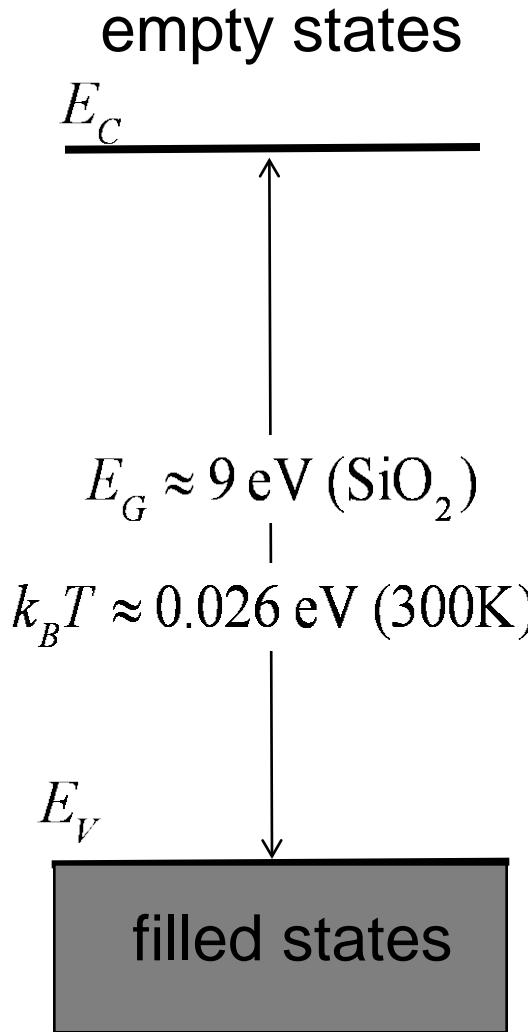


# P-type doping: Energy band view

---



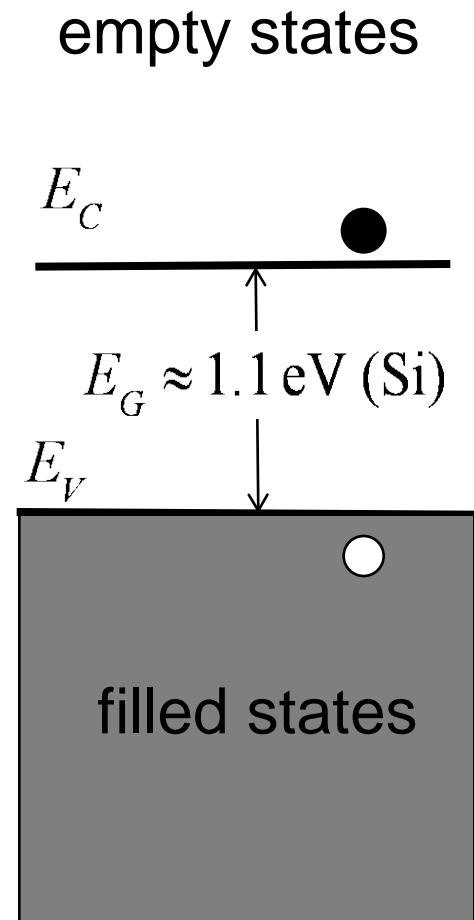
# Insulators



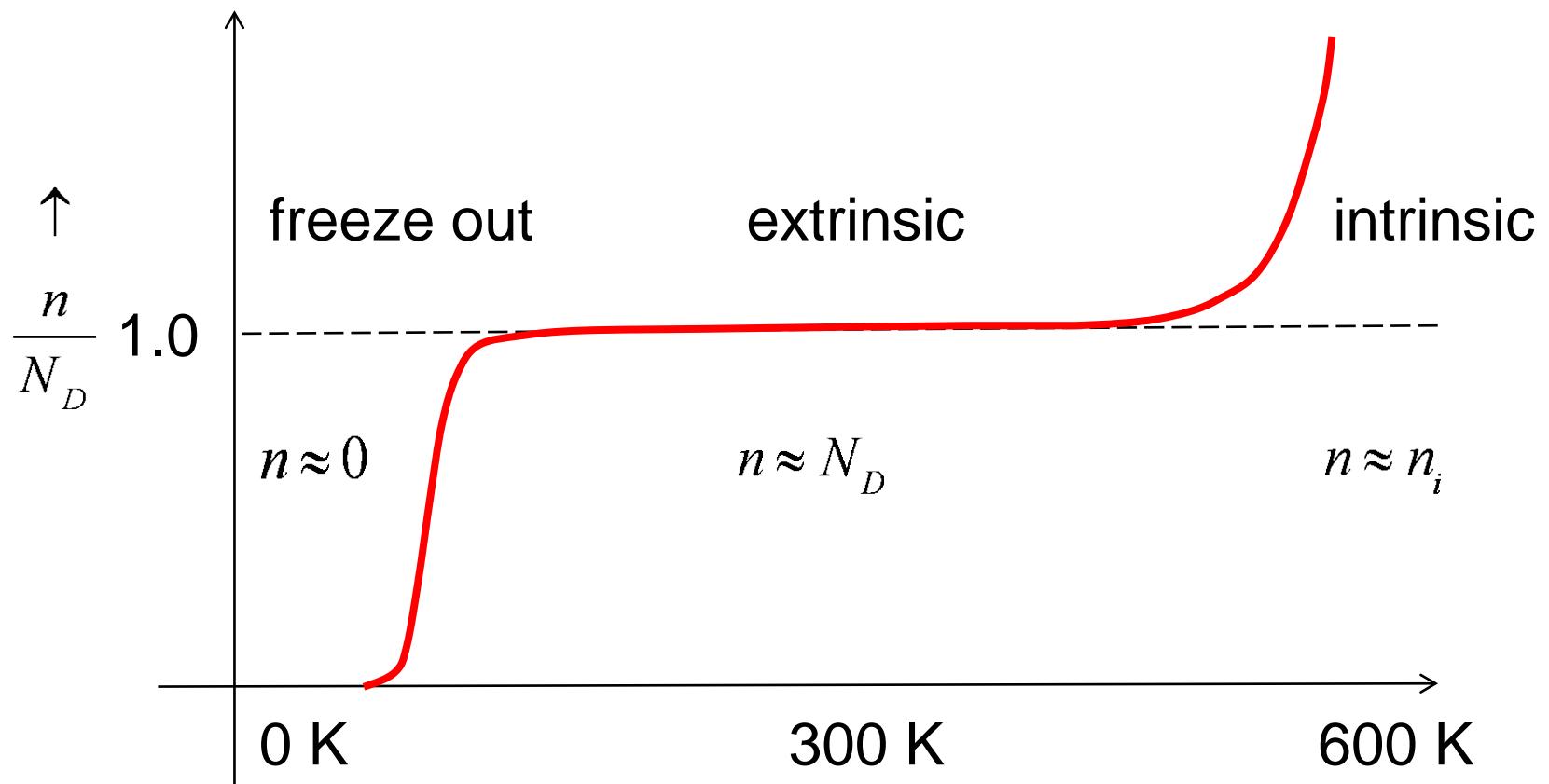
# Metals



# Semiconductors



# Carrier concentration vs. temperature



# Summary

---

1. Quantization of energy levels
2. Energy bands
3. Electrons and holes
4. Doping
5. Insulators, metals, and semiconductors

# Vocabulary

---

- 1) Crystalline
- 2) Amorphous
- 3) Polycrystalline
- 4) Bravais lattices
- 5) Unit cell
- 6) Primitive unit cell
- 7) Diamond lattice
- 8) Zinc blende lattice
- 9) Miller indices
- 10) Energy levels
- 11) Energy bands
- 12) Forbidden gap (bandgap)
- 13) Conduction band
- 14) Valence band
- 15) Electrons (in the conduction band)
- 16) Holes (in the valence band)
- 17) Optical generation
- 18) Thermal generation
- 19) Metal
- 20) Insulator
- 21) Semiconductor

# Primer on Semiconductors

## Unit 2: Quantum Mechanics

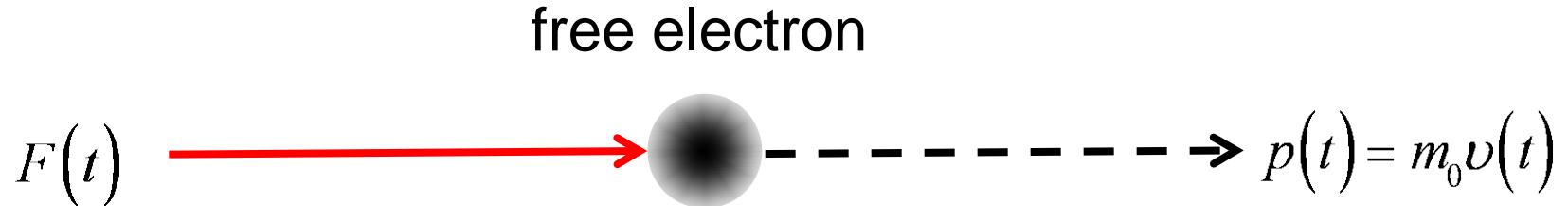
### Lecture 2.1: The wave equation

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Classical (Newtonian) mechanics

---



$$F = m_0 a = m_0 \frac{d^2 x}{dt^2} = m_0 \frac{dv}{dt}$$

$$F = \frac{dp}{dt}$$

Equations of motion:

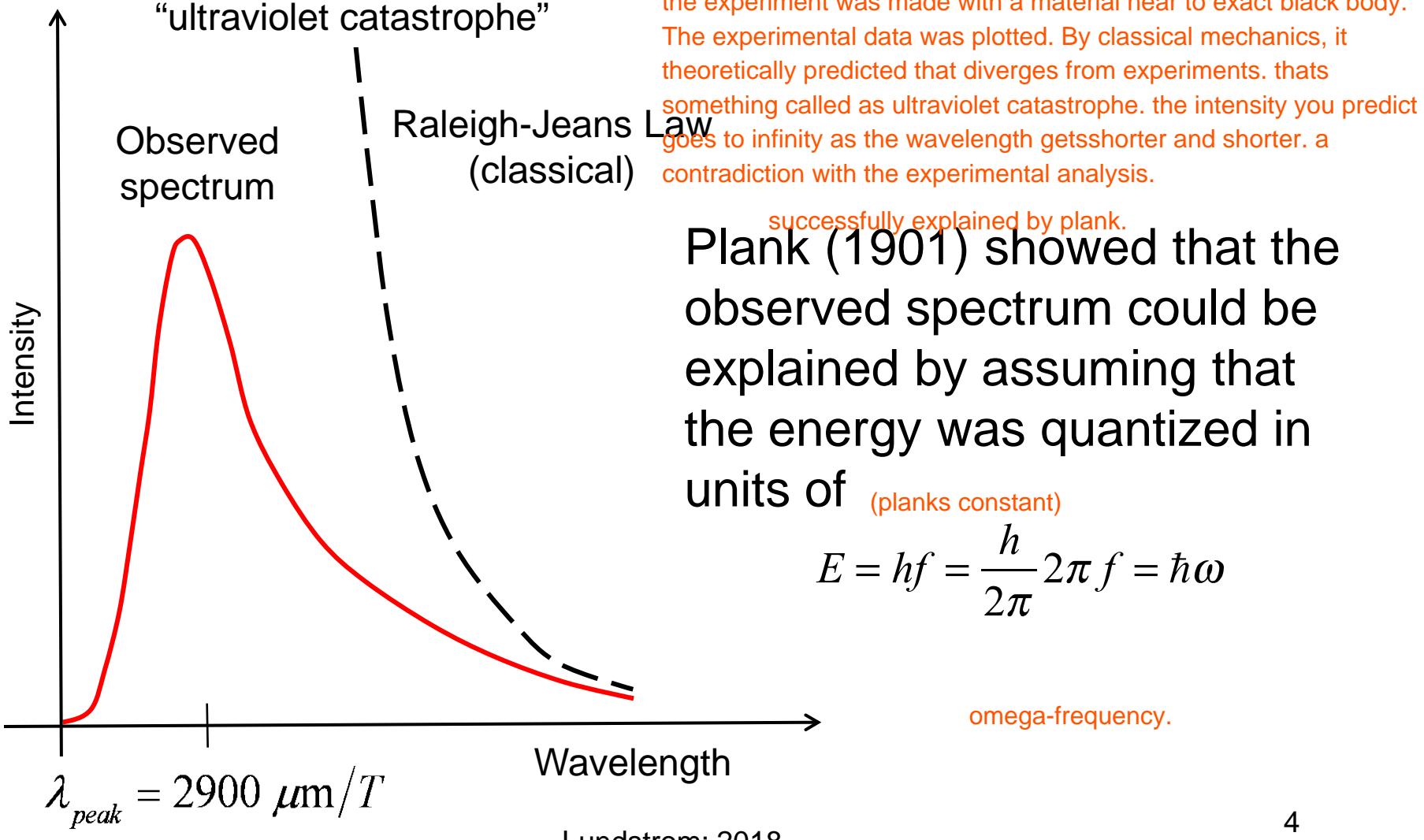
$$p(t) = p(0) + \int_0^t F(t') dt' \quad v(t) = v(0) + \frac{1}{m_0} \int_0^t F(t') dt' \quad x(t) = x(0) \int_0^t v(t') dt'$$

# The need to go beyond classical physics

---

- 1) Black body radiation (Planck, 1901)
- 1) Photoelectric effect (Einstein, 1905)
- 2) Atomic spectra (Bohr, 1913)
- 1) Wave-particle duality (de Broglie, 1924)

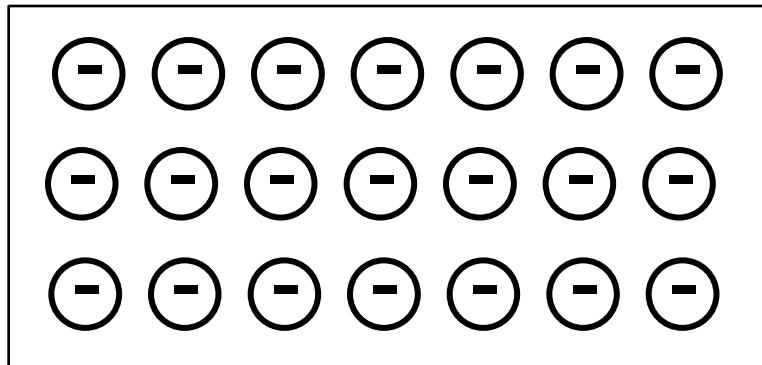
# Black body radiation



# Photoelectric effect

---

$$E = hf = \hbar\omega > \Phi_M$$

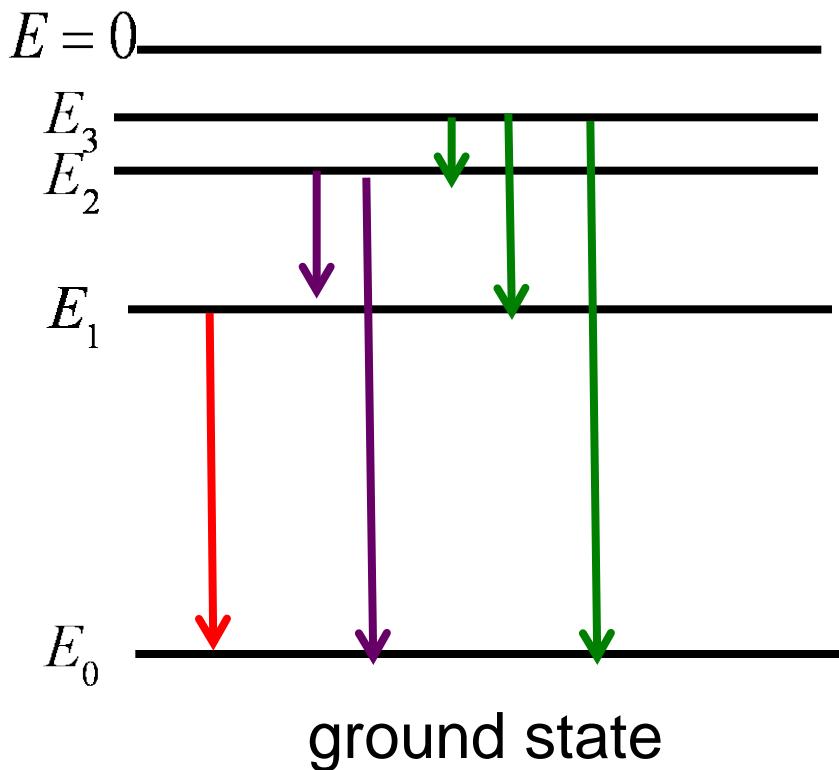


measured photons ejected per second per square centimeter, for ejection of electrons they need to above some critical frequency. when the energy of photon is higher than the work function of a metal, electrons were ejected.

Einstein (1904) showed that light should be thought of as **particles** with an energy

$$E = hf = \hbar\omega$$

# Atomic spectra



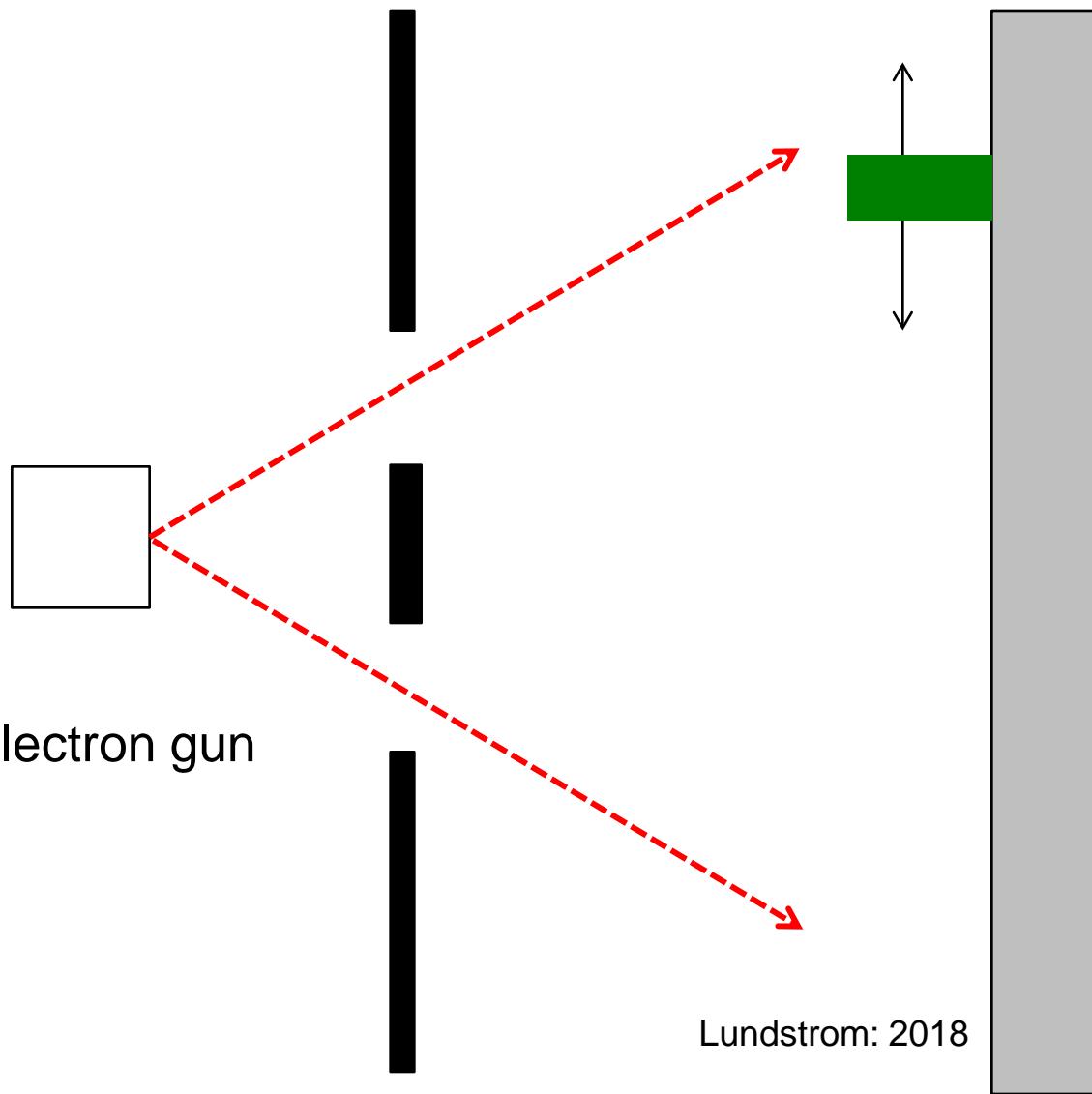
The light emitted by excited atoms comes in discrete colors.

Bohr (1913) showed that the light was produced by transitions between discrete energies:

$$\omega_{if} = \frac{E_i - E_f}{\hbar} \quad \text{initial-final}$$

Discrete energies can be explained if electrons are treated as **waves**.

# Wave particle duality



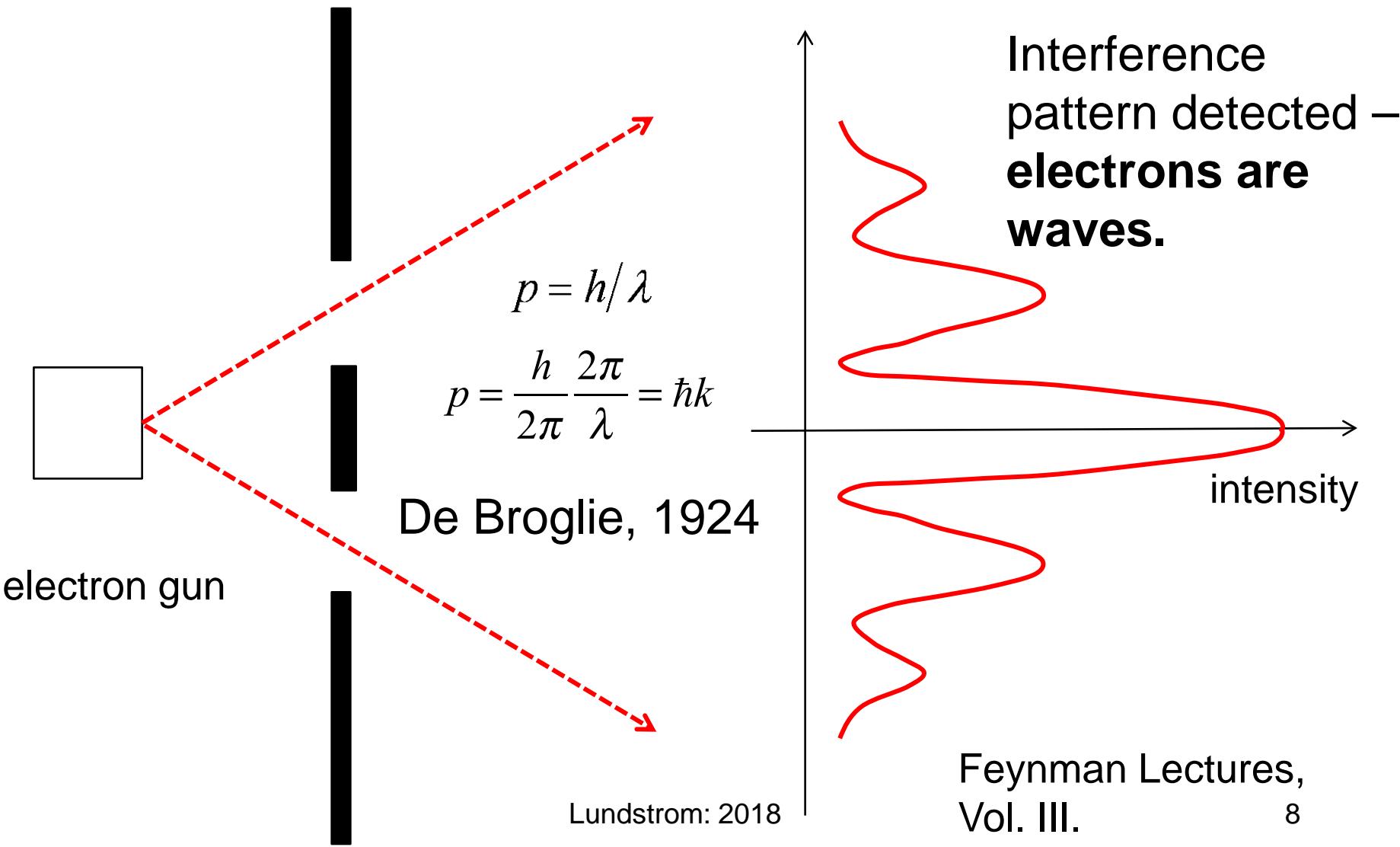
can detect whether no electron or single electron not as multiple parts of an electron.

detector

Only particles are detected –  
**electrons are particles.**

Feynman Lectures,  
Vol. III.

# Wave particle duality



# Experimental summary

---

- 1) Experimental evidence shows that energy is quantized (blackbody radiation, emission spectra of atoms).
- 2) Experimental evidence shows that waves can behave like particles (photoelectric effect) and particles like waves (electron diffraction experiments).

# Waves and particles

---

- 1) Waves show the effects of quantization when boundary conditions are applied.
- 2) Waves can be localized by adding up different wavelengths (wave packets)

**We need a wave equation for electrons!**

how particles behaves when they behave like a wave.

# Schrodinger wave equation

$$-\frac{\hbar}{i} \frac{\partial}{\partial t} \Psi(x, t) = -\frac{\hbar^2}{2m_0} \frac{\partial^2}{\partial x^2} \Psi(x, t) + U(x) \Psi(x, t)$$

To solve this equation, use “separation of variables”

$$\phi(t) = e^{-i\omega t}$$

$$E = \hbar\omega$$

$$\phi(t) = e^{-iE/\hbar}$$

$$\Psi(x, t) = \psi(x)\phi(t)$$

time alone (time dependent part alone)

$$\psi(x) = ?$$

position alone

(position dependent part)

Lundstrom: 2018

# Time-independent wave equation

---

$$-\frac{\hbar^2}{2m_0} \frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x)$$

space dependent equation

$$\Psi(x,t) = \psi(x)\phi(t) = \psi(x)e^{-i\omega t} \quad \omega = E/\hbar$$

The probability of finding an electron between  $x$  and  $x+dx$ , is:

$$P(x,t)dx = \Psi^*(x,t)\Psi(x,t)dx$$

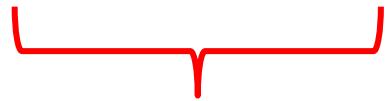
# Solving the time independent wave equation

---

$$-\frac{\hbar^2}{2m_0} \frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x)$$

— time independent

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2m_0}{\hbar^2} [E - U(x)]\psi(x) = 0$$



Solutions depend on whether  $E > U(x)$  or  $E < U(x)$

# Electron energy > potential energy

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m_0}{\hbar^2} [E - U(x)] \psi(x) = 0$$

$$E > U(x) \quad k^2 = \frac{2m_0}{\hbar^2} [E - U(x)] \quad \frac{d^2\psi(x)}{dx^2} + k^2 \psi(x) = 0$$

Solution:  $\psi(x) = A e^{\pm ikx}$

$$\Psi(x,t) = \psi(x)\phi(t)$$

This is a wave travelling in the +/- x direction.

$$\Psi(x,t) = A e^{\pm i(kx - \omega t)}$$

# Waves: phase velocity

$$\Psi(x,t) = A e^{i(kx - \omega t)} = A e^{i\theta}$$

$$U(x) = U_0$$

potential energy is constant meaning  $k$  is constant.

$$k(x) \text{ is constant}$$

Follow a point of constant phase:

$$\frac{d\theta}{dt} = 0$$

constant in position

$$\frac{d(kx - \omega t)}{dt} = 0 = k \frac{dx}{dt} - \omega$$

Phase velocity of the wave:

$$v_p = \frac{\omega}{k}$$

frequency / wave number

# Waves: wavelength

---

$$\Psi(x,t) = A e^{i(kx - \omega t)} = A e^{i\theta}$$
$$k = \frac{\sqrt{2m_0(E - U_0)}}{\hbar}$$

At a given time, the phase at a given  $x + 1$  wavelength must be  $2\pi$  plus the phase at  $x$ .

$$\theta(x + \lambda, t) = \theta(x, t) + 2\pi \quad k(x + \lambda) - \omega t = kx - \omega t + 2\pi \quad k\lambda = 2\pi$$

Wavelength:  $\lambda = \frac{2\pi}{k}$

Wavevector:  $k = \frac{2\pi}{\lambda}$

# Waves: momentum

---

$$p=mv$$

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m_0}{\hbar^2} [E - U(x)] \psi(x) = 0 \quad U(x) = U_0$$

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m_0}{\hbar^2} (E - U_0) \psi(x) = 0 \quad \psi(x) = A e^{ikx}$$

$$k^2 = \frac{2m_0}{\hbar^2} (E - U_0)$$

$$E = U_0 + \frac{\hbar^2 k^2}{2m_0} = U_0 + \frac{p^2}{2m_0} \rightarrow$$

$$p = \hbar k$$

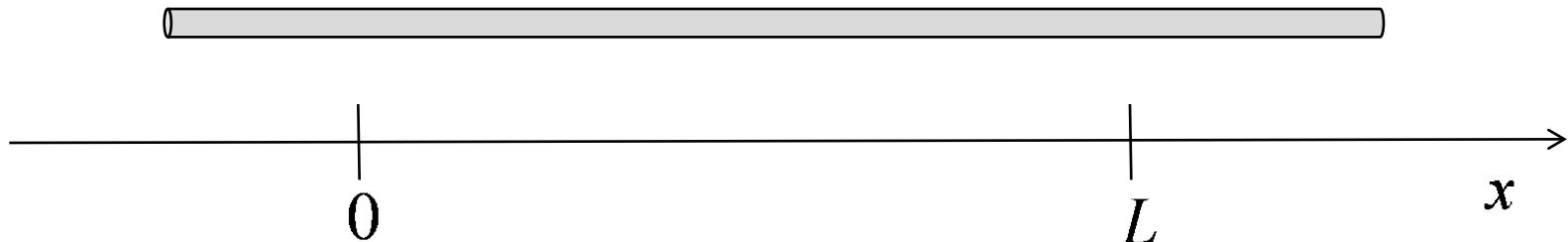
de Broglie  
(1924)

# Electron waves in 1D

where the electrons move as one dimensional particle.

nanowire

$$U(x) = U_0$$



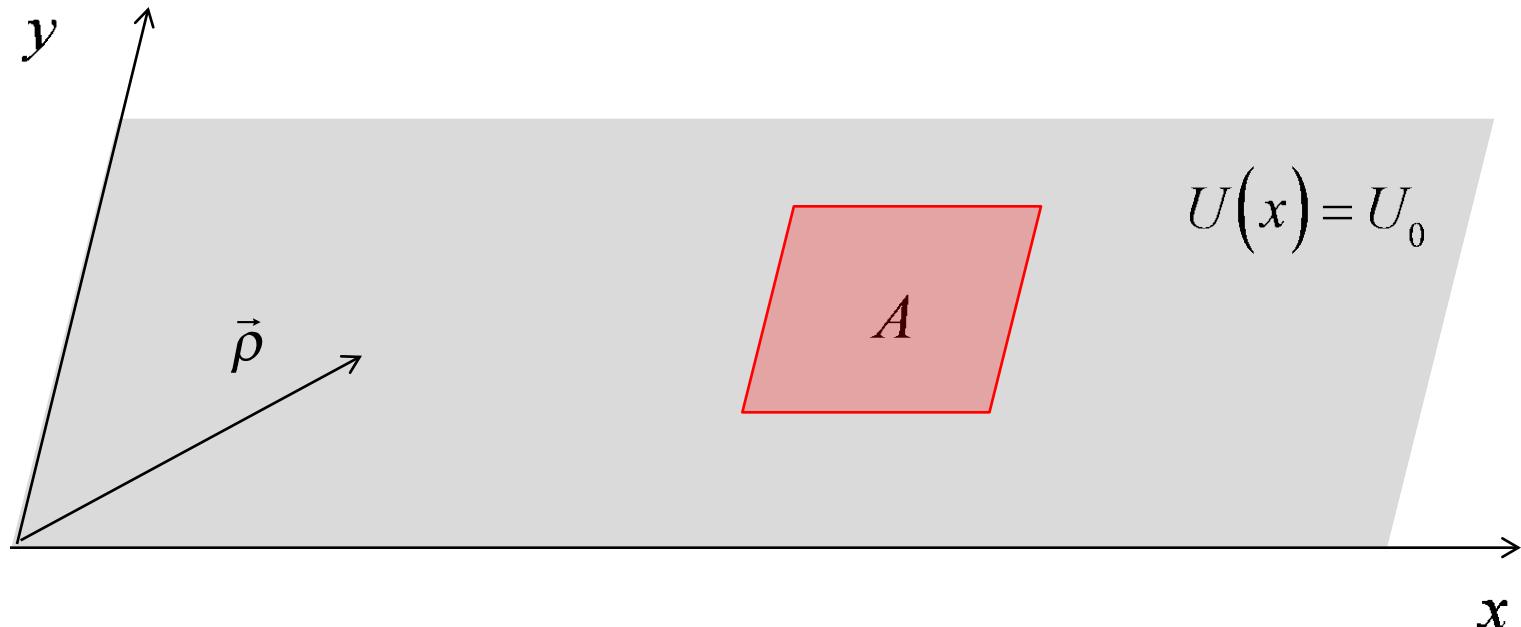
$$\psi(x) = A e^{\pm i k x}$$

assuming 1 electron is there bw 0 and L

$$\int_0^L \psi^*(x) \psi(x) dx = 1$$

$$\psi(x) = \frac{1}{\sqrt{L}} e^{ikx} \quad (\text{normalized in 1D})$$

# Electron waves in 2D



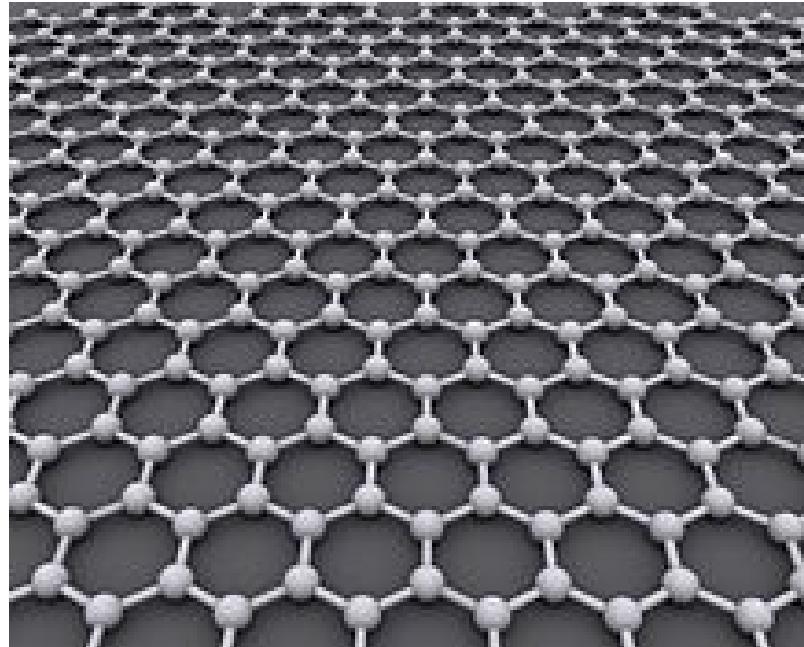
$$\psi(x, y) = A e^{\pm i(k_x x + k_y y)} = A e^{i \vec{k} \cdot \vec{\rho}}$$

$$\psi(\vec{\rho}) = \frac{1}{\sqrt{A}} e^{i \vec{k} \cdot \vec{\rho}} \quad (\text{normalized in 2D})$$

e.g. graphene

# Graphene and 2D materials

---

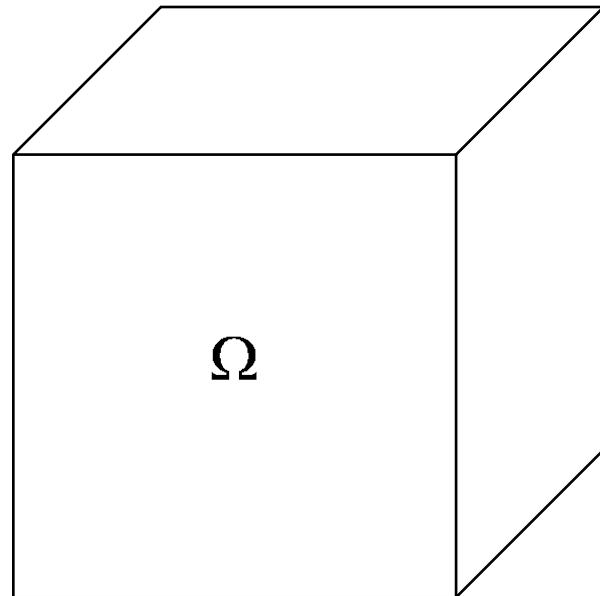


A 2D hexagonal lattice of carbon atoms

<https://en.wikipedia.org/wiki/Graphene>

# Electron waves in 3D

---

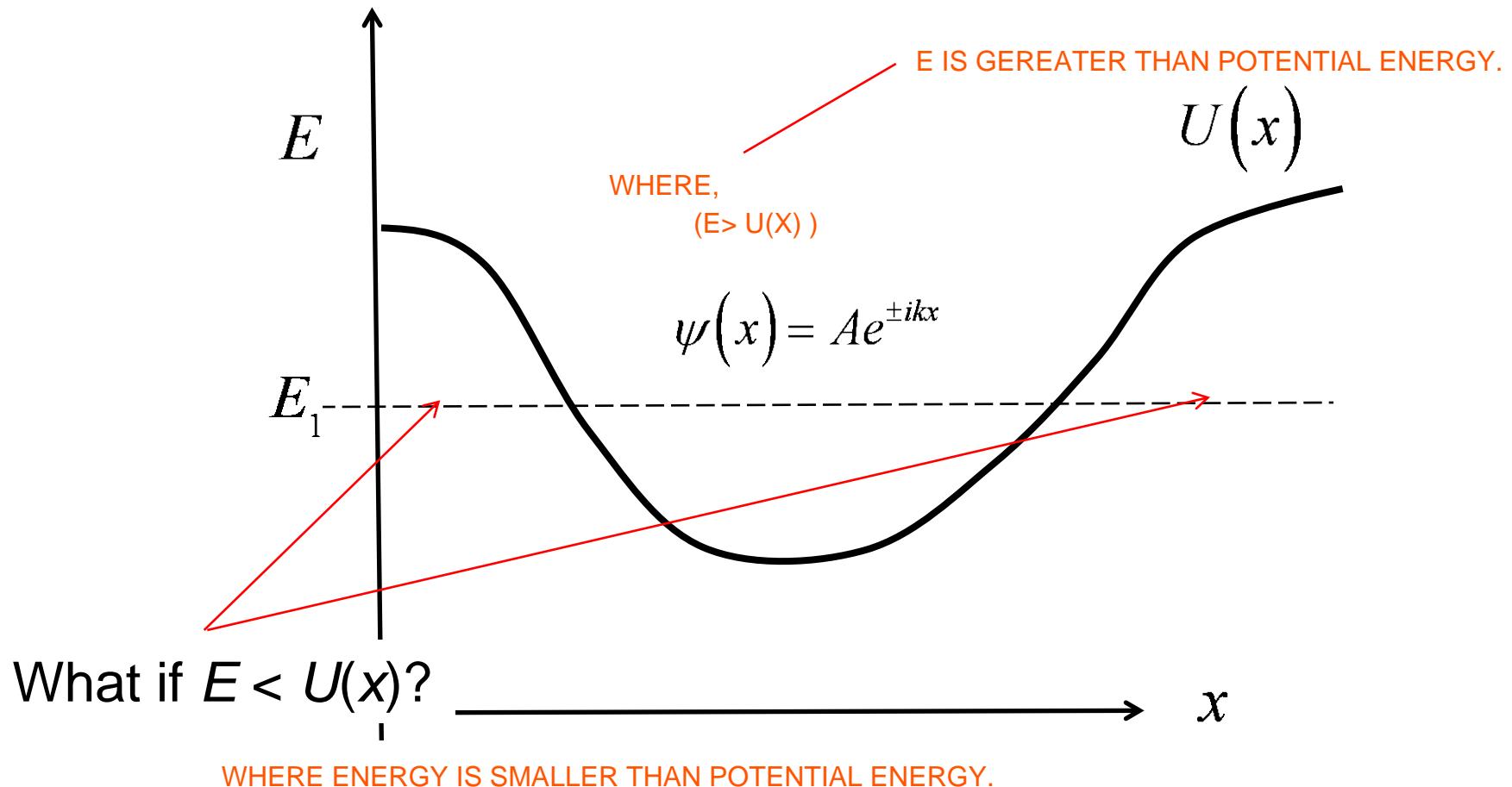


bulk solid

$$\psi(\vec{r}) = \frac{1}{\sqrt{\Omega}} e^{i(k_x x + k_y y + k_z z)} = \frac{1}{\sqrt{\Omega}} e^{i\vec{k} \cdot \vec{r}}$$

(normalized in 3D)

# Solutions of the wave equation



# Electron energy < potential energy

---

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m_0}{\hbar^2} [E - U(x)] \psi(x) = 0$$

$$E < U(x)$$

$$\alpha^2 = \frac{2m_0}{\hbar^2} [U(x) - E]$$

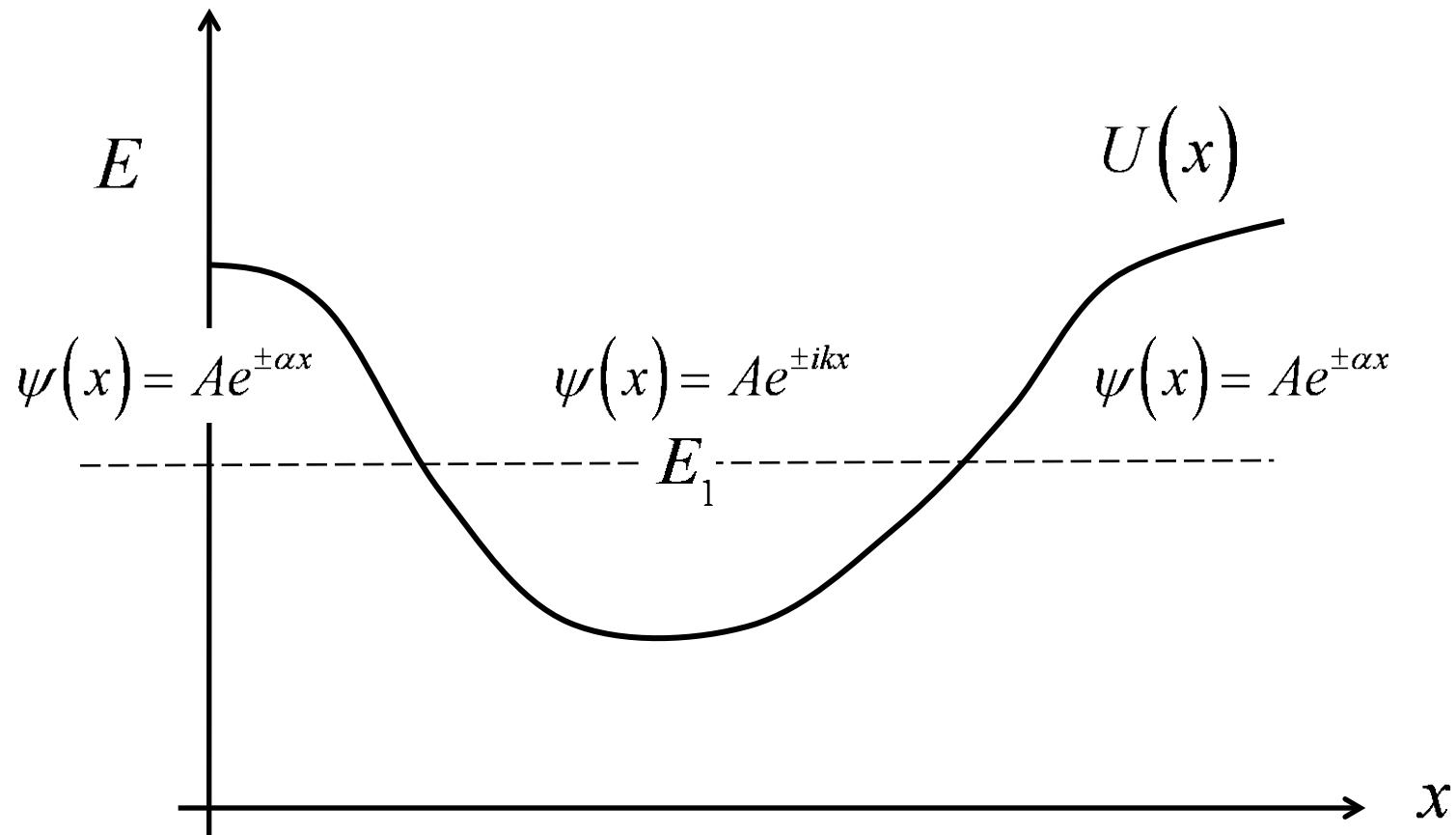
$$\frac{d^2\psi(x)}{dx^2} - \alpha^2 \psi(x) = 0$$

Solution:  $\psi(x) = A e^{\pm \alpha x}$

This is an exponentially decaying or growing solution.

# Solutions of the wave equation

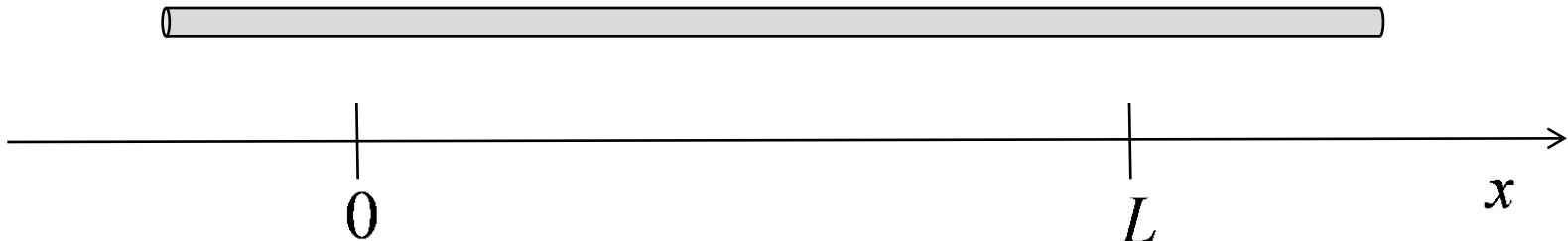
---



# Electrons are waves **and** particles

---

nanowire



$$\psi(x) = \frac{1}{\sqrt{L}} e^{ikx}$$

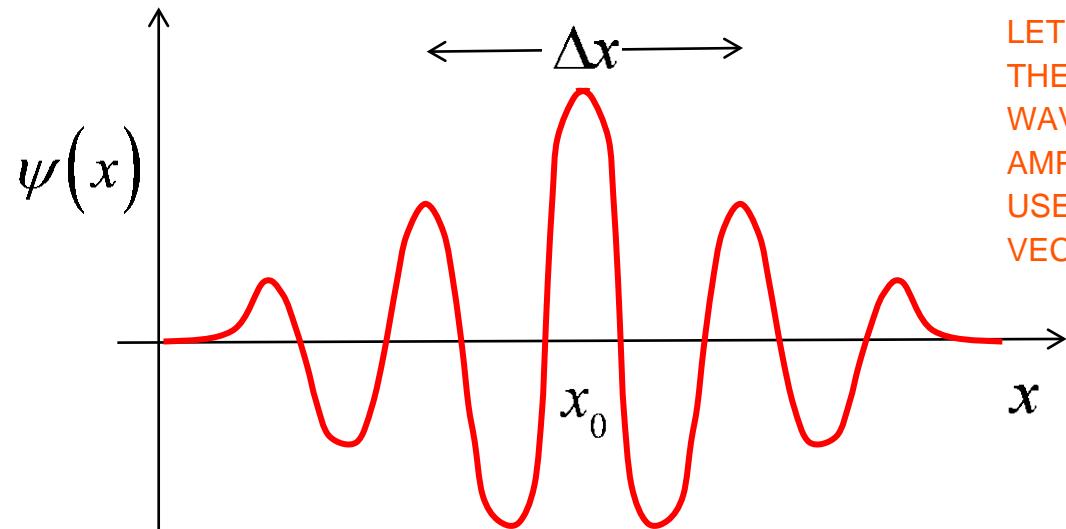
$$P(x)dx = \psi^*(x)\psi(x)dx = \frac{dx}{L}$$

## Waves are **everywhere!**

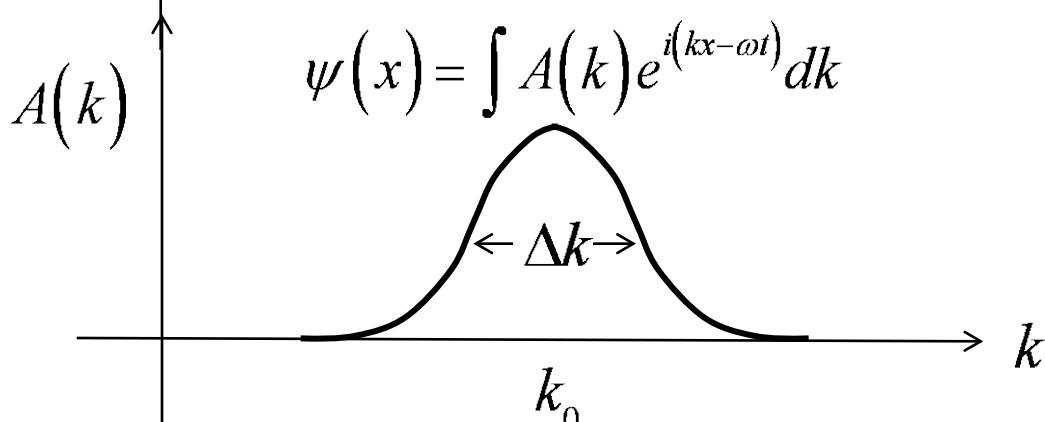
THEN HOW WE ARE ABLE TO PREDICT ELECTRON PARTICLES. (WE NEED TO FIND THE PROBABILITY OF FINDING THAT ELECTRON). THERE IS A WELL KNOWN PROCEDURE TO FIND THAT WHICH WORKS ON ANY TYPE OF WAVE TO LOCALIZE THE ENERGY IN A WAVE TO A PARTICULAR SPOT IN POSITION.

Lundstrom: 2018

# Wave packets



LET THE ELECTRON IS AT X<sub>0</sub> POSITION.  
THE WAY TO DO THAT IS TO ADD UP A BUNCH OF WAVES WITH DIFFERENT WAVELENGTHS AND THEIR AMPLITUDES SUCH THAT WE PUT TOGETHER ,IF WE USE ONE AMPLITUDE,WE HAVE ONE WAVE VECTOR,THE ELECTRON IS SPREADOUT EVERYWHERE.



THE WIDER THE SPREAD OF WAVE VECTORS K,  
THE MORE WE LOCALIZE THIS AT A PARTICULAR POSITION.  
THE NARROW THE SPREAD THE WIDER IT WILL.

Lundstrom: 2018

Particle:	$x = x_0$
Momentum:	$p = \hbar k_0$

$$\Delta k \Delta x = 1/2$$

BUT IF WE USE A NUMBER OF AMPLITUDES THEN THE WAVE VECTOR SPREADOUT IN DIFFERENT AMOUNTS OF AMPLITUDE,THEN WE CAN LOCALIZE THE ELECTRONS SUCH THAT THE WAVES INTERFERE CONSTRUCTIVELY NEAR X<sub>0</sub> BUT THEY INTERFERE DESTRUCTIVELY WHEN WE GET AWAY FROM THE PARTICULAR LOCATION.

# Uncertainty relations

---

A wave packet that is localized in space is spread out in k-space.

$$\Delta k \Delta x \geq 1/2 \rightarrow \Delta p \Delta x \geq \hbar/2 \quad (\text{UNCERTAINTY IN MOMENTUM AND POSITION. } p = \hbar k)$$

Similarly, a wave packet that is sharply defined in time, is spread out in frequency.

$$\Delta \omega \Delta t \geq 1/2 \rightarrow \Delta E \Delta t \geq \hbar/2 \quad (\text{ENERGY AND TIME } E = \hbar \omega)$$

# Uncertainty relations

---

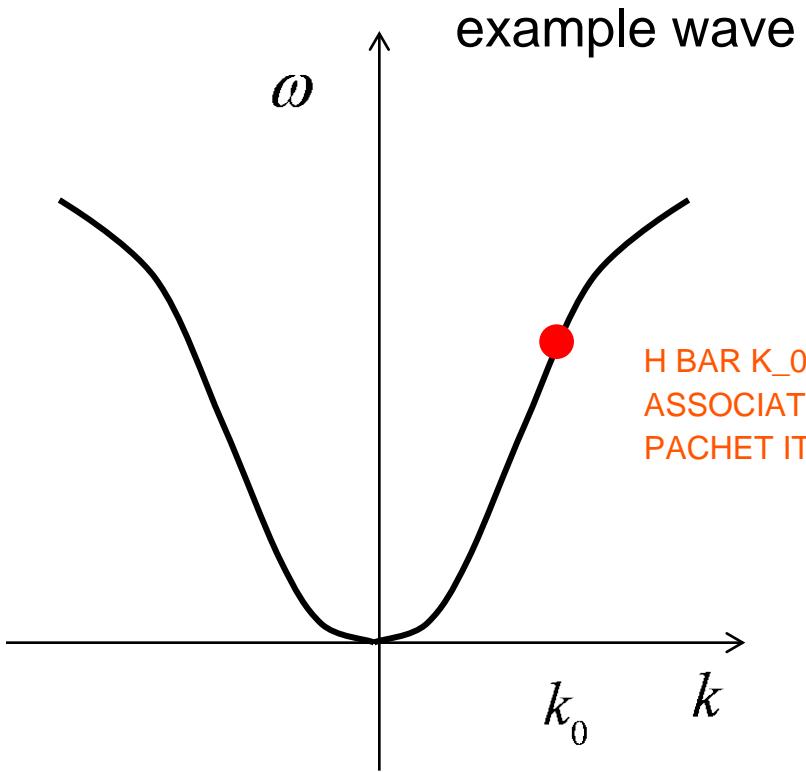
$$\Delta p \Delta x \geq \hbar/2$$

$$\Delta E \Delta t \geq \hbar/2$$

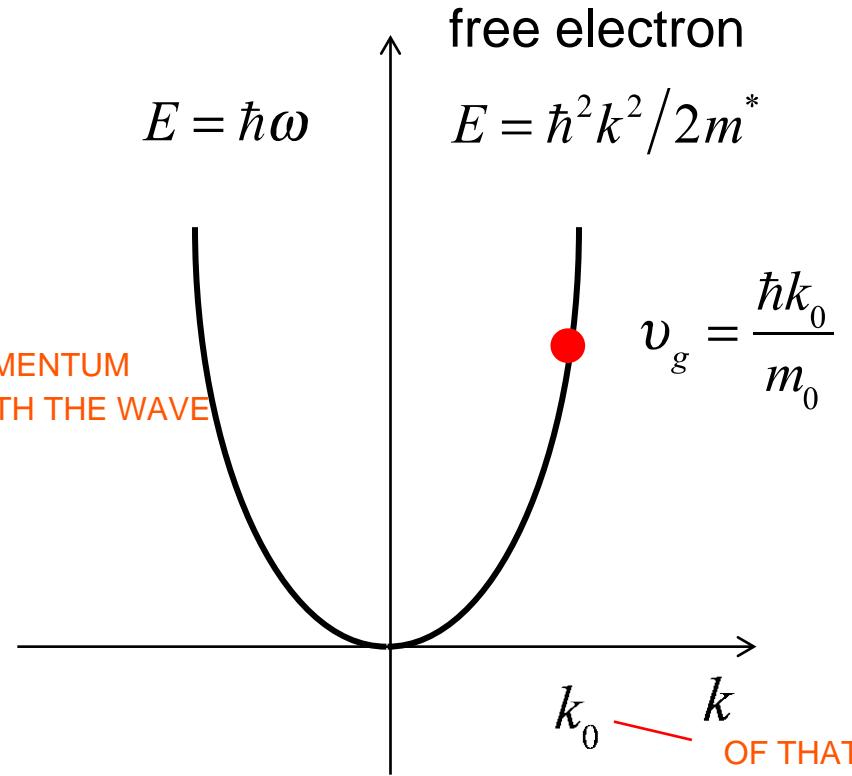
OFTEN USED TO DESCRIBE THE QUANTUM MECHANICAL PARTICLES.

WE CAN DESCRIBE A WAVE BY ITS DISPERSION.(HOW ITS FREQUENCY VARIES WITH WAVE NUMBER.)

## Wave packets: group velocity



H BAR K\_0 = MOMENTUM  
ASSOCIATED WITH THE WAVE  
PACHET ITSELF.



OF THAT  
WAVE  
PACKET.

For any wave:  $\omega(k)$  (dispersion)

$$v_g = d\omega/dk = (1/\hbar) dE/dk$$

Group velocity:  $v_g = d\omega/dk$

(GN BY SLOPE OF THE OMEGA.

Lundstrom: 2018  
THE CENTRE OF THE WAVE.

$$v_p = \omega/k \text{ PHASE VELOCITY}$$

# Summary

---

## Classical Mechanics

$$F = m_0 a$$

SPACE DEPENDENT PART   $\frac{\hbar^2}{2m_0} \frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x)$

$$\Psi(x,t) = \psi(x)e^{-i\omega t}$$

$$E = \hbar\omega = hf$$

$$P(x)dx = \psi^*(x)\psi(x)dx$$

$$\Delta p \Delta x \geq \hbar/2$$

$$\Delta E \Delta t \geq \hbar/2$$

# Primer on Semiconductors

## Unit 2: Quantum Mechanics

### Lecture 2.2: Quantum confinement

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Time-independent wave equation

---

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

The probability of finding an electron between  $x$  and  $x + dx$  is:

$$P(x)dx = \psi^*(x)\psi(x)dx$$

# Electron energy > potential energy

---

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E - U_0] \psi(x) = 0$$

$$E > U_0 \quad k^2 = \frac{2m}{\hbar^2} [E - U_0] \quad \frac{d^2\psi(x)}{dx^2} + k^2 \psi(x) = 0$$

Solution:  $\psi(x) = A e^{\pm ikx}$

Or:  $\psi(x) = A \sin(kx) + B \cos(kx)$

# 1D particle in a box

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi = 0$$

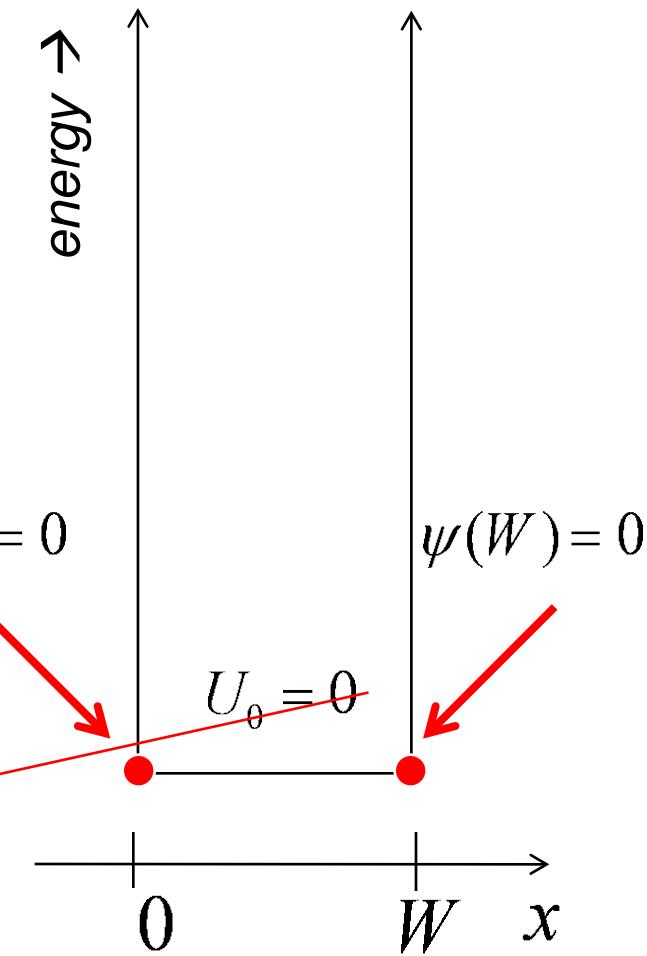
$$k^2 = \frac{2mE}{\hbar^2}$$

$$\psi(x) = A \sin(kx) + B \cos(kx)$$

boundary conditions:

$$\psi(x=0) = \psi(x=W) = 0$$

POTENTIAL ENERGY IS ZERO INSIDE THE BOX.



# Satisfying the boundary conditions

---

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi = 0 \quad k^2 = \frac{2mE}{\hbar^2}$$

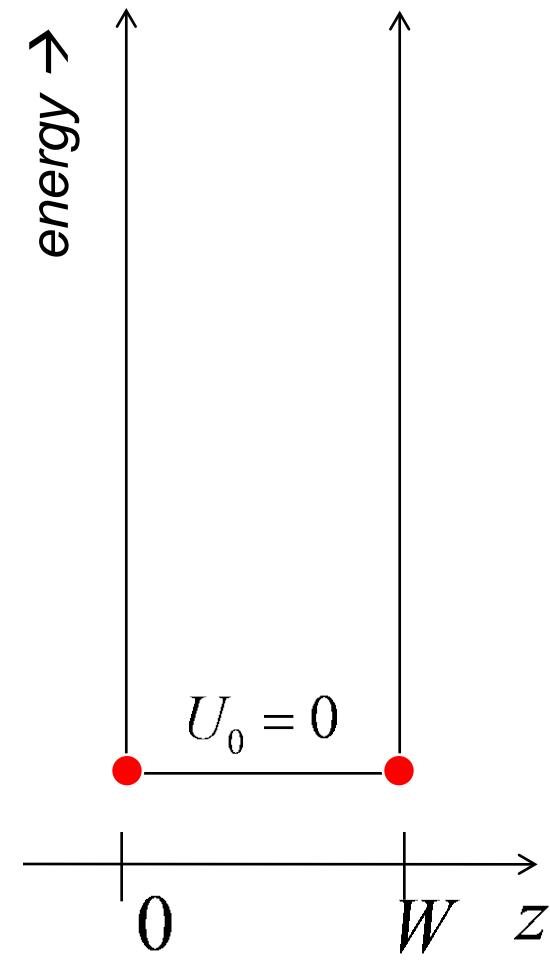
$$\psi(x) = A \sin kx$$

$$\psi(0) = 0 \quad \checkmark$$

$$\psi(W) = A \sin(kW) = 0$$

$$kW = j\pi \quad j = 1, 2, 3, \dots$$

$$k_j = j \frac{\pi}{W} \quad j = 1, 2, 3, \dots \quad \checkmark$$



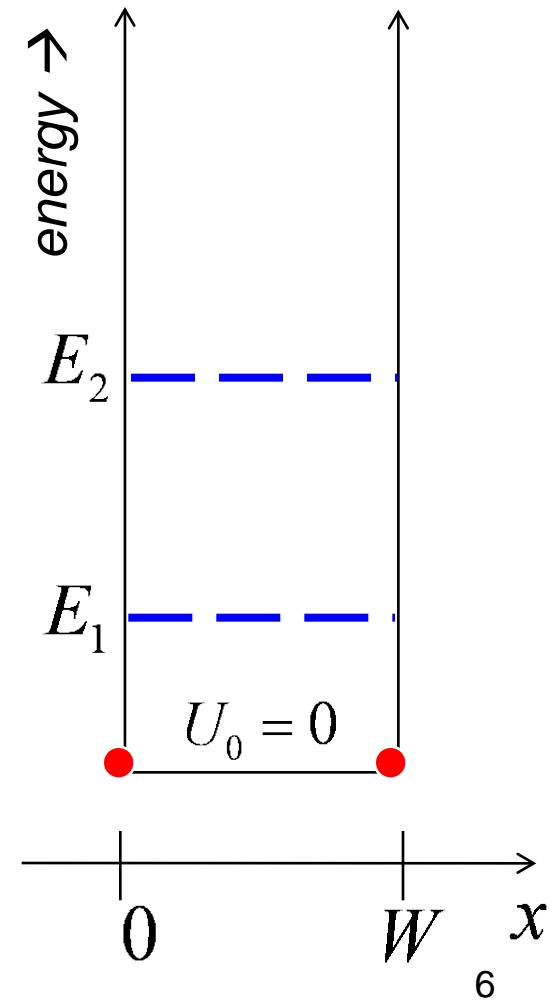
# Energy is quantized

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi = 0 \quad k^2 = \frac{2mE}{\hbar^2}$$

$$\psi(x) = \sin k_j x$$

$$k_j = \frac{\pi}{W} j \quad j = 1, 2, 3, \dots$$

$$E_j = \frac{\hbar^2 k_j^2}{2m} = \frac{\hbar^2 j^2 \pi^2}{2m W^2}$$



# 1D QW summary

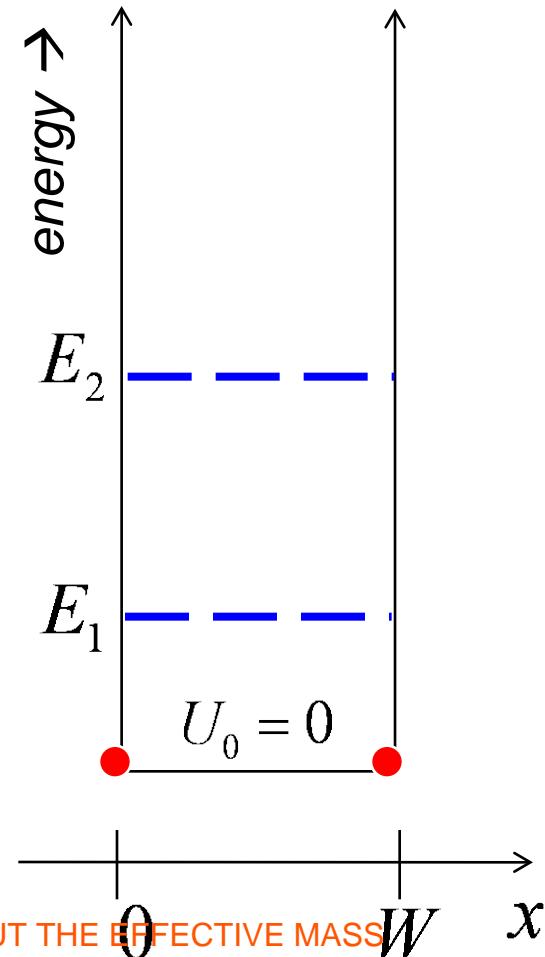
$$\psi(x) = A \sin k_j x \quad k_j = \frac{\pi}{W} j \quad j = 1, 2, 3, \dots$$

$$k^2 = \frac{2mE}{\hbar^2} \quad E_j = \frac{\hbar^2 k_j^2}{2m} = \frac{\hbar^2 j^2 \pi^2}{2m W^2}$$

- Confined electrons have quantized energies.
- Tighter confinement (smaller  $W$ ) leads to higher energies.
- Lighter masses lead to higher energies.

EFFECTIVE MASS OF Si IS LITTLE OVER 1 TIMES THE ELECTRON REST MASS, BUT THE EFFECTIVE MASS OF GERMANIUM IS MUCH, MUCH LIGHTER. SO WE EXPECT THE ENERGY LEVELS TO BE MUCH MUCH HIGHER IN GaAs.

Lundstrom: 2018



# Normalization of the wavefunction

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi = 0 \quad k^2 = \frac{2mE}{\hbar^2}$$

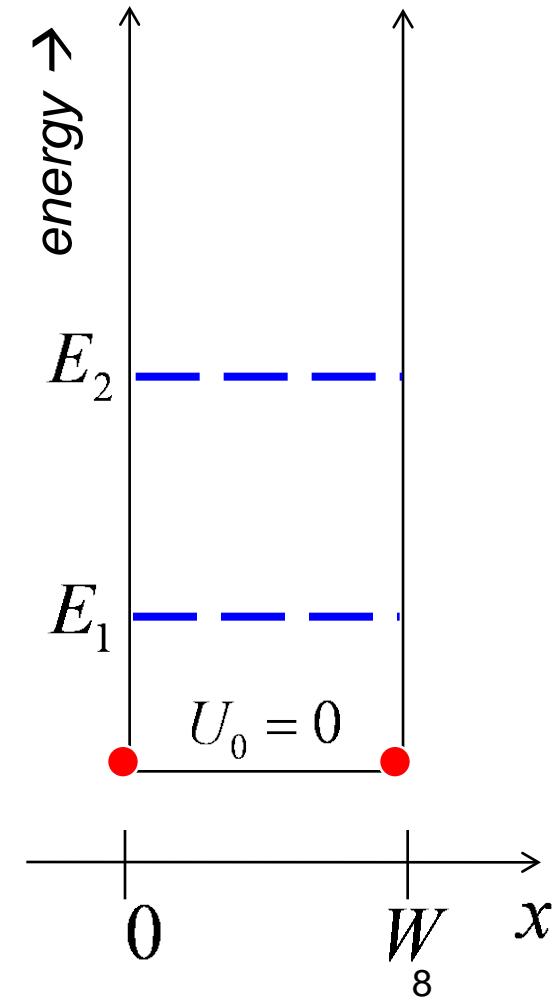
$$\psi(x) = A \sin k_j x \quad k_j = \frac{\pi}{W} j \quad j = 1, 2, 3, \dots$$

$$\int_0^W \psi^*(x)\psi(x)dx = 1$$

$$A^2 \int_0^W \sin^2(k_j x) dx = 1$$

$$A = \sqrt{2/W}$$

$$\psi(x) = \sqrt{\frac{2}{W}} \sin k_j x$$



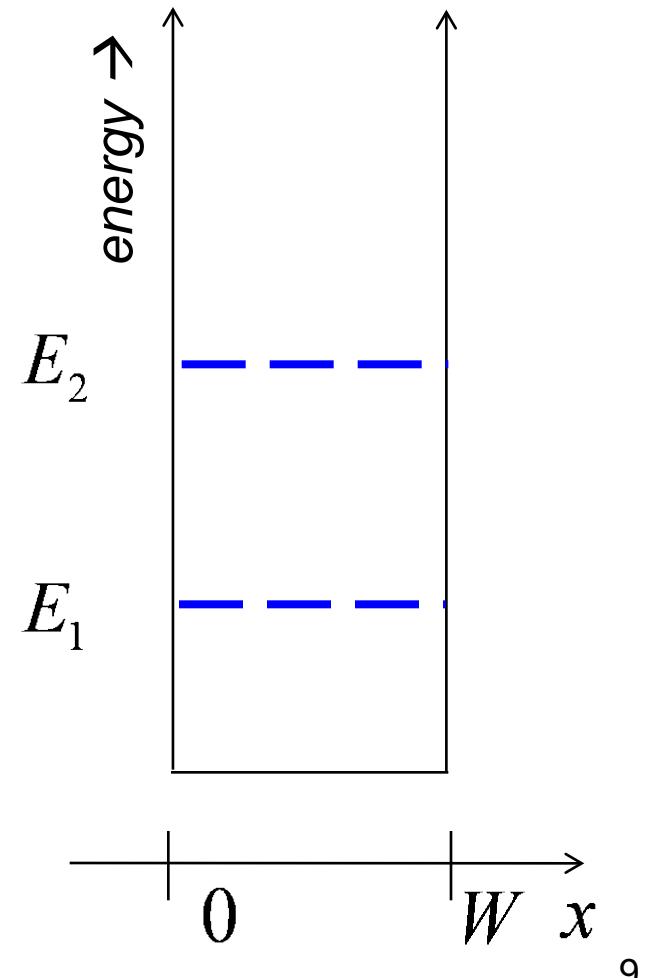
# Carrier densities in quantum wells

---

$$n(x) \propto \psi^*(x)\psi(x)$$

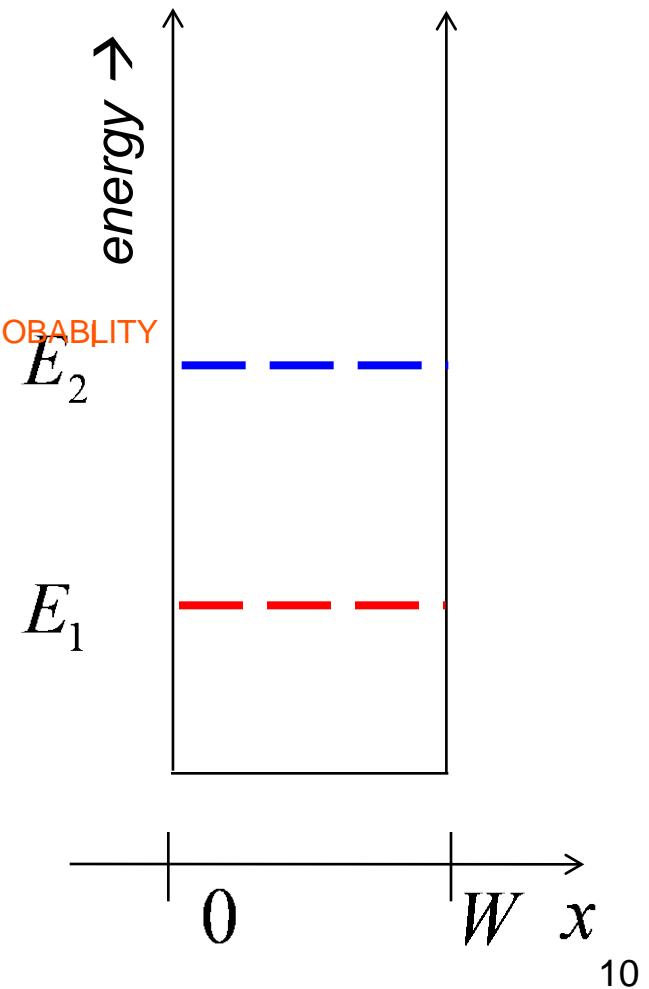
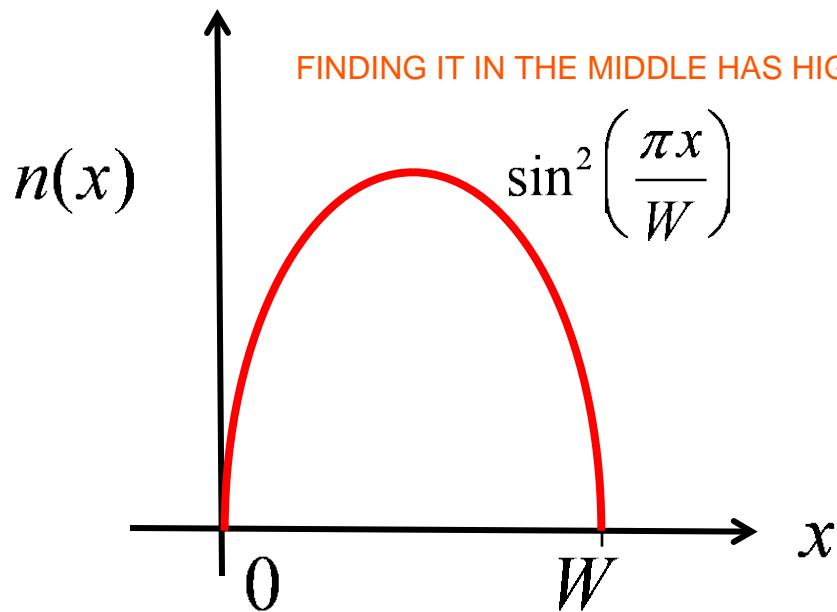
$$n(x) \propto \sin^2 k_j x$$

$$n(x) \propto \sin^2 \left( j \pi \frac{x}{W} \right)$$



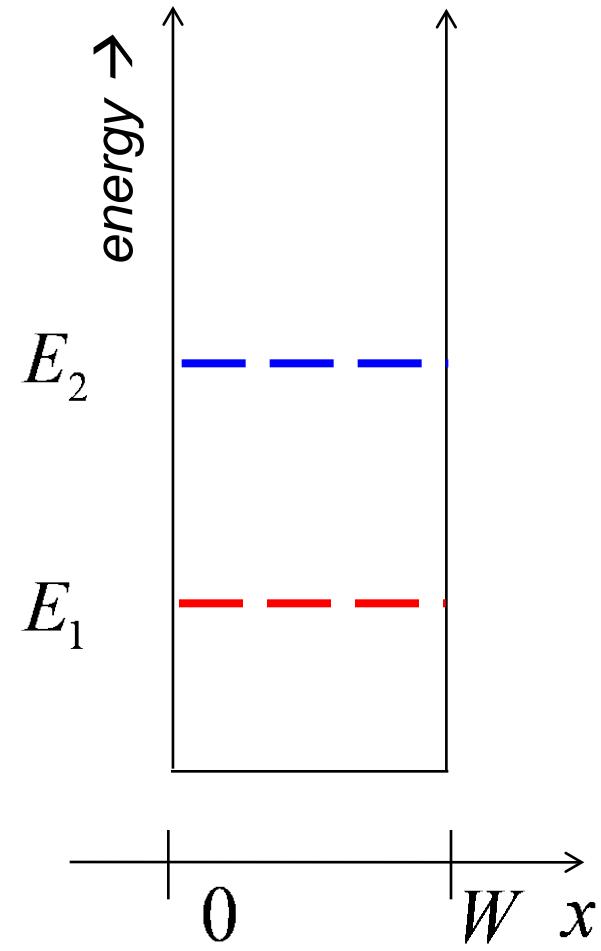
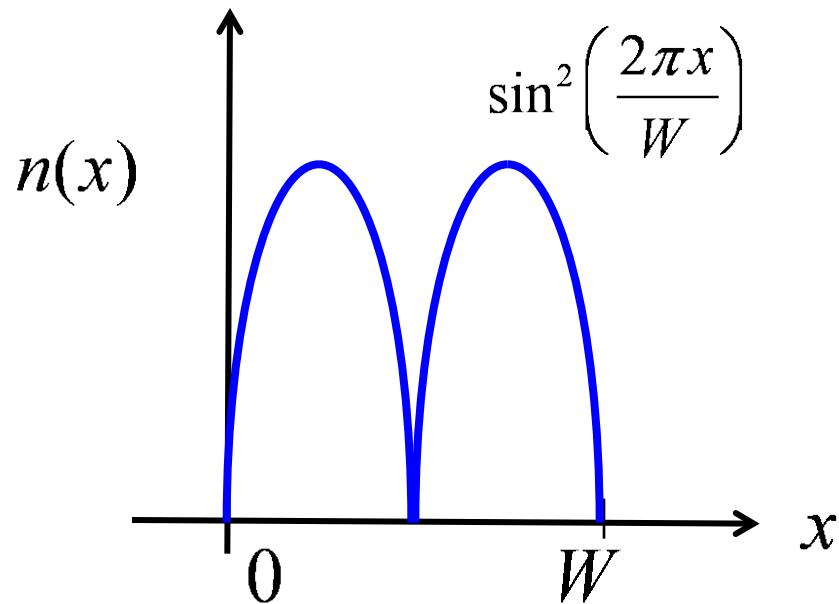
# Carrier density in subband 1

$$n(x) \propto \sin^2\left(j\pi \frac{x}{W}\right)$$



# Carrier density in subband 2

$$n(x) \propto \sin^2\left(j\pi \frac{x}{W}\right)$$



# Question

---

How narrow does the quantum well need to be in order to observe quantum effects?

**Answer:** When we confine electrons on the scale of their wavelength, we should expect quantum effects.

# de Broglie Wavelength

---

we need to form a 10 nm quantum well to see these effects.

What is the wavelength of a free (mobile) electron?

$$p = \hbar k = \hbar \frac{2\pi}{\lambda_B}$$

IF WE KNOW T AND m, we can solve

for p.  
 $E = \frac{p^2}{2m} \approx \frac{3}{2} k_B T$

$$\lambda_B = \sqrt{\frac{4\pi^2 \hbar^2}{3mk_B T}}$$

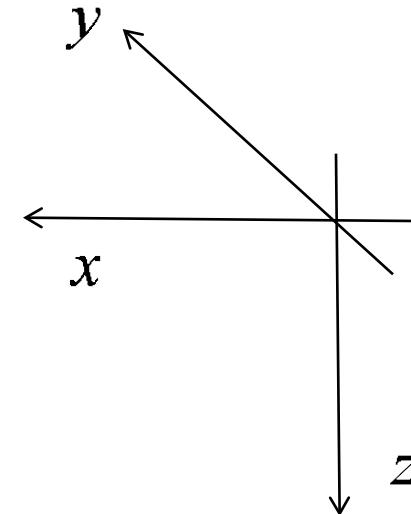
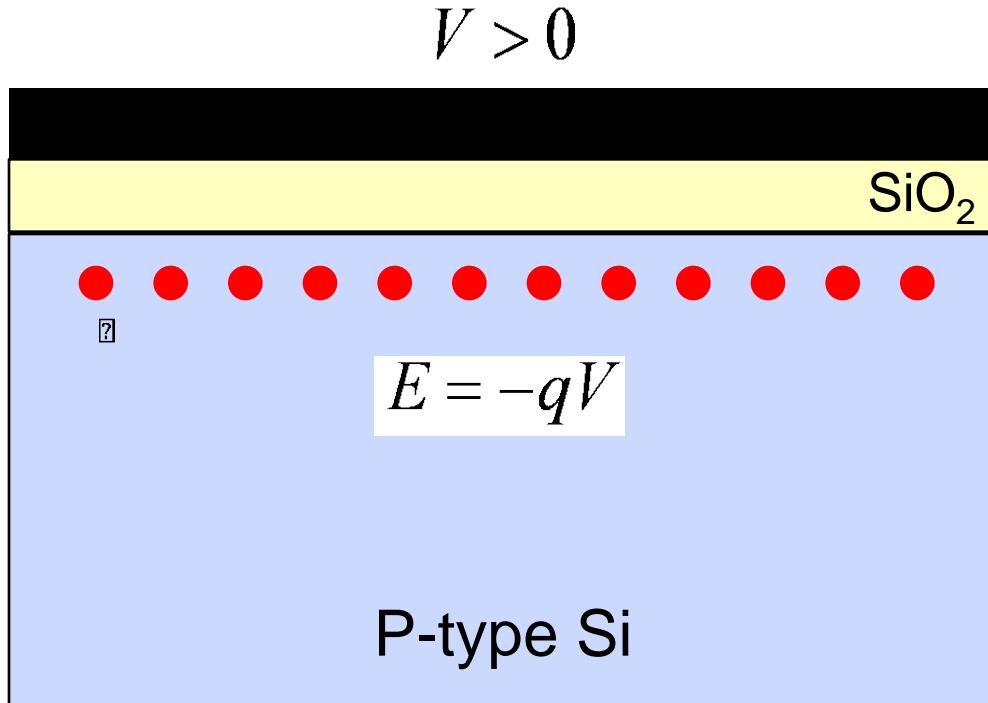
About 10 nm for electrons in silicon at room temperature

For lighter masses, confinement is felt in wider wells.

quantum well can be formed by electrostatic confinement.

## One way to produce a quantum well

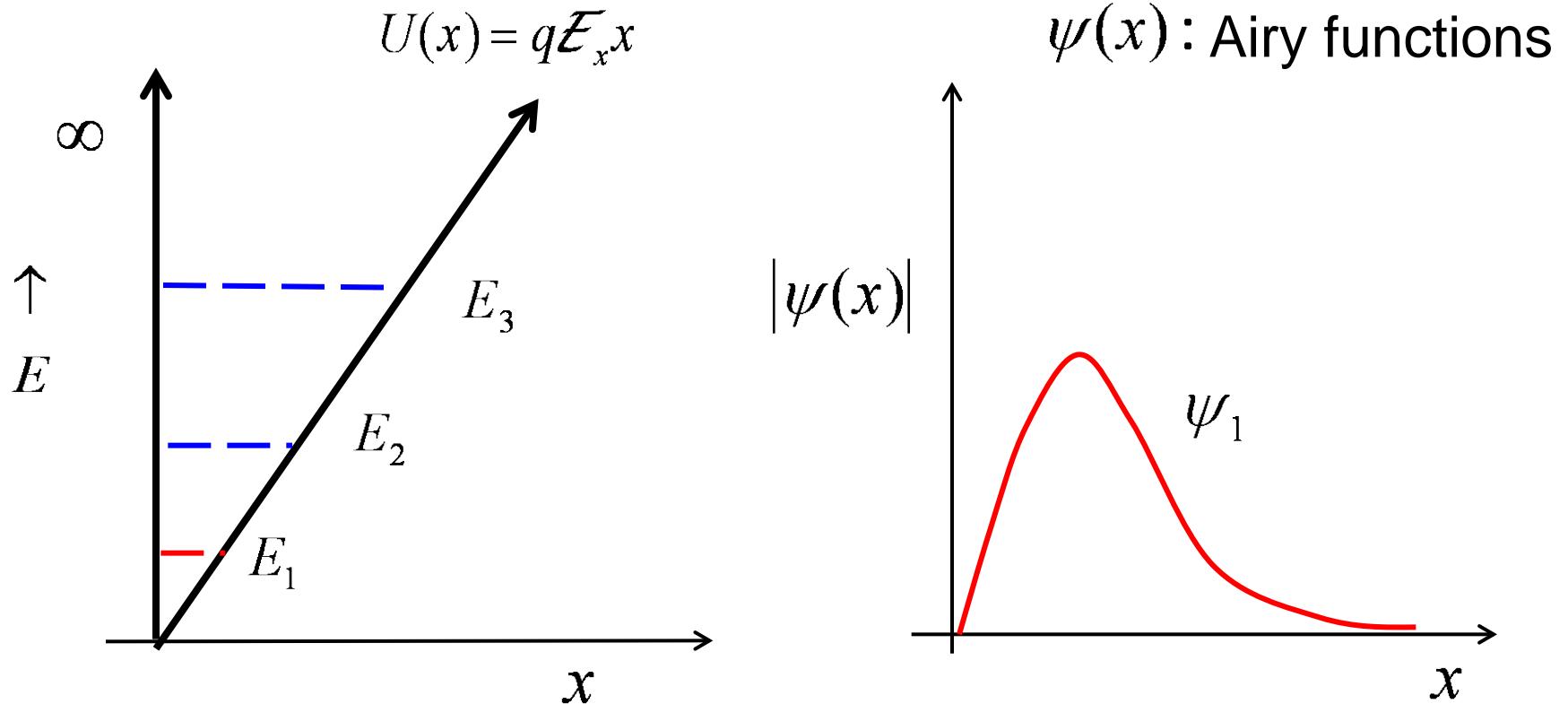
---



Electrons are confined in the  $z$ -direction,  
but free to move in the  $x$ - $y$  plane.

"electrostatic  
confinement"

# Triangular quantum well

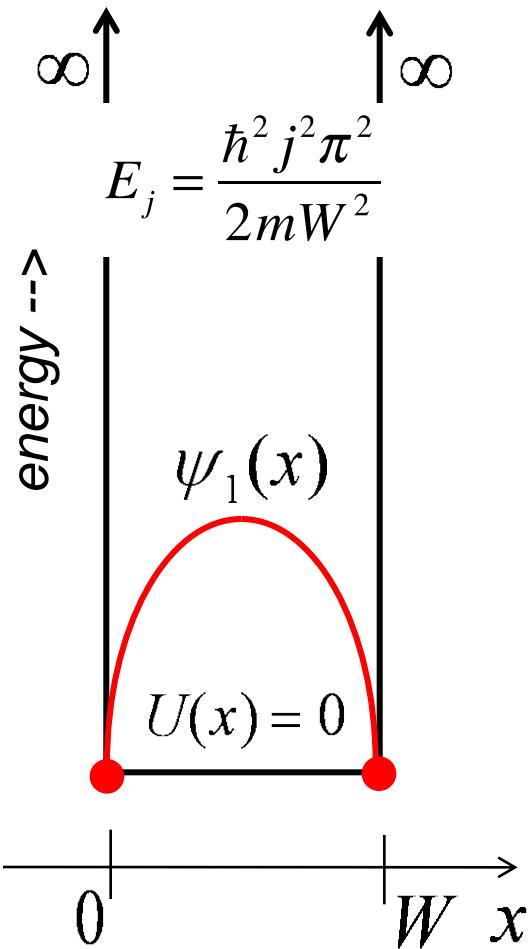


$$E_j = \left[ \frac{3hq\mathcal{E}_x}{4\sqrt{2m^*}} \left( j + 3/4 \right) \right]^{2/3} \quad j = 1, 2, 3, \dots$$

Lundstrom: 2018

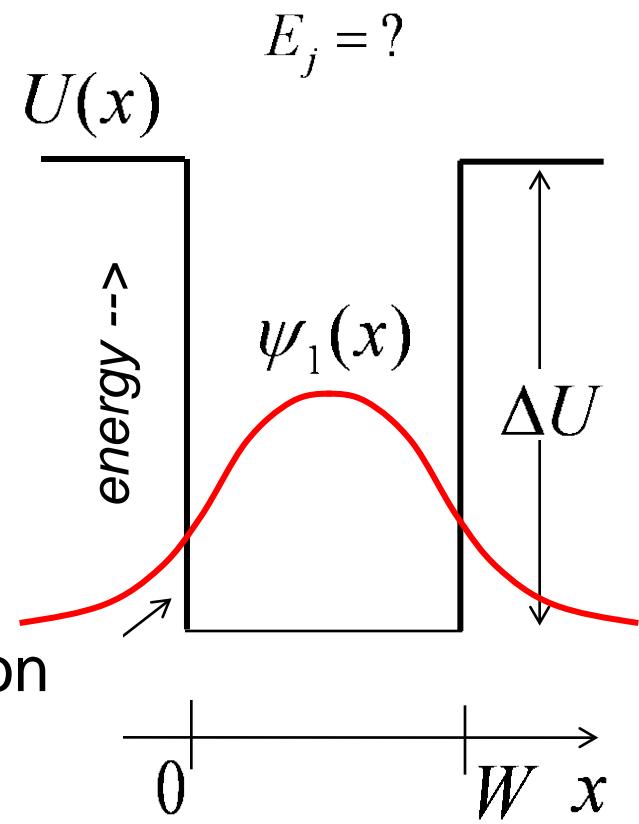
$$\langle x \rangle = \frac{2E_i}{3q\mathcal{E}}$$

# Infinite vs. finite quantum well

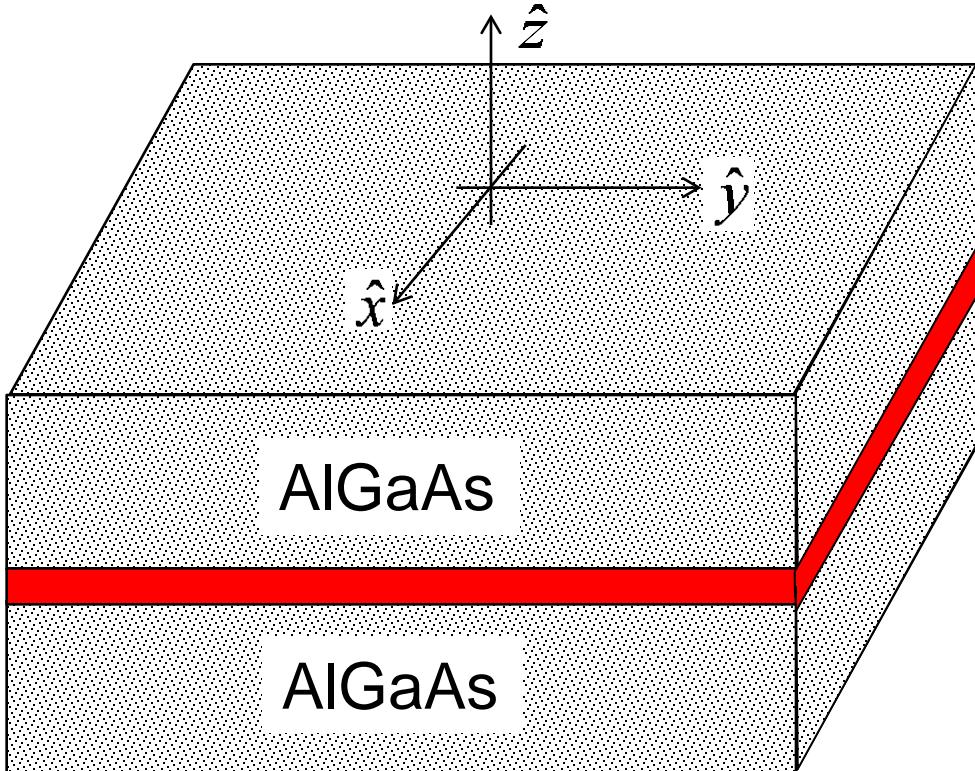


“wave function penetration”

they can leak out from the well in finite well.



# Quantum confinement with heterostructures



“GaAs quantum well”

epitaxy

GaAs

due to both AlGaAs a quantum well of around 10nm is formed in GaAs.

Electrons are confined in the z-direction, but free to move in the x-y plane.

$$\psi(x, y, z) = ?$$

# Wave function

---

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

extending to 3 dimensions

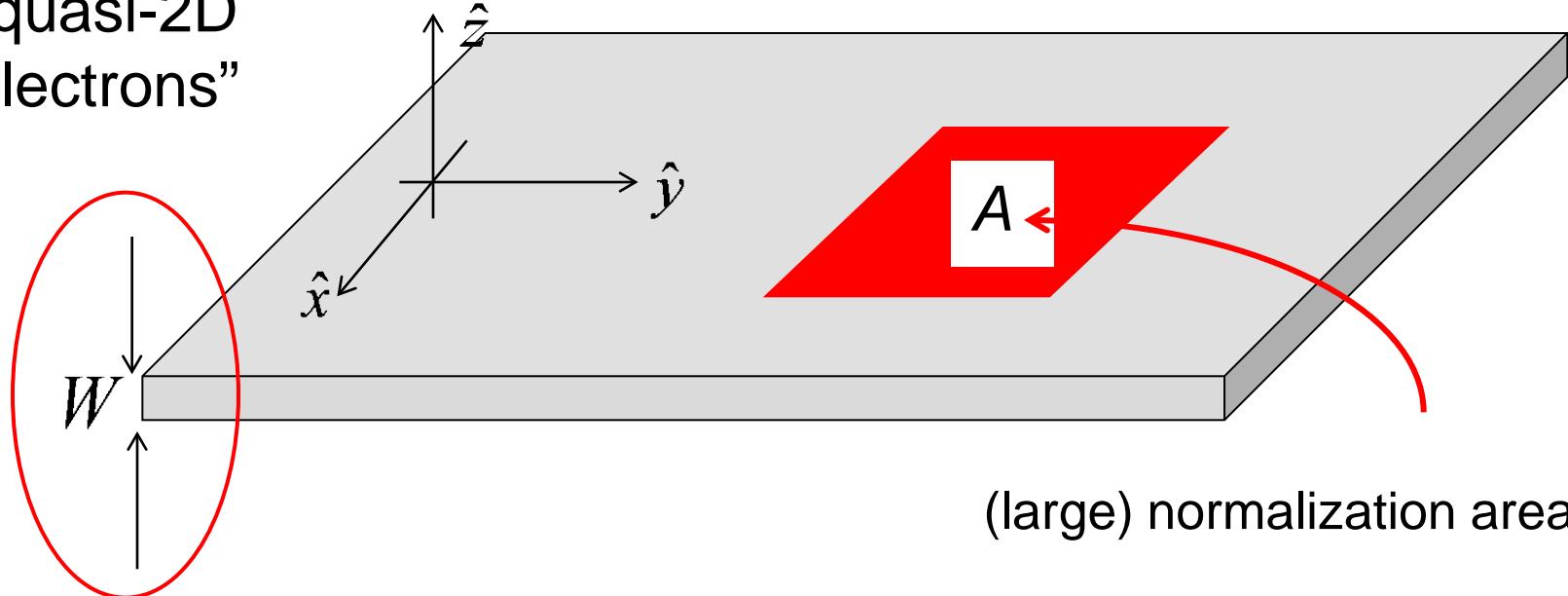
$$-\frac{\hbar^2}{2m} \nabla^2 \psi(x, y, z) + U(z)\psi(x, y, z) = E\psi(x, y, z)$$

$$\psi(x, y, z) = X(x)Y(y)Z(z)$$

$$\psi(x, y, z) \propto e^{\pm ik_x x} e^{\pm ik_y y} \phi(z) \quad \psi(x, y, z) \propto e^{\pm i \vec{k}_\parallel \bullet \vec{\rho}} \phi(z)$$

# 2D electrons

“quasi-2D  
electrons”



Semi-infinite in the x-y plane, but very thin in the z-direction.

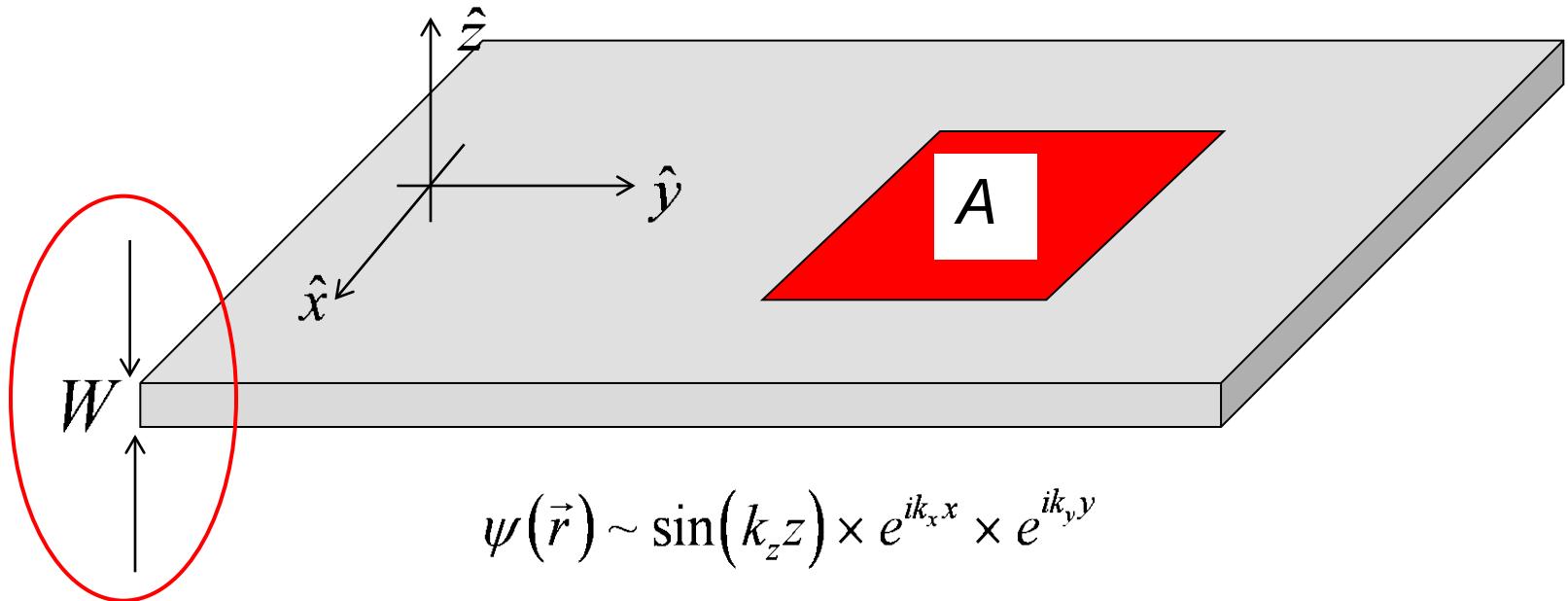
$$\psi(\vec{r}) \sim e^{i\vec{k} \cdot \vec{r}} \rightarrow \sin(k_z z) \times e^{ik_x x} \times e^{ik_y y}$$

$$\psi(\vec{r}) = \sqrt{2/W} \sin(k_z z) \times 1/\sqrt{A} e^{i(k_x x + k_y y)}$$

boundary conditions set the emergence of discrete energy levels.

## 2D electrons: subbands

---

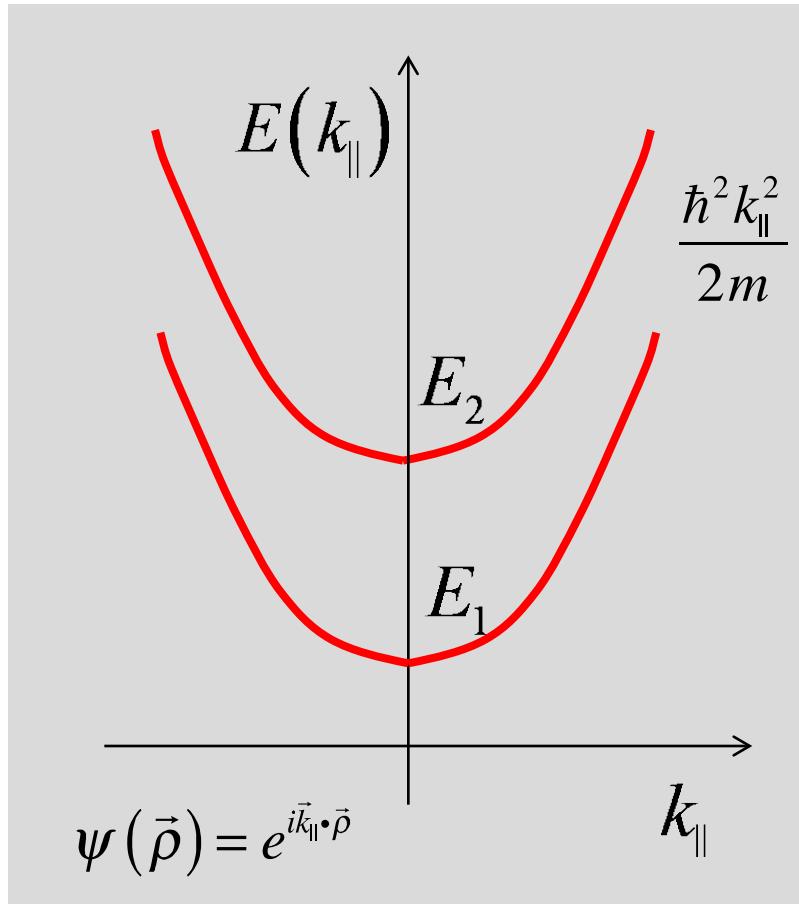


$$k_z = j \frac{\pi}{W} \quad E_j = \frac{\hbar^2 j^2 \pi^2}{2mW^2} \quad E = E_j + \frac{\hbar^2 k_{\parallel}^2}{2m}$$

$j$  is the subband index

# Subbands

additional energy



$$E_j = \frac{\hbar^2 j^2 \pi^2}{2mW^2}$$

$$k_{\parallel} = \sqrt{k_x^2 + k_y^2}$$

$$E = E_j + \frac{\hbar^2 k_{\parallel}^2}{2m}$$

# Summary

---

When electrons are confined, their energy is quantized and their wave functions change.

Quantum confinement can be produced in 3D materials with electric fields or by epitaxial growth.

Quantum confinement leads to “subbands”.

Specifics depend on the shape of the quantum well but the general features can be understood by analogy with the particle in a box solution.

# Primer on Semiconductors

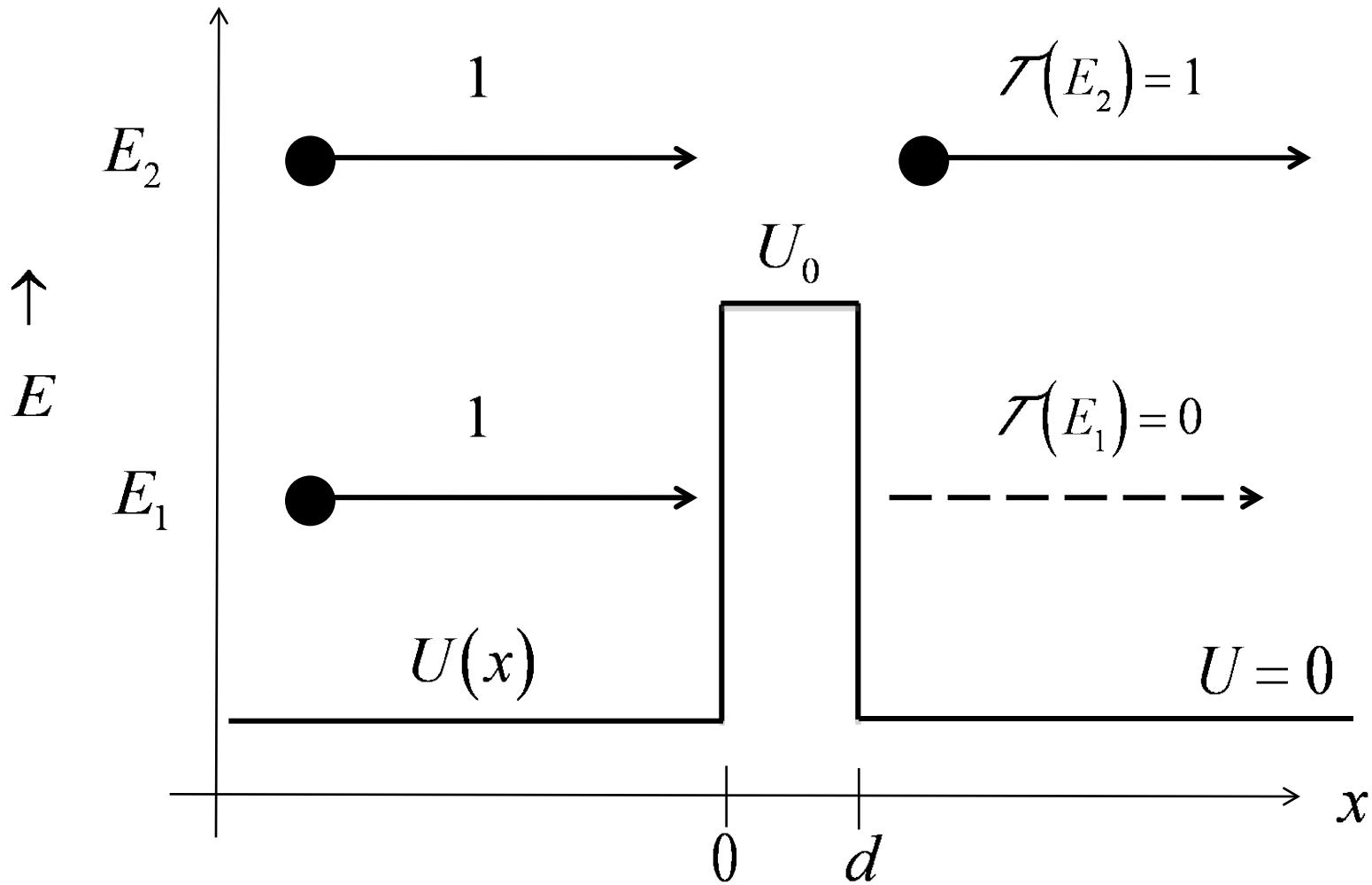
## Unit 2: Quantum Mechanics

### Lecture 2.3: Quantum tunneling and reflection

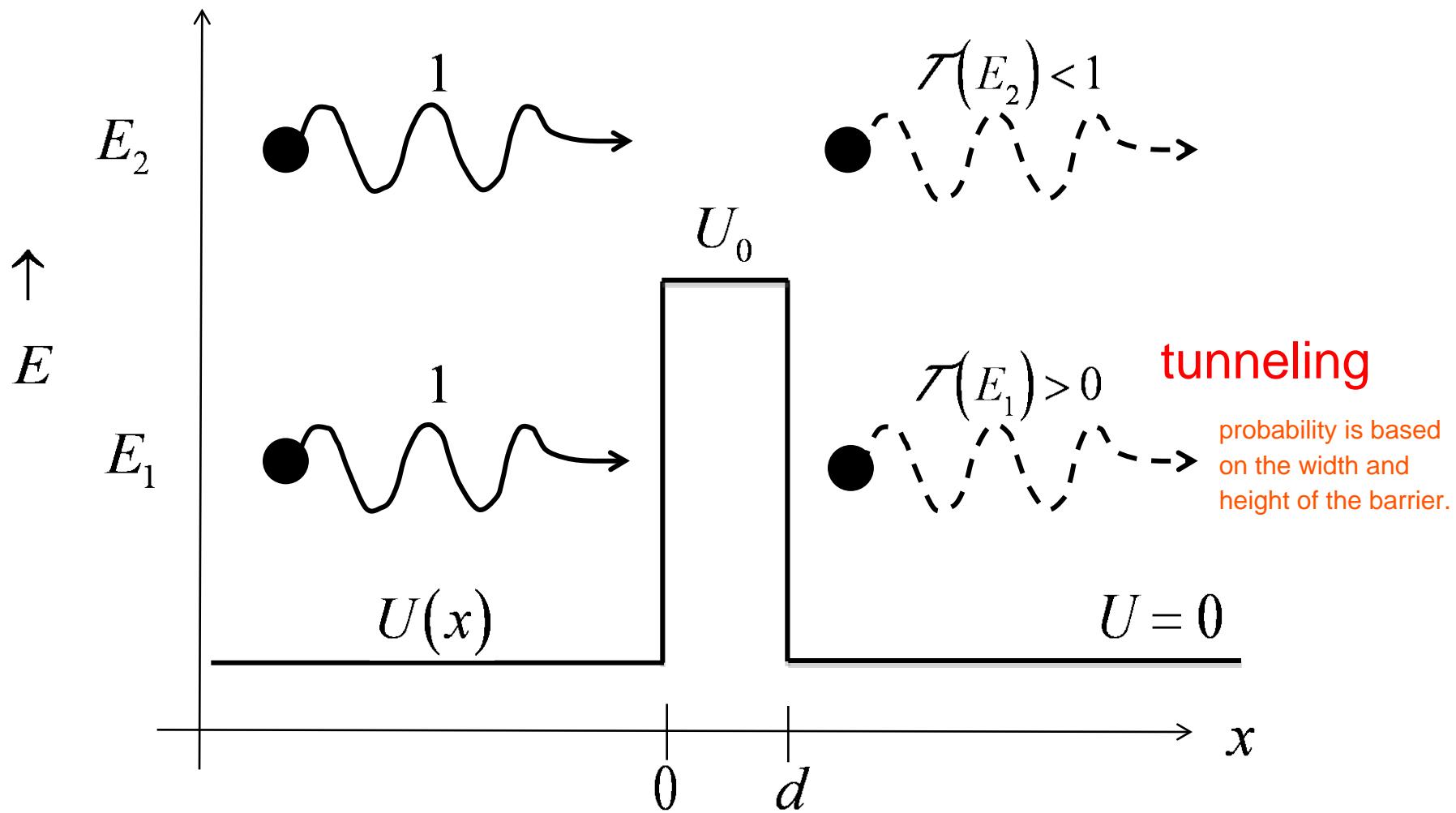
**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Classical vs. Quantum



# Classical vs. Quantum



# Solutions to the wave equation

---

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E - U_0] \psi(x) = 0$$

$$E > U_0 \quad k^2 = \frac{2m}{\hbar^2} [E - U_0]$$
$$\frac{d^2\psi(x)}{dx^2} + k^2 \psi(x) = 0$$
$$\psi(x) = A e^{+ikx} + B e^{-ikx}$$

# Solutions to the wave equation

---

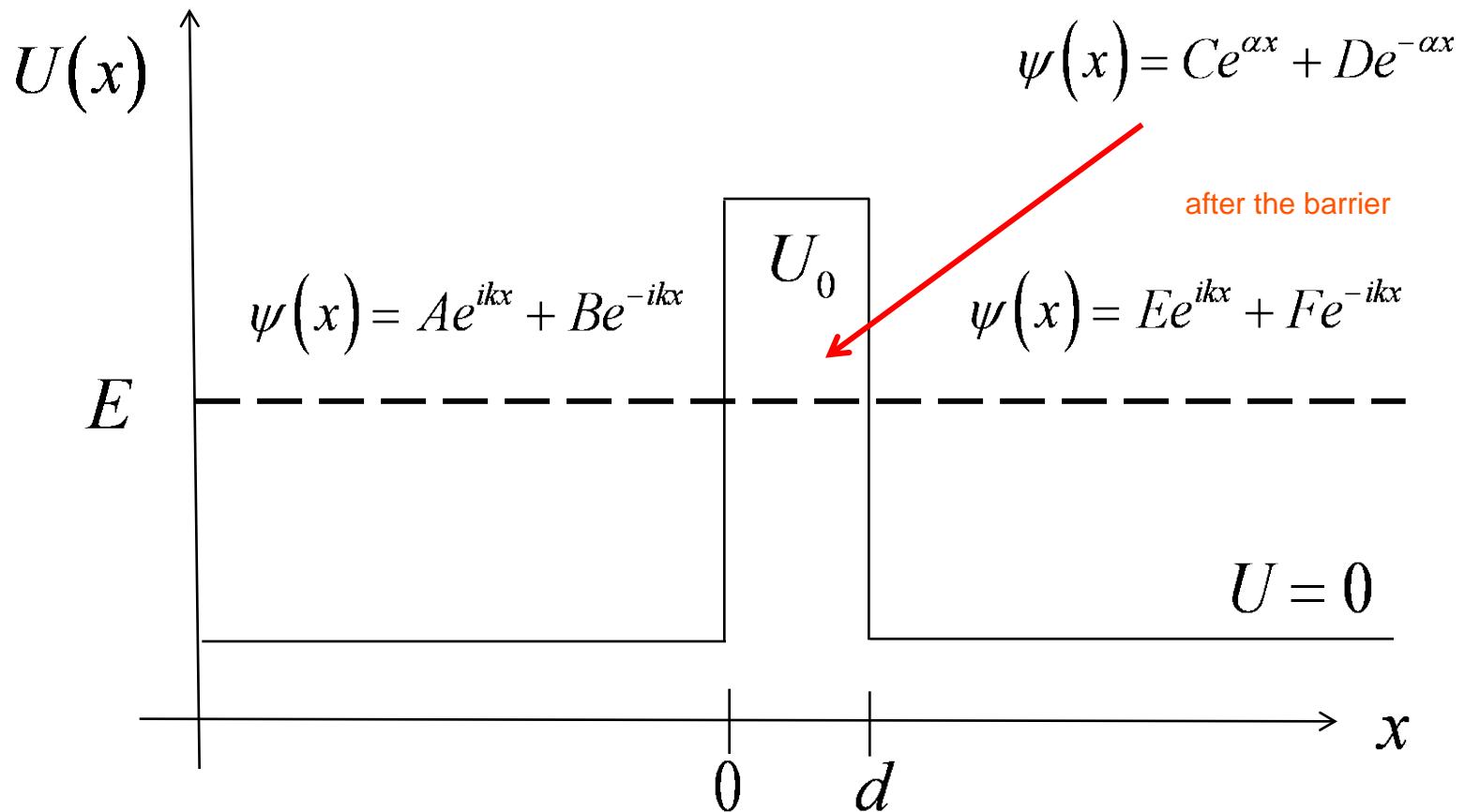
$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E - U_0] \psi(x) = 0$$

$$\alpha^2 = \frac{2m}{\hbar^2} [U_0 - E] \quad \frac{d^2\psi(x)}{dx^2} - \alpha^2 \psi(x) = 0$$

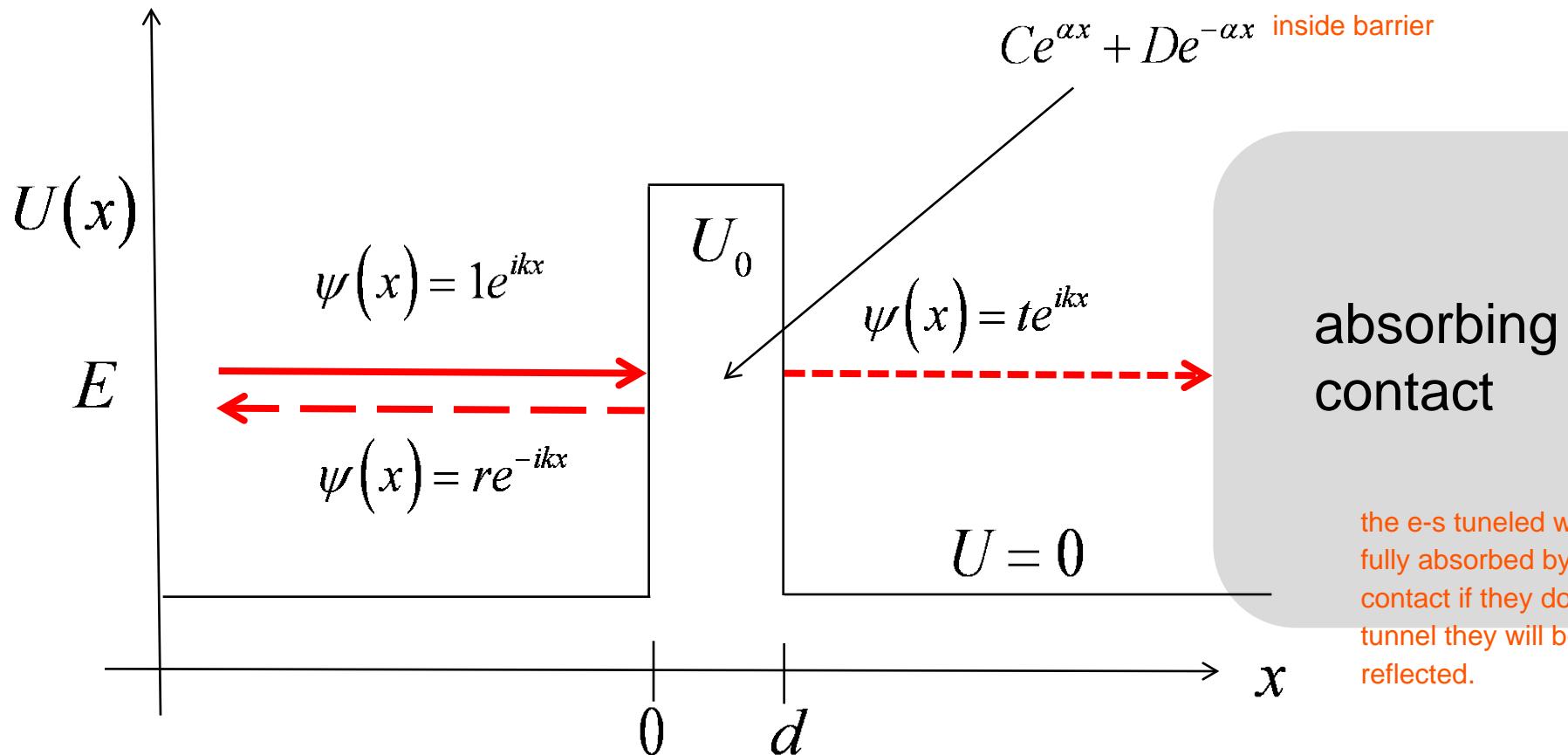
$$E < U_0$$

$$\psi(x) = Ce^{\alpha x} + De^{-\alpha x}$$

# Tunneling ( $E < U_0$ )

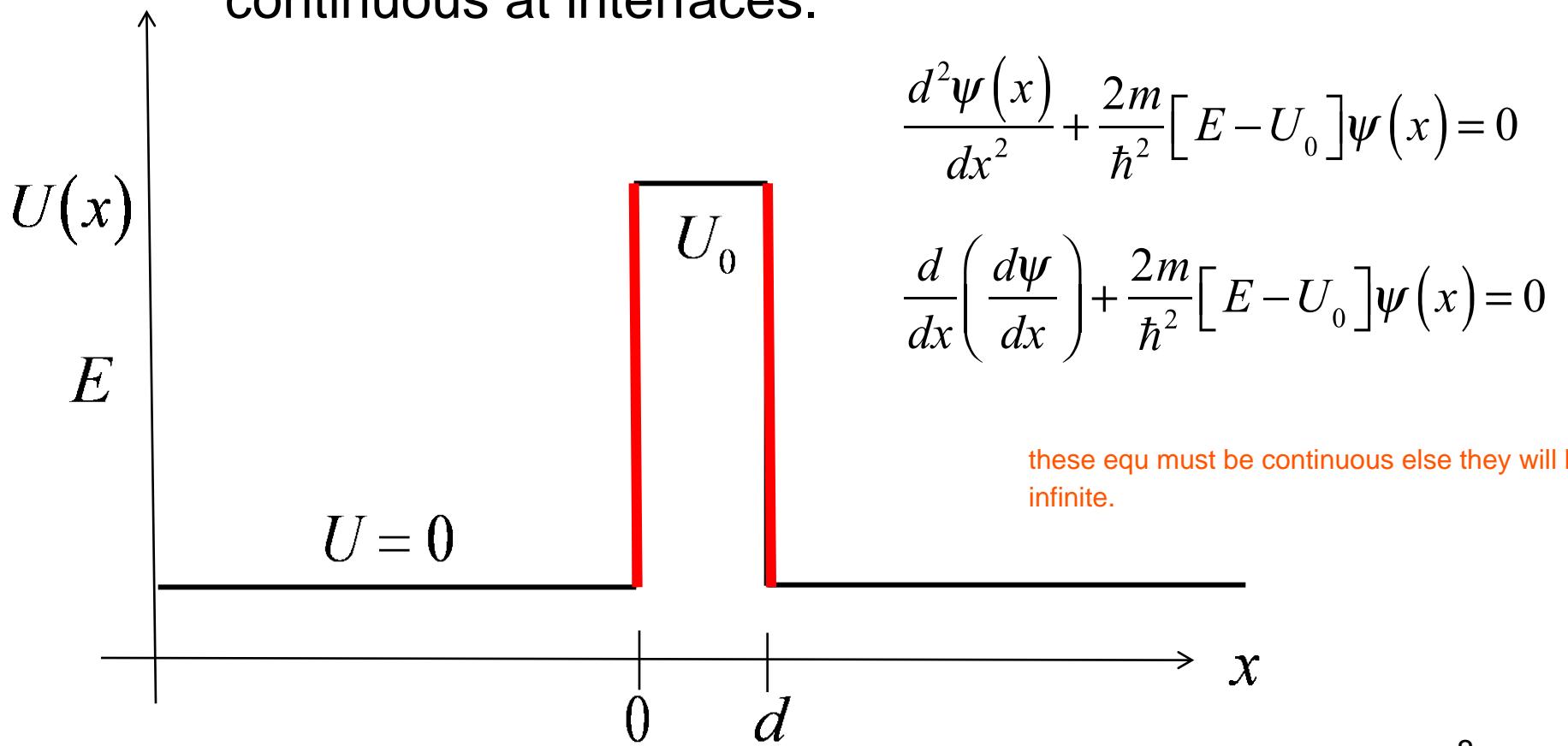


# Tunneling

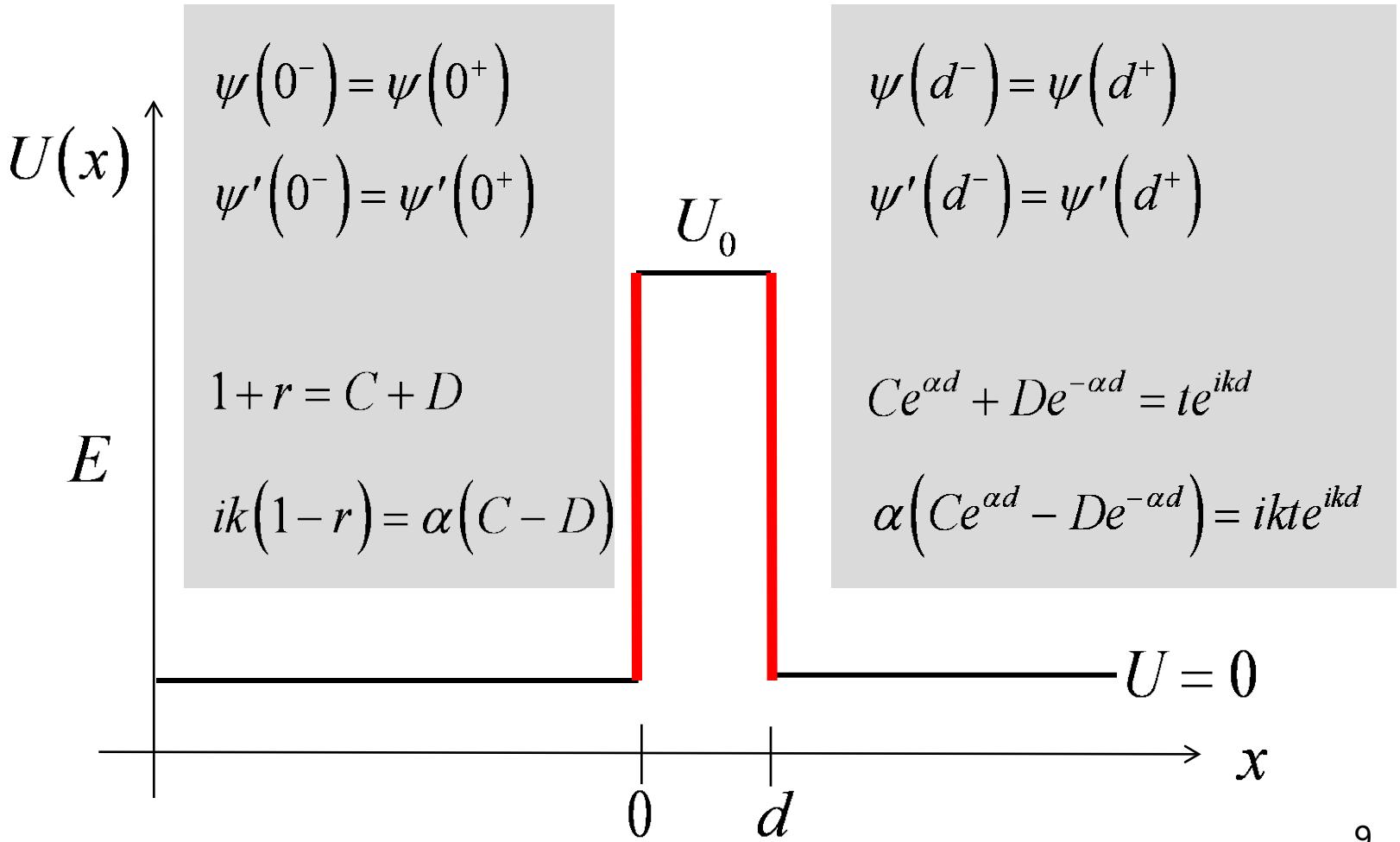


# Boundary conditions

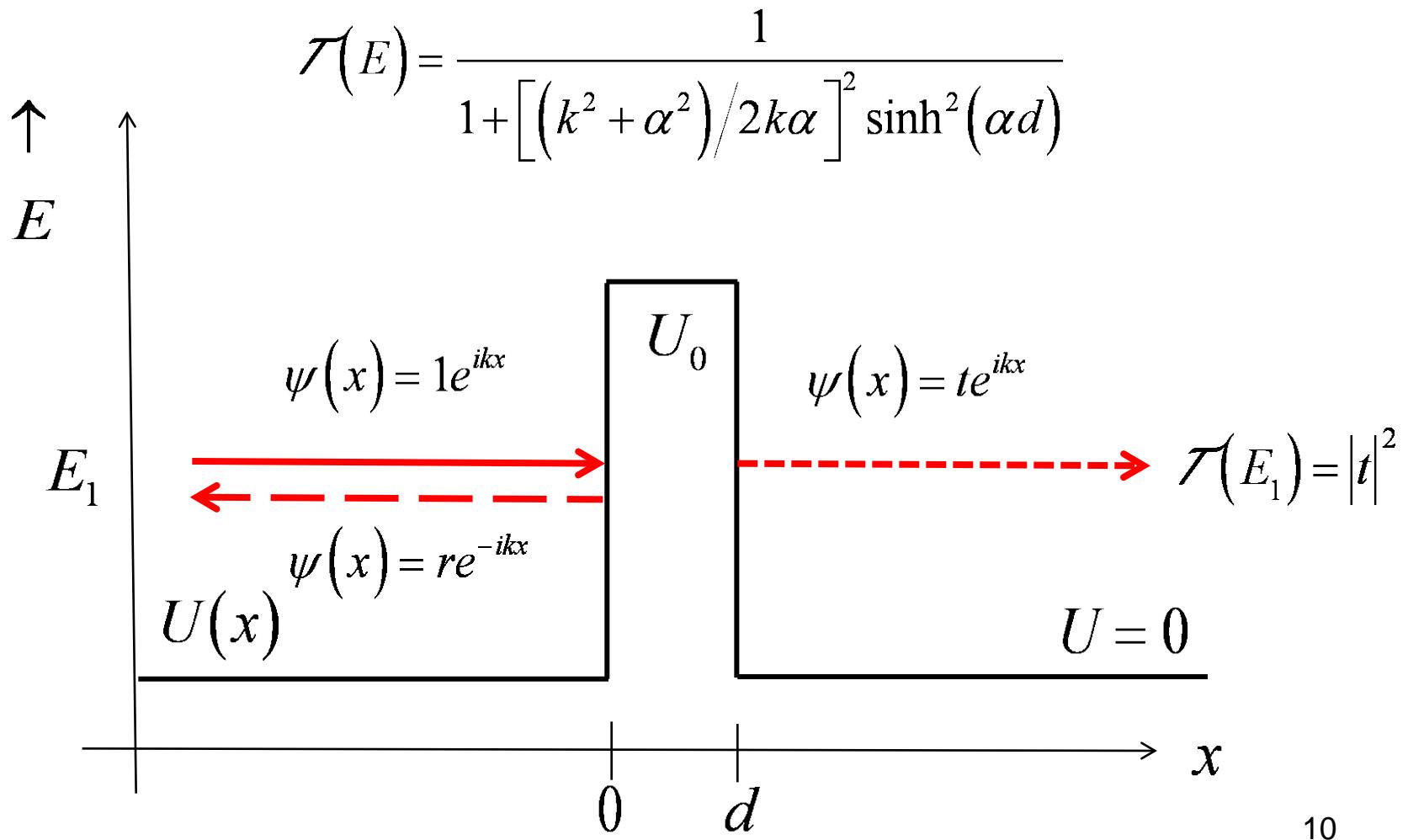
The wave function and its derivative must be continuous at interfaces.



# Boundary conditions



# Tunneling transmission



# Examine solution

---

$$\mathcal{T}(E) = \frac{1}{1 + \left[ (k^2 + \alpha^2)/2k\alpha \right]^2 \sinh^2(\alpha d)}$$

$$\sinh(\alpha d) = \frac{e^{\alpha d} - e^{-\alpha d}}{2} \approx \frac{e^{\alpha d}}{2} \quad \text{barrier is little bit thick}$$

$$\alpha^2 = \frac{2m}{\hbar^2} [U_0 - E]$$

$$\sinh^2(\alpha d) \approx \frac{e^{2\alpha d}}{4} \gg 1 \quad \text{alpha * d is large enough}$$

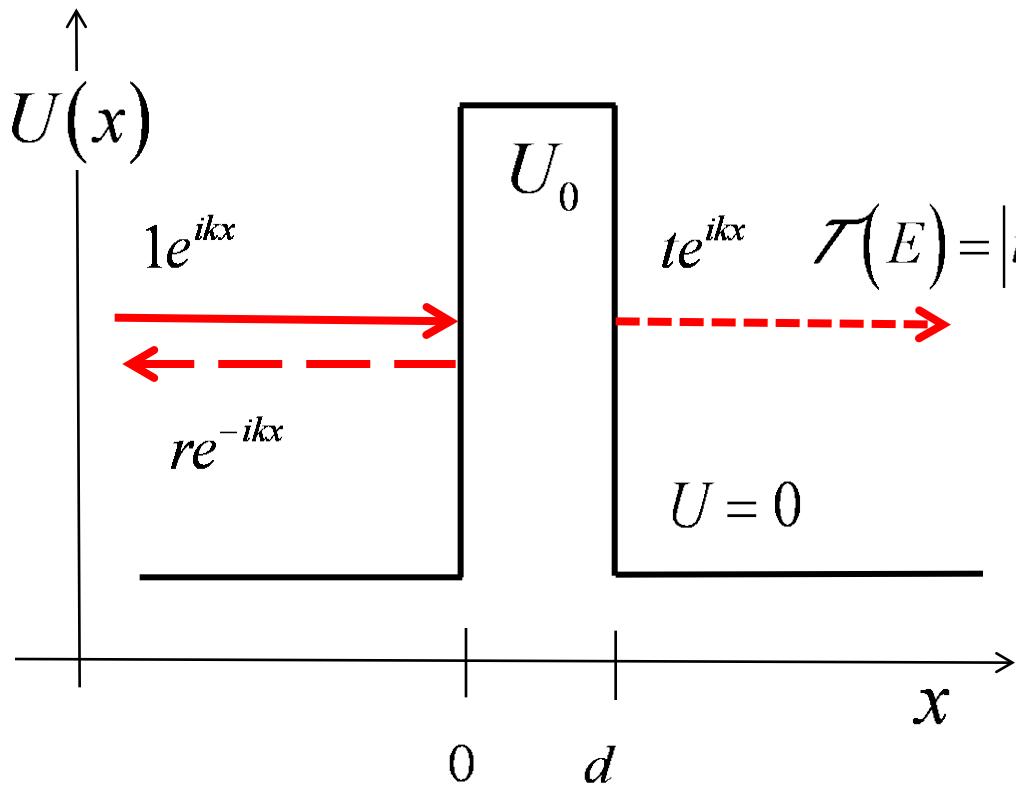
$$k^2 = \frac{2m}{\hbar^2} [E]$$

$$\mathcal{T}(E) \approx \left( \frac{16k\alpha}{k^2 + \alpha^2} \right)^2 e^{-2\alpha d}$$

$$\mathcal{T}(E) \propto \exp \left[ -2d \sqrt{2m^*(U_0 - E)/\hbar^2} \right]$$

# Tunneling: conclusions

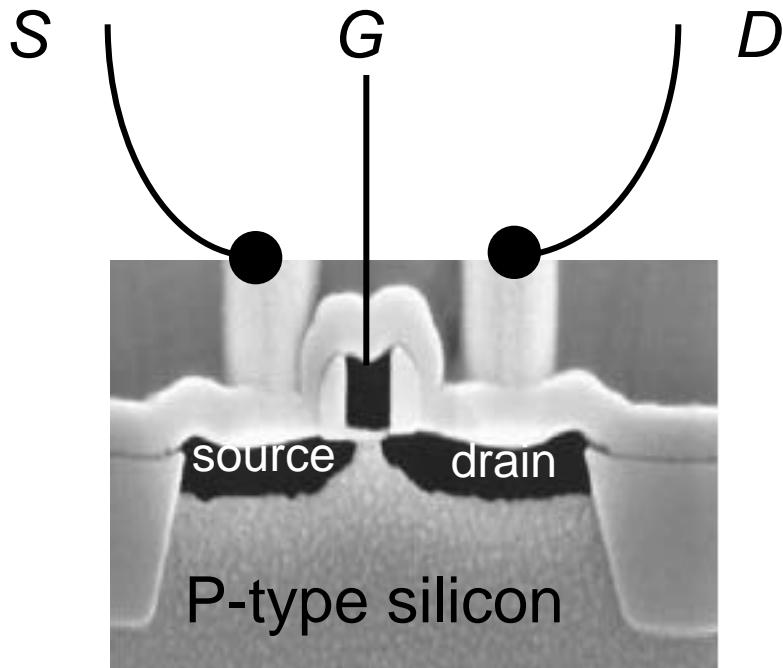
$$\mathcal{T}(E) \approx \exp\left(-2d\sqrt{2m(U_0 - E)/\hbar^2}\right)$$



- 1) Tunneling decreases exponentially with increasing barrier thickness.
- 2) Tunneling decreases exponentially with increasing barrier height.
- 3) Tunneling decreases exponentially with increasing mass.

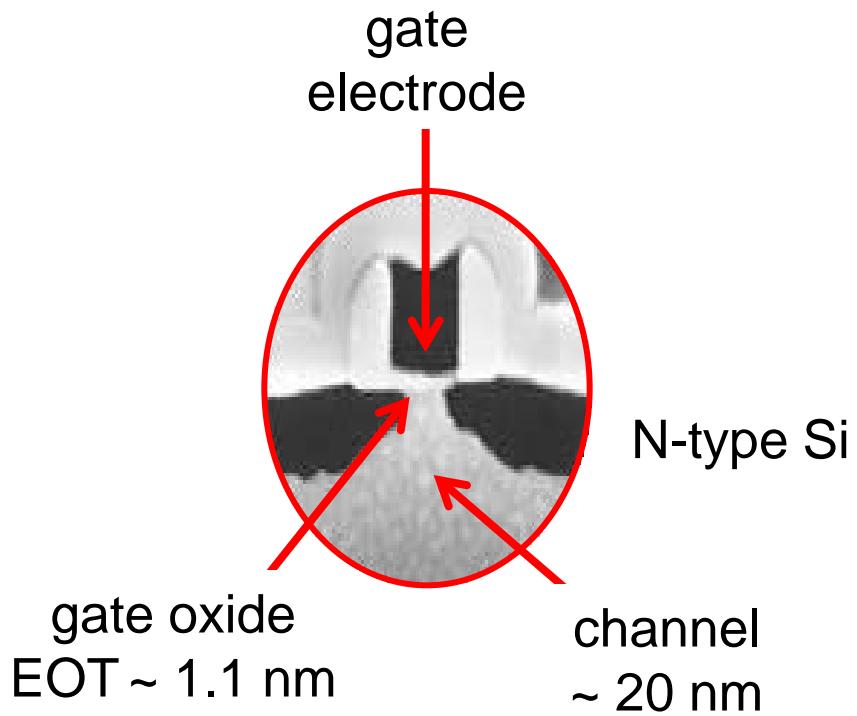
because light effective mass - we can expect more tunneling.

# Tunneling in CMOS technology



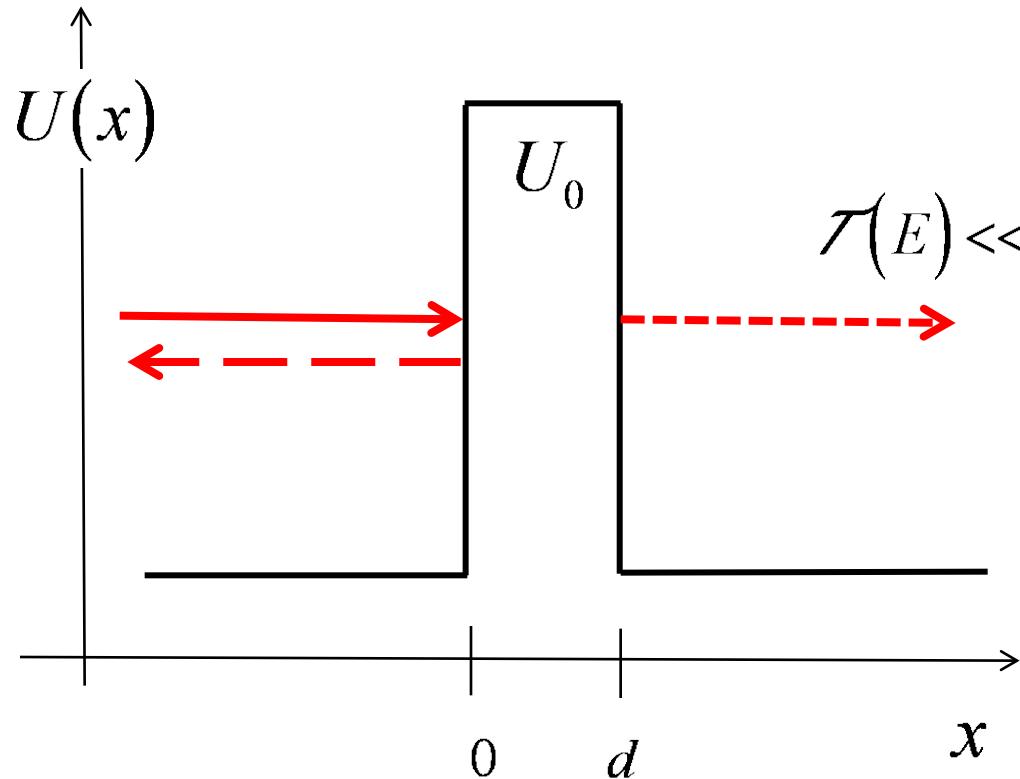
(Source: Texas Instruments, ~ 2000)

decrease in the gate oxide thickness (1nm) will increase tunneling and gate leakage current.. unaccepted function of nano devices.



# Resonant tunneling

---

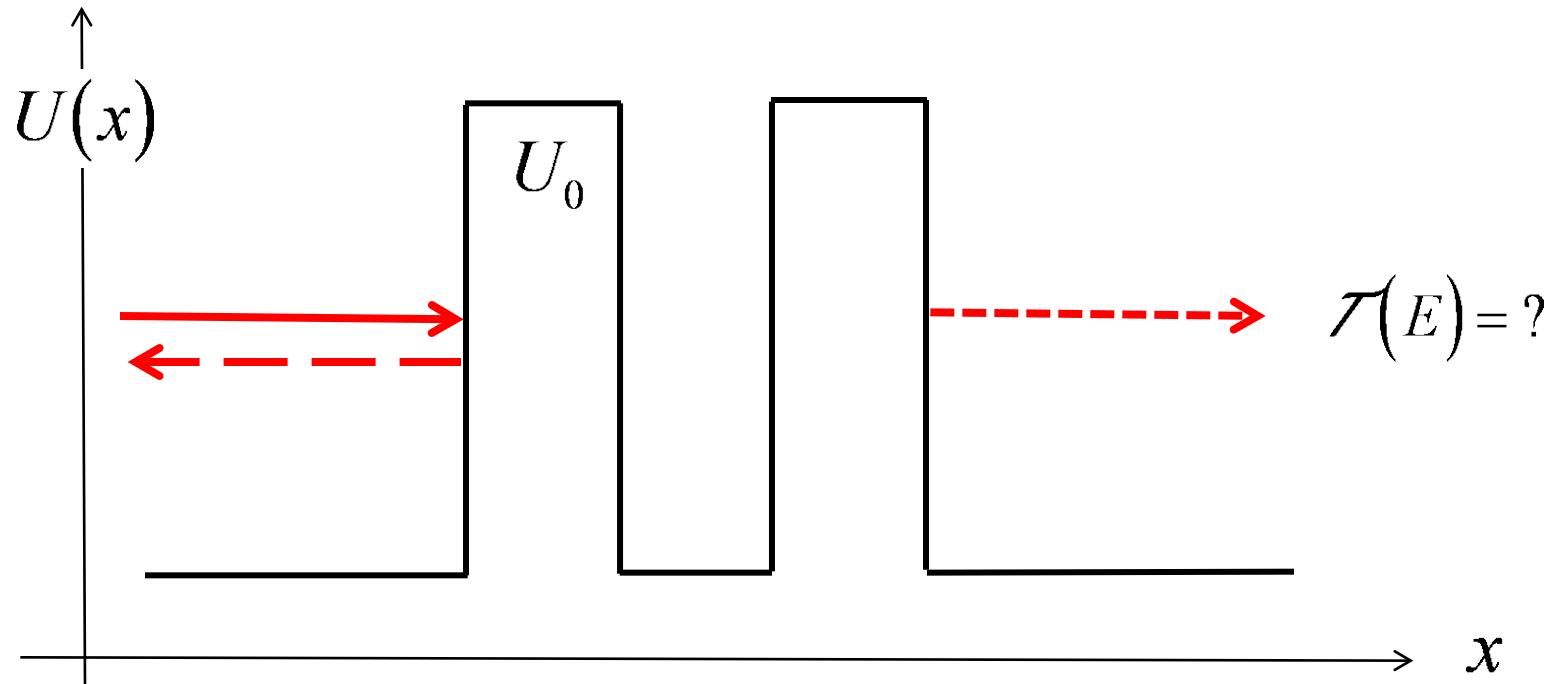


$$\tau(E) \ll 1$$

What happens if we put  
two barriers in series?

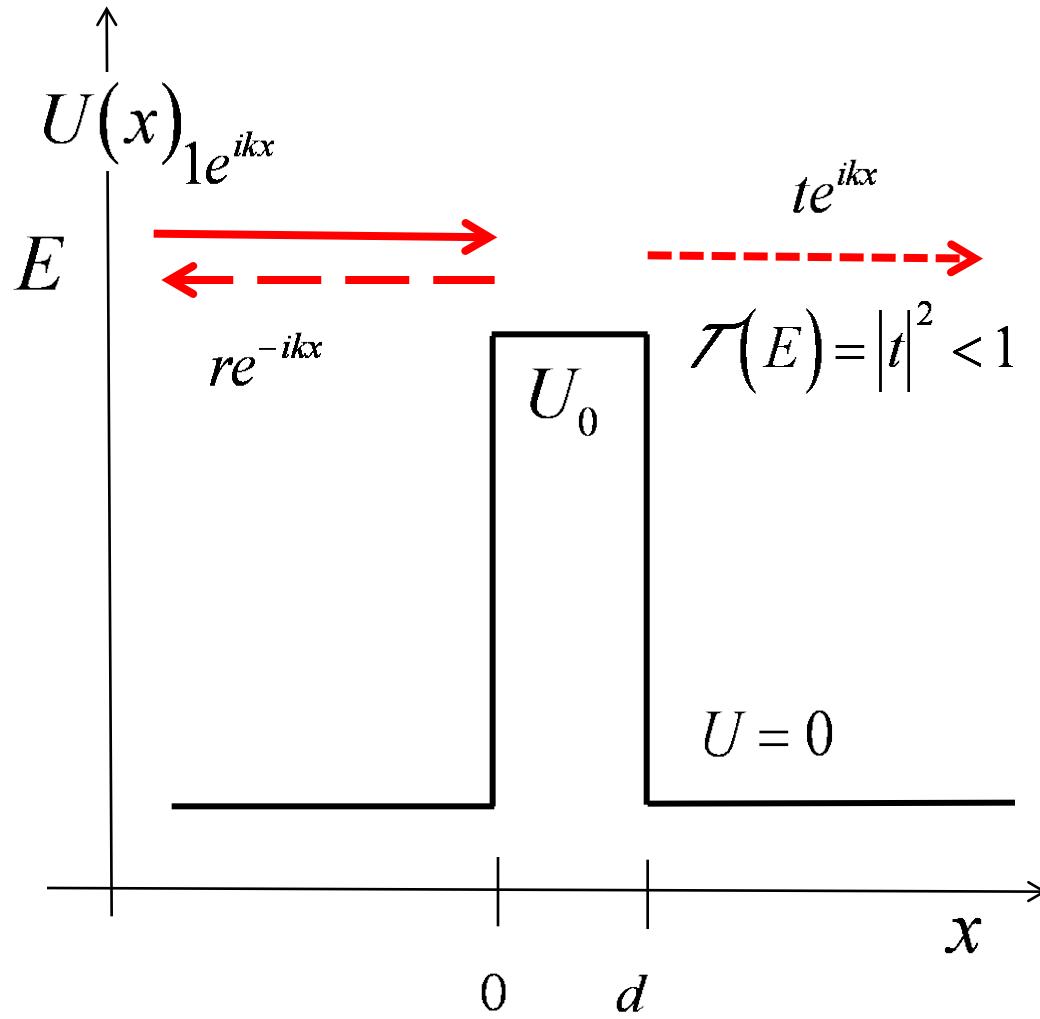
# Resonant tunneling

the probability of tunneling two will be less than 1



Surprisingly, the transmission can be **unity** at a specific energy, the **resonant energy**, at which all of the multiple reflections add up in phase.

# Quantum reflections



**The potential must change slowly** (on the scale of the electron's wavelength) to treat the electron as a classical particle.

# Summary

---

- 1) Classical particles can't get over a barrier unless they have enough energy, but quantum particles can tunnel through.
- 2) Tunneling decreases exponentially with increasing barrier thickness.
- 3) Tunneling decreases exponentially with increasing barrier height.
- 4) Tunneling decreases exponentially with increasing mass.
- 5) Particles with enough energy to get over the barrier can reflect, if the potential changes rapidly.

# Primer on Semiconductors

## Unit 2: Quantum Mechanics

### Lecture 2.4: Electron waves in crystals

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Wave equation in a constant potential

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E - U_0] \psi(x) = 0$$

$$E > U_0 \quad k^2 = \frac{2m_0}{\hbar^2} [E - U_0] \quad \frac{d^2\psi(x)}{dx^2} + k^2 \psi(x) = 0$$

Solution:  $\psi(x) = A e^{\pm ikx}$

This is a wave solution

$$\Psi(x, t) = \psi(x) \phi(t) \quad E(k) = U_0 + \frac{\hbar^2 k^2}{2m}$$

$$\Psi(x, t) = A e^{\pm i(kx - \omega t)} \quad p = \hbar k \quad v_g = \hbar k / m$$

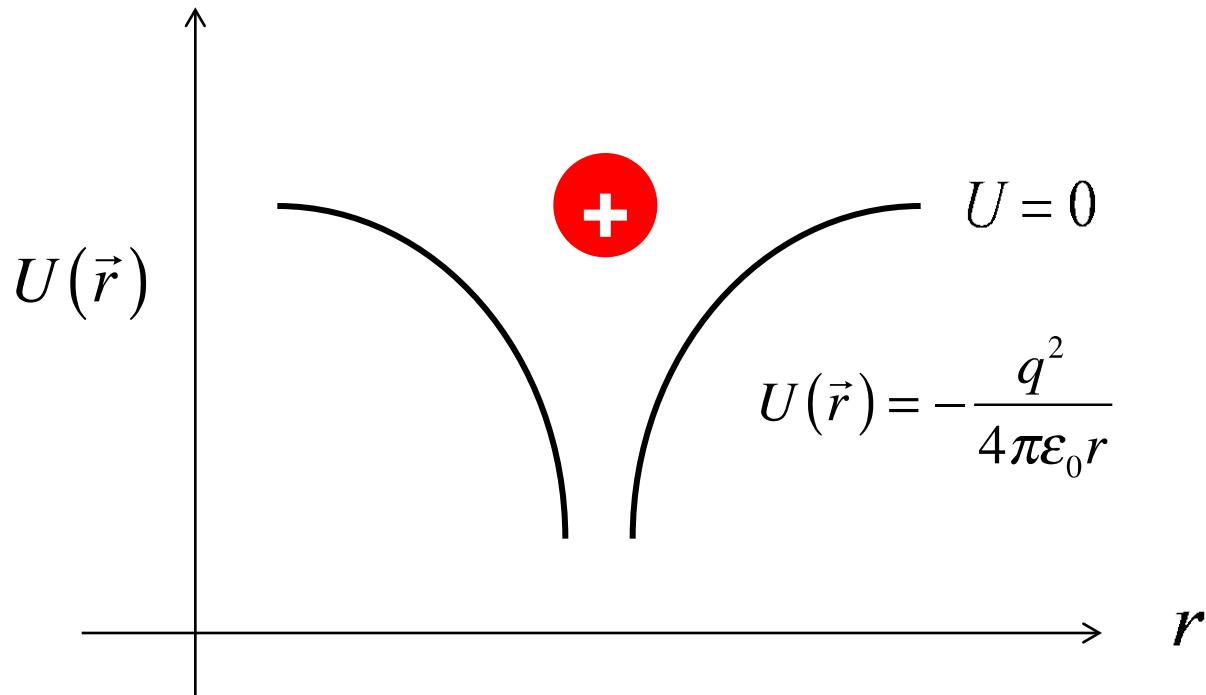
# Electrons in atoms

---

Hydrogen atom:

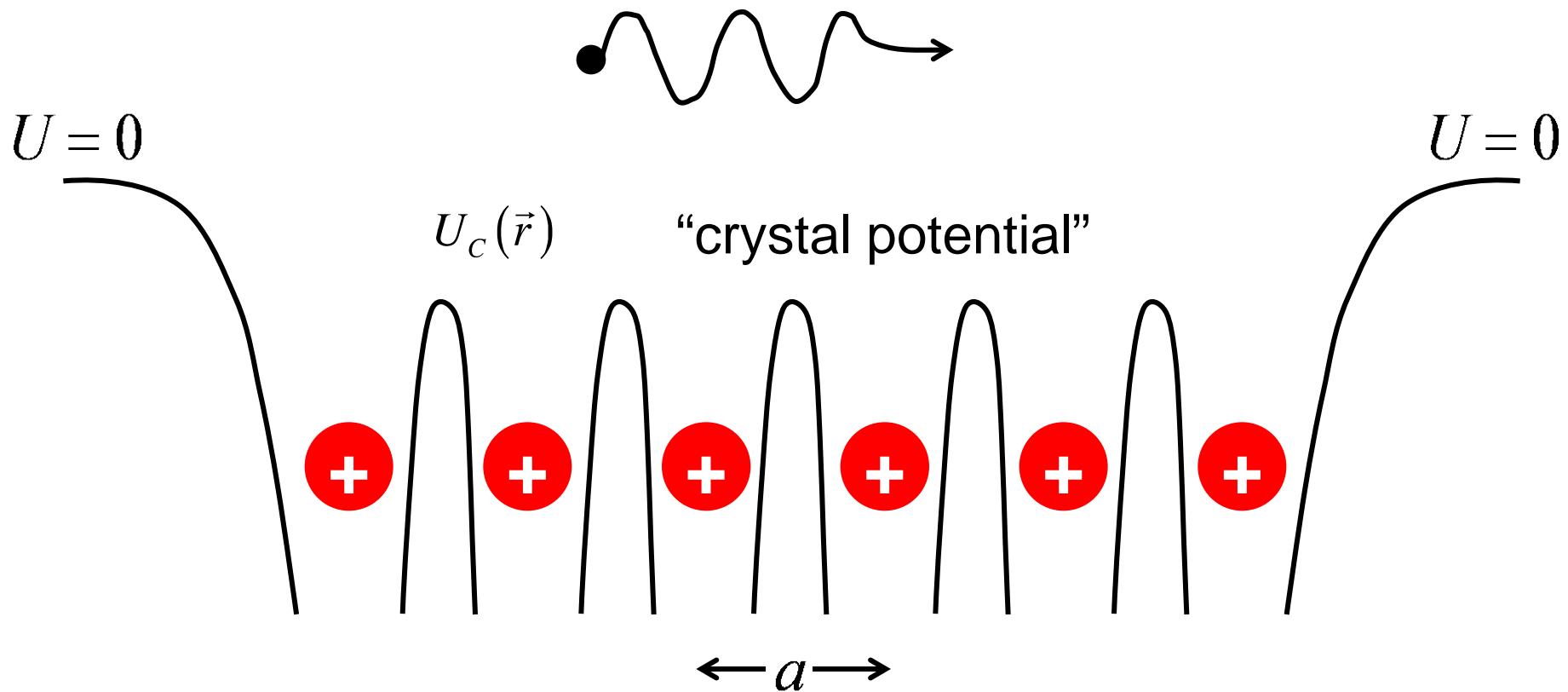
$$-\frac{\hbar^2}{2m_0} \nabla^2 \psi(\vec{r}) + U(\vec{r}) \psi(\vec{r}) = E \psi(\vec{r})$$

$$E_n = -\frac{13.6}{n^2} \text{ eV}$$



# Mobile electrons in crystals

---



# Electrons in crystals

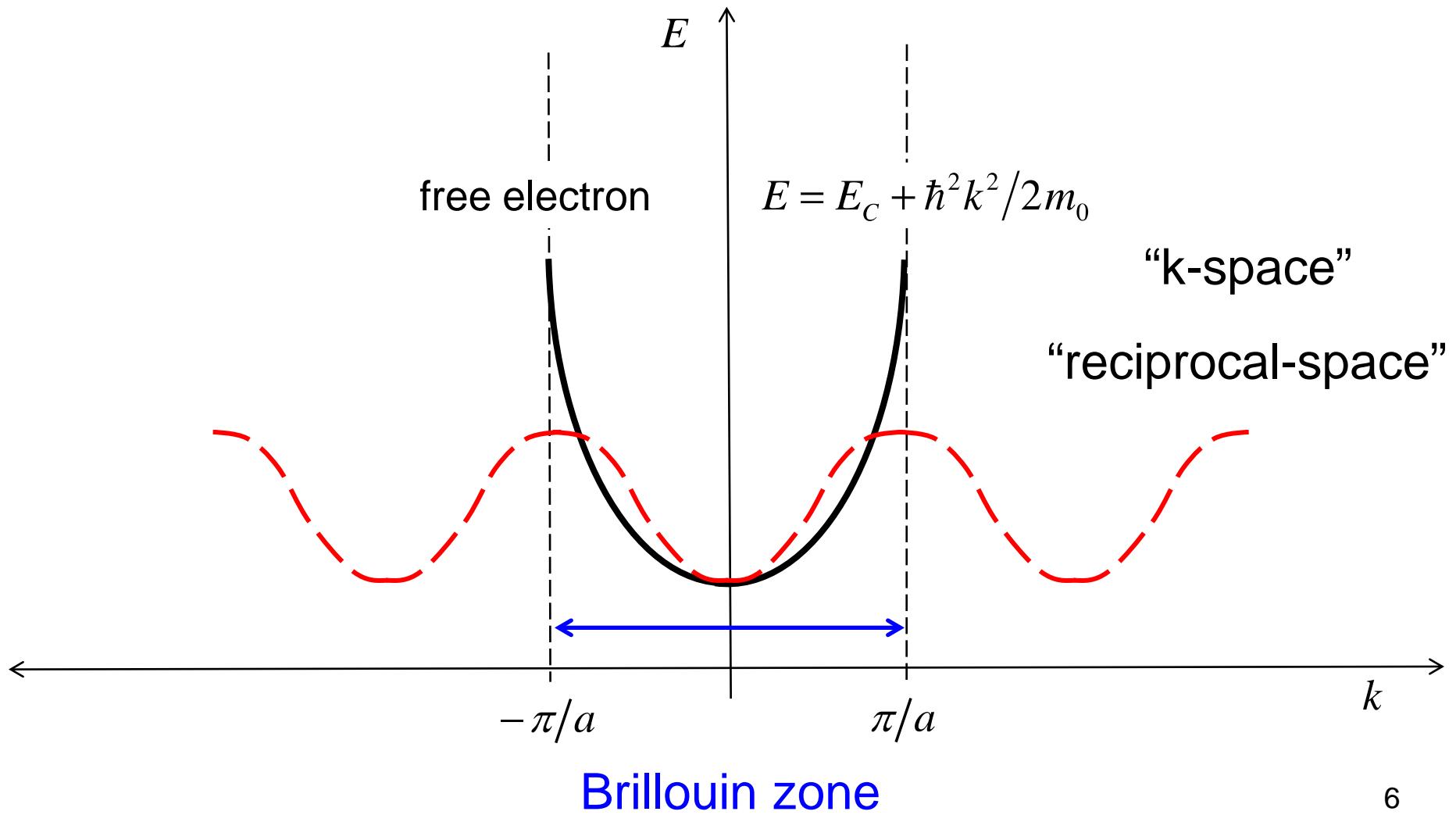
---

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + U_C(x)\psi(x) = E\psi(x) \quad U_C(\vec{r} + \vec{a}) = U_C(\vec{r})$$

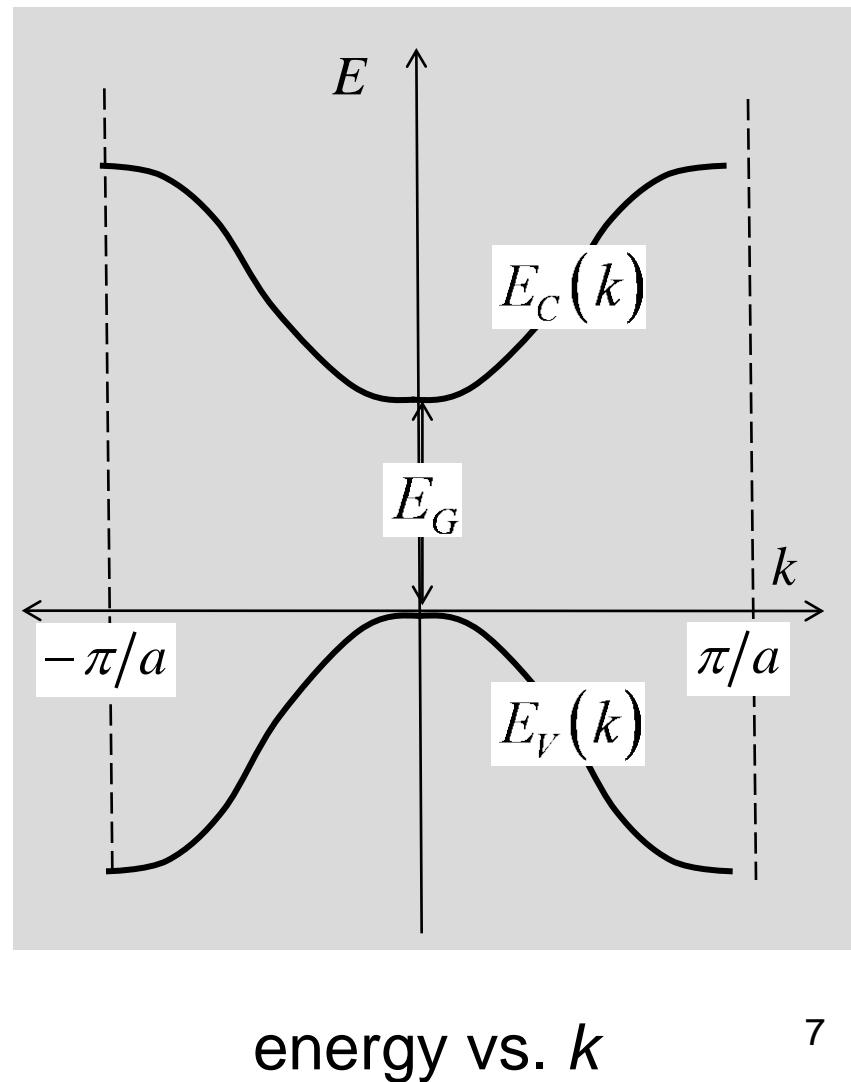
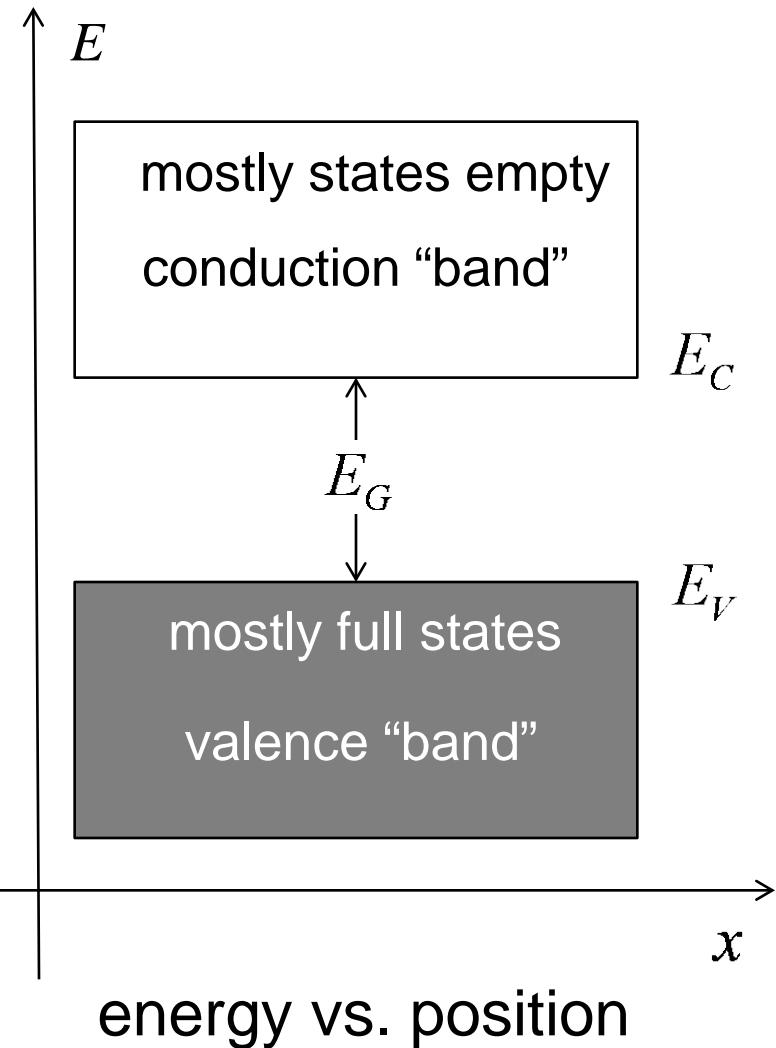
$$\psi(\vec{r}) = u_{\vec{k}}(\vec{r}) e^{i\vec{k}\cdot\vec{r}} \quad u_{\vec{k}}(\vec{r} + \vec{a}) = u_{\vec{k}}(\vec{r}) \quad \text{"Bloch wave"}$$

- Physical observables are periodic in the real space of a crystal lattice.
- Bloch functions are periodic in real space and k-space (reciprocal space).
- Wavefunctions are not periodic in real space but are periodic in k-space.

# Energy vs. momentum ( $k$ )



# Conduction and valence bands



# Crystal momentum

---

$$-\frac{\hbar^2}{2m_0} \frac{d^2\psi(x)}{dx^2} + U_C(x)\psi(x) = E\psi(x) \quad U_C(\vec{r} + \vec{a}) = U_C(\vec{r})$$

$$\psi(\vec{r}) = u_{\vec{k}}(\vec{r}) e^{i\vec{k}\cdot\vec{r}} \quad u_{\vec{k}}(\vec{r} + \vec{a}) = u_{\vec{k}}(\vec{r}) \quad k: \text{Brillouin zone}$$

“Bloch wave”

$\vec{p} \neq \hbar\vec{k}$     but....“crystal momentum”

$E(\vec{k})$     bandstructure (dispersion)     $E(\vec{k}) = \hbar\omega(\vec{k})$

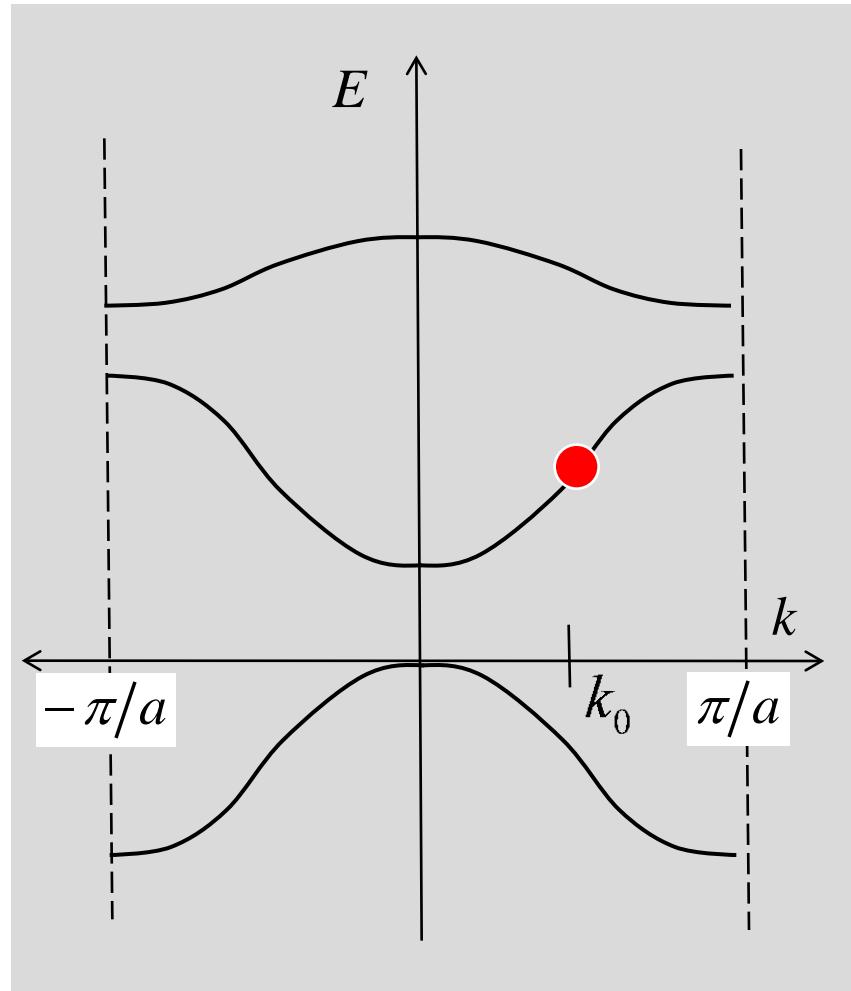
# Bandstructure basics

Particles described by a “wavepacket.”

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

The “group velocity” of a wavepacket is determined by the dispersion:

$$\vec{v}_g(\vec{k}) = \frac{1}{\hbar} \frac{dE}{dk}$$



# Parabolic bands

Near a band minimum or maximum,  $E(k)$  is a parabola.

$$E \approx E_C + \hbar^2 k^2 / 2m_n^*$$

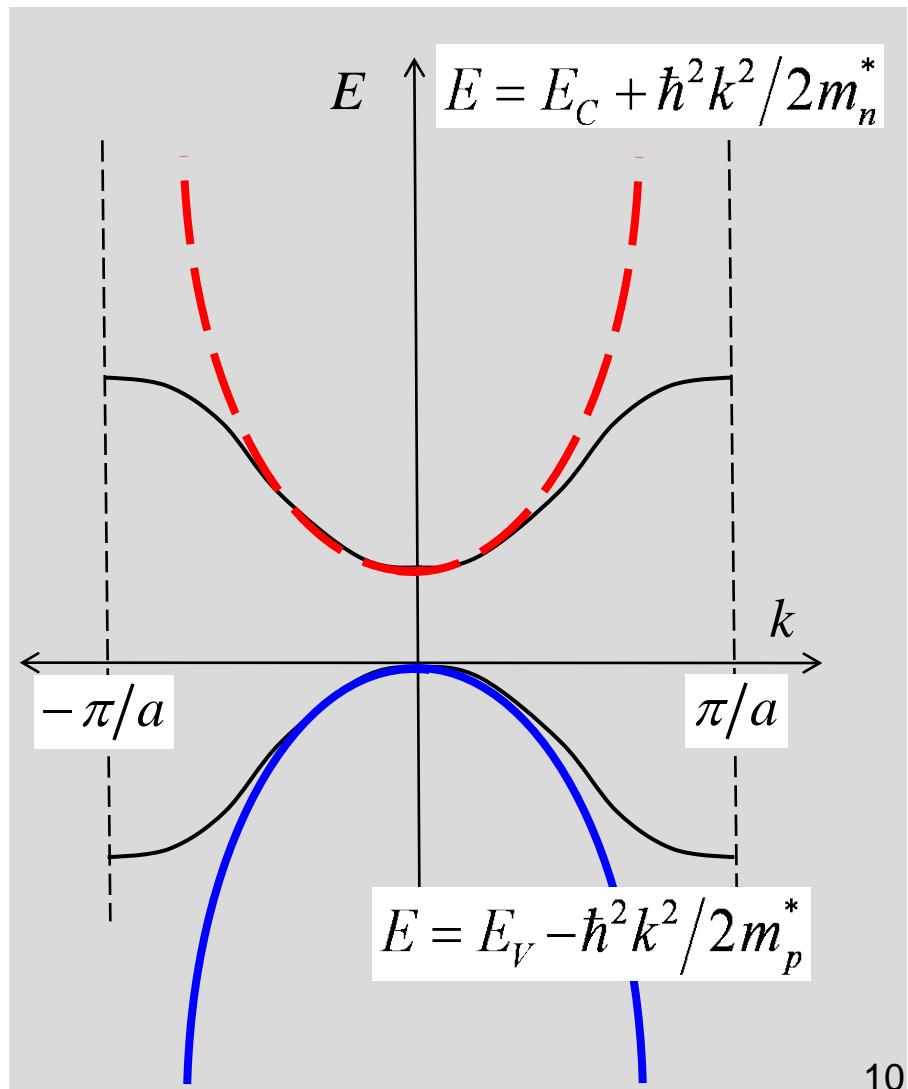
The curvature of the parabola is related to the **effective mass**.

$$m^* = \left( d^2 E / d(\hbar k)^2 \right)^{-1}$$

parabolic band assumption.

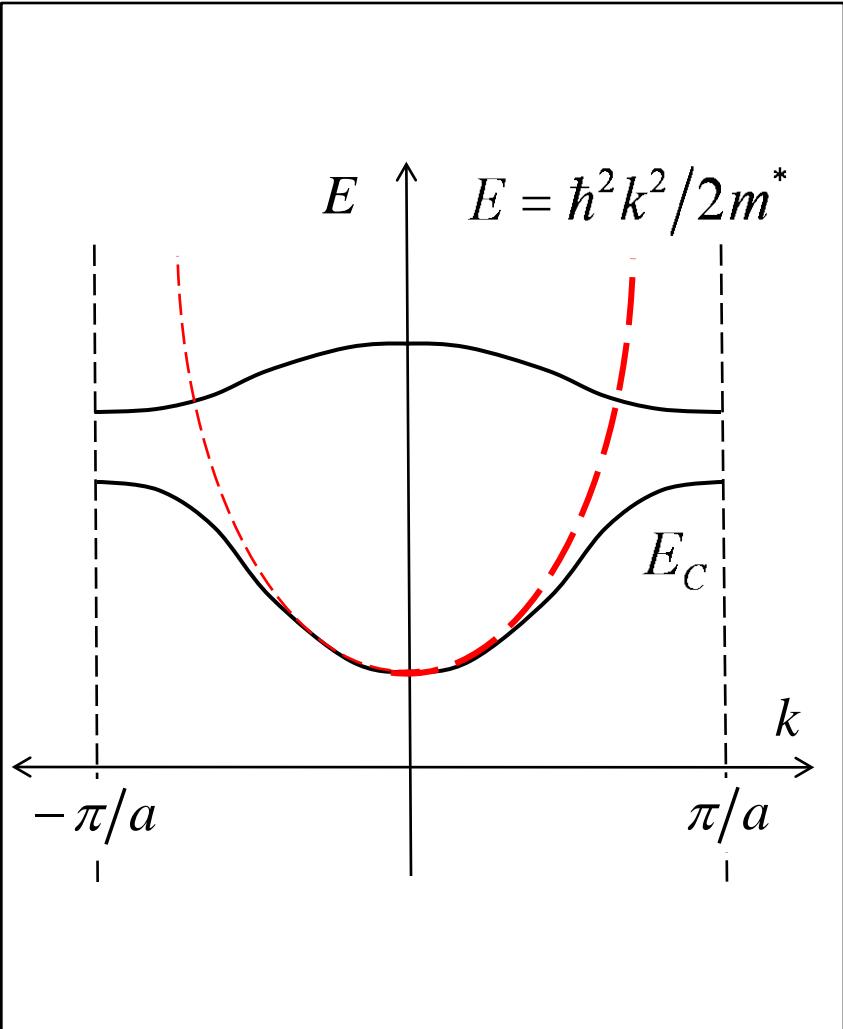
The **group velocity** is related to the crystal momentum and effective mass:

$$v_g(k) = \frac{1}{\hbar} \frac{dE(k)}{dk} = \frac{\hbar k}{m^*}$$



# Effective mass model for electrons

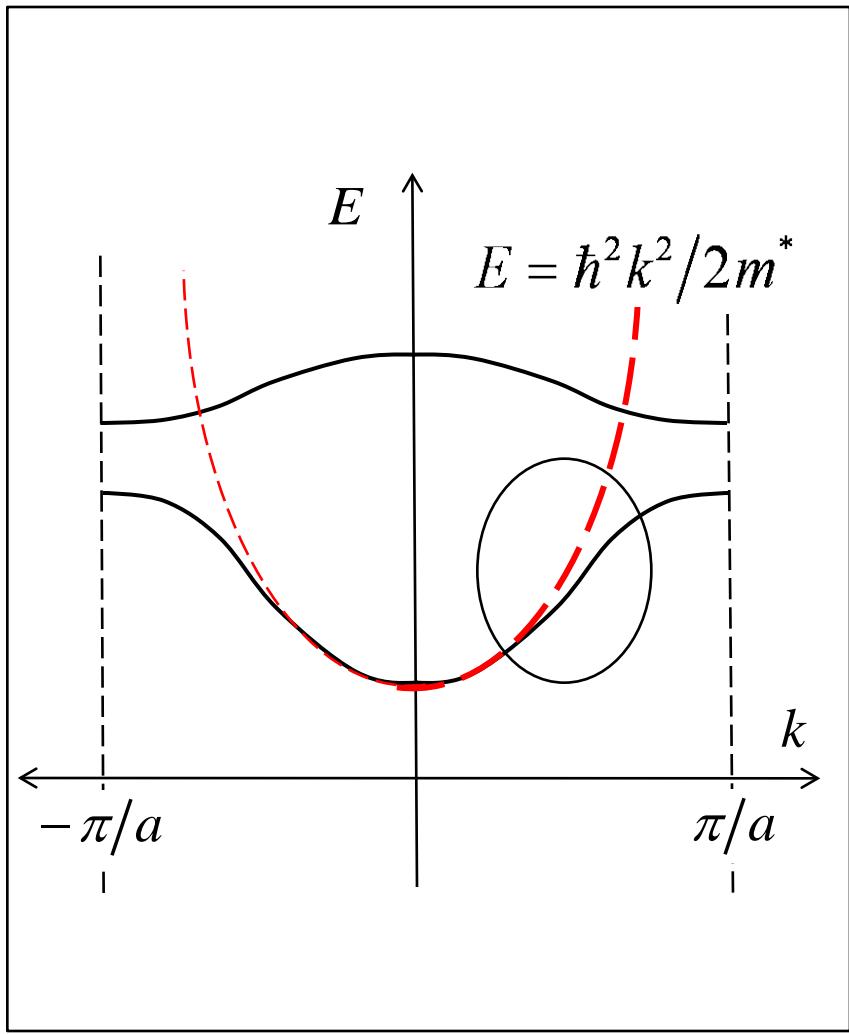
---



Typically, only states near the band edge matter, and these regions can be described by an effective mass approximation.

# First order correction for non-parabolicity

---



“Kane bands”

$$E(1 + \alpha E) = \frac{\hbar^2 k^2}{2m^*(0)}$$

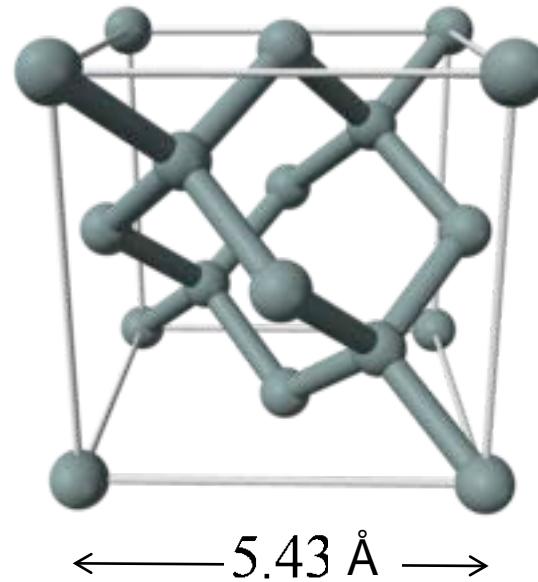
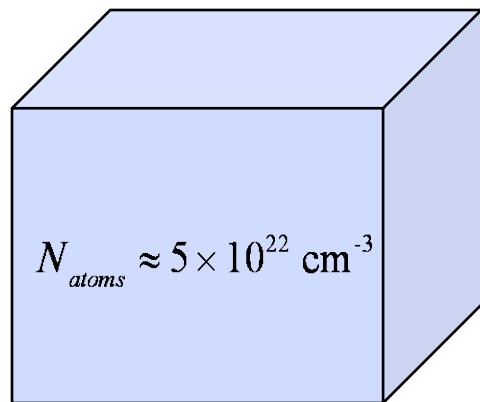
$$\alpha = 0.5 \text{ eV}^{-1} \quad \text{Si}$$

$$\alpha = 0.64 \text{ eV}^{-1} \quad \text{GaAs}$$

# 3D crystals

---

Silicon

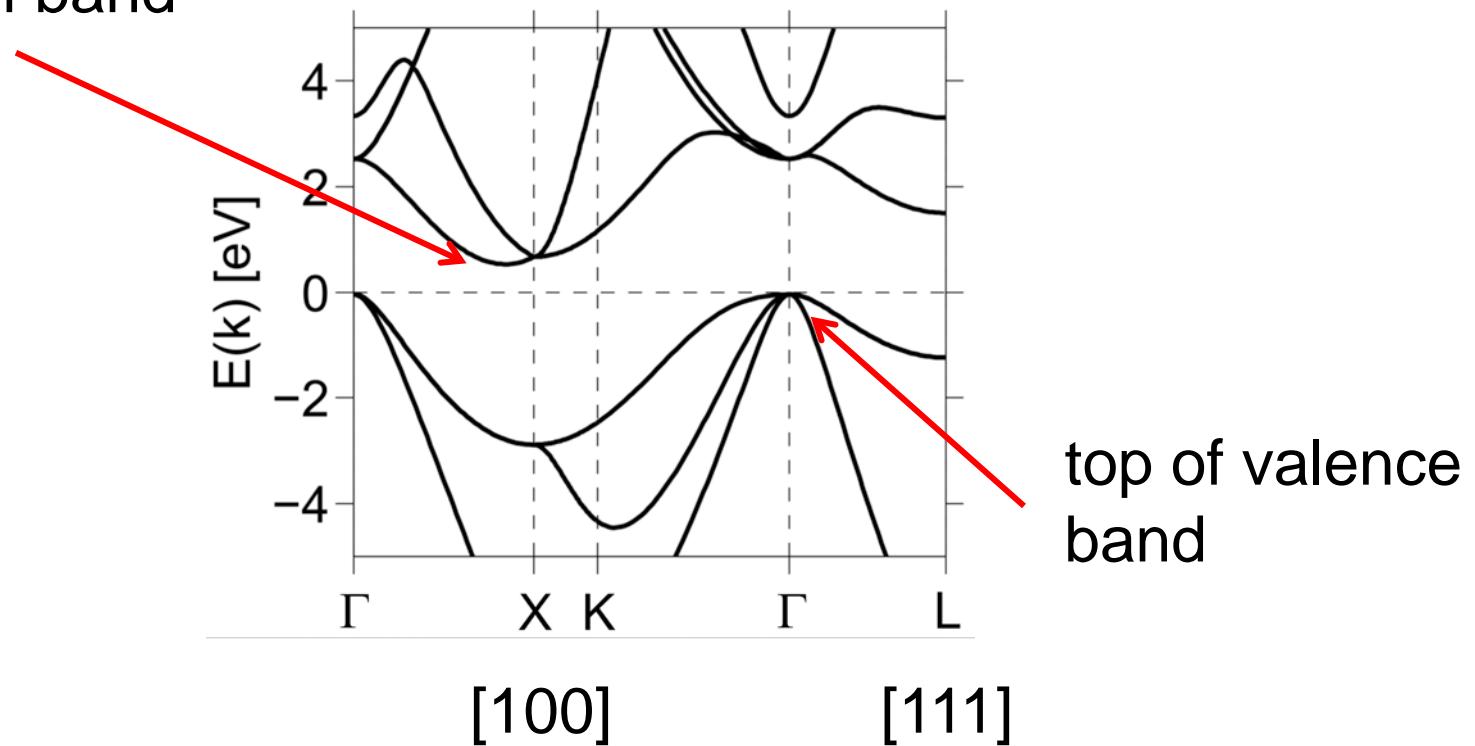


real space structure

# Band structure (electron dispersion)

bottom of  
conduction band

$E(k)$  for electrons in Si



# Constant energy surfaces

---

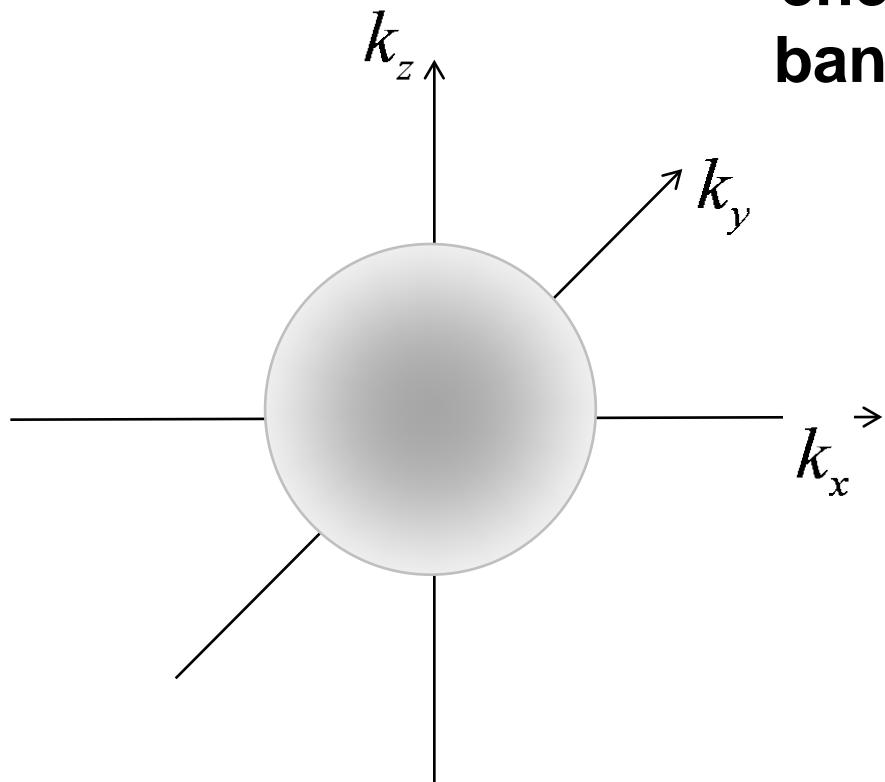
GaAs conduction band

**“spherical  
energy  
bands”**

$$E(\vec{k}) = \frac{\hbar^2 k_x^2}{2m_n^*} + \frac{\hbar^2 k_y^2}{2m_n^*} + \frac{\hbar^2 k_z^2}{2m_n^*}$$

equation of a sphere

$$m_n^* = 0.063m_0$$



# Constant energy surfaces

---

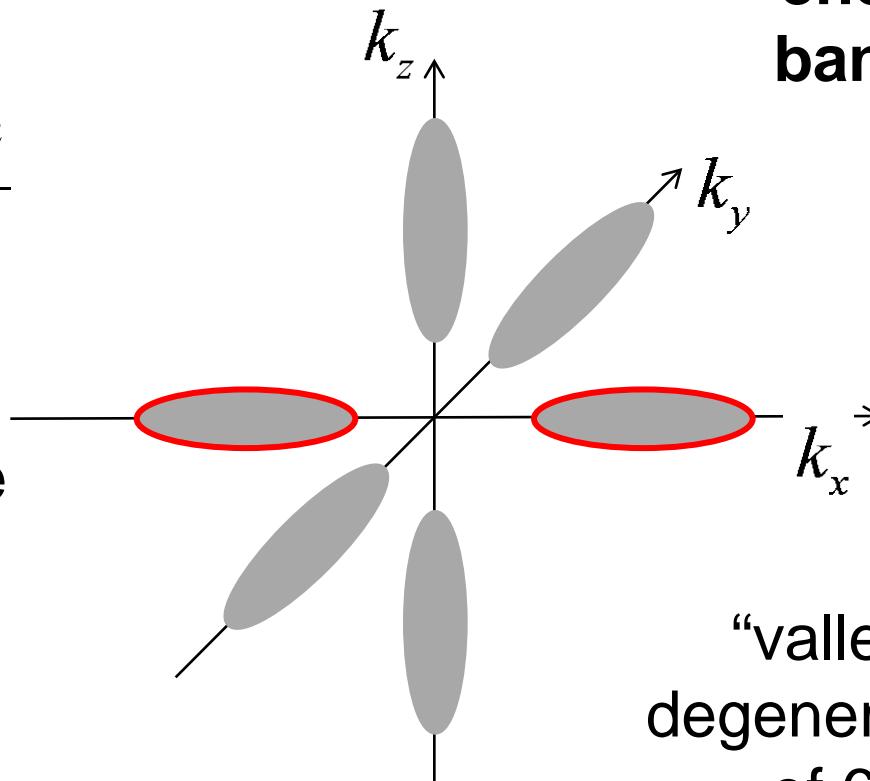
Si conduction band

$$E(\vec{k}) = \frac{\hbar^2 k_x^2}{2m_\ell^*} + \frac{\hbar^2 k_y^2}{2m_t^*} + \frac{\hbar^2 k_z^2}{2m_t^*}$$

equation of an ellipse

$$m_\ell^* = 0.9m_0$$

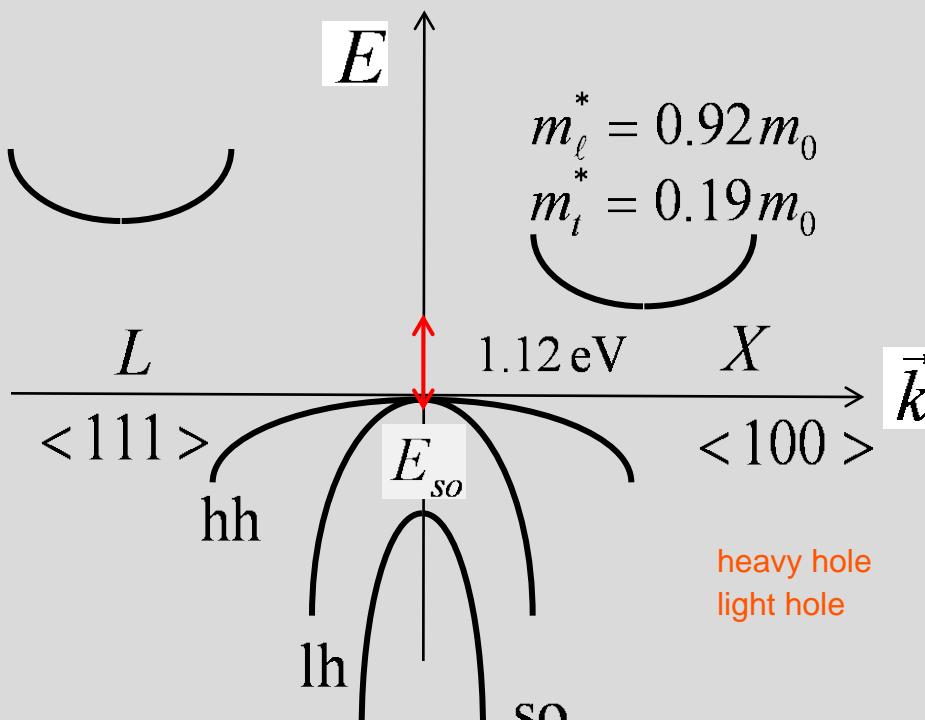
$$m_t^* = 0.19m_0$$



“ellipsoidal  
energy  
bands”

“valley  
degeneracy”  
of 6

# Model bandstructure for Si

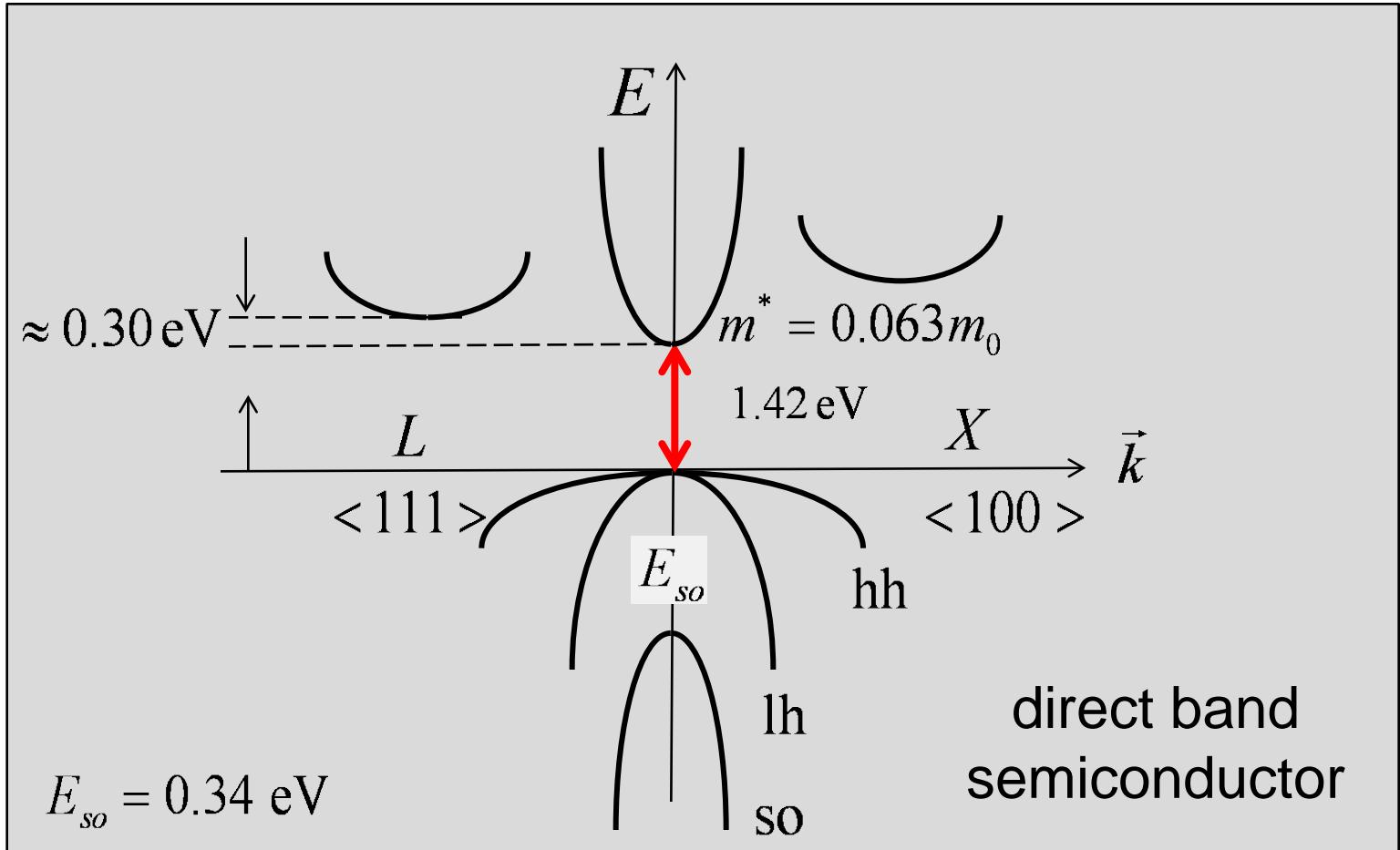


$$E(k) = E_C + \frac{\hbar^2 k^2}{2m_n^*}$$

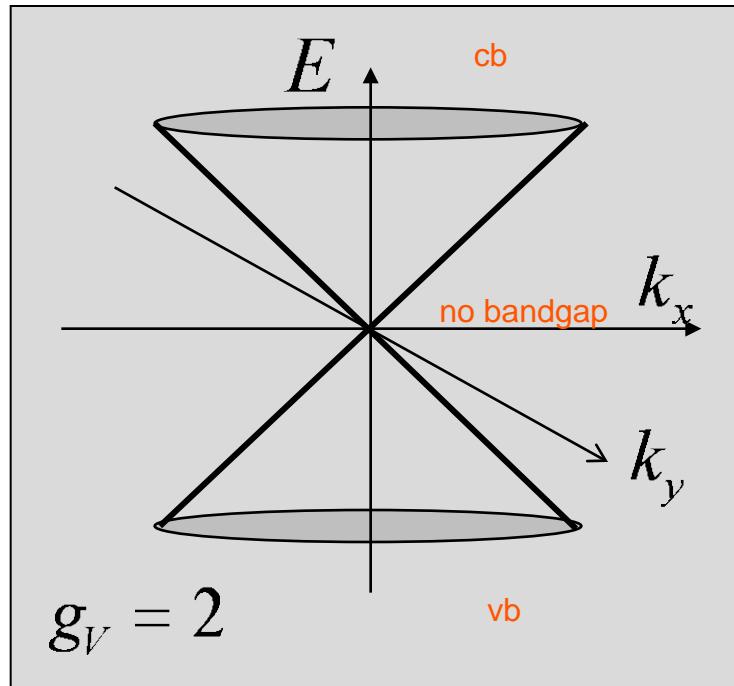
$$E(k) = E_V - \frac{\hbar^2 k^2}{2m_p^*}$$

“indirect” band semiconductor

# Model bandstructure: GaAs



# $E(k)$ for graphene



$$E(k) = \pm \hbar v_F \sqrt{k_x^2 + k_y^2} = \pm \hbar v_F k$$

Recall:

$$v_g(\vec{k}) = \frac{1}{\hbar} \frac{dE(k)}{dk}$$

For graphene:

$$v_g(\vec{k}) = v_F \approx 10^8 \text{ cm/s}$$

Also recall:

$$m^* = \left( \frac{1}{\hbar^2} \frac{d^2 E(k)}{dk^2} \right)^{-1}$$

For graphene:

$$m^* = ?$$

# Summary: Band structure

---

- 1) Electrons in a solid behave as both particles and as waves.
- 2) Electron waves are described by a band structure,  $E(k)$
- 3) Because the crystal is periodic, the dispersion is periodic in  $k$  (Brillouin zone).
- 4) Since electrons and holes are near the band minima and maxima, we can usually treat the bands as parabolic.
- 5) Electrons and holes can be treated as “semi-classical” particles with an effective mass and a crystal momentum.

# Summary: Mobile electrons in crystals

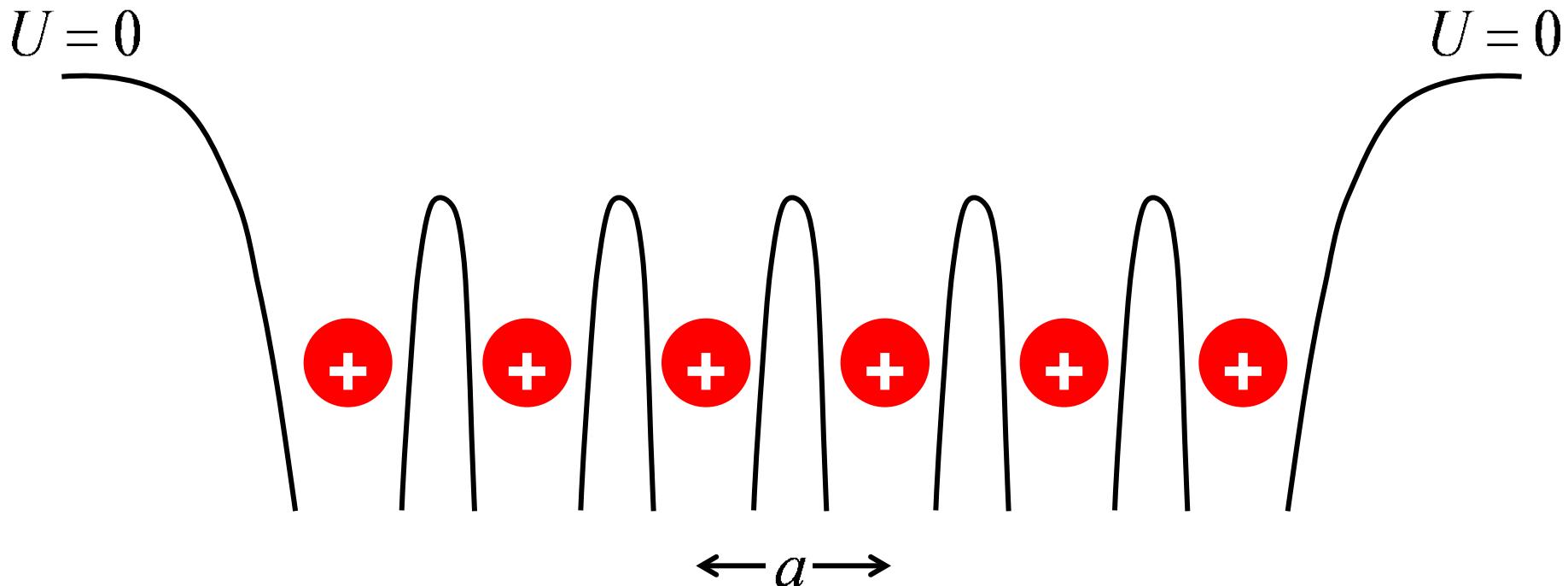


$$E(k) = \hbar^2 k^2 / 2m^*$$

$$p = \hbar k$$

$$v_g = (1/\hbar) dE/dk = \hbar k/m^*$$

$$F = dp/dt$$



# Primer on Semiconductors

## Unit 2: Quantum Mechanics

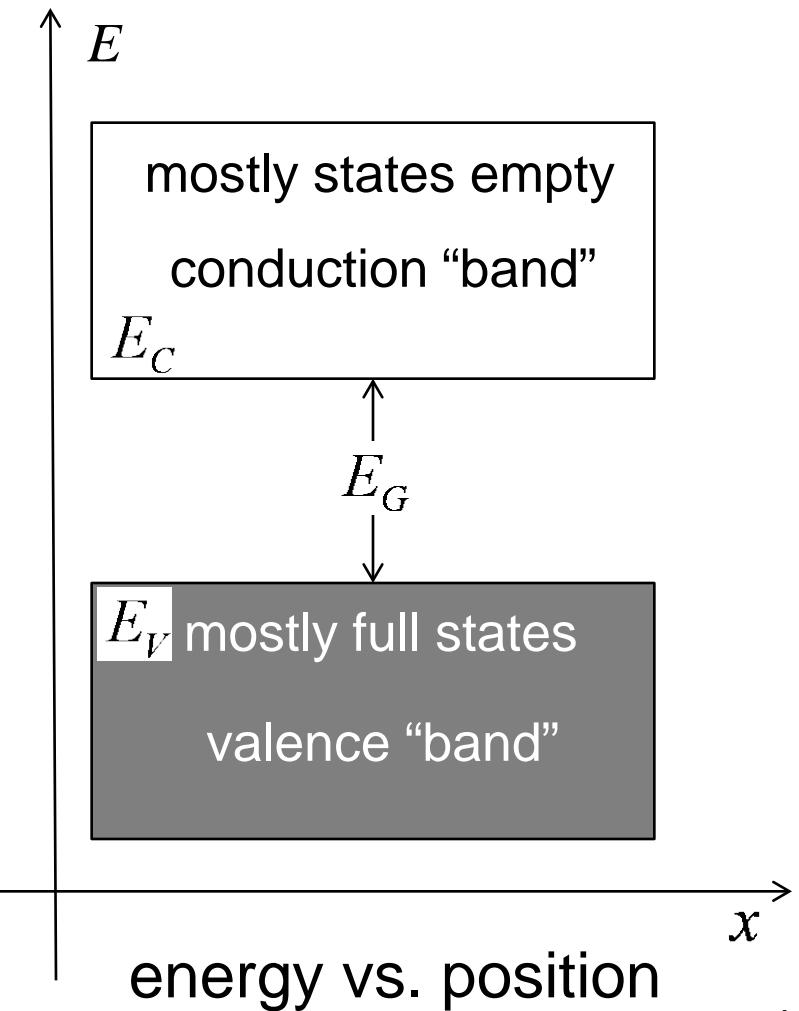
### Lecture 2.5: Density of states

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Conduction and valence bands

---



It will be important for us to know how the states are distributed in energy within the conduction and valence bands.

Most of the empty states (the holes) in the valence band are very near  $E_V$ .

Most of the filled states (the electrons) in the conduction band are very near  $E_C$ .

# Density of states

---

The number of states between  $E$  and  $E + dE$  is  $D(E)dE$ , where  $D(E)$  is the “density of states” (DOS).

In this lecture, we will calculate the DOS. This calculation is greatly simplified because only the region near the band edges are important, and in that region, the bands are often nearly parabolic:

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

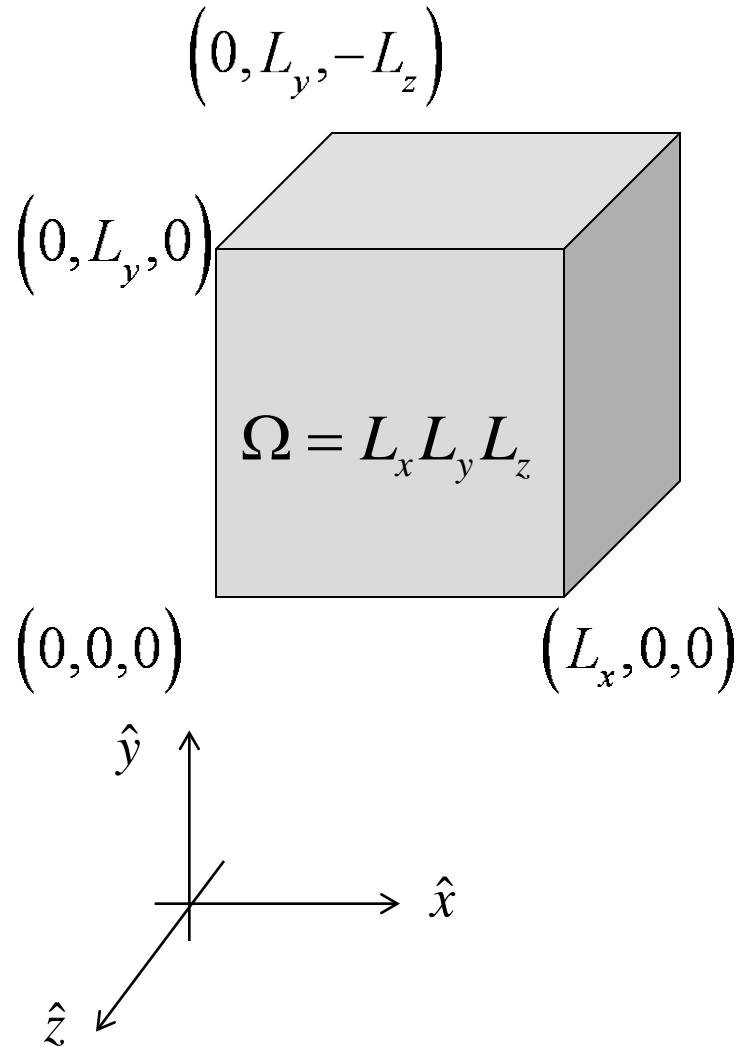
valence  
band

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

conduction band

# States in a finite volume of semiconductor

---



Finite volume,  $\Omega$   
**(part of an infinite volume)**

Finite number of states

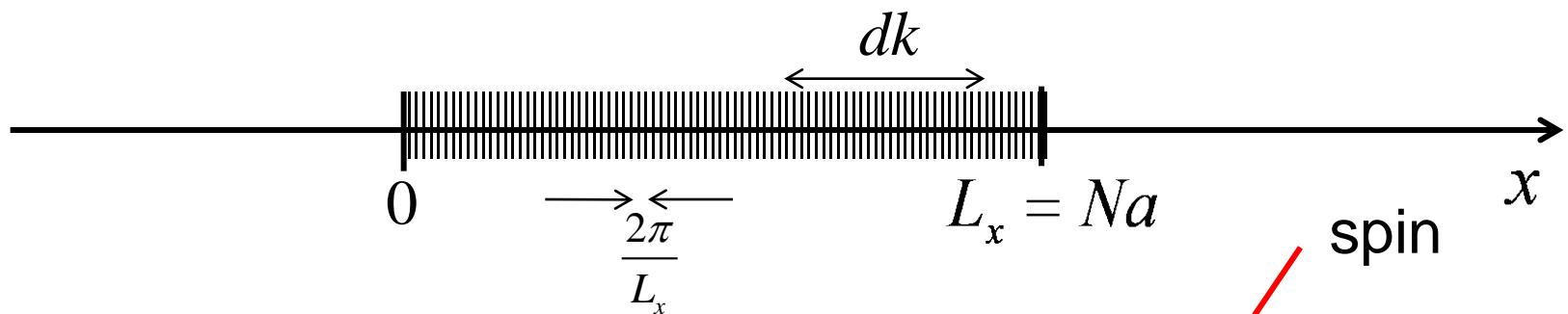
Periodic boundary conditions:

$$\psi(0,0,0) = \psi(L_x, 0, 0)$$

$$\psi(0,0,0) = \psi(0, L_y, 0)$$

$$\psi(0,0,0) = \psi(0,0, L_z)$$

# x-direction



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

$$\psi(0) = \psi(L_x) \rightarrow e^{ik_x L_x} = 1$$

$$k_x L_x = 2\pi j \quad j = 1, 2, 3, \dots$$

$$\# \text{ of states} = \frac{dk_x}{(2\pi/L_x)} \times 2 = N_k dk$$

$$N_k = \frac{L_x}{\pi} = \text{density of states in } k\text{-space}$$

$$k_x = \frac{2\pi}{L_x} j$$

$$L_x = Na \quad k_x = \frac{2\pi}{a} \frac{j}{N} \quad j_{\max} = N$$

“Brillouin zone”

$$0 < k < \frac{2\pi}{a}$$

$$k_{\max} = \frac{2\pi}{a}$$

# Density-of-states in k-space

---

1D:

$$N_k = 2 \times \left( \frac{L}{2\pi} \right) = \frac{L}{\pi} dk$$

2D:

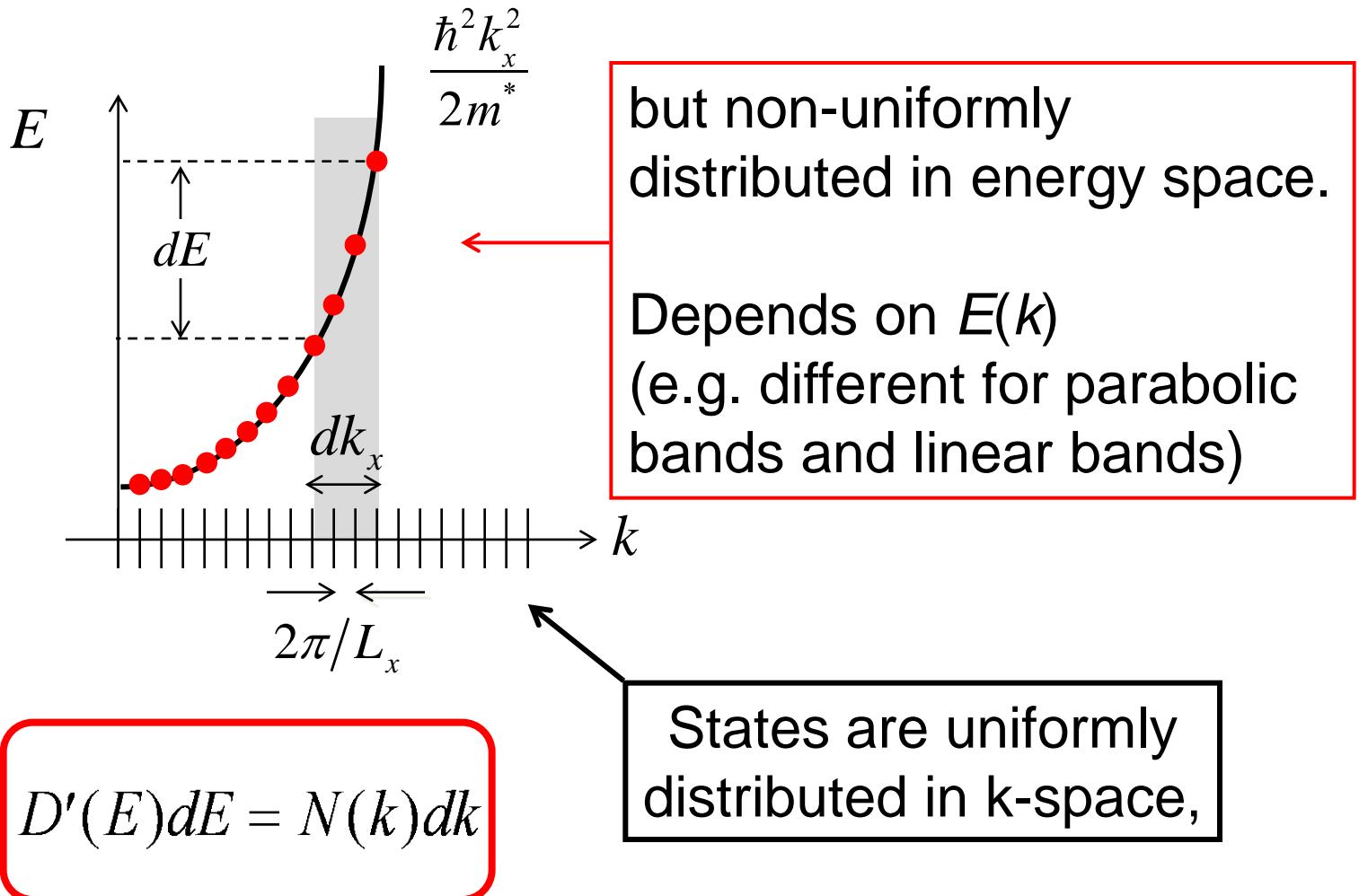
$$N_k = 2 \times \left( \frac{A}{4\pi^2} \right) = \frac{A}{2\pi^2} dk_x dk_y$$

independent of  $E(k)$

3D:

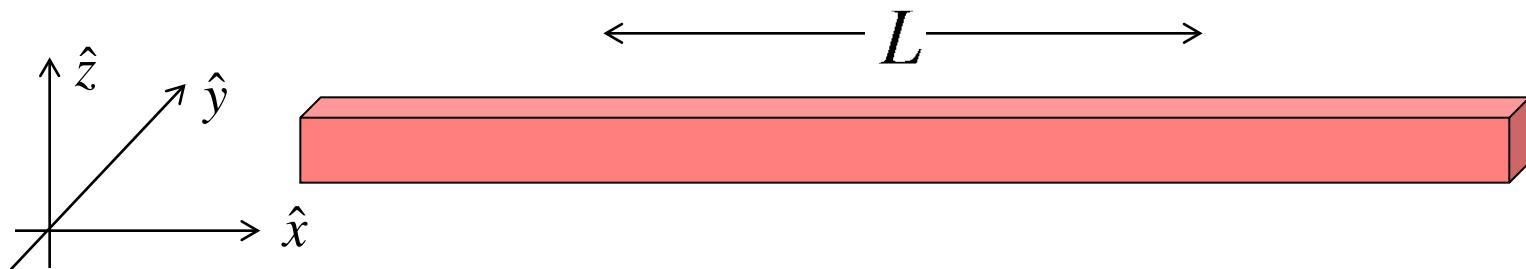
$$N_k = 2 \times \left( \frac{\Omega}{8\pi^3} \right) = \frac{\Omega}{4\pi^3} dk_x dk_y dk_z$$

# DOS: k-space vs. energy space



# Example 1: DOS(E) for 1D nanowire

---



Find DOS(E) per unit energy, per unit length, assuming a **single subband** and parabolic energy bands.

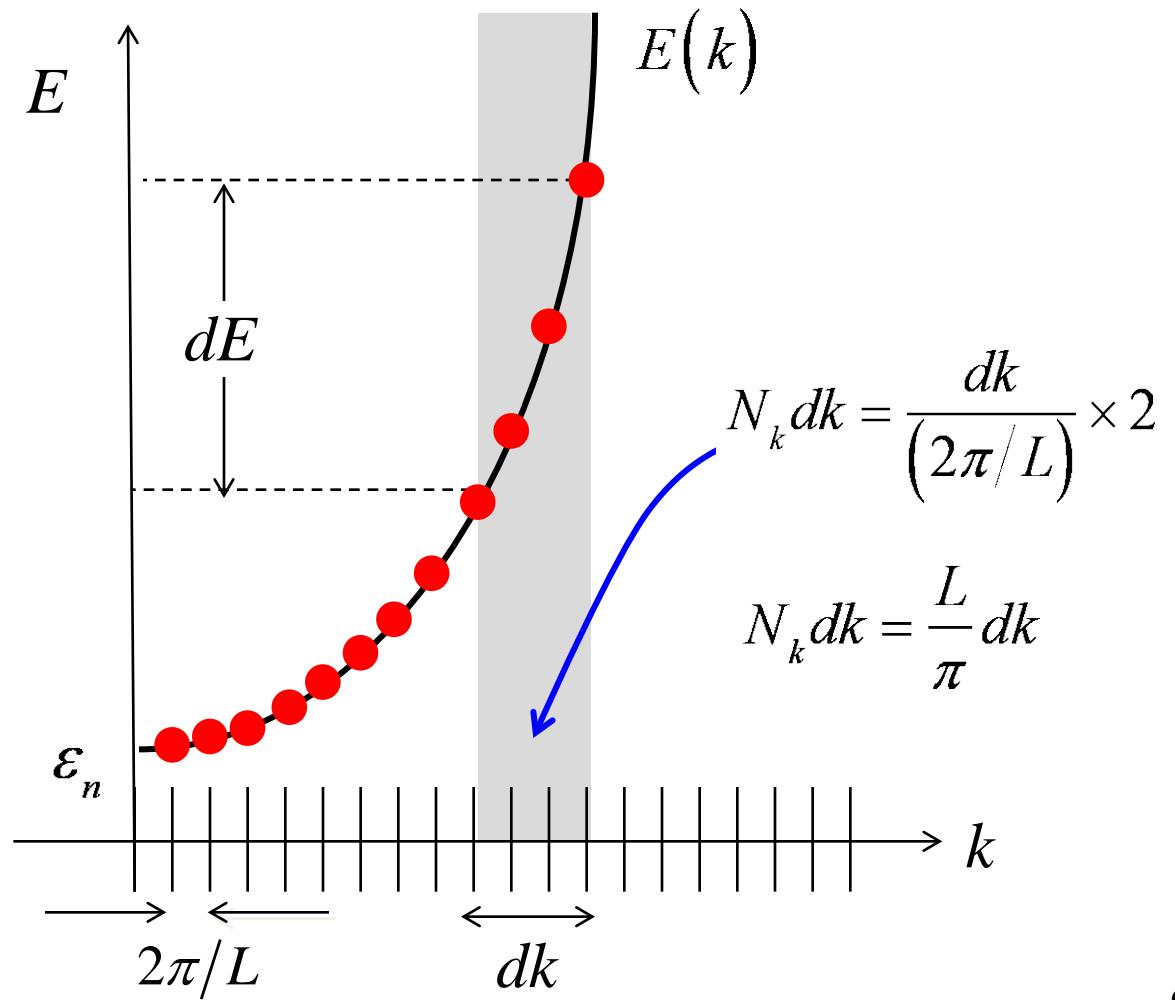
$$E = \varepsilon_n + \frac{\hbar^2 k_x^2}{2m^*}$$

# 1D (single subband)

$$D'_{1D}(E)dE = N_k dk$$

$$D_{1D}(E)dE = \frac{N_k dk}{L}$$

$$D_{1D}(E) \frac{\#}{\text{J-m}}$$



# 1D DOS

---

$$D_{1D}(E)dE = \frac{N_k dk}{L}$$

$$D_{1D}(E)dE = \frac{1}{\pi} dk$$

$$dE = \frac{\hbar^2 k dk}{m^*} \quad k = \frac{\sqrt{2m^*(E - \epsilon_n)}}{\hbar}$$

$$D_{1D}(E)dE = \frac{1}{\pi \hbar} \sqrt{\frac{m^*}{2(E - \epsilon_n)}} dE$$

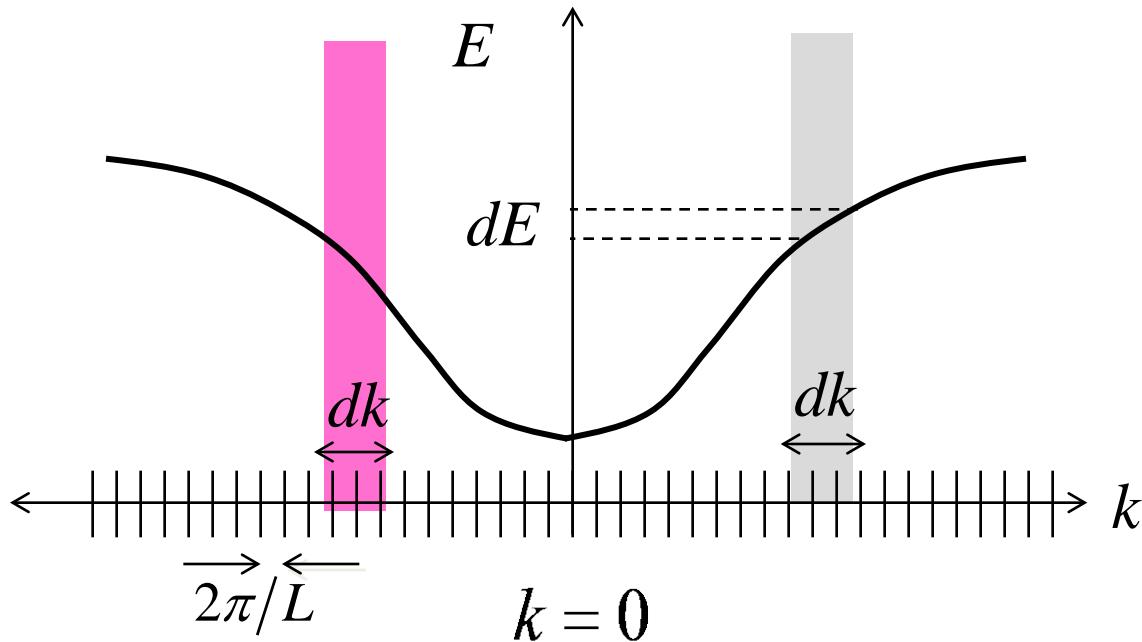
$E > \epsilon_n$       DOS in subband,  $n$ .  $n = 1, 2, 3\dots$

$$N_k dk = \frac{L}{\pi} dk$$

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

# Don't forget to multiply by 2

---



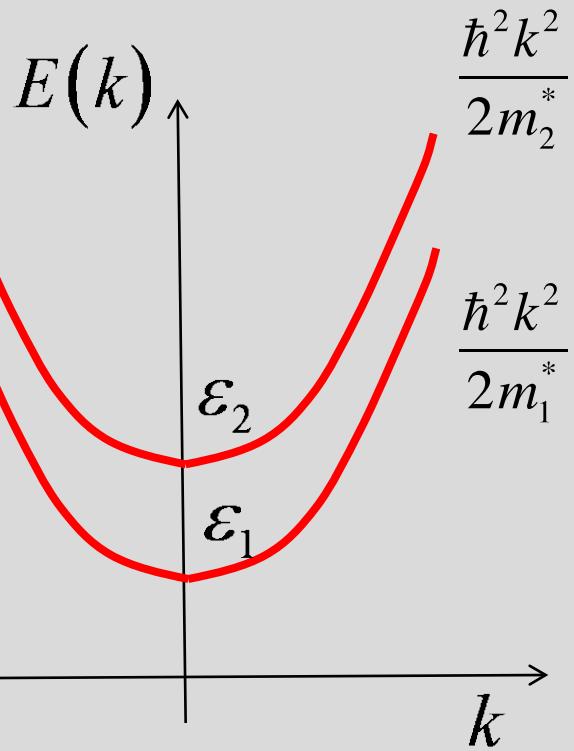
Multiply by 2 to account for the negative  $k$ -states.

$$D_{1D}(E)dE = \frac{2}{\pi\hbar} \sqrt{\frac{m^*}{2(E - \varepsilon_n)}} dE$$

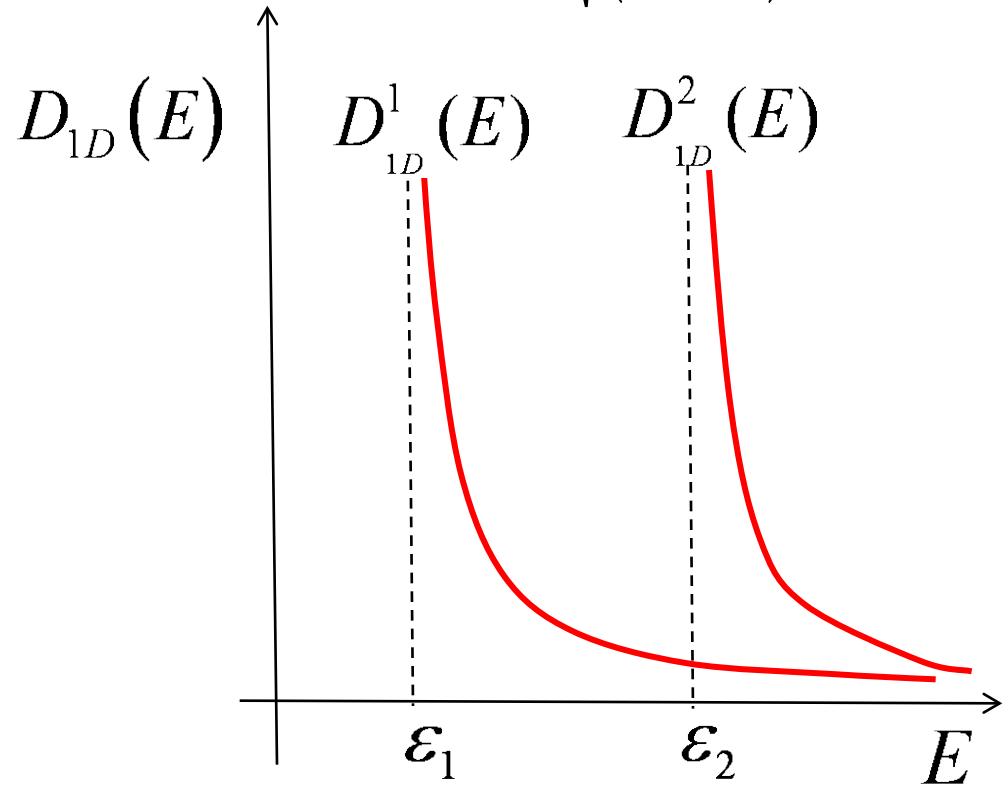
(parabolic energy bands)

# Multiple subbands

$$E = \epsilon_j + \frac{\hbar^2 k^2}{2m_j^*}$$

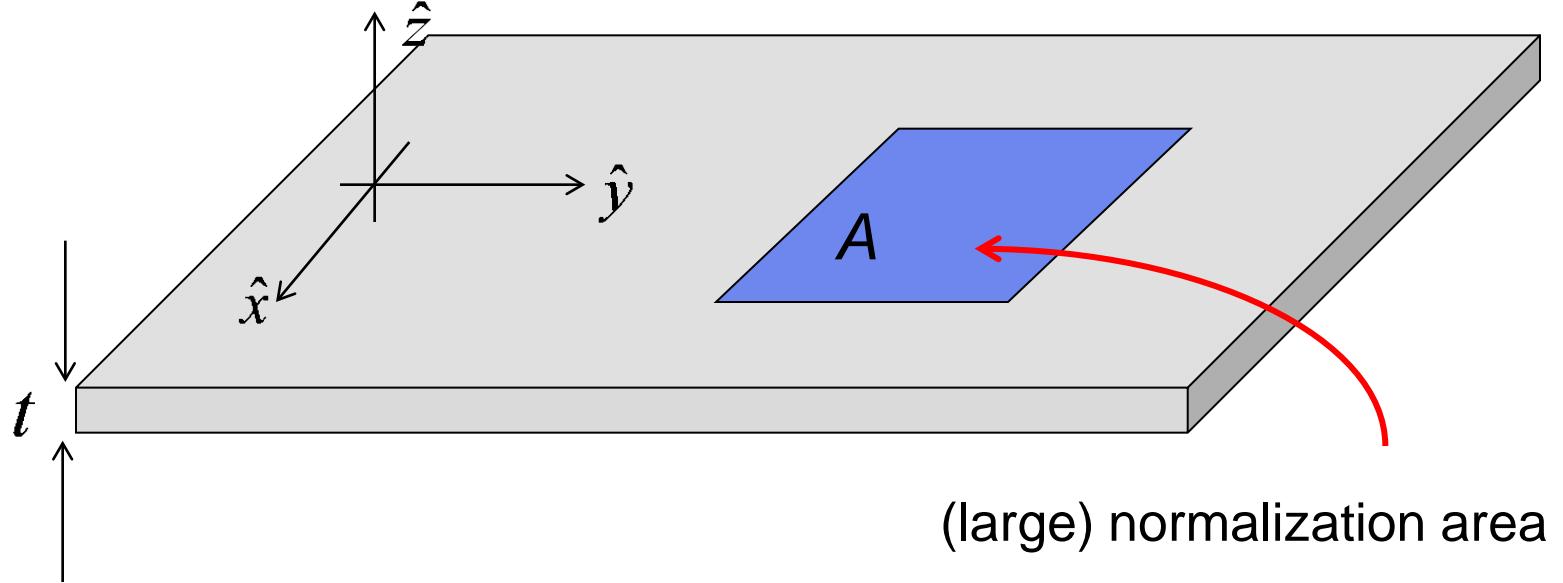


$$D_{1D}^j(E) = \frac{1}{\pi\hbar} \sqrt{\frac{2m_j^*}{(E - \epsilon_j)}}$$



## Example 2: DOS( $E$ ) for 2D electrons

---



Find DOS( $E$ ) per unit energy, per unit area, for a **single subband** assuming parabolic energy bands.

$$E = \varepsilon_j + \frac{\hbar^2 k_{\parallel}^2}{2m_j^*}$$

## Example 2: DOS(E) for 2D electrons

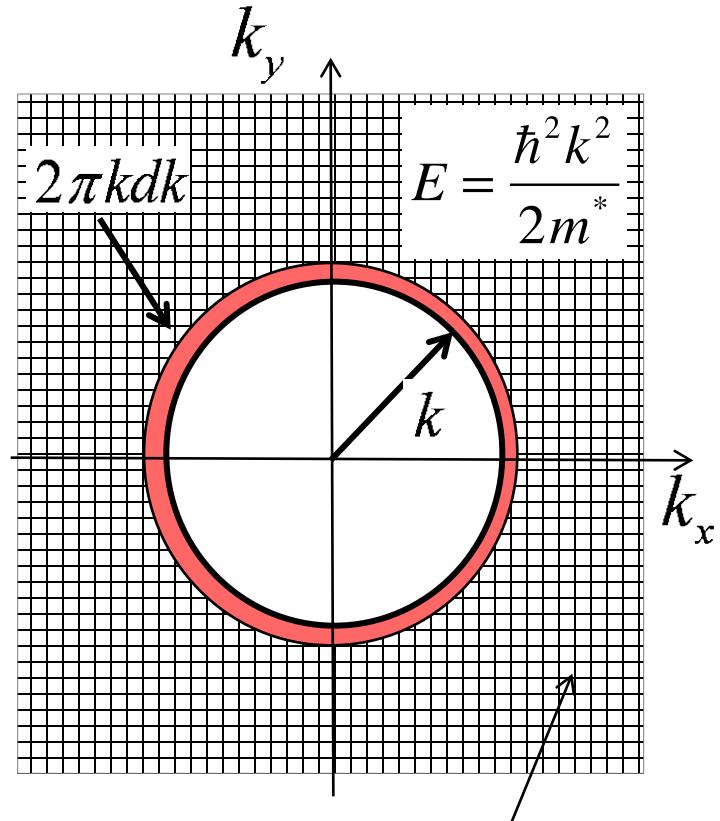
$$D(E)dE = \frac{N(k)}{A} dk^2$$

$$N_k = 2 \times \left( \frac{A}{4\pi^2} \right) = \frac{A}{2\pi^2}$$

$$D(E)dE = \frac{1}{2\pi^2} 2\pi kdk$$

$$E = \epsilon_n + \frac{\hbar^2 k^2}{2m^*} \quad dE = \epsilon_n + \frac{\hbar^2 kdk}{m^*}$$

$$D_{2D}(E) = \frac{m^*}{\pi \hbar^2} \quad E > E_C$$



Area of each state in k-space:  $\frac{4\pi^2}{A}$

## Example 3: DOS(E) for 3D electrons

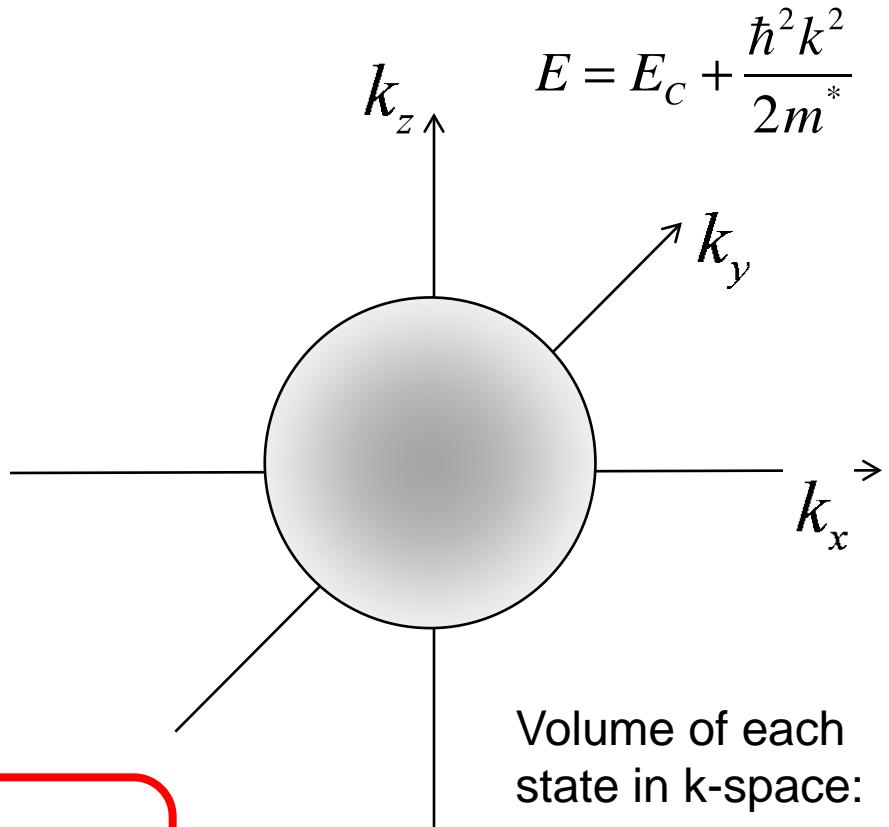
$$D(E)dE = \frac{N(k)}{\Omega} dk^3$$

$$N_k = 2 \times \left( \frac{\Omega}{8\pi^3} \right) = \frac{\Omega}{4\pi^3}$$

$$D(E)dE = \frac{1}{4\pi^3} 4\pi k^2 dk$$

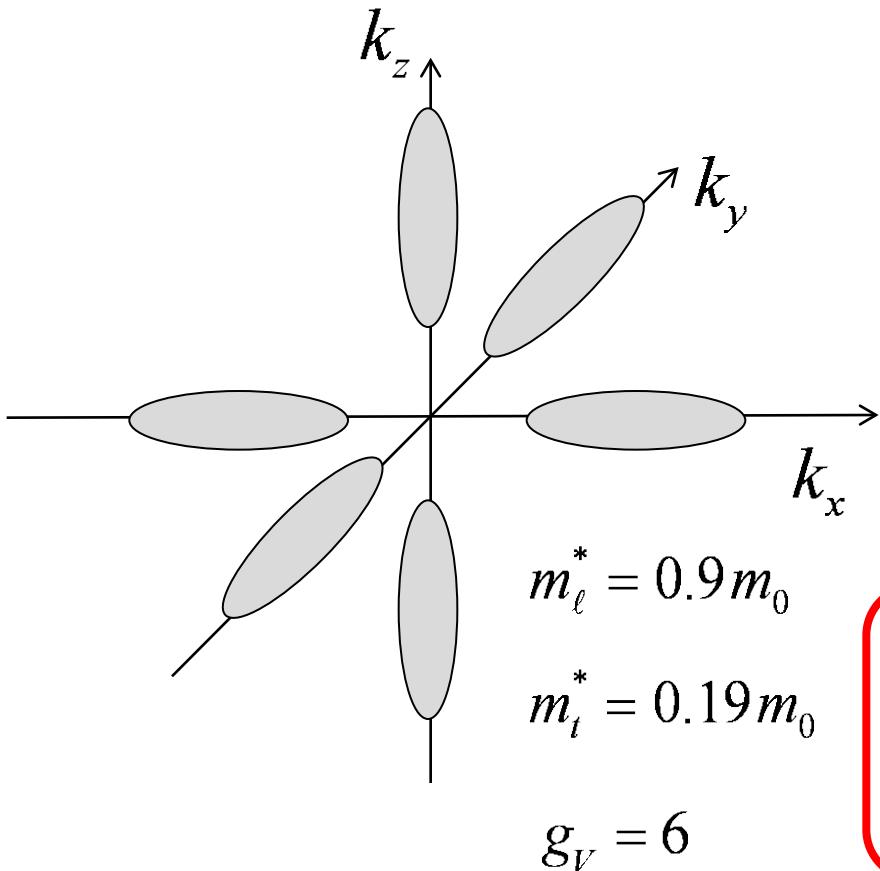
$$E = E_C + \frac{\hbar^2 k^2}{2m^*}$$

$$D_{3D}(E) = \frac{m^* \sqrt{2m^*(E - E_C)}}{\pi^2 \hbar^3} \quad E > E_C$$



$$\frac{8\pi^3}{\Omega}$$

# Ellipsoidal band and valley degeneracy



$$D_{3D}(E) = \frac{m^* \sqrt{2m^*(E - E_C)}}{\pi^2 \hbar^3} \quad m^* = ?$$

$$m_D^* \equiv 6^{2/3} (m_\ell m_t^2)^{1/3}$$

$$D_{3D}(E) = \frac{m_D^* \sqrt{2m_D^*(E - E_C)}}{\pi^2 \hbar^3}$$

Conduction band of Si:  
6 equivalent ellipsoidal valleys:

# Comments on 3D DOS

---

$$D_{3D}(E) = \frac{m_D^* \sqrt{2m_D^*(E - E_C)}}{\pi^2 \hbar^3}$$

For a bulk semiconductor with parabolic bands:

$$D_{3D}(E) \propto (m_D^*)^{3/2} \quad D_{3D}(E) \propto \sqrt{(E - E_C)}$$

Si:  $m_D^* = 1.182m_0$

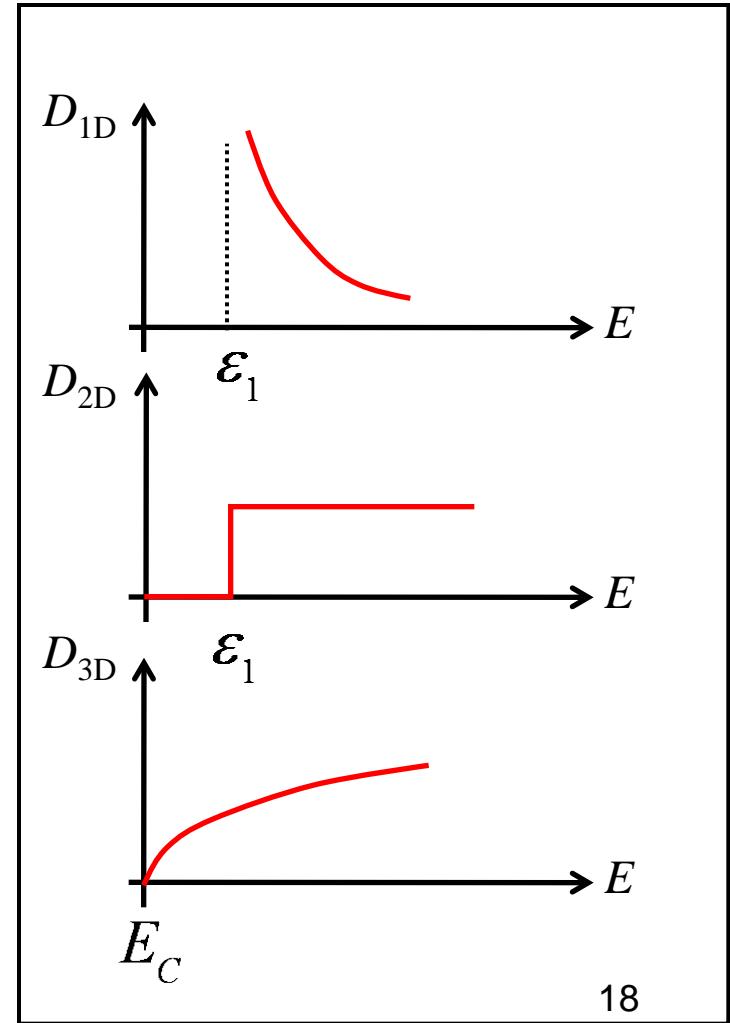
GaAs:  $m_D^* = 0.0655m_0$

# Parabolic bands: 1D, 2D, and 3D

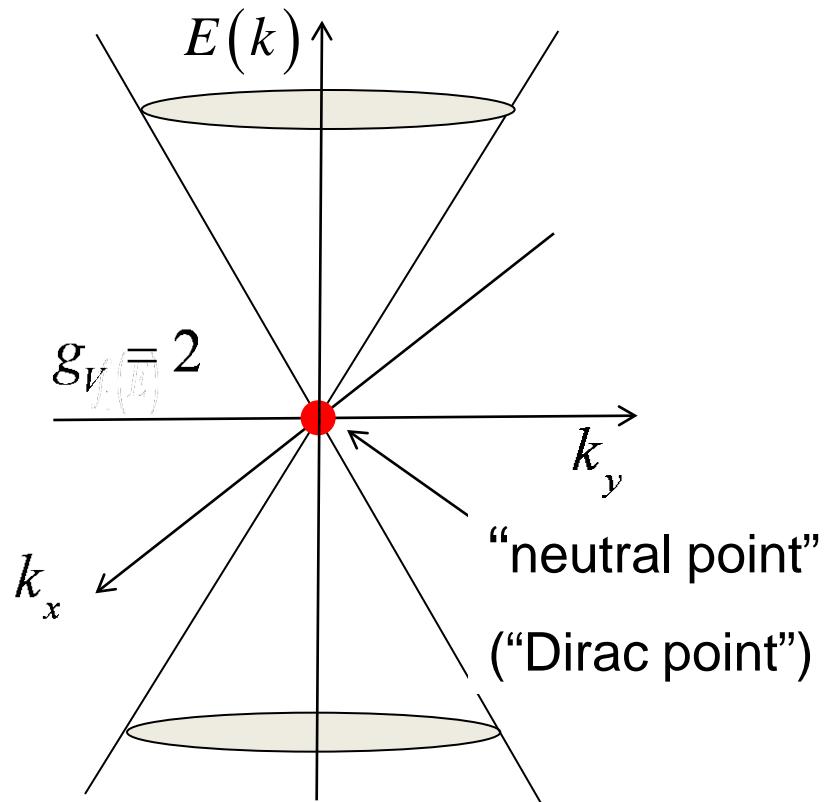
$$D_{1D}(E) = g_V \frac{1}{\pi \hbar} \sqrt{\frac{2m^*}{(E - \varepsilon_1)}} \Theta(E - \varepsilon_1)$$

$$D_{2D}(E) = g_V \frac{m^*}{\pi \hbar^2} \Theta(E - \varepsilon_1)$$

$$D_{3D}(E) = g_V \frac{m^* \sqrt{2m^*(E - E_C)}}{\pi^2 \hbar^3} \Theta(E - E_C)$$



# Exercise

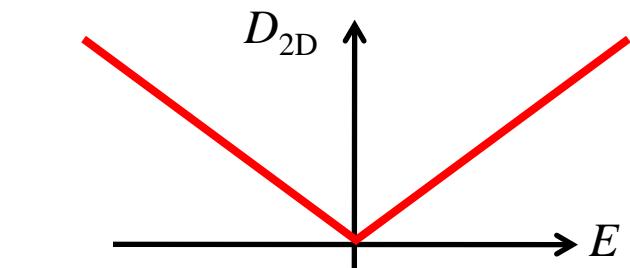


$$E(k) = \pm \hbar v_F k = \pm \hbar v_F \sqrt{k_x^2 + k_y^2}$$

19

Show that for graphene, the 2D DOS is:

$$D_{2D}(E) = g_V \frac{|E|}{\pi \hbar^2 v_F^2} = \frac{2|E|}{\pi \hbar^2 v_F^2}$$



19

# Summary

---

The DOS is an important concept – one that we will use frequently in the next unit.

The DOS depends on dimension.

$DOS(k)$  is independent of band structure, but  $DOS(E)$  depends on the band structure.

For 3D, bulk semiconductors with parabolic bands,  
 $DOS \sim (m^*)^{3/2}$  and  $DOS \sim \sqrt{E - E_C}$

# Primer on Semiconductors

## Unit 2: Quantum Mechanics

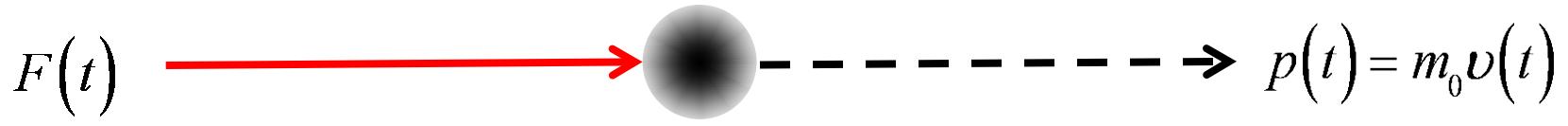
### Lecture 2.6: Unit 2 Recap

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Classical particles: Newton's Laws

---



$$F = m_0 a = m_0 \frac{d^2 x}{dt^2} = m_0 \frac{dv}{dt} \quad F = \frac{dp}{dt}$$

Equations of motion:

$$p(t) = p(0) + \int_0^t F(t') dt' \quad v(t) = v(0) + \frac{1}{m_0} \int_0^t F(t') dt' \quad x(t) = x(0) \int_0^t v(t') dt'$$

# Quantum particles: Wave equation

---

$$-\frac{\hbar}{i} \frac{\partial}{\partial t} \Psi(x, t) = -\frac{\hbar^2}{2m_0} \frac{\partial^2}{\partial x^2} \Psi(x, t) + U(x) \Psi(x, t)$$

$$\Psi(x, t) = \psi(x) \phi(t)$$

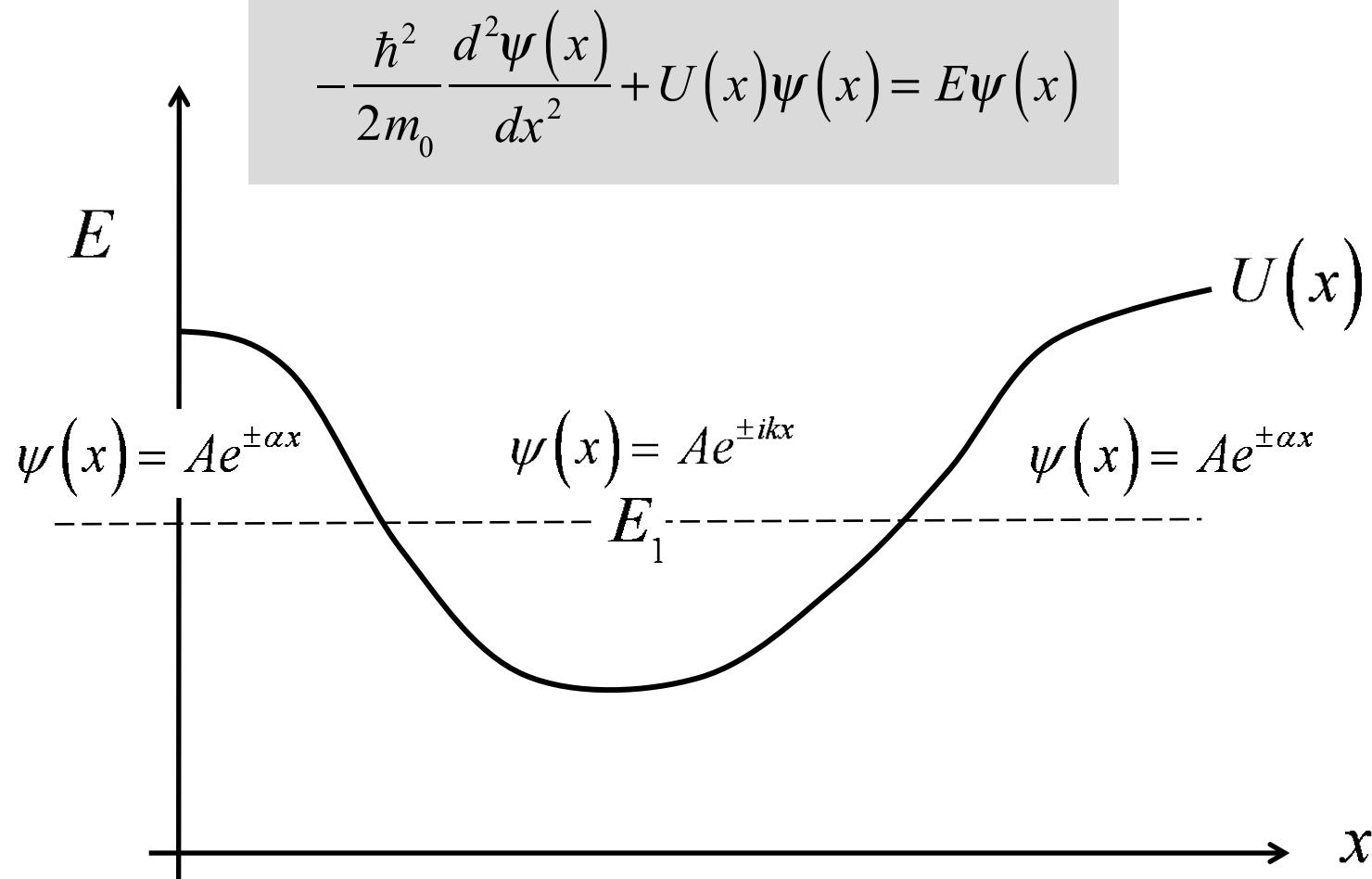
$$-\frac{\hbar^2}{2m_0} \frac{d^2 \psi(x)}{dx^2} + U(x) \psi(x) = E \psi(x)$$

$$\Psi(x, t) = \psi(x) \phi(t) = \psi(x) e^{-i\omega t} \quad \omega = E/\hbar$$

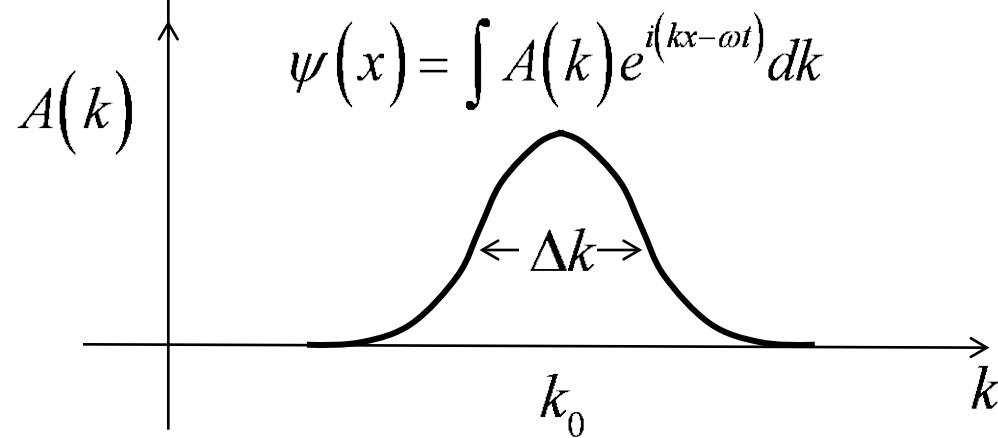
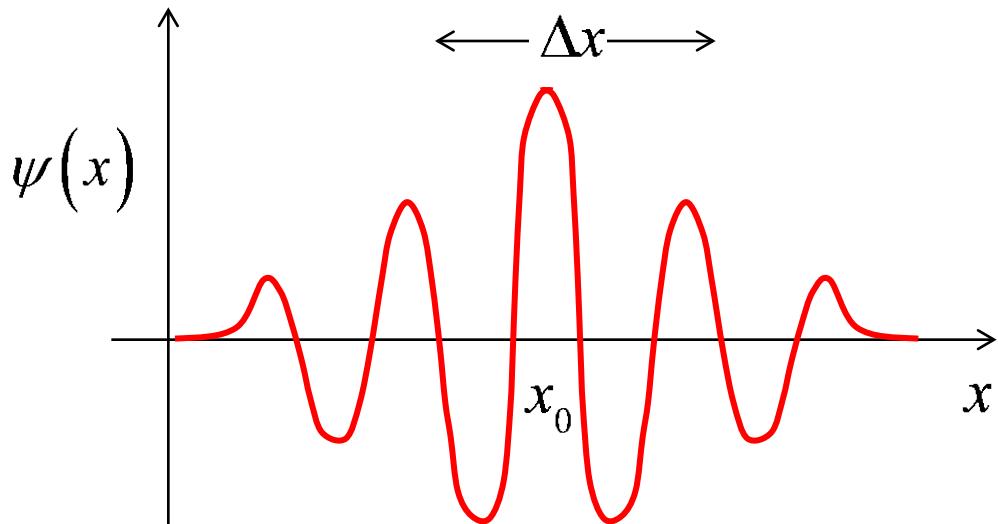
$$P(x, t) dx = \Psi^*(x, t) \Psi(x, t) dx$$

# Solutions of the time-independent wave equation

---



# Wave packets describe particles



Particle:  $x = x_0$

Momentum:  $p = \hbar k_0$

Velocity:  $v_g = \frac{1}{\hbar} \frac{dE}{dk} \Big|_{k=k_0}$

$$\Delta p \Delta x \geq \hbar/2$$

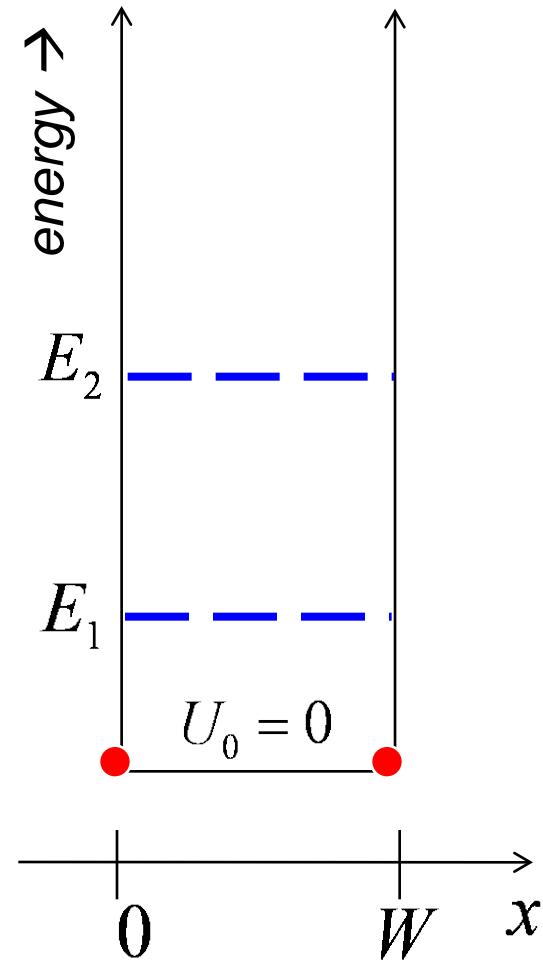
$$\Delta E \Delta t \geq \hbar/2$$

# 1D quantum well summary

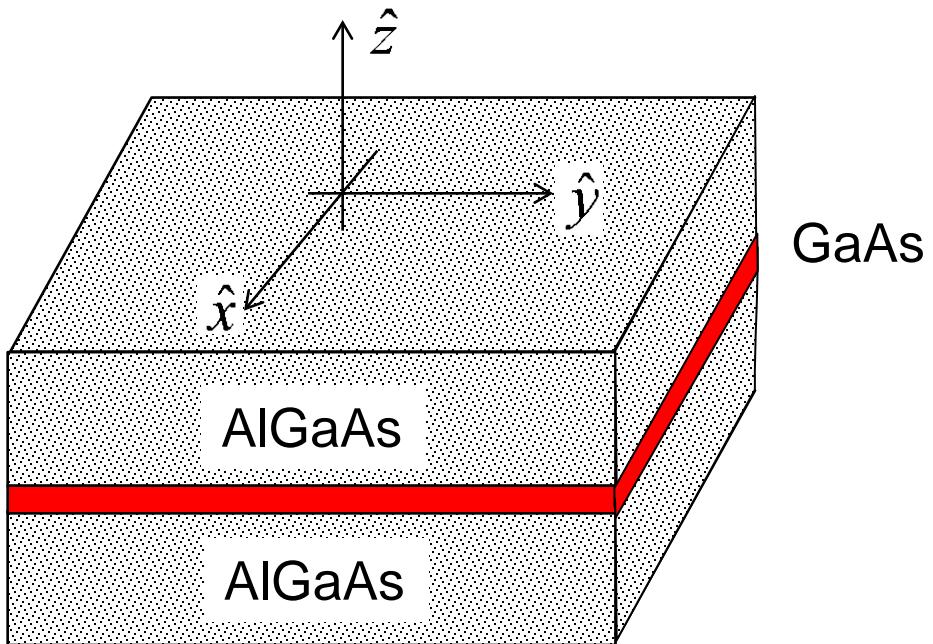
$$\psi(x) = A \sin k_j x \quad k_j = \frac{\pi}{W} j \quad j = 1, 2, 3 \dots$$

$$k^2 = \frac{2mE}{\hbar^2} \quad E_j = \frac{\hbar^2 k_j^2}{2m} = \frac{\hbar^2 j^2 \pi^2}{2mW^2}$$

- Confined electrons have quantized energies.
- Tighter confinement (smaller  $W$ ) leads to higher energies.
- Lighter masses leads to higher energies.



# Quantum confinement with heterostructures



Electrons are confined in the z-direction, but free to move in the x-y plane.

$$\psi(\vec{r}) \sim e^{i\vec{k} \cdot \vec{r}} \rightarrow \sin(k_z z) \times e^{ik_x x} \times e^{ik_y y}$$

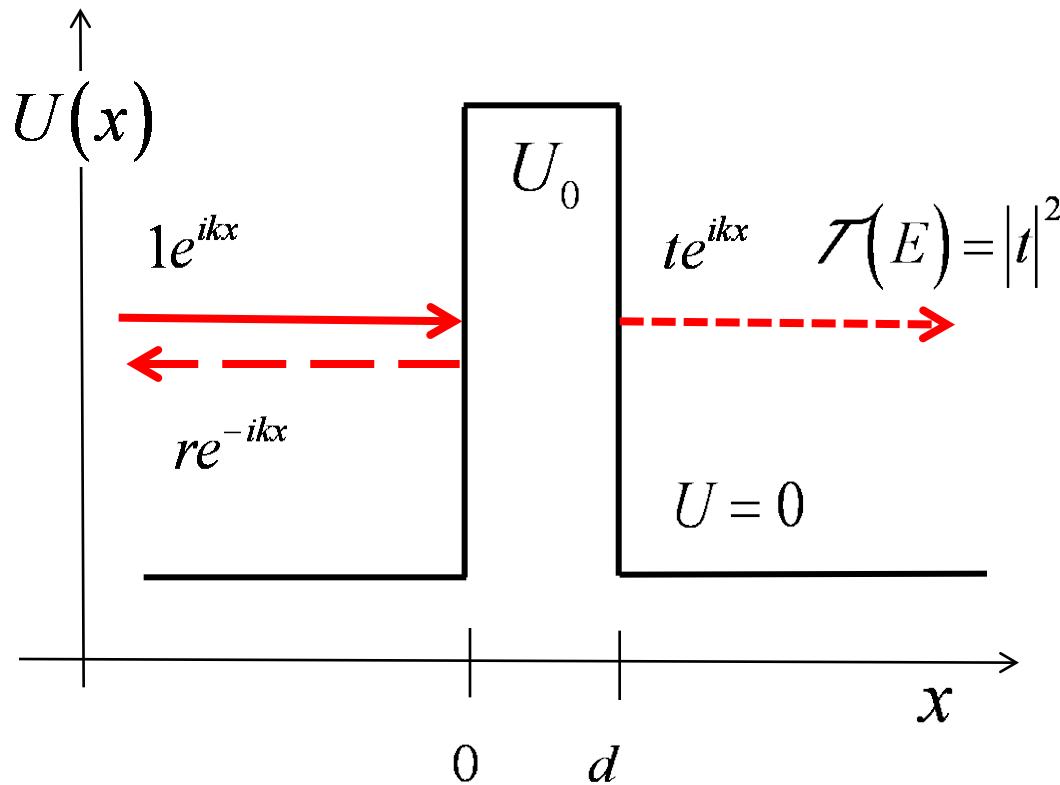
“GaAs quantum well”

$$k_{zj} = j \frac{\pi}{W} \quad E_j = \frac{\hbar^2 j^2 \pi^2}{2mW^2}$$

“subbands”     $E = E_j + \frac{\hbar^2 k_{||}^2}{2m}$

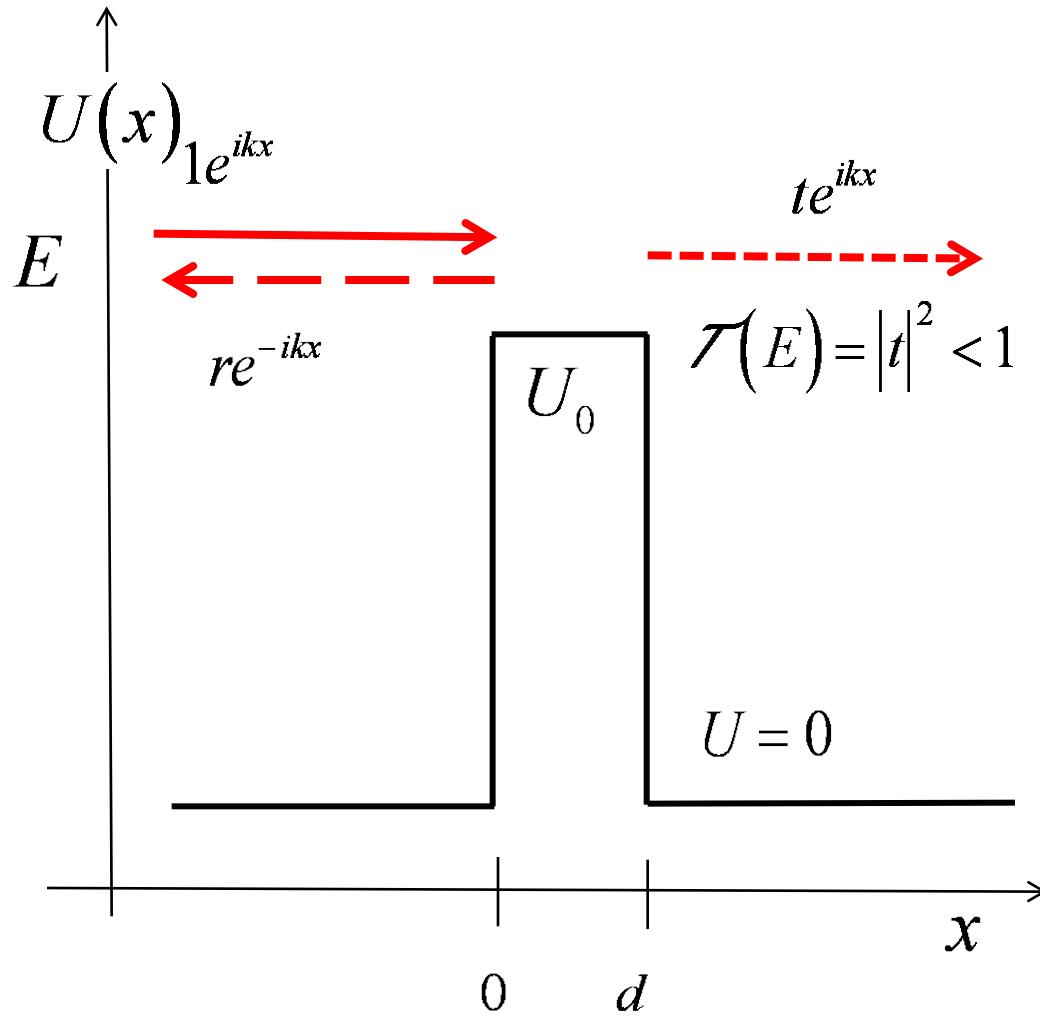
# Quantum tunneling

$$\mathcal{T}(E) \approx \exp\left(-2d\sqrt{2m(U_0 - E)/\hbar^2}\right)$$



- 1) Tunneling decreases exponentially with increasing barrier thickness.
- 2) Tunneling decreases exponentially with increasing barrier height.
- 3) Tunneling decreases exponentially with increasing mass.

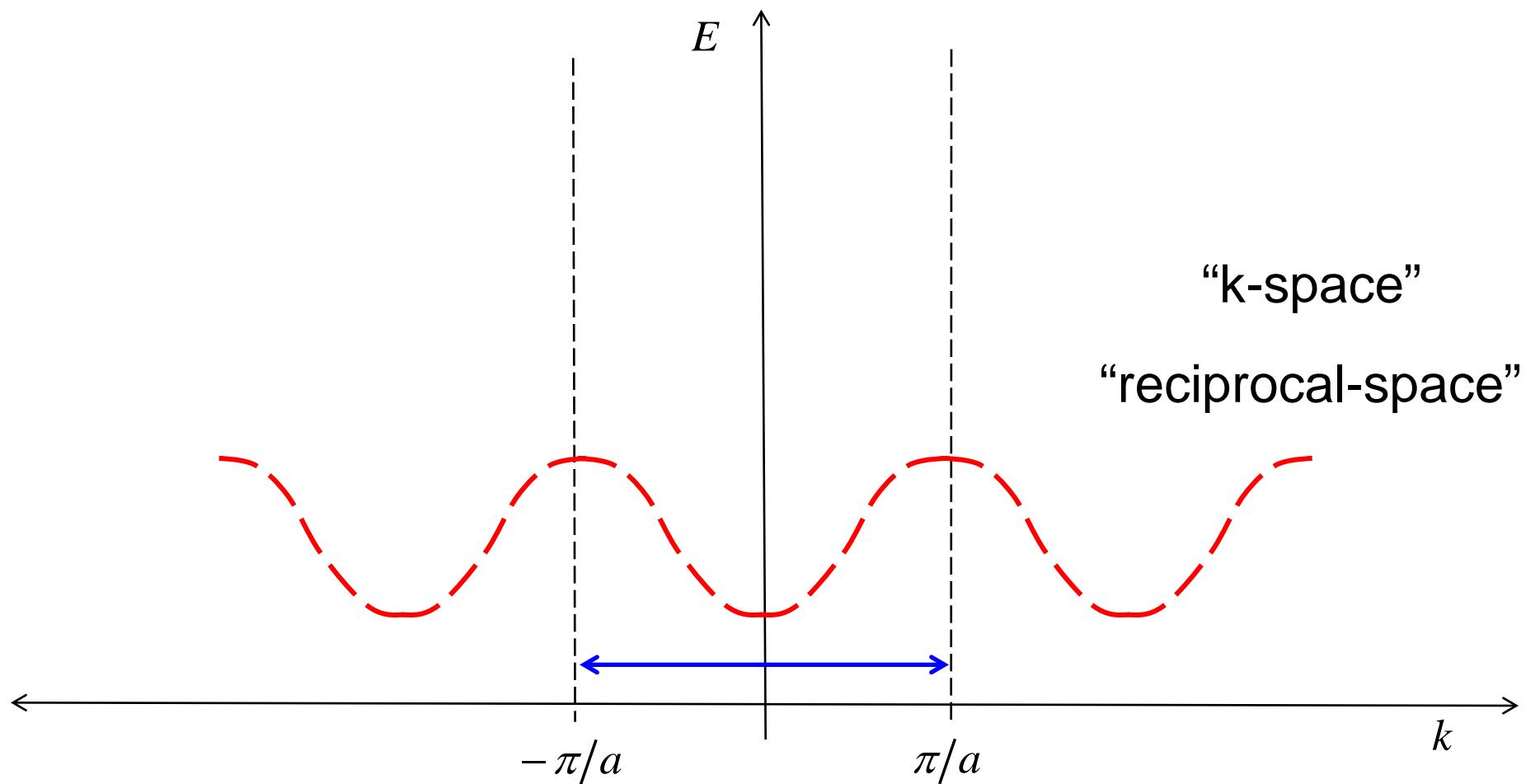
# Quantum reflection



**The potential must change slowly** (on the scale of the electron's wavelength) to treat the electron as a classical particle.

# Solutions are periodic in k-space

---



Brillouin zone

Lundstrom: 2018

# Reduced zone and effective mass

Near a band minimum or maximum,  $E(k)$  is a parabola.

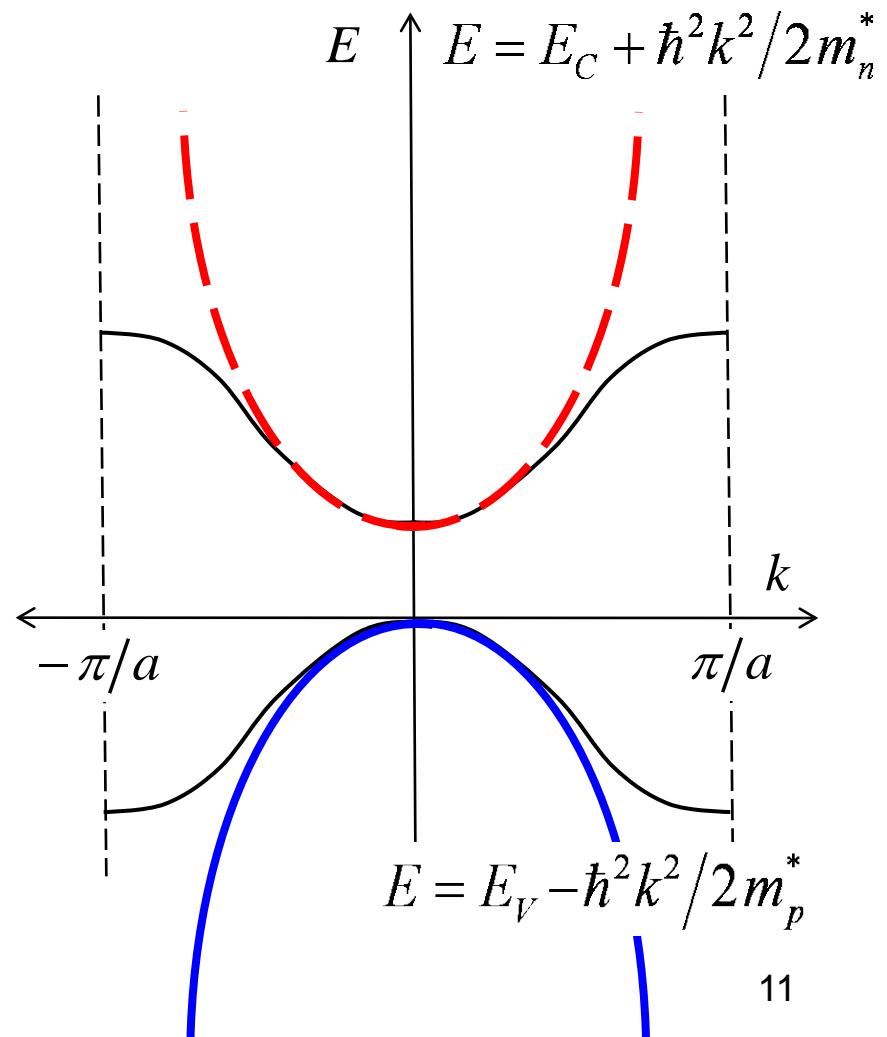
$$E \approx E_C + \hbar^2 k^2 / 2m_n^*$$

The curvature of the parabola is related to the **effective mass**.

$$m^* = \left( d^2 E / d(\hbar k)^2 \right)^{-1}$$

The **group velocity** is related to the crystal momentum and effective mass:

$$v_g(k) = \frac{1}{\hbar} \frac{dE(k)}{dk} = \frac{\hbar k}{m^*}$$



# Mobile electrons in crystals

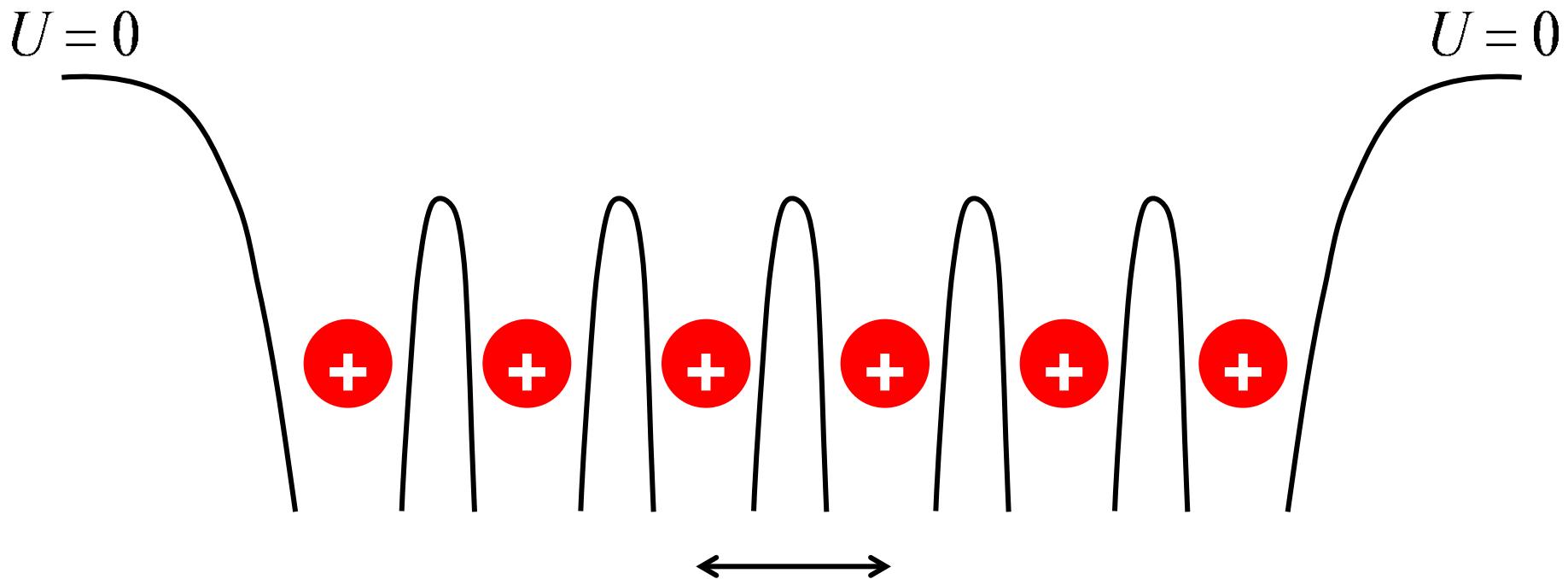


$$E(k) = \hbar^2 k^2 / 2m^*$$

$$p = \hbar k$$

$$v_g = (1/\hbar) dE/dk = \hbar k / m^*$$

$$F = dp/dt$$



# Summary

---

- 1) The crystal potential varies rapidly on an atomic scale. It determines the effective mass.
- 2) If the applied potential varies rapidly on the scale of the electron's wavelength, then we must solve a wave equation (e.g. semiconductor quantum wells)

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

- 3) If the applied potential varies slowly on the scale of the electron's wavelength, then we can treat electrons as classical particles with an effective mass.

$$E(k) = \hbar^2 k^2 / 2m^*$$

$$p = \hbar k$$

$$v_g = \hbar k / m^*$$

$$F = dp/dt$$

# Vocabulary

---

- |                          |                              |
|--------------------------|------------------------------|
| 1) Black body radiation  | 13) Brillouin zone           |
| 2) Photoelectric effect  | 14) Crystal momentum         |
| 3) De Broglie wavelength | 15) Band structure           |
| 4) Wave equation         | 16) Effective mass           |
| 5) Phase velocity        | 17) Kane bands               |
| 6) Group velocity        | 18) Spherical energy bands   |
| 7) Wavevector            | 19) Ellipsoidal energy bands |
| 8) Uncertainty relations | 20) Density of states (DOS)  |
| 9) Tunneling             | 21) Valley degeneracy        |
| 10) Quantum reflection   | 22) DOS effective mass       |
| 11) Crystal potential    |                              |
| 12) Bloch wave           |                              |

# Primer on Semiconductors

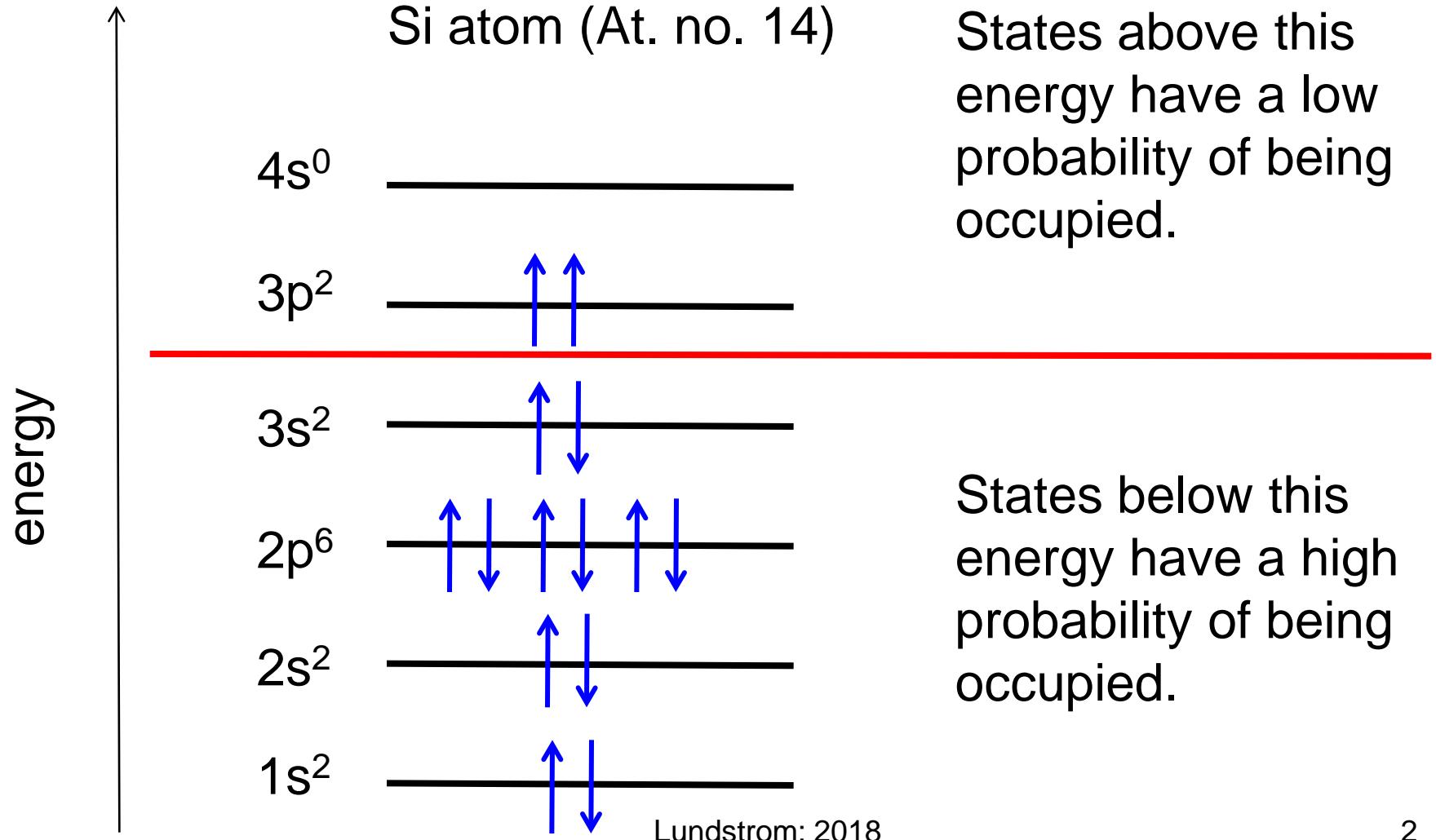
## Unit 3: Equilibrium Carrier Concentrations

### Lecture 3.1: The Fermi function

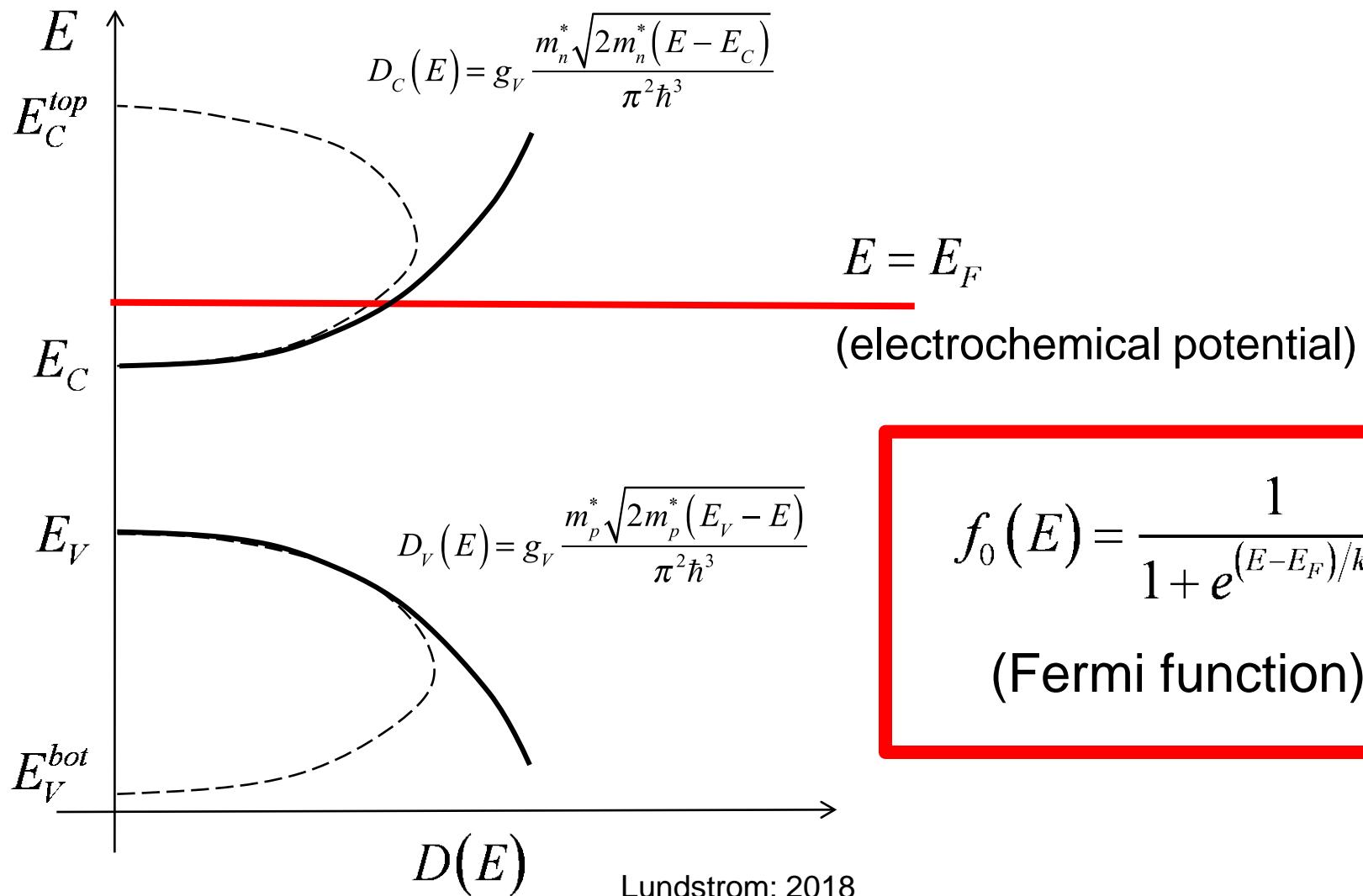
**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Occupation of states



# Fermi level

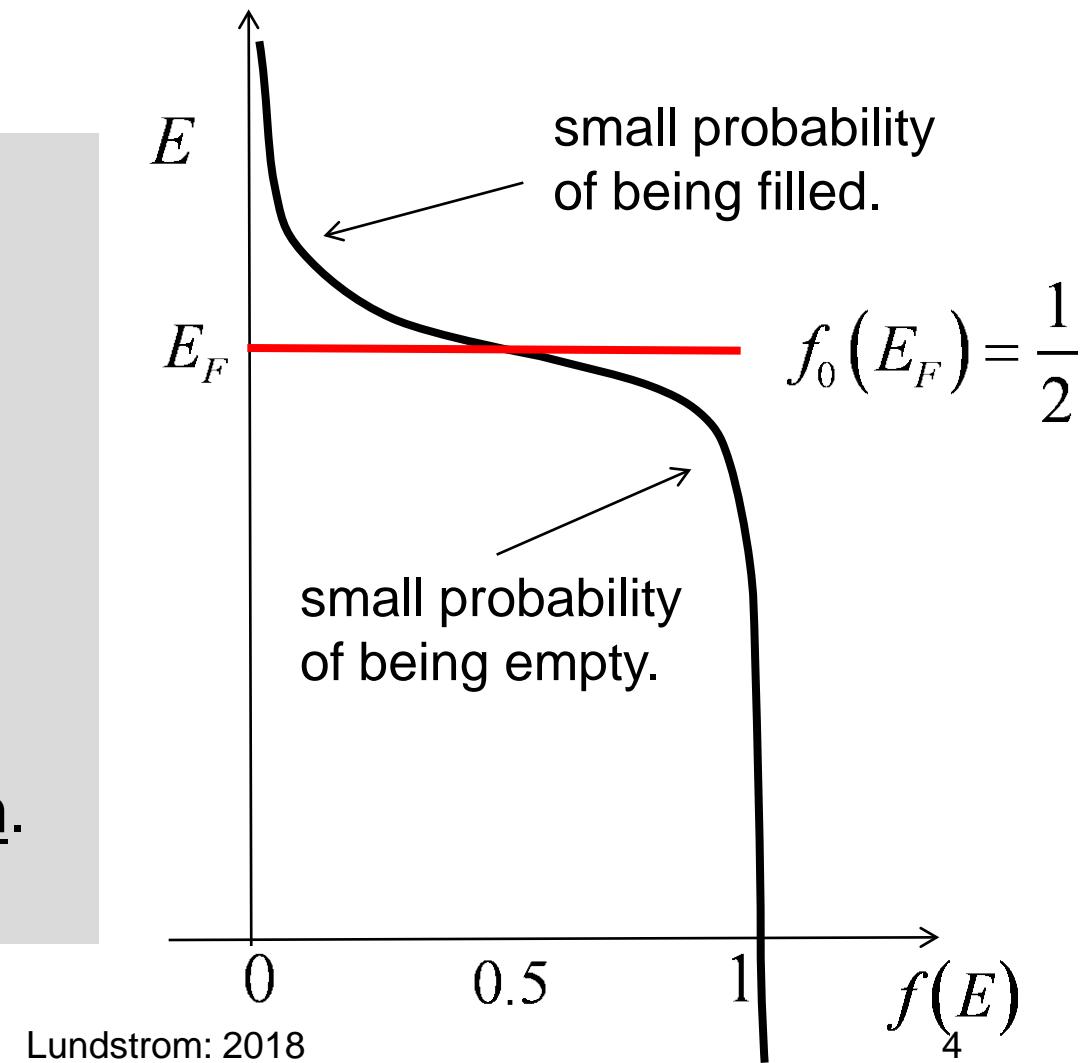


# The Fermi function

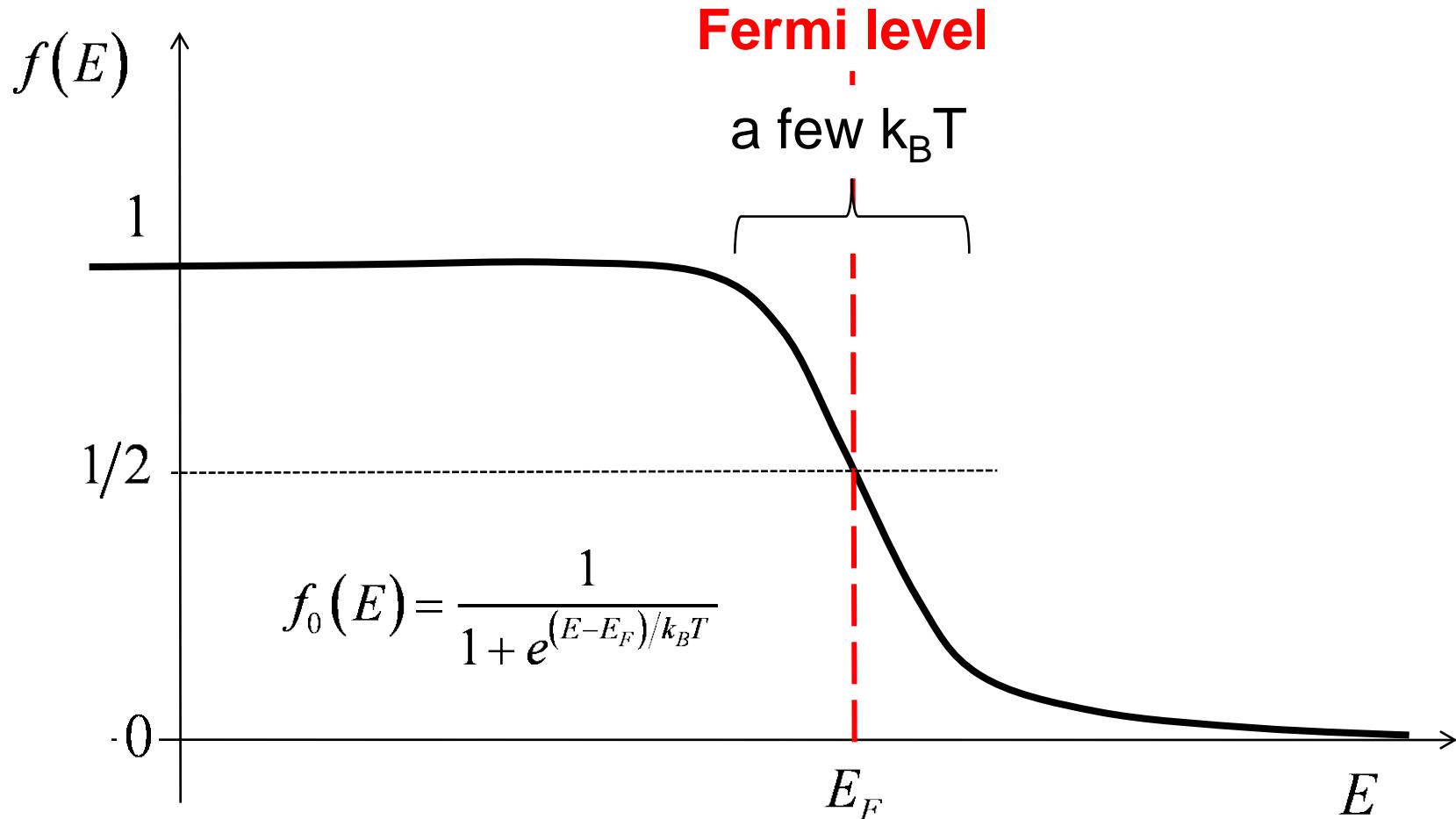
$$f_0(E) = \frac{1}{1 + e^{(E-E_F)/k_B T}}$$

## Fermi function

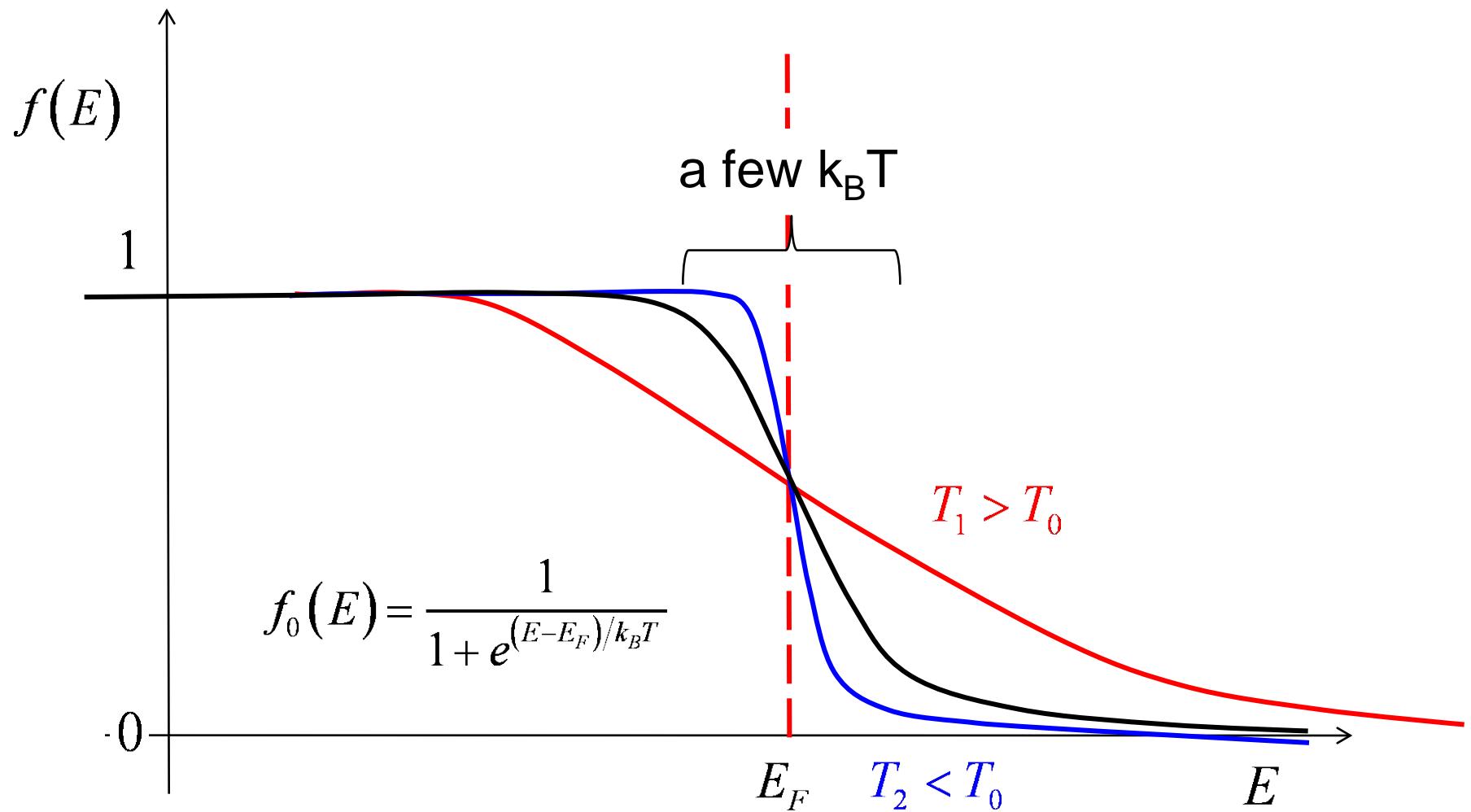
Probability that a state at energy,  $E$ , is occupied in equilibrium.



# More about the Fermi function



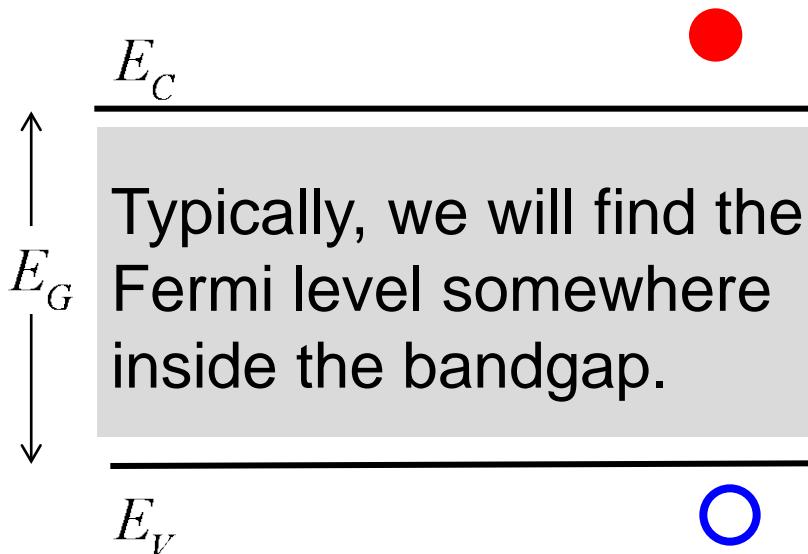
# Effect of temperature



# Electrons and holes

---

These states are way above the Fermi level.

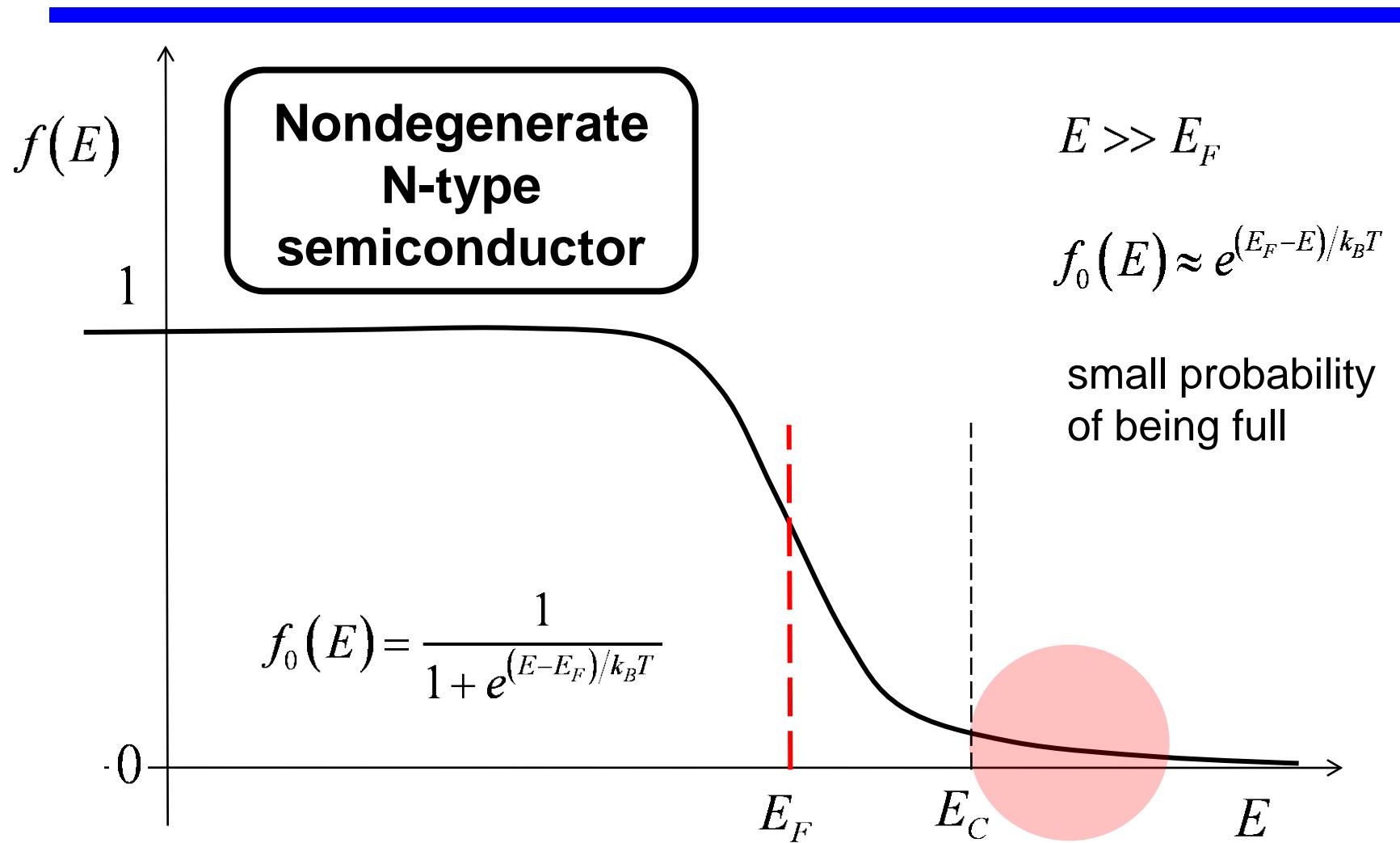


These states are way below the Fermi level.

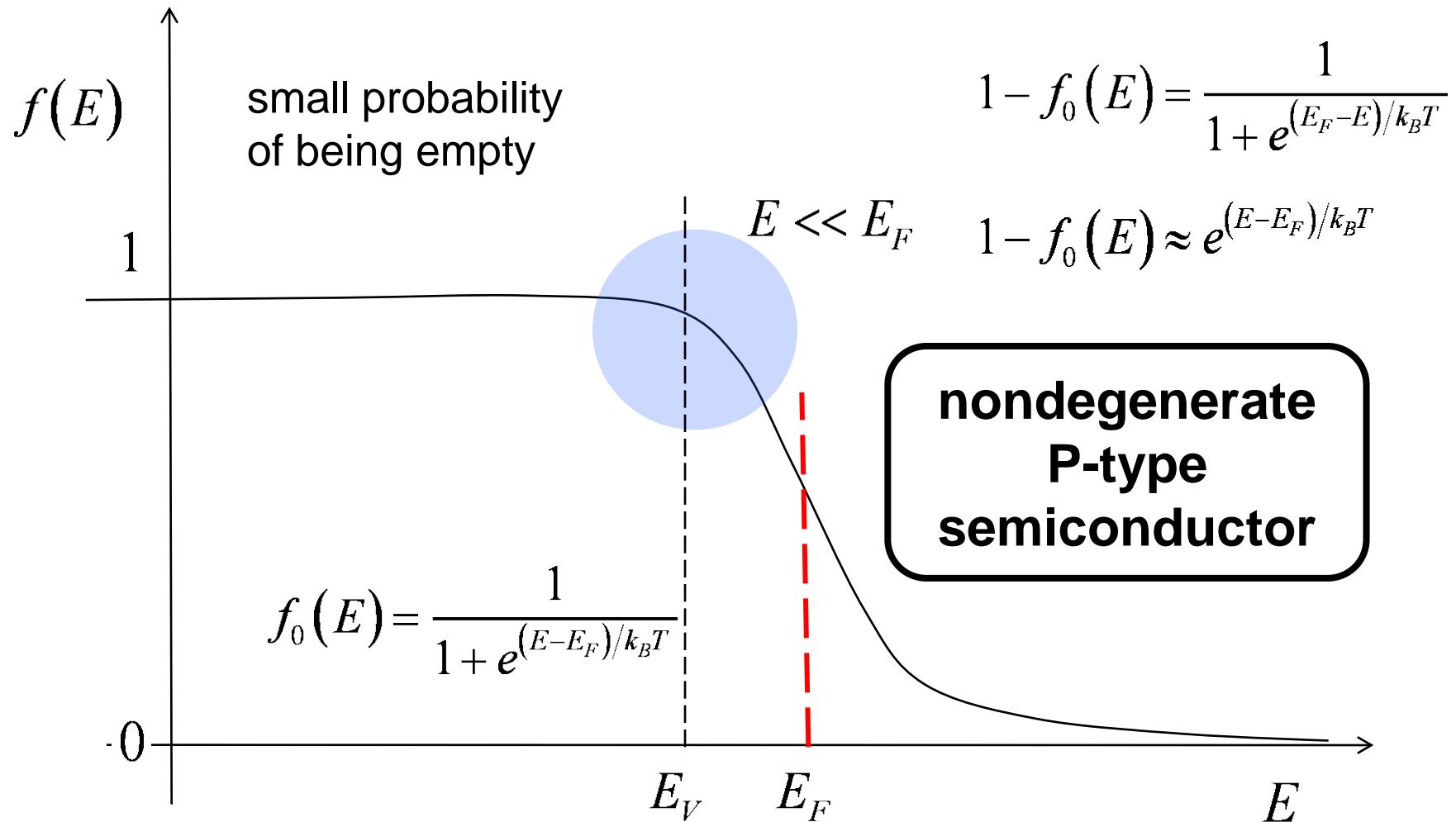
← A few states near  $E_C$  may be occupied.

← A few states near  $E_V$  may be empty.

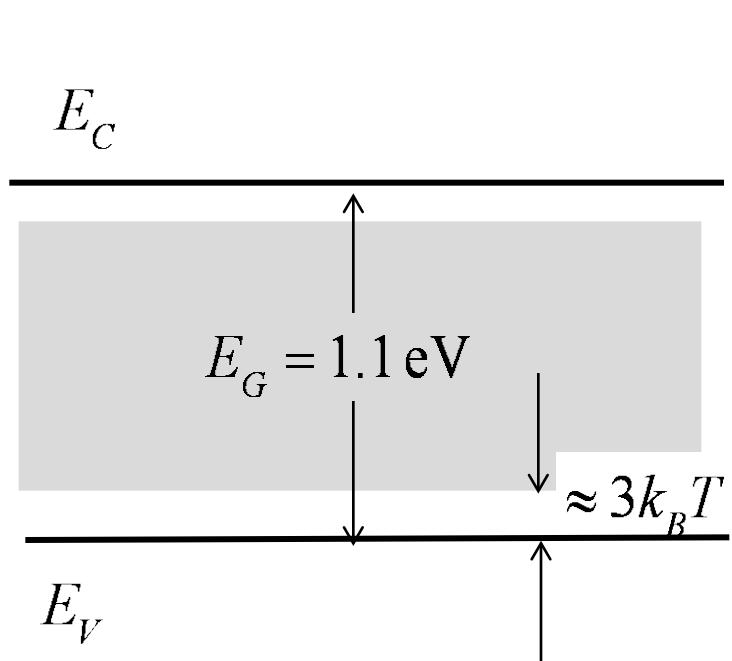
# Conduction band



# Valence band



# Nondegenerate semiconductors



$$f_0(E_C) = \frac{1}{1 + e^{(E_C - E_F)/k_B T}}$$

$$f_0(E_C) \approx e^{(E_F - E_C)/k_B T}$$

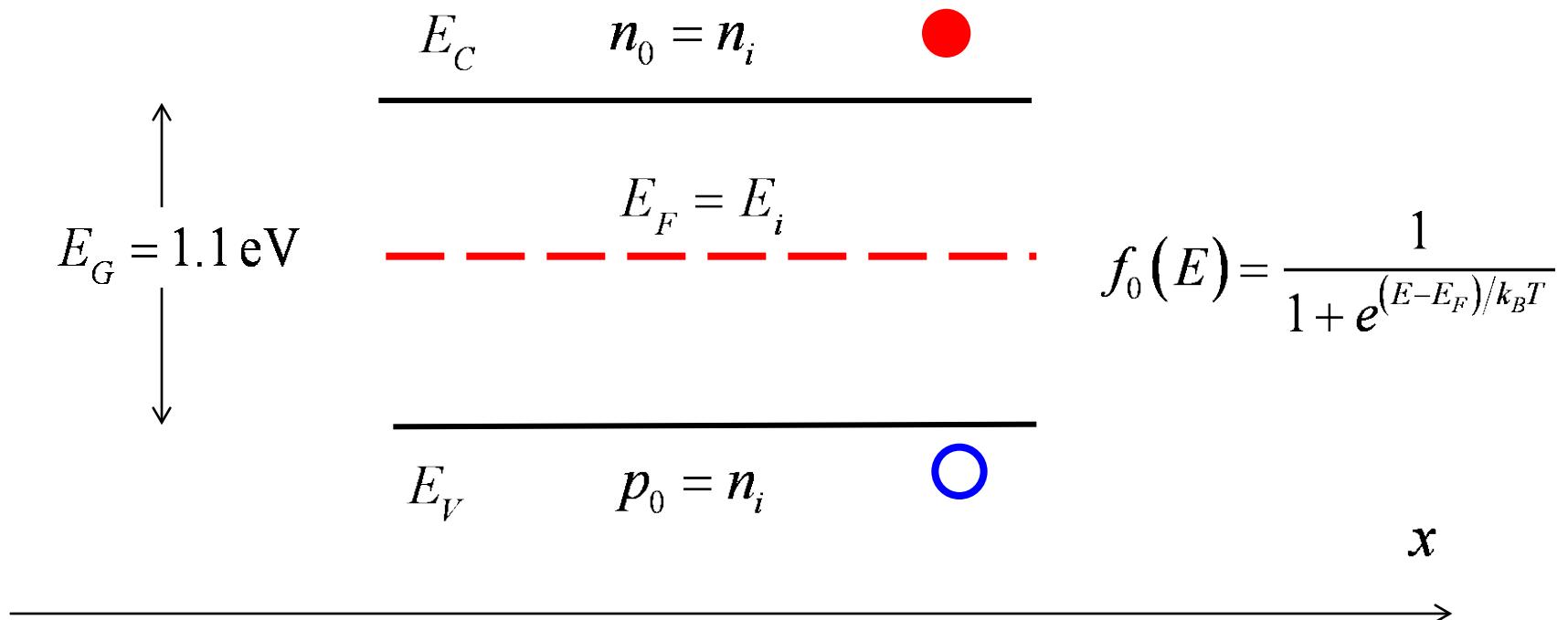
In a nondegenerate semiconductor, the Fermi level does not get too close to the band edges.

$$f_0(E_V) = \frac{1}{1 + e^{(E_V - E_F)/k_B T}}$$

$$1 - f_0(E_V) \approx e^{(E_V - E_F)/k_B T}$$

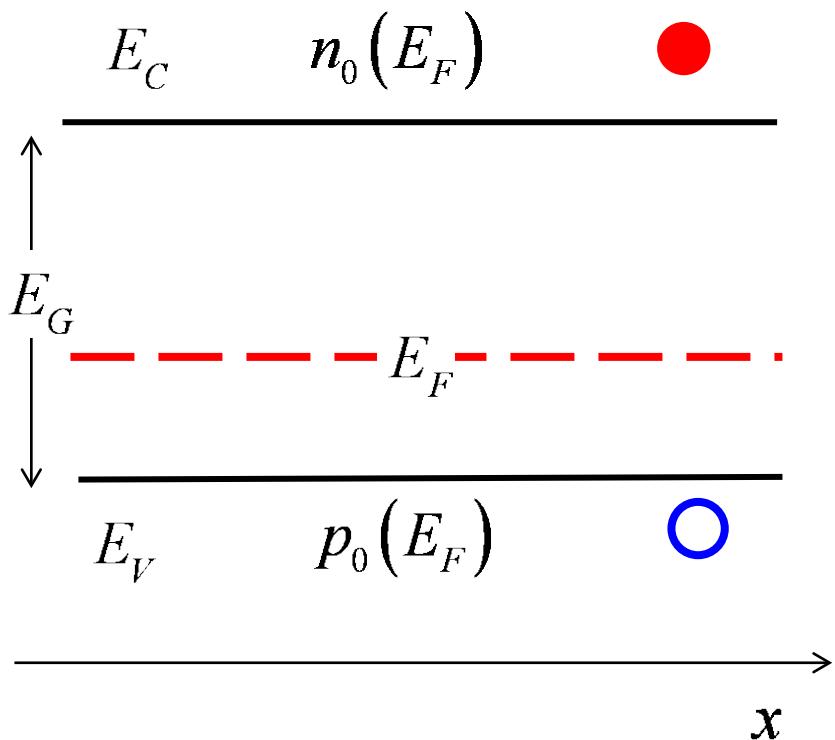
# Energy band diagram of an intrinsic semiconductor

---



# Energy band diagram and carrier densities

---



$$f_0(E) \approx e^{(E_F - E)/k_B T}$$

$$n_0 \propto e^{(E_F - E_C)/k_B T}$$

$$1 - f_0(E) \approx e^{(E_V - E_F)/k_B T}$$

$$p_0 \propto e^{(E_V - E_F)/k_B T}$$

# Summary

---

The Fermi function gives the probability that a state (if it exists) is occupied in equilibrium.

$$f_0(E) = \frac{1}{1 + e^{(E-E_F)/k_B T}}$$

(Fermi function)

The two key parameters in the Fermi function are the Fermi level and the temperature.

# Primer on Semiconductors

## Unit 3: Equilibrium Carrier Concentrations

### Lecture 3.2: Fermi-Dirac integrals

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# The Fermi function

---

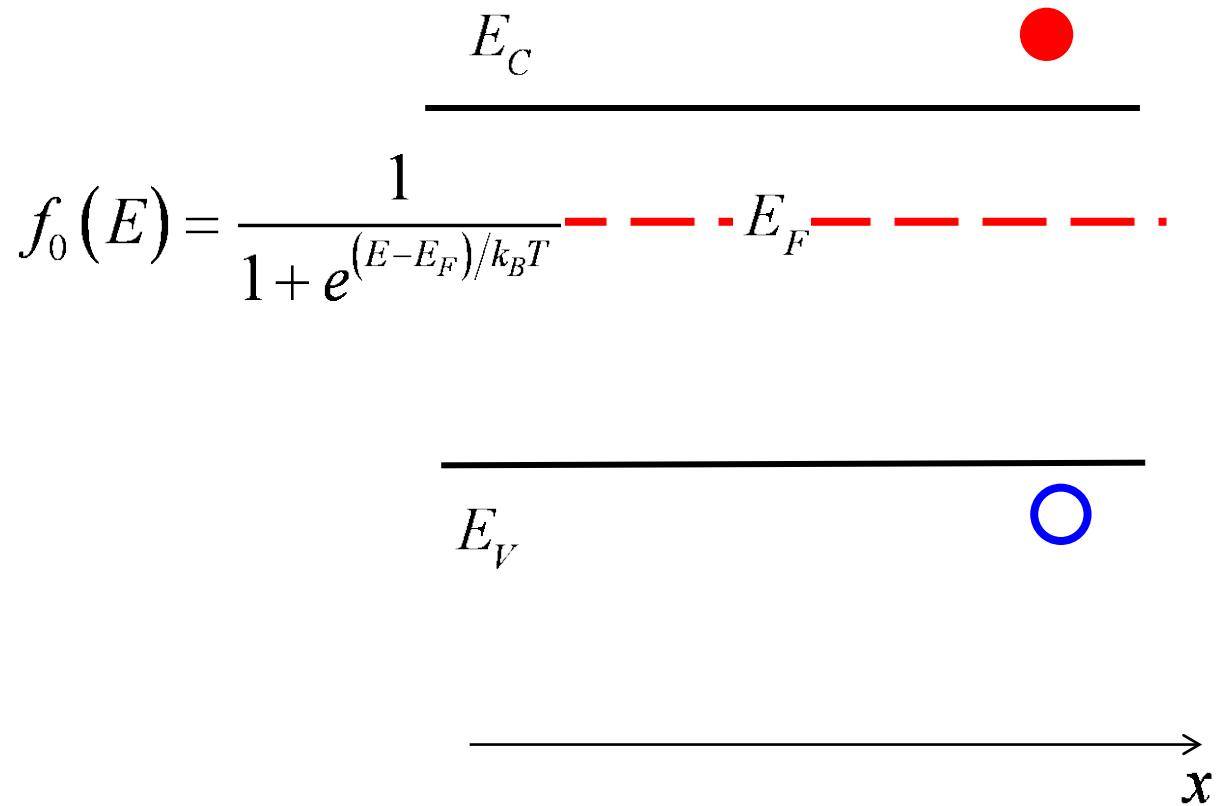
The Fermi function gives the probability that a state (if it exists) is occupied in equilibrium.

$$f_0(E) = \frac{1}{1 + e^{(E-E_F)/k_B T}}$$

(Fermi function)

The two key parameters in the Fermi function are the Fermi level and the temperature.

# Equilibrium carrier densities



nondegenerate  
semiconductor

# Two options

---

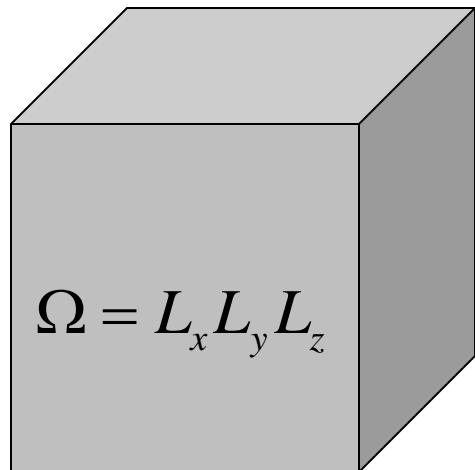
Our goal is to relate the equilibrium carrier density to the Fermi level and to the properties of the semiconductor.

We can do the calculation two ways:

- 1) In k-space
- 2) In energy space

# 3D bulk semiconductor: k-space

---

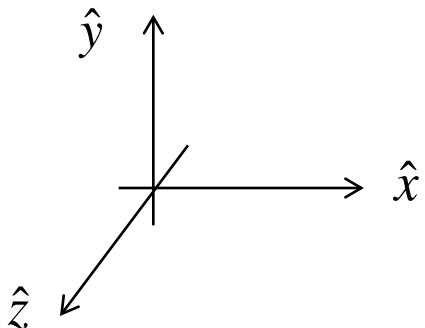


$$N = \sum_{\vec{k}} f_0(E_{\vec{k}})$$

$$n_0 = \frac{1}{\Omega} \sum_{\vec{k}} f_0(E_{\vec{k}})$$

$$\sum_{\vec{k}} \bullet \rightarrow \frac{\Omega}{4\pi^3} \int_{BZ} \bullet d^3k$$

$$n_0 = \frac{1}{\Omega} \int_{\vec{k}} f_0(E_{\vec{k}}) N_k d^3k$$



$$N_k = 2 \times \left( \frac{\Omega}{8\pi^3} \right) = \frac{\Omega}{4\pi^3}$$

# Density-of-states in k-space

---

1D:

$$N_k = 2 \times \left( \frac{L}{2\pi} \right) = \frac{L}{\pi} dk$$

2D:

$$N_k = 2 \times \left( \frac{A}{4\pi^2} \right) = \frac{A}{2\pi^2} dk_x dk_y$$

3D:

$$N_k = 2 \times \left( \frac{\Omega}{8\pi^3} \right) = \frac{\Omega}{4\pi^3} dk_x dk_y dk_z$$

**$N_k$   
independent of  $E(k)$**

$$\sum_{\vec{k}} \bullet \rightarrow N_k \int_{BZ} \bullet dk$$

(Should include valley degeneracy factor,  $g_V$ .)

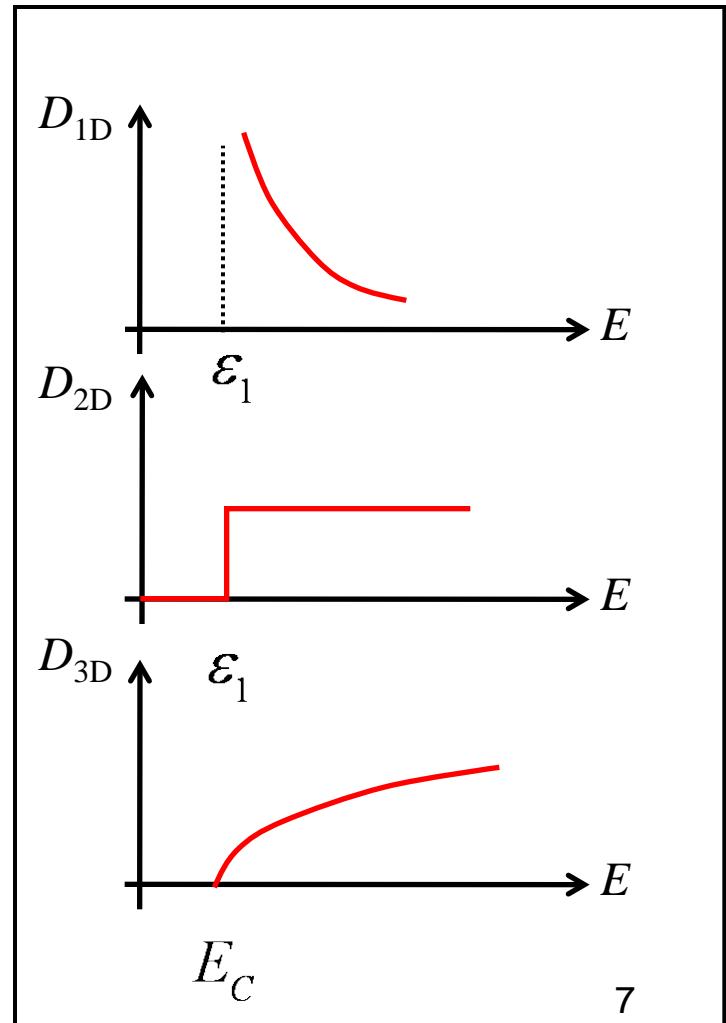
# Energy space (parabolic bands)

$$D_{1D}(E) = g_V \frac{1}{\pi \hbar} \sqrt{\frac{2m^*}{(E - \varepsilon_1)}} \Theta(E - \varepsilon_1)$$

$$D_{2D}(E) = g_V \frac{m^*}{\pi \hbar^2} \Theta(E - \varepsilon_1)$$

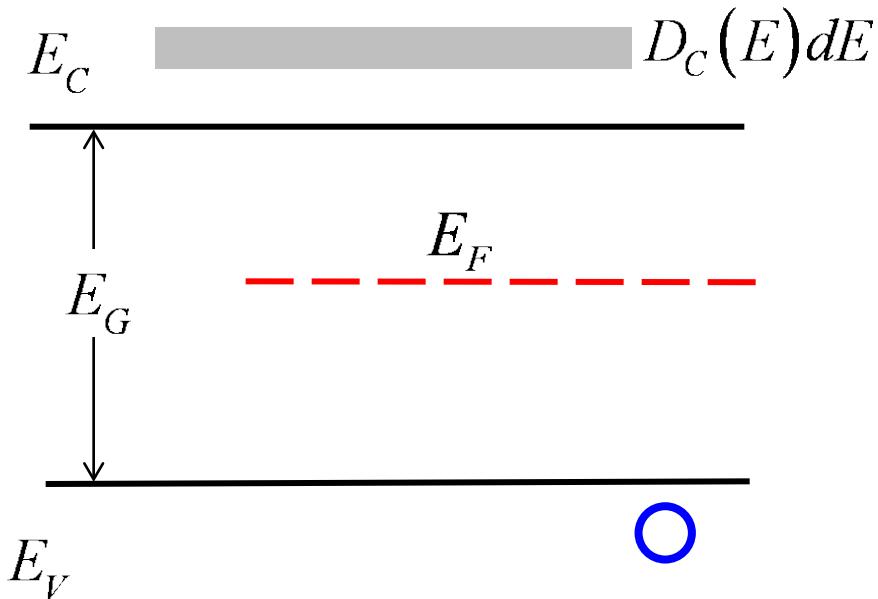
$$D_{3D}(E) = g_V \frac{m^* \sqrt{2m^*(E - E_C)}}{\pi^2 \hbar^3} \Theta(E - E_C)$$

$(E(k) = E_C + \hbar^2 k^2 / 2m^*)$  Lundstrom: 2018



# Distribution of electrons in the conduction band

---



$$n_0(E)dE = f_0(E)D_C(E)dE$$

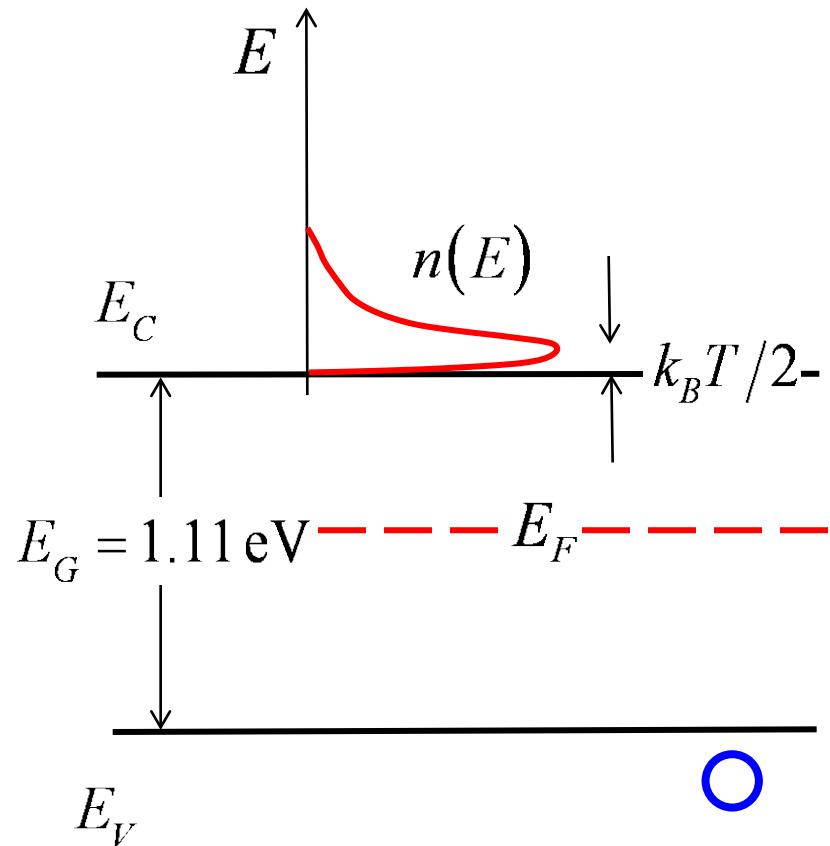
$$f_0(E) = \frac{1}{1 + e^{(E-E_F)/k_B T}}$$

$$f_0(E) \approx e^{-(E-E_F)/k_B T}$$

$$D_C(E) \propto \sqrt{E - E_C}$$

$$n_0(E)dE \propto \sqrt{E - E_C} e^{-(E-E_F)/k_B T} dE$$

# Distribution of electrons in the conduction band



***Electrons and holes are very near the band edges.***

$$n_0(E) \propto \sqrt{E - E_C} e^{-(E-E_F)/k_B T}$$

$$\frac{dn_0(E)}{dE} = 0$$

$$E = k_B T / 2$$

$$E = 0.013 \text{ eV} \quad T = 300 \text{ K}$$

# Compute the electron density

---

$$n_0 = \int_{E_C}^{\infty} n_0(E) dE = \int_{E_C}^{\infty} f_0(E) D_C(E) dE$$

$$f_0(E) = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

$$D_C(E) = g_V \frac{m_n^* \sqrt{2m_n^*(E - E_C)}}{\pi^2 \hbar^3}$$

Fermi level and  
temperature

effective mass and  
valley degeneracy

# Energy space (3D)

$$n_0 = \int_{E_C}^{\infty} f_0(E) D_C(E) dE$$

$$n_0 = \frac{(2m^*)^{3/2}}{2\pi^2 \hbar^3} \int_{E_C}^{\infty} \frac{(E - E_C)^{1/2}}{1 + e^{(E - E_F)/k_B T}} dE$$

$$n_0 = \frac{(2m^* k_B T)^{3/2}}{2\pi^2 \hbar^3} \int_0^{\infty} \frac{\eta^{1/2} d\eta}{1 + e^{\eta - \eta_F}}$$

$$n_0 = N_C \mathcal{F}_{1/2}(\eta_F) \text{cm}^{-3}$$

$$f_0(E) = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

$$D_C(E) = \frac{(2m^*)^{3/2}}{2\pi^2 \hbar^3} (E - E_C)^{1/2}$$

$$\eta_F = (E_F - E_C)/k_B T$$

$$\eta = (E - E_C)/k_B T$$

$$N_C = \frac{1}{4} \left( \frac{2m^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

# Fermi-Dirac integrals

---

$$\mathcal{F}_j(\eta_F) \equiv \frac{1}{\Gamma(j+1)} \int_0^{\infty} \frac{\eta^j d\eta}{1 + e^{\eta - \eta_F}}$$

$$\Gamma(n) = (n-1)! \quad (n \text{ integer})$$

$$\Gamma(1/2) = \sqrt{\pi}$$

$$\Gamma(p+1) = p\Gamma(p)$$

$$\mathcal{F}_j(\eta_F) \rightarrow e^{\eta_F} \quad \eta_F \ll 0$$

$$(E_F - E_C)/k_B T \ll 0$$

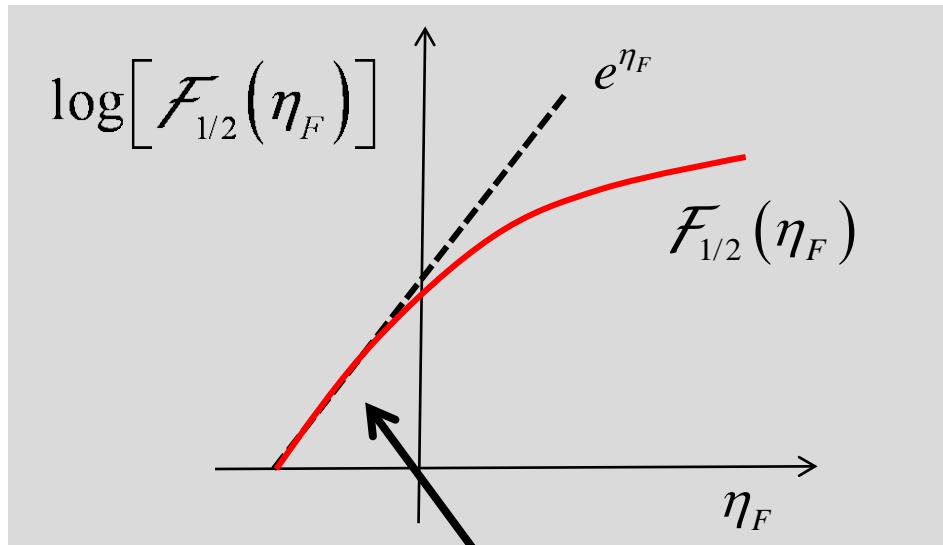
nondegenerate semiconductor

$$\frac{d\mathcal{F}_j}{d\eta_F} = \mathcal{F}_{j-1}$$

don't confuse with....  $F_j(\eta) = \int_0^{+\infty} \frac{x^j dx}{1 + e^{x-\eta}}$

For an introduction to Fermi-Dirac integrals, see: "Notes on Fermi-Dirac Integrals," 4rd Ed., by R. Kim and M. Lundstrom) <https://www.nanohub.org/resources/5475>

# Fermi-Dirac integral of order 1/2



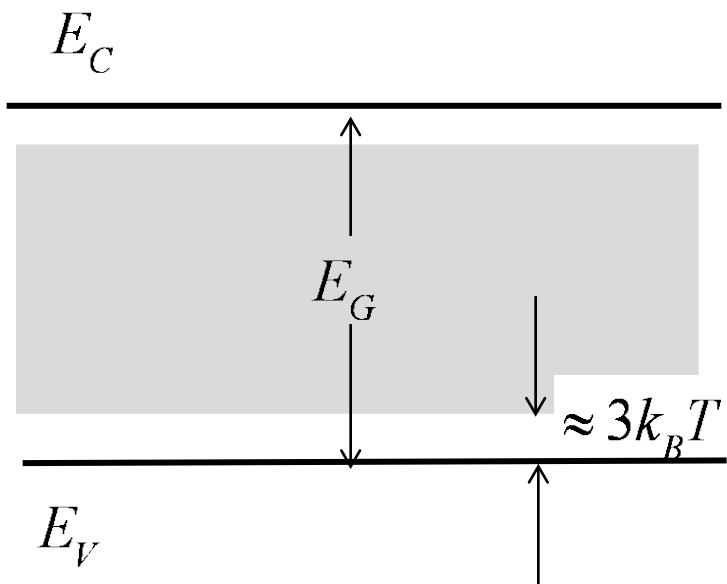
$$\mathcal{F}_{1/2}(\eta_F) \equiv \frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{\eta^{1/2} d\eta}{1 + e^{\eta - \eta_F}}$$
$$\eta_F = (E_F - E_C)/k_B T$$

$$\eta_F \ll 0 \quad E_F \ll E_C \quad \mathcal{F}_{1/2}(\eta_F) \rightarrow e^{\eta_F} \quad n_0 = N_C e^{\eta_F} \text{ cm}^{-3}$$

(nondegenerate semiconductor)

# Nondegenerate semiconductor

---



In a nondegenerate semiconductor, the Fermi level is well below the bottom of the conduction band and well above the top of the valence band.

# Compute the electron density

---

$$n_0 = N_C \mathcal{F}_{1/2}(\eta_F) \text{ cm}^{-3} \quad \eta_F = (E_F - E_C)/k_B T \quad N_C = \frac{1}{4} \left( \frac{2m^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

## Nondegenerate semiconductors:

$$\eta_F \ll 0$$

$$E_F \ll E_C$$

$$\mathcal{F}_{1/2}(\eta_F) \rightarrow e^{\eta_F}$$

$$n_0 = N_C e^{\eta_F} \text{ m}^{-3}$$

# Compute the hole density

$$p_0 = \int_{-\infty}^{E_V} [1 - f_0(E)] D_V(E) dE$$

$$f_0(E) = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

$$D_V(E) = g_V \frac{m_p^* \sqrt{2m_p^*(E_V - E)}}{\pi^2 \hbar^3}$$

$$p_0 = N_V \mathcal{F}_{1/2}(\eta_F) \text{ m}^{-3} \quad \eta_F = (E_V - E_F) / k_B T \quad N_V = \frac{1}{4} \left( \frac{2m_p^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

**Nondegenerate semiconductor:**

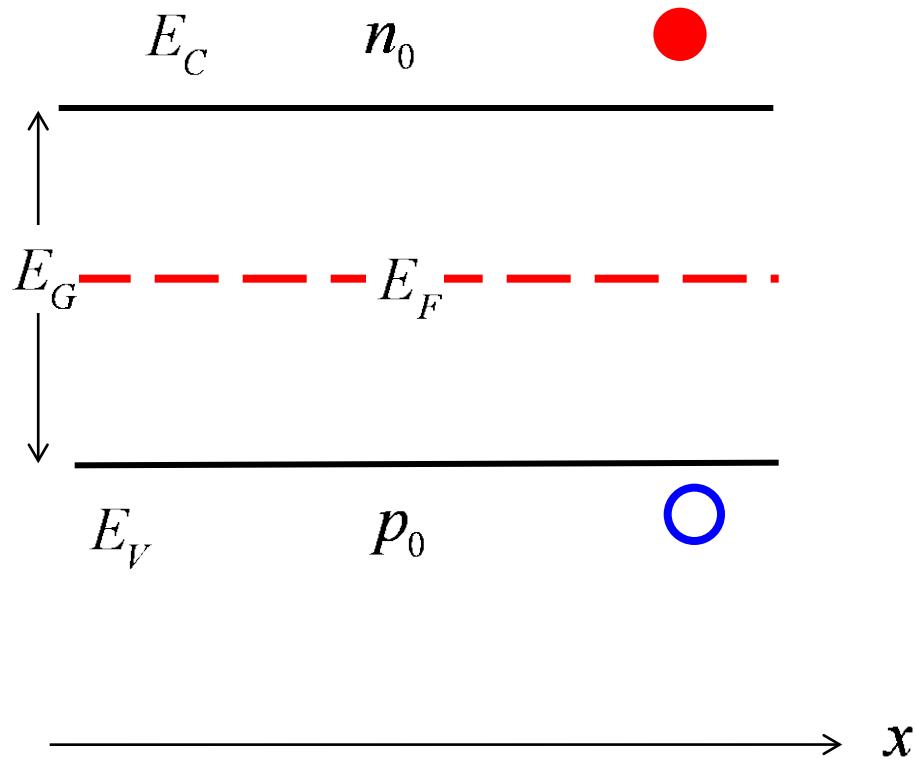
$$\eta_F \ll 0$$

$$E_F \gg E_V$$

$$\mathcal{F}_{1/2}(\eta_F) \rightarrow e^{\eta_F}$$

$$p_0 = N_V e^{\eta_F} \text{ m}^{-3}$$

# Summary



$$n_0 = N_C e^{(E_F - E_C)/k_B T}$$

$$p_0 = N_V e^{(E_V - E_F)/k_B T}$$

Nondegenerate  
semiconductor

# Primer on Semiconductors

## Unit 3: Equilibrium Carrier Concentrations

### Lecture 3.3: Carrier concentration vs. Fermi level

**Mark Lundstrom**

lundstro@purdue.edu

Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Carrier concentrations

Electrons

$$n_0 = N_C \mathcal{F}_{1/2} \left[ (E_F - E_C) / k_B T \right] \text{ m}^{-3}$$

$$N_C = \frac{1}{4} \left( \frac{2m_n^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

nondegenerate:

$$n_0 = N_C e^{(E_F - E_C) / k_B T}$$

Holes

$$p_0 = N_V \mathcal{F}_{1/2} \left[ (E_V - E_F) / k_B T \right] \text{ m}^{-3}$$

$$N_V = \frac{1}{4} \left( \frac{2m_p^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

nondegenerate:

$$p_0 = N_V e^{(E_V - E_F) / k_B T}$$

# Electron concentration

---

## Electrons

$$n_0 = N_C \mathcal{F}_{1/2} \left[ (E_F - E_C) / k_B T \right] \text{ m}^{-3}$$

$$N_C = \frac{1}{4} \left( \frac{2m_D^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

nondegenerate:

$$n_0 = N_C e^{(E_F - E_C) / k_B T}$$

For Si at  $T = 300\text{K}$ :

$$m_D^* = 1.182 m_0 \text{ (DOS effective mass)}$$

$$N_C = 3.23 \times 10^{19} \text{ cm}^{-3}$$

# Hole concentration

For Si at  $T = 300\text{K}$ :

$$m_p^* = 0.81m_0 \text{ (DOS effective mass)}$$

$$N_V = 1.83 \times 10^{19} \text{ cm}^{-3}$$

## Holes

$$p_0 = N_V \mathcal{F}_{1/2} \left[ (E_V - E_F) / k_B T \right] \text{ m}^{-3}$$

$$N_V = \frac{1}{4} \left( \frac{2m_p^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

nondegenerate:

$$p_0 = N_V e^{(E_V - E_F) / k_B T}$$

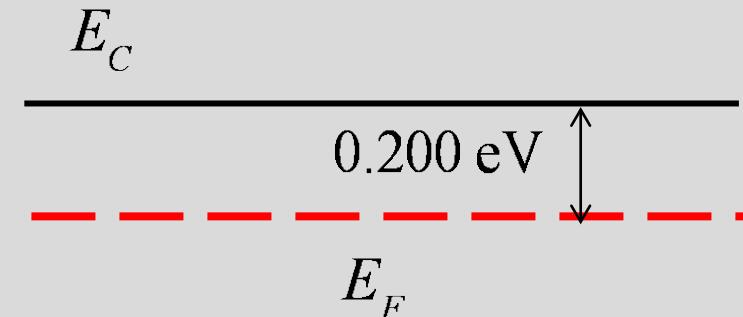
# Fermi level and electron concentration

Given the Fermi level, we can deduce the **electron** and hole concentrations.

$$n_0 = N_C \exp\left(\frac{(E_F - E_C)}{k_B T}\right)$$

$$N_C = 3.23 \times 10^{19} \text{ cm}^{-3}$$

(silicon at 300 K)



$$\begin{aligned} n_0 &= N_C \exp\left(\frac{-0.200}{0.026}\right) \\ &= N_C \exp(-7.69) \\ &= N_C \times 4.56 \times 10^{-4} \\ &= 1.47 \times 10^{16} \text{ cm}^{-3} \end{aligned}$$

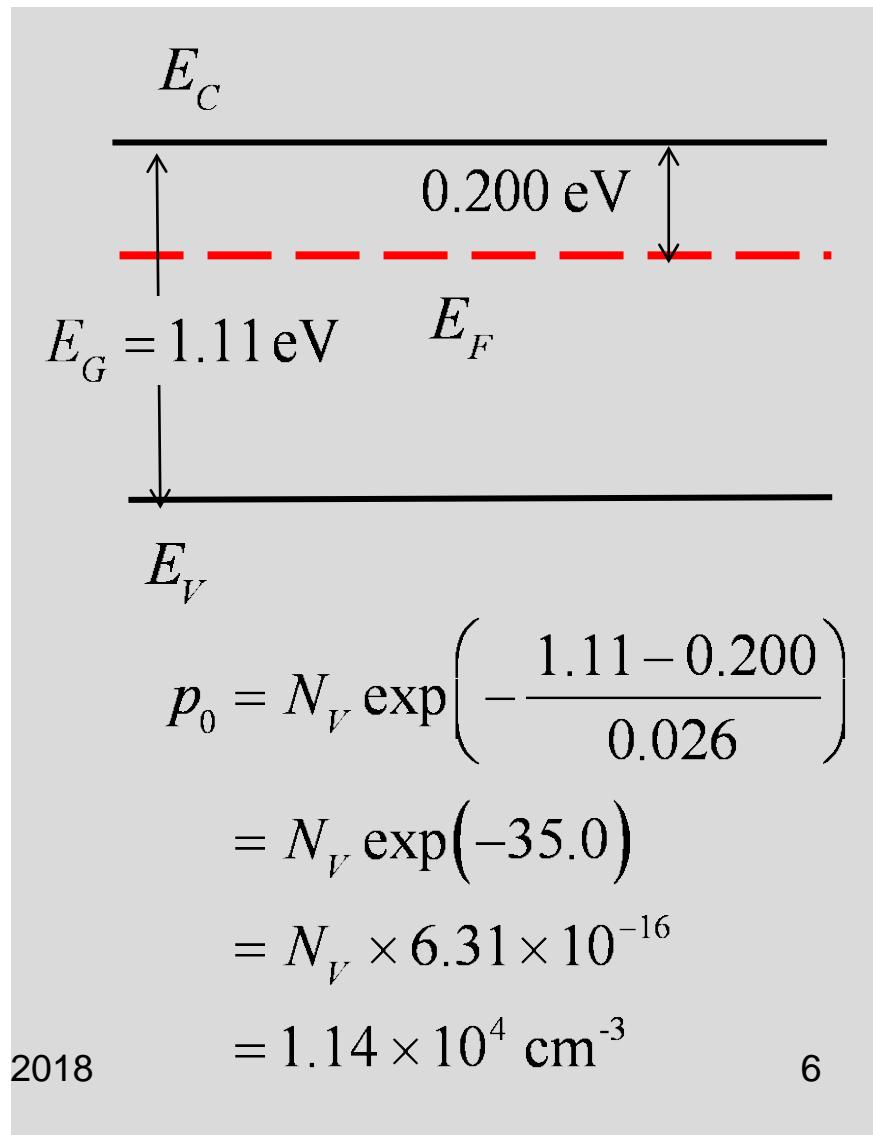
# Fermi level and hole concentration

Given the Fermi level, we can deduce the electron and **hole** concentrations.

$$p_0 = N_V \exp\left(\frac{(E_V - E_F)}{k_B T}\right)$$

$$N_V = 1.83 \times 10^{19} \text{ cm}^{-3}$$

(silicon at 300 K)



# From carrier concentration to Fermi level

---

If we are given  $n$ :

$$n_0 = N_C e^{(E_F - E_C)/k_B T}$$

$$p_0 = N_V e^{(E_V - E_F)/k_B T}$$

$$E_F = E_C + k_B T \ln\left(\frac{n_0}{N_C}\right)$$

If we are given  $p$ :

$$E_F = E_V - k_B T \ln\left(\frac{p_0}{N_V}\right)$$

# np product

---

The equilibrium product of the electron and hole concentrations is a **very important** quantity for a semiconductor.

# np product

---

$$n_0 p_0 = N_C e^{(E_F - E_C)/k_B T} N_V e^{(E_V - E_F)/k_B T}$$

$$n_0 p_0 = N_C N_V e^{(E_V - E_C)/k_B T}$$

$$n_0 p_0 = N_C N_V e^{-E_G/k_B T} = n_i^2$$

$$n_i = \sqrt{N_C N_V} e^{-E_G/2k_B T}$$

$$n_0 = N_C e^{(E_F - E_C)/k_B T}$$

$$p_0 = N_V e^{(E_V - E_F)/k_B T}$$

$$N_C = 2 \left[ \frac{(m_n^* k_B T)}{2\pi\hbar^2} \right]^{3/2}$$

$$N_V = 2 \left[ \frac{(m_p^* k_B T)}{2\pi\hbar^2} \right]^{3/2}$$

# np product

---

$$n_0 p_0 = n_i^2$$

$$n_i = \sqrt{N_C N_V} e^{-E_G/2k_B T}$$

- Independent of Fermi level (for nondegenerate semiconductor)
- Depends exponentially on band gap
- Depends exponentially on temperature
- For Si at 300 K

$$n_i = 1.0 \times 10^{10} \text{ cm}^{-3}$$

# Recall: Fermi level and hole concentration

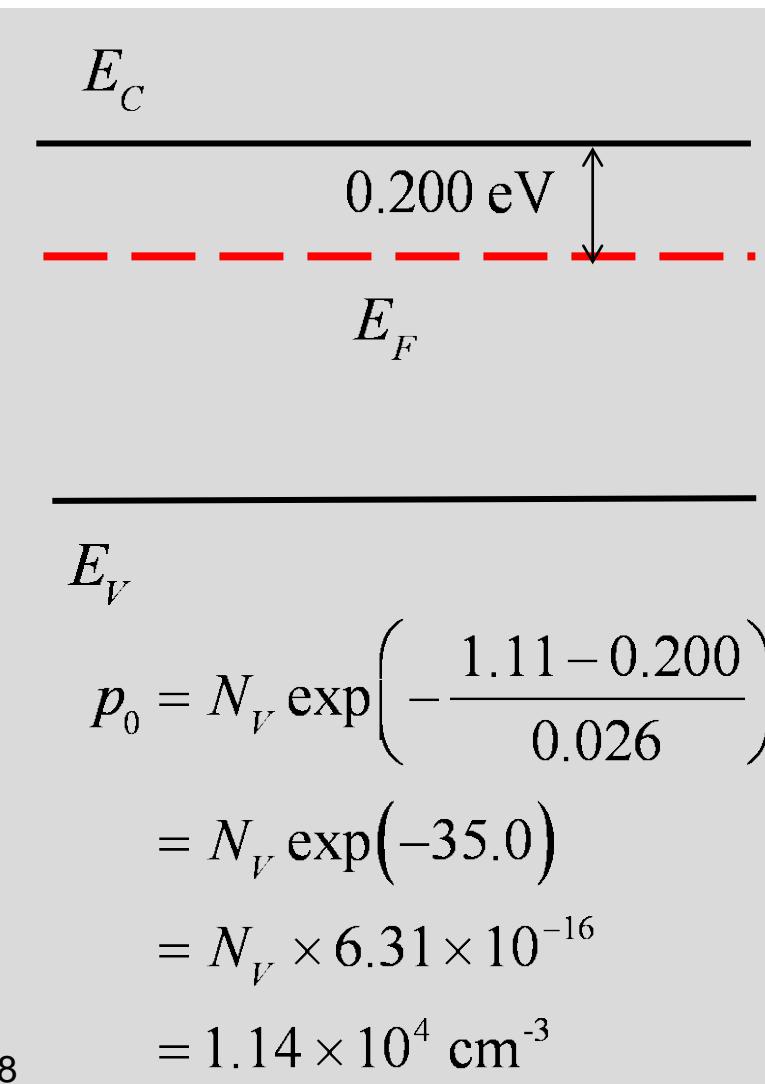
Given the Fermi level, we can deduce the electron and **hole** concentrations.

$$p_0 = N_V \exp\left(\frac{(E_V - E_F)}{k_B T}\right)$$

$$N_V = 1.83 \times 10^{19} \text{ cm}^{-3}$$

(silicon)

Lundstrom: 2018



## Another way

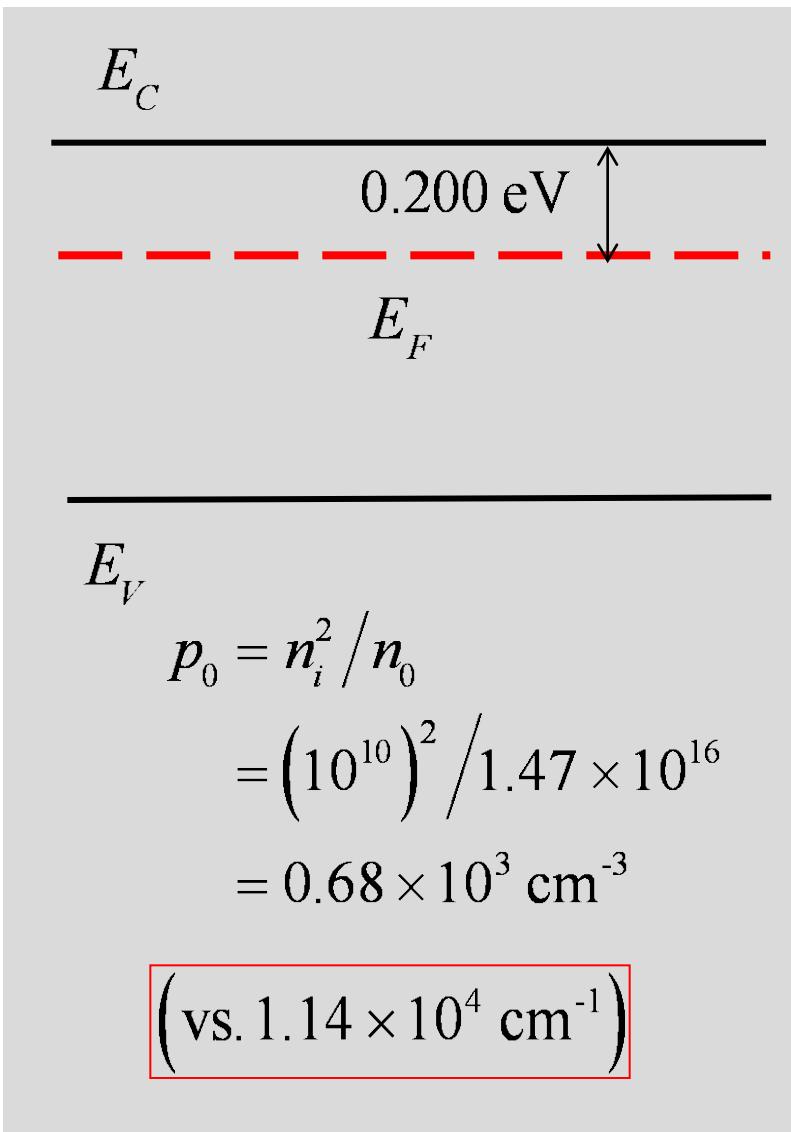
Find the electron concentration first.

$$n_0 = 1.47 \times 10^{16} \text{ cm}^{-3}$$

Then use

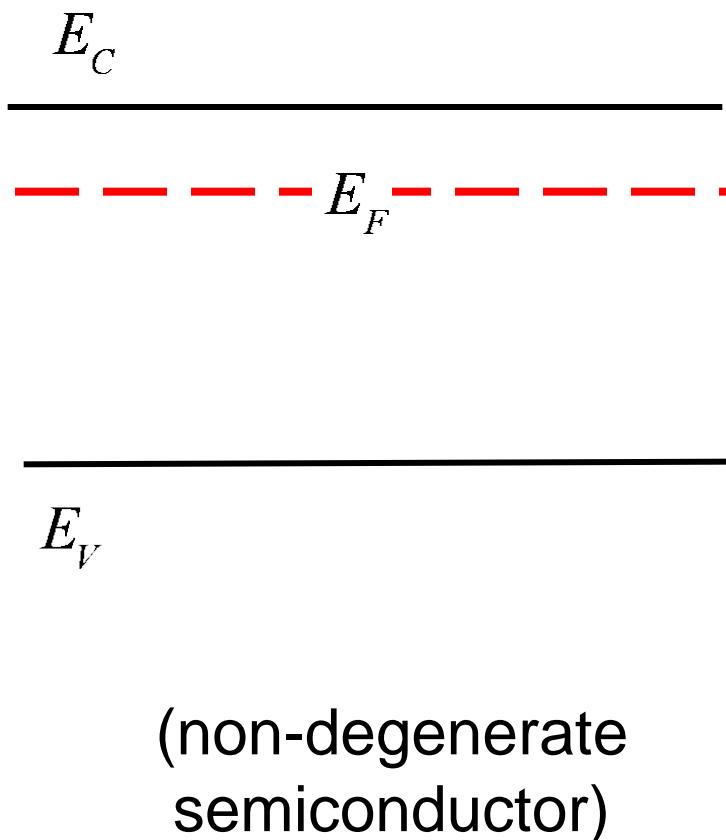
$$n_0 p_0 = n_i^2$$

$$n_i = \sqrt{N_C N_V} e^{-E_G/2k_B T} \neq 1.0 \times 10^{10} \text{ cm}^{-3}$$



# E-band diagram for N-type semiconductor

---



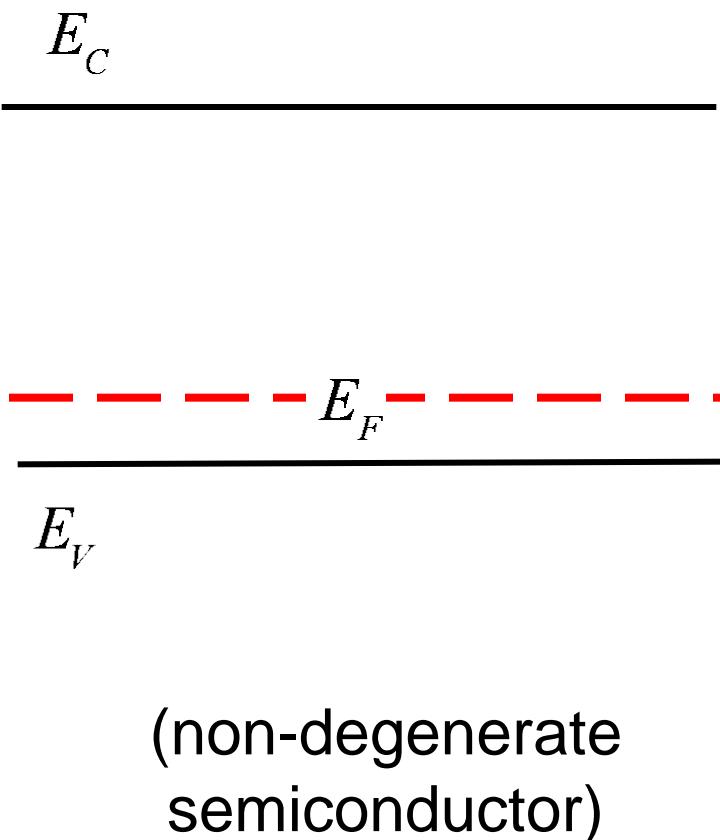
Fermi level is closer to the conduction band than to the valence band.

Electron concentration is greater than the hole concentration.  $n_0 > p_0$

But the  $np$  product does not change.  $n_0 p_0 = n_i^2$

# E-band diagram for P-type semiconductor

---



Fermi level is closer to the valence band than to the conduction band.

Hole concentration is greater than the electron concentration.  $p_0 > n_0$

But the  $np$  product does not change.  $n_0 p_0 = n_i^2$

# Intrinsic semiconductor

---

$E_C$

---

Fermi level is near the middle of the gap.

— — —  $E_F = E_i$  — — — .

---

Hole concentration is equal to the electron concentration.  $p_0 = n_0$

$E_V$

The  $np$  product is still the same.  $n_0 p_0 = n_i^2$

***Exactly where is the intrinsic Fermi level?***

# The intrinsic Fermi level

---

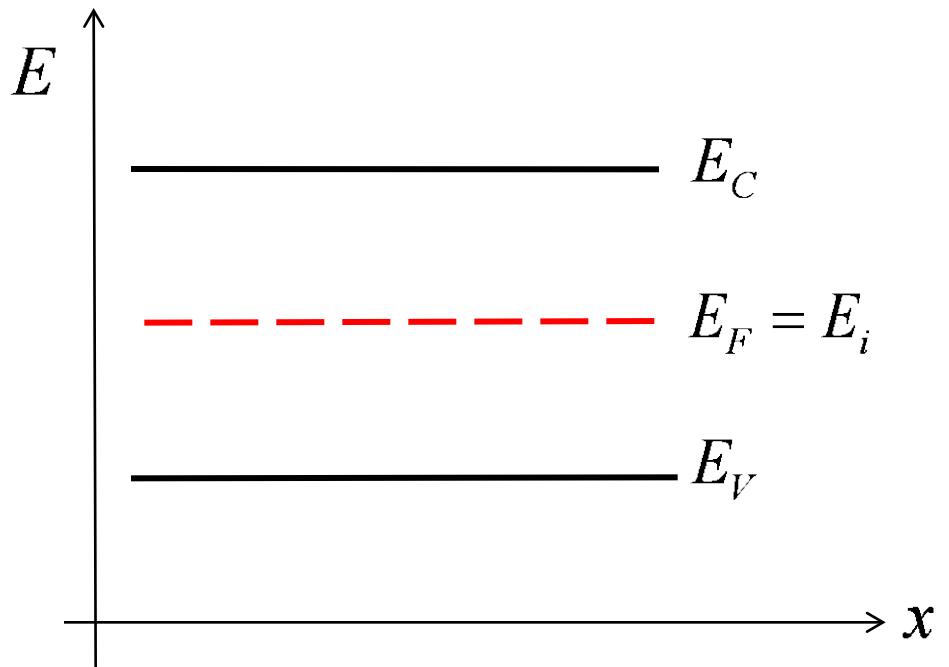
$$n_0 = N_C e^{(E_F - E_C)/k_B T}$$

$$p_0 = N_V e^{(E_V - E_F)/k_B T}$$

$$n_0 = p_0 = n_i \quad E_F = E_i$$

$$N_C e^{(E_i - E_C)/k_B T} = N_V e^{(E_V - E_i)/k_B T}$$

$$E_i = \frac{E_C + E_V}{2} + \frac{k_B T}{2} \ln\left(\frac{N_V}{N_C}\right)$$



# The intrinsic level: Silicon

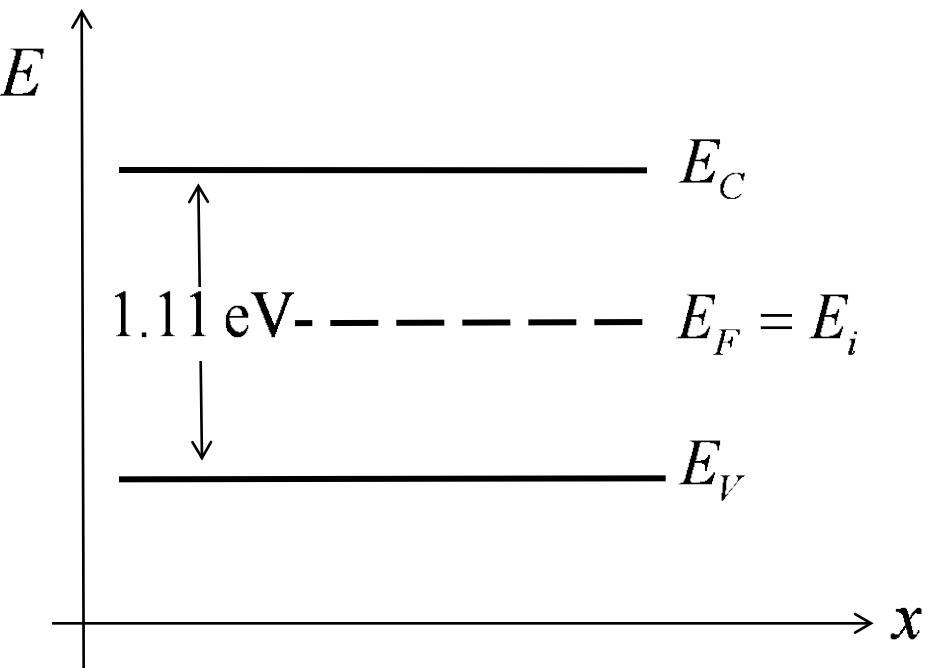
$$E_i = \frac{E_C + E_V}{2} + \frac{k_B T}{2} \ln\left(\frac{N_V}{N_C}\right)$$

$$N_C = 3.23 \times 10^{19} \text{ cm}^{-3}$$

$$N_V = 1.83 \times 10^{19} \text{ cm}^{-3}$$

$$T = 300 \text{ K}$$

$$E_i = \frac{E_C + E_V}{2} - 0.007 \text{ eV}$$



***The intrinsic level is very near the middle of the band gap.***

# Alternative expression for carrier densities

---

$$n_0 = N_C e^{(E_F - E_C)/k_B T}$$

$$p_0 = N_V e^{(E_V - E_F)/k_B T}$$

$$n_i = N_C e^{(E_i - E_C)/k_B T} \rightarrow N_C = n_i e^{-(E_i - E_C)/k_B T}$$

$$p_i = N_V e^{(E_V - E_i)/k_B T} \rightarrow N_V = n_i e^{-(E_V - E_i)/k_B T}$$

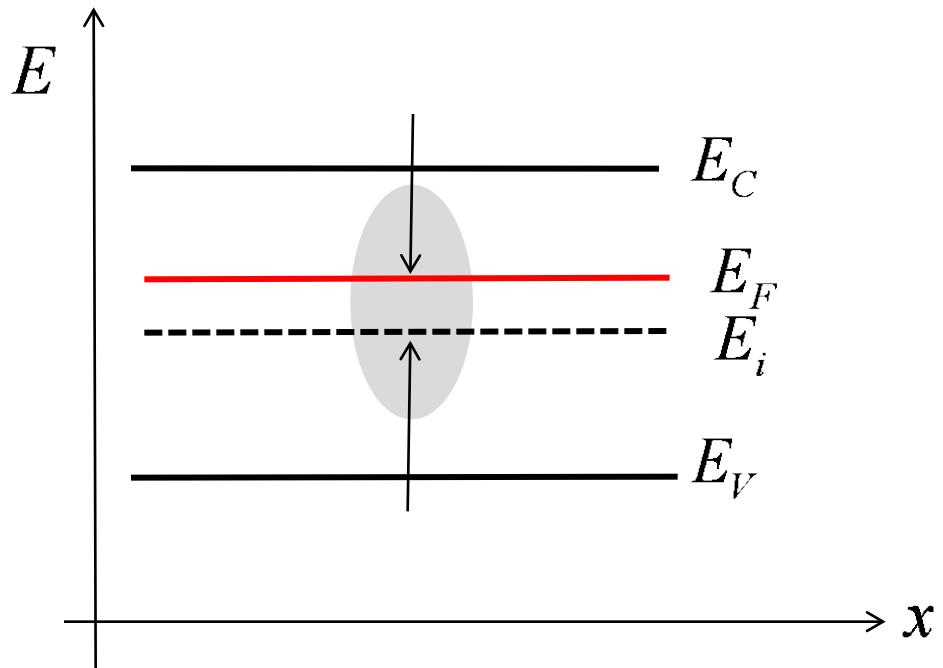
$$n_0 = n_i e^{(E_F - E_i)/k_B T}$$

$$p_0 = n_i e^{(E_i - E_F)/k_B T}$$

# “Reading” an E-band diagram

$$n_0 = n_i e^{(E_F - E_i)/k_B T}$$

$$p_0 = n_i e^{(E_i - E_F)/k_B T}$$



- Fermi level above  $E_i$ , n-type
- Fermi level below  $E_i$ , p-type

# Summary

---

$$n_0 = N_C e^{(E_F - E_C)/k_B T}$$

$$n_0 = n_i e^{(E_F - E_i)/k_B T}$$

$$p_0 = N_V e^{(E_V - E_F)/k_B T}$$

$$p_0 = n_i e^{(E_i - E_F)/k_B T}$$

$$N_C = \frac{1}{4} \left( \frac{2m_n^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

$$n_i = \sqrt{N_C N_V} e^{-E_G/2k_B T}$$

$$N_V = \frac{1}{4} \left( \frac{2m_p^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

$$n_0 p_0 = n_i^2$$

## Primer on Semiconductors

# Unit 3: Equilibrium Carrier Concentrations

## Lecture 3.4: Carrier concentration vs. doping density

**Mark Lundstrom**

[lundstro@purdue.edu](mailto:lundstro@purdue.edu)

Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Carrier concentrations vs. Fermi level

## Electrons

$$n_0 = N_C \mathcal{F}_{1/2} \left[ (E_F - E_C) / k_B T \right] \text{ m}^{-3}$$

$$N_C = \frac{1}{4} \left( \frac{2m_n^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

nondegenerate:

$$n_0 = N_C e^{(E_F - E_C) / k_B T}$$

$$n_0 = n_i e^{(E_F - E_i) / k_B T}$$

## Holes

$$p_0 = N_V \mathcal{F}_{1/2} \left[ (E_V - E_F) / k_B T \right] \text{ m}^{-3}$$

$$N_V = \frac{1}{4} \left( \frac{2m_p^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

nondegenerate:

$$p_0 = N_V e^{(E_V - E_F) / k_B T}$$

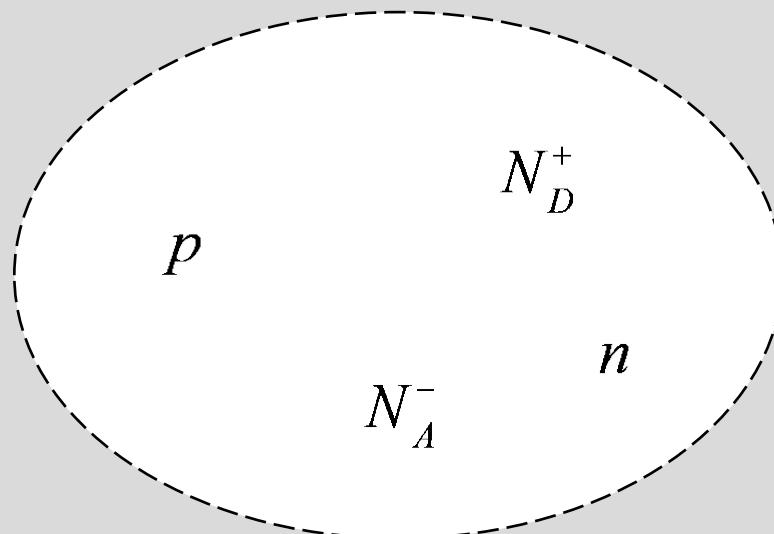
$$p_0 = n_i e^{(E_i - E_F) / k_B T}$$

# Space charge density

---

What is the net charge in this region?

$$\rho = q \left[ p - n + N_D^+ - N_A^- \right] \text{ C/m}^3$$



bulk, uniform semiconductor

# Space charge neutrality

---

Nature abhors a vacuum. Nature also abhors a charge.

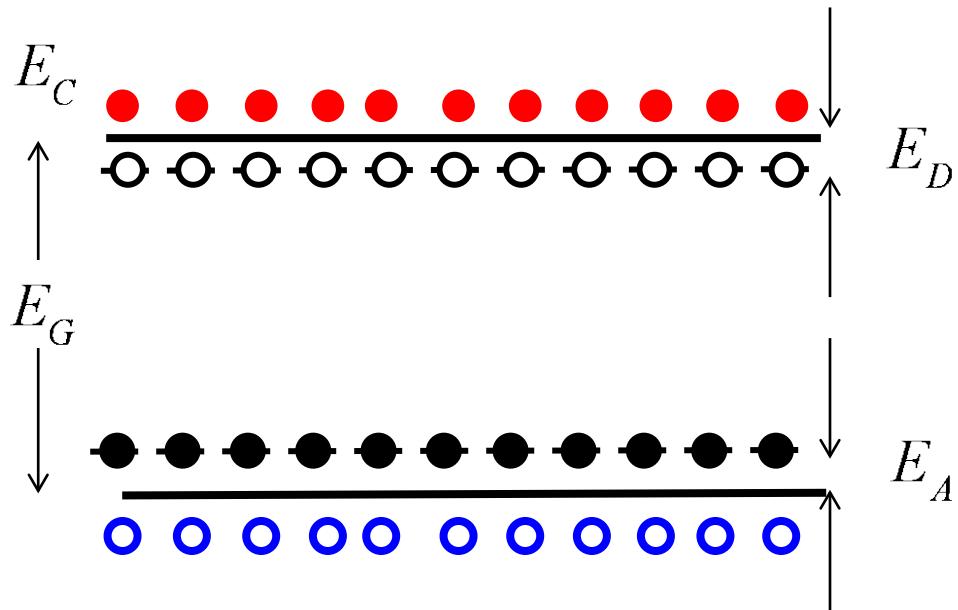
Mobile charges (electrons and holes) will be attracted to the immobile ionized dopants), so that the net charge is zero.

$$\rho = q \left[ p - n + N_D^+ - N_A^- \right] = 0$$

Almost uniform semiconductors will be nearly neutral, but with strong non-uniformities (e.g. PN junctions), there will be a space charge.

# Fully ionized dopants

---



All donors have donated their electrons to the conduction band and are now positively charged.

$$N_D^+ = N_D \quad N_A^- = N_A$$

All acceptors have accepted an electron from the valence band and are now negatively charged.

## Space charge neutrality again

---

$$\rho = q \left[ p - n + N_D^+ - N_A^- \right] = 0$$

Assume **fully ionized dopants** (this will typically be the case for good dopants near and above room temperature).

$$\rho = q \left[ p_0 - n_0 + N_D - N_A \right] = 0 \quad n_0 p_0 = n_i^2$$

Assuming that we know how many dopants we introduced into the semiconductor, these are two equations in two unknowns –  $p$  and  $n$ .

# Solving for the carrier density in equilibrium

---

1) charge neutrality:  $p_0 - n_0 + N_D^+ - N_A^- = 0$

2) Fully ionized dopants:  $p_0 - n_0 + N_D - N_A = 0$

3) np product:  $n_0 p_0 = n_i^2$  (equilibrium)

4) result:  $\frac{n_i^2}{n_0} - n_0 + N_D - N_A = 0$

$$p_0 - \frac{n_i^2}{p_0} + N_D - N_A = 0$$

# Result: N-type

---

$$\frac{n_i^2}{n_0} - n_0 + N_D - N_A = 0$$

$$n_0 = \frac{N_D - N_A}{2} + \left[ \left( \frac{N_D - N_A}{2} \right)^2 + n_i^2 \right]^{1/2}$$

$$p_0 = \frac{n_i^2}{n_0}$$

# Result: P-type

---

$$p_0 - \frac{n_i^2}{p_0} + N_D - N_A = 0$$

$$p_0 = \frac{N_A - N_D}{2} + \left[ \left( \frac{N_A - N_D}{2} \right)^2 + n_i^2 \right]^{1/2}$$

$$n_0 = \frac{n_i^2}{p_0}$$

## Example 1

---

Consider Si doped with phosphorus at  $N_D = 2.00 \times 10^{15} \text{ cm}^{-3}$   
The temperature is 300 K. What are  $n$  and  $p$ ?

Recall that at 300 K in Si,  $n_i = 1.00 \times 10^{10} \text{ cm}^{-3}$

Assume that the donors are fully ionized.

$$n_0 = \frac{N_D - N_A}{2} + \left[ \left( \frac{N_D - N_A}{2} \right)^2 + n_i^2 \right]^{1/2} = \frac{N_D}{2} + \left[ \left( \frac{N_D}{2} \right)^2 + n_i^2 \right]^{1/2}$$

$$N_D \gg n_i$$

$$n_0 = N_D = 2.00 \times 10^{15} \text{ cm}^{-3}$$

$$p_0 = n_i^2 / n_0$$

$$p_0 = (10^{10})^2 / 2 \times 10^{15} = 5 \times 10^4 \text{ cm}^{-3}$$

## Example 2

---

Consider Si doped with phosphorus at  $N_D = 2.00 \times 10^{15} \text{ cm}^{-3}$  and Boron at  $N_A = 1.00 \times 10^{15} \text{ cm}^{-3}$ .

The temperature is 300 K. What are  $n$  and  $p$ ?

$$n_0 = \frac{N_D - N_A}{2} + \left[ \left( \frac{N_D - N_A}{2} \right)^2 + n_i^2 \right]^{1/2}$$

$$N_D - N_A \gg n_i \quad n_0 = N_D - N_A$$

$$n_0 = 1.00 \times 10^{15} \text{ cm}^{-3}$$

$$p_0 = n_i^2 / n_0 \quad p_0 = (10^{10})^2 / 1 \times 10^{15} = 1 \times 10^5 \text{ cm}^{-3}$$

# Conclusion

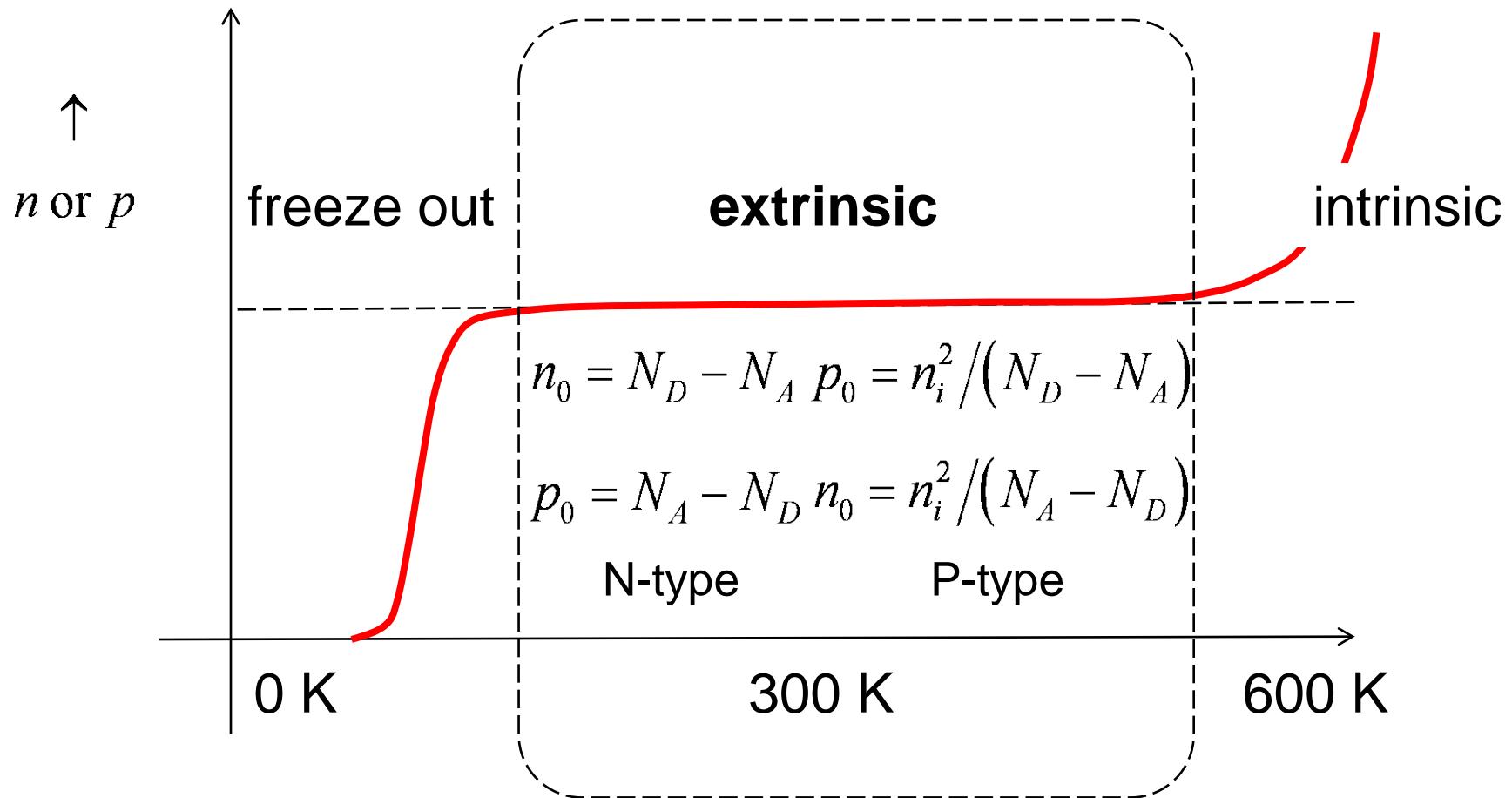
---

When the net doping density is much greater than the intrinsic carrier concentration and the dopants are fully ionized, then

$$n_0 = N_D - N_A \quad p_0 = n_i^2 / (N_D - N_A) \quad \text{N-type} \quad N_D > N_A$$

$$p_0 = N_A - N_D \quad n_0 = n_i^2 / (N_A - N_D) \quad \text{P-type} \quad N_A > N_D$$

# Summary



# Primer on Semiconductors

## Unit 3: Equilibrium Carrier Concentrations

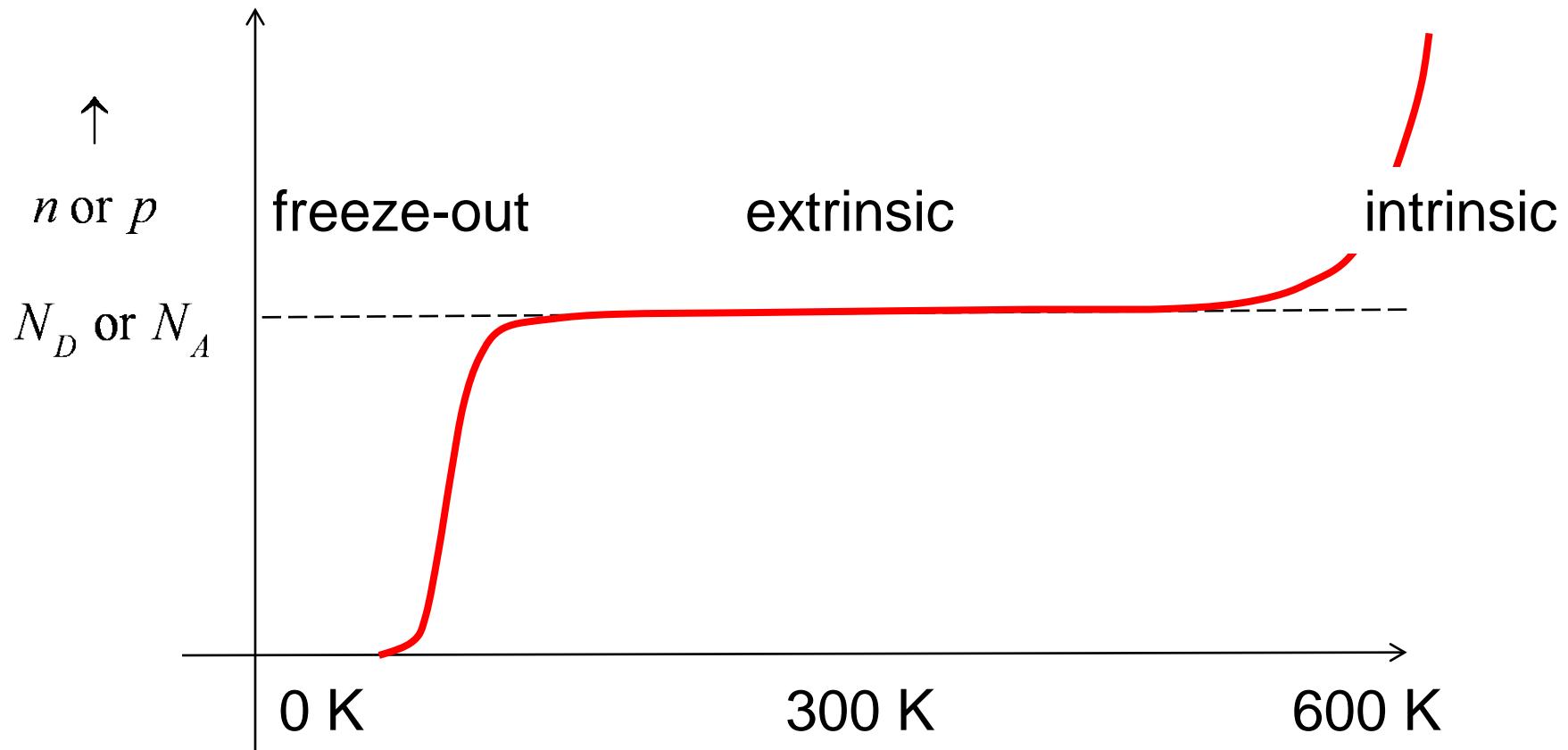
### Lecture 3.5: Carrier concentration vs. temperature

**Mark Lundstrom**

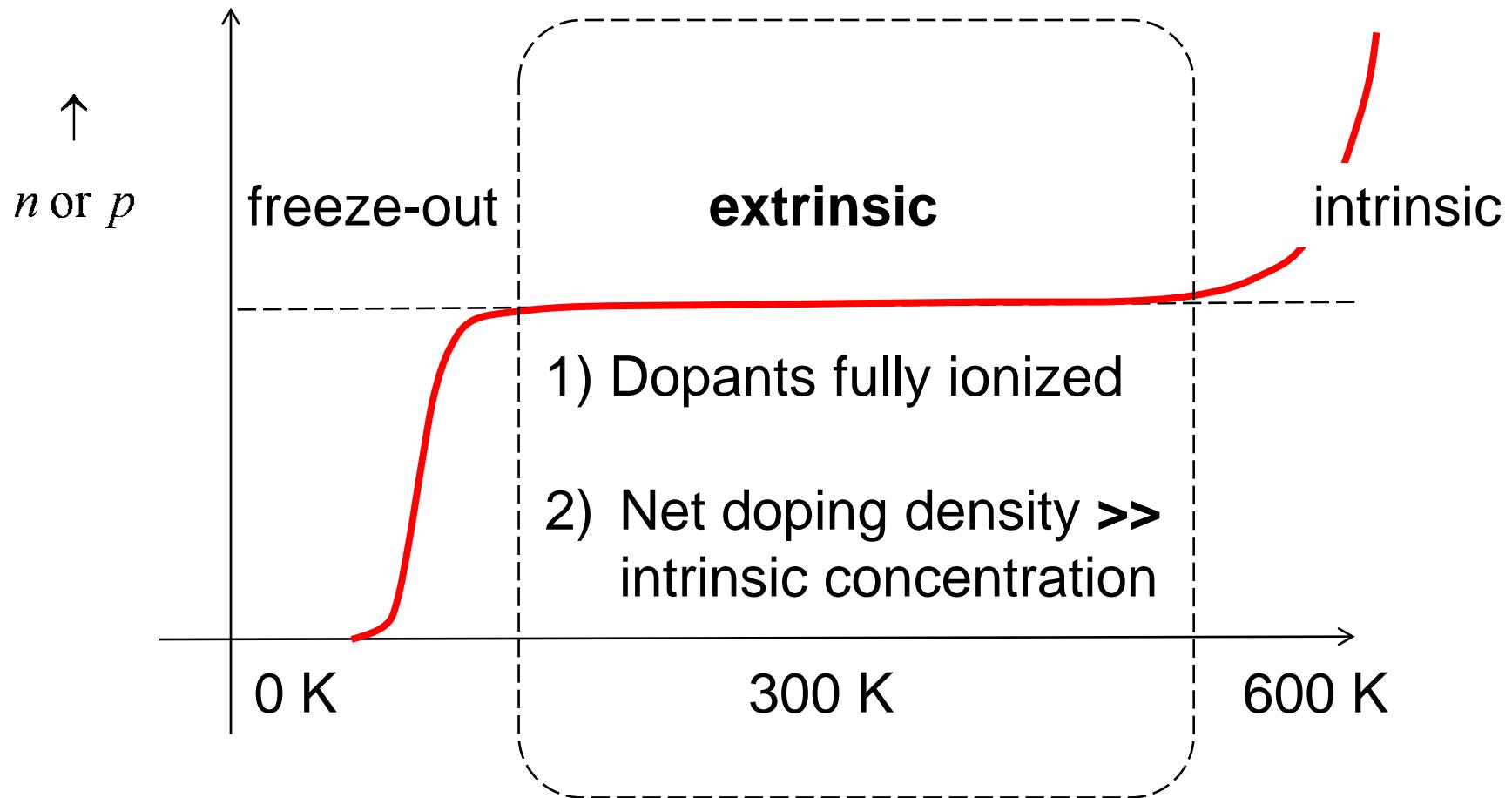
[lundstro@purdue.edu](mailto:lundstro@purdue.edu)

Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Carrier concentration vs. temperature



# The extrinsic region



# The extrinsic region (equilibrium)

---

N-type

$$N_D - N_A \gg n_i$$

$$n_0 = N_D - N_A$$

$$p_0 = \frac{n_i^2}{n_0}$$

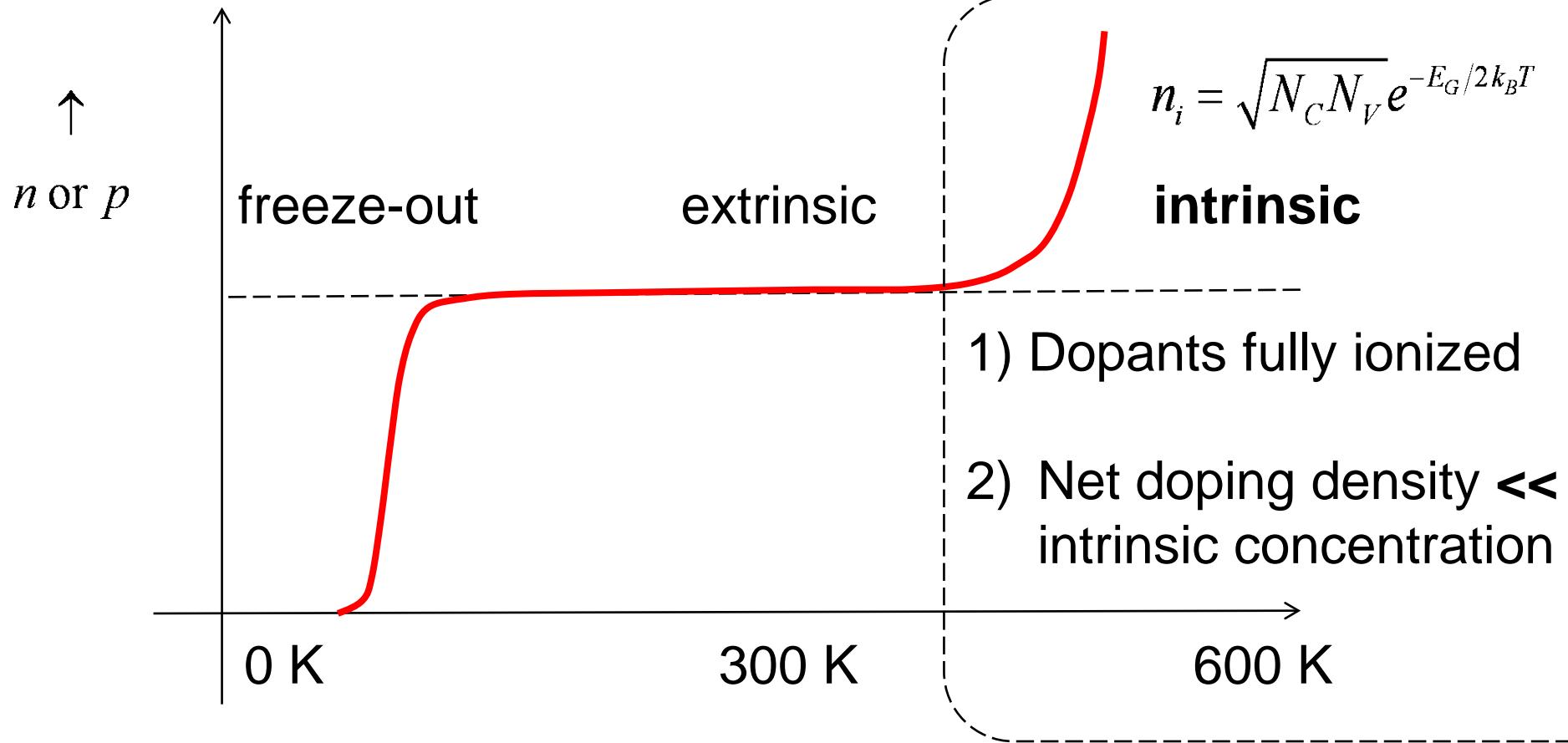
P-type

$$N_A - N_D \gg n_i$$

$$p_0 = N_A - N_D$$

$$n_0 = \frac{n_i^2}{p_0}$$

# The intrinsic region



# N-type at high temperatures

---

$$\frac{n_i^2}{n_0} - n_0 + N_D - N_A = 0$$

$$n_0 = \frac{N_D - N_A}{2} + \left[ \left( \frac{N_D - N_A}{2} \right)^2 + n_i^2 \right]^{1/2}$$

$$p_0 = \frac{n_i^2}{n_0}$$

cannot be  
neglected



# P-type at high temperatures

---

$$p_0 - \frac{n_i^2}{p_0} + N_D - N_A = 0$$

$$p_0 = \frac{N_A - N_D}{2} + \left[ \left( \frac{N_A - N_D}{2} \right)^2 + n_i^2 \right]^{1/2}$$

$$n_0 = \frac{n_i^2}{p_0}$$

cannot be  
neglected

## Example 3

---

Consider Si doped with phosphorus at  $N_D = 2.00 \times 10^{15} \text{ cm}^{-3}$   
The temperature is **600 K**. What are  $n$  and  $p$ ?

Recall that at 300 K in Si,  $n_i = 1.00 \times 10^{10} \text{ cm}^{-3}$

$$n_i = \sqrt{N_C N_V} e^{-E_G/2k_B T}$$

$$N_C = 2 \left[ \frac{(m_n^* k_B T)^{3/2}}{2\pi\hbar^2} \right]$$

Computing  $n_i$  requires a careful treatment of the temperature dependence of the band gap and effective masses.

$$N_V = 2 \left[ \frac{(m_p^* k_B T)^{3/2}}{2\pi\hbar^2} \right]$$

## Example 3 (cont.)

---

$$n_i (T = 600 \text{ K}) = 4 \times 10^{15} \text{ cm}^{-3}$$

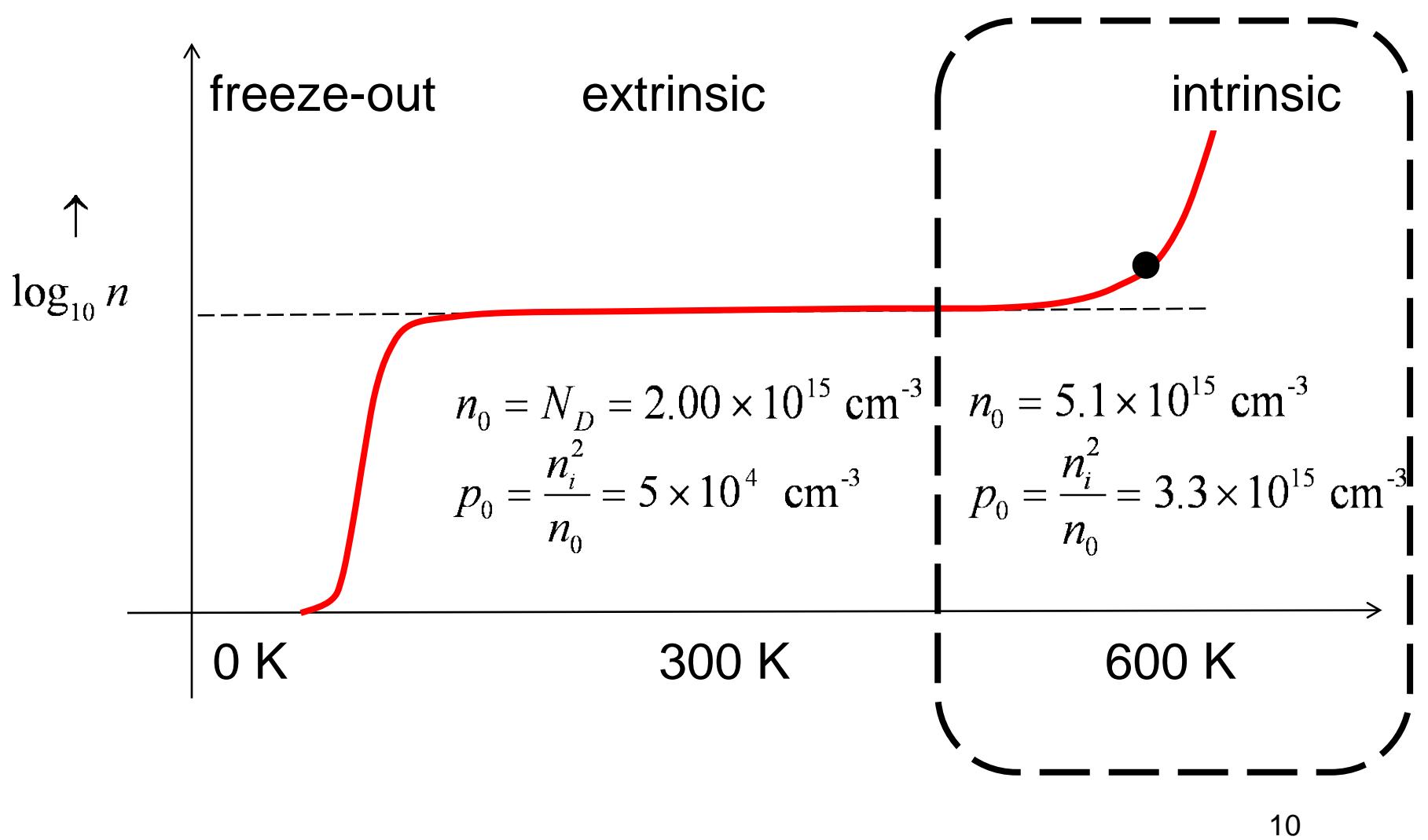
From Fig. 4.17, of R.F. Pierret, *Advanced Semiconductor Fundamentals*, 2<sup>nd</sup> Ed., Prentice Hall, 2003.

$$n_0 = \frac{N_D}{2} + \left[ \left( \frac{N_D}{2} \right)^2 + n_i^2 \right]^{1/2} \quad N_D = 2 \times 10^{15} \text{ cm}^{-3}$$

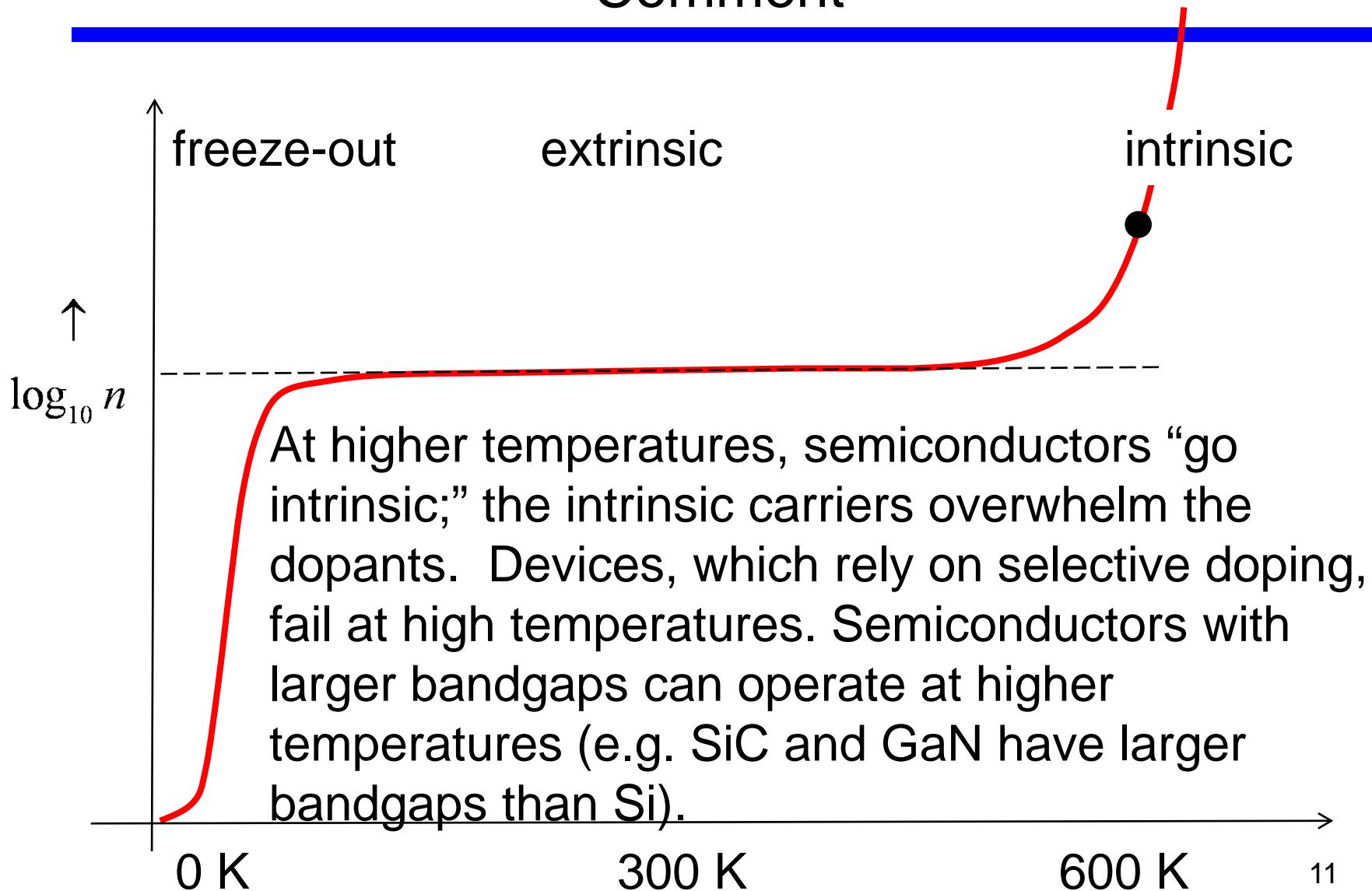
$$n_0 = 1.0 \times 10^{15} + \left[ (1.0 \times 10^{15})^2 + (4.0 \times 10^{15})^2 \right]^{1/2} = 5.1 \times 10^{15} \text{ cm}^{-3}$$

$$p_0 = \frac{n_i^2}{n_0} = \frac{(4.0 \times 10^{15})^2}{5.1 \times 10^{15}} = 3.3 \times 10^{15} \text{ cm}^{-3}$$

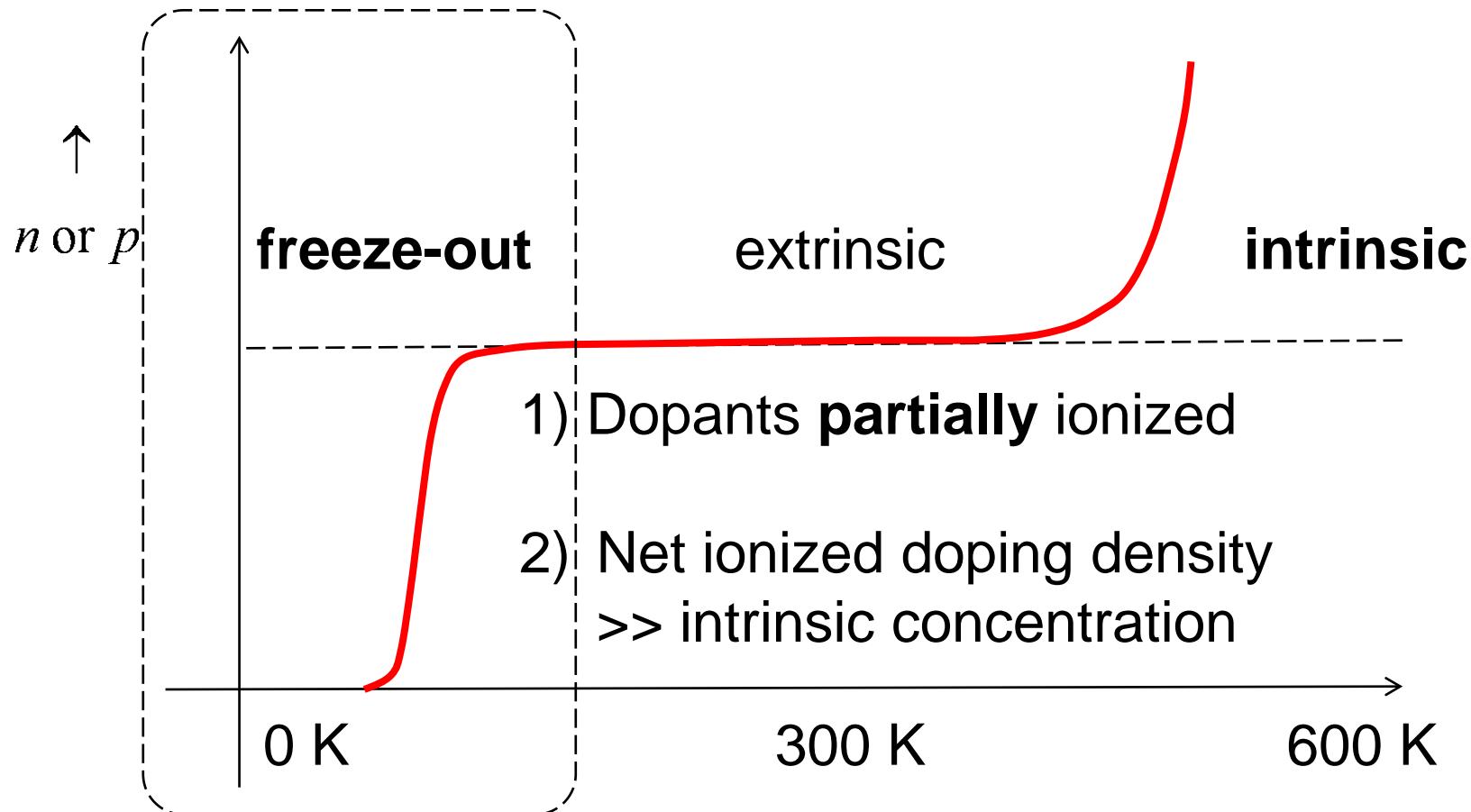
## Example 3



## Comment



# The freeze-out region



# Solving for the carrier density: N-type

---

1) charge neutrality:  $p_0 - n_0 + N_D^+ - N_A^- = 0$

2) Neglect minority carriers:  $n_0 p_0 = n_i^2 \rightarrow p_0 = n_i^2 / n_0 \ll n_0$

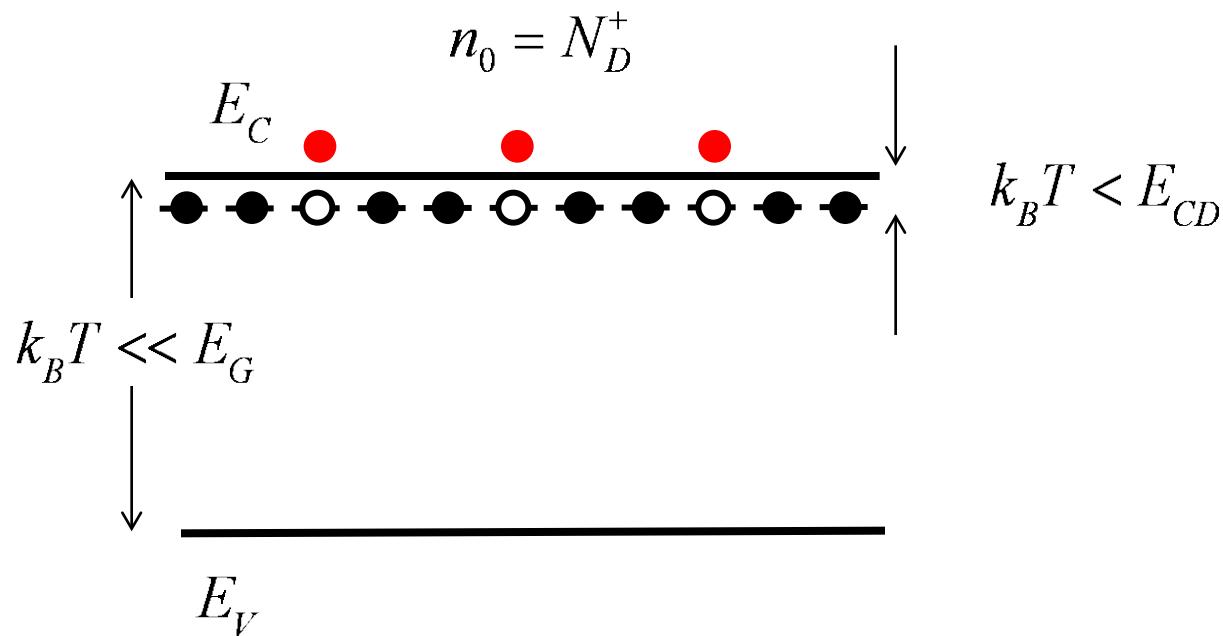
3) result:  $n_0 = N_D^+ - N_A^-$

We just need to compute the net concentration of ionized dopants.

# Low temperature

---

$T > 0 \text{ K}$

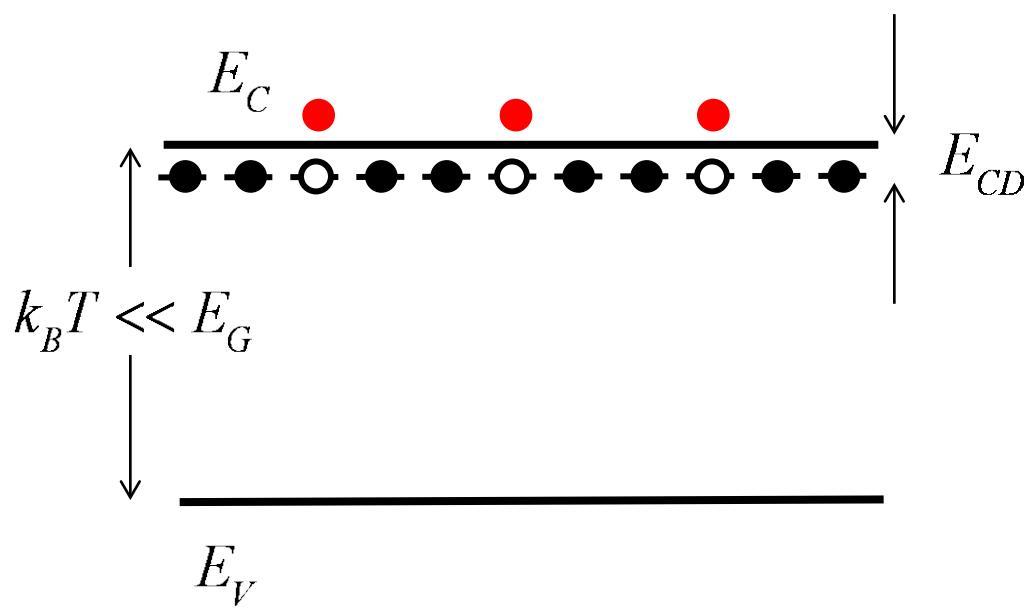


A few extrinsic carriers due to doping, but no intrinsic carriers due to thermal excitation across the band gap.

# Ionized donor concentration

---

$T > 0 \text{ K}$



fraction of donor level  
occupied:

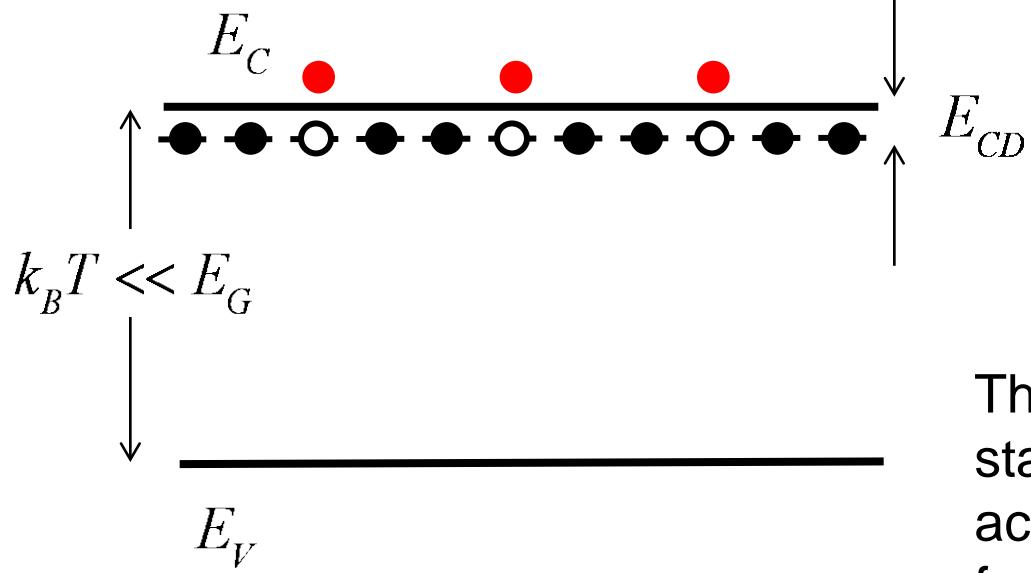
$$\frac{N_D^0}{N_D} = f_0(E_D)$$

$$\frac{N_D^+}{N_D} = 1 - \frac{N_D^0}{N_D} = 1 - f_0(E_D)$$

$$f_0(E_D) = \frac{1}{1 + e^{(E_D - E_F)/k_B T}}$$

# Ionized donor concentration

$T > 0 \text{ K}$



$$\frac{N_D^+}{N_D} = 1 - f_0(E_D)$$

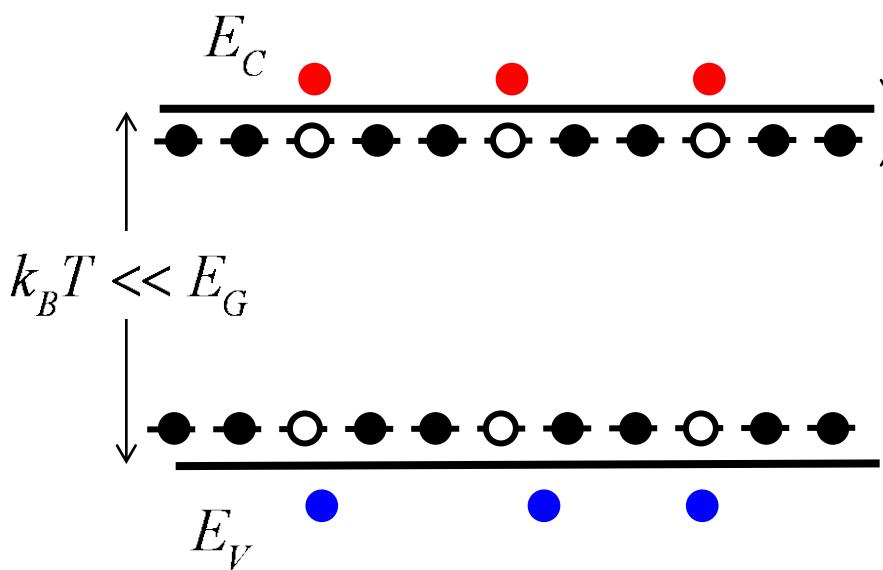
$$\frac{N_D^+}{N_D} = \frac{1}{1 + e^{(E_F - E_D)/k_B T}}$$

This is **almost correct**. The statistics of occupying donor (and acceptor) levels are a bit different from occupying band states.

$$\frac{N_D^+}{N_D} = \frac{1}{1 + g_D e^{(E_F - E_D)/k_B T}}$$

# Ionized dopant concentration

$T > 0 \text{ K}$



$$\frac{N_D^+}{N_D} = \frac{1}{1 + g_D e^{(E_F - E_D)/k_B T}}$$

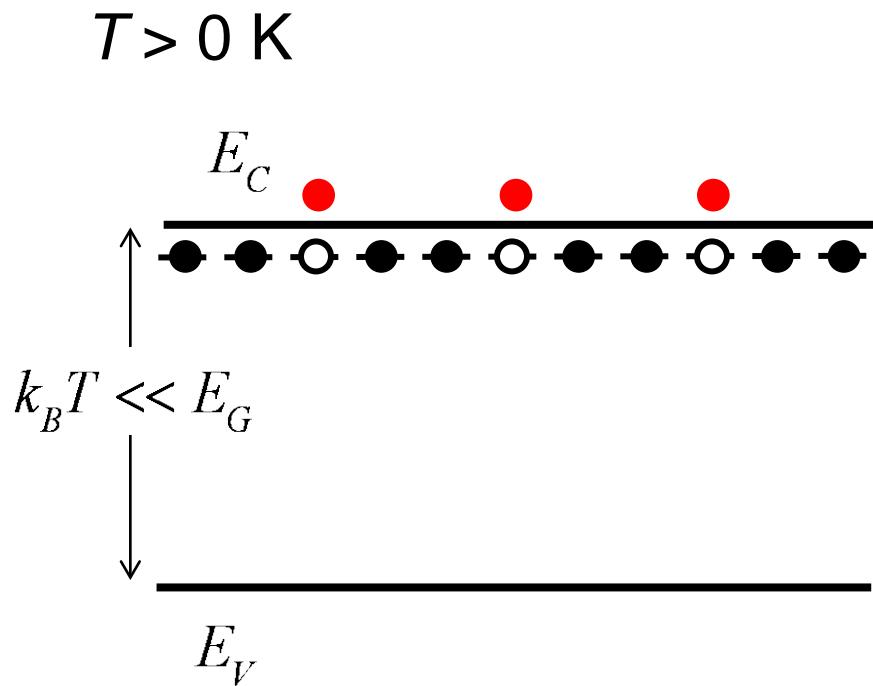
$$g_D = 2 \quad (\text{standard value})$$

$$\frac{N_A^-}{N_A} = \frac{1}{1 + g_A e^{(E_A - E_F)/k_B T}}$$

$$g_A = 4 \quad (\text{standard value})$$

See R.F. Pierret, *Advanced Semiconductor Fundamentals*, Sec. 4.4.4 for a discussion.

## Example: N-type sample



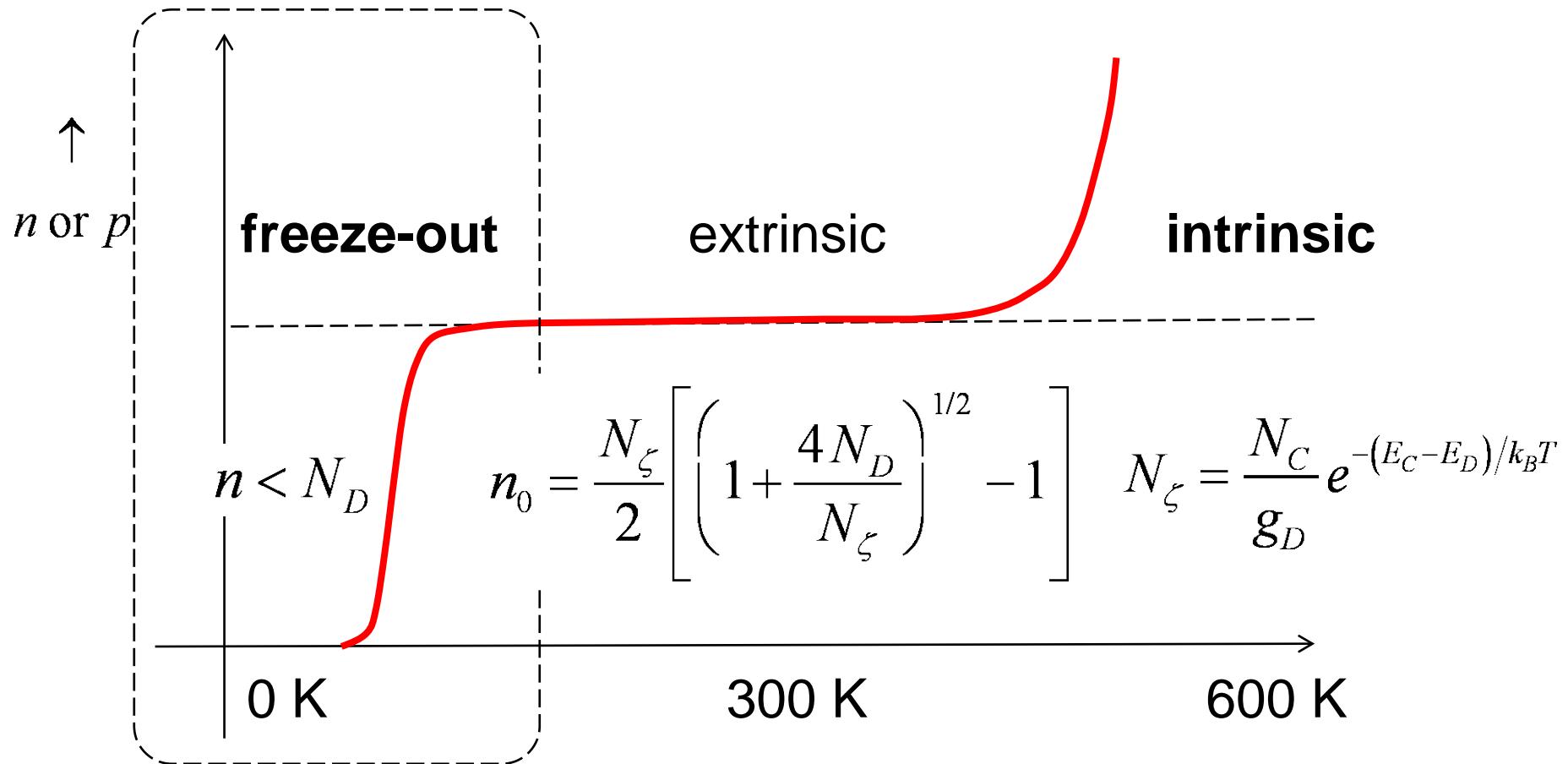
$$\frac{N_D^+}{N_D} = \frac{1}{1 + g_D e^{(E_F - E_D)/k_B T}}$$

$$n_0 = N_D^+ = \frac{N_D}{1 + g_D e^{(E_F - E_D)/k_B T}}$$

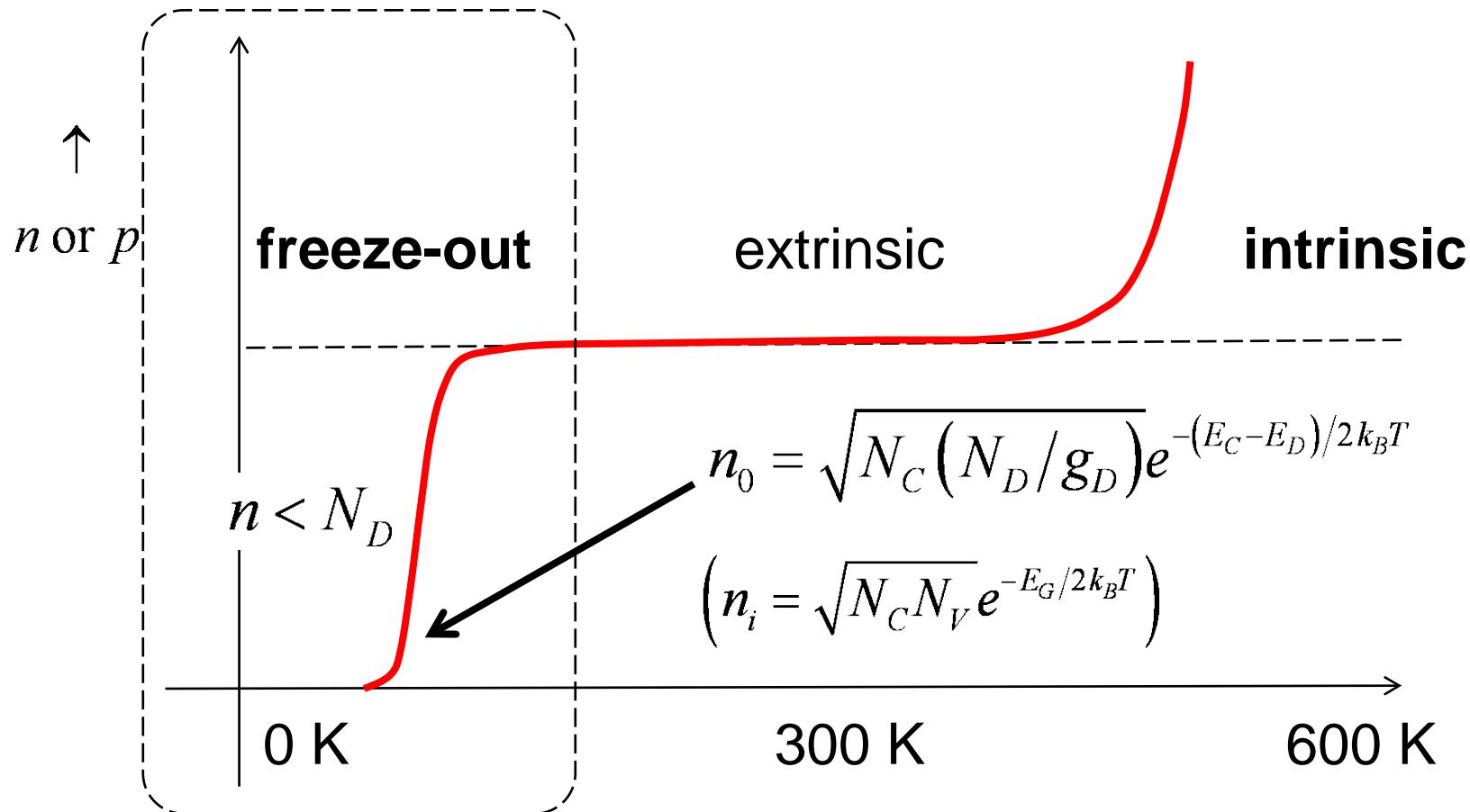
$$n_0 = N_C e^{(E_F - E_C)/k_B T}$$

These two equations can be solved for  $n_0(T)$  – see R.F. Pierret, *Advanced Semiconductor Fundamentals*, 2<sup>nd</sup> Ed. Sec. 4.5.2.

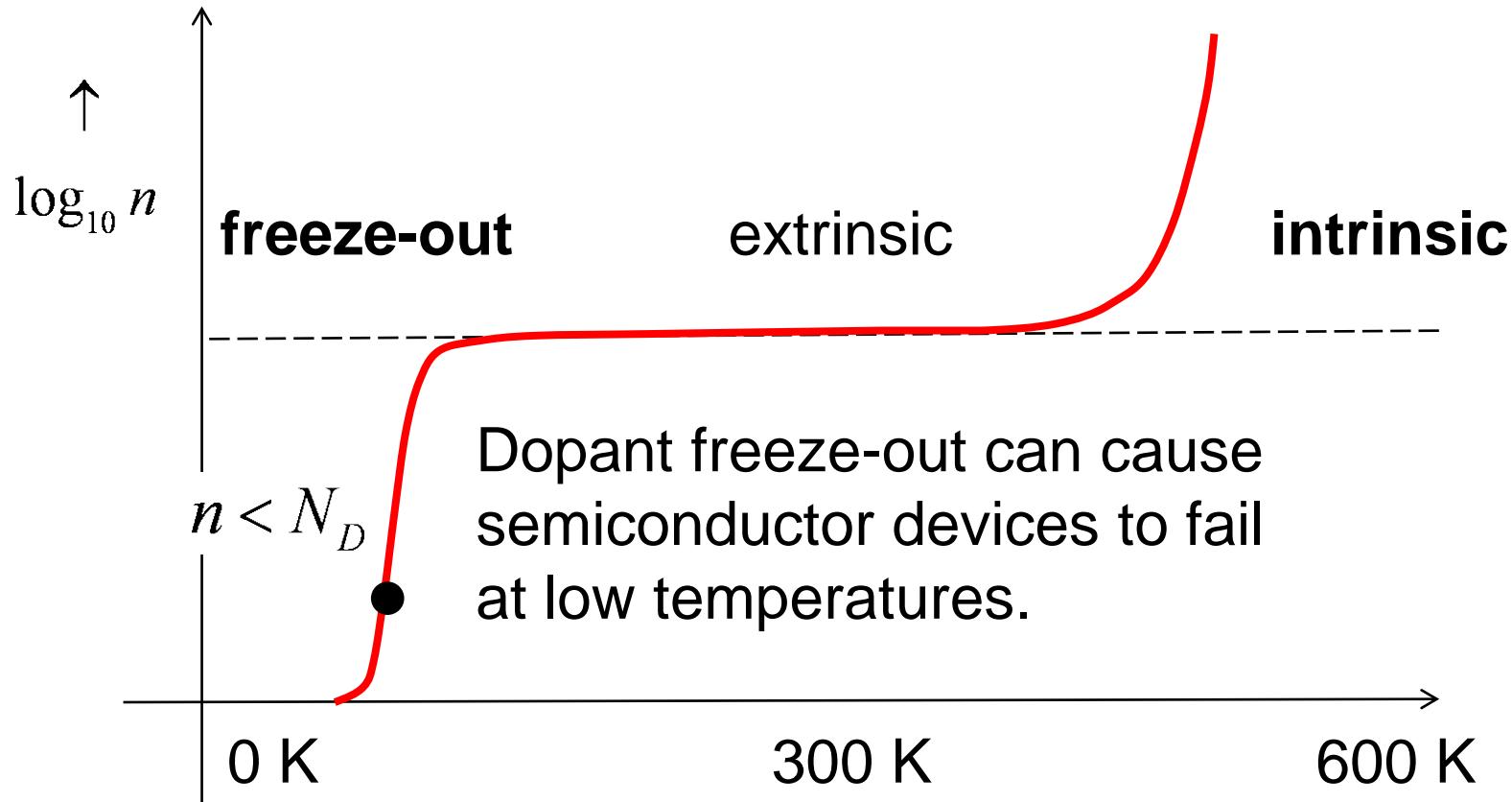
# The freeze-out region



# The freeze-out region

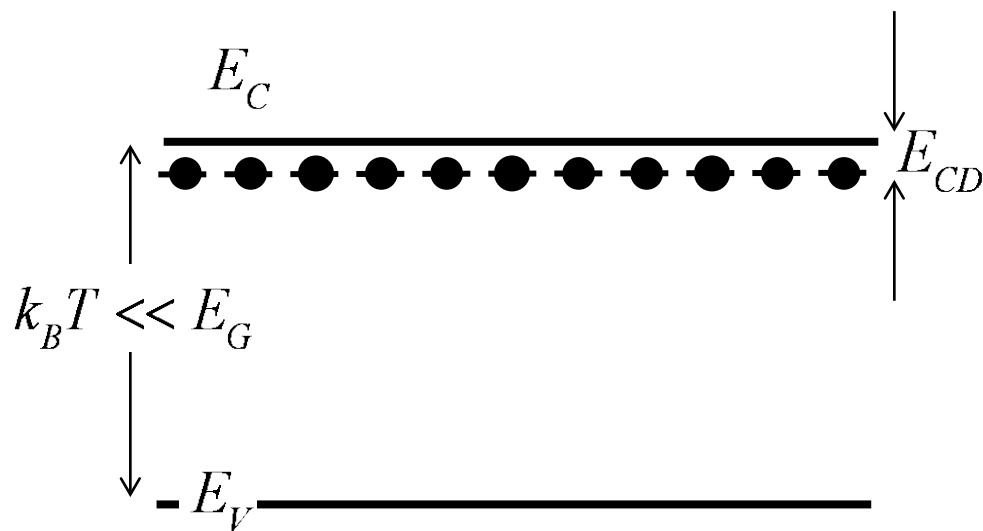


## Comment



# Metal-insulator transition

$T = 0 \text{ K}$



Metals conduct electricity at 0 K.

Semiconductors become insulators at 0 K because of freeze-out.

**Heavily doped semiconductors are different.**

When the dopants are close to each other, their wave functions overlap. Impurity levels become impurity bands.

**Freeze-out does not occur in heavily doped semiconductors.**

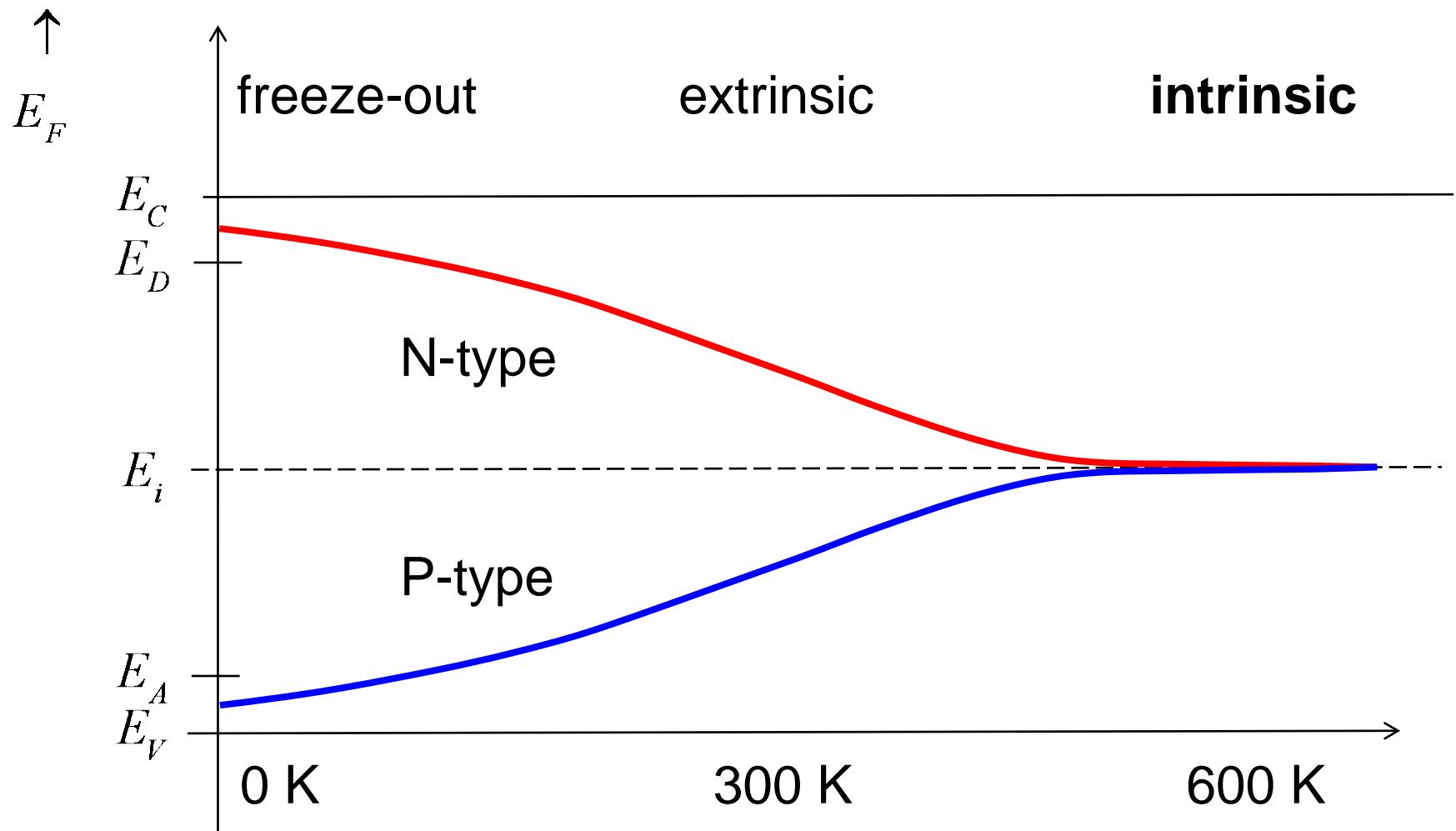
In Si, for  $N_D > 10^{19} \text{ cm}^{-3}$ , the impurity band merges with the conduction band.

# Question

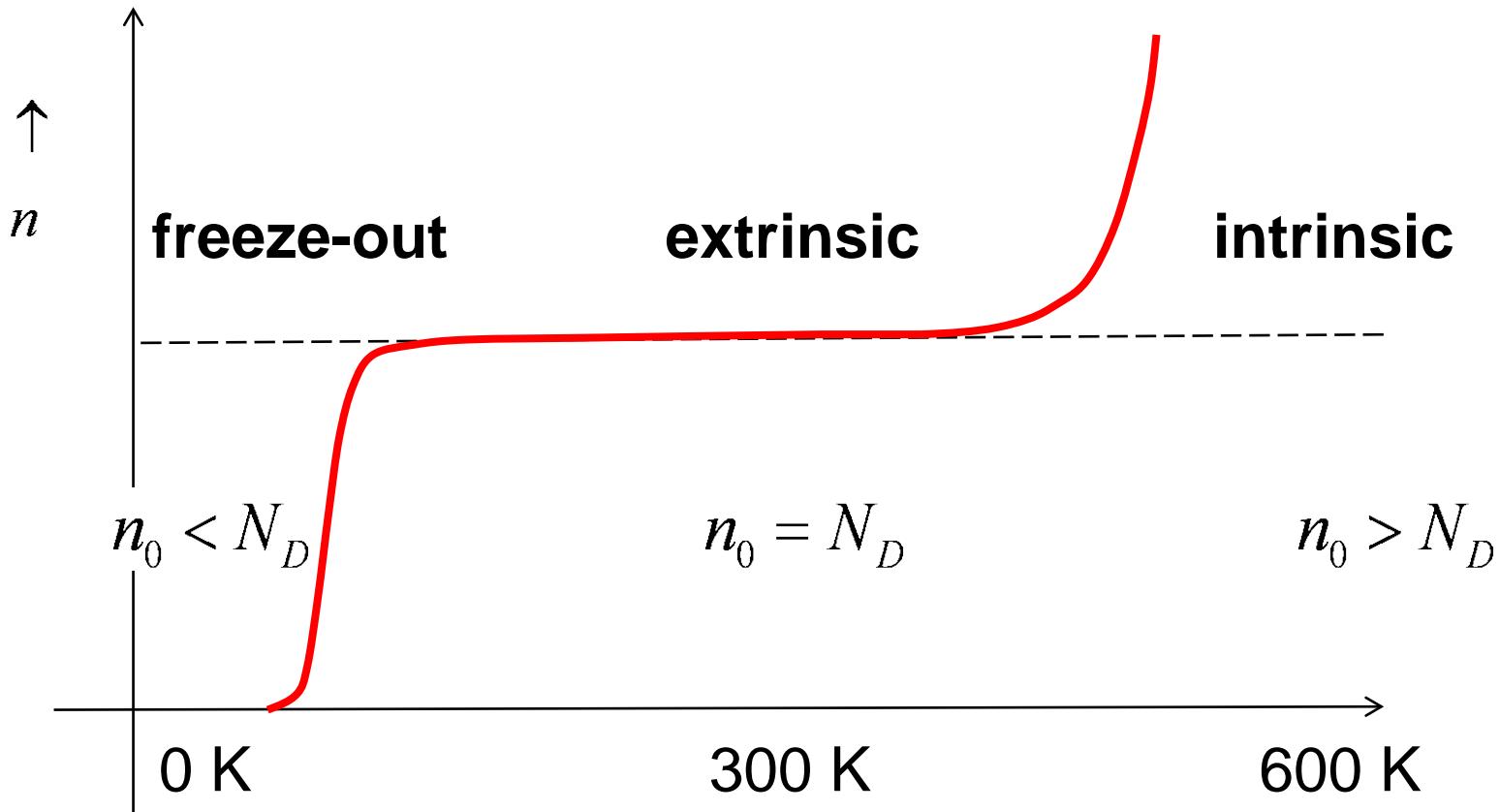
---

We now understand how the carrier concentration varies with temperature. How does the Fermi level vary with temperature?

# Fermi level vs. temperature



# Summary



You should also understand  $E_F$  vs.  $T$  qualitatively.

# Primer on Semiconductors

## Unit 3: Equilibrium Carrier Concentrations

### Lecture 3.6: Unit 3 Recap

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Fermi function

---

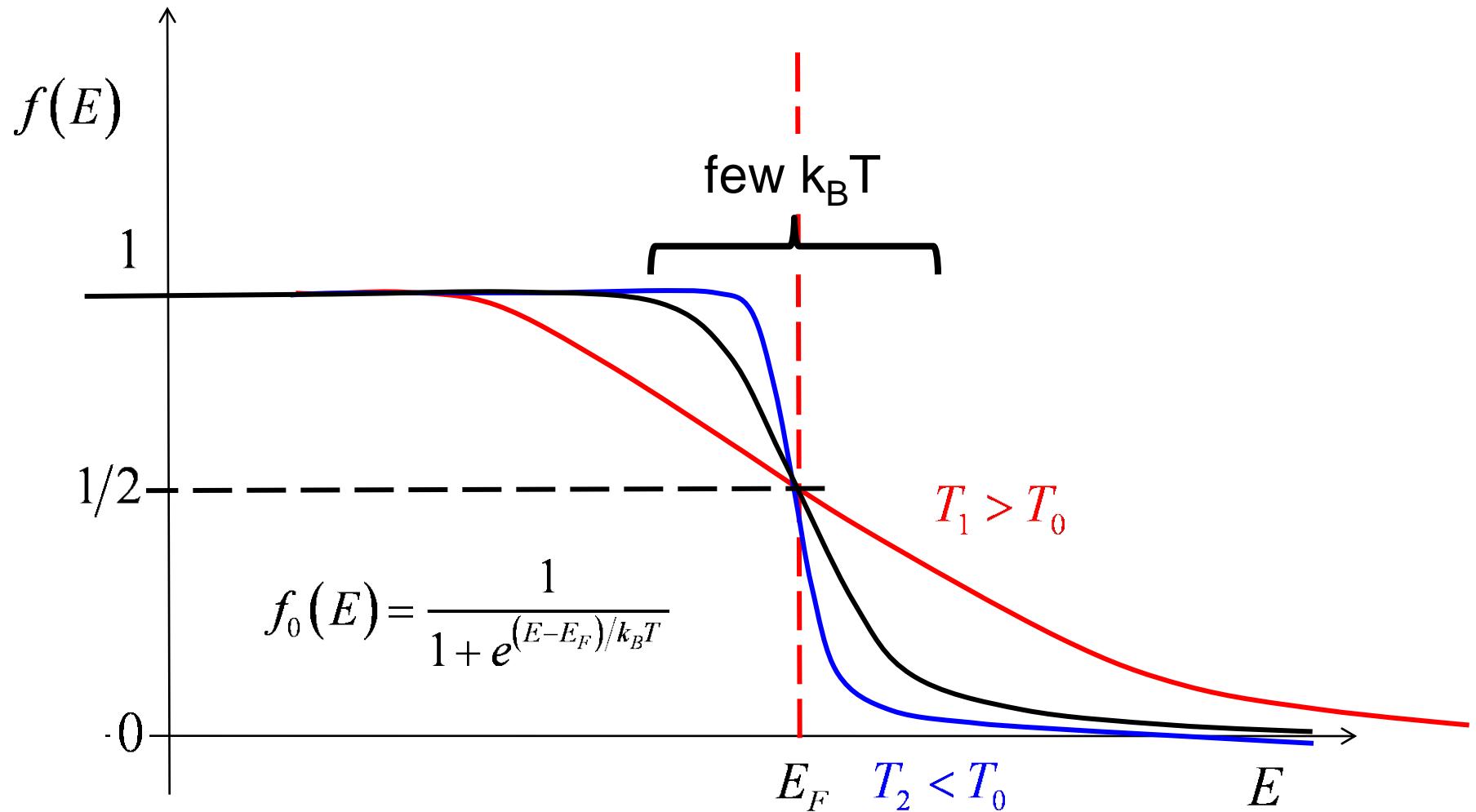
The Fermi function gives the probability that a state (if it exists) is occupied in equilibrium.

$$f_0(E) = \frac{1}{1 + e^{(E-E_F)/k_B T}}$$

(Fermi function)

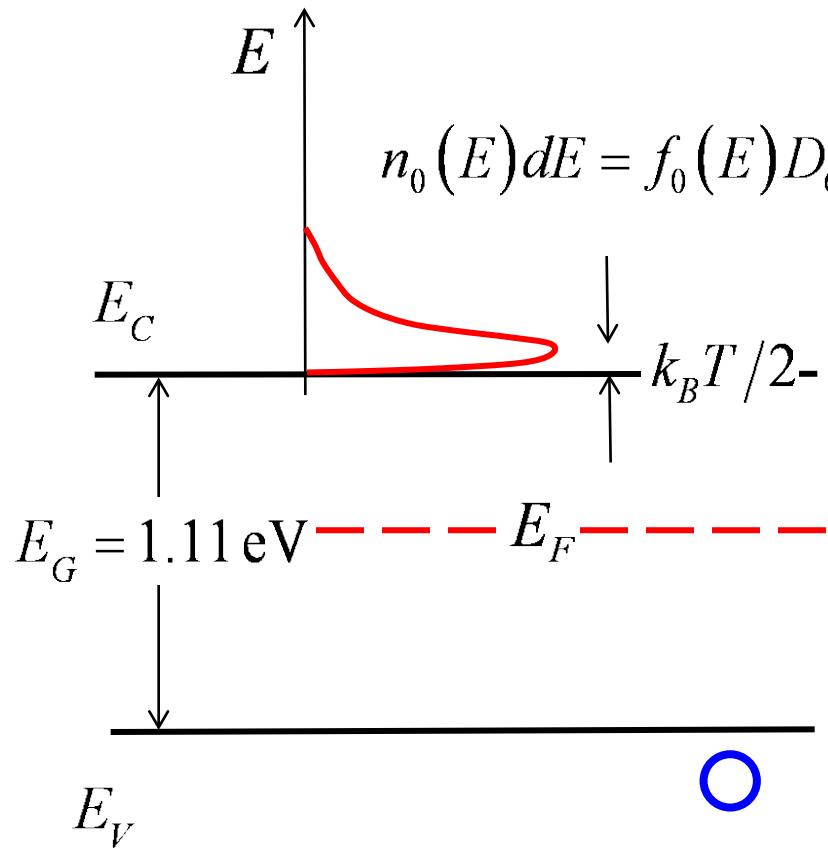
The two key parameters in the Fermi function are the Fermi level and the temperature.

# Fermi level and temperature



# Distribution of carriers in the bands

---



non-degenerate semiconductor)

***Electrons and holes are very near the band edges.***

# Fermi-Dirac integrals

---

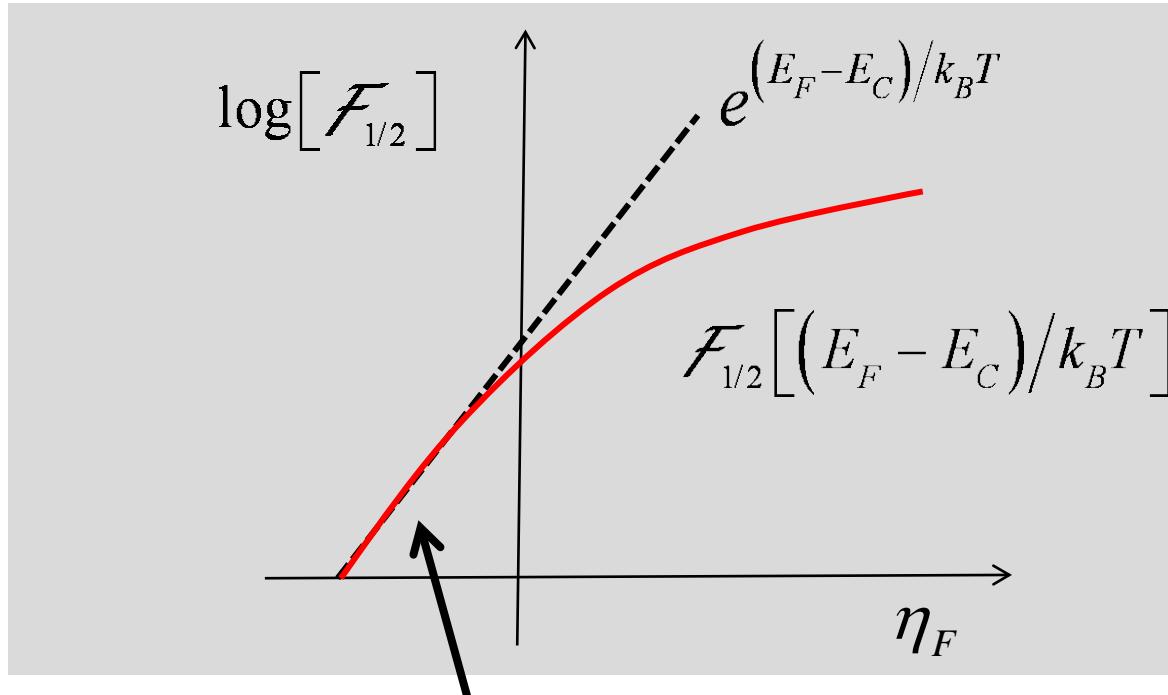
$$n_0 = \int_{E_C}^{\infty} n_0(E) dE = \int_{E_C}^{\infty} f_0(E) D_C(E) dE$$

$$n_0 = N_C \mathcal{F}_{1/2} \left[ (E_F - E_C) / k_B T \right] \text{cm}^{-3}$$

$$N_C = \frac{1}{4} \left( \frac{2m^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

# FD integrals and exponentials

---

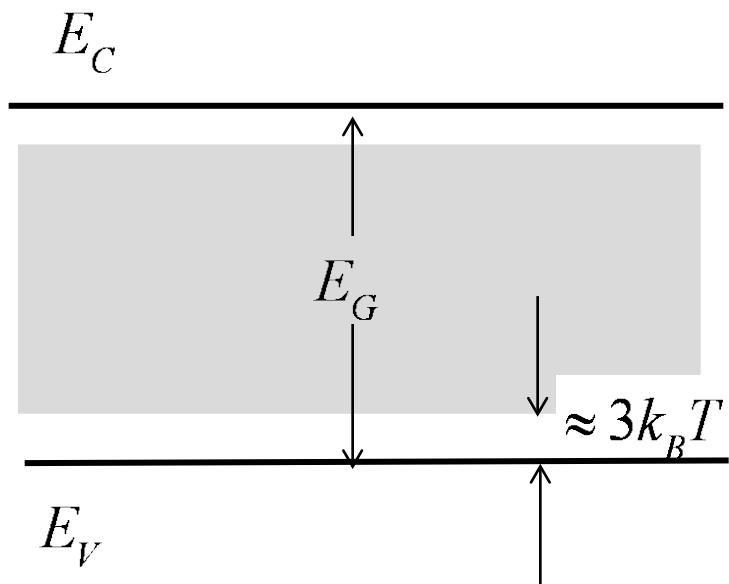


$$E_F < E_C \quad \mathcal{F}_{1/2}(E_F - E_C)/k_B T \rightarrow e^{(E_F - E_C)/k_B T}$$

(nondegenerate semiconductor)

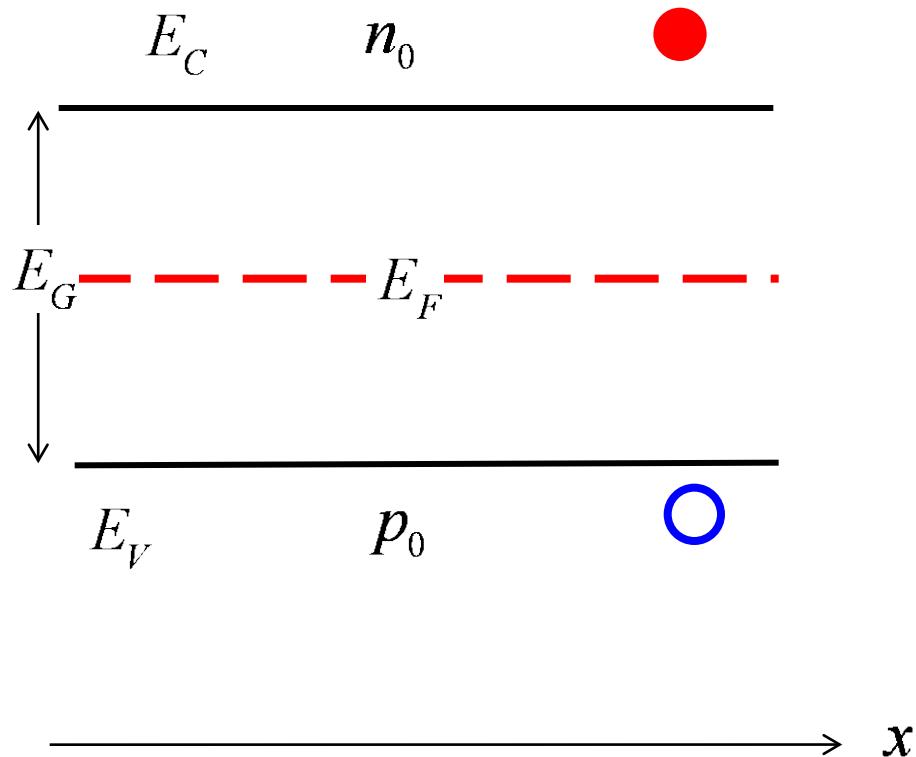
# Nondegenerate semiconductors

---



In a nondegenerate semiconductor, the Fermi level is well below the bottom of the conduction band and well above the top of the valence band.

# Carrier densities for nondegenerate semiconductors



$$n_0 = N_C e^{(E_F - E_C)/k_B T}$$

$$p_0 = N_V e^{(E_V - E_F)/k_B T}$$

Nondegenerate  
semiconductor

# Equilibrium np product

---

$$n_0 p_0 = n_i^2$$

$$n_i = \sqrt{N_C N_V} e^{-E_G/2k_B T}$$

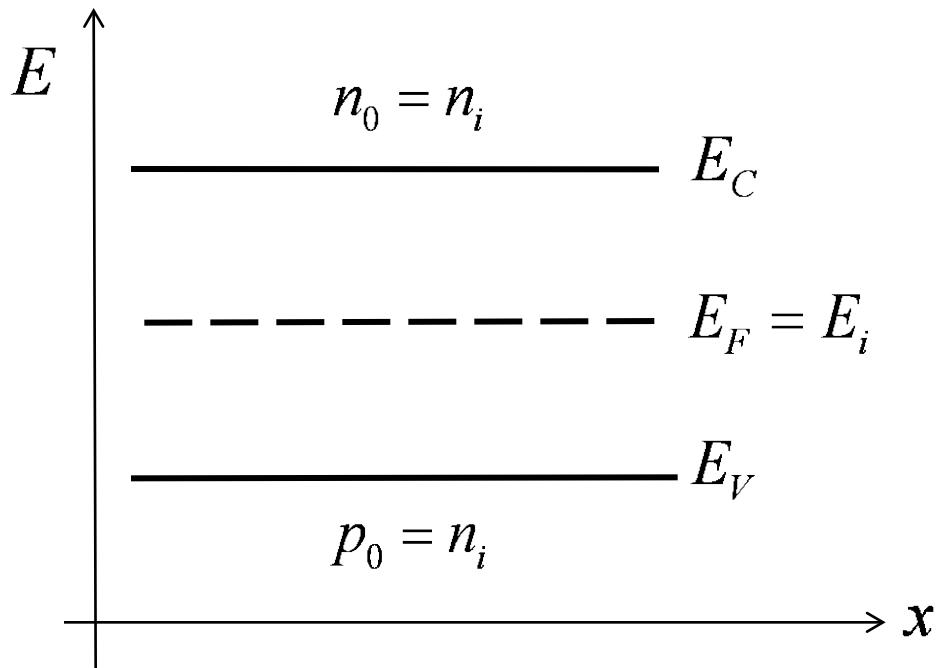
- Independent of Fermi level (for nondegenerate semiconductor)
- Depends exponentially on band gap
- Depends exponentially on temperature
- For Si at 300 K

$$n_i = 1.0 \times 10^{10} \text{ cm}^{-3}$$

# The intrinsic Fermi level

---

$$E_i = \frac{E_C + E_V}{2} + \frac{k_B T}{2} \ln\left(\frac{N_V}{N_C}\right)$$



# Carrier concentration relations (nondegenerate)

$$n_0 = N_C e^{(E_F - E_C)/k_B T}$$

$$n_0 = n_i e^{(E_F - E_i)/k_B T}$$

$$p_0 = N_V e^{(E_V - E_F)/k_B T}$$

$$p_0 = n_i e^{(E_i - E_F)/k_B T}$$

$$N_C = \frac{1}{4} \left( \frac{2m_n^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

$$n_i = \sqrt{N_C N_V} e^{-E_G/2k_B T}$$

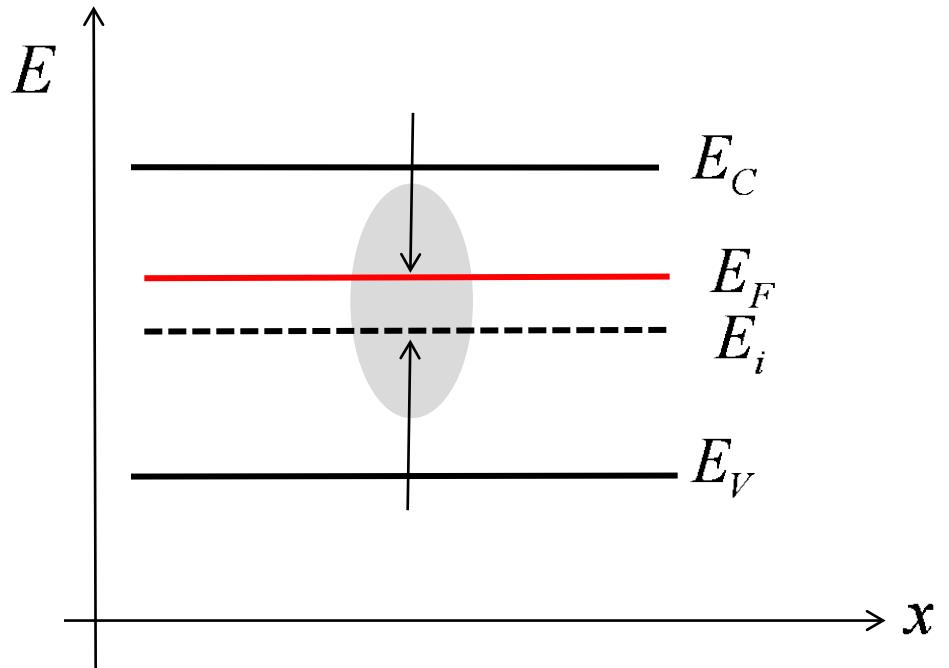
$$N_V = \frac{1}{4} \left( \frac{2m_p^* k_B T}{\pi \hbar^2} \right)^{3/2}$$

$$n_0 p = n_i^2$$

# Reading an e-band diagram

$$n_0 = n_i e^{(E_F - E_i)/k_B T}$$

$$p_0 = n_i e^{(E_i - E_F)/k_B T}$$



- Fermi level above  $E_i$ , N-type
- Fermi level below  $E_i$ , P-type

# Carrier concentration vs. doping

$$p_0 - n_0 + N_D - N_A = 0 \quad (\text{SCN})$$

$$n_0 p_0 = n_i^2$$

$$n_0 = \frac{N_D - N_A}{2} + \left[ \left( \frac{N_D - N_A}{2} \right)^2 + n_i^2 \right]^{1/2}$$

$$p_0 = \frac{n_i^2}{n_0}$$

$$p_0 = \frac{N_A - N_D}{2} + \left[ \left( \frac{N_A - N_D}{2} \right)^2 + n_i^2 \right]^{1/2}$$

$$n_0 = \frac{n_i^2}{p_0}$$

## Extrinsic region

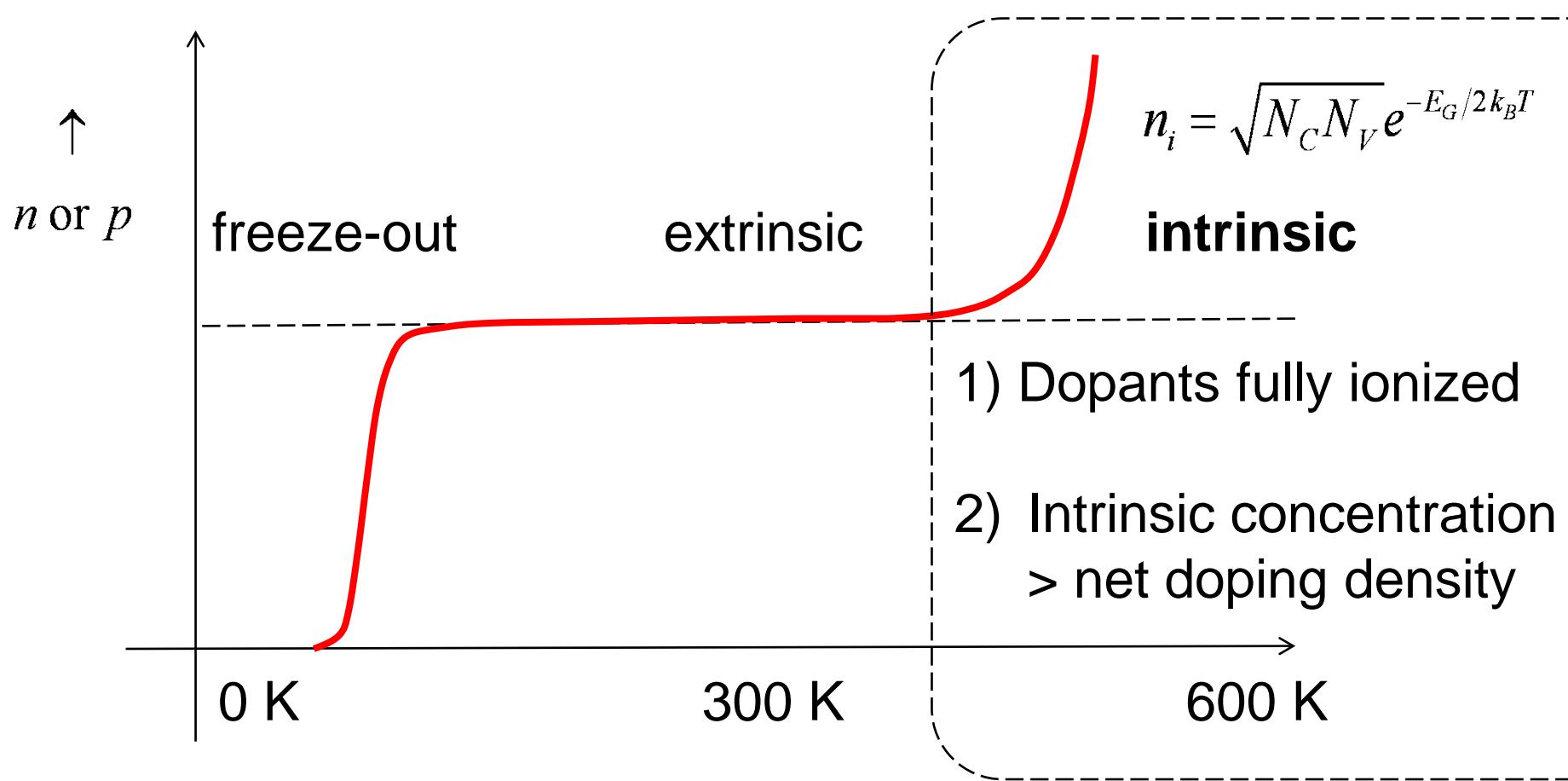
---

When the net doping density is much greater than the intrinsic carrier concentration and the dopants are fully ionized, then

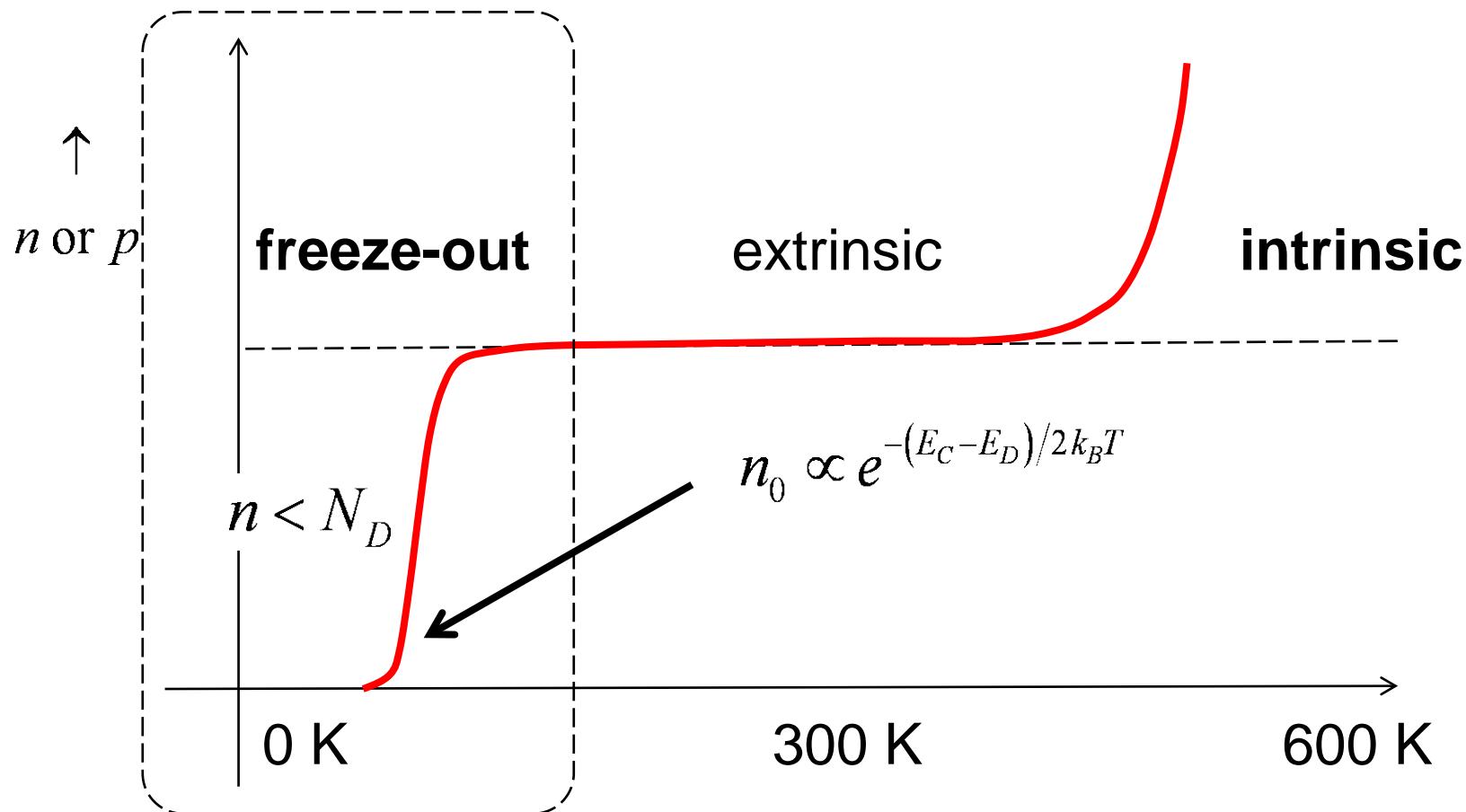
$$n_0 = N_D - N_A \quad p_0 = n_i^2 / (N_D - N_A) \quad \text{N-type} \quad N_D > N_A$$

$$p_0 = N_A - N_D \quad n_0 = n_i^2 / (N_A - N_D) \quad \text{P-type} \quad N_A > N_D$$

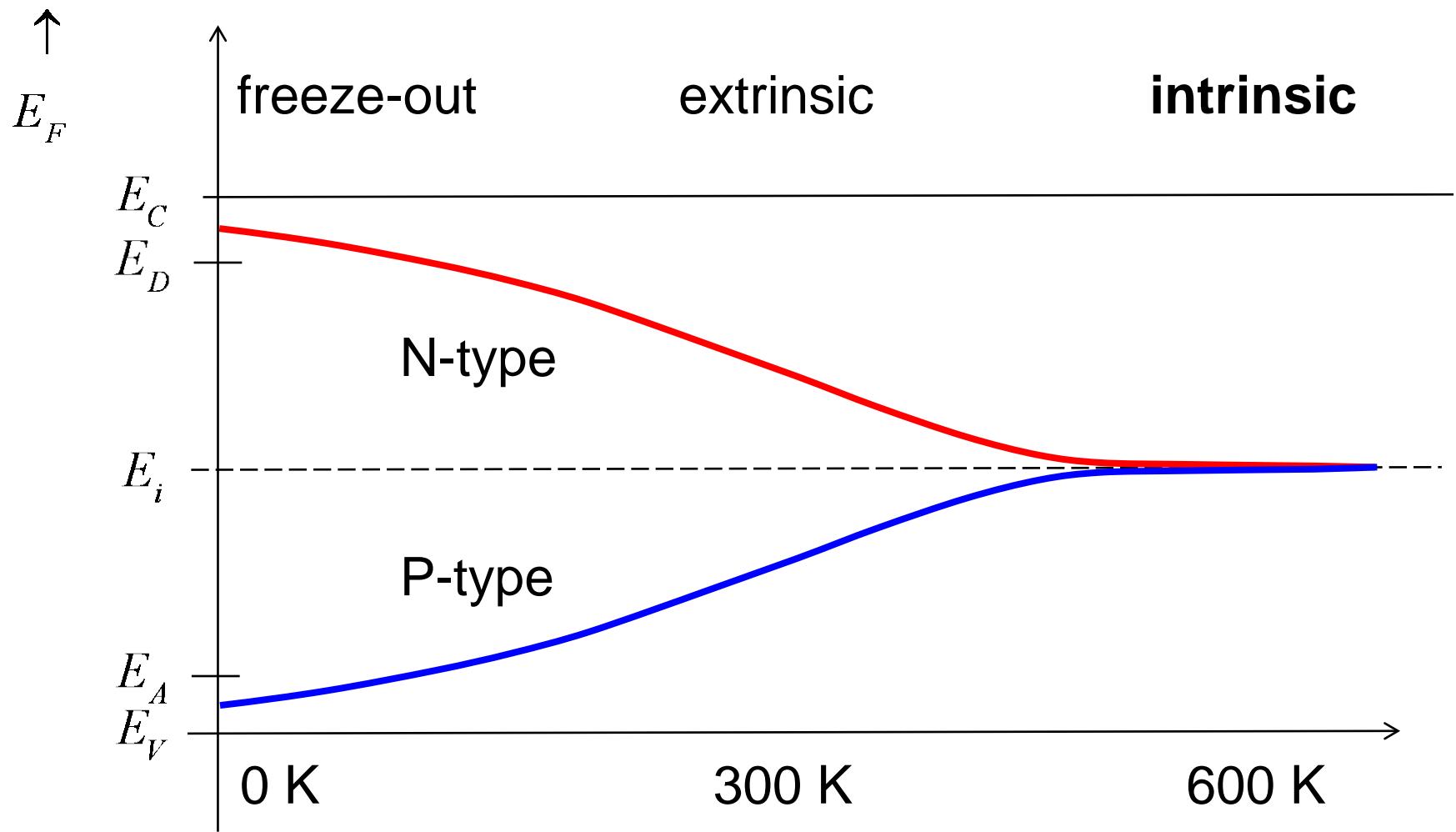
# The intrinsic region



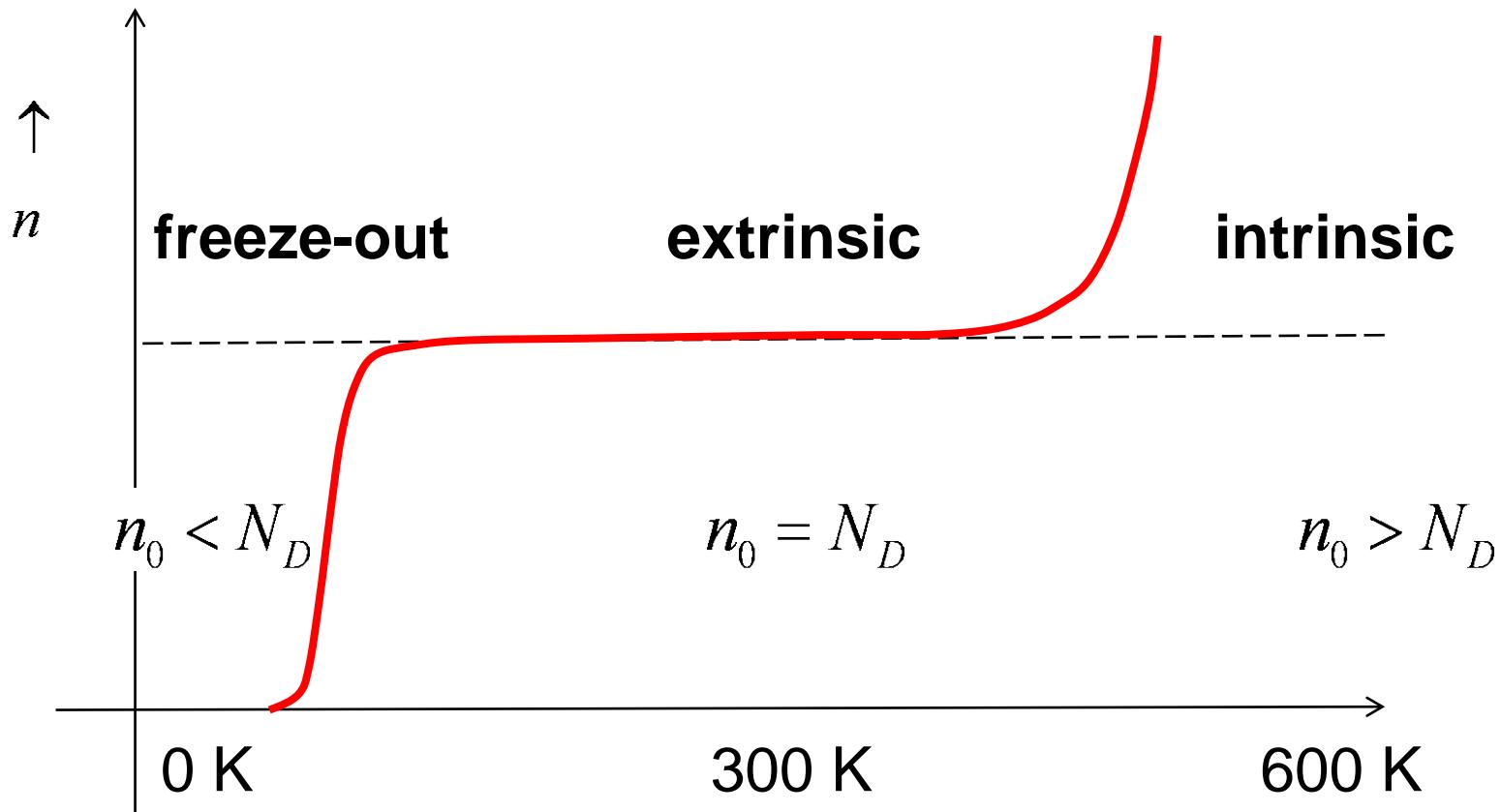
# The freeze out region



# Fermi level vs. temperature



# Unit summary



You should understand this quantitatively  
and  $E_F$  vs.  $T$  qualitatively.

# Vocabulary

---

- 1) Fermi level
- 2) Fermi function
- 3) Nondegenerate
- 4) Fermi-Dirac integral
- 5) Effective DOS
- 6) np product
- 7) Intrinsic concentration
- 8) Intrinsic Fermi level
- 9) Majority carrier
- 10) Minority carrier
- 11) Freeze-out
- 12) Extrinsic semiconductor
- 13) Intrinsic semiconductor
- 14) Donor degeneracy factor
- 15) Acceptor degeneracy factor
- 16) Metal-insulator transition

# Primer on Semiconductors

## Unit 4: Carrier Transport, Recombination, and Generation

### Lecture 4.1: The Landauer Approach

**Mark Lundstrom**

lundstro@purdue.edu

Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Carrier transport

---

The flow of charge carriers produces currents, which can be controlled to produce electronic devices.

Our goal is to understand the flow of charge carriers.

In learning chemistry, we begin with the simplest atom – the hydrogen atom and then to proceed to more complex atoms, molecules, compounds, etc.

We will take a similar approach - begin by understanding the current in a small, nanodevice, and then extend that understanding to large, bulk semiconductors.

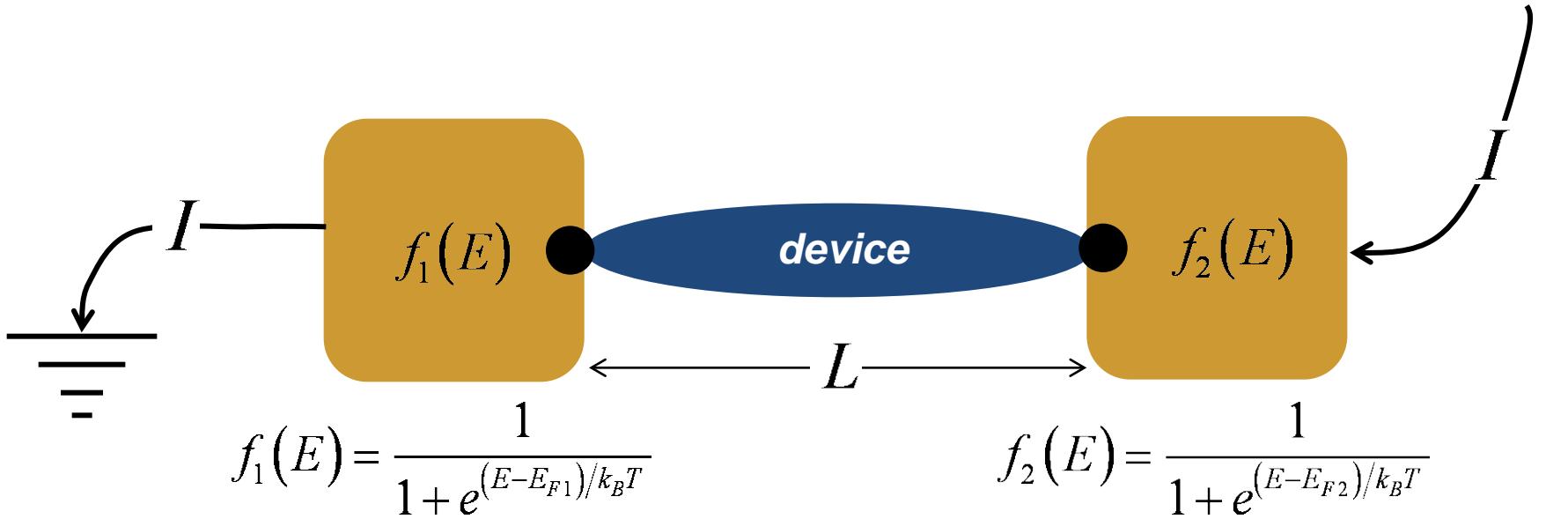
## Comments

---

Our approach will be very simple, intuitive, and descriptive. Those who want a deeper understanding, should consult:

Supriyo Datta, *Lessons from Nanoelectronics*, 2<sup>nd</sup> Ed., Part A: Basic Concepts, World Scientific Publishing Co., Singapore, 2017.

# Current in a nano device



How does the current that flows in contact 2, depend on the voltages on the two contacts?

# Current

---

$$I = \frac{2q}{h} \int T(E) M(E) (f_1(E) - f_2(E)) dE$$

Fundamental constants

Transmission:

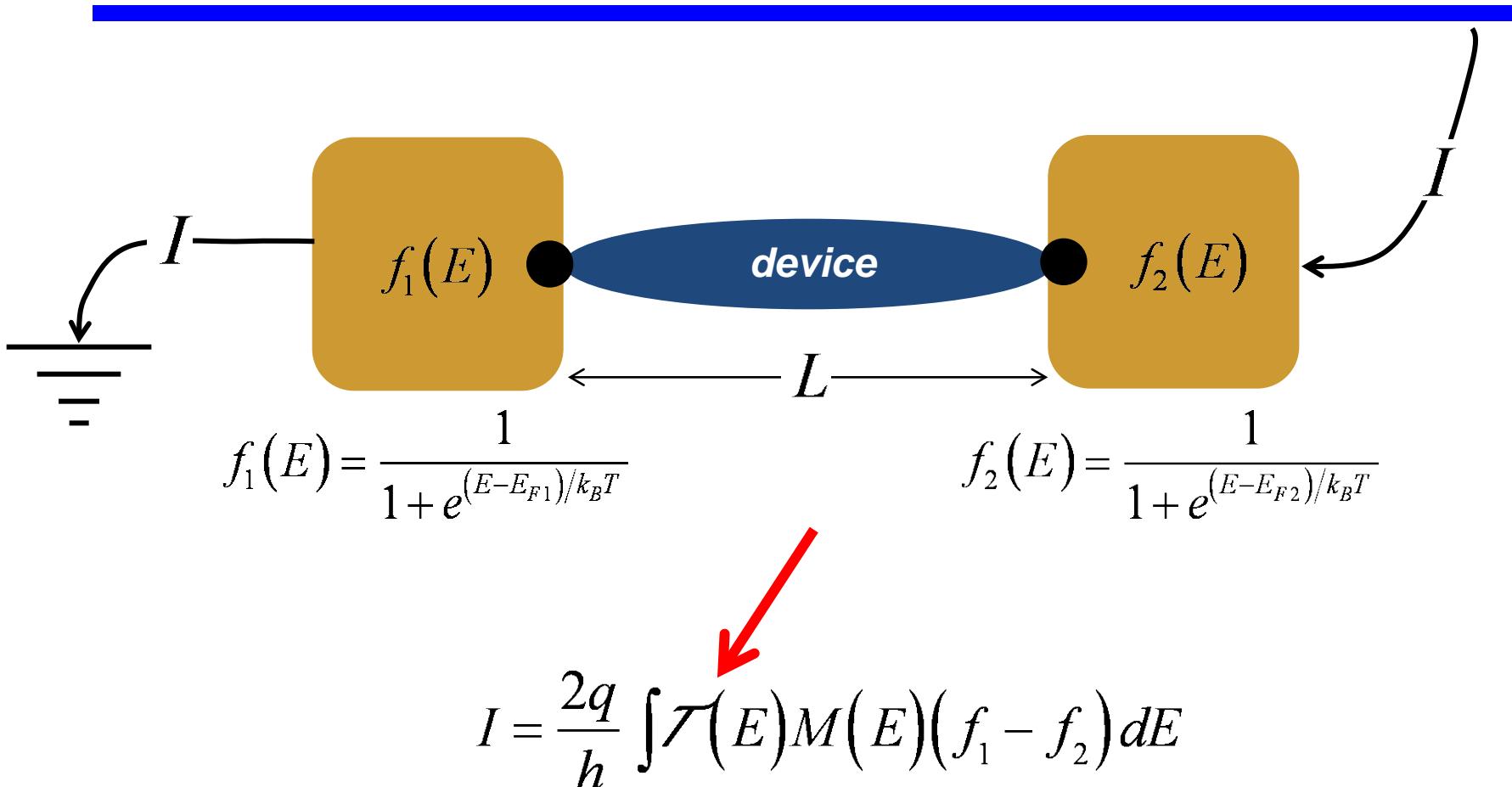
$$0 < T(E) < 1$$

No. of Channels

Ideal “Landauer” contacts

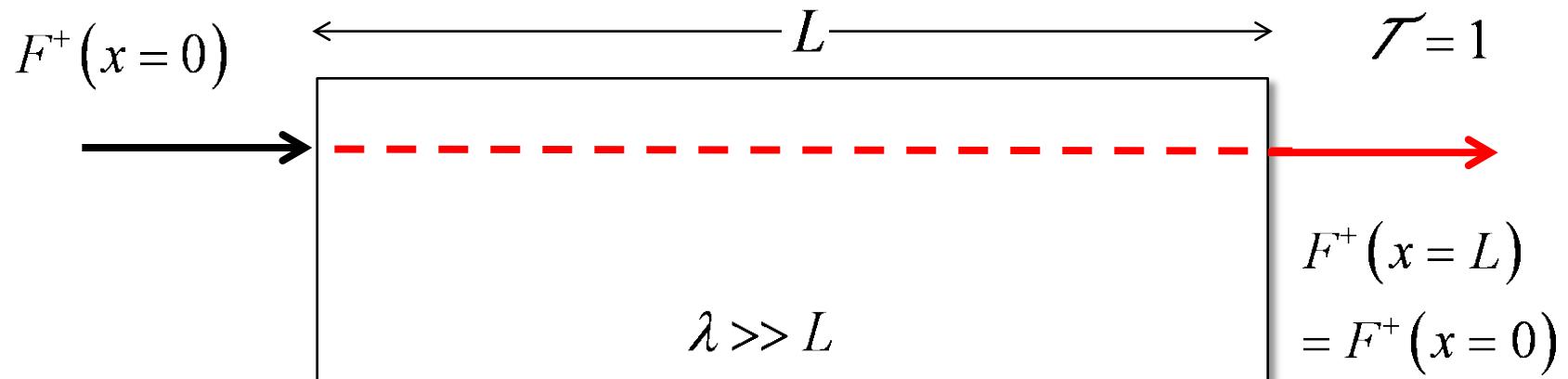
Can be derived from rigorous transport theory (the Boltzmann equation), but this expression is intuitively easy to understand.

# What is transmission?



# Transmission (ballistic)

without any distraction flow will reach the other end.



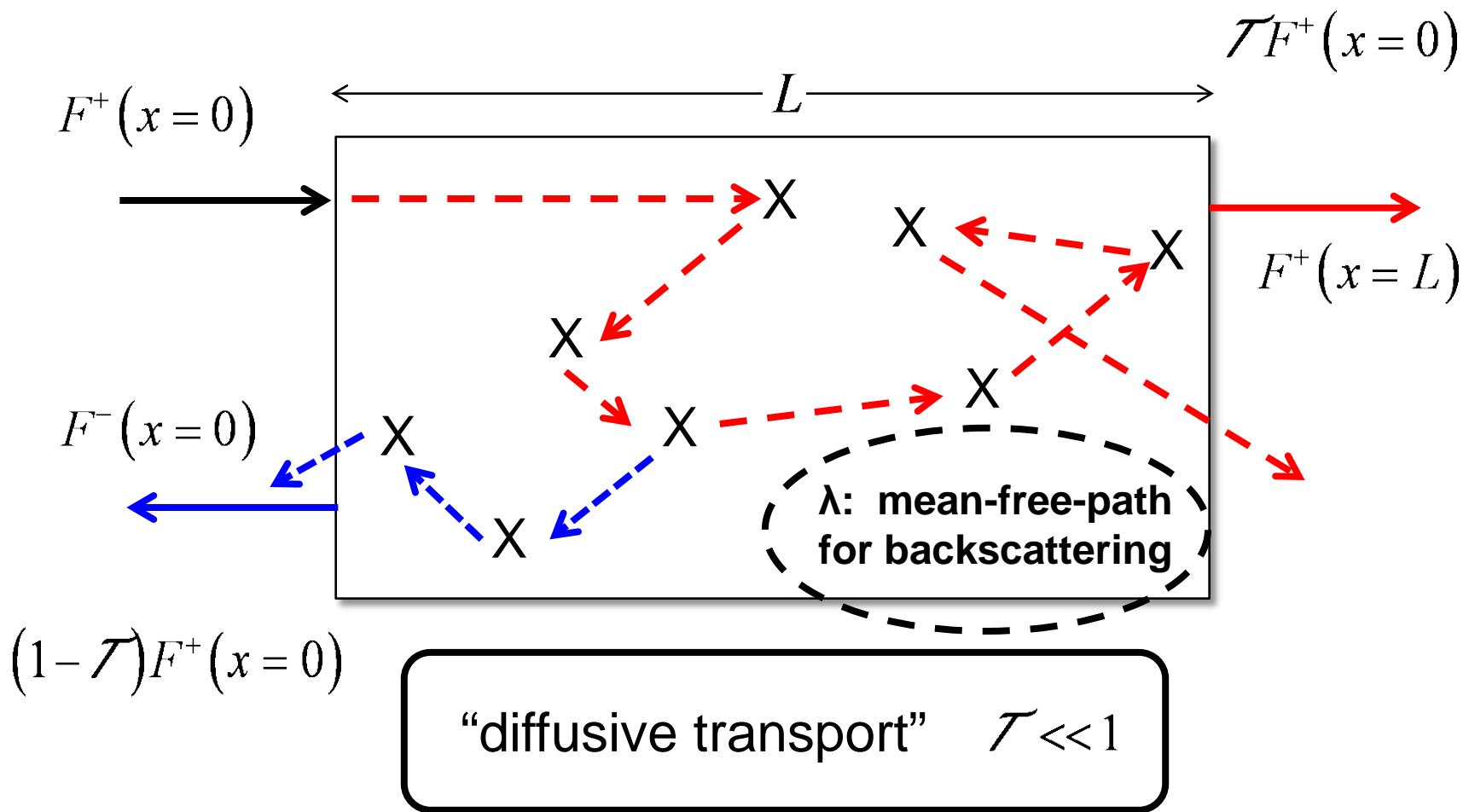
$\lambda \gg L$

$F^-(x = 0) = 0$

$\lambda$ : mean-free-path for backscattering

ballistic transport:  $\mathcal{T} = 1$

# Transmission (diffusive)



# Transmission

---

$$\mathcal{T}(E) = \frac{\lambda(E)}{\lambda(E) + L}$$

$\lambda$  is the “mean-free-path for backscattering”

This expression can be derived with relatively few assumptions.

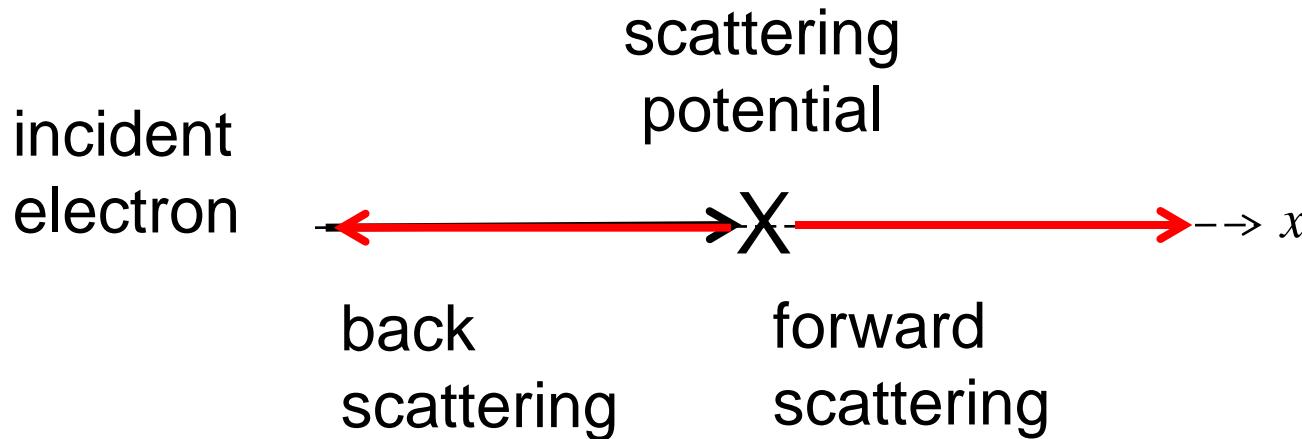
1) Diffusive:  $L \gg \lambda$   $\mathcal{T} = \frac{\lambda}{L} \ll 1$

2) Ballistic:  $L \ll \lambda$   $\mathcal{T} = 1$

$$\lambda(E) \neq v(E)\tau(E) = \Lambda$$

# MFP for backscattering in 1D

---



If we assume that the scattering is ***isotropic*** (equal probability of scattering forward or back) then average time between **backscattering** events is  $2\tau$ .

$$\lambda(E) = 2v(E)\tau(E) \quad \left\{ \Lambda(E) = v(E)\tau(E) \right\}$$

# MFP and diffusion coefficient

---

Recall Fick's Law of Diffusion:

$$F = -D \frac{dc}{dx} \frac{\#}{\text{cm}^2\text{-s}}$$

Concentration of  
diffusing particles:  $c \frac{1}{\text{cm}^3}$

Diffusion coefficient:  $D \frac{\text{cm}^2}{\text{s}}$

It turns out that there is a simple relation  
between the MFP and the diffusion coefficient:

$$D = \frac{\nu_T \lambda_0}{2}$$

# MFP and diffusion coefficient

---

$$D = \frac{v_T \lambda_0}{2}$$

The MFP,  $\lambda_0$ , is assumed to be independent of energy.

Nondegenerate conditions are assumed.

$$v_T = \sqrt{\frac{2k_B T}{\pi m^*}}$$

The uni-directional thermal velocity is the average velocity of electrons travelling on the  $+x$ , or  $-x$ , etc. direction in equilibrium.

# MFP and diffusion coefficient

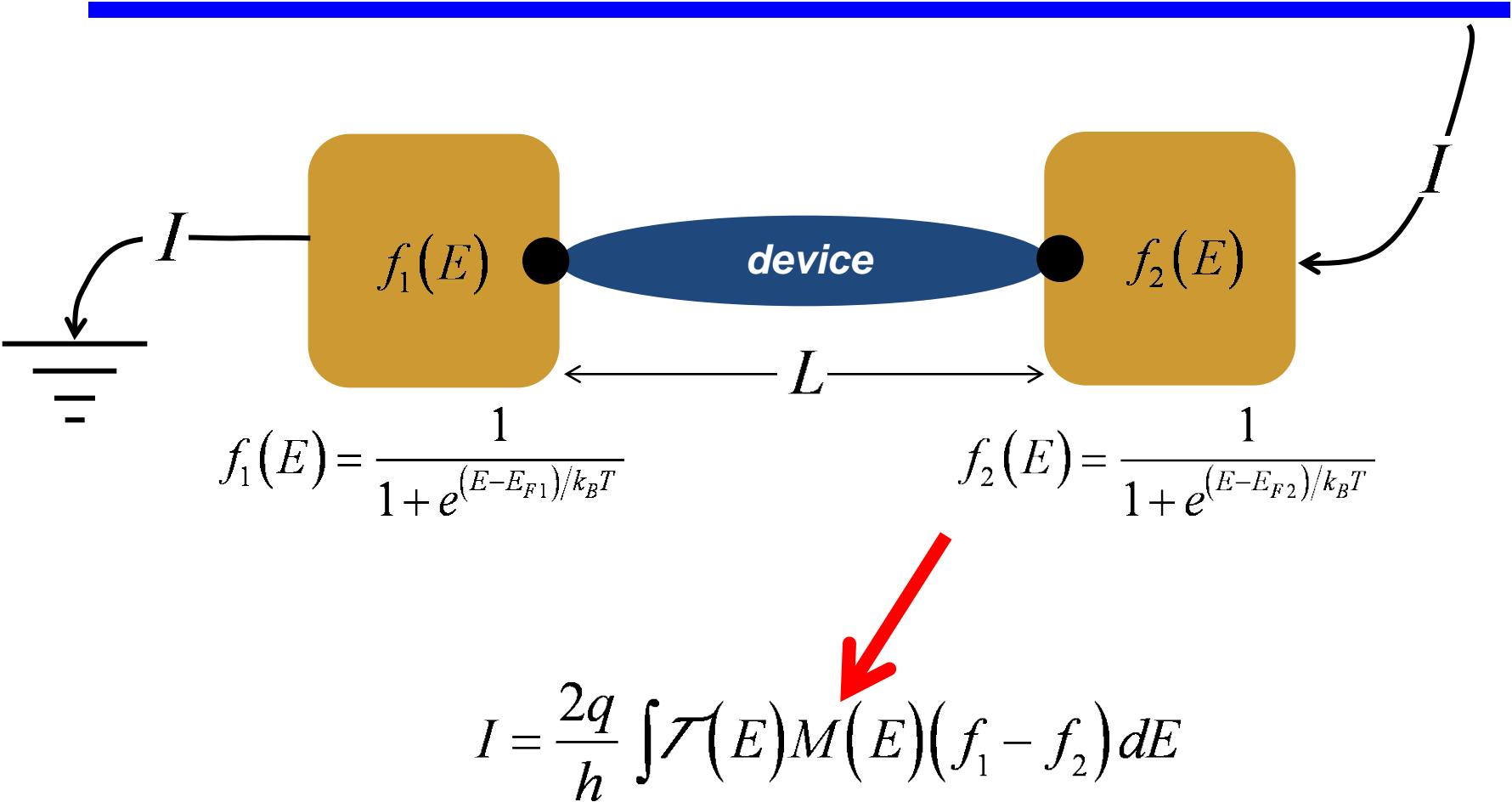
---

$$D = \frac{v_T \lambda_0}{2}$$

This is a useful formula because it allows us to deduce the MFP from a measured  $D$ .

For more discussion, see Sec. 6.2 in Mark Lundstrom and Changwook Jeong, *Near-Equilibrium Transport*, World Scientific, 2013.

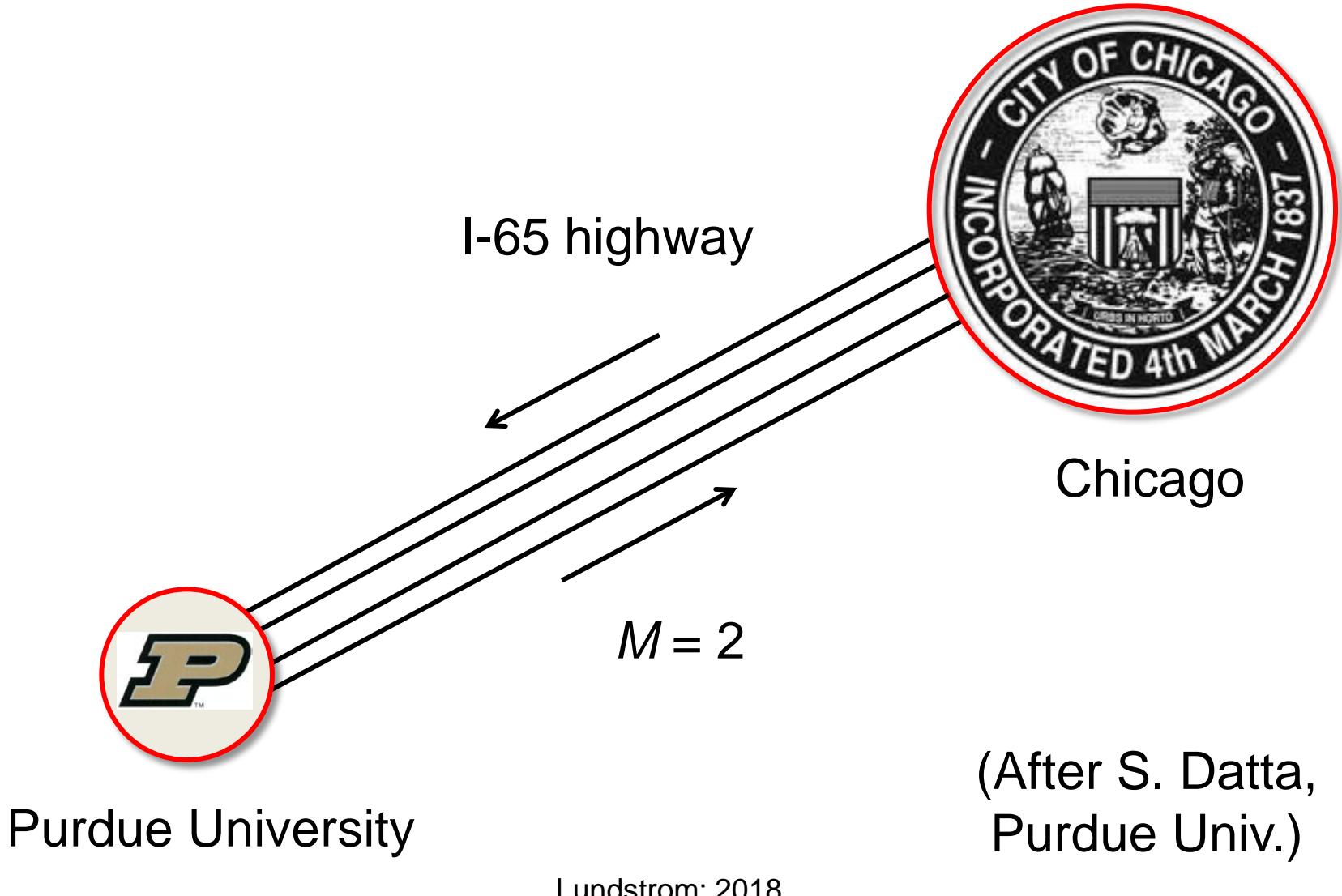
# What is a channel?



(channels are also called “modes”)

# Channels are like lanes on a highway

---



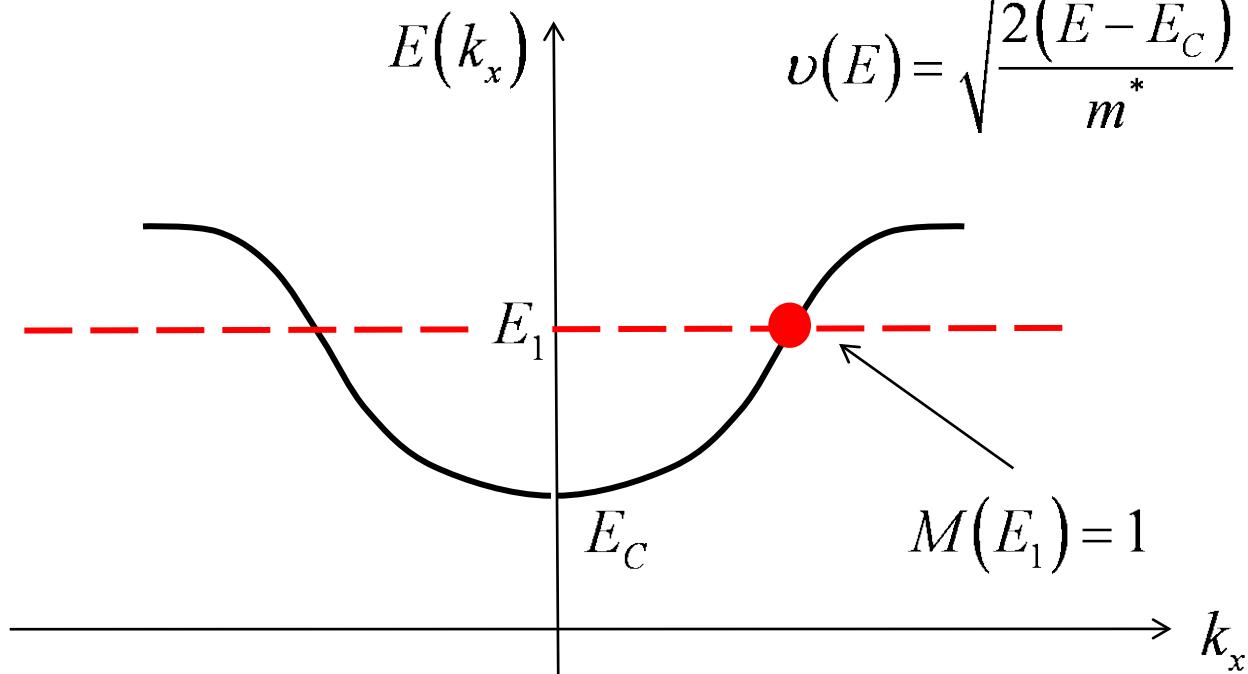
# Channels (modes) from $E(k)$

---

**A channel is a state with a velocity.**

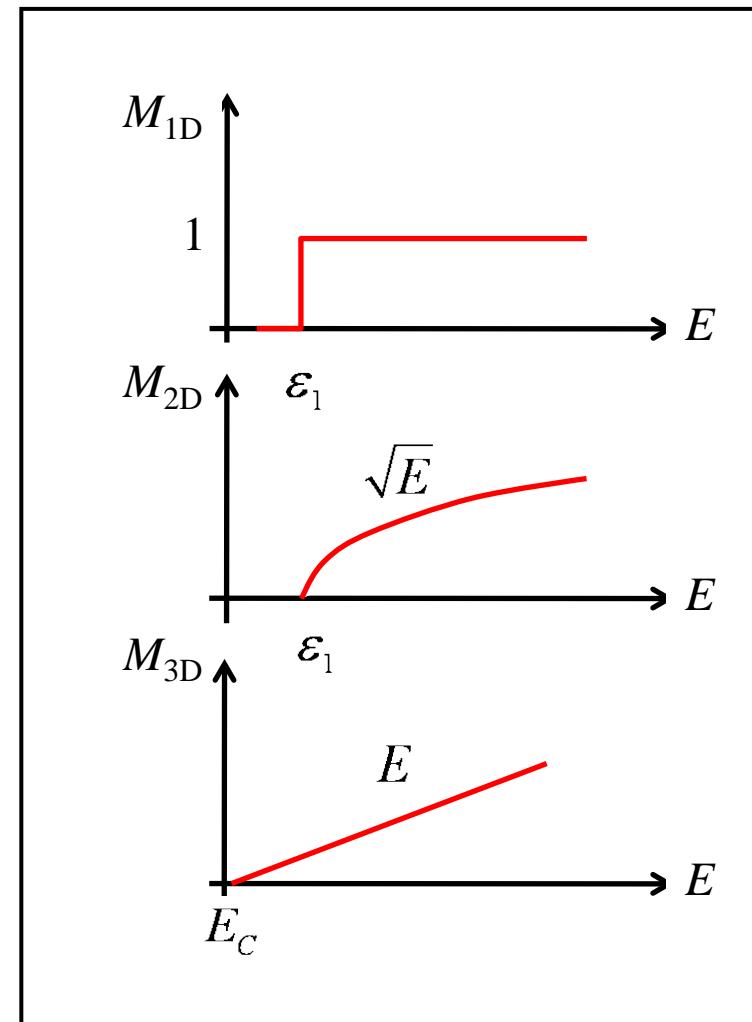
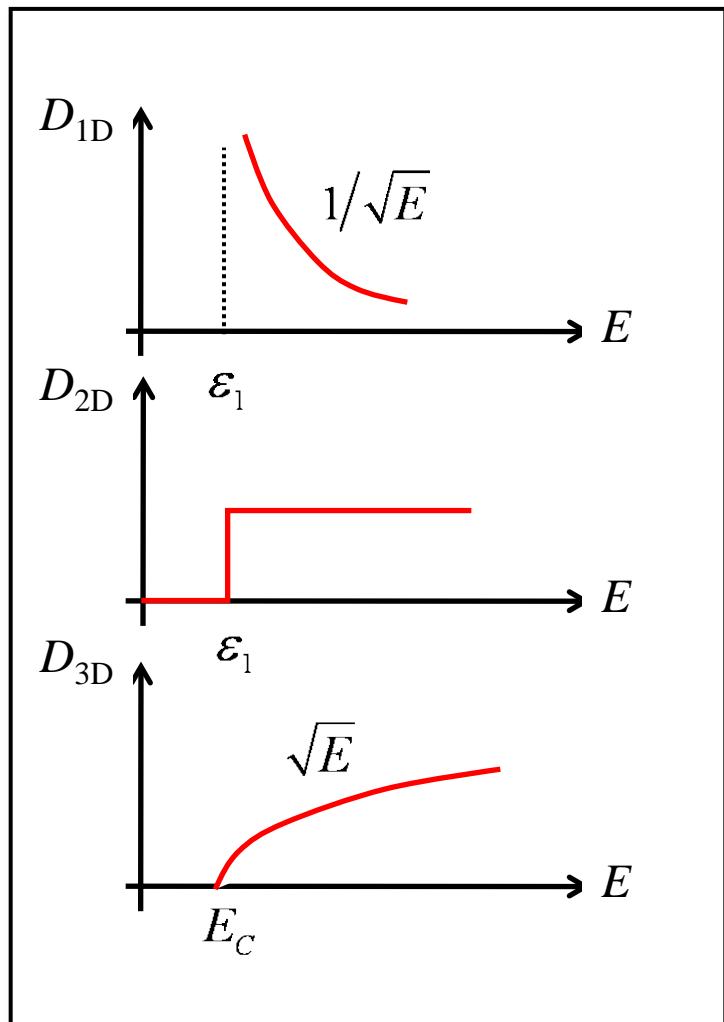
$$M(E) = A \frac{\hbar}{4} \langle v_x^+(E) \rangle D_{3D}(E)$$

$$v(E) = \sqrt{\frac{2(E - E_C)}{m^*}}$$



(Easily generalized to arbitrary band structures in 2D and 3D.)

# $M(E)$ vs. $DOS(E)$ (parabolic bands)



# Channels, transmission, and MFP

$$\mathcal{T}(E) = \frac{\lambda(E)}{\lambda(E) + L}$$

1D       $M(E) = 1$   
(per subband)

$$\lambda(E) = 2\Lambda(E)$$

2D       $M(E) = W \frac{\sqrt{2m^*(E - E_c)}}{\pi\hbar}$

$$\lambda(E) = \frac{\pi}{2} \Lambda(E)$$

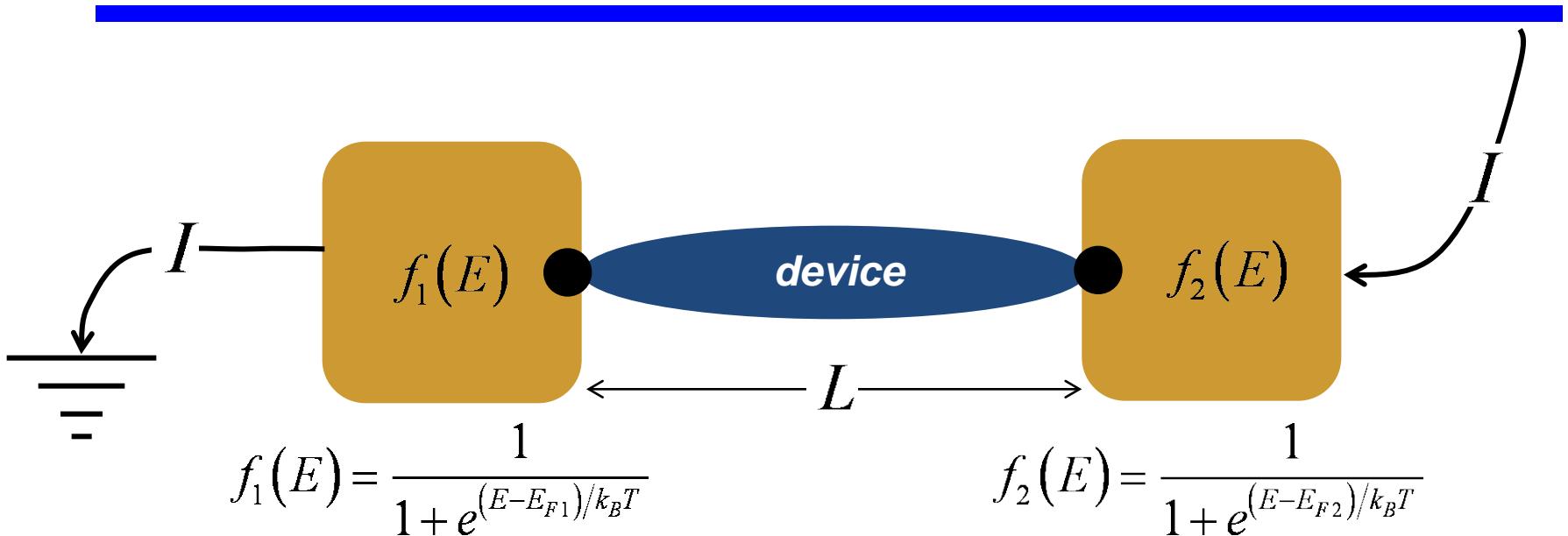
3D       $M(E) = A \frac{m^*}{2\pi\hbar^2} (E - E_c)$

$$\lambda(E) = \frac{4}{3} \Lambda(E)$$

Parabolic bands + large  
structures with many channels.

$$\Lambda(E) = v(E) \tau(E)_{18}$$

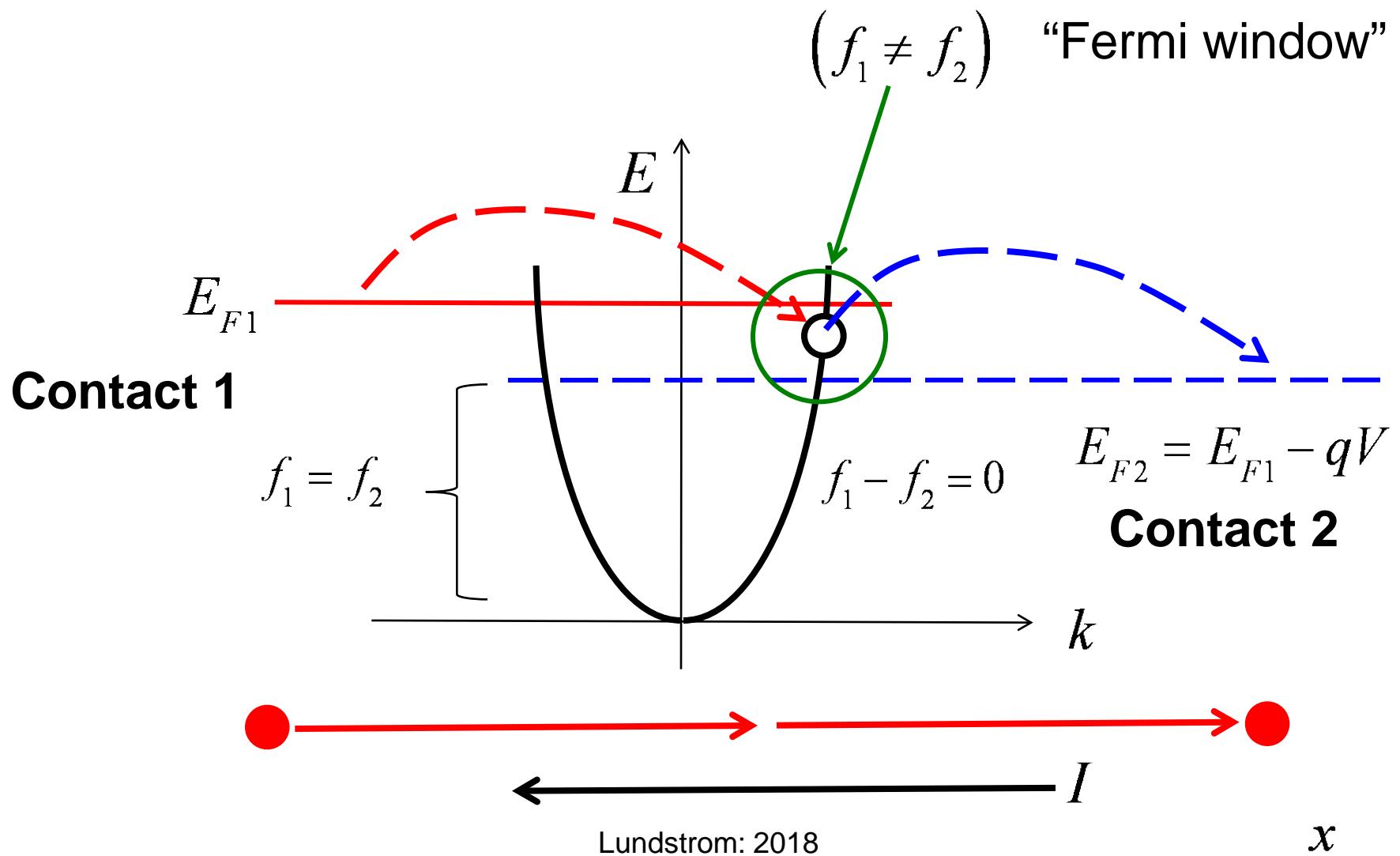
# Fermi window



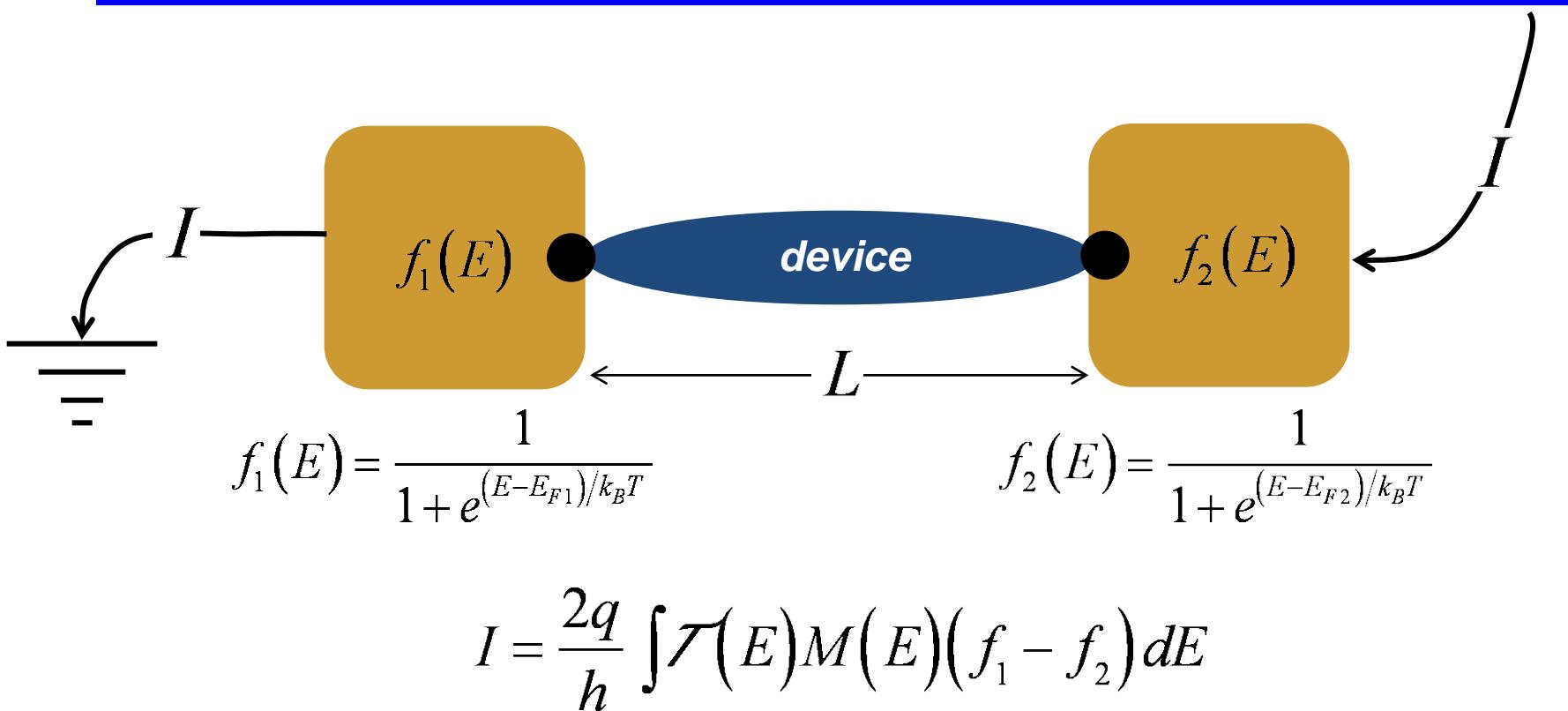
$$I = \frac{2q}{h} \int \mathcal{T}(E) M(E) (f_1 - f_2) dE$$

The range of energies over which  $(f_1 - f_2) \neq 0$

# How current flows ( $T = 0$ K)



# Summary



Can be used to describe the current in small and large devices and in short to long devices.

# Primer on Semiconductors

## Unit 4: Carrier Transport, Recombination, and Generation

### Lecture 4.2: Current from the nanoscale to macroscale

**Mark Lundstrom**

[lundstro@purdue.edu](mailto:lundstro@purdue.edu)

Electrical and Computer Engineering

Purdue University

West Lafayette, Indiana USA

# Carrier transport

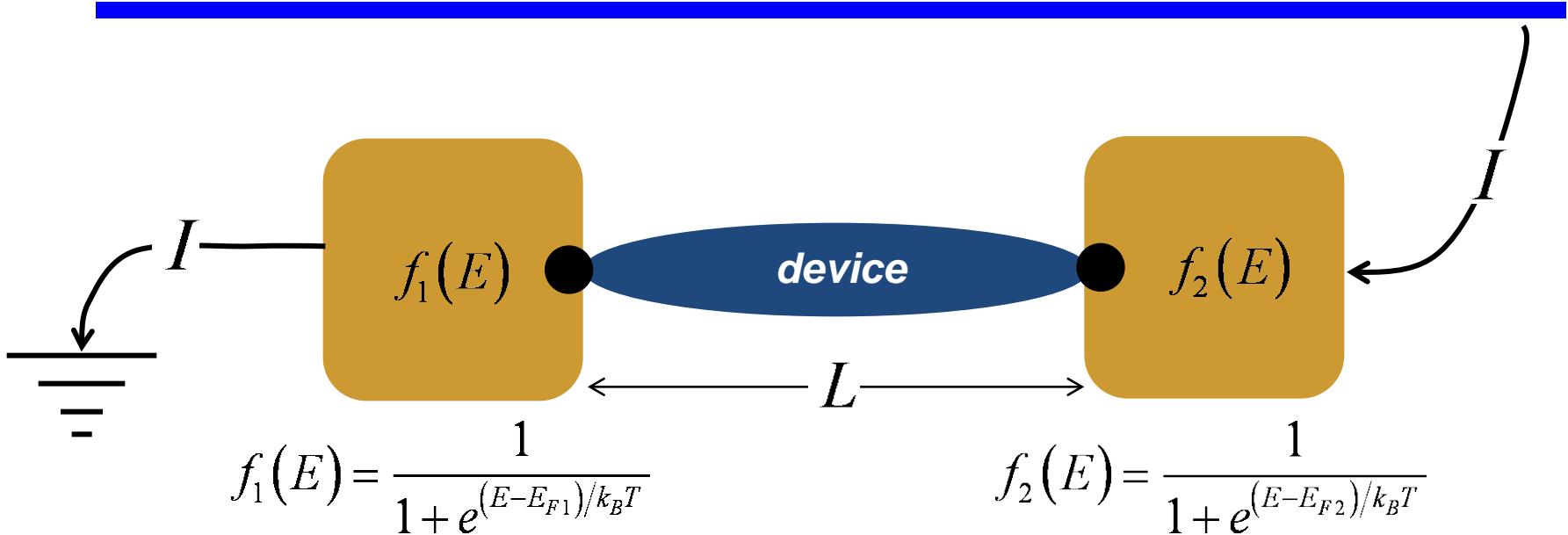
---

Our goals in this lecture are:

- 1) To understand the current in a nano-device and the important concept of **quantized conductance**.
- 2) To use the Landauer Approach to derive a current equation for bulk (i.e. large) semiconductors.

Comment: Traditional semiconductor device physics is based on a current equation for bulk semiconductors. Nano-devices are increasingly important, but the macroscopic current equation continues to provide the overall framework for understanding semiconductor devices.

# Landauer approach to current flow



$$I = \frac{2q}{h} \int \mathcal{T}(E) M(E) (f_1 - f_2) dE$$

Can be used to describe the current in small and large devices and in short to long devices.

## Comment

---

We will restrict our attention to small applied voltages (or small electric fields in bulk semiconductors).

Things become more complicated at high electric fields, but we can often describe the effects by modifying the small electric field results.

# Fermi window (small bias)

---

$$I = \frac{2q}{h} \int \mathcal{T}(E) M(E) \left( f_1(E) - \underline{f_2(E)} \right) dE$$

$$f_1(E) = \frac{1}{1 + e^{(E-E_{F1})/k_B T}} = f_0(E) \quad \delta E_F = -qV$$

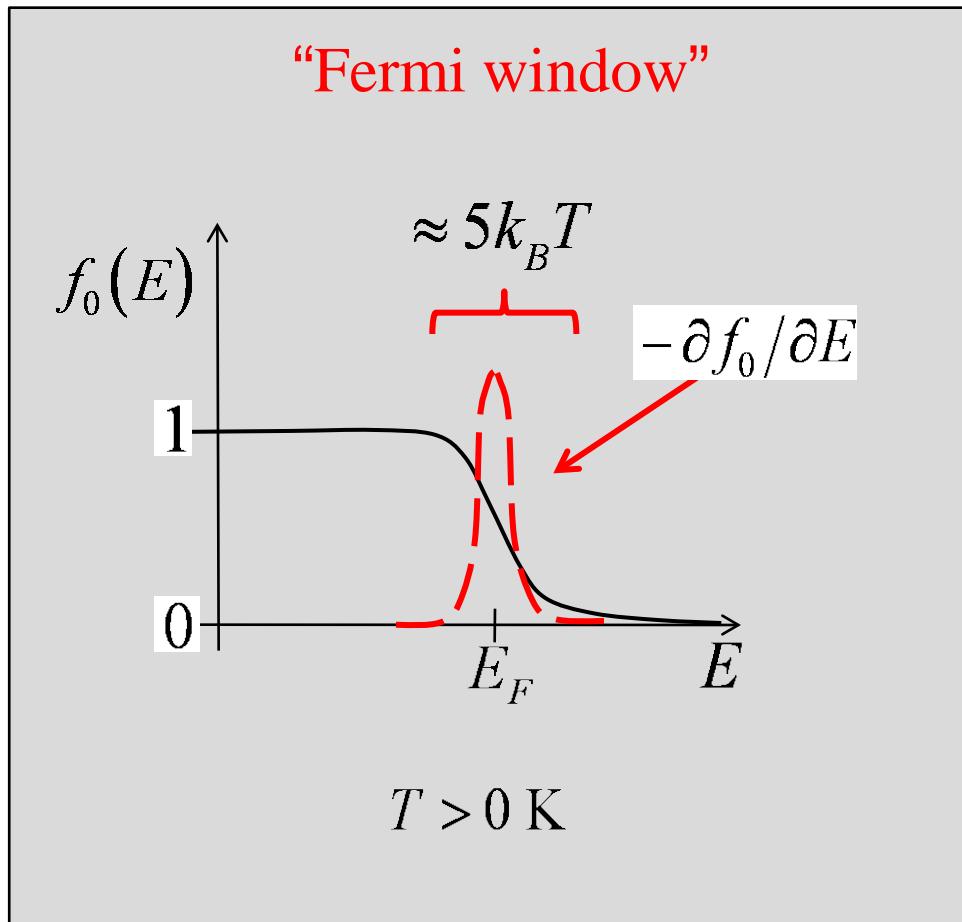
$$f_2(E) \approx f_1(E) + \frac{\partial f_1}{\partial E_F} \delta E_F$$

$$f_2(E) \approx f_1(E) + \left( -\frac{\partial f_1}{\partial E} \right) \delta E_F$$

$$f_1(E) - f_2(E) = \left( -\frac{\partial f_0}{\partial E} \right) (qV)$$

$$f_1(E) - f_2(E) \approx -\left( -\frac{\partial f_1}{\partial E} \right) \delta E_F \quad \text{Lundstrom: 2018}$$

# Fermi window: small bias

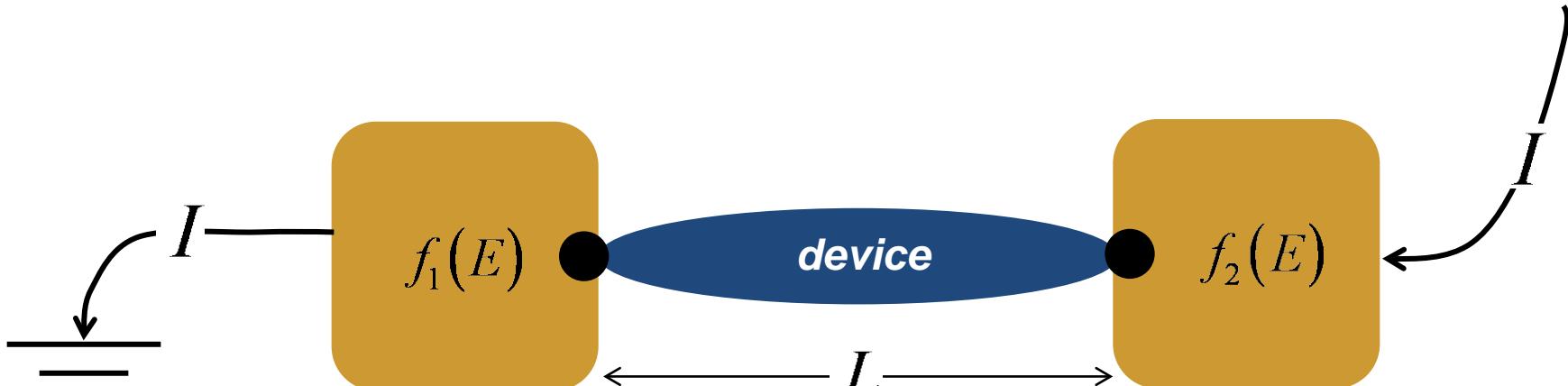


$$W_F(E) = \left( -\frac{\partial f_0}{\partial E} \right)$$

$$\int W_F(E) dE = 1$$

# Current for a small voltage difference

---



$$f_1(E) = \frac{1}{1 + e^{(E-E_{F1})/k_B T}}$$

$$f_2(E) = \frac{1}{1 + e^{(E-E_{F2})/k_B T}}$$

$$I = \frac{2q}{h} \int \mathcal{T}(E) M(E) (f_1 - f_2) dE$$

$$f_1(E) - f_2(E) \rightarrow \left( -\frac{\partial f_1}{\partial E} \right) (qV) \Rightarrow I = GV$$

# Small bias conductance

---

$$I = GV \quad \text{A}$$

$$G = \frac{2q^2}{h} \int \mathcal{T}(E) M(E) \left( -\frac{\partial f_0}{\partial E} \right) dE \quad \text{S}$$

# Conductance at $T = 0$ K

$$G = \frac{2q^2}{h} \int \mathcal{T}(E) M(E) \left( -\frac{\partial f_0}{\partial E} \right) dE \quad S$$

$T = 0$  K:

$$\left( -\frac{\partial f_0}{\partial E} \right) = \delta(E_F)$$

$$G(T = 0 \text{ K}) = \frac{2q^2}{h} \mathcal{T}(E_F) M(E_F)$$

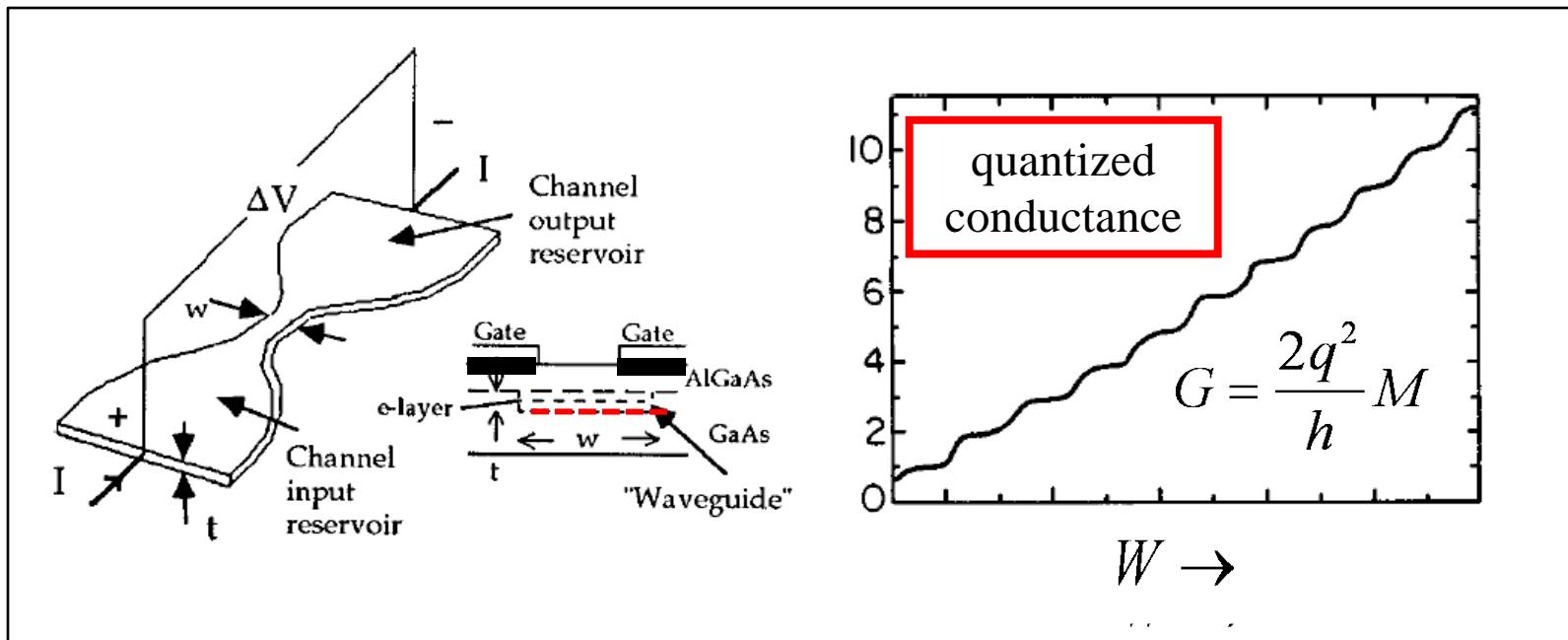
2D conductor

$$M(E) = W g_v \frac{\sqrt{2m^* E}}{\pi \hbar}$$

For large  $W$ ,  $M$  is  $\sim W$

For small  $W$ ,  $M$  comes in discrete units.

# Quantized conductance

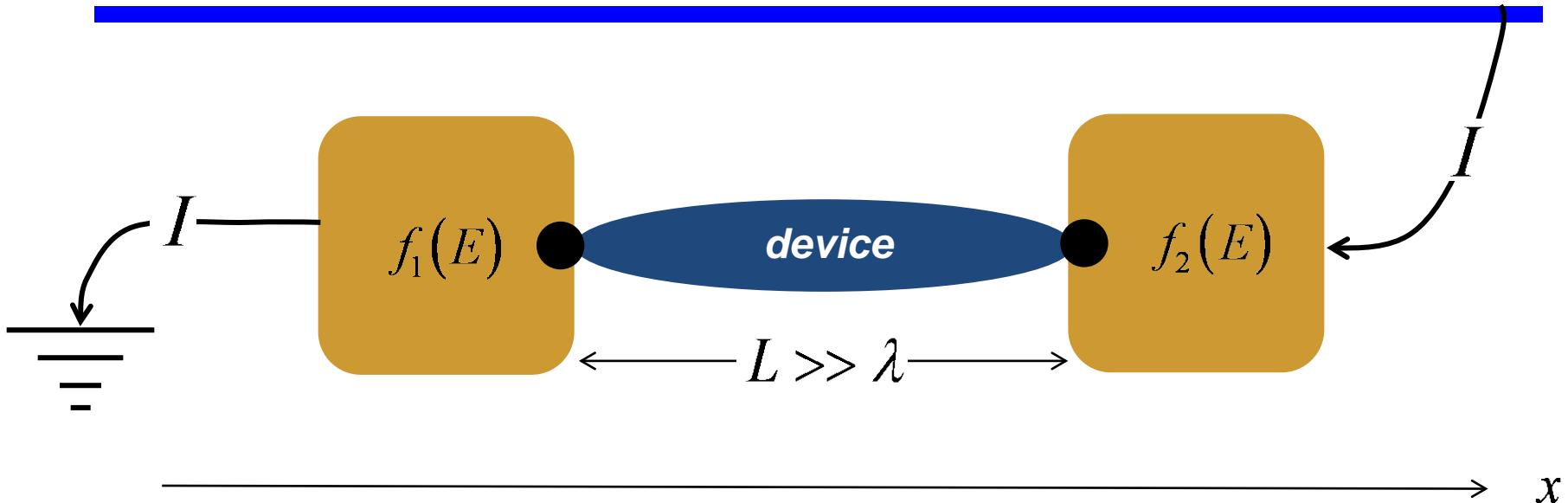


Ohm's Law (1827)

D. Holcomb, *American J. Physics*, **67**, pp. 278-297 1999.

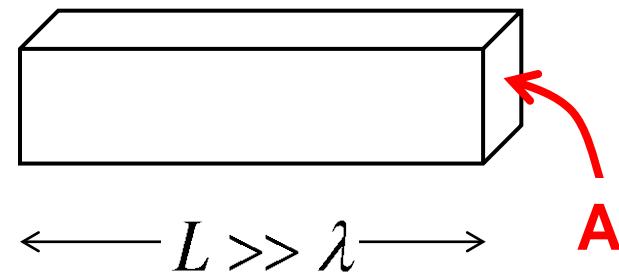
Data from: B. J. van Wees, et al., *Phys. Rev. Lett.* **60**, 848851, 1988.

# Landauer Approach to bulk transport



We seek an equation for the current density in the +x direction.

$$\text{In 3D: } J_x = -I/A$$



# Current equation in the bulk

$$G = \frac{2q^2}{h} \int \mathcal{T}(E) M(E) \left( -\frac{\partial f_0}{\partial E} \right) dE \quad \mathcal{T}(E) = \frac{\lambda(E)}{\lambda(E) + L} \rightarrow \frac{\lambda(E)}{L}$$

diffusive

$$J_x = -I/A = \left\{ \frac{2q^2}{h} \int \frac{\lambda(E) M(E)}{L} \left( -\frac{\partial f_0}{\partial E} \right) dE \right\}_V \quad \frac{qV}{L} = -\frac{dF_n}{dx}$$

$$J_x = \sigma_n \frac{d(F_n/q)}{dx} \quad \sigma_n = \frac{2q^2}{h} \int \lambda(E) (M(E)/A) \left( -\frac{\partial f_0}{\partial E} \right) dE$$

# Current equation (3D bulk)

---

$$J_x = \sigma_n \frac{d(F_n/q)}{dx}$$

$\sigma_n$ : Conductivity (S/m)       $\rho_n = 1/\sigma_n$ : Resistivity (Ohm-m)

$n$ : electron density

$\sigma_n \equiv nq\mu_n$        $q$ : magnitude of the electronic charge

$\mu_n$ : mobility m<sup>2</sup>/V-s

$$J_x = n\mu_n \frac{dF_n}{dx}$$

# The quasi-Fermi level or electrochemical potential

---

“electrochemical potential”

$$J_x = \sigma_n \frac{d(F_n/q)}{dx}$$

“quasi-Fermi level”

The quantity,  $F_n$ , is analogous to the Fermi level, but it is defined out of equilibrium and reduces to the Fermi level in equilibrium.

$$n_0 = N_C e^{(E_F - E_C)/k_B T} \rightarrow n = N_C e^{(F_n - E_C)/k_B T}$$

In equilibrium, the current is zero:  $J_x = 0 = \sigma_n \frac{d(F_n/q)}{dx} \rightarrow \frac{dE_F}{dx} = 0$

**The Fermi level is constant, independent of position, in equilibrium.**

# The mobility

---

$$J_x = \sigma_n \frac{d(F_n/q)}{dx} \quad J_x = n\mu_n \frac{dF_n}{dx}$$

The fundamental quantity is the **conductivity** – mobility is a derived quantity.

To relate the mobility to material properties, we should begin by evaluating the conductivity.

# Landauer derivation of the mobility

---

$$\sigma_n = \frac{2q^2}{h} \int \lambda(E) \left( M(E)/A \right) \left( -\frac{\partial f_0}{\partial E} \right) dE$$

$$\lambda(E) = \lambda_0 \quad M(E)/A = \frac{m^*}{2\pi\hbar^2} (E - E_C) \quad f_0(E) = \frac{1}{1 + e^{(E_E - E_F)/k_B T}}$$

$$\sigma_n = \frac{2q^2}{h} \lambda_0 \left( \frac{m^* k_B T}{2\pi\hbar^2} \right) e^{(E_F - E_C)/k_B T} \quad (\text{nondegenerate})$$

$$n_0 = \frac{1}{4} \left( \frac{2m_n^* k_B T}{\pi\hbar^2} \right)^{3/2} e^{(E_F - E_C)/k_B T}$$

# Mobility

---

$$\sigma_n = n_0 q \left( \frac{v_T \lambda_0}{2(k_B T / q)} \right) = n_0 q \mu_n$$

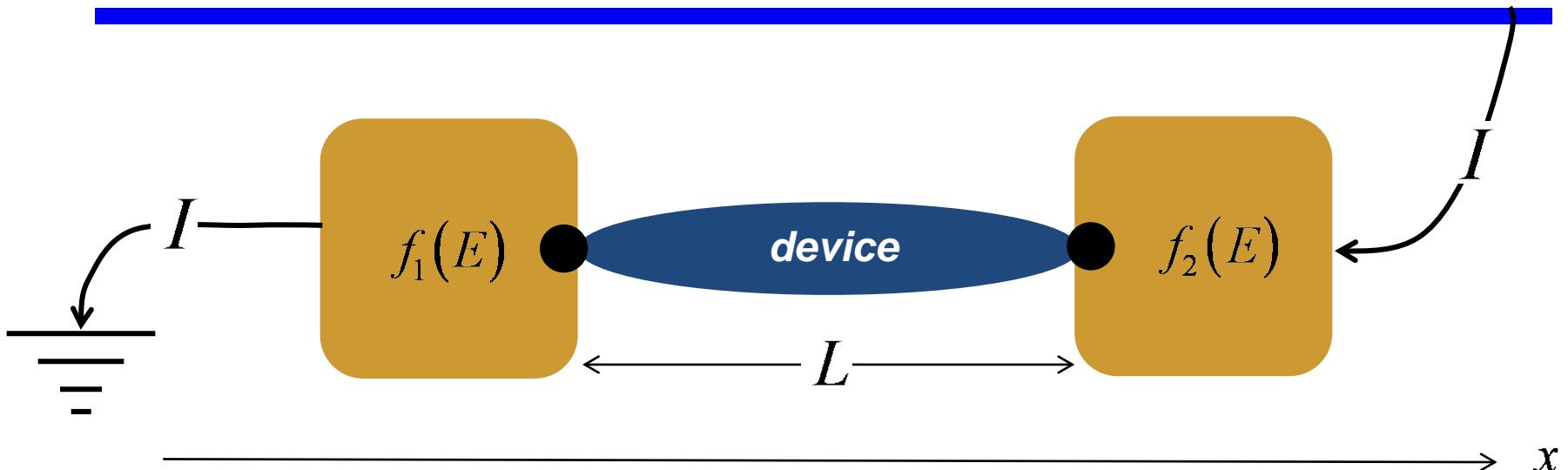
$$\mu_n \equiv \left( \frac{v_T \lambda_0}{2(k_B T / q)} \right) \text{ cm}^2/\text{V-s}$$

$$v_T = \sqrt{\frac{2k_B T}{\pi m^*}} \text{ cm/s}$$

uni-directional thermal velocity

**Note:**  $(k_B T / q) \mu_n = \left( \frac{v_T \lambda_0}{2} \right) = D_n \text{ cm}^2/\text{s}$  (the diffusion coefficient discussed earlier.)

# Summary



$$I = \frac{2q}{h} \int \mathcal{T}(E) M(E) (f_1 - f_2) dE$$

$$J_x = n \mu_n \frac{dF_n}{dx}$$

For small devices,  $M$  is countable

For short devices,  $T=1$ , ballistic.

A special case for large and long devices.

# Primer on Semiconductors

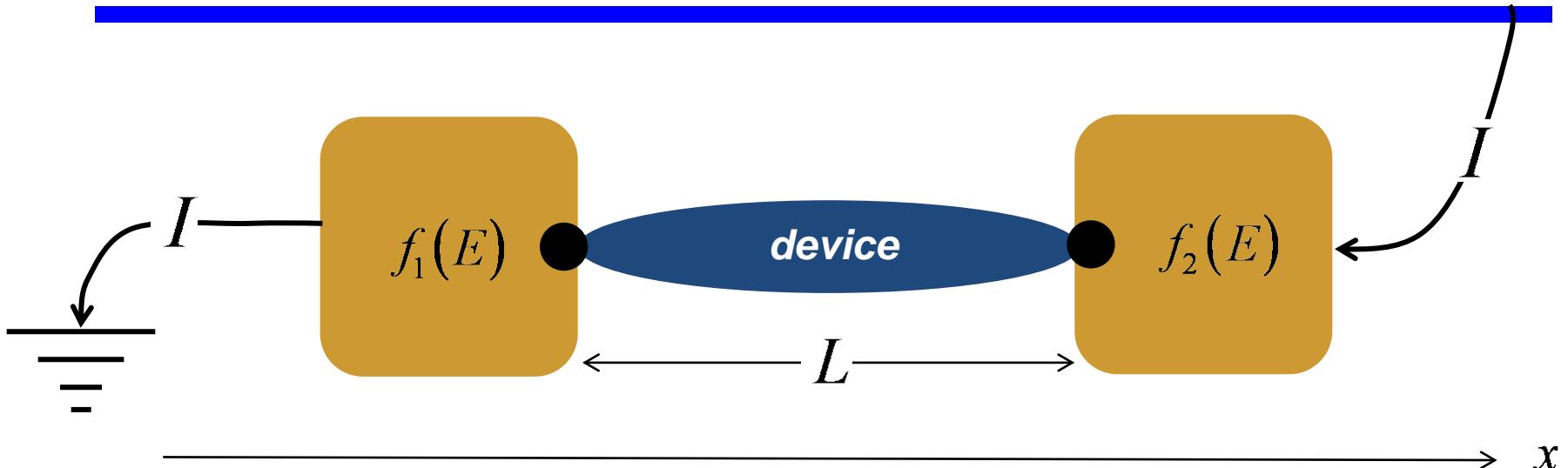
## Unit 4: Carrier Transport, Recombination, and Generation

### Lecture 4.3: Drift-diffusion equation

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Review



$$I = \frac{2q}{h} \int \mathcal{T}(E) M(E) (f_1 - f_2) dE$$

$$J_x = n \mu_n \frac{dF_n}{dx}$$

For small devices,  $M$  is countable

For short devices,  $T=1$ , ballistic.

A special case for large and long devices.

# Current equation for bulk semiconductors

---

$$J_x = n \mu_n \frac{dF_n}{dx}$$

$$n = N_C e^{(F_n - E_C)/k_B T}$$

$$E_C(x) = E_{ref} - qV(x)$$

$$F_n = E_C + k_B T \ln\left(\frac{n}{N_C}\right)$$

$$\frac{dE_C}{dx} = -q \frac{dV}{dx} = q\mathcal{E}$$

$$\frac{dF_n}{dx} = \frac{dE_C}{dx} + k_B T \frac{1}{n} \frac{dn}{dx}$$

$$k_B T \mu_n = q D_n \quad D_n / \mu_n = k_B T / q$$

$$J_x = n \mu_n \frac{dE_C}{dx} + k_B T \mu_n \frac{dn}{dx}$$

$$J_x = n q \mu_n \mathcal{E} + q D_n \frac{dn}{dx}$$

# The drift-diffusion equation

$$J_x = nq\mu_n \mathcal{E} + qD_n \frac{dn}{dx}$$

$$D_n/\mu_n = k_B T/q$$

(Einstein relation)

$$J_{drift} = nq\mu_n \mathcal{E}$$

current due to **drift**  
in an electric field



$$F_e = -q\mathcal{E}$$

$$\mu_n \frac{\text{m}^2}{\text{V}\cdot\text{s}} \quad \text{"mobility"}$$

$$J_{diff} = qD_n \frac{dn}{dx}$$

current due to  
**diffusion** in a  
concentration gradient

$$D_n/\mu_n = k_B T/q$$

$$D_n \frac{\text{m}^2}{\text{s}} \quad \text{"diffusion coefficient"}$$

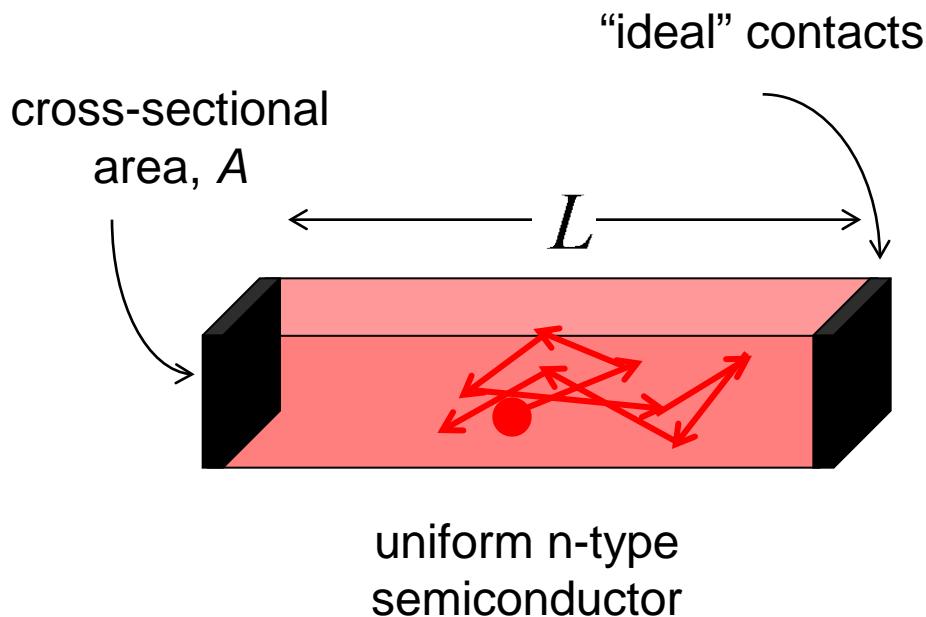
# Drift and Diffusion

---

In the next few slides, we will briefly discuss the drift and diffusion currents separately.

# Semiconductor in equilibrium

---



$$\langle KE \rangle = \frac{3}{2} k_B T$$

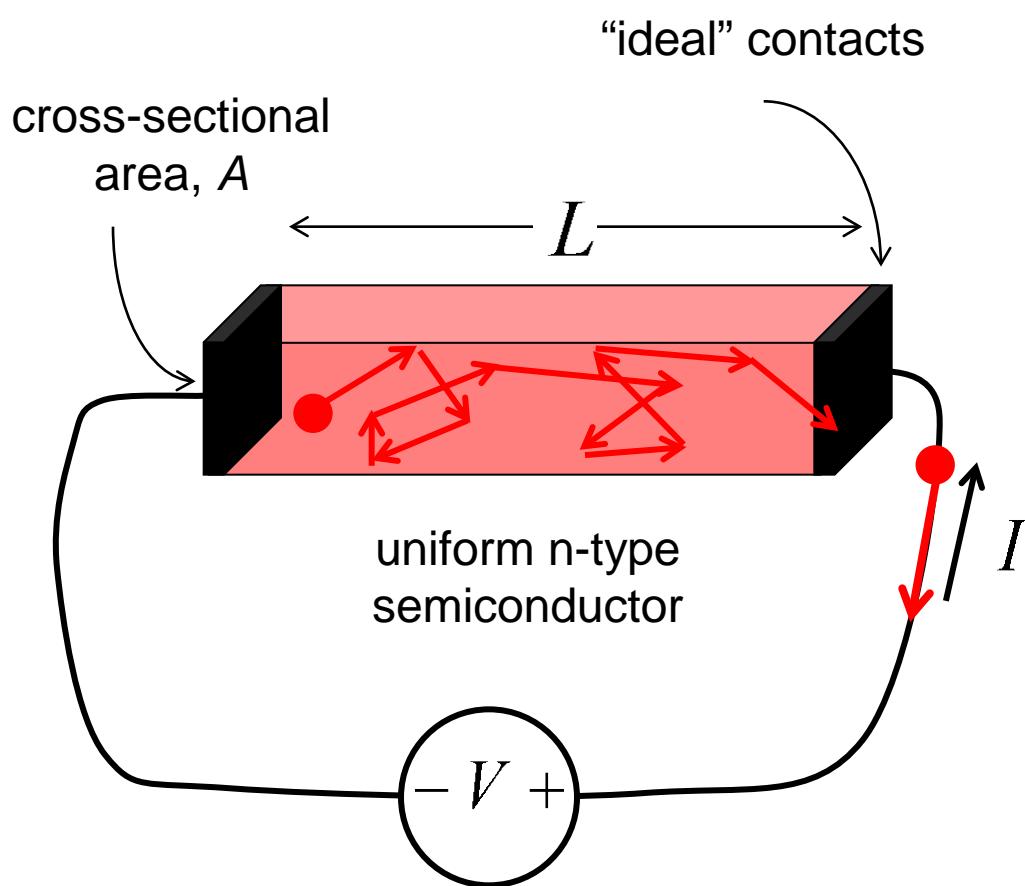
$$\langle KE \rangle = \frac{1}{2} m_n^* \langle v^2 \rangle$$

$$\sqrt{\langle v^2 \rangle} = v_{rms} = \sqrt{\frac{3k_B T}{m_n^*}}$$

$$v_{rms} \approx 10^7 \text{ cm/s} (300 \text{ K})$$

$$v_{rms} \propto \sqrt{T}$$

# Semiconductor under bias

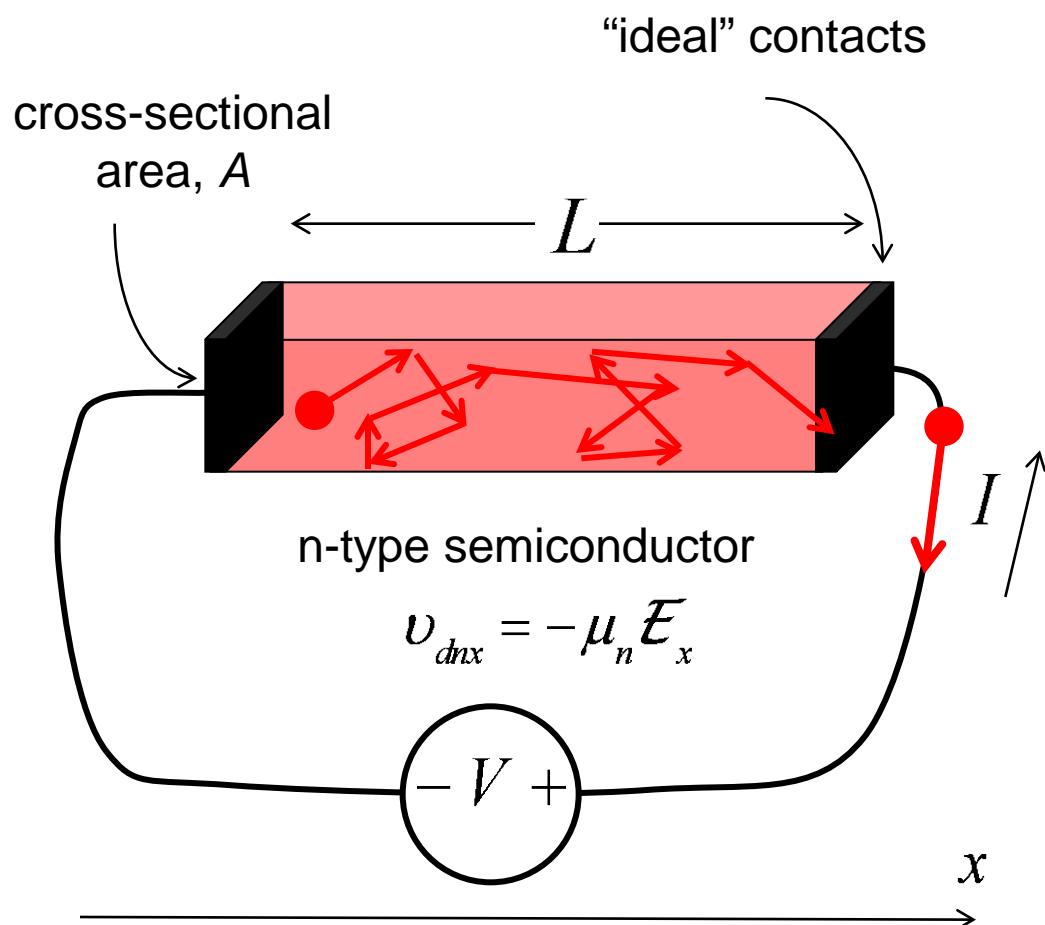


- 1) random walk with a small bias from left to right
- 2) assume that electrons “drift” to the right at an average velocity,  $v_d$

$$v_{dnx} = -\mu_n \mathcal{E}_x$$

- 3) what is  $I$ ?

# Drift current and drift velocity



$$I = -Q/t_t$$

$$Q = -qnAL$$

$$t_t = L/v_{dnx}$$

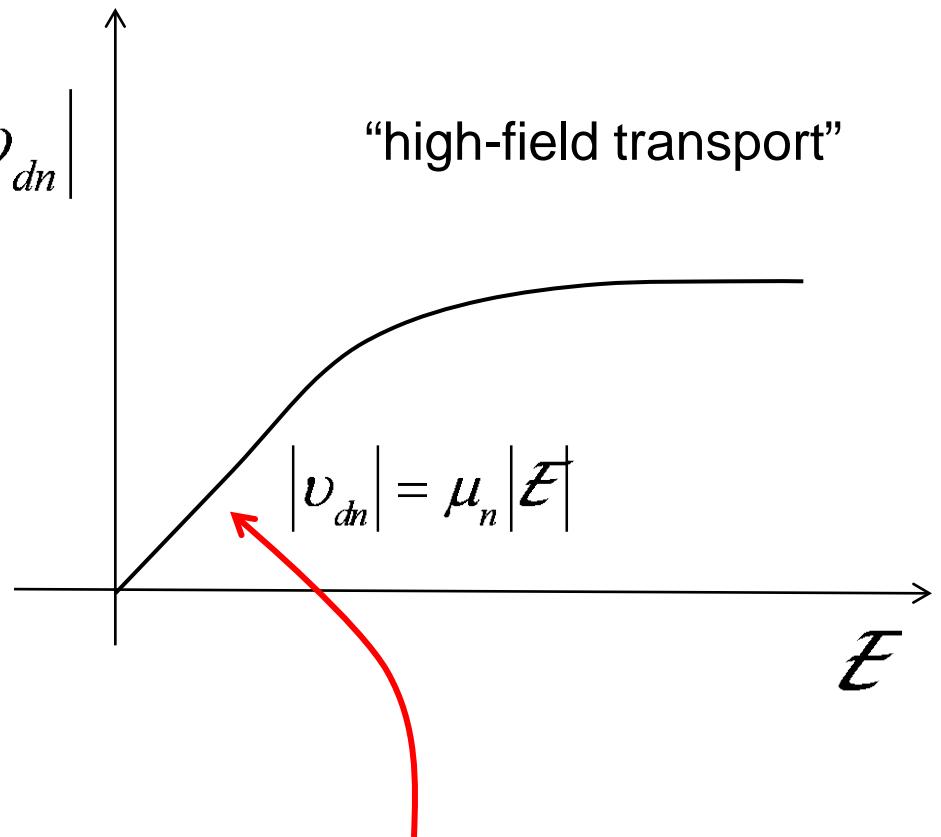
$$I = nqv_{dnx}A$$

$$J_{nx} = -nqv_{dnx} A/m^2$$

$$J_{px} = +pqv_{dnx} A/m^2$$

# Velocity and electric field

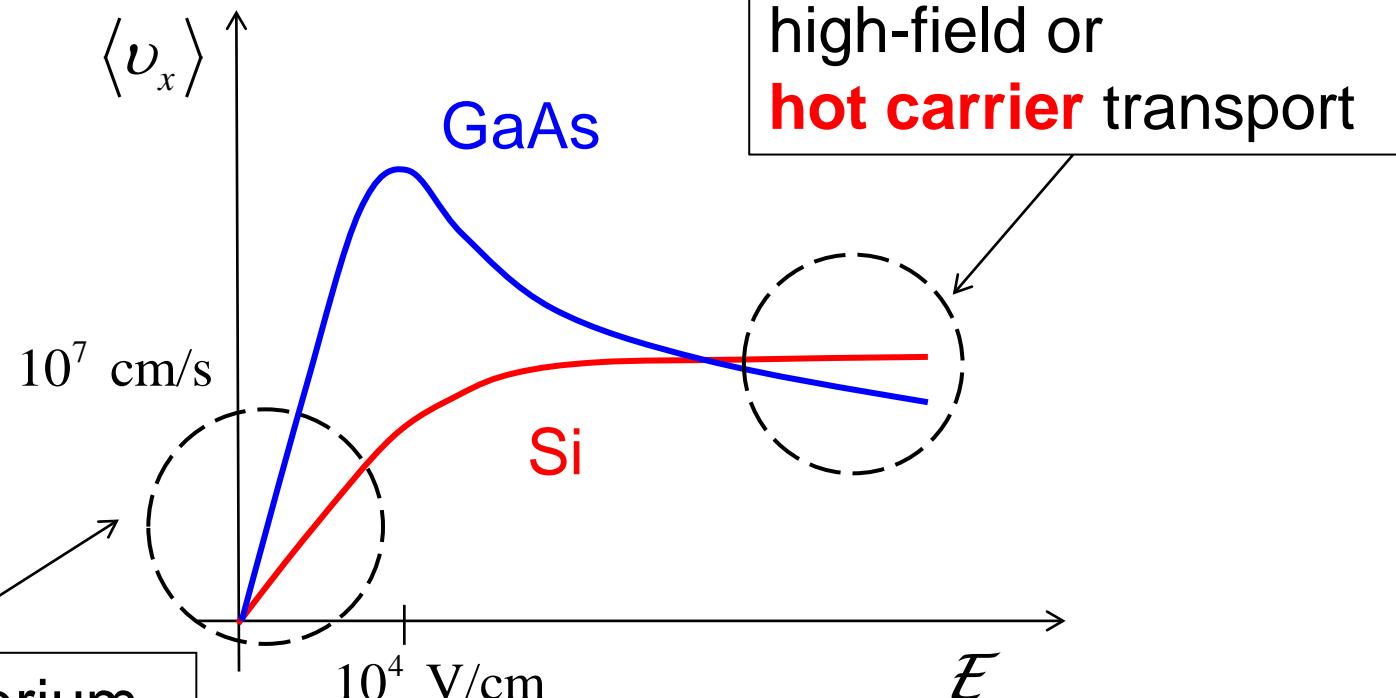
$$v_{dn} = -\mu_n \mathcal{E}$$
$$\mu_n \equiv \left( \frac{v_T \lambda_0}{2(k_B T / q)} \right) \text{ cm}^2/\text{V-s}$$
$$\mu_n = \left( \frac{q \tau}{m_n^*} \right) \text{ cm}^2/\text{V-s}$$



"low-field" or "near-equilibrium"  
or "linear" transport

# Velocity vs. electric field

(bulk semiconductors assumed)



near-equilibrium  
(or “linear”  
transport

Lundstrom: 2018

# Drift current

---

$$v_{dn} = -\mu_n \mathcal{E}$$

$$v_{dp} = +\mu_p \mathcal{E}$$

$$J_n = -nq v_{dn} A/m^2$$

$$J_p = pq v_{dp} A/m^2$$

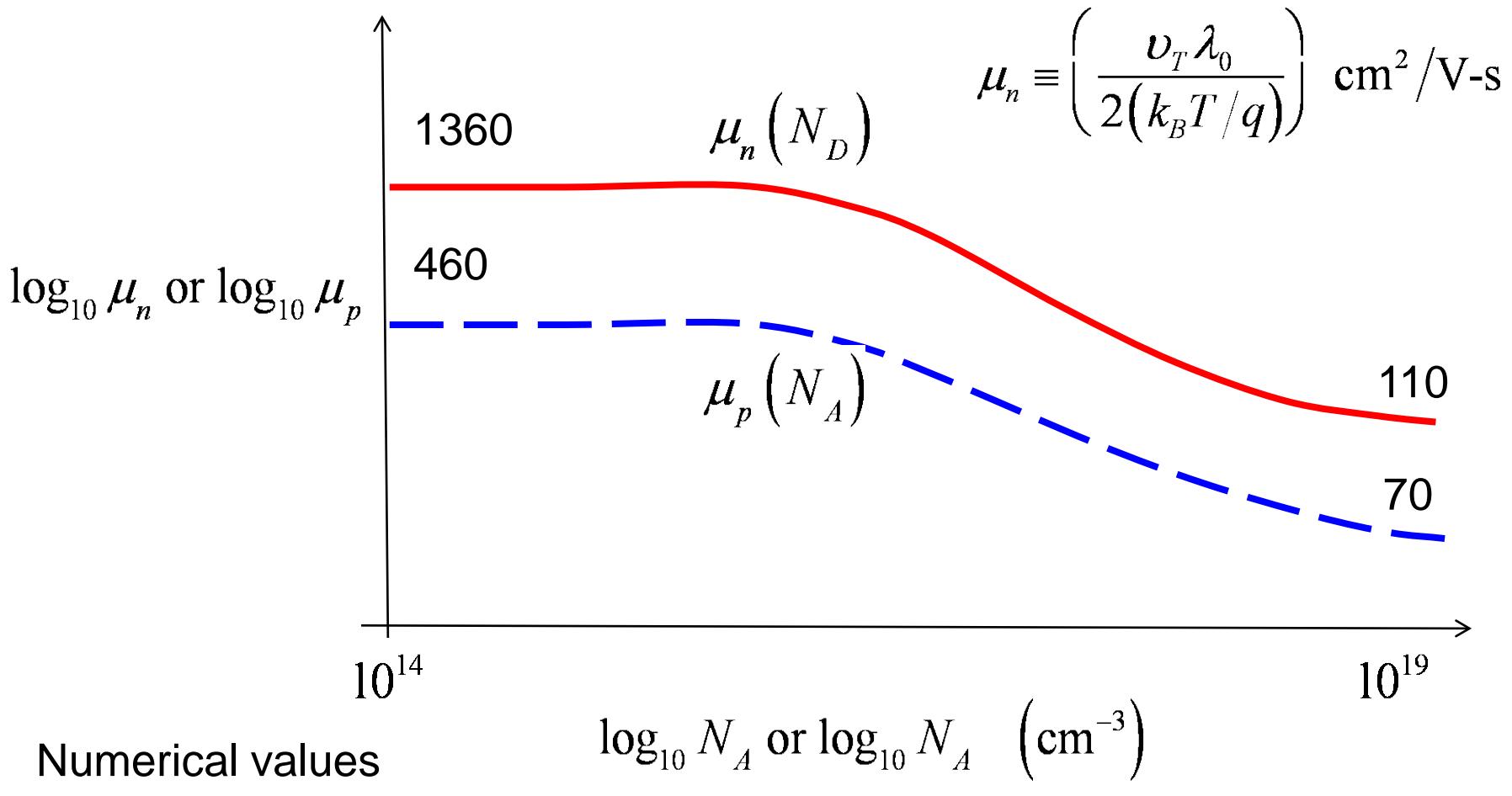
$$J_n = nq \mu_n \mathcal{E} A/m^2$$

$$J_p = pq \mu_p \mathcal{E} A/m^2$$

To describe high-field transport:

$$\mu_n, \mu_p \rightarrow \mu_n(\mathcal{E}), \mu_p(\mathcal{E})$$

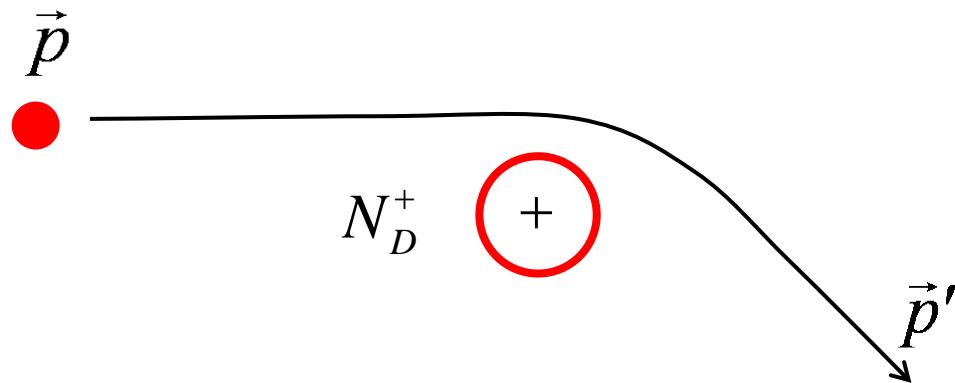
# Mobility vs. doping



# Ionized impurity scattering

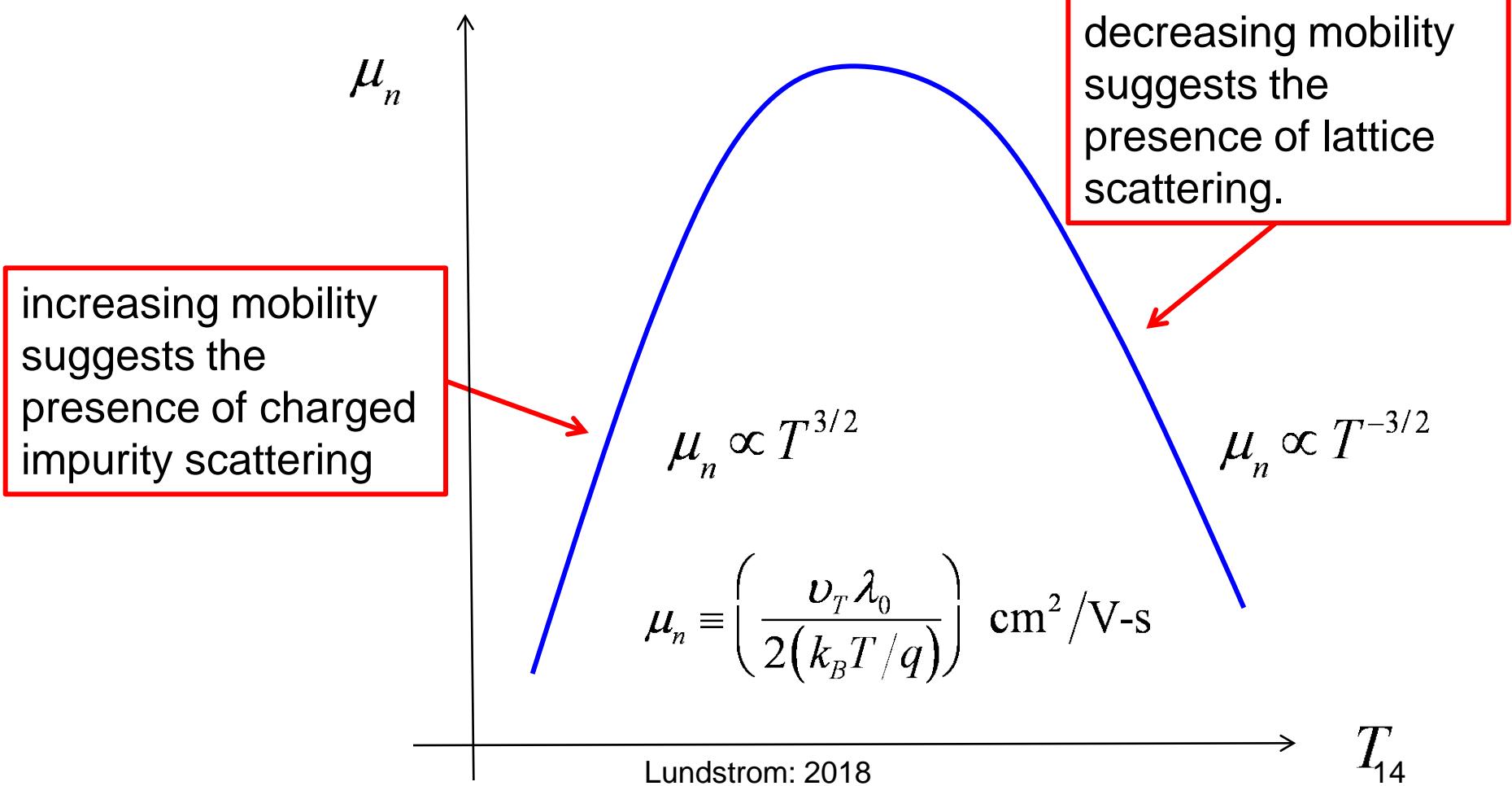
---

electrons in N-type material



Donors provide electrons to the conduction band, but ionized donors can “scatter” those electrons.

# Mobility vs. temperature



# Drift current, conductivity, resistivity

---

$$J_n = nq\mu_n \mathcal{E} \text{ A/m}^2$$

$$J_n = \sigma_n \mathcal{E} \text{ A/m}^2$$

$$\sigma_n = nq\mu_n (\text{units?})$$

$$J_p = pq\mu_p \mathcal{E} \text{ A/m}^2$$

$$J_p = \sigma_p \mathcal{E} \text{ A/m}^2$$

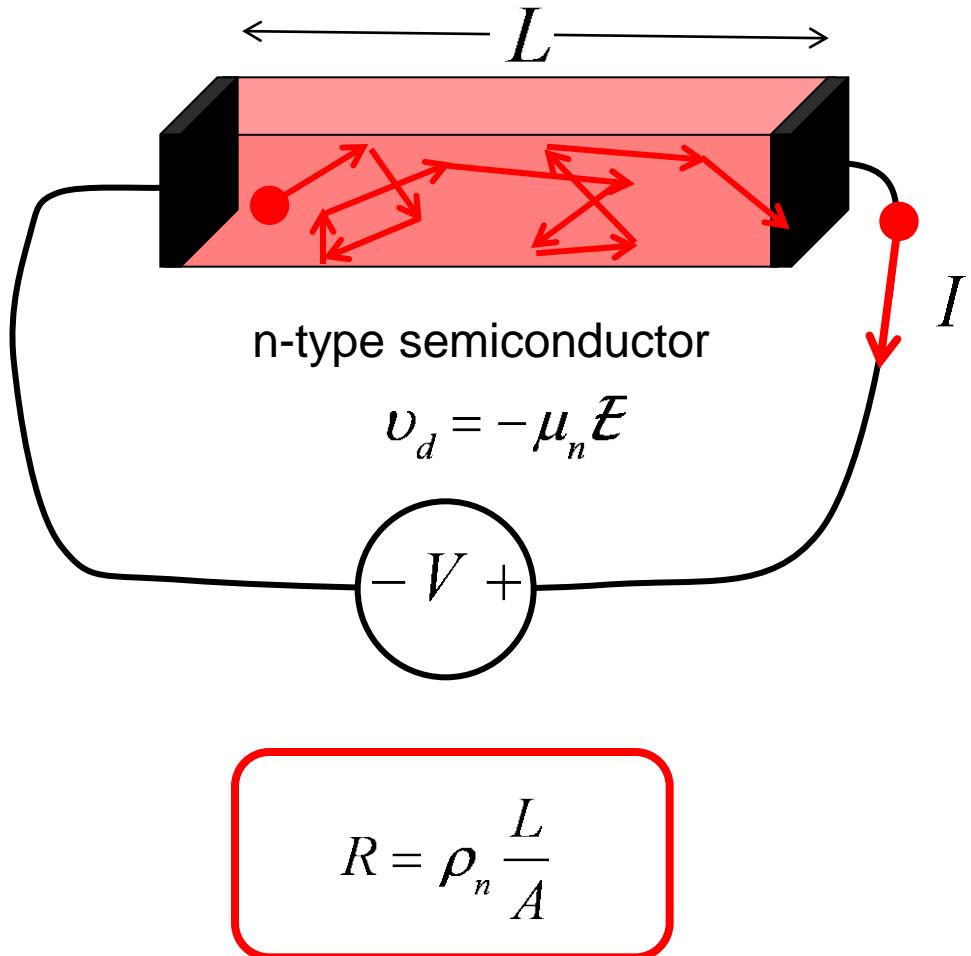
$$\sigma_p = pq\mu_p$$

$$J_{tot} = J_n + J_p = (\sigma_n + \sigma_p) \mathcal{E} = \sigma \mathcal{E} \text{ A/m}^2$$

$$J_{tot} = \sigma \mathcal{E} \text{ A/m}^2$$

$$\rho = \frac{1}{\sigma} = \frac{1}{\sigma_n + \sigma_p} = \frac{1}{nq\mu_n + pq\mu_p} \Omega\text{-cm}$$

# Resistance



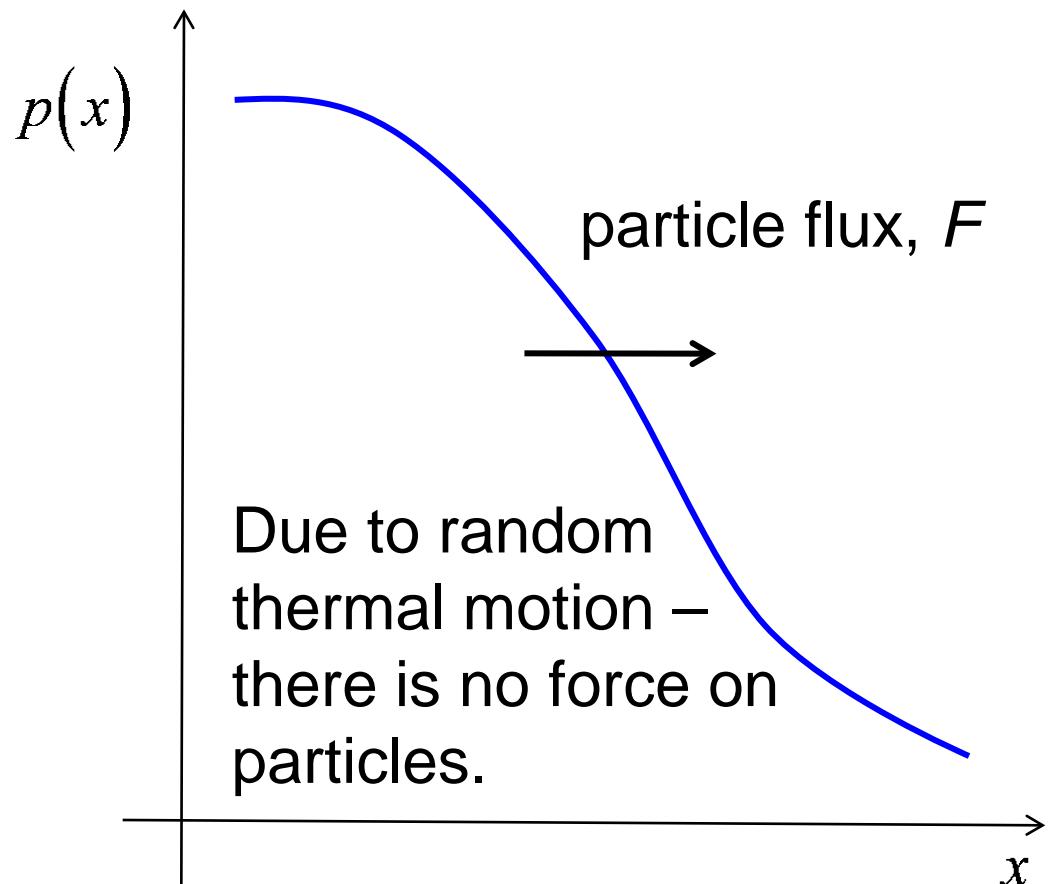
$$J_n = \sigma_n \mathcal{E} \text{ A/m}^2$$

$$I = AJ_n = \sigma_n A \mathcal{E} \text{ Amps}$$

$$I = \sigma_n A \frac{V}{L}$$

$$I = \left( \sigma_n \frac{A}{L} \right) V = GV = \frac{1}{R} V$$

# Fick's Law of diffusion



$$F = \frac{J_p}{q} = -D \frac{dp}{dx} \quad \frac{\#}{\text{cm}^2\text{-s}}$$

$$D \quad \text{cm}^2/\text{s}$$

(Adolph Fick, 1855)

# Diffusion currents

---

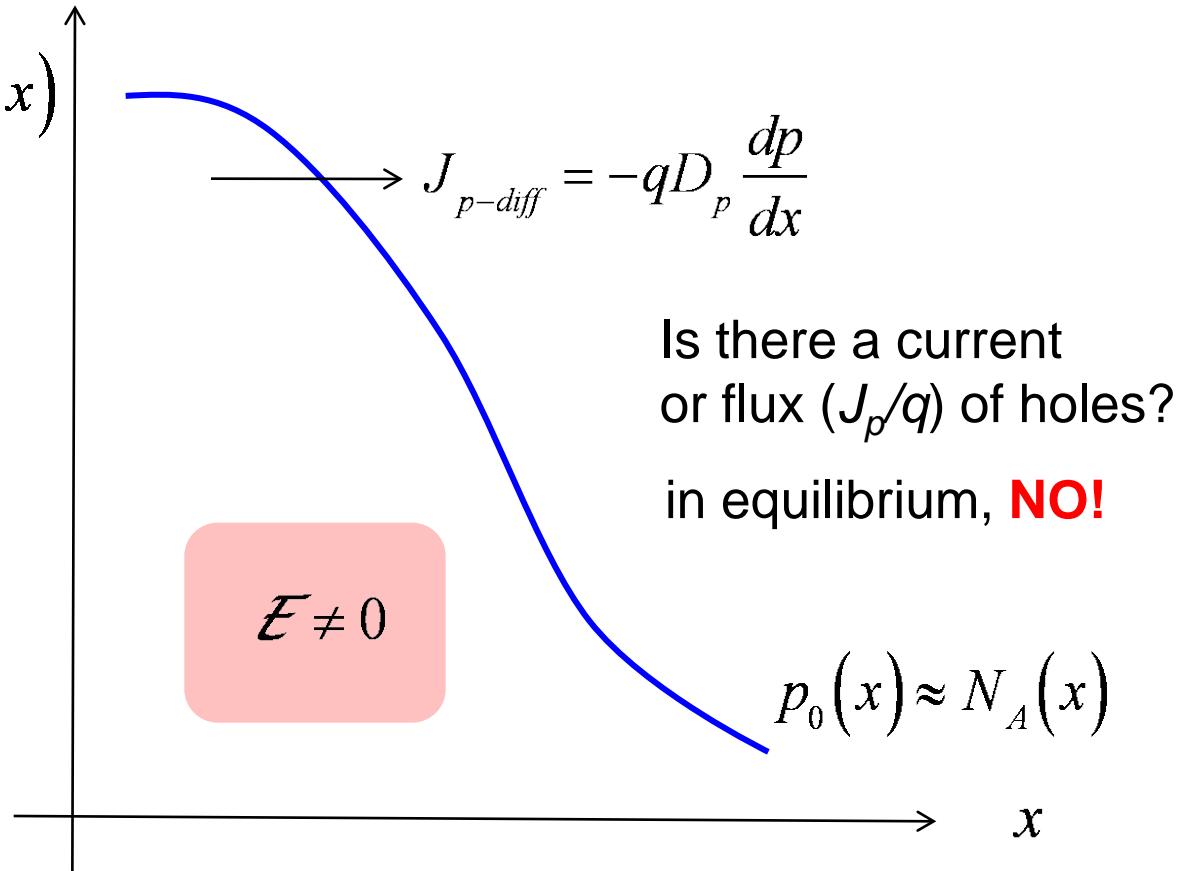
$$J_{p-diff} = -qD_p \frac{dp}{dx} \quad J_{n-diff} = +qD_n \frac{dn}{dx}$$

Whenever there is a concentration gradient, there is a diffusion current.

# Nonuniformly doped semiconductor in equilibrium

What direction is the electric field?

- a) To the right?
- b) To the left?



There must be a drift current that exactly cancels the diffusion current.

# Summary: Drift- diffusion equation

---

$$J_{px} = p\mu_p \vec{\nabla} F_p \quad \vec{J}_p = \vec{J}_{p-drift} + \vec{J}_{p-diff} = pq\mu_p \vec{E} - qD_p \vec{\nabla} p$$

current = drift current + diffusion current

$$J_{nx} = n\mu_n \vec{\nabla} F_n \quad \vec{J}_n = \vec{J}_{n-drift} + \vec{J}_{n-diff} = nq\mu_n \vec{E} + qD_n \vec{\nabla} n$$

total current = electron current + hole current

$$\vec{J} = \vec{J}_p + \vec{J}_n$$

$$\mu_p = \frac{v_T \lambda_0}{2(k_B T/q)} = \frac{q\tau}{m_p^*}$$

$$D_p/\mu_p = D_n/\mu_n = k_B T/q$$

(Einstein, 1905)

# Primer on Semiconductors

## Unit 4: Carrier Transport, Recombination, and Generation

### Lecture 4.4: Carrier recombination

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Equilibrium and non-equilibrium

---

**In equilibrium:**

$$n_0 = N_C e^{(E_F - E_C)/k_B T} \quad p_0 = N_V e^{(E_V - E_F)/k_B T}$$

**Out of equilibrium**, there can be additional “excess carriers”:

$$n = n_0 + \Delta n \quad p = p_0 + \Delta p$$

(The excess carrier concentrations can be positive or negative.)

**Question:** How do the excess carrier concentrations vary with time?

# Carrier recombination

---

P-type, equilibrium

$$\Delta n(t = 0)$$

$$p_0 = 10^{17} \text{ cm}^{-3} \quad n_0 = n_i^2 / p_0 = 10^3 \text{ cm}^{-3}$$

**Expect:**

$$\Delta n(t) = \Delta n(t = 0) e^{-t/\tau} \quad \Delta n \text{ may be either positive or negative.}$$

**Goal:** Understand the recombination lifetime,  $\tau_n$ .

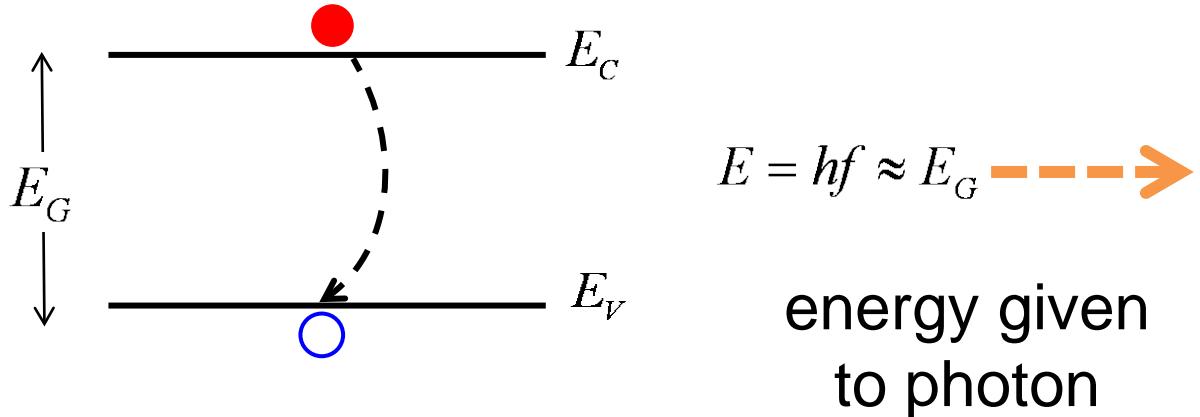
# How can excess carriers recombine?

---

We will discuss three different ways:

- 1) Band-to-band (radiative) recombination
- 2) Auger recombination
- 3) SRH (defect-assisted) recombination

# 1) Band-to-band (radiative) recombination



$$\left. \frac{\partial n}{\partial t} \right|_{b-b} = \left. \frac{\partial p}{\partial t} \right|_{b-b} = -B(n_p - n_i^2) \quad (n_0 p_0 = n_i^2)$$

(Note that this is zero in equilibrium – as it should be.)

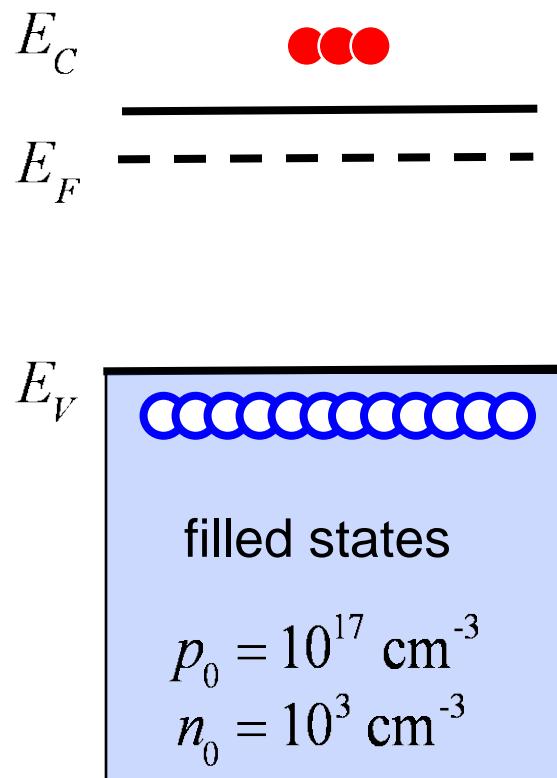
# Low level injection

---

the doping injection conc is small compared to majority conc and large compared to the minority carrier conc.

The term “low level injection” means that the excess carrier concentration is **orders of magnitude smaller than the equilibrium majority carrier concentration** but **orders of magnitude larger than the equilibrium minority carrier concentration**.

# Example: Low level injection in a p-type semiconductor



$$n = n_0 + \Delta n$$

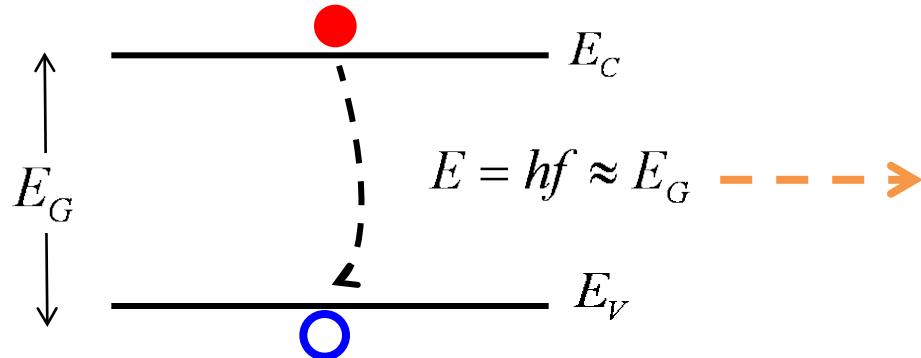
$$p = p_0 + \Delta p$$

$$\Delta n \approx \Delta p$$

$$\Delta n = 10^8 \text{ cm}^{-3} \gg n_0$$

$$\Delta p \approx \Delta n = 10^8 \text{ cm}^{-3} \ll p_0$$

# Low level injection in a p-type semi



$$\left. \frac{\partial n}{\partial t} \right|_{b-b} = -B(n_p - n_i^2)$$

$$n = n_0 + \Delta n \approx \Delta n$$

$$p = p_0 + \Delta p \approx N_A$$
$$\left. \frac{\partial \Delta n}{\partial t} \right|_{b-b} \approx -BN_A \Delta n = -\frac{\Delta n}{\tau_{bb}}$$

$$np \approx \Delta n N_A \gg n_i^2$$

$$\tau_{bb} = \frac{1}{BN_A}$$

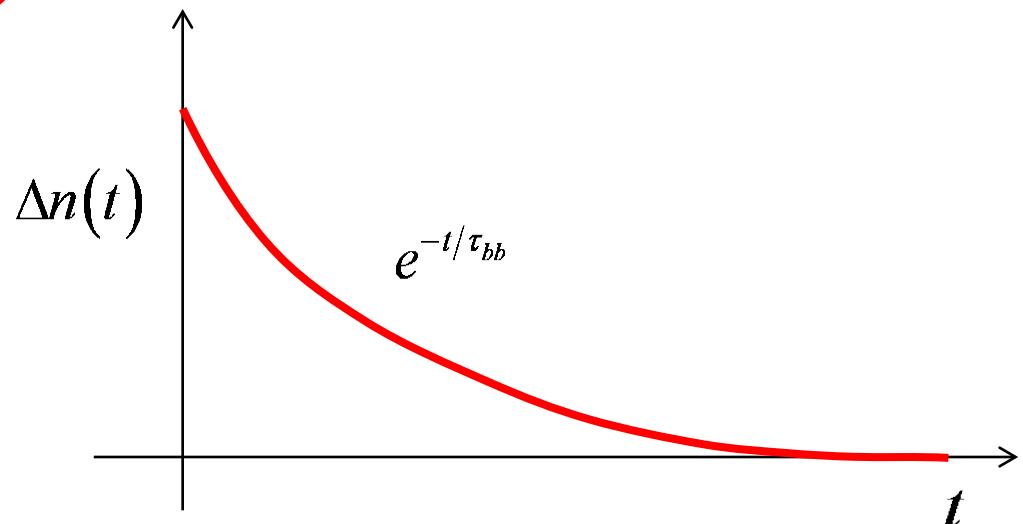
# Excess carrier concentration vs. time

$$\left. \frac{\partial n}{\partial t} \right|_{b-b} = -B(np - n_i^2)$$

$$\left. \frac{\partial \Delta n}{\partial t} \right|_{b-b} \approx -\frac{\Delta n}{\tau_{bb}}$$

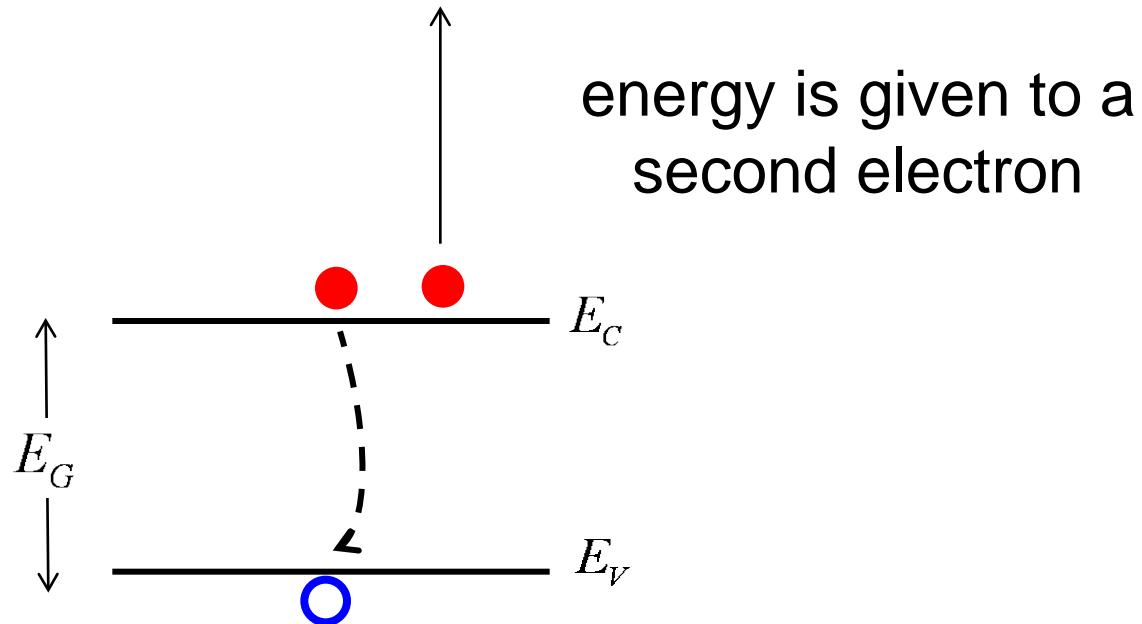
$$\tau_{bb} = \frac{1}{BN_A}$$

$$\Delta n(t) = Ce^{-t/\tau_{bb}}$$



## 2) Auger recombination

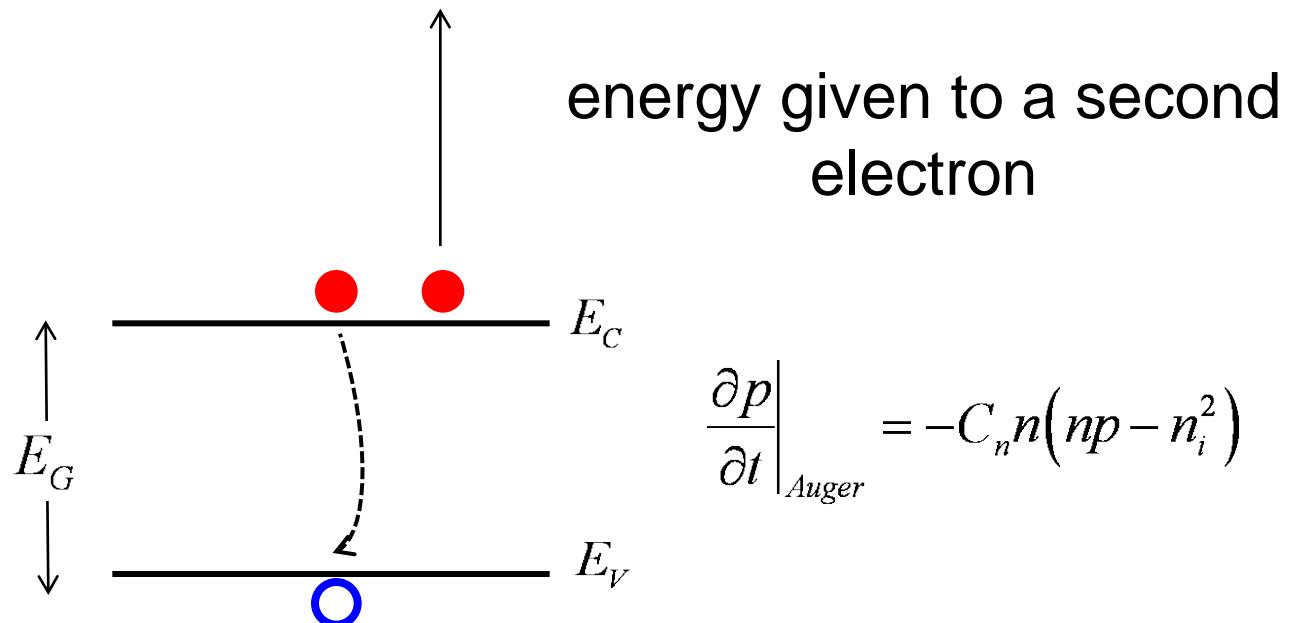
---



$$\left. \frac{\partial p}{\partial t} \right|_{Auger} = C_n n (np - n_i^2) + C_p p (np - n_i^2)$$

(Note that this is zero in equilibrium – as it should be.)

# Low level injection in an n-type semiconductor



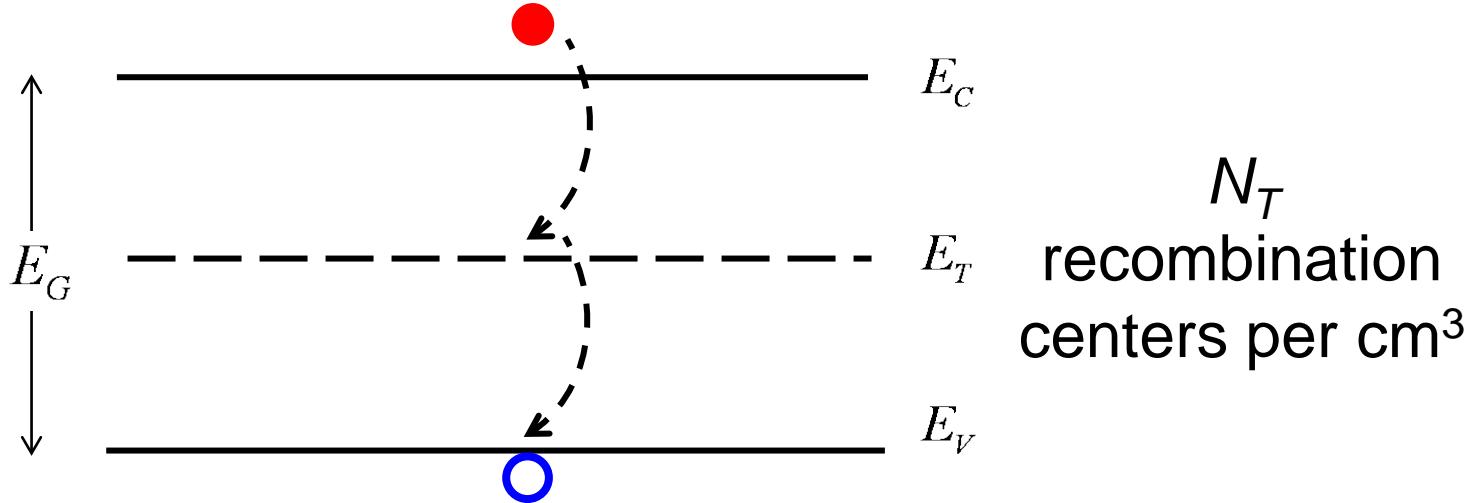
$$n = n_0 + \Delta n \approx N_D$$

$$p = p_0 + \Delta p \approx \Delta p$$
$$\left. \frac{\partial \Delta p}{\partial t} \right|_{Auger} \approx -C_n N_D^2 \Delta p = -\frac{\Delta p}{\tau_{Auger}}$$

$$np \approx \Delta p N_D \gg n_i^2$$

$$\tau_{Auger} = \frac{1}{C_n N_D^2}$$

### 3) SRH (defect-assisted) recombination



energy released as thermal energy

$$\frac{\partial n}{\partial t} \Big|_{SRH} = \frac{\partial p}{\partial t} \Big|_{SRH} = \frac{- (np - n_i^2)}{\tau_p (n + n_1) + \tau_n (p + p_1)}$$

$$\tau_n = 1/c_n N_T$$

$$\tau_p = 1/c_p N_T$$

$$n_1, p_1 \approx n_i$$

(Shockley Read Hall recombination)

# Low level injection in a p-type semiconductor

---

$$\frac{\partial n}{\partial t} \Big|_{SRH} = \frac{\partial p}{\partial t} \Big|_{SRH} = \frac{- (np - n_i^2)}{\tau_p (n + n_1) + \tau_n (p + p_1)}$$

$$n = n_0 + \Delta n \approx \Delta n$$

$$p + p_1 \gg n + n_1$$

$$p = p_0 + \Delta p \approx N_A$$

$$p \gg p_1$$

$$np \approx \Delta n N_A \gg n_i^2$$

$$\frac{\partial \Delta n}{\partial t} \Big|_{SRH} = - \frac{\Delta n}{\tau_n}$$

$$\tau_{SRH} = \frac{1}{c_n N_T}$$

# Recombination under low level injection

band-band

$$\frac{\partial \Delta n}{\partial t} \Big|_{b-b} = -\frac{\Delta n}{\tau_{b-b}} \quad \tau_{b-b} = \frac{1}{BN_A}$$

Auger

$$\frac{\partial \Delta n}{\partial t} \Big|_{Auger} = -\frac{\Delta n}{\tau_{Auger}} \quad \tau_{Auger} = \frac{1}{C_p N_A^2}$$

SRH

$$\frac{\partial \Delta n}{\partial t} \Big|_{SRH} = -\frac{\Delta n}{\tau_n} \quad \tau_n = \frac{1}{c_n N_T}$$

The minority carrier lifetime is a key parameter for solar cells, bipolar transistors, etc.

# Multiple recombination processes

$$\frac{\partial \Delta n}{\partial t} \Big|_{tot} = -\frac{\Delta n}{\tau_{eff}} \quad \frac{1}{\tau_{eff}} = \frac{1}{\tau_{b-b}} + \frac{1}{\tau_{Auger}} + \frac{1}{\tau_{SRH}}$$

Total  
recombination rate

rates add

$$\Delta n(t) = \Delta n(0) e^{-t/\tau_{eff}}$$

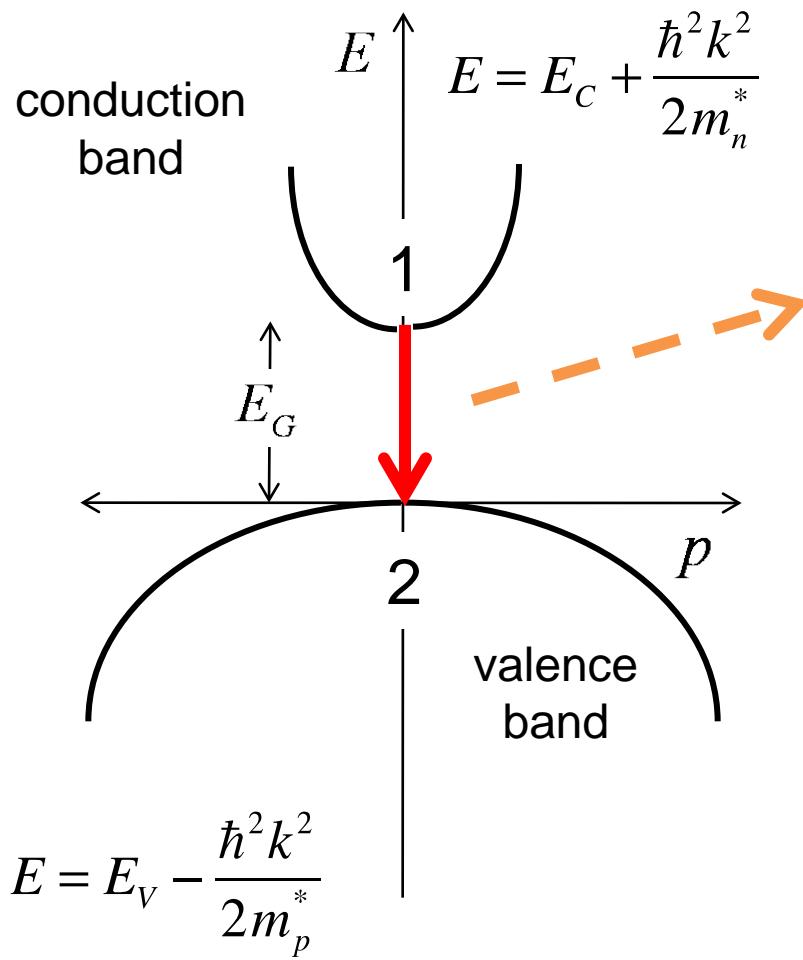
# Discussion

---

When are the various recombination processes dominant?

- 1) Auger: For heavily doped semiconductors  $\tau_{Auger} = \frac{1}{C_p N_A^2}$
- 2) SRH: When defects are present and other effects don't dominate.
- 3) Radiative: **Only for direct gap semiconductors**  $\tau_{b-b} = \frac{1}{BN_A}$

# BB recombination in **direct gap** semiconductors



Conservation of energy:

$$E_{ph} = hf \approx E_G$$

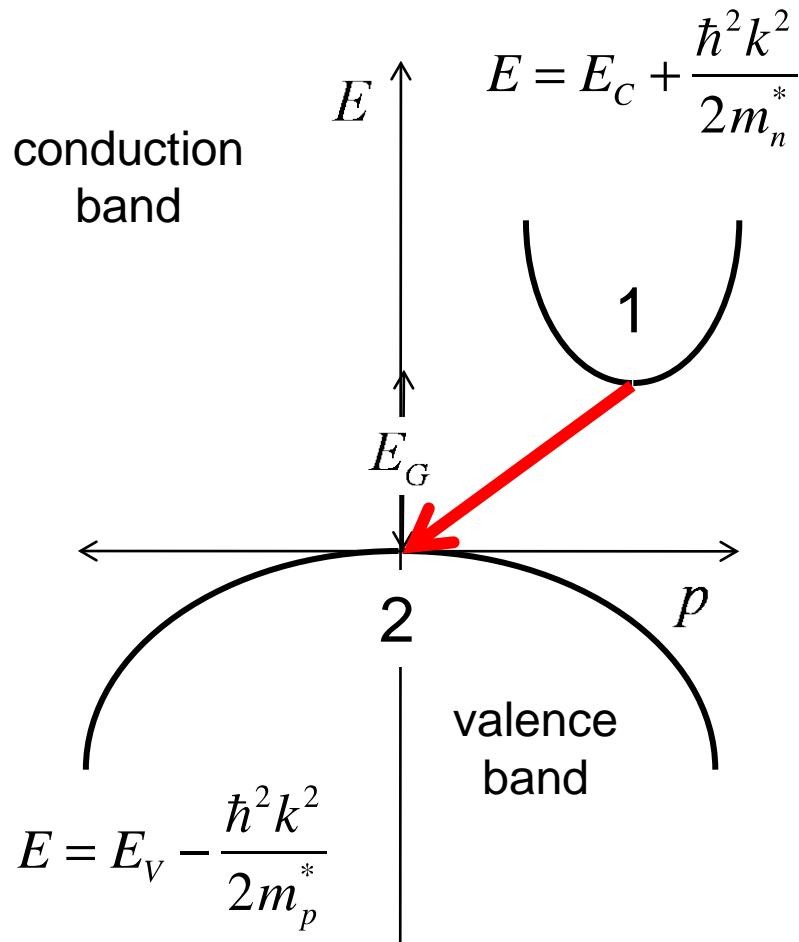
Conservation of momentum:

$$\hbar k_1 - \hbar k_2 = \hbar k_{ph} \approx 0$$

$$k_1 \approx k_2$$

("vertical transitions"  
photons have very little  
momentum)

# BB recombination in **indirect** gap semiconductors



Conservation of energy:

$$E_{ph} = hf = E_G \pm \hbar\omega_{lv}$$

Conservation of momentum:

$$\hbar k_1 - \hbar k_2 = \hbar k_{ph} + \hbar k_{lv}$$

(must involve a lattice vibration (lv) with the right momentum)

**BB recombination in indirect semiconductors is very weak!**

# Three type of recombination

---

## 1) Band-to-band radiative recombination

dominates in direct gap semiconductors  
makes lasers and LEDs possible

## 2) Auger recombination

dominates when the carrier densities are very high  
(heavily doped semiconductors or lasers)

## 3) SRH recombination

dominates in indirect gap semiconductors  
and in low quality direct gap semiconductors

# Recombination-generation

$$R = X(np - n_i^2)$$

$$X = B$$

band-to-band  
radiative

$$X = C_n n + C_p p$$

Auger

$$X = \frac{1}{\tau_p(n+n_1) + \tau_n(p+p_1)}$$

SRH

$$(np > n_i^2)$$

net recombination

$$(np < n_i^2)$$

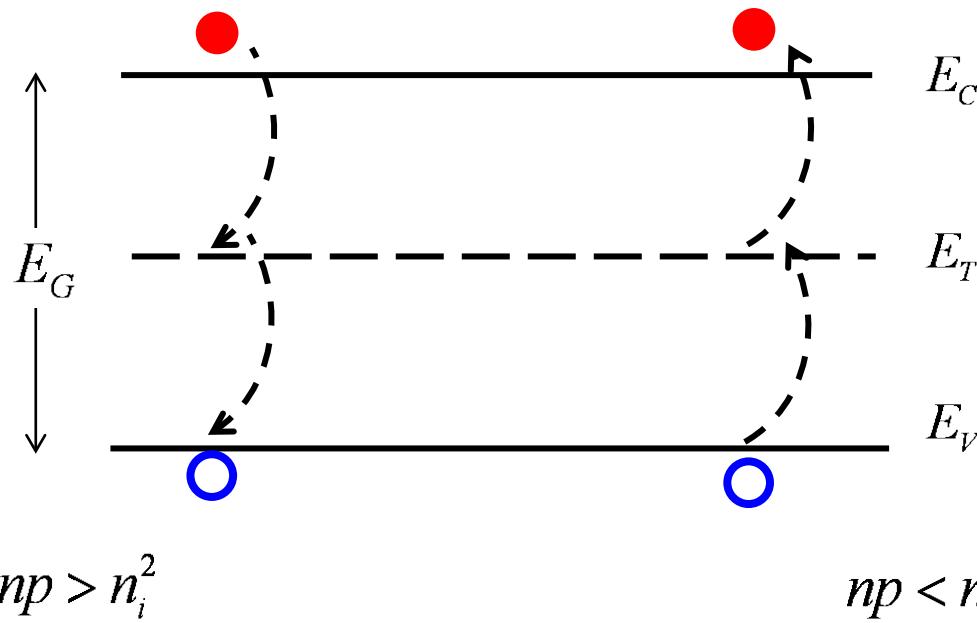
**net generation**

### 3) SRH (defect-assisted) **generation**

---

$R > 0$ :  
recombination

$R < 0$ :  
generation



releases thermal energy

requires thermal energy

# Summary

---

When excess carriers are introduced, a semiconductor responds by trying to restore equilibrium.

In the simplest, and quite common case, the perturbation decays exponentially with time.

$$\Delta n(t) = \Delta n(t=0)e^{-t/\tau_n}$$

(low level injection)

The minority carrier lifetime is controlled by radiative, Auger, or defect-assisted process – or by some combination of these.

# Primer on Semiconductors

## Unit 4: Carrier Transport, Recombination, and Generation

### Lecture 4.5: Carrier generation

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Recombination and generation

---

$$\Delta n(t) = \Delta n(t=0)e^{-t/\tau_n}$$

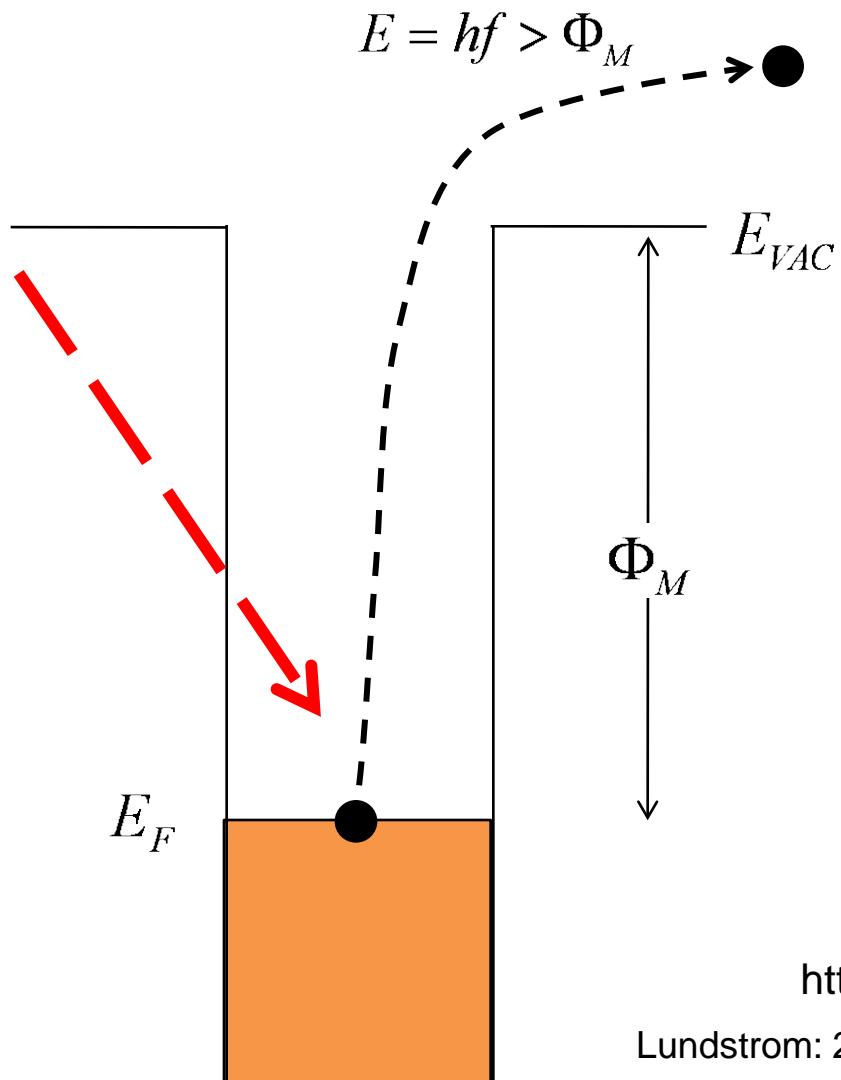
(low level injection)

The minority carrier lifetime is controlled by radiative, Auger, or defect-assisted recombination process – or by some combination of these.

**Generation processes** are the inverses of the recombination processes.

# Photoelectric effect (optical generation)

---



Einstein, in 1905, when he wrote  
the [Annus Mirabilis](#) papers

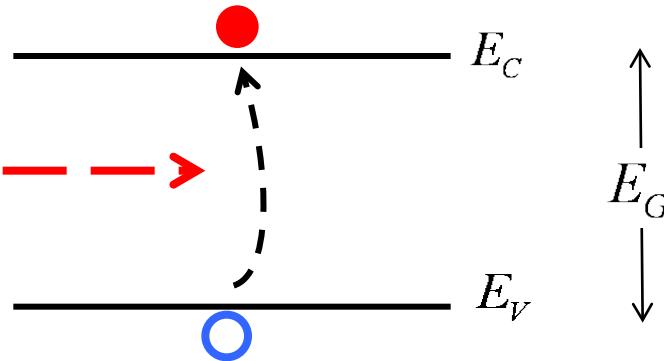
[http://en.wikipedia.org/wiki/Photoelectric\\_effect](http://en.wikipedia.org/wiki/Photoelectric_effect)

# Optical generation in semiconductors

---

$$\lambda < \frac{hc}{E_G}$$

$$E = hf > E_G$$



$$f\lambda = c$$

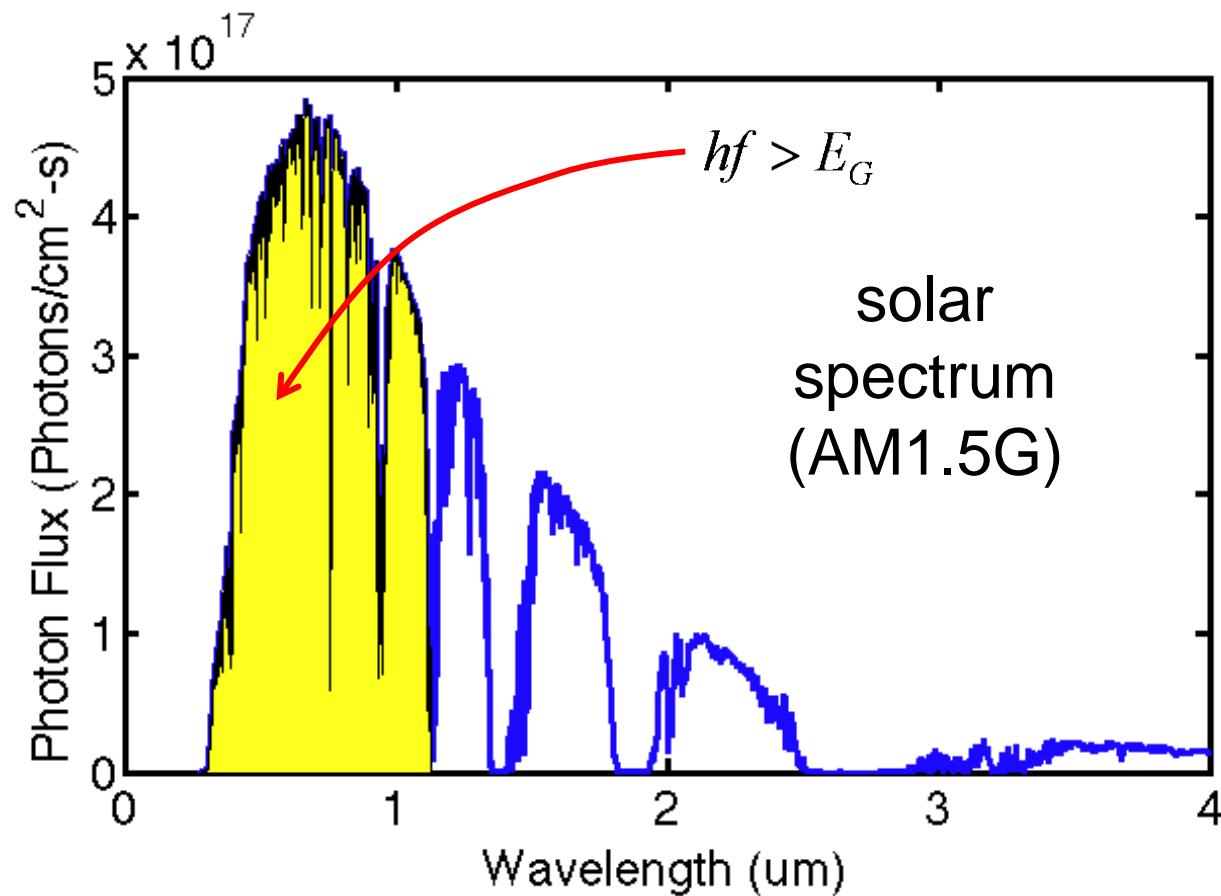
$$f = \frac{c}{\lambda}$$

$$E = hf = \frac{hc}{\lambda}$$

# Carrier generation from a solar spectrum

---

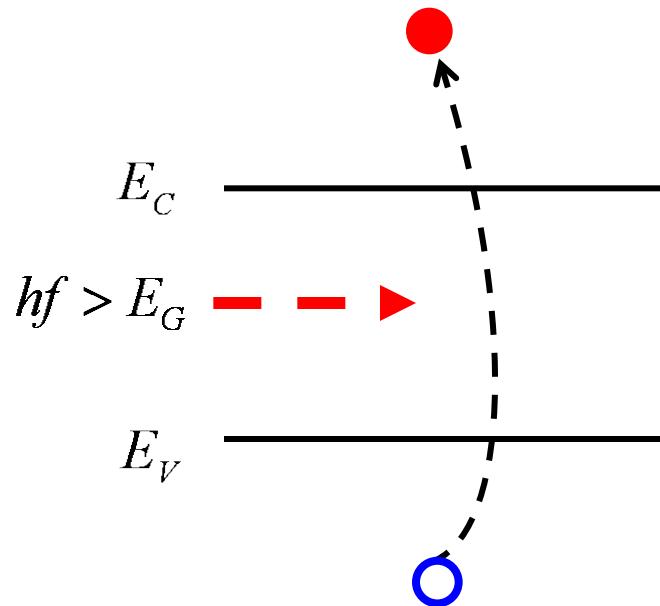
Example: Silicon  $E_G = 1.1$  eV. Only photons with a wavelength smaller than 1.13  $\mu\text{m}$  will be absorbed.



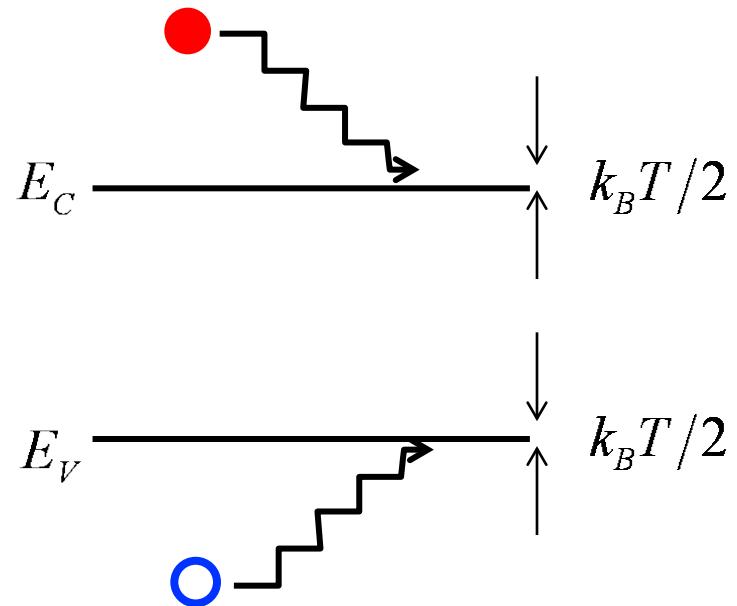
# Thermalization

---

Energy is lost for photons with energies greater than the bandgap.

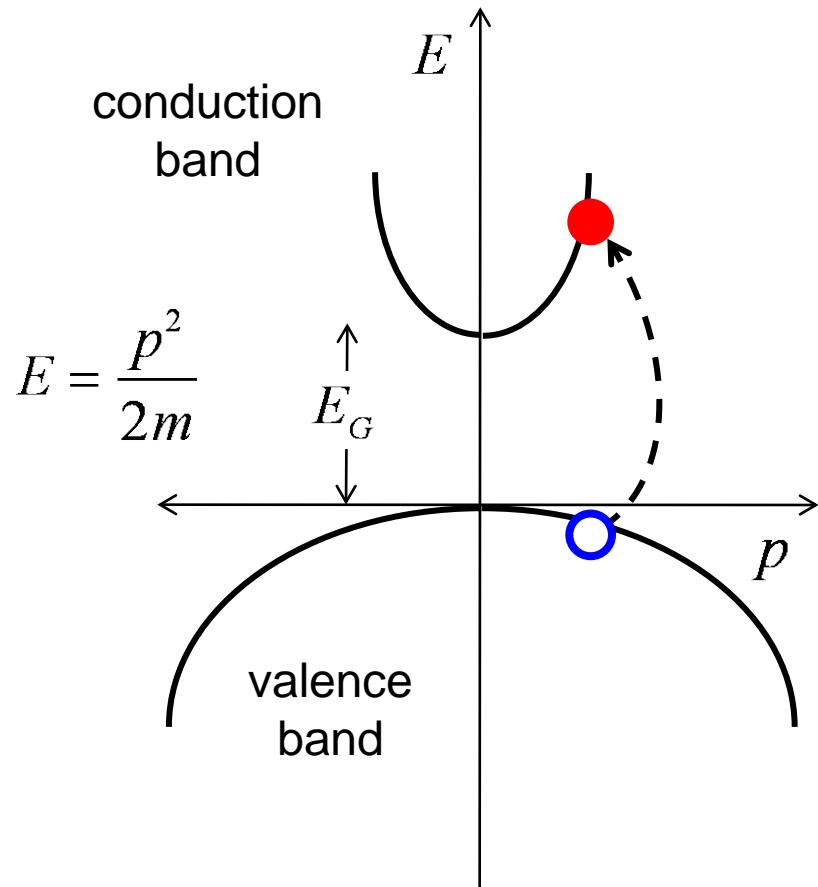


Carriers are created with excess energy.



Extra energy is lost due to thermalization as carrier relax back to the band edge.

# Thermalization on an $E(k)$ diagram



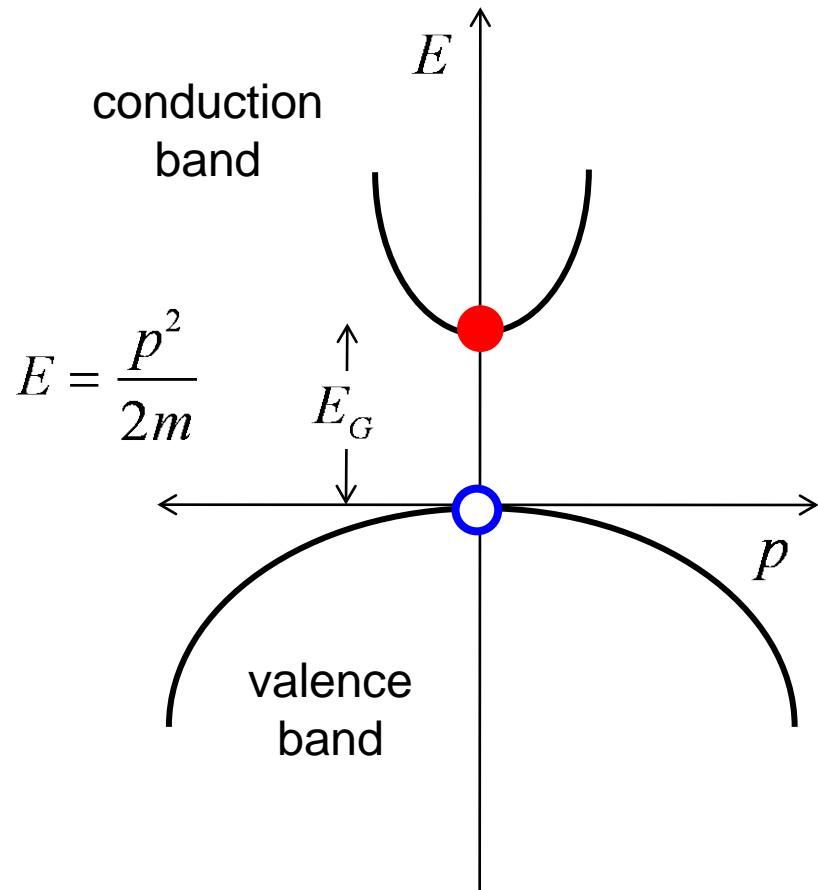
Electrons move downhill to lower their energy.

Holes move up to lower their energy.

(This is an electron energy diagram)

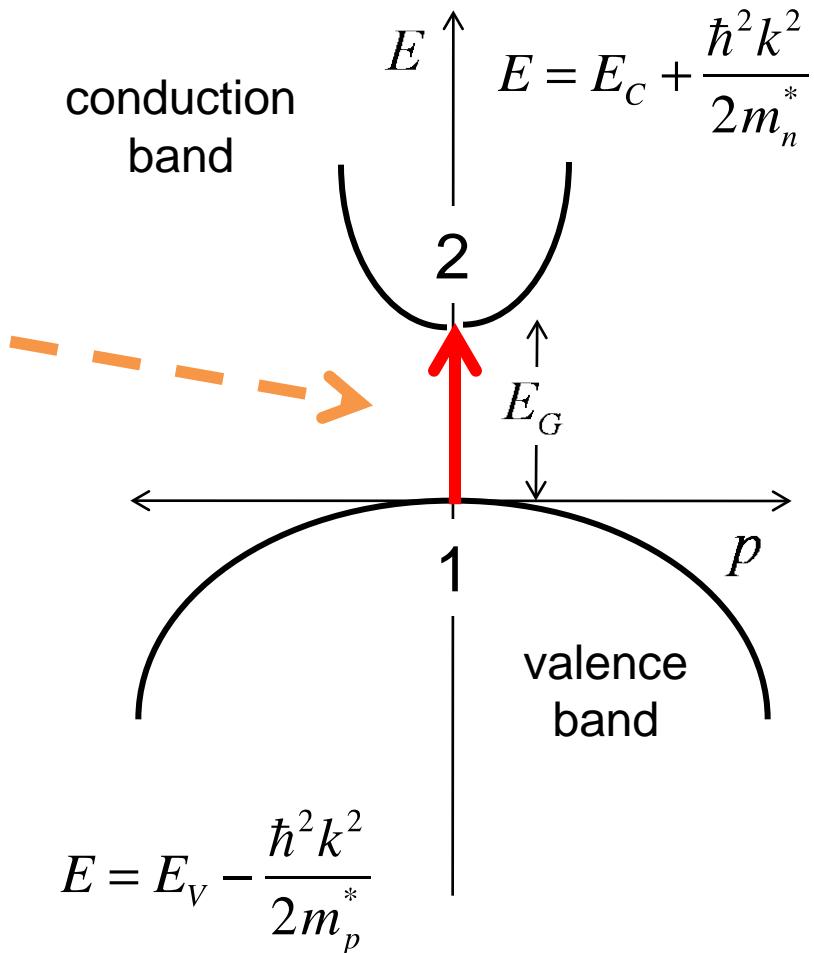
# Thermalization on an $E(k)$ diagram

---



The excess energy is released as heat.

# Optical absorption in a **direct gap** semiconductor



Conservation of energy:

$$E_{ph} = hf \approx E_G$$

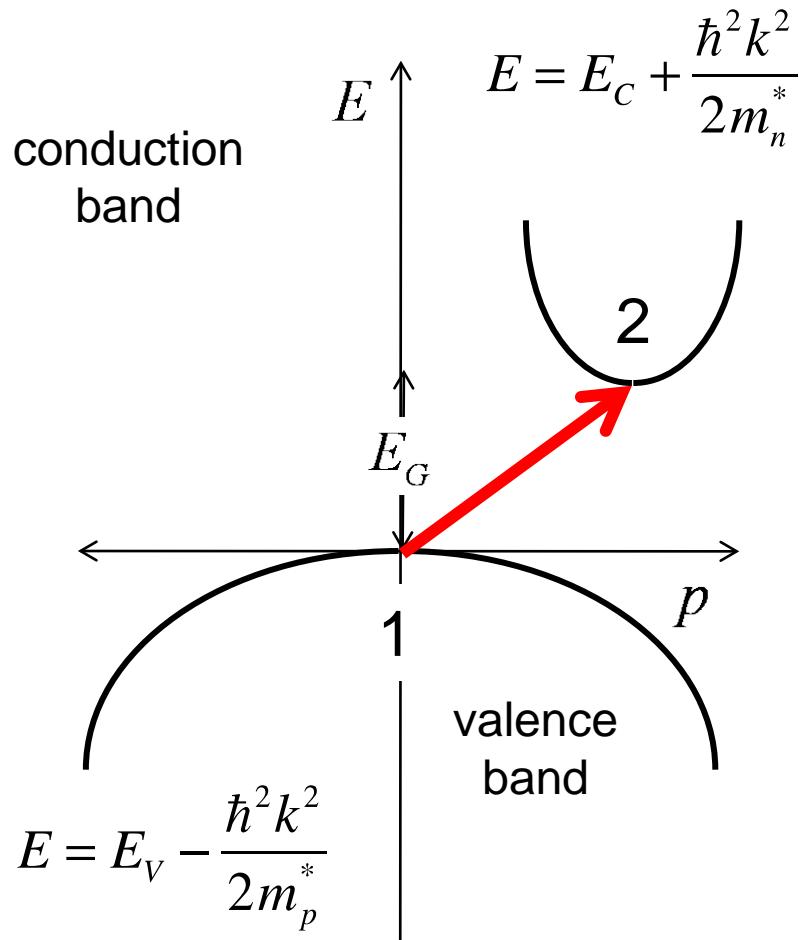
Conservation of momentum:

$$\hbar k_1 - \hbar k_2 = \hbar k_{ph} \approx 0$$

$$k_1 \approx k_2$$

("vertical transitions"  
because photons have  
very little momentum)

# Optical absorption in an **indirect gap** semiconductor



Conservation of energy:

$$E_{ph} = hf \approx E_G \pm \hbar\omega_{lv}$$

Conservation of momentum:

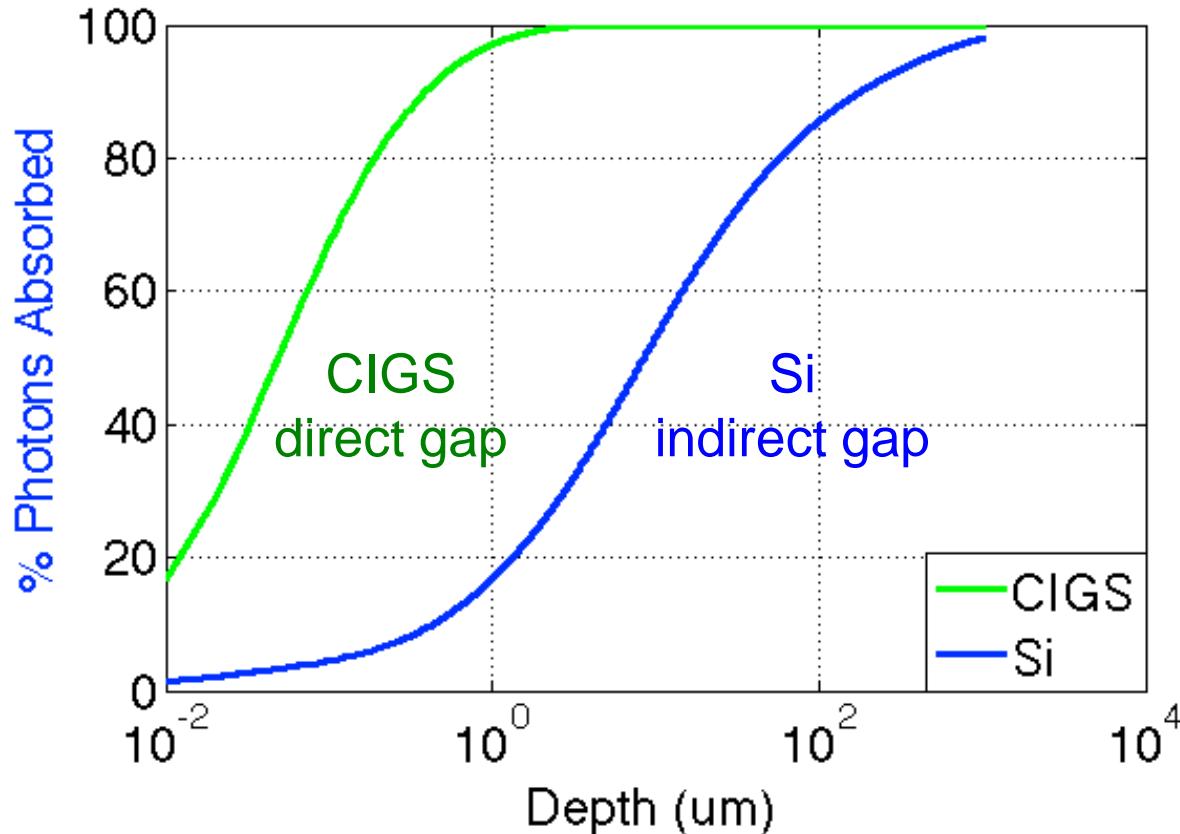
$$\hbar k_1 - \hbar k_2 = \hbar k_{ph} + \hbar k_{lv}$$

(must involve a lattice vibration with the right momentum)

**BB absorption in indirect semiconductors is very weak!**  
**(just as BB recombination is)**

# Optical absorption vs. semiconductor thickness

The direct bandgap of CIGS (Copper Indium Gallium Selenide) allows it to absorb light much faster than Silicon. A layer of silicon must be  $10^4$  microns thick to absorb ~100% of the light, while CIGS need only be about 2 microns thick.



# Absorption coefficient

---

Incident flux:  $\Phi_0$

Flux at position,  $x$ :  $\Phi(x) = \Phi_0 e^{-\alpha(\lambda)x}$

optical absorption coefficient:

$$\alpha(\lambda) > 0 \quad \text{for} \quad E > E_G \quad (\lambda < hc/E_G)$$

Generation rate at position,  $x$

:

$$G(x) = -\frac{d\Phi(x)}{dx} = \Phi_0 \alpha(\lambda) e^{-\alpha(\lambda)x}$$

$\alpha(\lambda)$       direct gap  $\rightarrow$  higher alpha

# Types of generation

---

1) Optical generation

“Inverse of radiative recombination”

2) Thermal generation

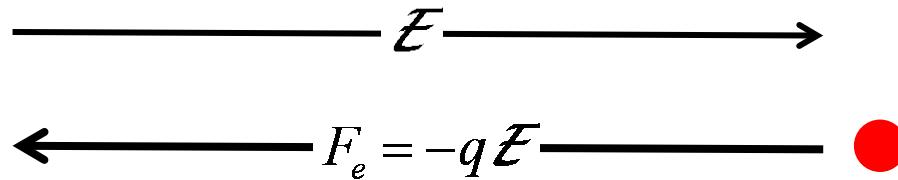
“Inverse of SRH recombination”

3) Impact ionization

“Inverse of Auger recombination”

# Impact ionization

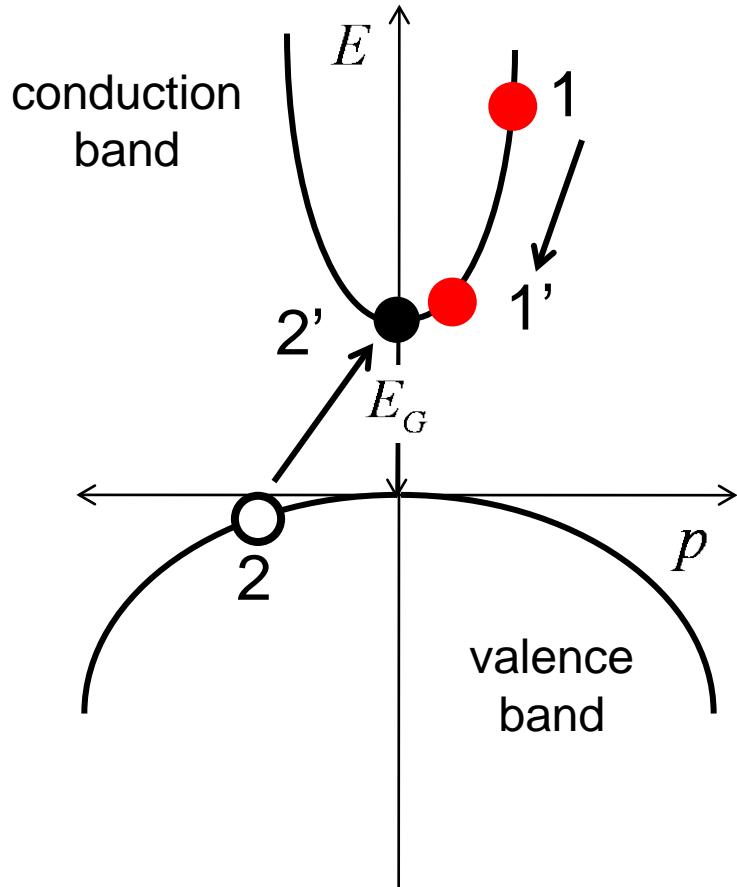
---



Under large electric fields, electrons can gain a lot of kinetic energy.

If the kinetic energy exceeds the band gap, then a collision with an atom in the lattice can produce an electron and hole.

# Impact ionization: $E(k)$ picture



Energetic electron 1 produces and e-h pair, 2 and 2'

Electrons 1' and 2' can now gain energy in the strong electric field, and produce 2 more e-h pairs.

As the process continues, the number of e-h pairs multiples.

# Impact ionization

---

The process we have described is called **avalanche multiplication** and can lead to “breakdown” in semiconductor devices under high voltages.

Wider bandgap semiconductors have less impact ionization and, therefore, higher breakdown voltages.

**Avalanche multiplication** is also used to produce sensitive photodetectors – avalanche photodetectors.

# Generation

---

1) Optical generation

Inverse of radiative recombination

2) Thermal generation

Inverse of SRH recombination

3) Impact ionization

Inverse of Auger recombination

# Primer on Semiconductors

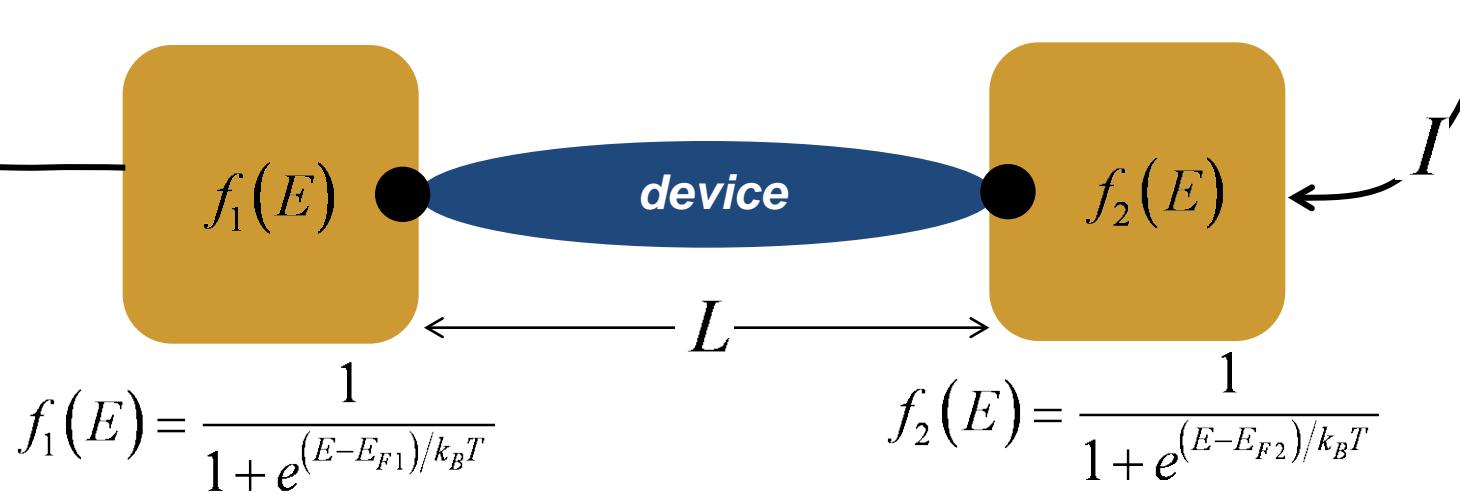
## Unit 4: Carrier Transport, Recombination, and Generation

### Lecture 4.6: Unit 4 Recap

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Landauer approach



Fundamental  
constants

Transmission:

$$0 < \mathcal{T}(E) < 1$$

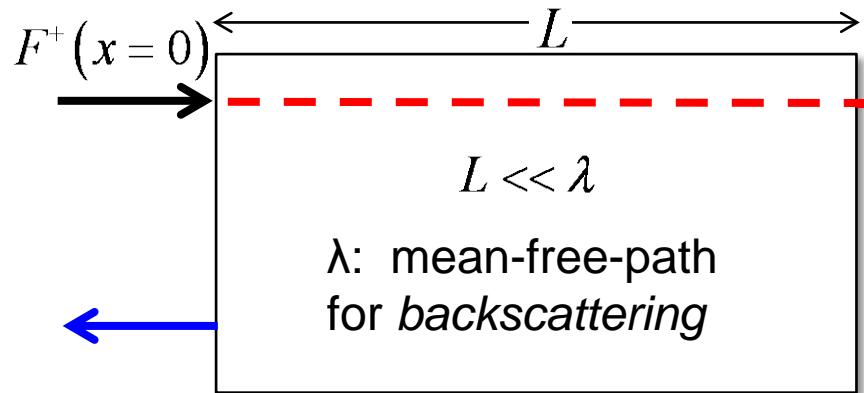
No. of  
Channels

Lundstrom: 2018

Ideal  
“Landauer”  
contacts

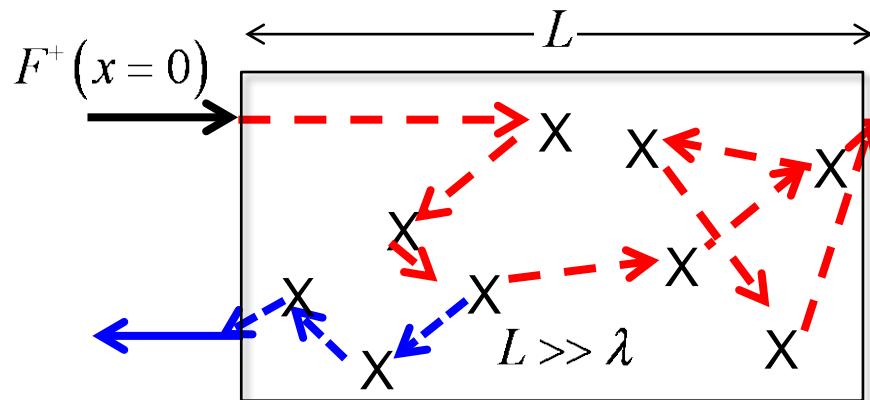
$$I = \frac{2q}{h} \int \mathcal{T}(E) M(E) (f_1(E) - f_2(E)) dE$$

# Transmission



ballistic transport:  $\mathcal{T}=1$

$$\mathcal{T}(E) = \frac{\lambda(E)}{\lambda(E) + L}$$

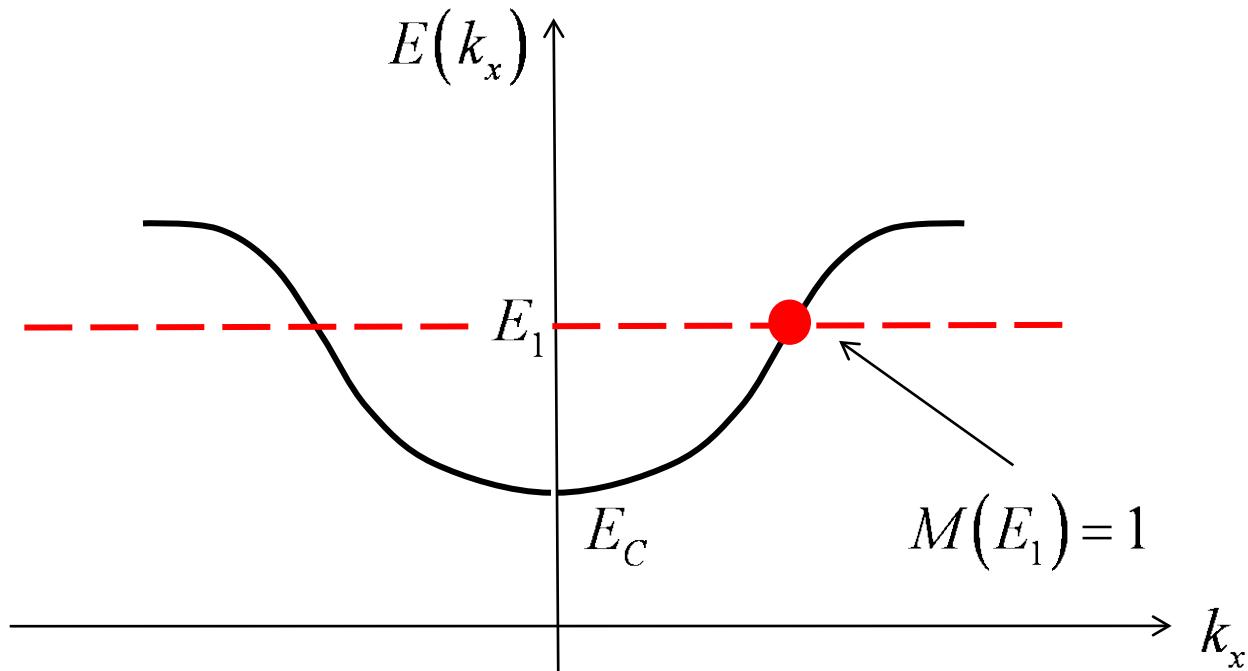


“diffusive transport”  $\mathcal{T} \ll 1$

# Channels

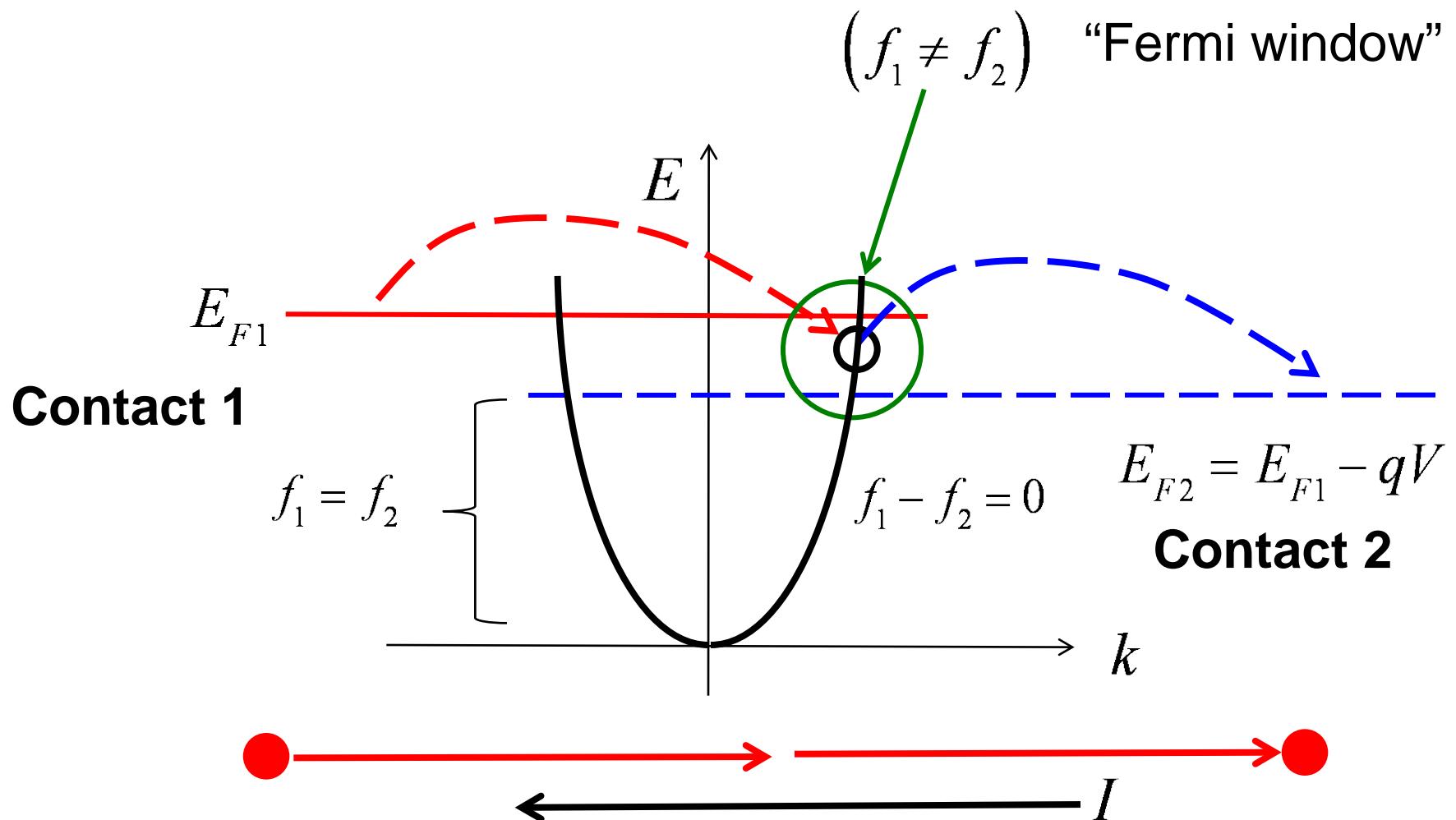
---

**A channel is a state with a velocity.**



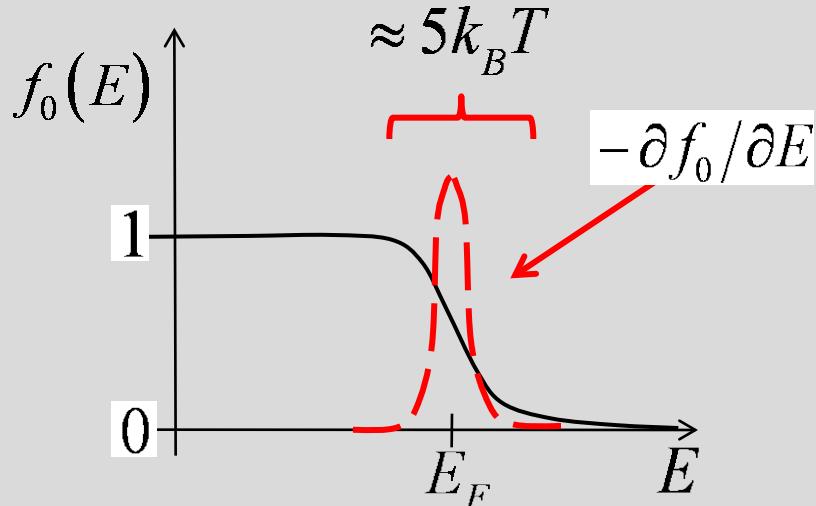
(Easily generalized to arbitrary band structures in 2D and 3D.)

# How current flows ( $T = 0$ K)



# Fermi window under small bias

“Fermi window”



$$T > 0 \text{ K}$$

$$(f_1 - f_2) \approx \left( -\frac{\partial f_0}{\partial E} \right) qV$$

$$W_F(E) = \left( -\frac{\partial f_0}{\partial E} \right)$$

$$\int W_F(E) dE = 1$$

# Small bias conductance

---

$$I = GV \quad \text{A}$$

$$G = \frac{2q^2}{h} \int \mathcal{T}(E) M(E) \left( -\frac{\partial f_0}{\partial E} \right) dE \quad \text{S}$$

$$G = \frac{2q^2}{h} \mathcal{T}(E_F) M(E_F) \quad (T = 0 \text{ K})$$

$$G = \frac{2q^2}{h} M(E_F) \quad (T = 0 \text{ K and ballistic})$$

Quantized conductance in nanostructures.

# Small bias conductance in the diffusive limit

---

$$\tau(E) = \frac{\lambda(E)}{\lambda(E) + L} \rightarrow \frac{\lambda(E)}{L} \rightarrow J_n = \sigma_n \frac{d(F_n/q)}{dx}$$

$\sigma_n$ : Conductivity (S/m)       $\rho_n = 1/\sigma_n$ : Resistivity (Ohm-m)

$n$ : electron density

$\sigma_n \equiv nq\mu_n$        $q$ : magnitude of the electronic charge

$\mu_n$ : mobility m<sup>2</sup>/V-s

$$J_x = n\mu_n \frac{dF_n}{dx}$$

# Drift-diffusion equation

---

$$J_x = n\mu_n \frac{dF_n}{dx}$$

$$n = N_C e^{(F_n - E_C)/k_B T}$$

$$J_x = nq\mu_n \mathcal{E} + qD_n \frac{dn}{dx}$$

$$D_n/\mu_n = k_B T/q$$

Einstein Relation

# Drift-diffusion equation

---

$$J_{px} = p\mu_p \vec{\nabla} F_p \quad \vec{J}_p = \vec{J}_{p-drift} + \vec{J}_{p-diff} = pq\mu_p \vec{E} - qD_p \vec{\nabla} p$$

current = drift current + diffusion current

$$J_{nx} = n\mu_n \vec{\nabla} F_n \quad \vec{J}_n = \vec{J}_{n-drift} + \vec{J}_{n-diff} = nq\mu_n \vec{E} + qD_n \vec{\nabla} n$$

total current = electron current + hole current

$$\vec{J} = \vec{J}_p + \vec{J}_n$$

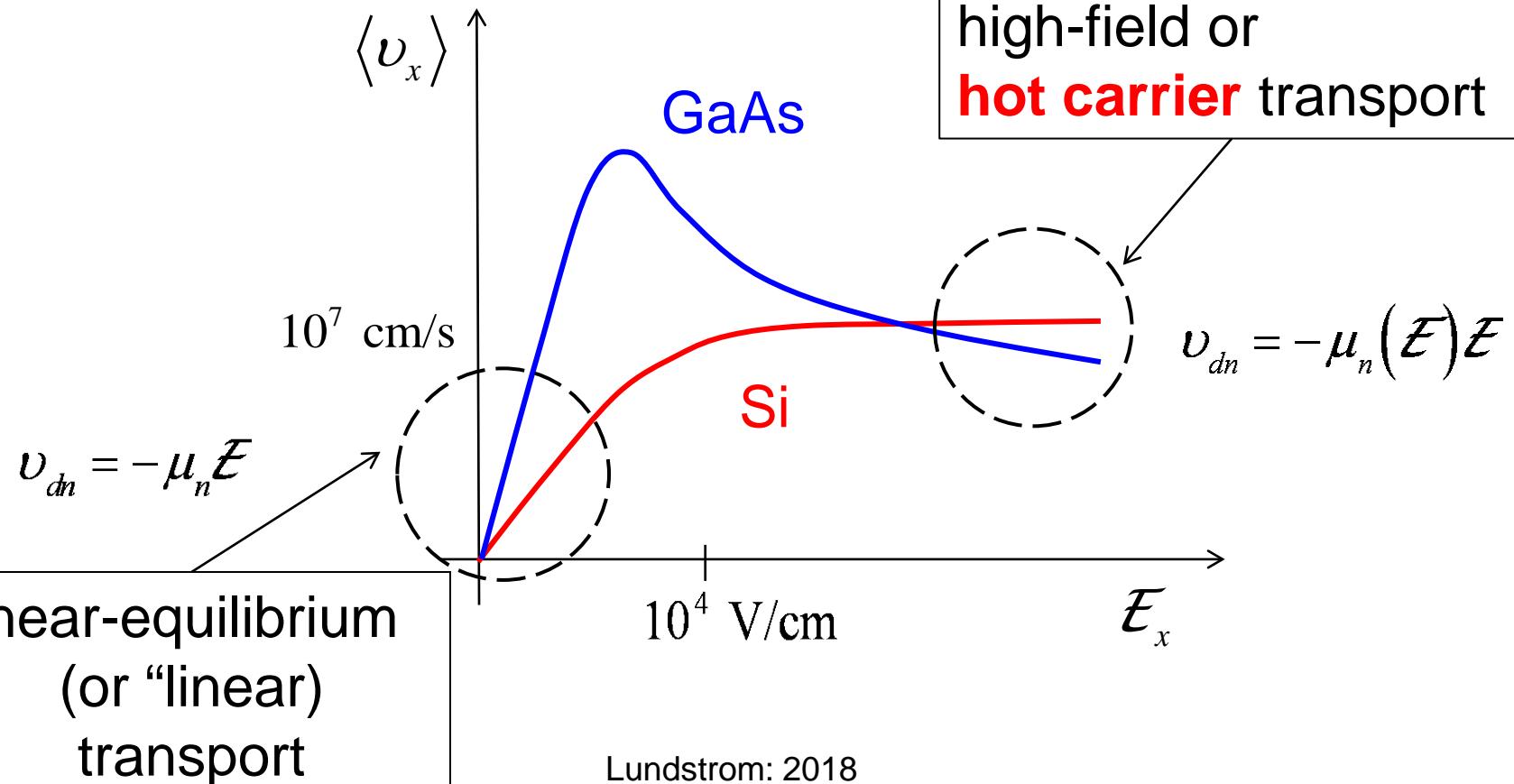
$$\mu_p = \frac{v_T \lambda_0}{2(k_B T / q)} = \frac{q\tau}{m_p^*}$$

$$D_p / \mu_p = D_n / \mu_n = k_B T / q$$

(Einstein, 1905)

# Velocity vs. field characteristic

(**bulk** semiconductors assumed)



# Recombination

---

When excess carriers are introduced, a semiconductor responds by trying to restore equilibrium.

$$\Delta n(t) = \Delta n(t = 0) e^{-t/\tau_n}$$

(low level injection)

The minority carrier lifetime is controlled by **radiative**, **Auger**, or **defect-assisted** processes – or by some combination of these.

# Recombination processes

---

## 1) Band-to-band radiative recombination

dominates in direct gap semiconductors  
makes lasers and LEDs possible

## 2) Auger recombination

dominates when the carrier densities are very high  
(heavily doped semiconductors or lasers)

## 3) SRH recombination

dominates in high quality, indirect gap semiconductors  
and in low quality direct gap semiconductors

# Generation processes

---

1) Optical generation

Inverse of radiative recombination

2) Thermal generation

Inverse of SRH recombination

3) Impact ionization

Inverse of Auger recombination

# Unit 4 summary

---

1) Out of equilibrium, currents can flow:

$$J_{nx} = n\mu_n \vec{\nabla} F_n \quad \vec{J}_n = nq\mu_n \vec{E} + qD_n \vec{\nabla} n$$

2) Out of equilibrium, excess carriers recombine:

$$\Delta n(t) = \Delta n(t=0) e^{-t/\tau_n}$$

3) Out of equilibrium, carriers can be generated by processes such as optical absorption and impact ionization.

# Vocabulary

---

Absorption coefficient

Auger recombination

Ballistic transport

Band-to-band recombination

Channels

Conductivity

Diffusive transport

Drift-diffusion equation

Drift velocity

Einstein relation

Electrochemical potential

Excess carriers

Impact ionization

Landauer approach

Mobility

Fermi window

Fick's Law

Low level injection

Minority carrier lifetime

Mean-free-path (MFP)

MFP for backscattering

Modes

Quantized conductance

Quasi-Fermi level

Radiative recombination

Resistivity

SRH recombination

Thermal velocity

## Vocabulary (cont.)

---

Thermalization

Transmission

Velocity vs. field characteristic

Vertical transition

## Primer on Semiconductors

# Unit 5: The Semiconductor Equations

## Lecture 5.1: Mathematical formulation

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Solving semiconductor problems

---

For a uniform semiconductor in equilibrium, we can assume space-charge neutrality:

$$\rho_0 = q(p_0 - n_0 + N_D^+ - N_A^-) = 0$$

We also know that in equilibrium:

$$n_0 p_0 = n_i^2$$

In general, neither one of the above equations is valid, so how do we solve for the electron and hole concentrations and for the electric field too?

# Equilibrium vs. non-equilibrium

equilibrium

$$n_0 = n_i e^{(E_F - E_i)/k_B T}$$

$$p_0 = n_i e^{(E_i - E_F)/k_B T}$$

$$n_0 p_0 = n_i^2$$

$$f_0 = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

non-equilibrium

$$n = n_i e^{(F_n - E_i)/k_B T}$$

$$p = n_i e^{(E_i - F_p)/k_B T}$$

$$np \neq n_i^2$$

$$f_c = \frac{1}{1 + e^{(E - F_n)/k_B T}}$$

$$1 - f_v = 1 - \frac{1}{1 + e^{(E - F_p)/k_B T}}$$

# The unknowns

---

$$p(\vec{r}) = n_i e^{(E_i(\vec{r}) - F_p(\vec{r})) / k_B T}$$

$$n(\vec{r}) = n_i e^{(F_n(\vec{r}) - E_i(\vec{r})) / k_B T}$$

$$E_i(\vec{r}) = E_i^{\text{ref}} - qV(\vec{r})$$

3 unknowns

$$p(\vec{r}), n(\vec{r}), V(\vec{r})$$

or

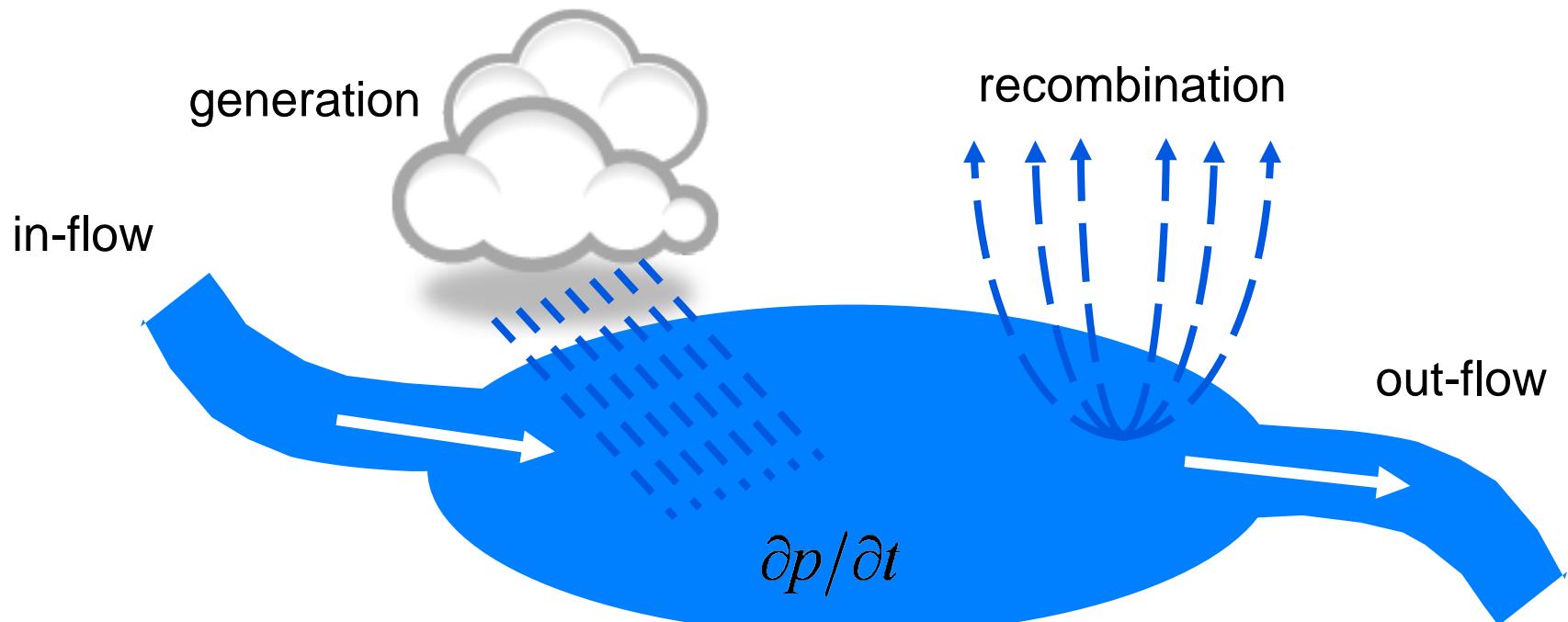
$$F_p(\vec{r}), F_n(\vec{r}), V(\vec{r})$$

We need to formulate 3 equations in 3 unknowns.

# First equation: Continuity equation for holes

$$\frac{\partial p}{\partial t} = \text{in-flow} - \text{out-flow} + G - R$$

$$\frac{\partial p}{\partial t} = -\nabla \cdot \frac{\vec{J}_p}{q} + G_p - R_p$$



# One equation in 3 unknowns

---

$$\frac{\partial p}{\partial t} = -\nabla \cdot \frac{\vec{J}_p}{q} + G_p - R_p$$

$$\vec{J}_p = pq\mu_p \vec{\mathcal{E}} - qD_p \vec{\nabla} p$$

optical generation  
or impact ionization

Need equation  
for the electric  
field

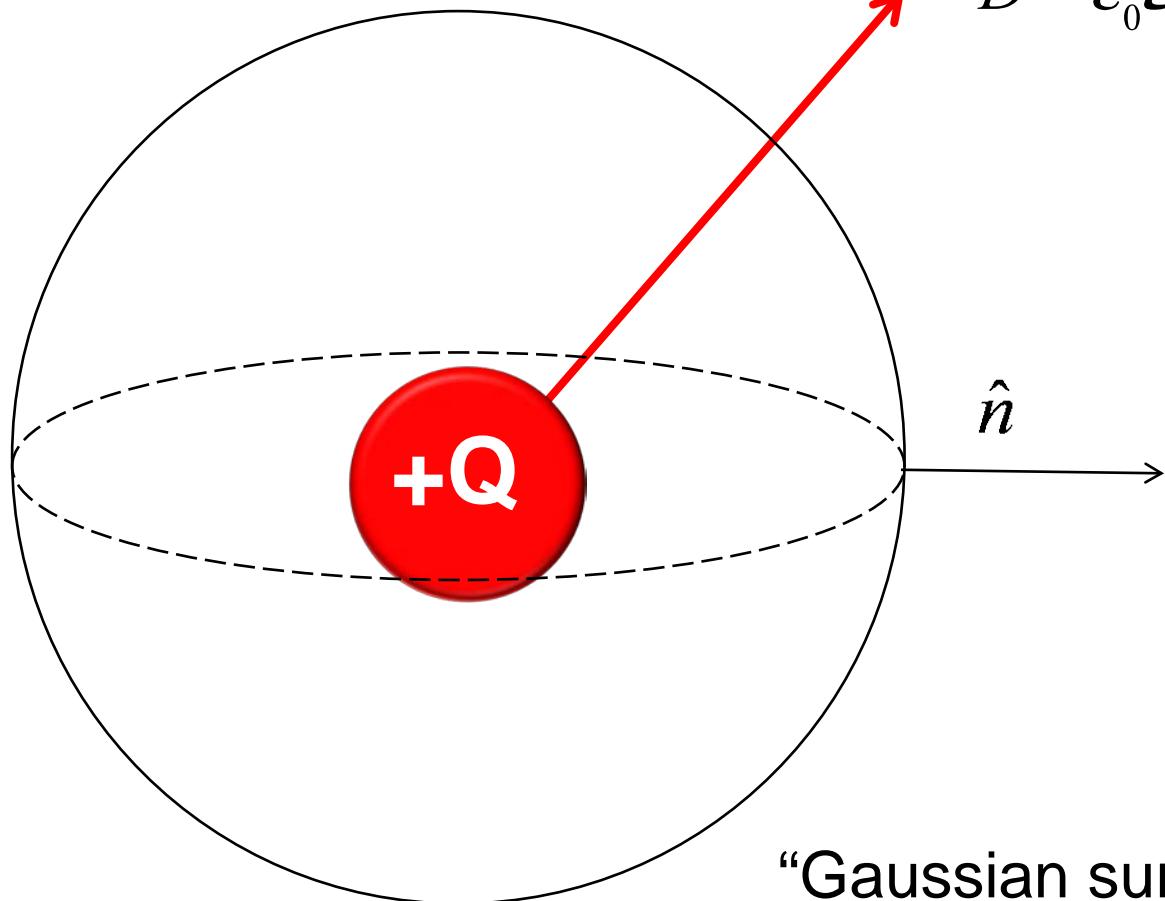
$$R_p \propto np$$

Radiative, Auger  
or defect-assisted  
processes

Need equation  
for electrons

# Gauss's Law

---



$$\vec{D} = \epsilon_0 \vec{E}$$

$$\vec{D} = K_s \epsilon_0 \vec{E}$$

$$\oint \vec{D} \cdot d\vec{S} = Q$$

“Gaussian surface”

# Gauss's Law in 1D

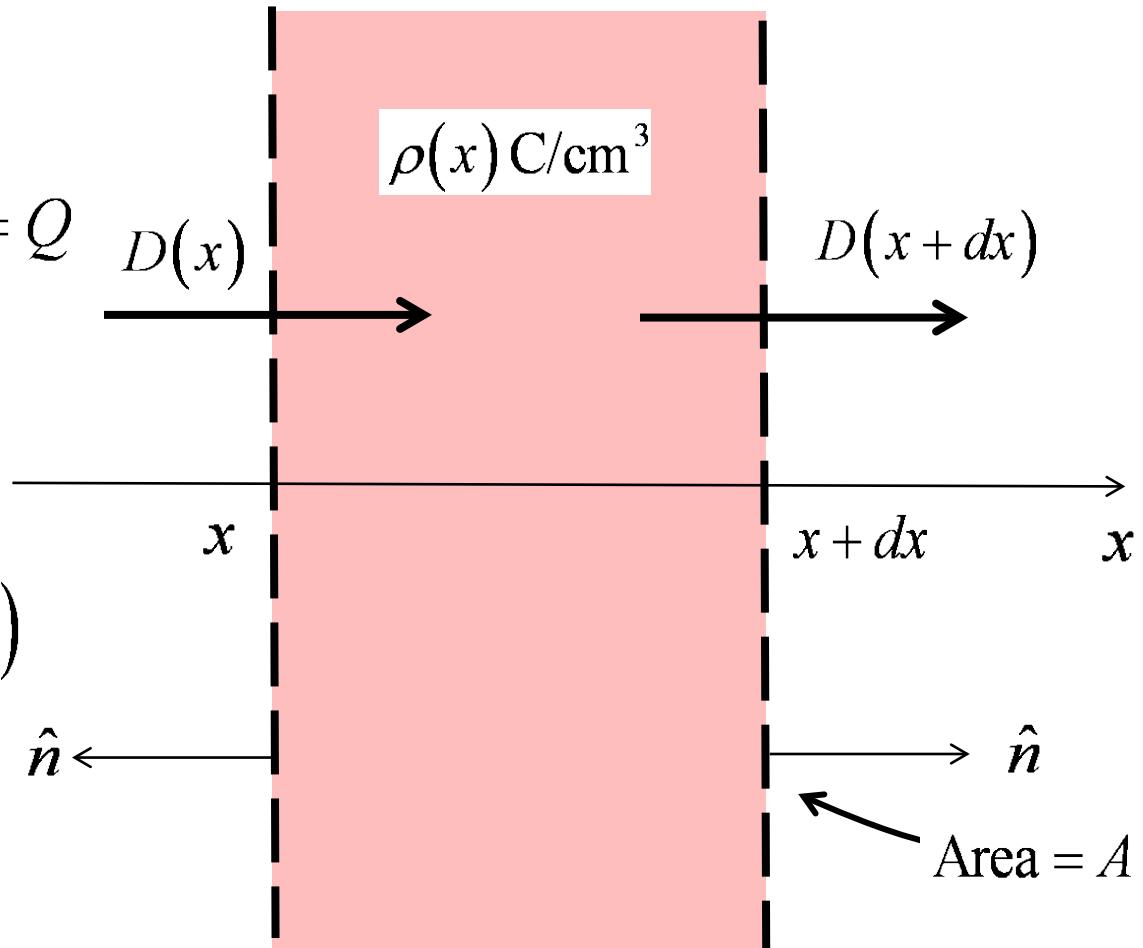
$$\oint \vec{D} \cdot d\vec{S} = Q$$

$$-D(x)A + D(x+dx)A = Q$$

$$Q = \rho(x)Adx$$

$$\frac{D(x+dx) - D(x)}{dx} = \rho(x)$$

$$\frac{dD}{dx} = \rho(x)$$



# The Poisson equation

---

$$\oint \vec{D} \cdot d\vec{S} = Q \iff \nabla \cdot \vec{D} = \rho(x)$$

$$D = K_s \epsilon_0 \vec{\epsilon}$$

$$\nabla \cdot (K_s \epsilon_0 \vec{\epsilon}) = \rho(\vec{r})$$

$$\rho(\vec{r}) = q [ p(\vec{r}) - n(\vec{r}) + N_D^+(\vec{r}) - N_A^-(\vec{r}) ]$$

# The “semiconductor equations”

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$

$$\frac{\partial n}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_n}{-q} \right) + G_n - R_n$$

$$\nabla \cdot (K_s \epsilon_0 \vec{\mathcal{E}}) = \rho$$

Three equations in three unknowns:

$$p(\vec{r}), n(\vec{r}), V(\vec{r})$$

$$\{F_p(\vec{r}), F_n(\vec{r}), V(\vec{r})\}$$

$$\vec{J}_p = p \mu_p \vec{\nabla} F_p = pq \mu_p \vec{\mathcal{E}} - q D_p \vec{\nabla} p$$

$$\rho = q(p - n + N_D^+ - N_A^-)$$

$$\vec{J}_n = n \mu_n \vec{\nabla} F_n = nq \mu_n \vec{\mathcal{E}} + q D_n \vec{\nabla} n$$

$$\vec{\mathcal{E}}(\vec{r}) = \nabla V(\vec{r})$$

# Semiconductor equations

---

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$

$$\frac{\partial n}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_n}{-q} \right) + G_n - R_n$$

$$\nabla \cdot (K_s \epsilon_0 \vec{\mathcal{E}}) = \rho$$

Not as fundamental as Maxwell's equations, but these equations are the starting point for the analysis of most semiconductor devices.

# Discussion: Equilibrium

---

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$

$$0 = -\nabla \cdot \left( \frac{0}{q} \right) + 0 - 0$$

$$\frac{\partial n}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_n}{-q} \right) + G_n - R_n$$



$$0 = -\nabla \cdot \left( \frac{0}{-q} \right) + 0 - 0$$

$$\nabla \cdot (K_s \epsilon_0 \vec{\mathcal{E}}) = \rho$$

$$\nabla \cdot (K_s \epsilon_0 \vec{\mathcal{E}}) = \rho_0$$

What can we learn from equilibrium?

$$p_0 = n_i e^{(E_i - E_F)/k_B T}$$

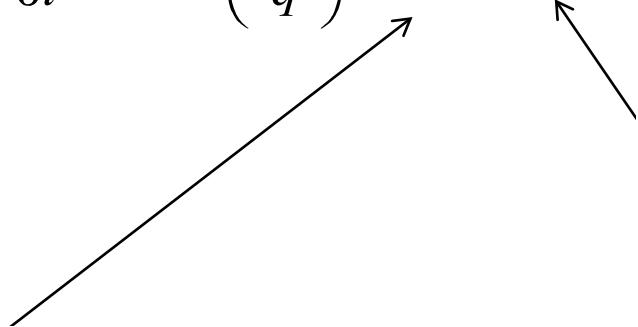
$$n_0 = n_i e^{(E_F - E_i)/k_B T}$$

$$n_0 p_0 = n_i^2$$

# Reminder: Generation and recombination

---

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$



other generation processes

e.g. optical generation  
impact ionization

Band-to-band  
SRH  
Auger

recombination:

$$R_p > 0$$

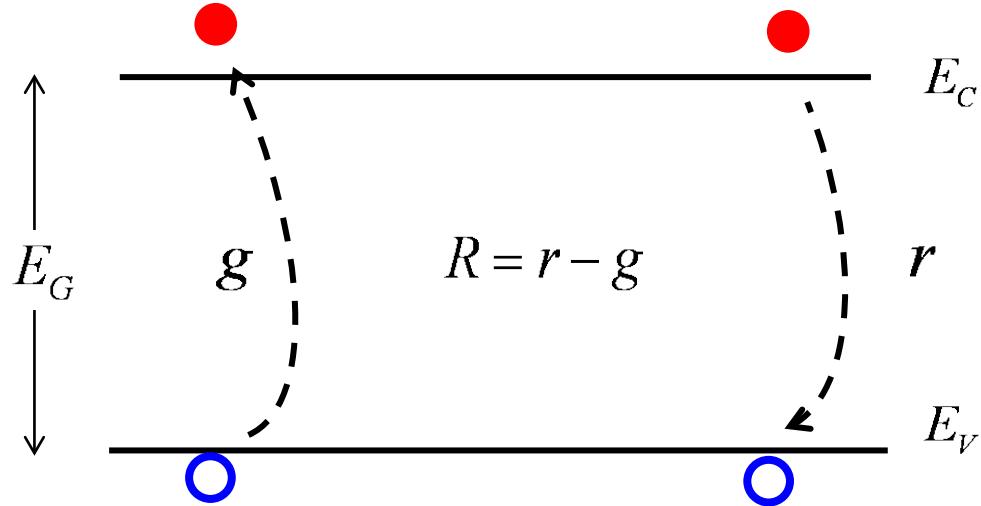
generation:

$$R_p < 0$$

steady-state:

$$R_p = R_n = R$$

# Discussion



$$R_p = R_n = R < 0$$

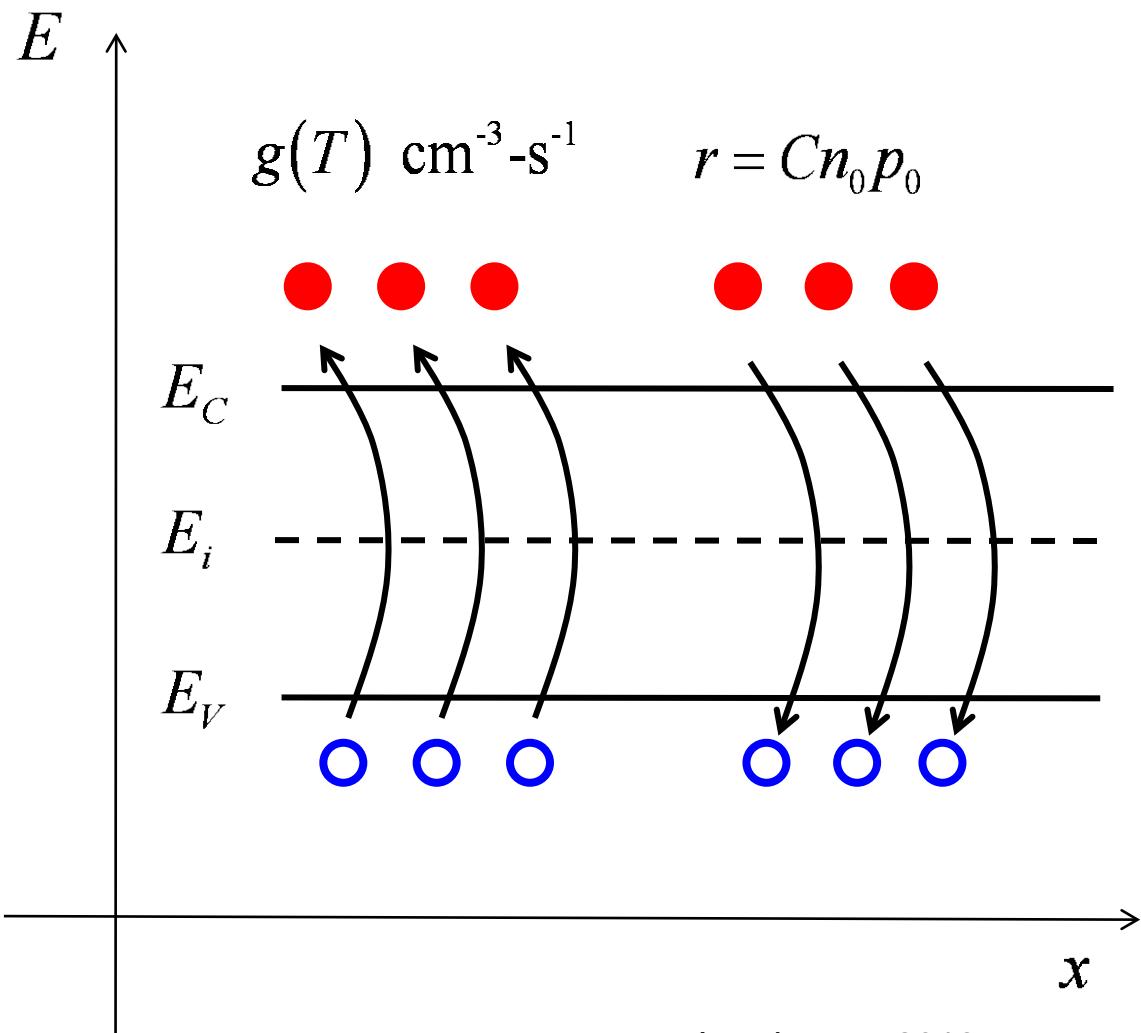
requires energy to  
break covalent bonds

$$R_p = R_n = R > 0$$

releases energy

**In equilibrium:  $R = 0$**

# Why is $n_0 p_0 = n_i^2$ ?



In equilibrium:

$$g = r$$

$$n_0 p_0 = \frac{g(T)}{C} = n_i^2(T)$$

$$n_0 p_0 = n_i^2(T)$$

# Summary: The “semiconductor equations”

---

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$

$$\frac{\partial n}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_n}{-q} \right) + G_n - R_n$$

$$\nabla \cdot (K_s \epsilon_0 \vec{\mathcal{E}}) = \rho$$

Three equations in three unknowns:

$$p(\vec{r}), n(\vec{r}), V(\vec{r})$$

$$\{F_p(\vec{r}), F_n(\vec{r}), V(\vec{r})\}$$

$$\vec{J}_p = p \mu_p \vec{\nabla} F_p = pq \mu_p \vec{\mathcal{E}} - q D_p \vec{\nabla} p$$

$$\rho = q(p - n + N_D^+ - N_A^-)$$

$$\vec{J}_n = n \mu_n \vec{\nabla} F_n = nq \mu_n \vec{\mathcal{E}} + q D_n \vec{\nabla} n$$

$$\vec{\mathcal{E}}(\vec{r}) = \nabla V(\vec{r})$$

## Primer on Semiconductors

# Unit 5: The Semiconductor Equations

## Lecture 5.2: Energy band diagrams

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Summary: The “semiconductor equations”

---

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$

$$\frac{\partial n}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_n}{-q} \right) + G_n - R_n$$

$$\nabla \cdot (K_s \epsilon_0 \vec{\mathcal{E}}) = \rho$$

Three equations in three unknowns:

$$p(\vec{r}), n(\vec{r}), V(\vec{r})$$

$$\{F_p(\vec{r}), F_n(\vec{r}), V(\vec{r})\}$$

$$\vec{J}_p = p \mu_p \vec{\nabla} F_p = pq \mu_p \vec{\mathcal{E}} - q D_p \vec{\nabla} p$$

$$\rho = q(p - n + N_D^+ - N_A^-)$$

$$\vec{J}_n = n \mu_n \vec{\nabla} F_n = nq \mu_n \vec{\mathcal{E}} + q D_n \vec{\nabla} n$$

$$\vec{\mathcal{E}}(\vec{r}) = \nabla V(\vec{r})$$

# Energy band diagrams

---

An energy band diagram is a plot of the bottom of the conduction band and the top of the valence band vs. position.

Energy band diagrams are a powerful tool for understanding semiconductor devices because they provide **qualitative solutions to the semiconductor equations**.

# Kroemer's lemma of proven ignorance

---

“Whenever I teach my semiconductor device physics course, one of the central messages I try to get across early is the importance of energy band diagrams. I often put this in the form of “Kroemer’s lemma of proven ignorance:

If, in discussing a semiconductor problem, you cannot draw an **Energy Band Diagram**, this shows that **you** don’t know what you are talking about.”

(Nobel Lecture, 2000)

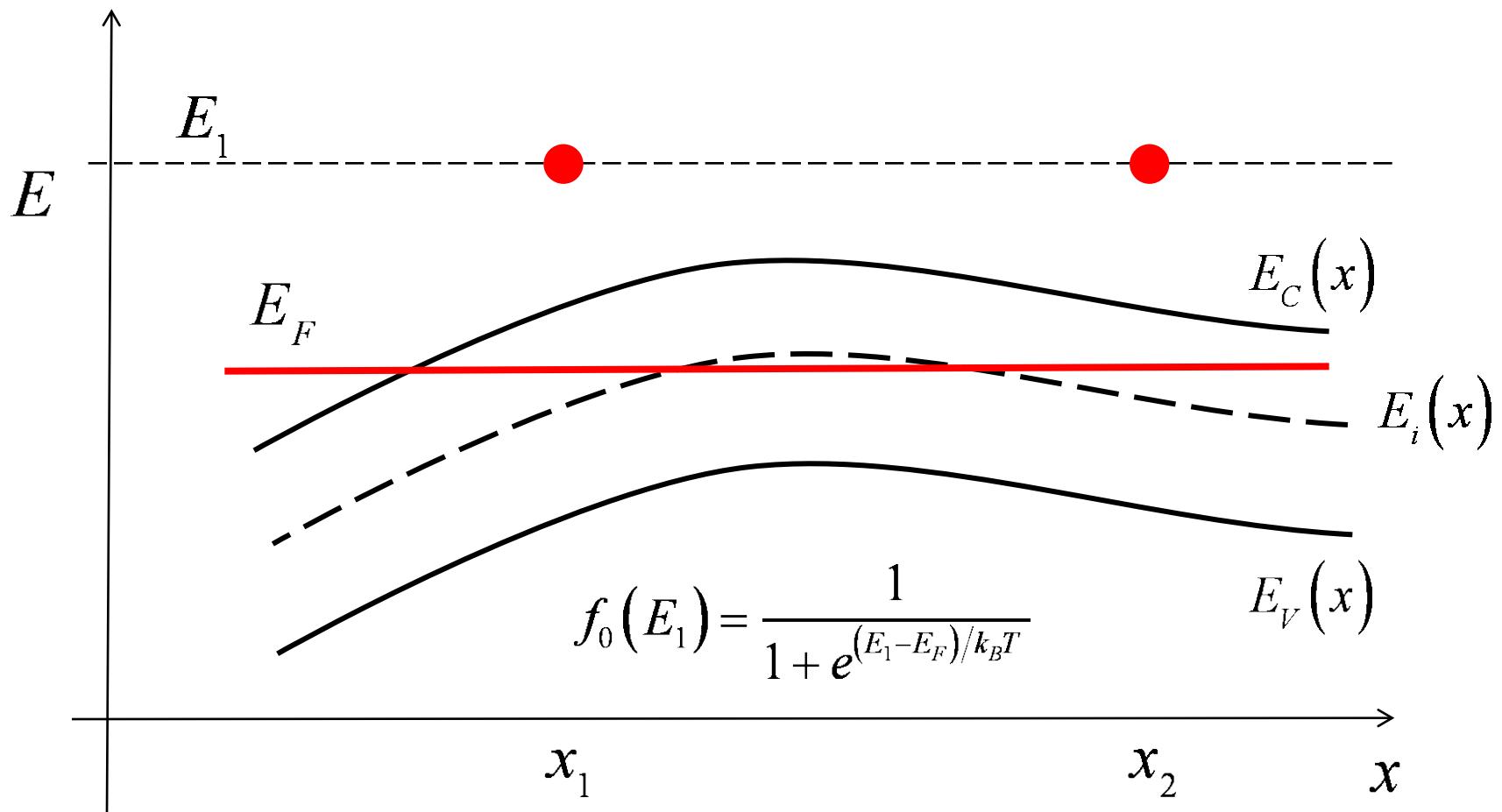
# Kroemer's corollary

---

If you can draw one, but don't, then **your audience** won't know what you are talking about.”

(Nobel Lecture, 2000)

# An important principle (in equilibrium)



# The Fermi level in equilibrium

---

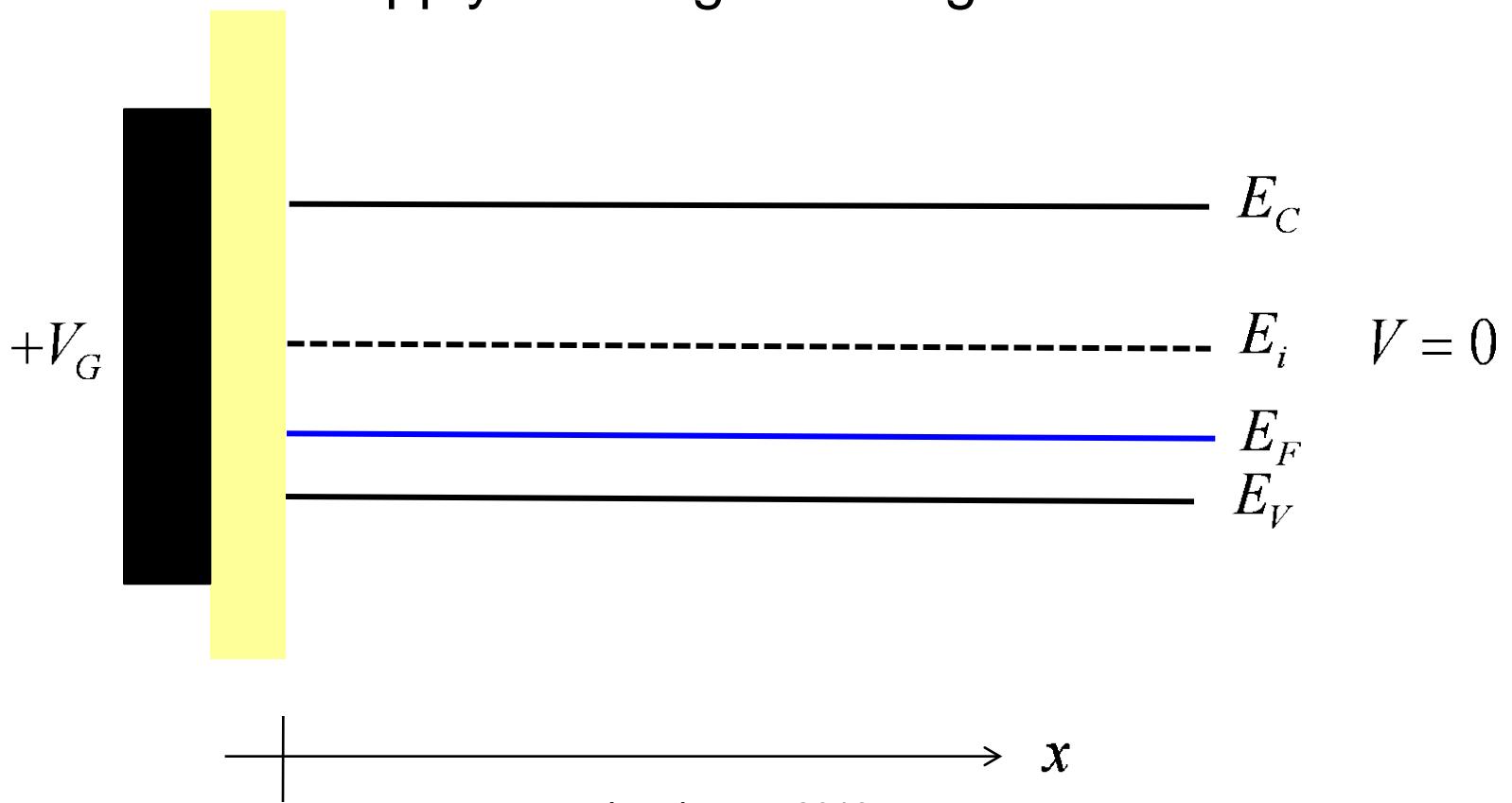
The Fermi level is constant in equilibrium.

$$J_n = n\mu_n \frac{dF_n}{dx} = 0 = n\mu_n \frac{dE_F}{dx} \rightarrow E_F \text{ is constant}$$

# Band bending

---

What happens when we apply a voltage to the gate?



# Voltage and electron potential energy

---

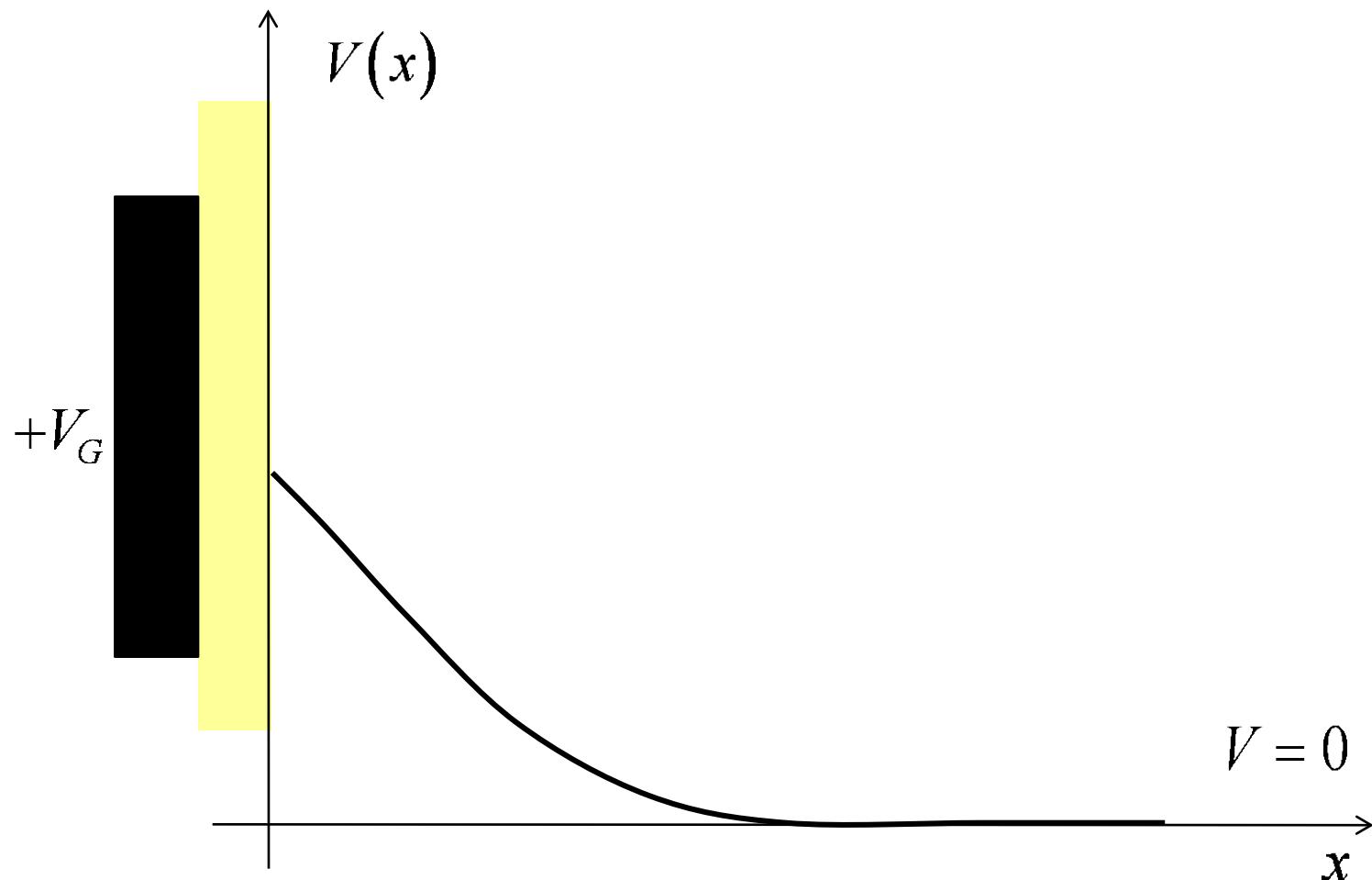
$$E = -qV$$



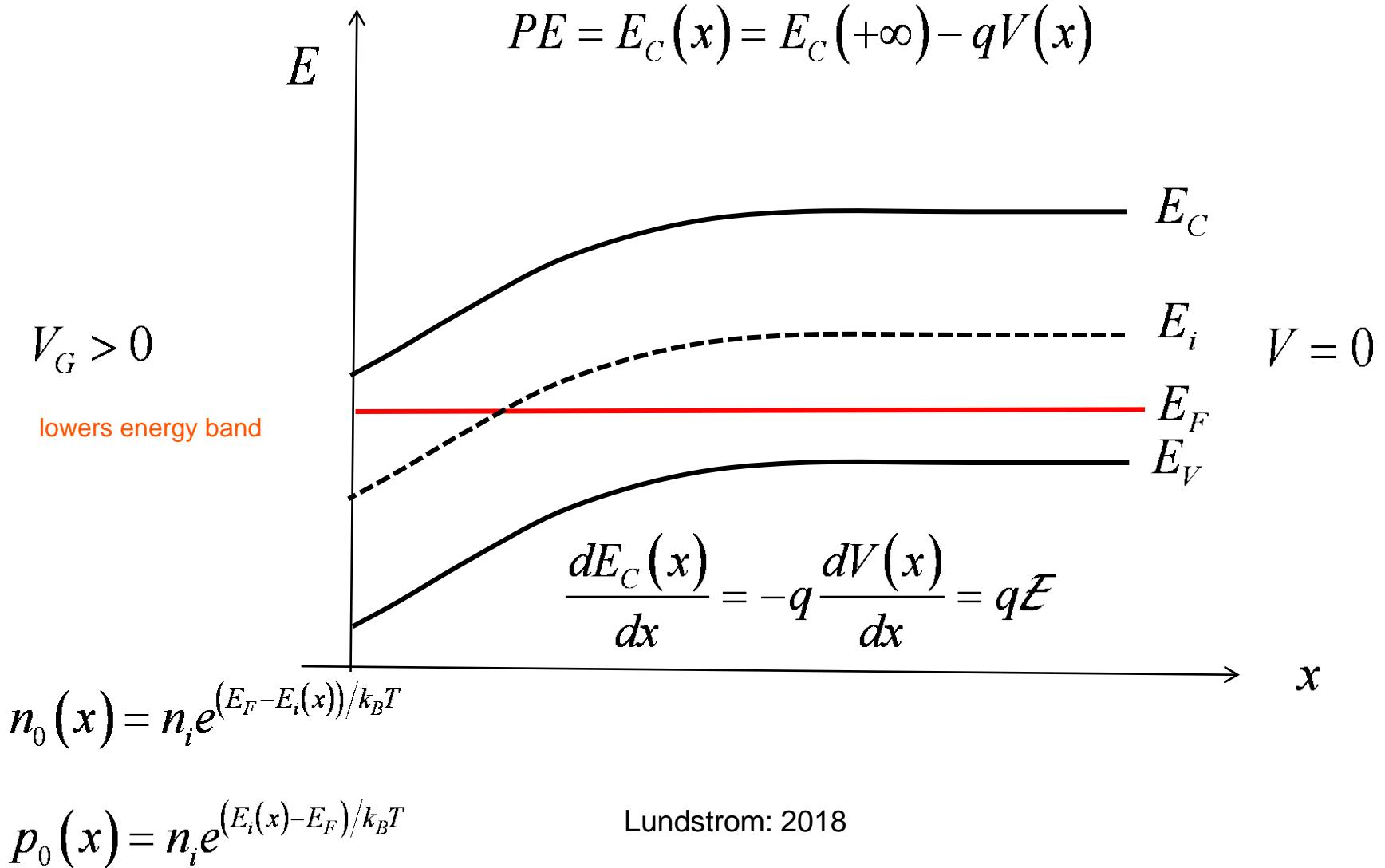
$$+V$$

A positive potential **lowers** the energy of an electron.

# Electrostatic potential vs. position

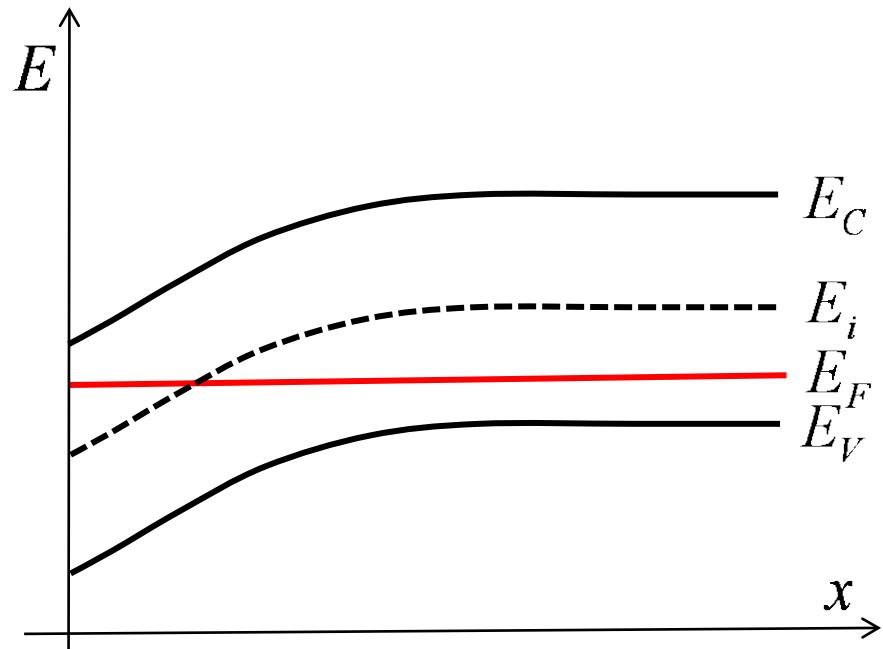


# Electrostatic potential causes band bending



# Band diagrams

Drawing the band diagram



$$\frac{d\mathcal{E}}{dx} = \frac{\rho(x)}{K_S \epsilon_0}$$

Reading the band diagram

$$V(x) \propto -E_C(x)$$

$$\mathcal{E} \propto dE_C(x)/dx$$

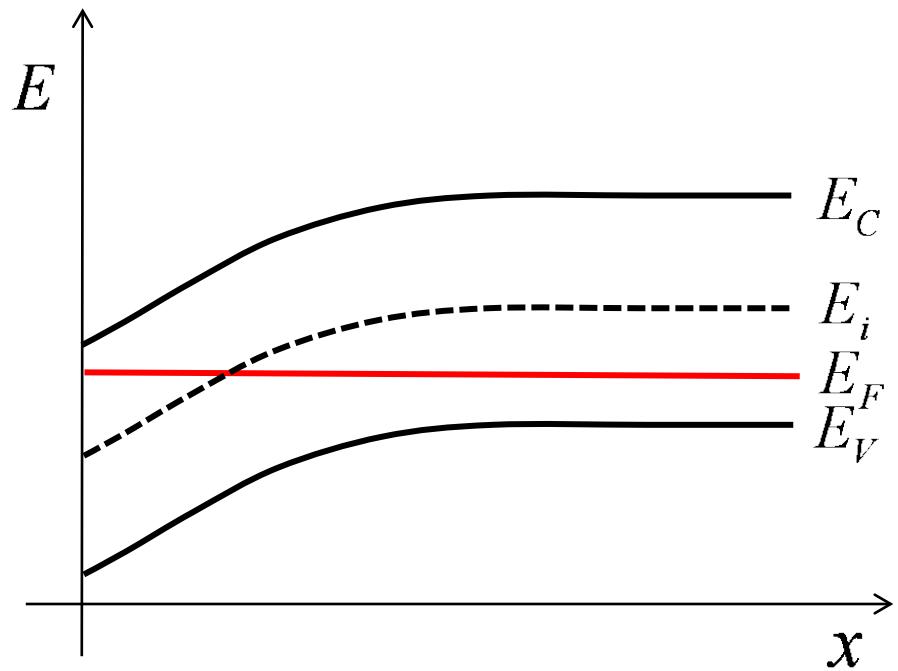
$$\log n(x) \propto E_F - E_i(x)$$

$$\log p(x) \propto E_i(x) - E_F$$

$$\rho(x) \propto d^2E_C/dx^2$$

# Practice

---



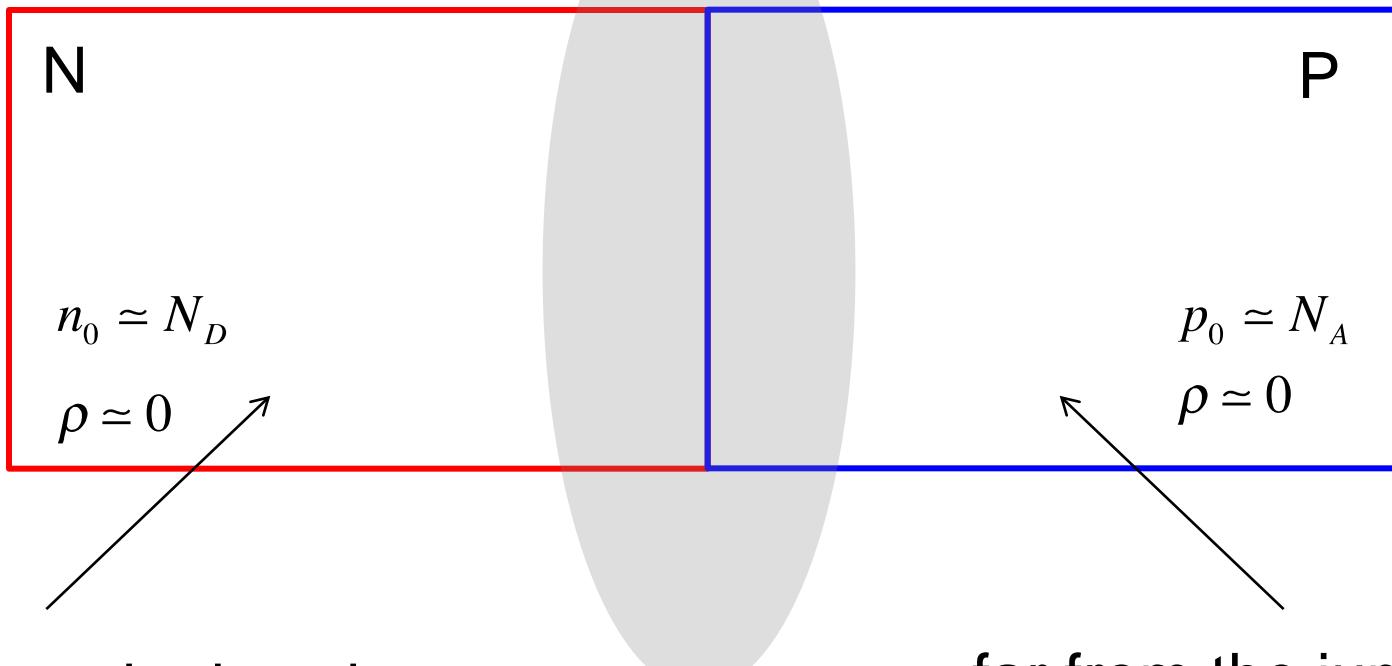
Sketch vs. position:

- Electrostatic potential
- Electric field
- Electron density
- Hole density
- Space charge density

## Another example: NP junction in equilibrium

---

the bands will bend  
near the junction



far from the junction,  
the bands will be flat

far from the junction,  
the bands will be flat

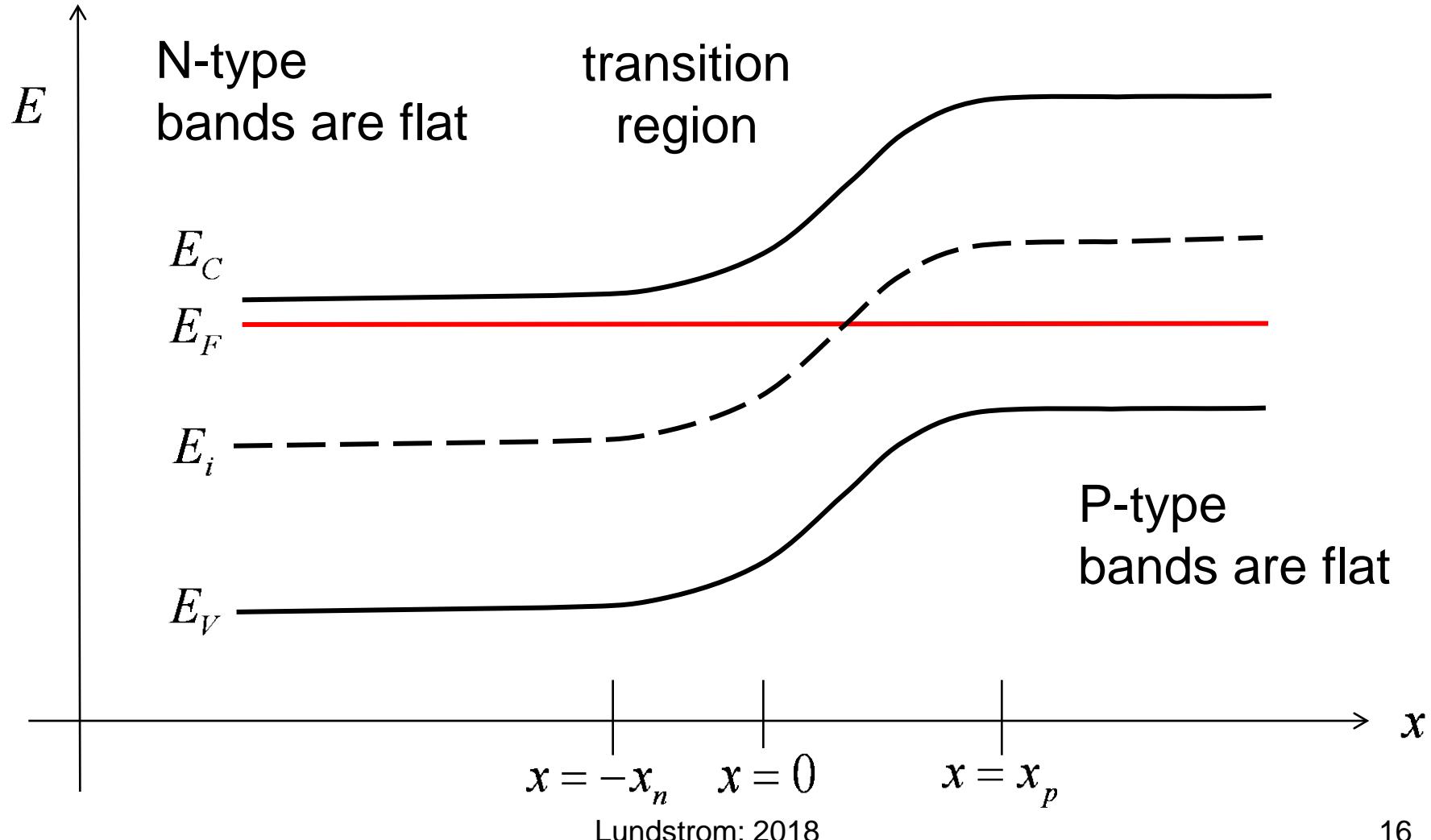
# Procedure: Equilibrium energy band diagram

---



- 1) Begin with  $E_F$
- 2) Draw the E-bands where you know the carrier density then connect the two regions.
- 3) Then “read” the energy band diagram to obtain the electrostatic potential, electric field, carrier densities, and space charge density vs. position.

# Energy band diagram

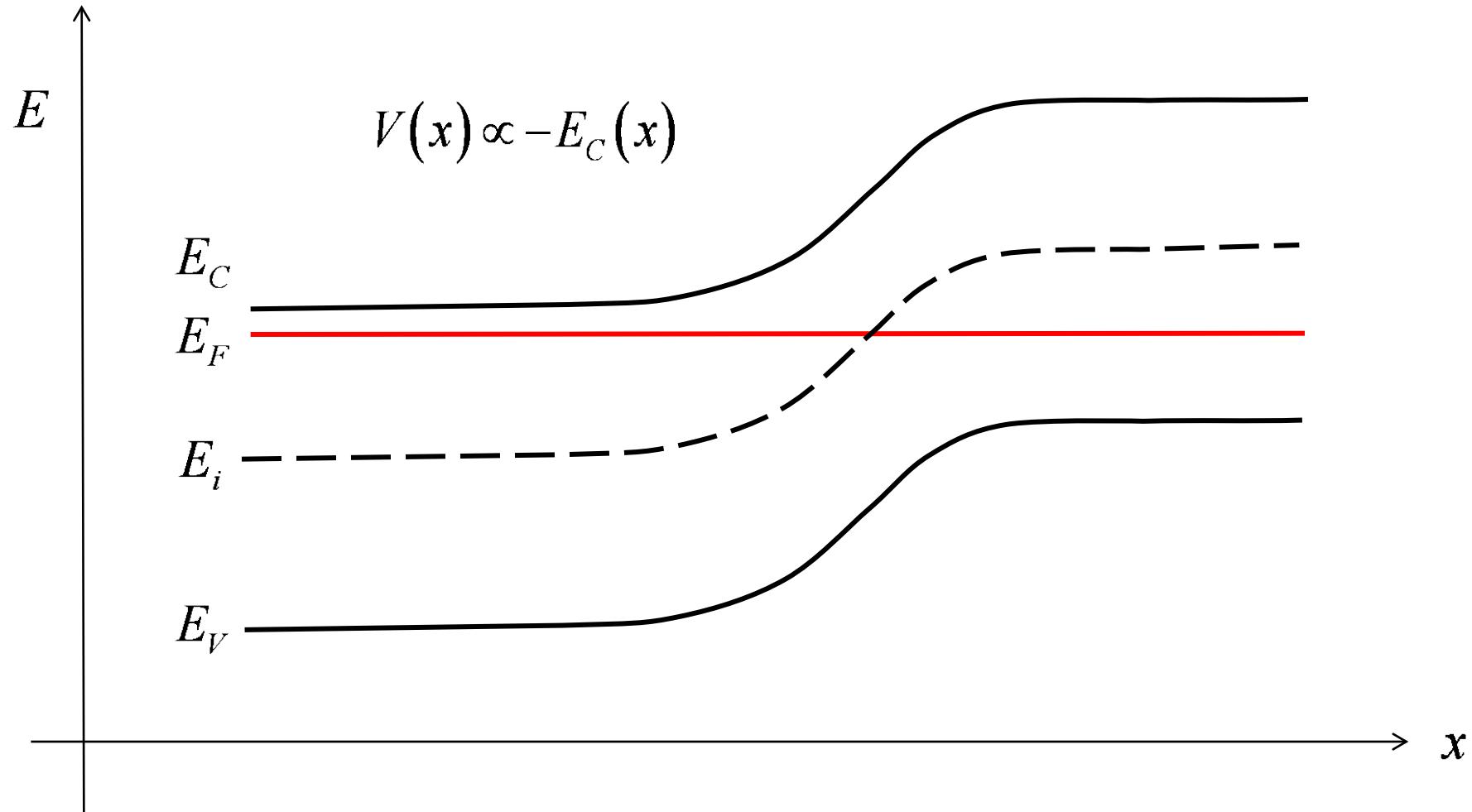


Now, “read” the e-band diagram

---

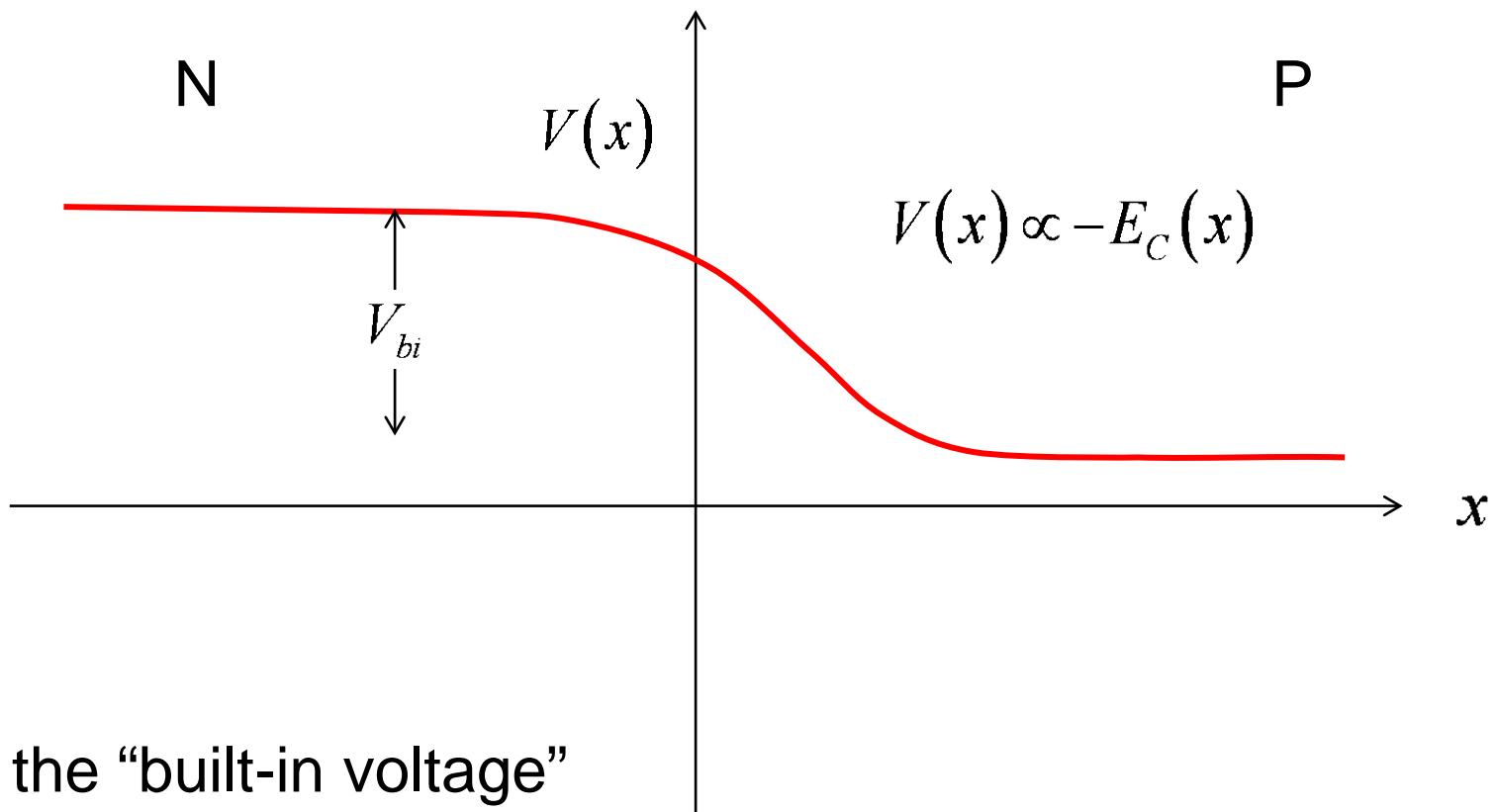
- 1) Electrostatic potential vs. position
- 2) Electric field vs. position
- 3) Electron and hole densities vs. position
- 4) Space-charge density vs. position

# Electrostatic potential?

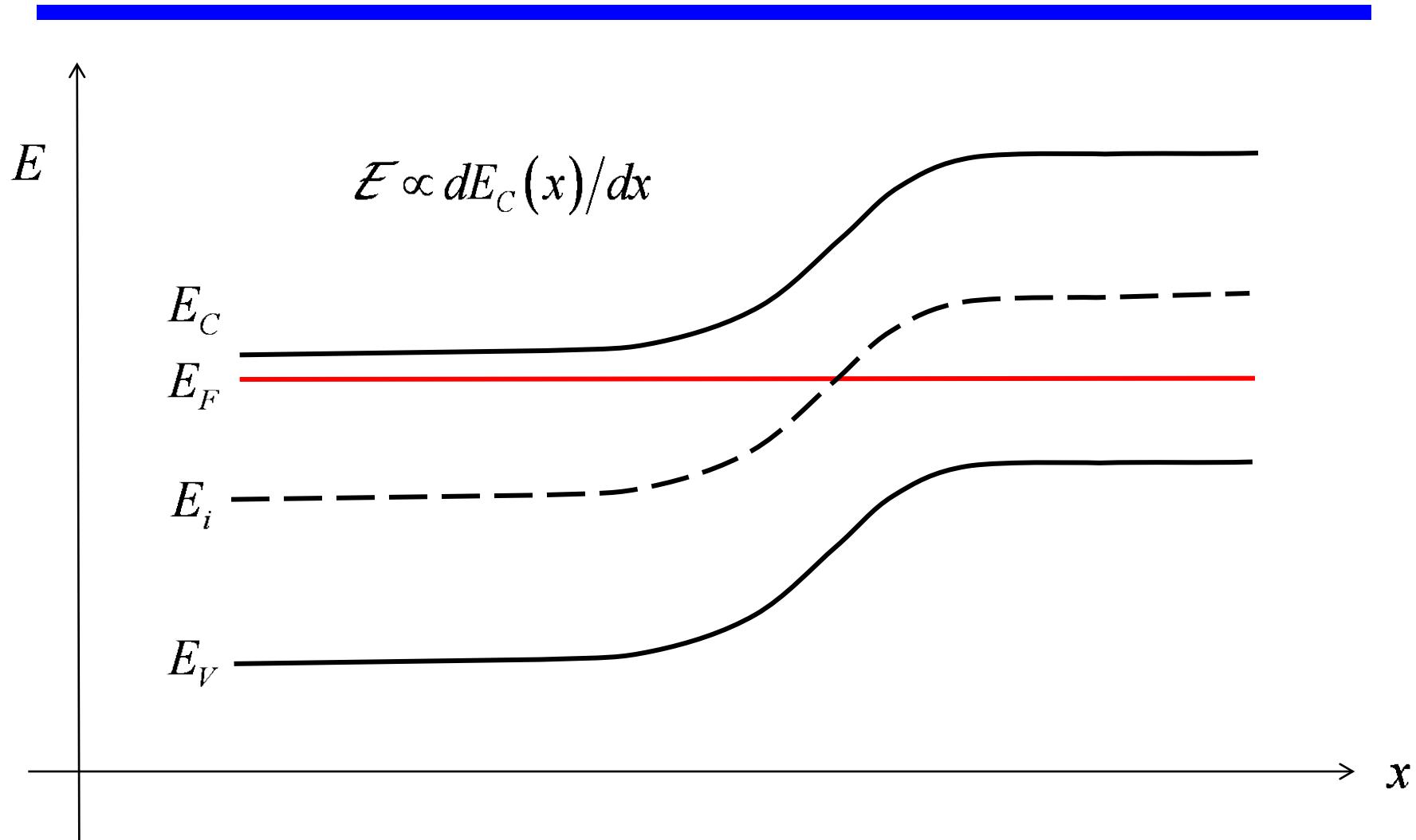


# Electrostatics: $V(x)$

---

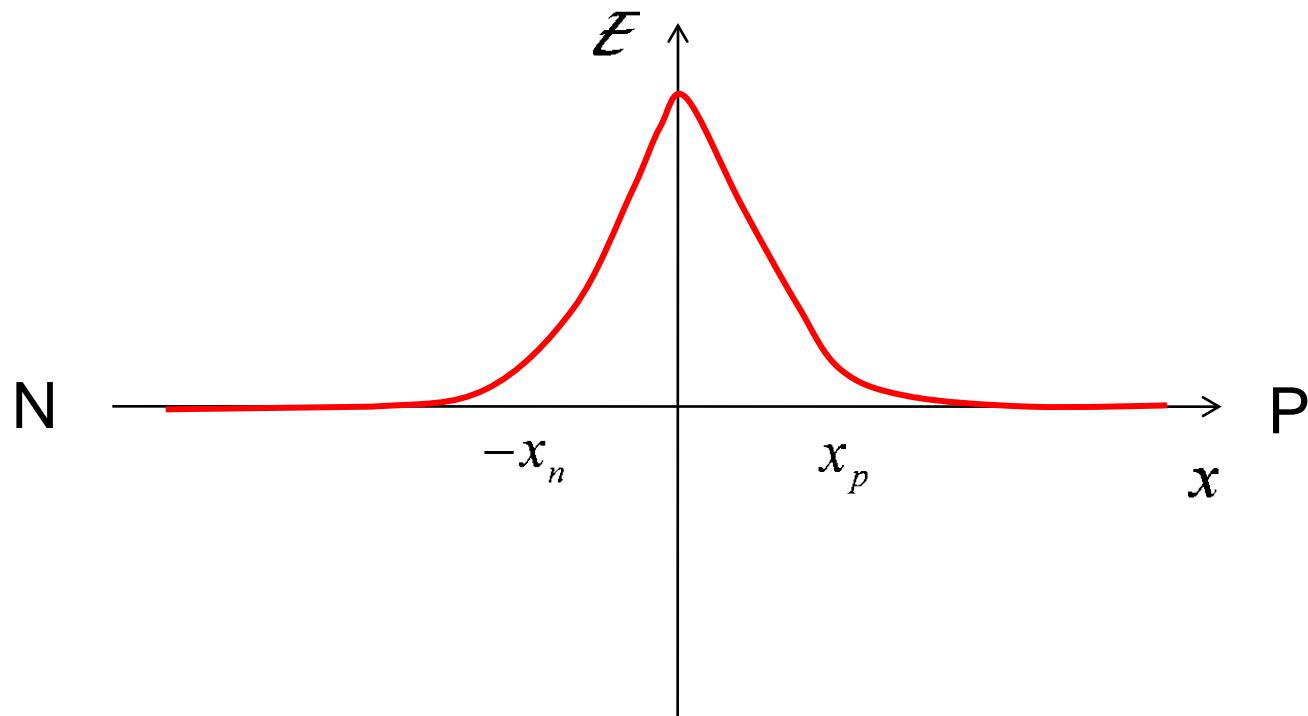


# Electric field?

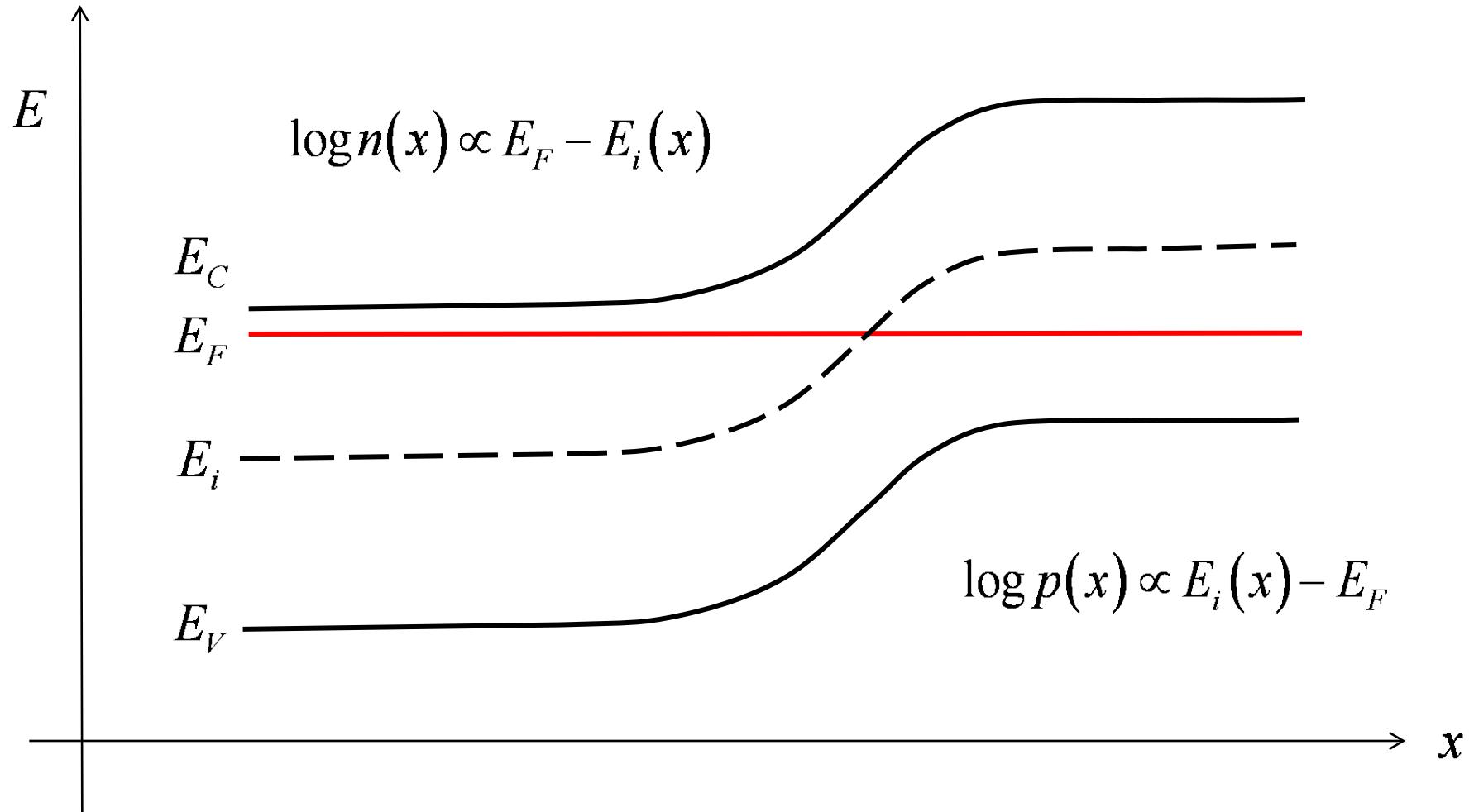


# Electric field: $\mathcal{E}(x)$

---

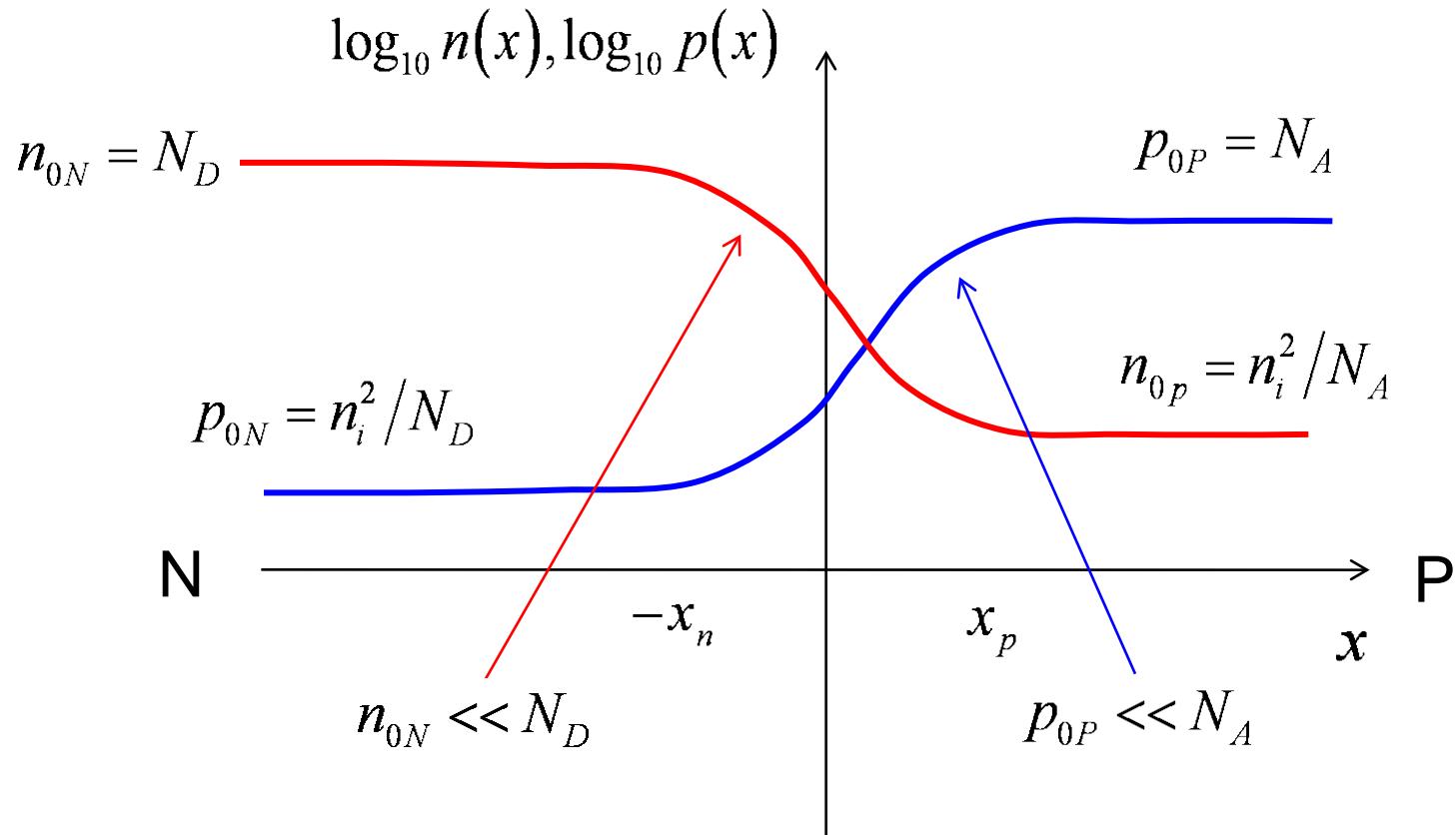


# Carrier densities?

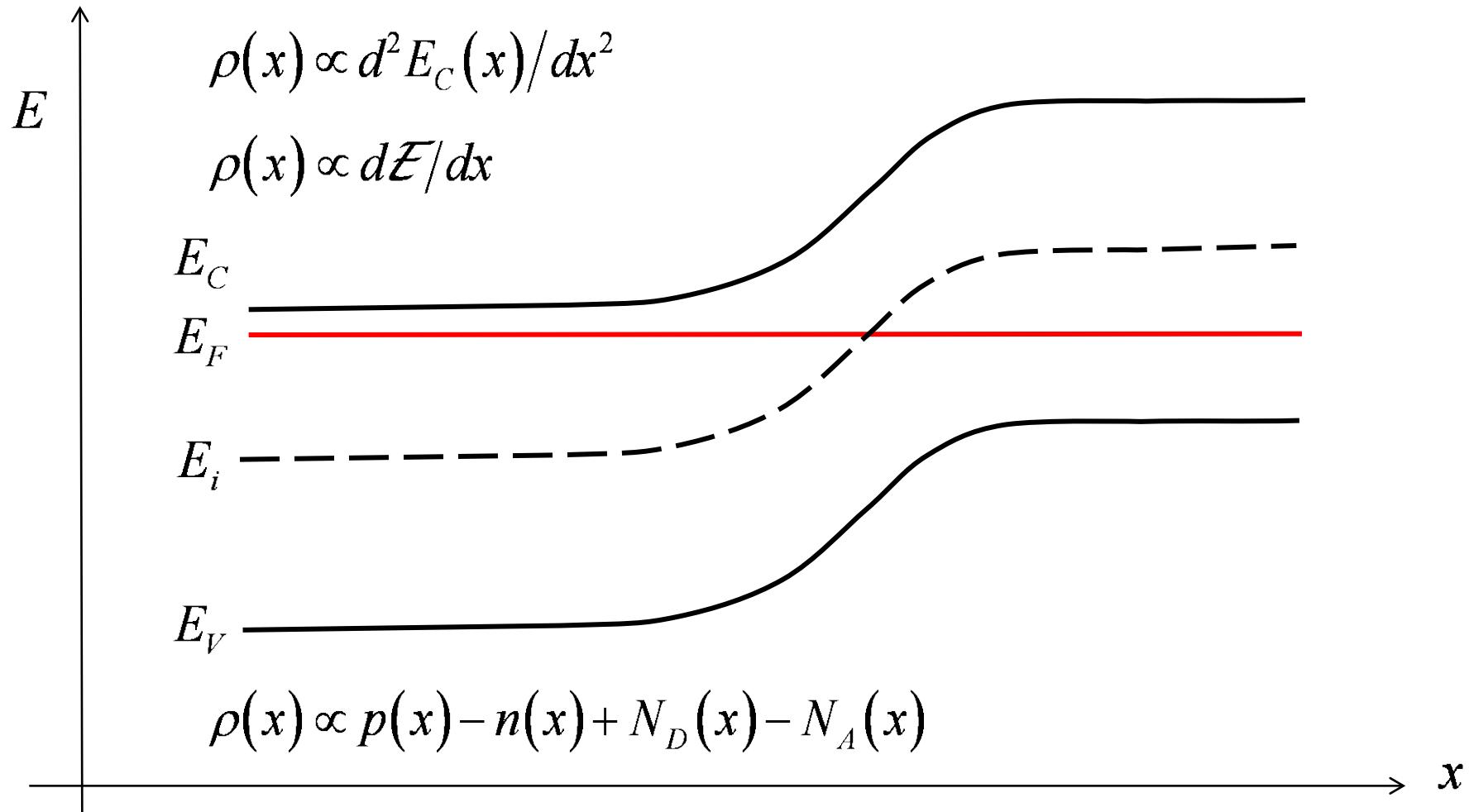


# Carrier densities vs. $x$

---

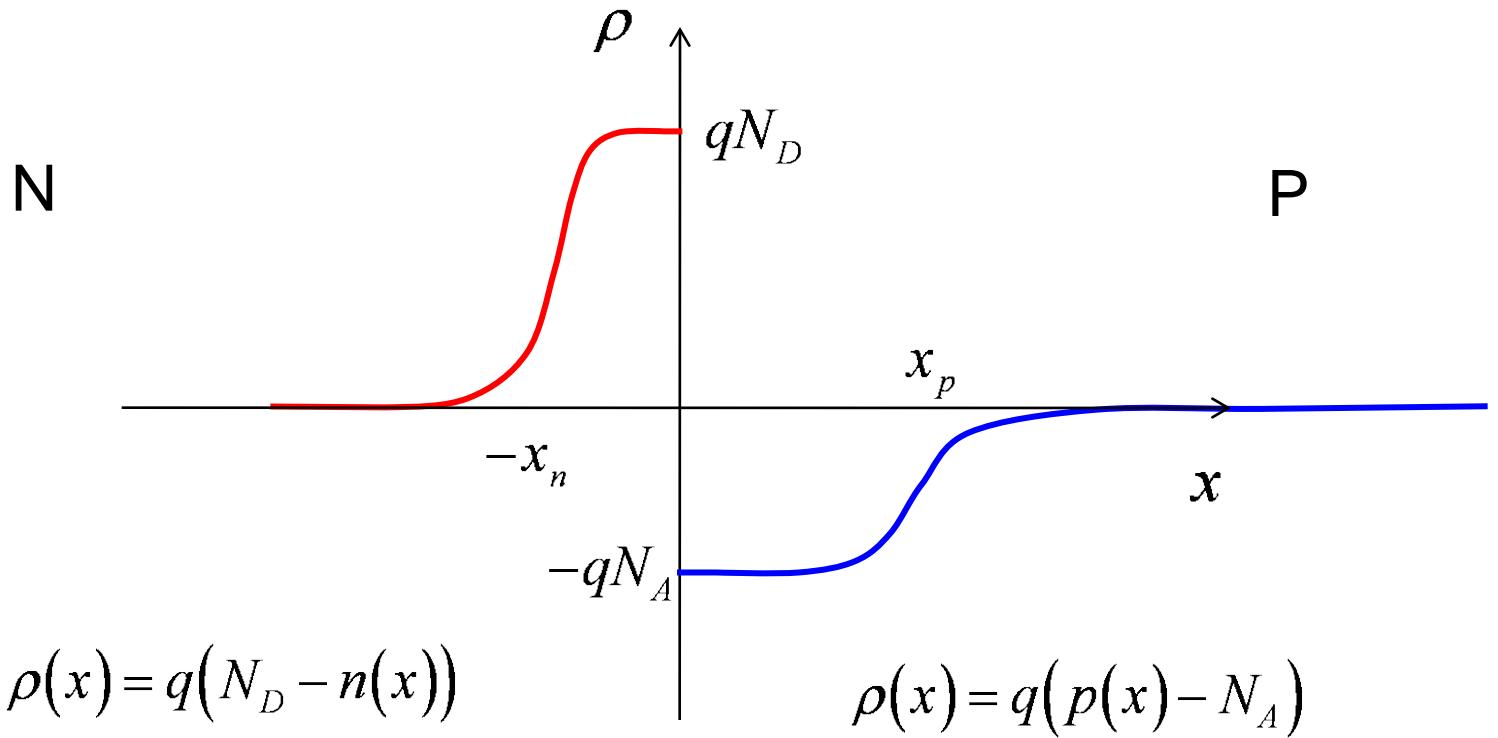


# Space charge?



# Electrostatics: rho(x)

---



# NP junction electrostatics

---

**Question:** How would we actually **calculate**  $\rho(x)$ ,  $E(x)$ ,  $V(x)$ ,  $n(x)$ , and  $p(x)$ ?

**Answer:** Solve the semiconductor equations.

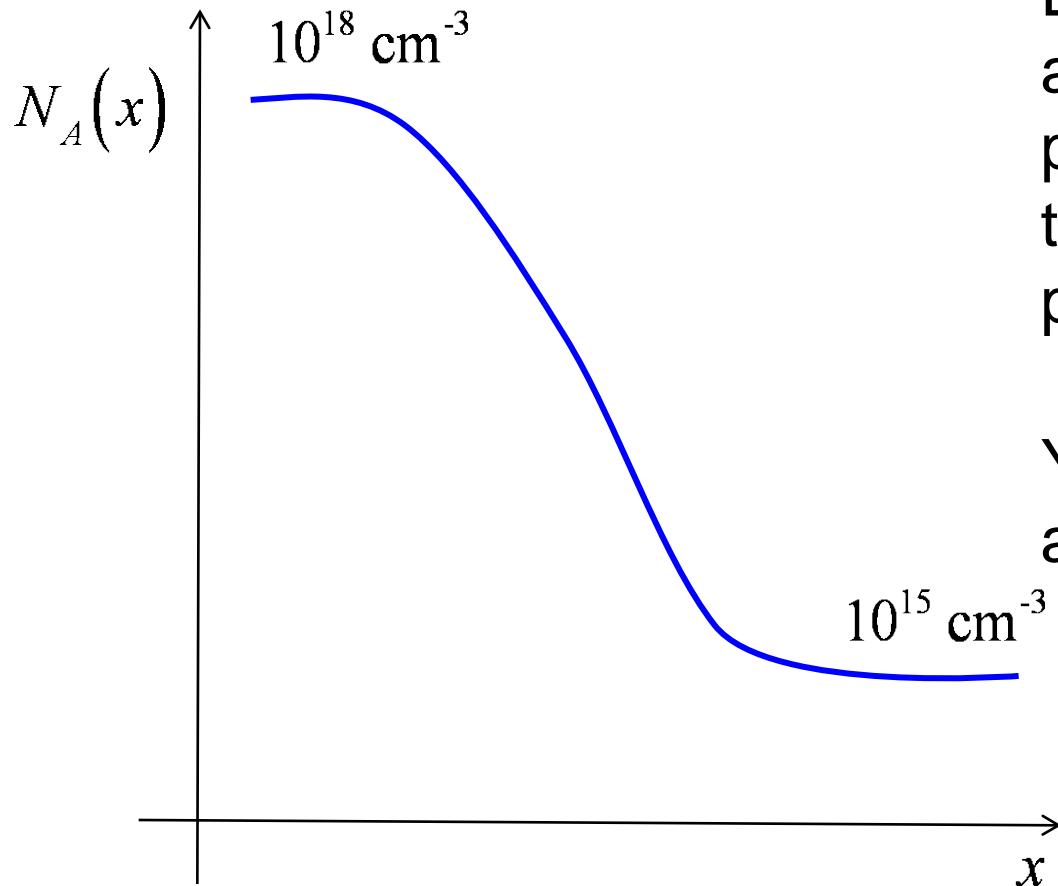
$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$

$$\frac{\partial n}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_n}{-q} \right) + G_n - R_n$$

$$\nabla \cdot (K_s \epsilon_0 \vec{E}) = \rho$$

## More practice

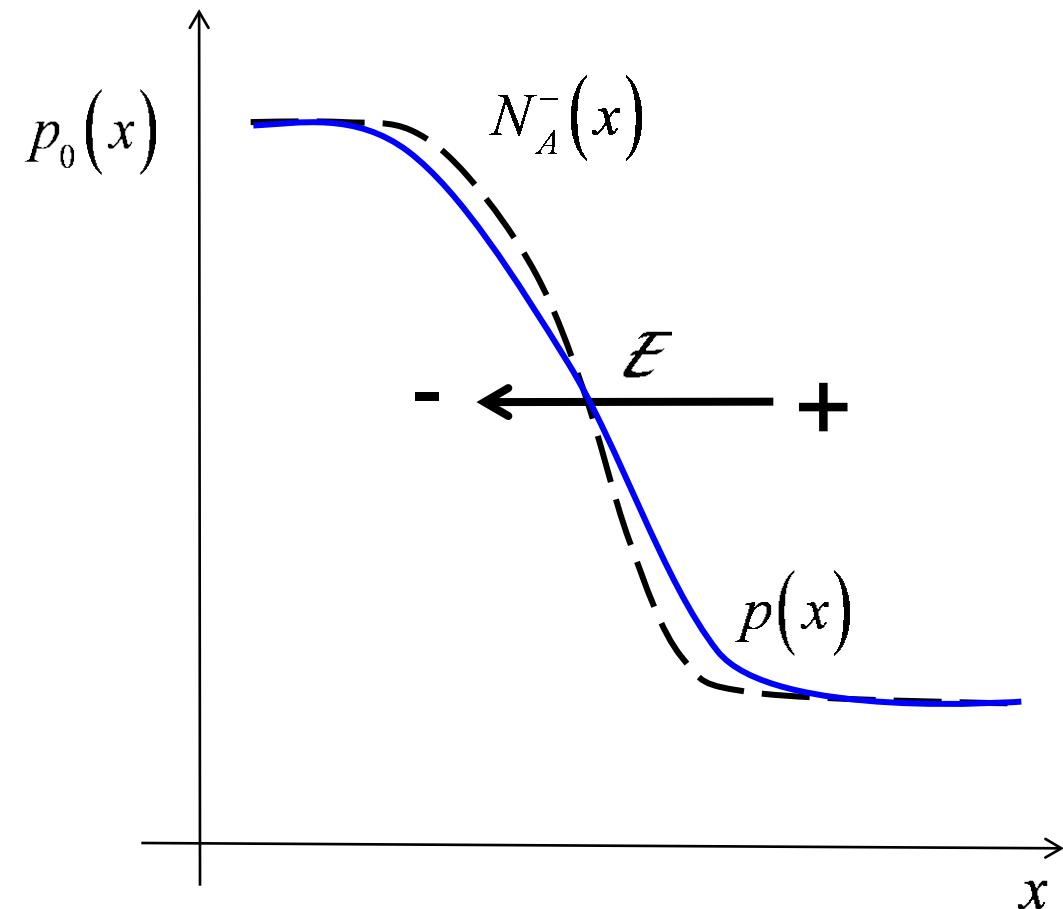
---



Draw the e-band diagram and find the electrostatic potential vs. position and the electric field vs. position.

You will find that there is an electric field.

# Where does the electric-field come from?



$$p_0(x) \approx N_A^-(x)$$

“quasi-neutral”

The result is a drift current equal and opposite to the diffusion current so that the total current is zero in equilibrium.

# Summary

---

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$

$$\frac{\partial n}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_n}{-q} \right) + G_n - R_n$$

$$\nabla \cdot (K_s \epsilon_0 \vec{\mathcal{E}}) = \rho$$

Three coupled, nonlinear PDE's in three unknowns:

$$p(\vec{r}), n(\vec{r}), V(\vec{r})$$

**Drawing and then reading an E-band diagram gives us a qualitative solution to these equations.**

## Primer on Semiconductors

# Unit 5: The Semiconductor Equations

## Lecture 5.3: Quasi-Fermi levels

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Equilibrium vs. non-equilibrium

equilibrium

$$n_0 = n_i e^{(E_F - E_i)/k_B T}$$

$$p_0 = n_i e^{(E_i - E_F)/k_B T}$$

$$n_0 p_0 = n_i^2$$

$$f_0 = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

non-equilibrium

$$n = n_i e^{(F_n - E_i)/k_B T}$$

$$p = n_i e^{(E_i - F_p)/k_B T}$$

$$np \neq n_i^2$$

$$f_c = \frac{1}{1 + e^{(E - F_n)/k_B T}}$$

$$1 - f_v = 1 - \frac{1}{1 + e^{(E - F_p)/k_B T}}$$

# The semiconductor equations

---

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$

$$\frac{\partial n}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_n}{-q} \right) + G_n - R_n$$

$$\nabla^2 V = -\rho / K_S \epsilon_0$$

Three equations in  
three unknowns:

$$p(\vec{r}), n(\vec{r}), V(\vec{r})$$

or:

$$F_p(\vec{r}), F_n(\vec{r}), V(\vec{r})$$

$$\vec{J}_p = p \mu_p \vec{\nabla} F_p$$

$$\rho = q(p - n + N_D^+ - N_A^-)$$

$$\vec{J}_n = n \mu_n \vec{\nabla} F_n$$

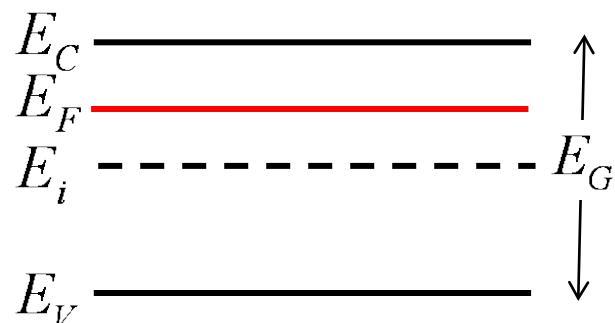
$$\vec{\mathcal{E}}(\vec{r}) = \nabla V(\vec{r})$$

# Where is the Fermi level?

---

N-type silicon in **equilibrium**

$$n_0 = N_D = 10^{17} \text{ cm}^{-3}$$



$$p_0 = \frac{n_i^2}{n_0} = 10^3 \text{ cm}^{-3}$$

$$n_0 = n_i e^{(E_F - E_i)/k_B T}$$

$$p_0 = n_i e^{(E_i - E_F)/k_B T}$$

Given either carrier density, we can determine the Fermi level

# Now where is the Fermi level?

---

Now assume that there are  $10^{14} \text{ cm}^{-3}$  **excess carriers**.

$$n \approx n_0 = 10^{17} \text{ cm}^{-3}$$

The diagram shows two horizontal lines representing energy bands. The top line is labeled  $E_C$  and the bottom line is labeled  $E_V$ . A vertical double-headed arrow between them is labeled  $E_G$ , representing the band gap.

$$p = \Delta p = 10^{14} \text{ cm}^{-3} \gg p_0$$

- a) Where it was in equilibrium
- b) Closer to the conduction band
- c) Closer to the valence band
- d) Near the middle of the band
- e) None of the above

**Same # of electrons, more holes -> need 2 Fermi levels!**

# Quasi-Fermi levels

---

$$\begin{array}{c} n = 10^{17} \text{ cm}^{-3} \\ E_C \xrightarrow{\quad\quad\quad} F_n \approx E_F \\ E_i \xrightarrow{\quad\quad\quad} F_p \\ E_V \xrightarrow{\quad\quad\quad} p = 10^{14} \text{ cm}^{-3} \end{array}$$

Non-equilibrium  
(low level injection)

$$n = n_i e^{(F_n - E_i)/k_B T} \approx n_0$$

$$F_n = E_F$$

$$p = n_i e^{(E_i - F_p)/k_B T} \gg p_0$$

$$F_p < E_F$$

# Non-equilibrium

---

$$\begin{array}{c} n = 10^{17} \text{ cm}^{-3} \\ E_C \hline F_n \approx E_F \\ E_i \hline F_p \\ E_V \hline p = 10^{14} \text{ cm}^{-3} \end{array}$$

**When the QFL's are split,  
the semiconductor is out  
of equilibrium.**

In equilibrium:  $F_n = F_p = E_F$

# NP product

---

Equilibrium

$$n_0 = n_i e^{(E_F - E_i)/k_B T}$$

$$p_0 = n_i e^{(E_i - E_F)/k_B T}$$

$$n_0 p_0 = n_i^2$$

Out of equilibrium

$$n = n_i e^{(F_n - E_i)/k_B T}$$

$$p = n_i e^{(E_i - F_p)/k_B T}$$

$$np = n_i^2 e^{(F_n - F_p)/k_B T}$$

$$F_n > F_p \rightarrow np > n_i^2$$

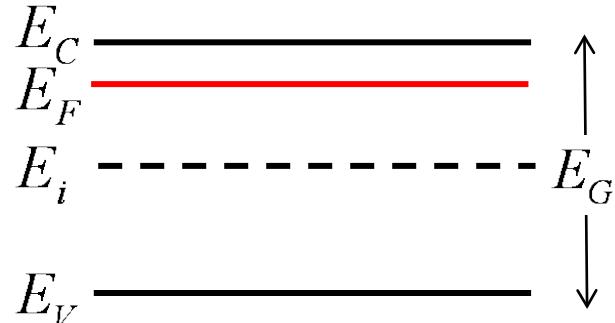
$$F_n < F_p \rightarrow np < n_i^2$$

# Some numbers (equilibrium)

---

## N-type silicon in equilibrium

$$n_0 = N_D = 10^{17} \text{ cm}^{-3}$$



$$p_0 = \frac{n_i^2}{n_0} = 10^3 \text{ cm}^{-3}$$

$$n_0 = n_i e^{(E_F - E_i)/k_B T}$$

$$p_0 = n_i e^{(E_i - E_F)/k_B T}$$

$$(E_F - E_i) = k_B T \ln\left(\frac{n}{n_i}\right)$$

$$(E_F - E_i) = 0.026 \ln\left(\frac{10^{17}}{10^{10}}\right) \text{ eV}$$

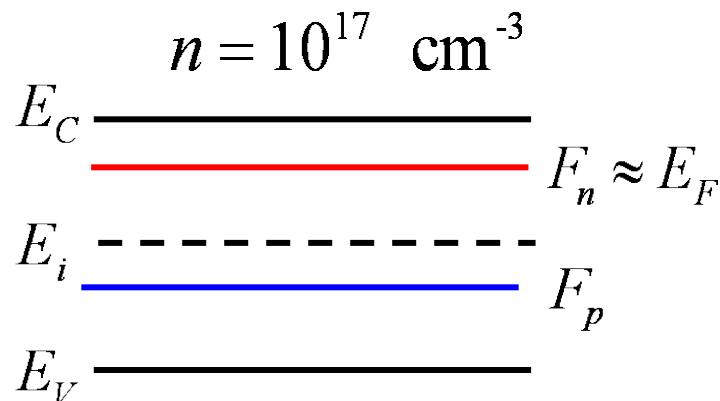
$$(E_F - E_i) = 0.42 \text{ eV}$$

# Some numbers (LL injection)

---

$$n = n_i e^{(F_n - E_i)/k_B T}$$

$$p = n_i e^{(E_i - F_p)/k_B T}$$



$$(F_n - E_i) = k_B T \ln\left(\frac{n}{n_i}\right) = 0.026 \ln(10^7)$$

$$(F_n - E_i) = 0.42 \text{ eV}$$

$$(E_i - F_p) = k_B T \ln\left(\frac{p}{n_i}\right) = 0.026 \ln(10^4)$$

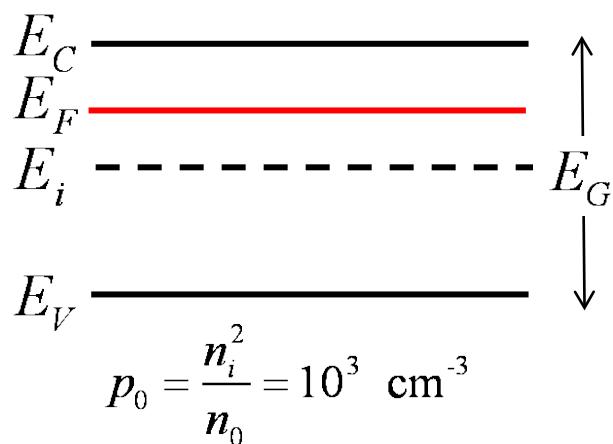
$$(E_i - F_p) = 0.24 \text{ eV}$$

# Discussion

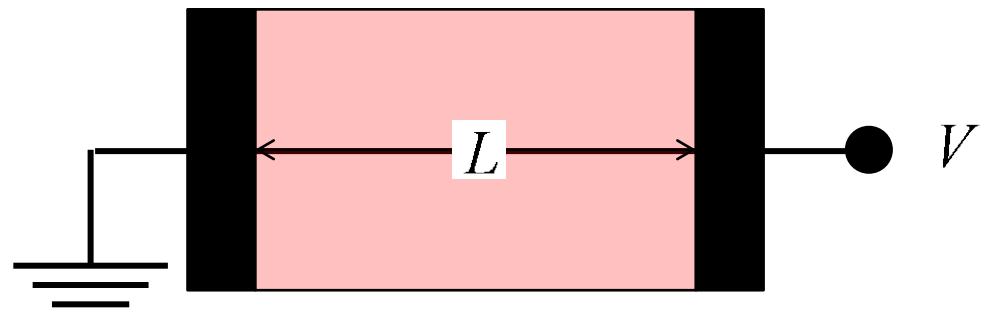
---

Note that it is possible for a semiconductor to be out of equilibrium (e.g. with current flowing), but with  $F_n = F_p$ .

$$n_0 = N_D = 10^{17} \text{ cm}^{-3}$$



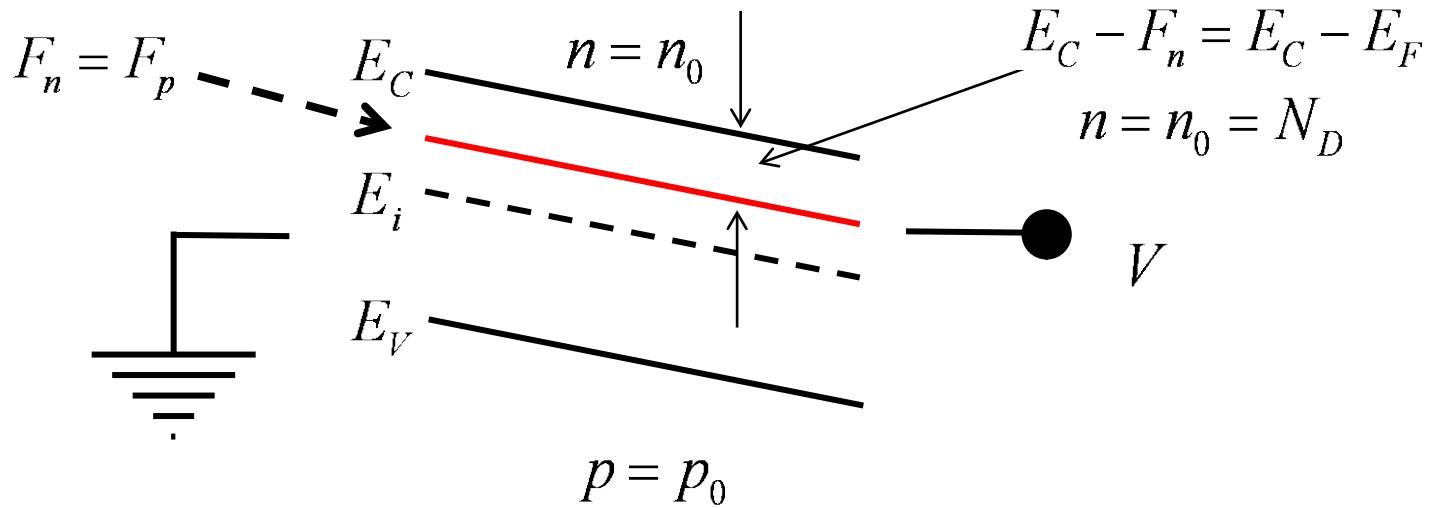
N-type semiconductor  
in equilibrium



N-type semiconductor  
resistor under bias

# E-band diagram of an N-type resistor

Note that it is possible for a semiconductor to be out of equilibrium (e.g. with current flowing), but with  $F_n = F_p$ .



No excess carriers,  $np = n_i^2$   
but current is flowing.

# Assumptions

---

What assumption is involved in replacing the equilibrium Fermi level with two quasi-Fermi levels out of equilibrium?

In equilibrium, the probability that a state is occupied is given by:

$$f_0(E) = \frac{1}{1 + e^{(E-E_F)/k_B T}}$$

We assume that the **same function** describes the occupation of states in the conduction and valence bands if we simply replace the Fermi level by the appropriate QFL:

$$f_C(E) = \frac{1}{1 + e^{(E-F_n)/k_B T}}$$

$$1 - f_V(E) = 1 - \frac{1}{1 + e^{(E-F_p)/k_B T}}$$

# Summary

---

Equilibrium:

$$E_F$$

$$f_0(E) = \frac{1}{1 + e^{(E-E_F)/k_B T}}$$

Out of Equilibrium:

$$F_n$$

$$f_C(E) = \frac{1}{1 + e^{(E-F_n)/k_B T}}$$

$$F_p$$

$$1 - f_V(E) = 1 - \frac{1}{1 + e^{(E-F_p)/k_B T}}$$

This assumption can be expected to work if we are “close enough” to equilibrium.

## Primer on Semiconductors

# Unit 5: The Semiconductor Equations

## Lecture 5.4: Minority carrier diffusion equation

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# Semiconductor equations

---

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$

$$\frac{\partial n}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_n}{-q} \right) + G_n - R_n$$

$$\nabla \cdot (K_s \epsilon_0 \vec{\mathcal{E}}) = \rho$$

Although not as fundamental as Maxwell's equations, these equations are the starting point for the analysis of most semiconductor devices.

# Solving the semiconductor equations

---

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$

$$\frac{\partial n}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_n}{-q} \right) + G_n - R_n$$

$$\nabla \cdot (K_s \epsilon_0 \vec{\mathcal{E}}) = \rho$$

- 1) Direct, numerical solutions
- 2) Qualitative solutions with energy band diagrams
- 3) Simplify the equations, then solve analytically

# Outline of the lecture

---

Analyzing semiconductor problems involving minority carriers usually comes down to solving the **minority carrier diffusion equation** (MCDE), a simplification of the semiconductor equations.

Minority carrier devices include solar cells, bipolar transistors, and light-emitting diodes.

In this lecture, I will discuss several examples, which illustrate solving the MCDE for several common situations.

# Minority carrier diffusion equation

---

$$n = n_0 = N_D$$

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$

(N-type semiconductor in low level injection)

(hole continuity equation)

$$\frac{\partial p}{\partial t} = -\frac{d}{dx} \left( \frac{J_{px}}{q} \right) + G_L - R_p$$

(1D, generation by light)

$$\frac{\partial \Delta p}{\partial t} = -\frac{d}{dx} \left( \frac{-qD_p d\Delta p / dx}{q} \right) + G_L - \frac{\Delta p}{\tau_p}$$

(low-level injection,  $\Delta p \gg p_0$ , no electric field)

$$\frac{\partial \Delta p}{\partial t} = D_p \frac{d^2 \Delta p}{dx^2} - \frac{\Delta p}{\tau_p} + G_L$$

( $D_p$  spatially uniform)

# Minority carrier diffusion equation

---

$$\frac{\partial \Delta p(x,t)}{\partial t} = D_p \frac{d^2 \Delta p(x,t)}{dx^2} - \frac{\Delta p(x,t)}{\tau_p} + G_L$$

To use the MCDE to solve a problem, **first check** to be sure that the simplifying assumptions needed to derive the MCDE from the continuity equation apply.

**Then simplify** the MCDE (if possible), **specify the initial condition** (if necessary) and the **two boundary conditions** (if necessary).

# Reminder: Low level injection

---

N-type semiconductor:

$$n(x,t) \approx n_0 = N_D$$

$$p(x,t) \approx \Delta p(x,t) \gg p_0 = n_i^2/n_0$$

$$\frac{\partial \Delta p(x,t)}{\partial t} = D_p \frac{d^2 \Delta p(x,t)}{dx^2} - \frac{\Delta p(x,t)}{\tau_p} + G_L$$

P-type semiconductor:

$$p(x,t) \approx p_0 = N_A$$

$$n(x,t) \approx \Delta n(x,t) \gg n_0 = n_i^2/p_0$$

$$\frac{\partial \Delta n(x,t)}{\partial t} = D_n \frac{d^2 \Delta n(x,t)}{dx^2} - \frac{\Delta n(x,t)}{\tau_n} + G_L$$

# Example: MCDE for electrons in Si

---

P-type Si at  $T = 300$  K

$$N_A = 10^{17} \text{ cm}^{-3} = p_0$$

$$\mu_n = 300 \text{ cm}^2/\text{V-s}$$

$$D_n = \left( \frac{k_B T}{q} \right) \mu_n = 7.8 \text{ cm}^2/\text{s}$$

$$\tau_n = 10^{-6} \text{ s}$$

$$L_n = \sqrt{D_n \tau_n} = 28 \text{ } \mu\text{m}$$

MCDE for electrons

$$\frac{\partial \Delta n(x,t)}{\partial t} = D_n \frac{d^2 \Delta n(x,t)}{dx^2} - \frac{\Delta n(x,t)}{\tau_n} + G_L$$

“diffusion length”

# Example 1: Steady-state, uniform illumination

---

Steady-state, uniform generation (no spatial variation)

$$G_L = 10^{20} \text{ cm}^{-3}\text{s}^{-1}$$

Solve for  $\Delta n$  and for the QFL's.

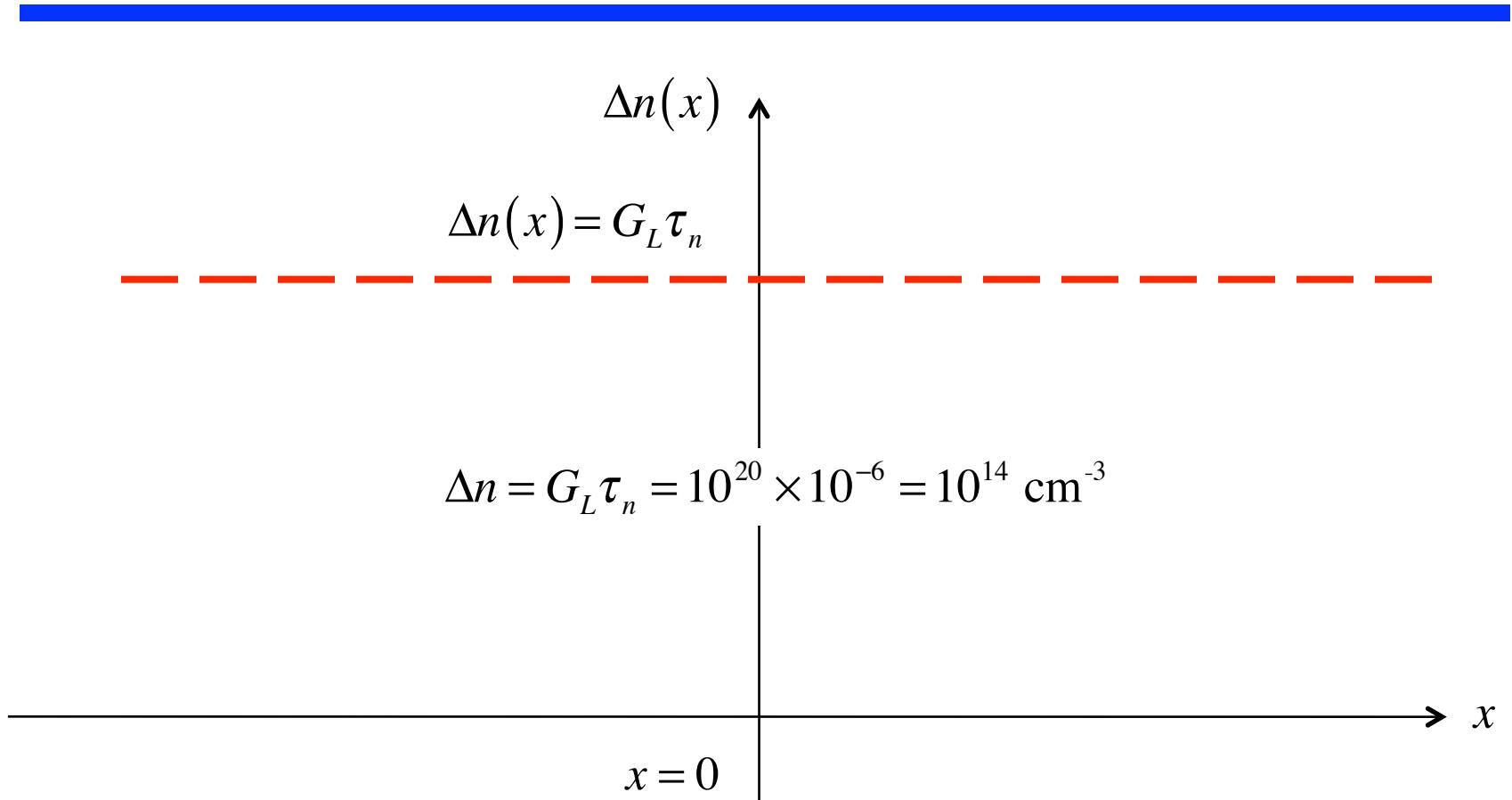
- 1) Simplify the MCDE
- 2) Solve the MCDE for  $\Delta n$
- 3) Deduce  $F_n$  from  $\Delta n$

$$\frac{\partial \Delta n}{\partial t} = D_n \frac{d^2 \Delta n}{dx^2} - \frac{\Delta n}{\tau_n} + G_L$$

$$0 = 0 - \frac{\Delta n}{\tau_n} + G_L$$

$$\boxed{\Delta n = G_L \tau_n}$$

# Example 1: Solution



Steady-state, uniform generation, no spatial variation

# Example 1: Equilibrium Fermi level

---

P-type / equilibrium

$$n_0 = \frac{n_i^2}{p_0} = 10^3 \text{ cm}^{-3}$$

$$E_C \text{ ——————}$$

$$\begin{array}{c} E_i \\ \text{--- --- --- --- ---} \\ E_V \text{ ——————} \quad E_F \end{array}$$

$$p_0 = 10^{17} \text{ cm}^{-3}$$

$$p_0 = n_i e^{(E_i - E_F)/k_B T}$$

$$10^{17} = 10^{10} e^{(E_i - E_F)/k_B T}$$

$$E_F = E_i - 0.41 \text{ eV}$$

# Example 1: Quasi-Fermi levels

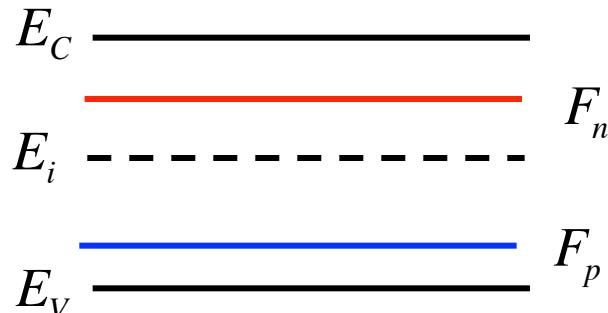
---

P-type / low-level injection

$$F_p = E_i - 0.41 \text{ eV}$$

$$\Delta n = 10^{14} \text{ cm}^{-3} \gg n_0$$

$$n \approx \Delta n = n_i e^{(F_n - E_i)/k_B T}$$



$$10^{14} = 10^{10} e^{(F_n - E_i)/k_B T}$$

$$F_n = E_i + 0.24 \text{ eV}$$

$$p_0 = 10^{17} \text{ cm}^{-3}$$

Steady-state, uniform generation, no spatial variation

## Example 2: Transient decay to equilibrium

---

Now turn off the light.

Transient, no generation, no spatial variation

Solve for  $\Delta n(t)$  and for the QFL's.

- 1) Simplify the MCDE
- 2) Solve the MCDE for  $\Delta n$
- 3) Deduce  $F_n$  from  $\Delta n$

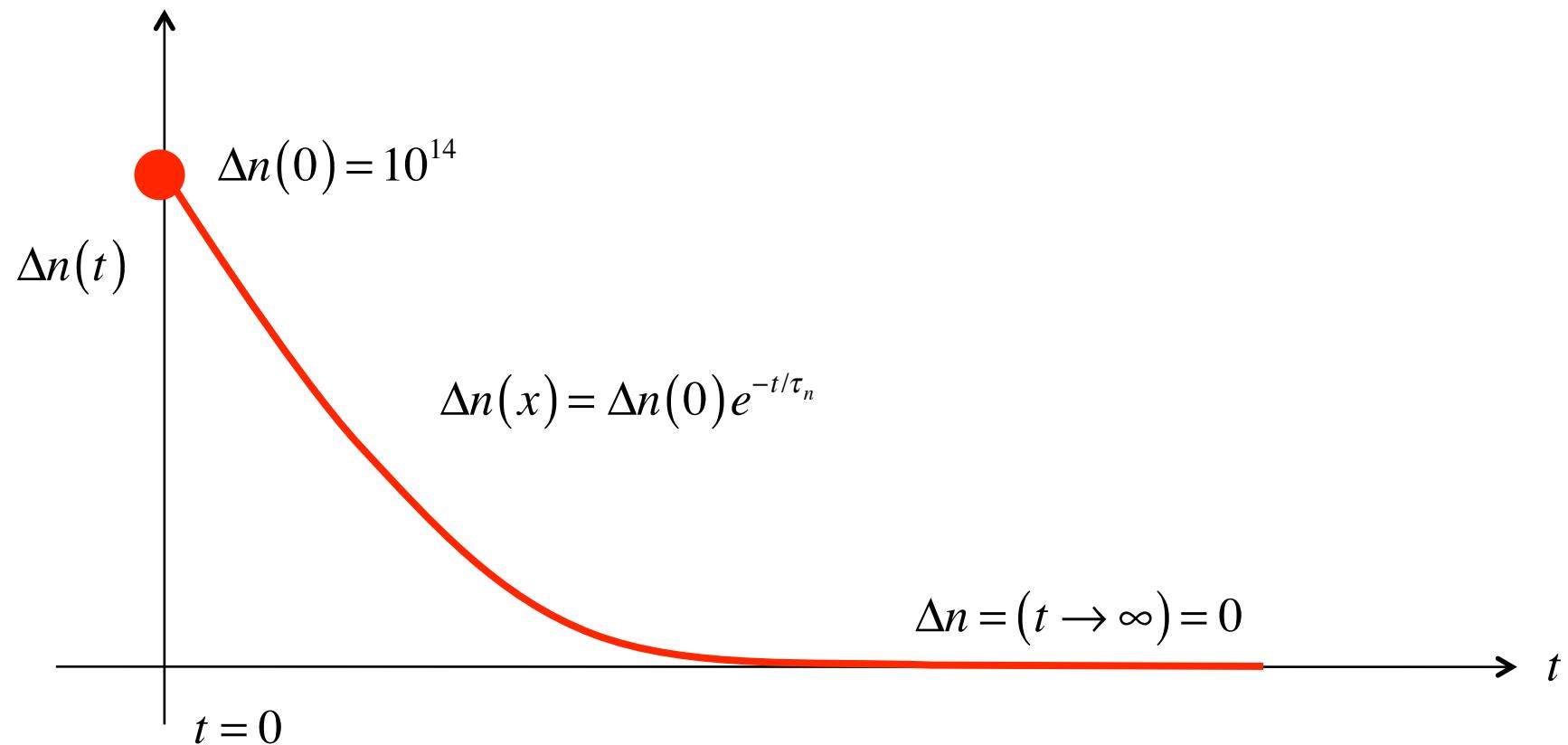
$$\frac{\partial \Delta n(x,t)}{\partial t} = D_n \frac{d^2 \Delta n(x,t)}{dx^2} - \frac{\Delta n(x,t)}{\tau_n} + G_L$$

$$\frac{\partial \Delta n}{\partial t} = 0 - \frac{\Delta n}{\tau_n} + 0$$

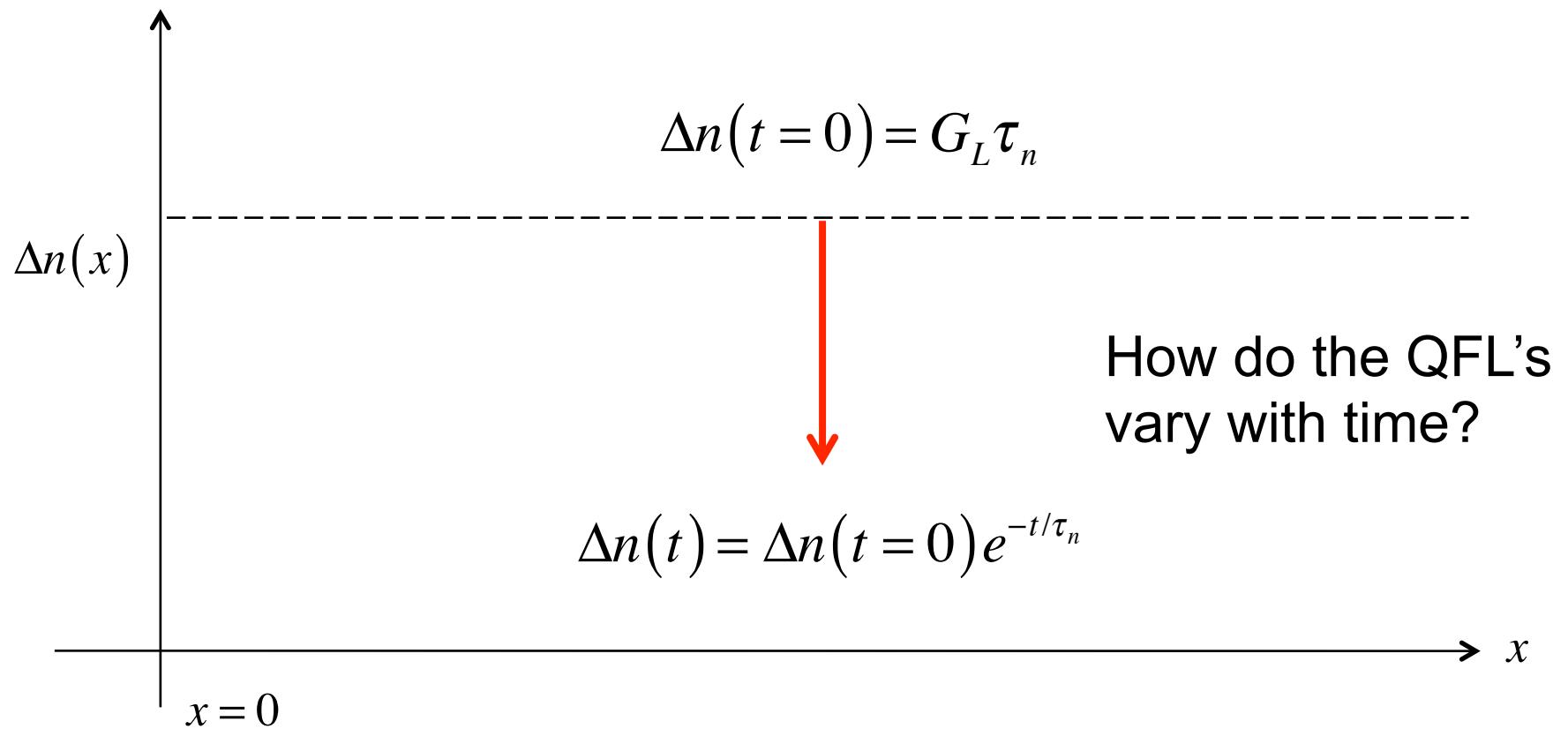
$$\frac{\partial \Delta n}{\partial t} = - \frac{\Delta n}{\tau_p}$$

$$\Delta n(t) = \Delta n(0) e^{-t/\tau_n} = 10^{14} e^{-t/\tau_n}$$

## Example 2: Solution



## Example 2: Solution



transient, no generation, no spatial variation

## Example 2: Solution

---

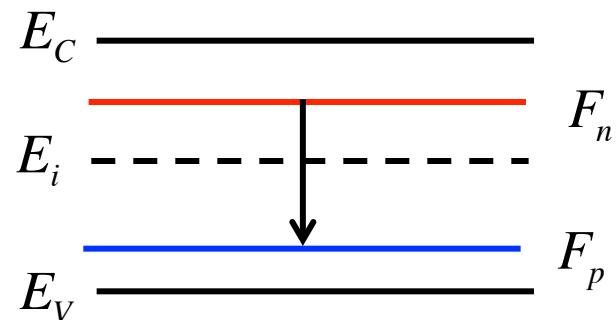
$$F_p = E_i - 0.41 \text{ eV}$$

$$n(t) \approx \Delta n(t) = n_i e^{(F_n(t) - E_i)/k_B T}$$

$$10^{14} e^{-t/\tau_n} = 10^{10} e^{(F_n(t) - E_i)/k_B T}$$

$$F_n(t) = E_i + k_B T \ln(10^4) - k_B T \frac{t}{\tau_n}$$

$$F_n(t) = F_n(t=0) - k_B T \frac{t}{\tau_n}$$



For long times,  $F_n$  should approach the equilibrium Fermi level.  
Explain what is wrong with our answer in the long time limit.

## Example 3: SS diffusion in a long sample

---

Steady-state, sample is long ( 200 micrometers) compared to the diffusion length. No generation.

$$\begin{aligned}\Delta n(x=0) &= 10^{12} \text{ cm}^{-3} && \text{fixed} \\ \Delta n(x=L) &= 0 \text{ cm}^{-3}\end{aligned}$$

$$\frac{\partial \Delta n}{\partial t} = D_p \frac{d^2 \Delta n}{dx^2} - \frac{\Delta n}{\tau_n} + G_L$$

$$0 = D_p \frac{d^2 \Delta n}{dx^2} - \frac{\Delta n}{\tau_n} + 0$$

Solve for  $\Delta n$  and for the QFL's.

- 1) Simplify the MCDE
- 2) Solve the MCDE for  $\Delta n$
- 3) Deduce  $F_n$  from  $\Delta n$

$$\frac{d^2 \Delta n}{dx^2} - \frac{\Delta n}{D_p \tau_n} = 0$$

$$\frac{d^2 \Delta n}{dx^2} - \frac{\Delta n}{L_n^2} = 0 \quad L_n \equiv \sqrt{D_n \tau_n}$$

## Example 3: Continued

---

Steady-state, sample **long** compared to the diffusion length.  
No generation.

$$\Delta n(x=0) = 10^{12} \text{ cm}^{-3}$$

fixed

$$\Delta n(x=L) = 0 \text{ cm}^{-3}$$

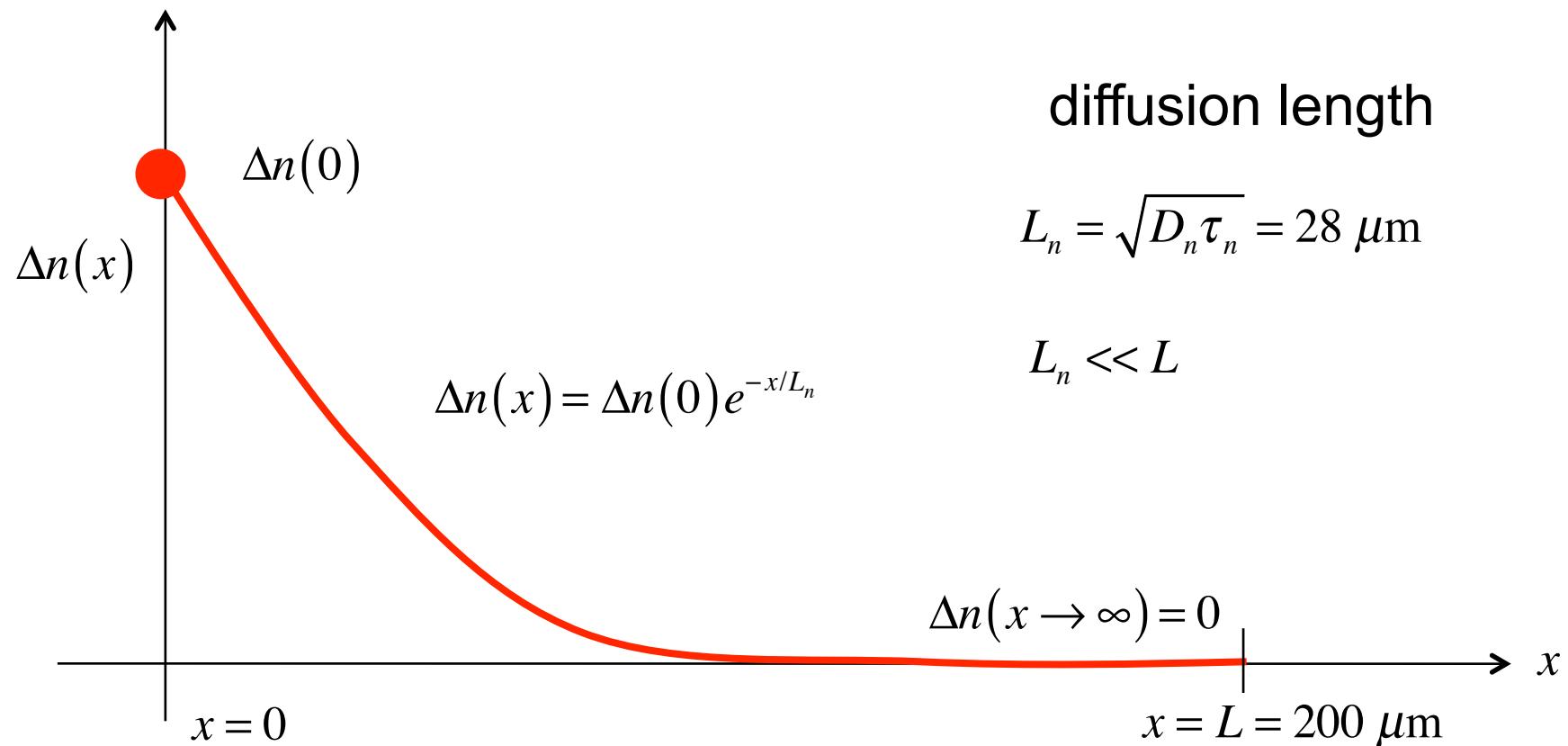
$$\frac{d^2 \Delta n(x)}{dx^2} - \frac{\Delta n(x)}{L_n^2} = 0 \quad L_n \equiv \sqrt{D_n \tau_n}$$

$$\Delta n(x) = A e^{-x/L_n} + B e^{+x/L_n}$$

$$\Delta n(x) = A e^{-x/L_n}$$

$$\Delta n(x) = \Delta n(0) e^{-x/L_n} = 10^{12} e^{-x/L_n}$$

## Example 3: Solution



Steady-state, sample **long** compared to the diffusion length.

## Example 3: Suggested exercise

---

Draw the energy band diagram with the QFL's. Is there an electron current?

## Example 4: SS diffusion in a **short** sample

---

Steady-state, sample is **5 micrometers long**. No generation.

$$\Delta n(x=0) = 10^{12} \text{ cm}^{-3}$$

fixed

$$\Delta n(x = 5 \mu\text{m}) = 0$$

$$\frac{\partial \Delta n}{\partial t} = D_p \frac{d^2 \Delta n}{dx^2} - \frac{\Delta n}{\tau_n} + G_L$$

$$\frac{d^2 \Delta n}{dx^2} - \frac{\Delta n}{L_n^2} = 0 \quad L_n \equiv \sqrt{D_n \tau_n}$$

- 1) Simplify the MCDE
- 2) Solve the MCDE for  $\Delta n$
- 3) Deduce  $F_n$  from  $\Delta n$

$$L_n = 28 \mu\text{m} \gg L = 5 \mu\text{m}$$

$$\frac{d^2 \Delta n}{dx^2} = 0$$

## Example 4: Continued

---

Steady-state, sample is **5 micrometers long**. No generation.

$$\Delta n(x=0) = 10^{12} \text{ cm}^{-3} \quad \text{fixed}$$

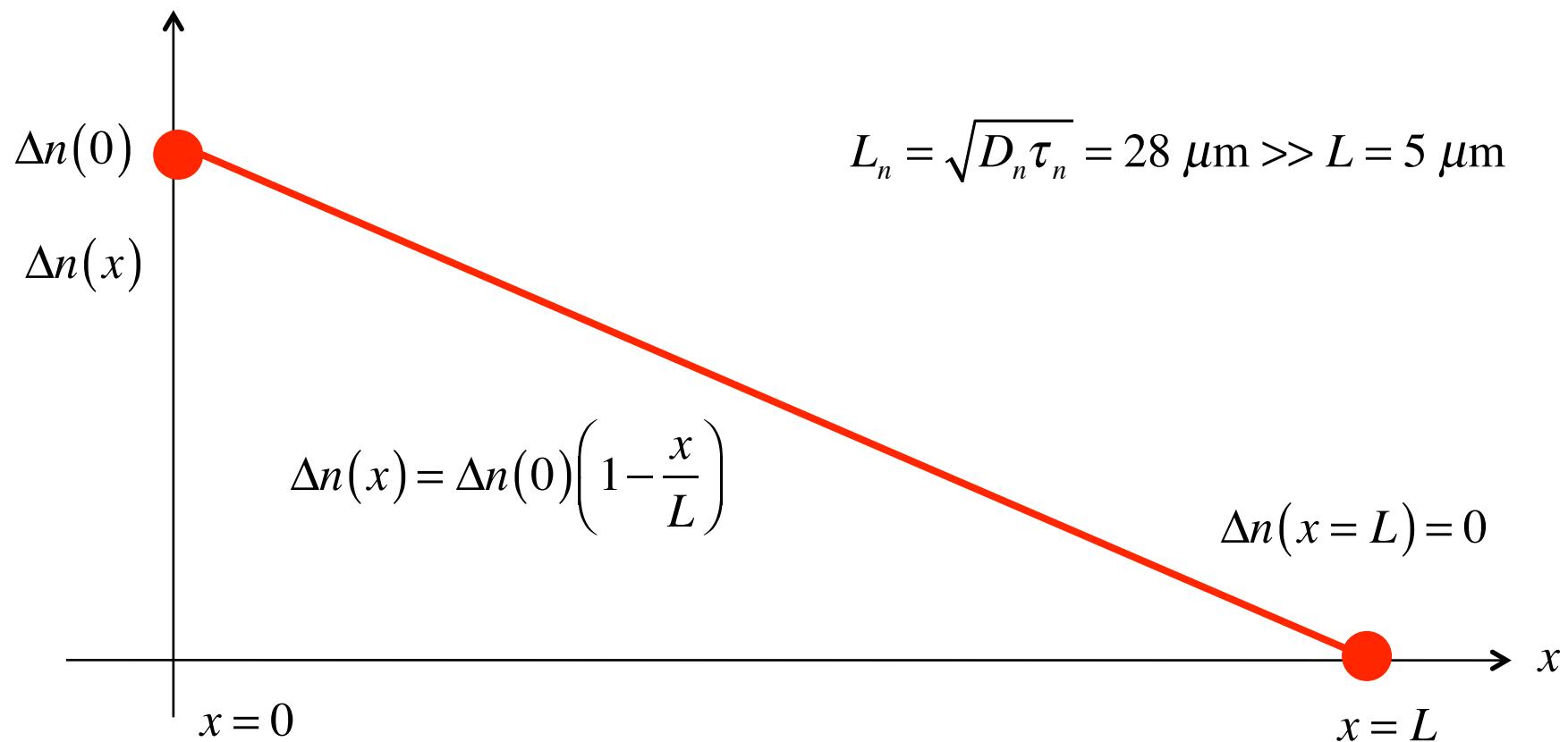
$$\frac{d^2 \Delta n(x)}{dx^2} = 0$$

$$\Delta n(x=5 \mu\text{m}) = 0$$

$$\Delta n(x) = Ax + B$$

$$\boxed{\Delta n(x) = \Delta n(0) \left( 1 - \frac{x}{L} \right)}$$

## Example 4: Solution



Steady-state, sample **short** compared to the diffusion length.

## Example 5

---

Steady-state, sample is **30 micrometers long**. No generation.

$$\Delta n(x=0) = 10^{12} \text{ cm}^{-3}$$

fixed

$$\Delta n(x=30 \mu\text{m}) = 0$$

$$\frac{\partial \Delta n}{\partial t} = D_p \frac{d^2 \Delta n}{dx^2} - \frac{\Delta n}{\tau_n} + G_L$$

$$0 = D_p \frac{d^2 \Delta n}{dx^2} - \frac{\Delta n}{\tau_n} + 0$$

- 1) Simplify the MCDE
- 2) Solve the MCDE from  $\Delta n$
- 3) Deduce  $F_n$  from  $\Delta n$

$$\frac{d^2 \Delta n}{dx^2} - \frac{\Delta n}{L_n^2} = 0 \quad L_n \equiv \sqrt{D_n \tau_n}$$

$$L_n = 28 \mu\text{m} \quad L = 30 \mu\text{m}$$

## Example 5: Solution

---

Steady-state, sample is **30 micrometers long**. No generation.

$$\Delta n(x = 0) = 10^{12} \text{ cm}^{-3} \text{ fixed}$$

$$\frac{d^2 \Delta n}{dx^2} - \frac{\Delta n}{L_n^2} = 0$$

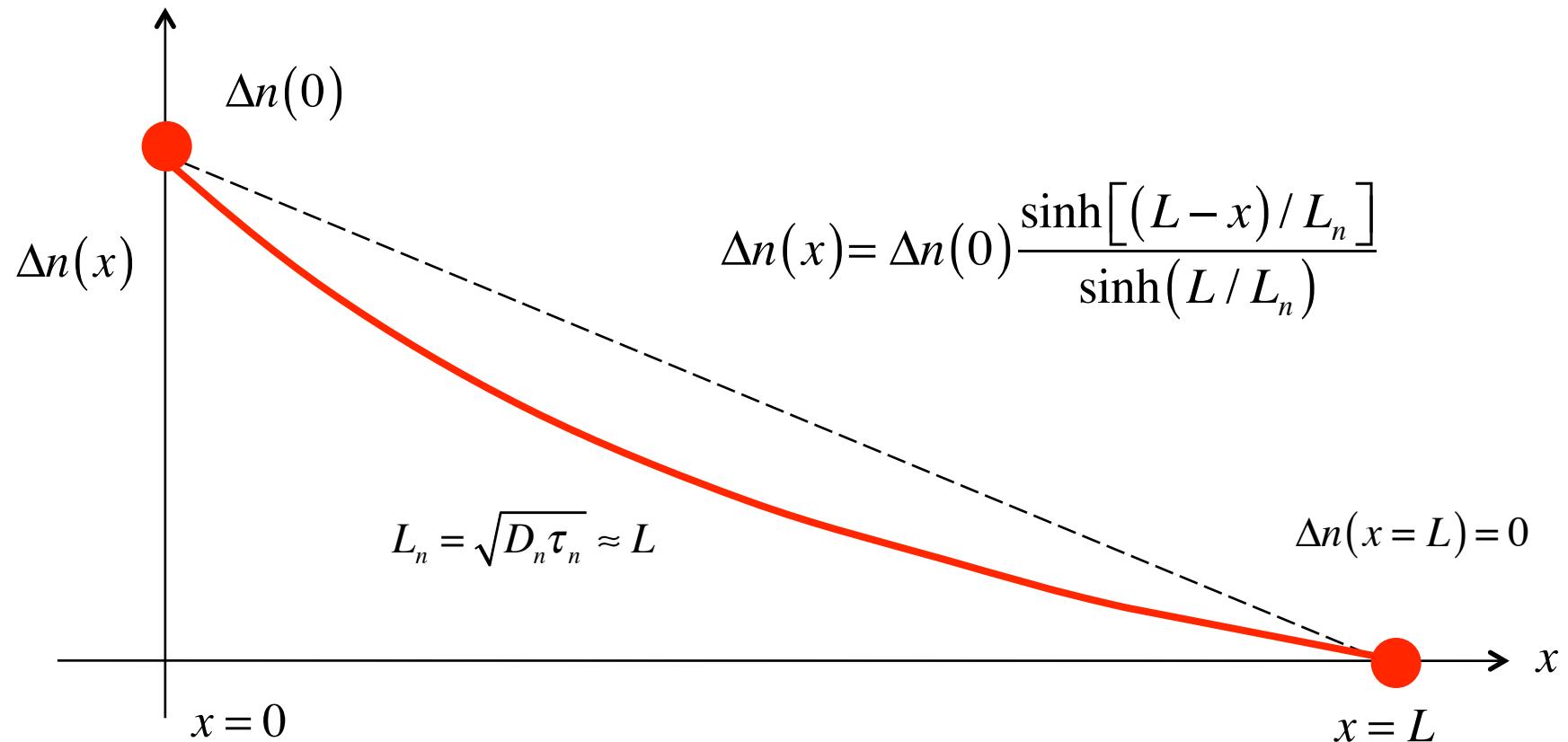
$$\Delta n(x = 30 \mu\text{m}) = 0$$

$$\Delta n(x) = A e^{-x/L_n} + B e^{+x/L_n}$$

$$\Delta n(0) = A + B = 10^{12}$$

$$\Delta n(L) = A e^{-L/L_n} + B e^{+L/L_n} = 0$$

## Example 5: Solution



Steady-state, sample **neither long nor short** compared to the diffusion length.

## Example 6:

---

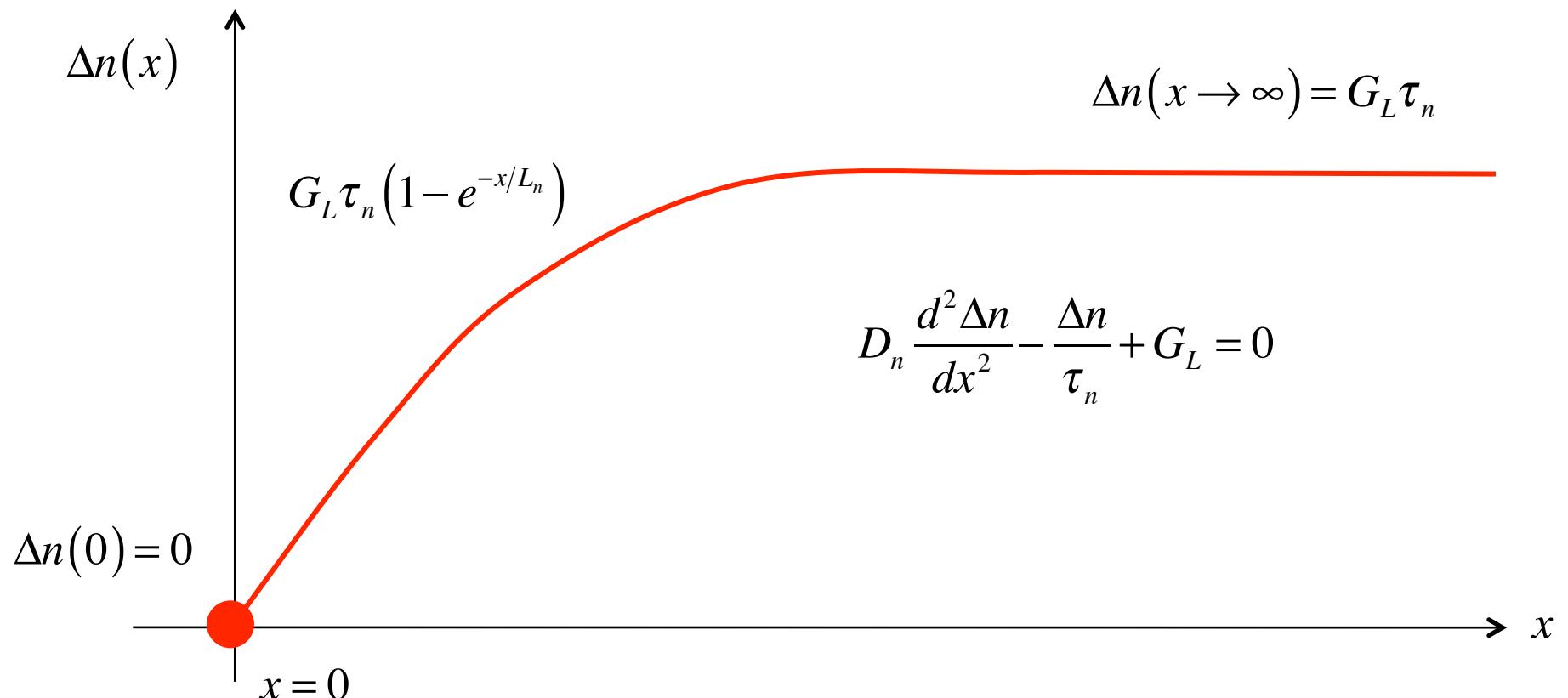
An infinitely long sample is uniformly illuminated with light for a long time. The optical generation rate  $G_L = 1 \times 10^{20} \text{ cm}^{-3} \text{ sec}^{-1}$ . The minority carrier lifetime is 1 microsecond. The surface at  $x = 0$  is highly defective, with a high density of R-G centers, so that  $\Delta n(0) = 0$ .

Find the s.s. excess minority carrier concentration vs. position.

$$D_n \frac{d^2 \Delta n}{dx^2} - \frac{\Delta n}{\tau_n} + G_L = 0$$

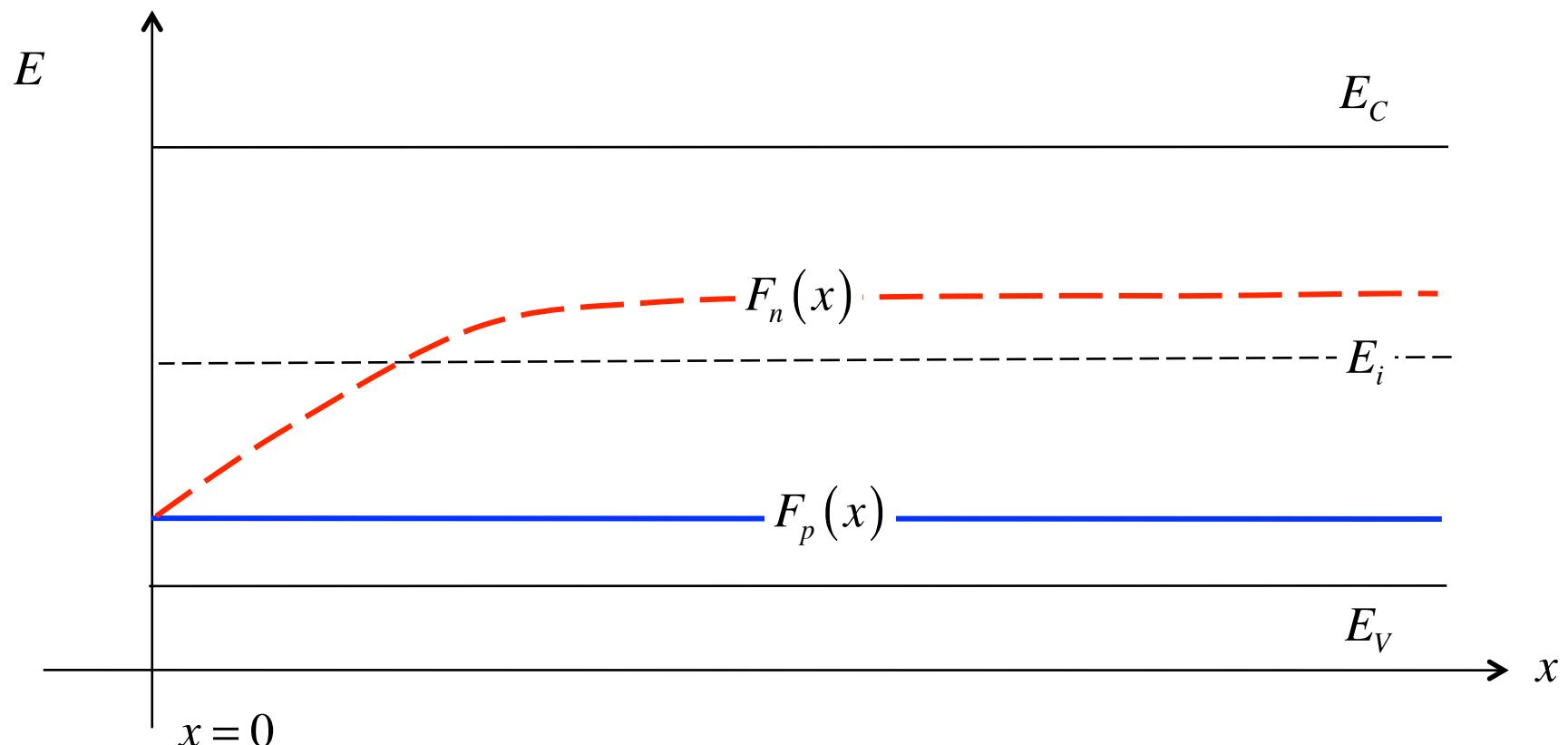
**Can we guess the solution?**

## Example 6: Solution



What does the energy band diagram look like?

## Example 6: Energy band diagram



What does a gradient in the QFL mean?

# Summary (i)

---

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$

$$\frac{\partial n}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_n}{-q} \right) + G_n - R_n$$

$$\nabla \cdot (K_s \epsilon_0 \vec{\mathcal{E}}) = \rho$$

$$\frac{\partial \Delta p(x,t)}{\partial t} = D_p \frac{d^2 \Delta p(x,t)}{dx^2} - \frac{\Delta p(x,t)}{\tau_p} + G_L$$

$$\frac{\partial \Delta n(x,t)}{\partial t} = D_n \frac{d^2 \Delta n(x,t)}{dx^2} - \frac{\Delta n(x,t)}{\tau_n} + G_L$$

LL injection in an N-type material  
(no electric field)

LL injection in a P-type material  
(no electric field)

## Summary (ii)

---

$$\frac{\partial \Delta p(x,t)}{\partial t} = D_p \frac{d^2 \Delta p(x,t)}{dx^2} - \frac{\Delta p(x,t)}{\tau_p} + G_L \quad \frac{\partial \Delta n(x,t)}{\partial t} = D_n \frac{d^2 \Delta n(x,t)}{dx^2} - \frac{\Delta n(x,t)}{\tau_n} + G_L$$

General features of the solutions:

Transient solutions goes as  $\exp[-t/\tau_n]$

For long regions, steady-state spatial solutions go as  $\exp[-x/L_n]$  in a long region

For short regions, steady-state solutions are linear.

## Primer on Semiconductors

# Unit 5: The Semiconductor Equations

## Lecture 5.5: Unit 5 Recap

**Mark Lundstrom**

lundstro@purdue.edu  
Electrical and Computer Engineering  
Purdue University  
West Lafayette, Indiana USA

# The unknowns

---

3 unknowns

$$p(\vec{r}), n(\vec{r}), V(\vec{r})$$

or

$$F_p(\vec{r}), F_n(\vec{r}), V(\vec{r})$$

We need to formulate 3 equations in 3 unknowns.

# Continuity equation

---

$$\frac{\partial p}{\partial t} = -\nabla \cdot \frac{\vec{J}_p}{q} + G_p - R_p$$

$$\vec{J}_p = pq\mu_p \vec{\mathcal{E}} - qD_p \vec{\nabla} p$$

optical generation  
or impact ionization

Radiative,  
Auger, or defect-  
assisted

**Need an equation for the electric field**

# Electrostatics

---

$$\oint \vec{D} \cdot d\vec{S} = Q$$

Gauss's Law

$$\nabla \cdot \vec{D} = \rho(x)$$

Poisson equation

$$\vec{D} = K_s \epsilon_0 \vec{\mathcal{E}}$$

$$\nabla \cdot (K_s \epsilon_0 \vec{\mathcal{E}}) = \rho(r)$$

$$\rho(r) = q [ p(r) - n(r) + N_D^+(r) - N_A^-(r) ]$$

# The “semiconductor equations”

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$

$$\frac{\partial n}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_n}{-q} \right) + G_n - R_n$$

$$\nabla \cdot (K_s \epsilon_0 \vec{\mathcal{E}}) = \rho$$

Three equations in three unknowns:

$$p(\vec{r}), n(\vec{r}), V(\vec{r})$$

or

$$F_p(\vec{r}), F_n(\vec{r}), V(\vec{r})$$

$$\vec{J}_p = pq\mu_p \vec{\mathcal{E}} - qD_p \vec{\nabla} p = p\mu_p \vec{\nabla} F_p$$

$$\rho = q(p - n + N_D^+ - N_A^-)$$

$$\vec{J}_n = nq\mu_n \vec{\mathcal{E}} + qD_n \vec{\nabla} n = n\mu_n \vec{\nabla} F_n$$

$$\vec{\mathcal{E}}(\vec{r}) = \nabla V(\vec{r})$$

# Energy band diagrams

---

An energy band diagram is a plot of the bottom of the conduction band and the top of the valence band vs. position.

An energy band diagram is a powerful tool for understanding semiconductor devices because they provide **qualitative solutions to the semiconductor equations**.

# An important principle

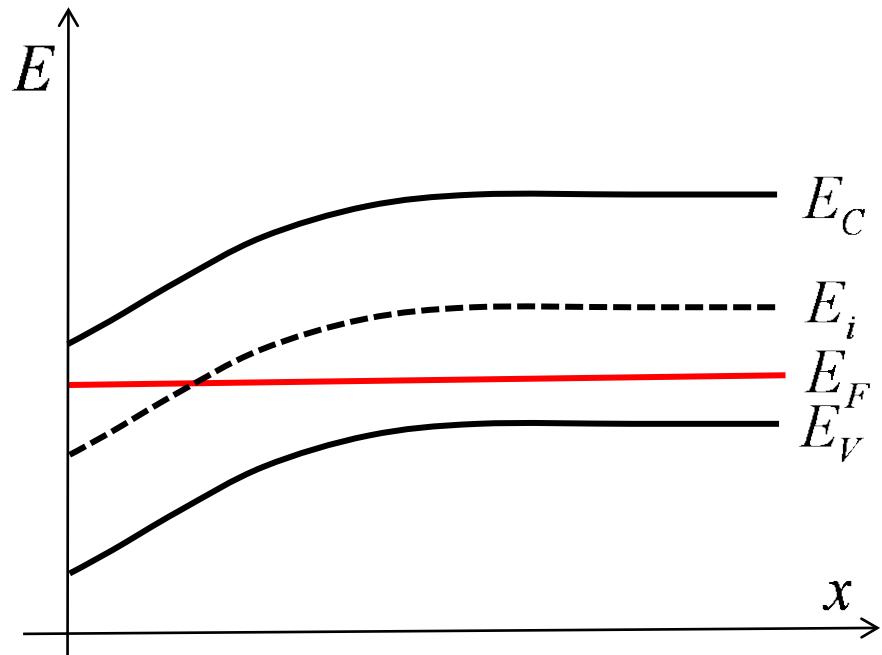
---

The Fermi level is constant in equilibrium.

The starting point for drawing energy band diagrams.

# Band diagrams

Drawing the band diagram



Reading the band diagram

$$V(x) \propto -E_C(x)$$

$$\mathcal{E} \propto dE_C(x)/dx$$

$$\log n(x) \propto E_F - E_i(x)$$

$$\log p(x) \propto E_i(x) - E_F$$

$$\rho(x) \propto d^2E_C/dx^2$$

# Drawing equilibrium band diagrams

---



- 1) Begin with  $E_F$
- 2) Draw the E-bands where you know the carrier density
- 3) Then add the rest

# Equilibrium vs. non-equilibrium

equilibrium

$$n_0 = n_i e^{(E_F - E_i)/k_B T}$$

$$p_0 = n_i e^{(E_i - E_F)/k_B T}$$

$$n_0 p_0 = n_i^2$$

$$f_0 = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

non-equilibrium

$$n = n_i e^{(F_n - E_i)/k_B T}$$

$$p = n_i e^{(E_i - F_p)/k_B T}$$

$$np = n_i^2 e^{(F_n - F_p)/k_B T}$$

$$f_c = \frac{1}{1 + e^{(E - F_n)/k_B T}}$$

$$1 - f_v = 1 - \frac{1}{1 + e^{(E - F_p)/k_B T}}$$

# Solving the semiconductor equations

---

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$

$$\frac{\partial n}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_n}{-q} \right) + G_n - R_n$$

$$\nabla \cdot (K_s \epsilon_0 \vec{\mathcal{E}}) = \rho$$

For problems that focus on minority carriers in low-level injections, these equations can be simplified, so that we only need to solve the minority carrier diffusion equation (MCDE).

# Example: Minority hole diffusion equation

---

$$n = n_0 = N_D$$

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$

(N-type semiconductor in  
low level injection)

(hole continuity equation)

$$\frac{\partial p}{\partial t} = -\frac{d}{dx} \left( \frac{J_{px}}{q} \right) + G_L - R_p$$

(1D, generation by light)

$$\frac{\partial \Delta p}{\partial t} = -\frac{d}{dx} \left( \frac{-q D_p d\Delta p / dx}{q} \right) + G_L - \frac{\Delta p}{\tau_p}$$

(low-level injection, no  
electric field)

$$\frac{\partial \Delta p}{\partial t} = D_p \frac{d^2 \Delta p}{dx^2} - \frac{\Delta p}{\tau_p} + G_L$$

( $D_p$  spatially uniform)

# General procedure

---

- 1) Write down the MCDE

N-type      
$$\frac{\partial \Delta p(x,t)}{\partial t} = D_p \frac{d^2 \Delta p(x,t)}{dx^2} - \frac{\Delta p(x,t)}{\tau_p} + G_L$$

P-type      
$$\frac{\partial \Delta n(x,t)}{\partial t} = D_n \frac{d^2 \Delta n(x,t)}{dx^2} - \frac{\Delta n(x,t)}{\tau_n} + G_L$$

- 2) Simplify the MCDE for the specific problem
- 3) Solve the MCDE for the excess minority carrier density
- 4) Deduce QFL from the excess minority carrier density

# General features of MCDE solutions

---

Transient solutions goes as  $\exp[-t/\tau_n]$

For long regions, steady-state spatial solutions go as  $\exp[-x/L_n]$  in a long region

For short regions, steady-state solutions are linear.

# Summary

---

$$\frac{\partial p}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_p}{q} \right) + G_p - R_p$$

$$\frac{\partial n}{\partial t} = -\nabla \cdot \left( \frac{\vec{J}_n}{-q} \right) + G_n - R_n$$

$$\nabla \cdot (K_s \epsilon_0 \vec{\mathcal{E}}) = \rho$$

$$\vec{J}_p = p \mu_p \vec{\nabla} F_p = pq \mu_p \vec{\mathcal{E}} - q D_p \vec{\nabla} p$$

$$\vec{J}_n = n \mu_n \vec{\nabla} F_n = nq \mu_n \vec{\mathcal{E}} + q D_n \vec{\nabla} n$$

$$\rho = q(p - n + N_D^+ - N_A^-)$$

$$\vec{\mathcal{E}}(\vec{r}) = \nabla V(\vec{r})$$

- 1) Direct, numerical solutions
- 2) Qualitative solutions with energy band diagrams
- 3) Simplified, analytical solutions.

# Vocabulary

---

Built-in potential

Continuity equation

Diffusion length

Einstein relation

Energy band diagram

Gauss's Law

Low level injection

Minority carrier diffusion equation

Poisson equation

Relative dielectric constant

Quasi-Fermi levels

Quasi-neutrality

Semiconductor equations