

## Section 14 Doping

### 14.2 Statistics of donor and acceptor levels

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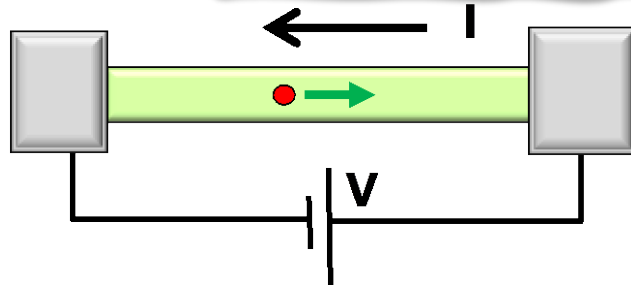


School of Electrical and  
Computer Engineering

# Section 14

## Doping

Not Enough Electrons available

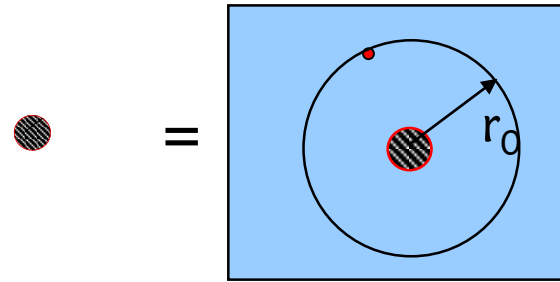
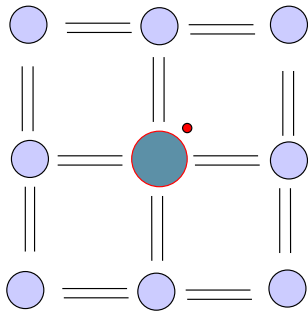


$$I = G \times V$$

$$= q \times n \times v \times A$$

↑ charge density   
 ↑ velocity   
 area

- 14.1 Basic concepts of donors and acceptors

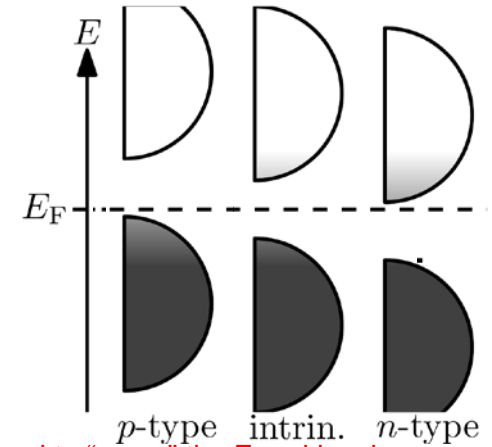


A doping atom behaves like a H-atom, except that the dielectric constant and effective masses are given by those of the host atom.

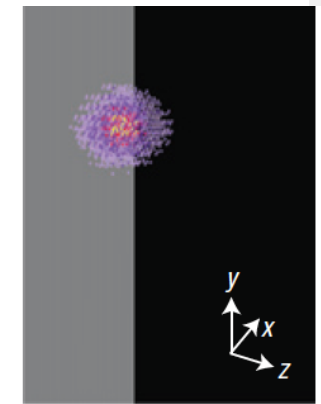
- 14.2 Statistics of donor and acceptor levels

- 14.3

- 14.4



- » Need to "move" the Fermi level
- » "add" electrons – n-type doping –  $E_F$  close to  $E_c$
- » "add" holes – p-type doping –  $E_F$  close to  $E_v$



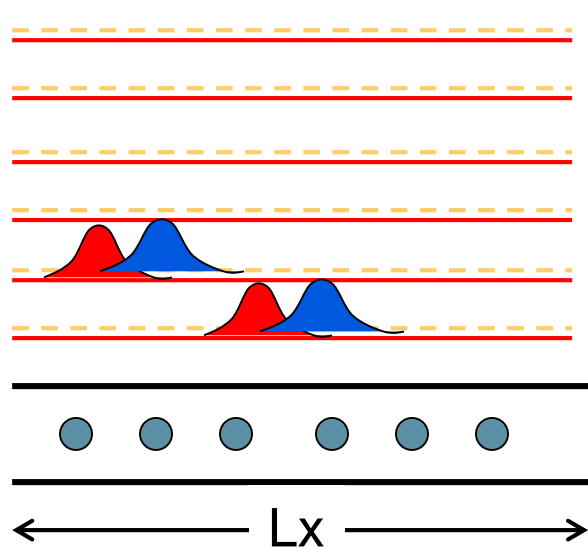
Video

Video

Video

Video

# Localized vs. Band Electrons



$$E_6 \leftarrow 12\pi/L_x$$

$$E_5 \leftarrow 10\pi/L_x$$

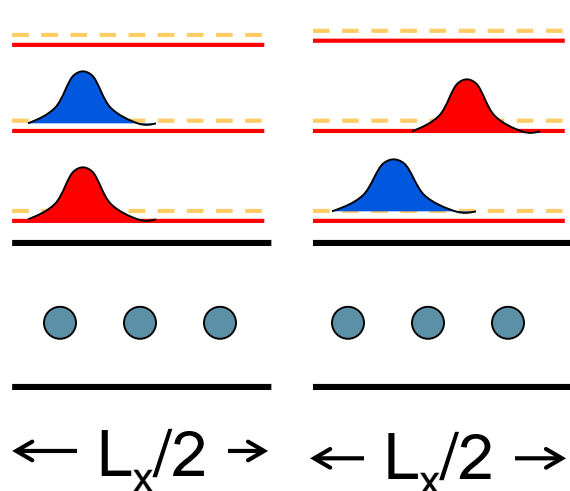
$$E_4 \leftarrow 8\pi/L_x$$

$$E_3 \leftarrow 6\pi/L_x$$

$$E_2 \leftarrow 4\pi/L_x$$

$$E_1 \leftarrow 2\pi/L_x$$

Two electrons (even with opposite spin) can not be at the same position and same energy because of electrostatic repulsion



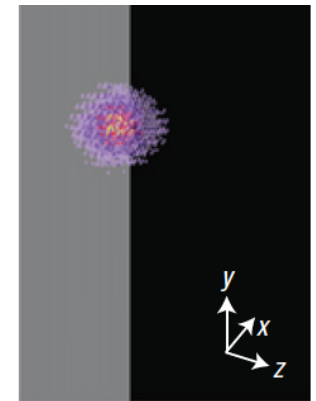
$$E_{3'} \leftarrow 6\pi/(L_x/2)$$

$$E_{2'} \leftarrow 4\pi/(L_x/2)$$

$$E_{1'} \leftarrow 2\pi/(L_x/2)$$

Band electrons (with opposite spin) need not be at the same position, so they can share occupy same energy level.

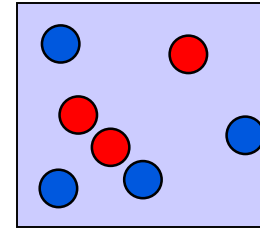
When we divide space by a factor of 2, the number of states (e.g. 6 here) does not change.



# Looking ahead: Carrier-Density w/Doping

A bulk material must be charge neutral over all ...

$$\int [p - n + N_D^+ - N_A^-] dV = 0$$



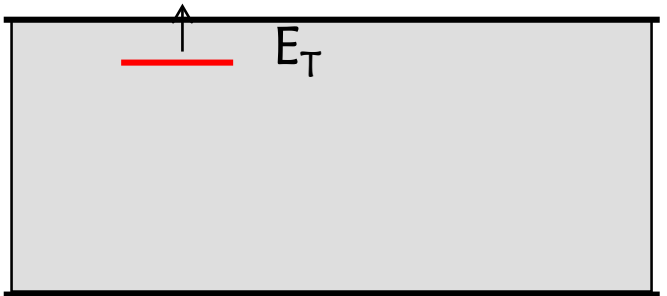
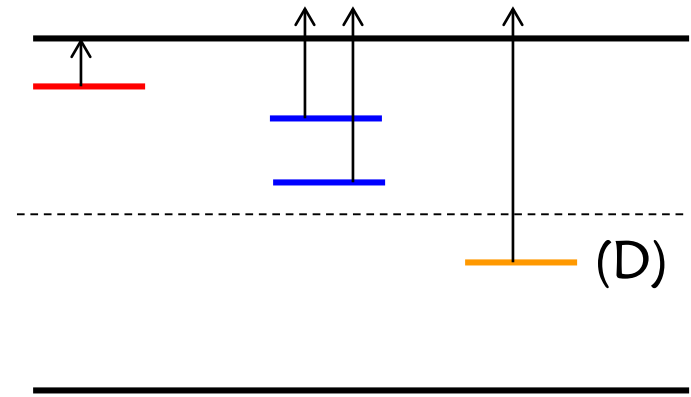
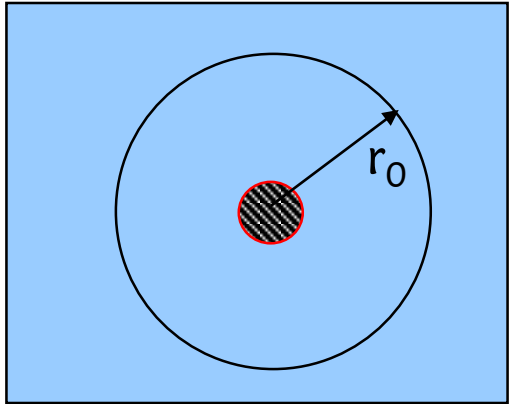
Further if the material is *spatially homogenous*

$$p - n + N_D^+ - N_A^- = 0$$

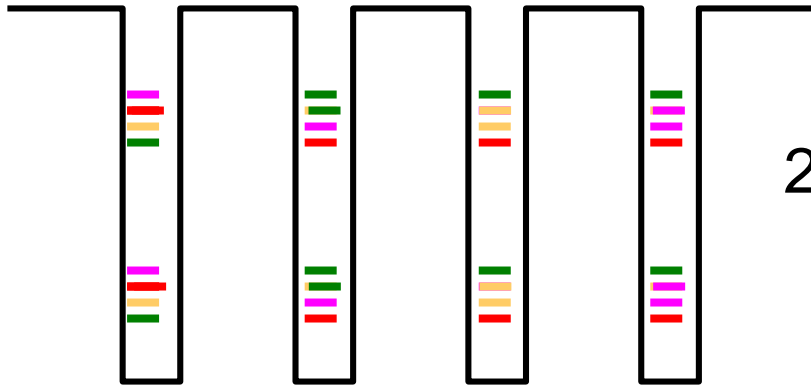
$$N_V e^{-(E_F - E_V)/k_B T} - N_C e^{-(E_C - E_F)/k_B T} + \frac{N_D}{1 + 2e^{(E_F - E_D)/k_B T}} - \frac{N_A}{1 + 4e^{(E_A - E_F)/k_B T}} = 0$$

Let us see how the formula comes about ...

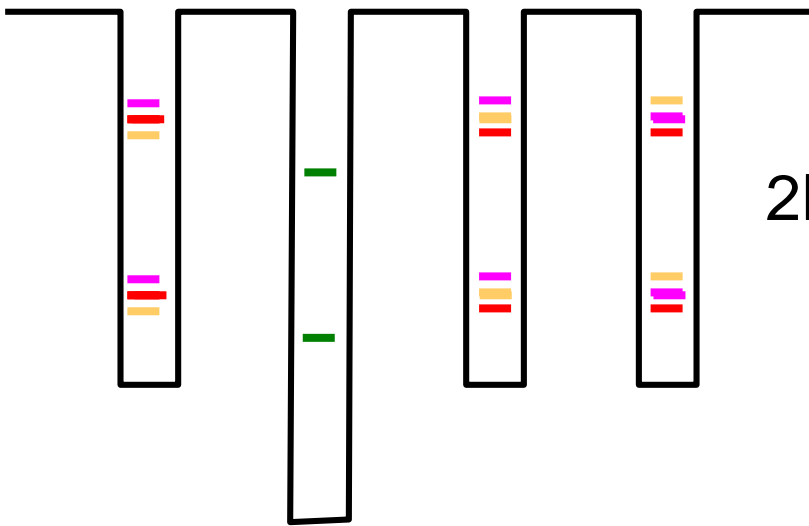
# Characteristics of Donor Atoms



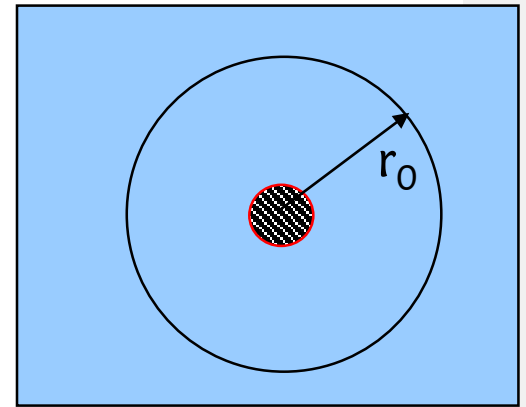
# Localized vs. Delocalized States



$2N$  states/per-band (with spin)

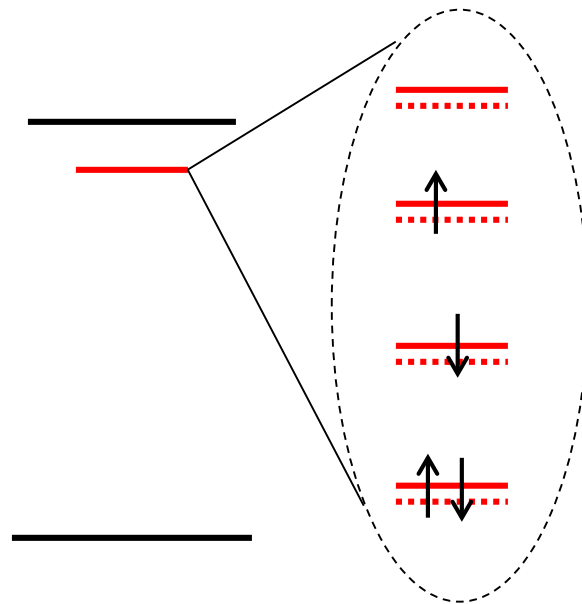


$2N-2$  states/per-band (with spin)



# Statistics of Donor Levels

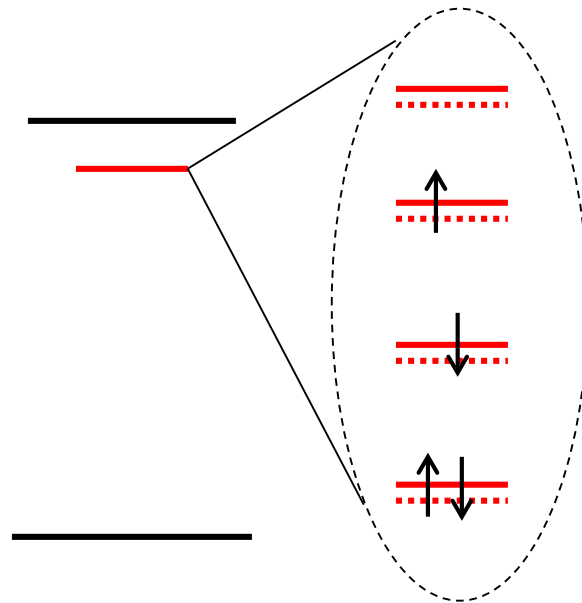
$$P_i = \frac{e^{-(E_i - N_i E_F)/k_B T}}{\sum_i e^{-(E_i - N_i E_F)/k_B T}} \equiv \frac{e^{-(E_i - N_i E_F)/k_B T}}{Z}$$



$u/d$	$E_i$	$N_i$	$P_i$
0/0	0	0	1/Z

# Statistics of Donor Levels

$$P_i = \frac{e^{-(E_i - N_i E_F) / k_B T}}{\sum_i e^{-(E_i - N_i E_F) / k_B T}} \equiv \frac{e^{-(E_i - N_i E_F) / k_B T}}{Z}$$



$u/d$	$E_i$	$N_i$	$P_i$
0/0	0	0	$1/Z$
1/0	1	1	$e^{-\frac{(E_i - E_F)}{k_B T}} / Z$
0/1	1	1	$e^{-\frac{(E_i - E_F)}{k_B T}} / Z$

**1/1**    **x**    **x**

x Coulomb interaction forbids this configuration



# Statistics of Donor Levels

$u/d$	$E_i$	$N_i$	$P_i$
0/0	0	0	$1/Z$
0/1	1	1	$e^{-\frac{(E_i - E_F)}{k_B T}} / Z$
1/0	1	1	$e^{-\frac{(E_i - E_F)}{k_B T}} / Z$

Probability that the donor is empty (charged)

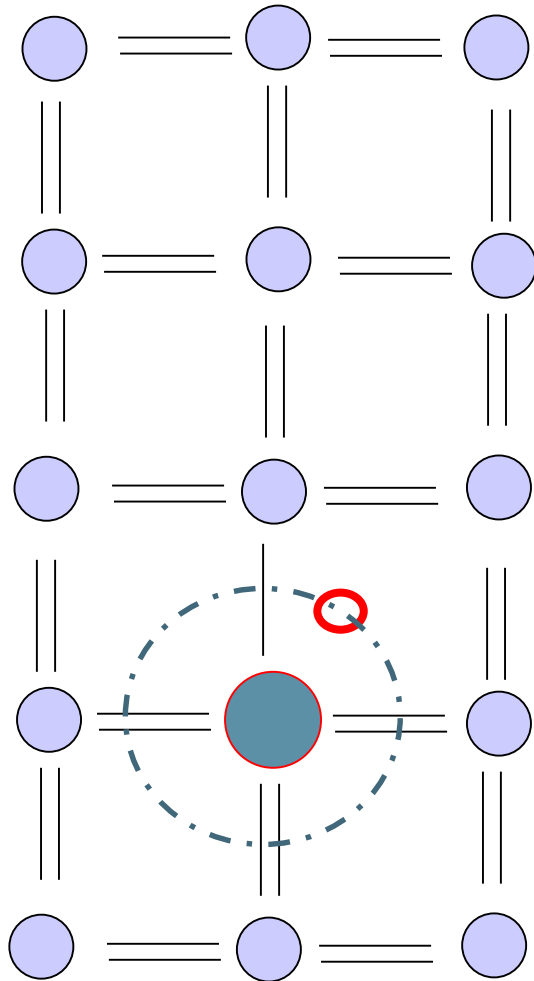
$$f_{00} = \frac{P_{00}}{P_{00} + P_{01} + P_{10}} = \frac{1/Z}{1/Z + 2e^{-(E_i - E_F)/k_B T} / Z} = \frac{1}{1 + 2e^{(E_F - E_i)/k_B T}}$$

Probability that the donor is filled with at least one electron (neutral)

$$1 - f_{00} = 1 - \frac{1}{1 + 2e^{(E_F - E_i)/k_B T}} = \frac{1}{1 + \frac{1}{2}e^{(E_i - E_F)/k_B T}}$$

Note the extra factor ...

# Acceptor Atoms

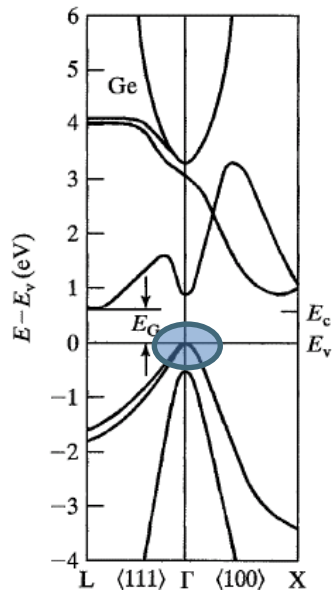
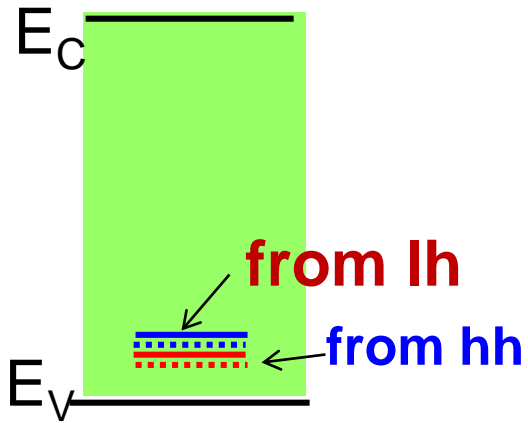


II	III	IV	V	VI
4 Be	5 B	6 C	7 N	8 O
12 Mg	13 Al	14 Si	15 P	16 S
30 Zn	31 Ga	32 Ge	33 As	34 Se
48 Cd	49 In	50 Sn	51 Sb	52 Te
80 Hg	81 Tl	82 Pb	83 Bi	84 Po

State [1] ... Hole present ...  $N-1$  charges

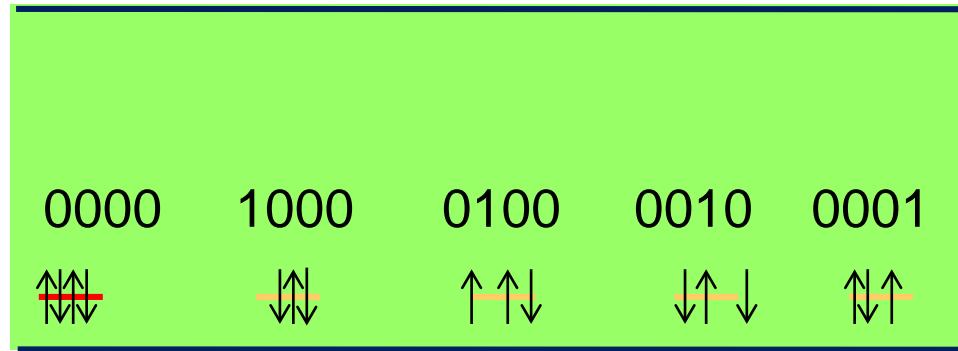
State [0] ... Hole filled ...  $N$  charges

# Statistics of Acceptor Levels in Si and Ge



1. Each atom contributes 2 states (up & down spin) to a band, therefore a band has  $2N$  states.
2. Every time a host atom is replaced by a impurity atom, 2 states disappear per a band and appear as localized states (sort of).
3. Therefore an acceptor atom close to hh and lh bands removes four states from those bands.
4. Because of Coulomb interaction only 1 hole can seat in these 4 states: the states are 0000, 0001, 0010, 0100, 1000.
5. One now uses  $P_i$  to compute the occupation of acceptors.

# Number and Energy Considerations ...



4N-4 States  
In HH/LH bands

- 1) [0000] is the charged state as it has N electrons, but N-1 protons.
- 2) Single hole configuration [0001] is uncharged, as we have N-1 electrons, and N-1 protons ... same is true for [0010], [0100], [1000] states.
- 3) Going from [0000] to [0001] states, the number of electrons goes down by 1 ( $N_i = -1$ ).
- 4) Going from [0000] to [0001] states energy goes down by  $-E_A$ , because one electron is no longer occupying the high energy level at  $E_A$ .

# Statistics of Acceptor Levels

$$P_{0000} = \frac{e^{-(0-0)E_F)/k_B T}}{\sum_i e^{-(E_i - N_i E_F)/k_B T}} \equiv \frac{1}{Z}$$

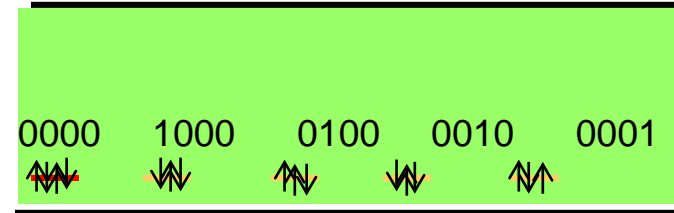


$$P_{0001} = P_{0010} = P_{0100} = P_{1000} = \frac{e^{-(-E_A - (-1)E_F)/k_B T}}{\sum_i e^{-(E_i - N_i E_F)/k_B T}} \equiv \frac{e^{(E_A - E_F)/k_B T}}{Z}$$

$$f_{0000} = \frac{P_{0000}}{P_{0000} + P_{1000} + P_{0100} + P_{0010} + P_{0001}} = \frac{1}{1 + 4e^{(E_A - E_F)/k_B T}}$$

# Filled and empty Donor/Acceptor Levels

$$N_A^{filled} \equiv N_A^- = N_A [f_{0000}] = N_A \frac{1}{1 + 4e^{(E_A - E_F)/k_B T}}$$



$$f_{0000} = \frac{1}{1 + 4e^{(E_A - E_F)/k_B T}}$$

4N-4 States

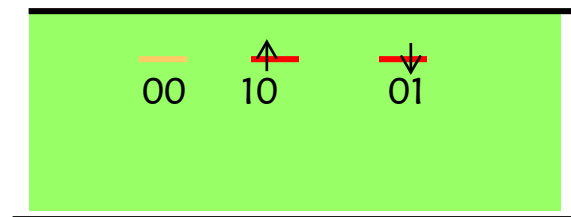
In HH/LH bands

(Two holes can not seat together)

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

$$N_D^{empty} \equiv N_D^+ = N_D f_{00} = N_D \frac{1}{1 + 2e^{(E_F - E_i)/k_B T}}$$

2N-2 states



# Distributions are physical ... Define an effective donor level

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

Degeneracy factor ...

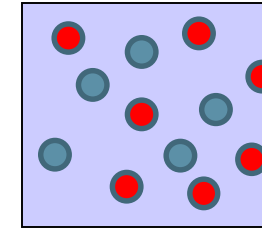
$$f_D = \frac{N_D}{1 + e^{\epsilon/k_B T} e^{(E_F - E_D)/k_B T}} = \frac{N_D}{1 + e^{(E_F - E_D')/k_B T}}$$

Effective donor level

# Carrier-density with Uniform Doping

A bulk material must be charge neutral over all ...

$$\int [p - n + N_D^+ + N_A^-] dV = 0$$



Further if the doping is **spatially homogenous**

$$p - n + N_D^+ + N_A^- = 0$$

**FD integral vs. FD function ?**

$$N_V \frac{2}{\sqrt{\pi}} F_{1/2} [\beta(E_F - E_V)] - N_A \frac{2}{\sqrt{\pi}} F_{1/2} [\beta(E_C - E_F)] + \frac{N_D}{1 + 2e^{\beta(E_F - E_D)}} - \frac{N_A}{1 + 4e^{\beta(E_A - E_F)}} = 0$$

$$N_V e^{-(E_F - E_V)/k_B T} - N_C e^{-(E_C - E_F)/k_B T} + \frac{N_D}{1 + 2e^{(E_F - E_D)/k_B T}} - \frac{N_A}{1 + 4e^{(E_A - E_F)/k_B T}} = 0 \quad (\text{approx.})$$

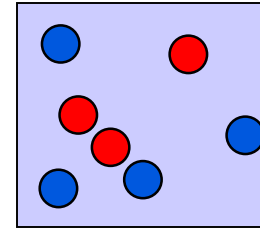
Once you know  $E_F$ , you can calculate  $n$ ,  $p$ ,  $N_D^+$ ,  $N_A^-$ .



# Summary ...

A bulk material must be charge neutral over all ...

$$\int [p - n + N_D^+ + N_A^-] dV = 0$$



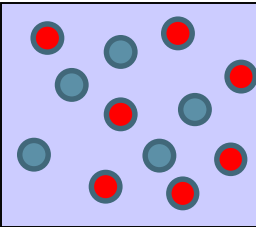
Further if the material is *spatially homogenous*

$$p - n + N_D^+ + N_A^- = 0$$

$$N_V e^{-(E_F - E_V)/k_B T} - N_C e^{-(E_C - E_F)/k_B T} + \frac{N_D}{1 + 2e^{(E_F - E_D)/k_B T}} - \frac{N_A}{1 + 4e^{(E_A - E_F)/k_B T}} = 0$$

# Intrinsic Concentration

$$p - n + N_D^+ + N_A^- = 0$$

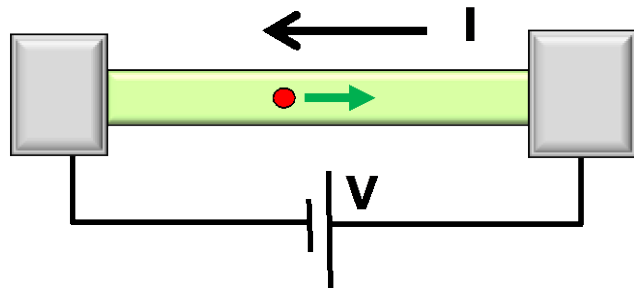


$$N_V e^{-(E_F - E_V)/k_B T} - N_C e^{-(E_C - E_F)/k_B T} + \frac{N_D}{1 + 2e^{(E_F - E_D)/k_B T}} - \frac{N_A}{1 + 4e^{(E_A - E_F)/k_B T}} = 0$$

$$n - p = 0 \Rightarrow N_C e^{-\beta(E_C - E_F)} = N_V e^{+\beta(E_V - E_F)}$$

$$E_F \equiv E_i = \frac{E_G}{2} + \frac{1}{2\beta} \ln \frac{N_V}{N_C}$$

# Section 14 Doping

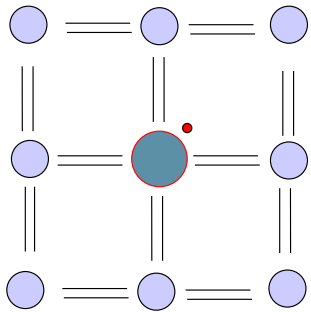


$$I = G \times V$$

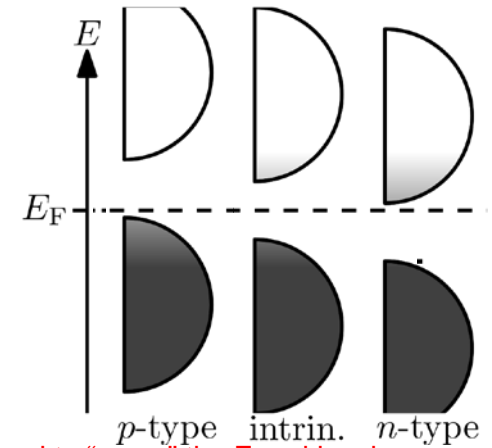
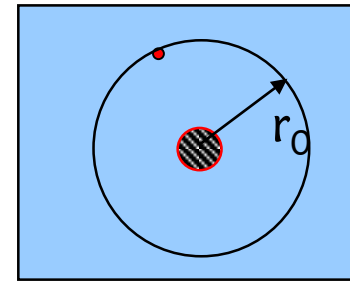
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↑ charge density   
 ↑ velocity   
 area

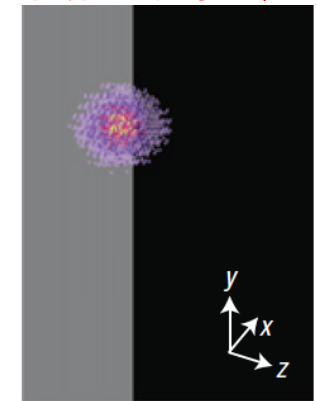
## • 14.1 Basic concepts of donors and acceptors



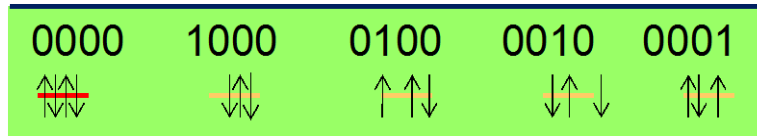
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- » Need to "move" the Fermi level
- » "add" electrons – n-type doping –  $E_F$  close to  $E_c$
- » "add" holes – p-type doping –  $E_F$  close to  $E_v$



## • 14.2 Statistics of donor and acceptor levels



$$N_V e^{-(E_F - E_V)/k_B T} - N_C e^{-(E_C - E_F)/k_B T} + \frac{N_D}{1 + 2e^{(E_F - E_D)/k_B T}} - \frac{N_A}{1 + 4e^{(E_A - E_F)/k_B T}} = 0$$

## • 14.3

## • 14.4



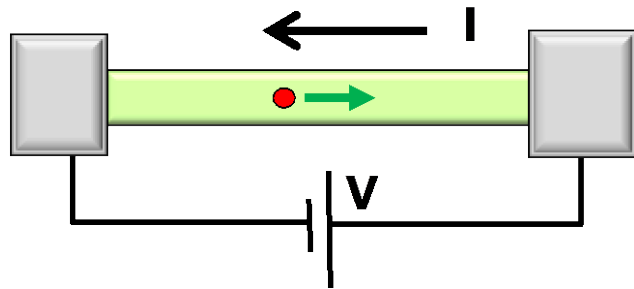
Video

Video

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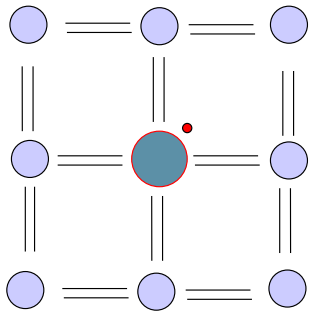


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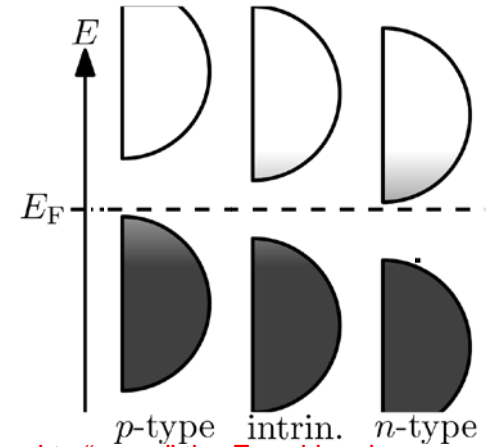
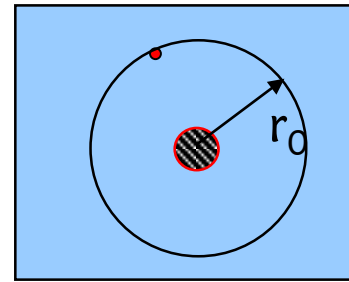
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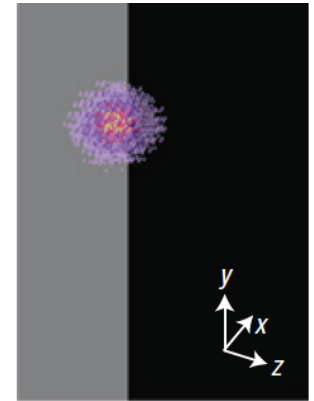
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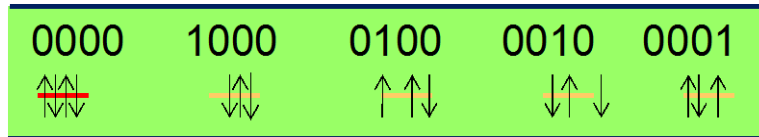
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## • 14.2 Statistics of donor and acceptor levels



$$N_V e^{-(E_F - E_V)/k_B T} - N_C e^{-(E_C - E_F)/k_B T} + \frac{N_D}{1 + 2e^{(E_F - E_D)/k_B T}} - \frac{N_A}{1 + 4e^{(E_A - E_F)/k_B T}} = 0$$

## • 14.3 Temperature dependence of carrier concentration

## • 14.4



Video

Video

Video

Video