Section 12
Occupation of States

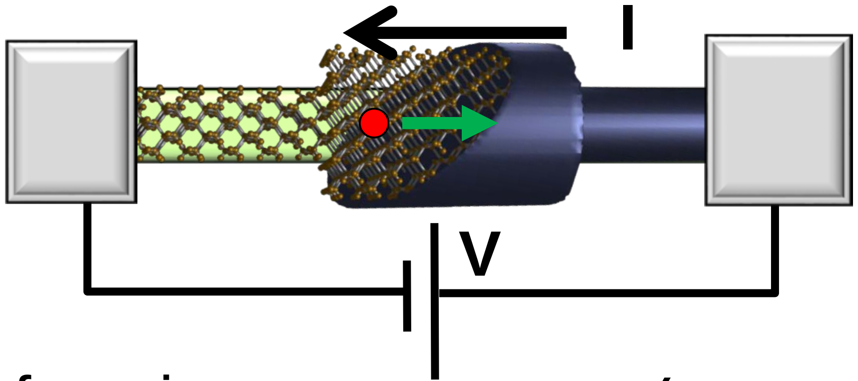
Gerhard Klimeck

gekco@purdue.edu

PURDUE UNIVERSITY

School of Electrical and Computer Engineering

Section 12
Occupation of States



$I = G \times V$

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

charge density velocity area

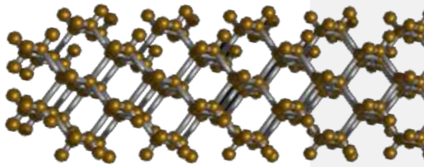
II	III	IV	V	VI
4 Be	5 B	6 C	7 N	8 O
12 Mg	13 **Al**	14 **Si**	15 **P**	16 S
30 **Zn**	31 **Ga**	32 Ge	33 **As**	34 **Se**
48 Cd	49 In	50 Sn	51 Sb	52 Te
80 Hg	81 Tl	82 Pb	83 Bi	84 Po

$$n \neq \rho \times N$$

Number of carriers available for conduction

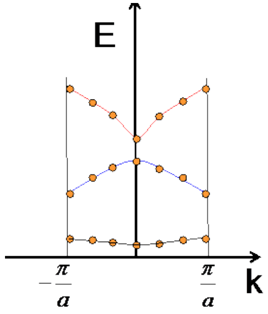
Number of electrons/atoms

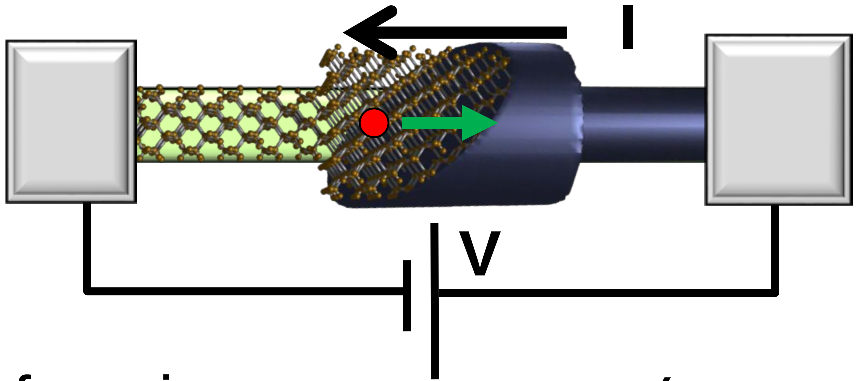
Number of atoms/volume from crystal structure



- **Materials, composition, crystals**
- Tabulated for “known” bulk materials
- At nm-scale properties change with geometry => theory

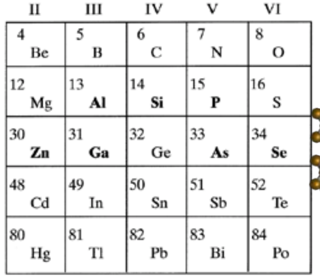
Section 12
Occupation of States



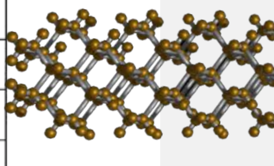


$$I = G \times V$$
$$= q \times n \times v \times A$$

charge density velocity area



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

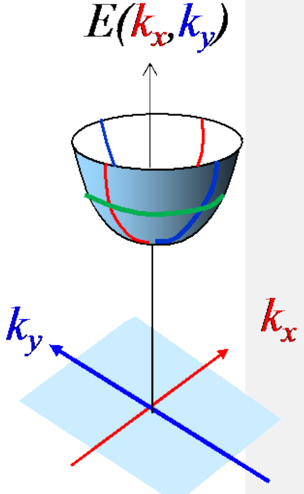


Number of carriers available for conduction

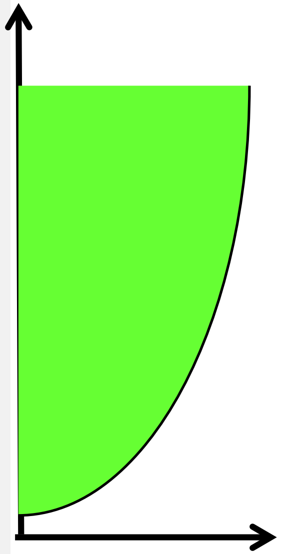
$$n \neq \rho \times N$$

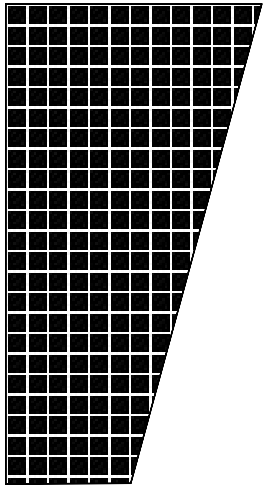
Number of electrons/atoms

Number of atoms/volume from crystal structure



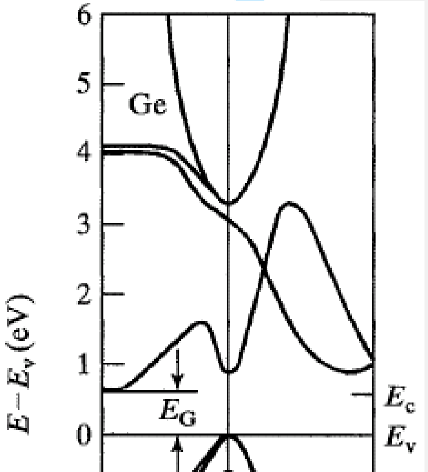
Number of states



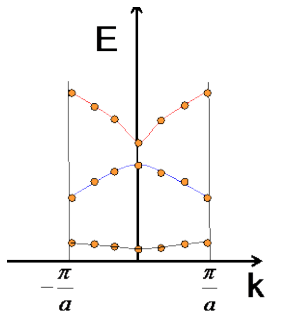


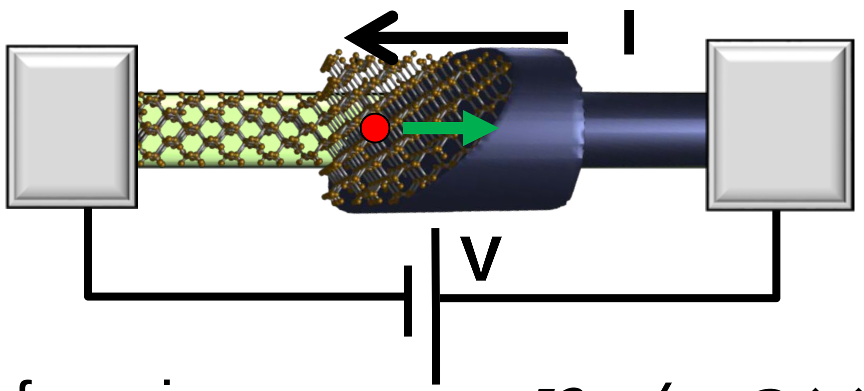
- **Materials, composition, crystals**
- Tabulated for “known” bulk materials
- At nm-scale properties change with geometry => theory

⇒ **Quantum Mechanics Mechanics**
- Concepts of density of states and masses



Section 12
Occupation of States

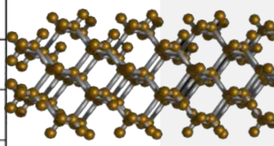




$$I = G \times V$$
$$= q \times n \times v \times A$$

charge density velocity area

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

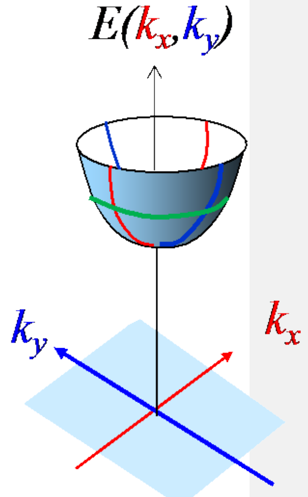


Number of carriers available for conduction

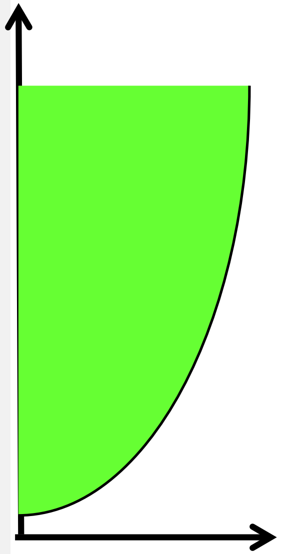
$$n \neq \rho \times N$$

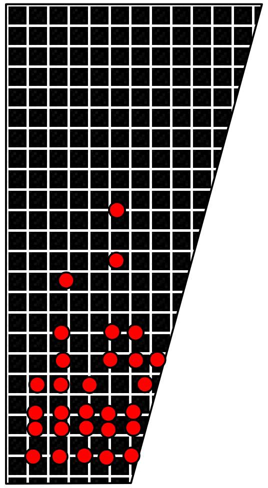
Number of electrons/atoms

Number of atoms/volume from crystal structure



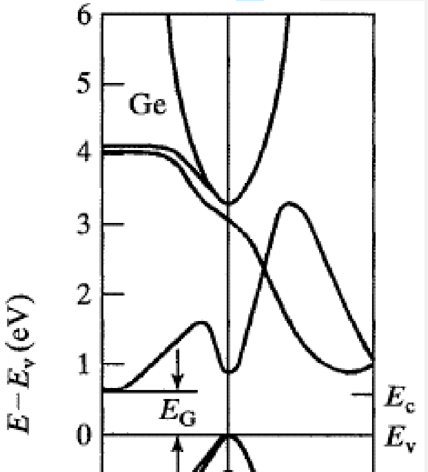
Number of states



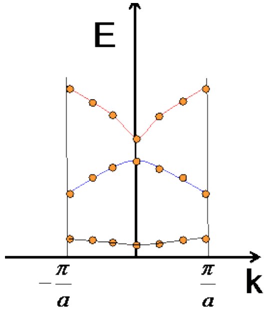


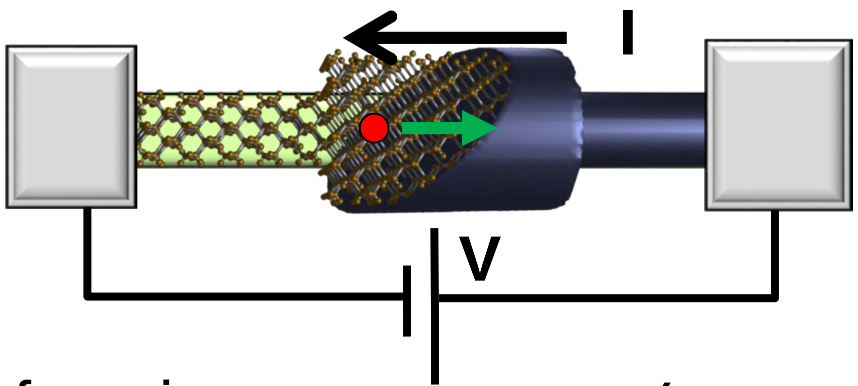
- **Materials, composition, crystals**
- Tabulated for “known” bulk materials
- At nm-scale properties change with geometry => theory

$\Rightarrow$ **Quantum Mechanics Mechanics**
- Concepts of density of states and masses



Section 12
Occupation of States

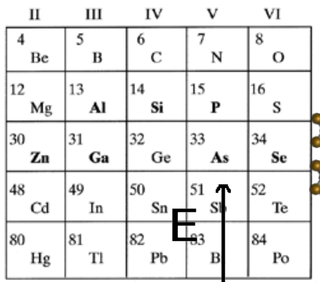


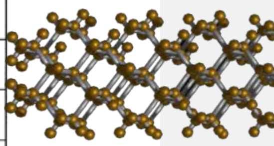


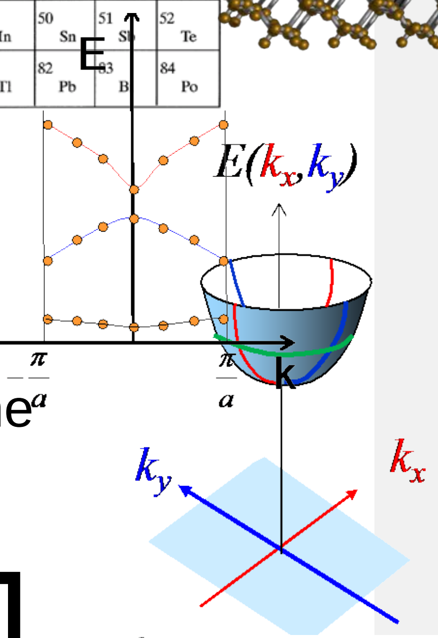
$I = G \times V$

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

charge density velocity area







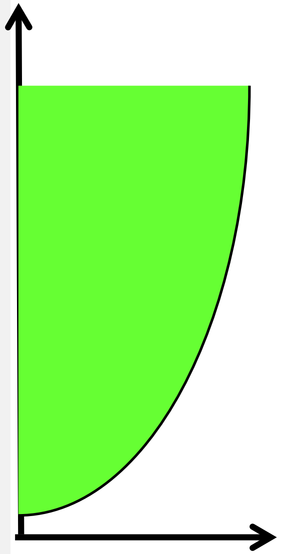
Number of carriers available for conduction

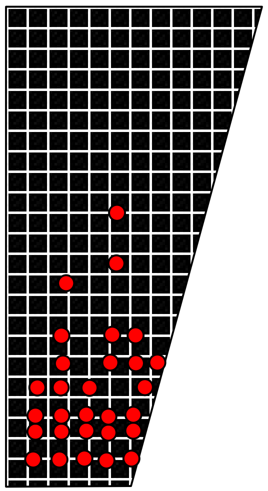
$$n \neq \rho \times N$$

Number of electrons/atoms

Number of atoms/volume from crystal structure

Carrier number = Number of states x ***filling factor***





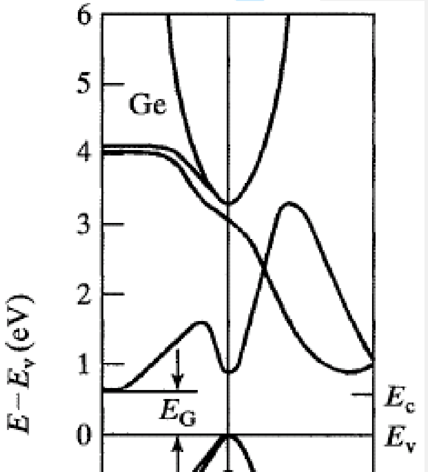
- **Materials, composition, crystals**
- Tabulated for “known” bulk materials
- At nm-scale properties change with geometry => theory

$\Rightarrow$ **Quantum Mechanics Mechanics**

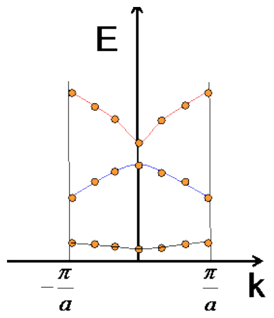
- Concepts of density of states and masses

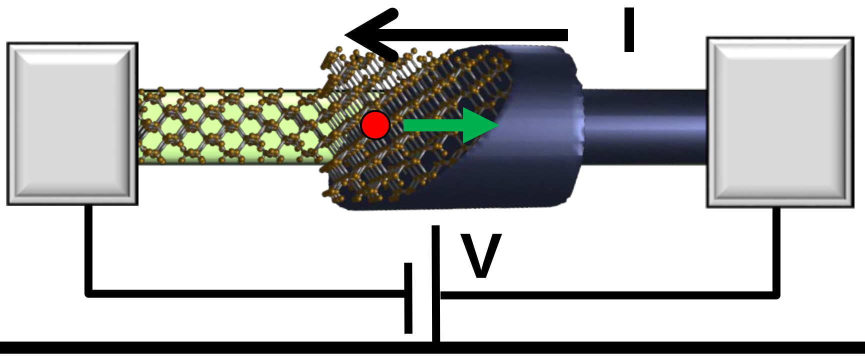
$\Rightarrow$ **Equilibrium Statistical Mechanics**

- Occupation factors



Section 12
Occupation of States





$$I = G \times V$$
$$= q \times n \times v \times A$$

charge density velocity area

- **Materials, composition, crystals**
- Tabulated for "known" bulk materials
- At nm-scale properties change with geometry => theory

$\Rightarrow$ **Quantum Mechanics Mechanics**
- Concepts of density of states and masses

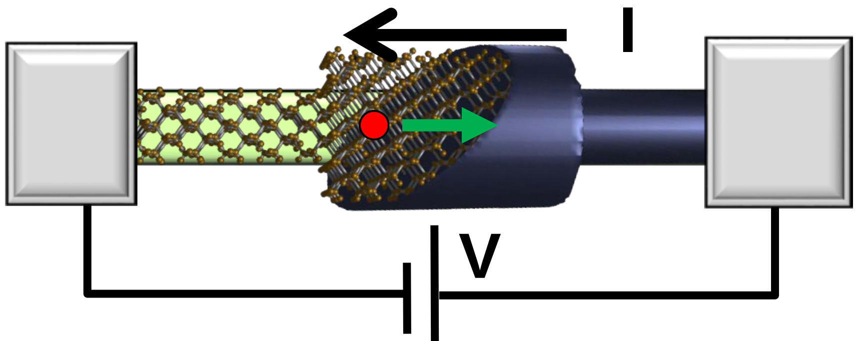
$\Rightarrow$ **Equilibrium Statistical Mechanics**
- Occupation factors

Transport with scattering, non-equilibrium Statistical Mechanics
- Drift-diffusion equation with recombination-generation

Carrier number =
Number of states x ***filling factor***

Understanding transport in concrete devices
- Diodes, BJT/HBT, MOS

Section 12
Occupation of States



$I = G \times V$

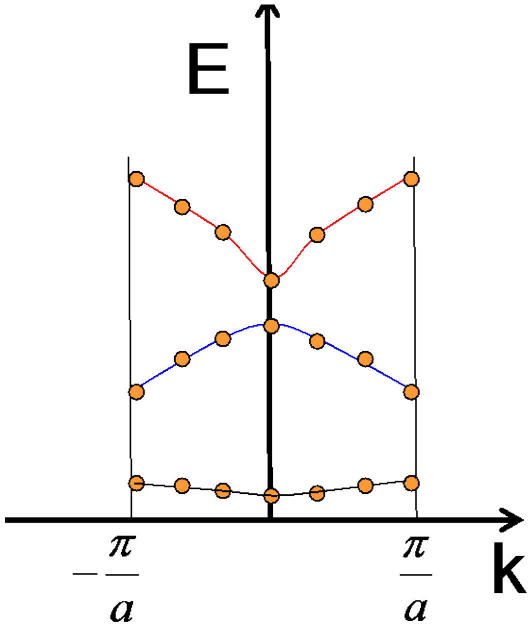
$= q \times n \times v \times A$

charge density velocity area

- **Materials, composition, crystals**
- Tabulated for "known" bulk materials
- At nm-scale properties change with geometry => theory

$\Rightarrow$ **Quantum Mechanics Mechanics**
- Concepts of density of states and masses

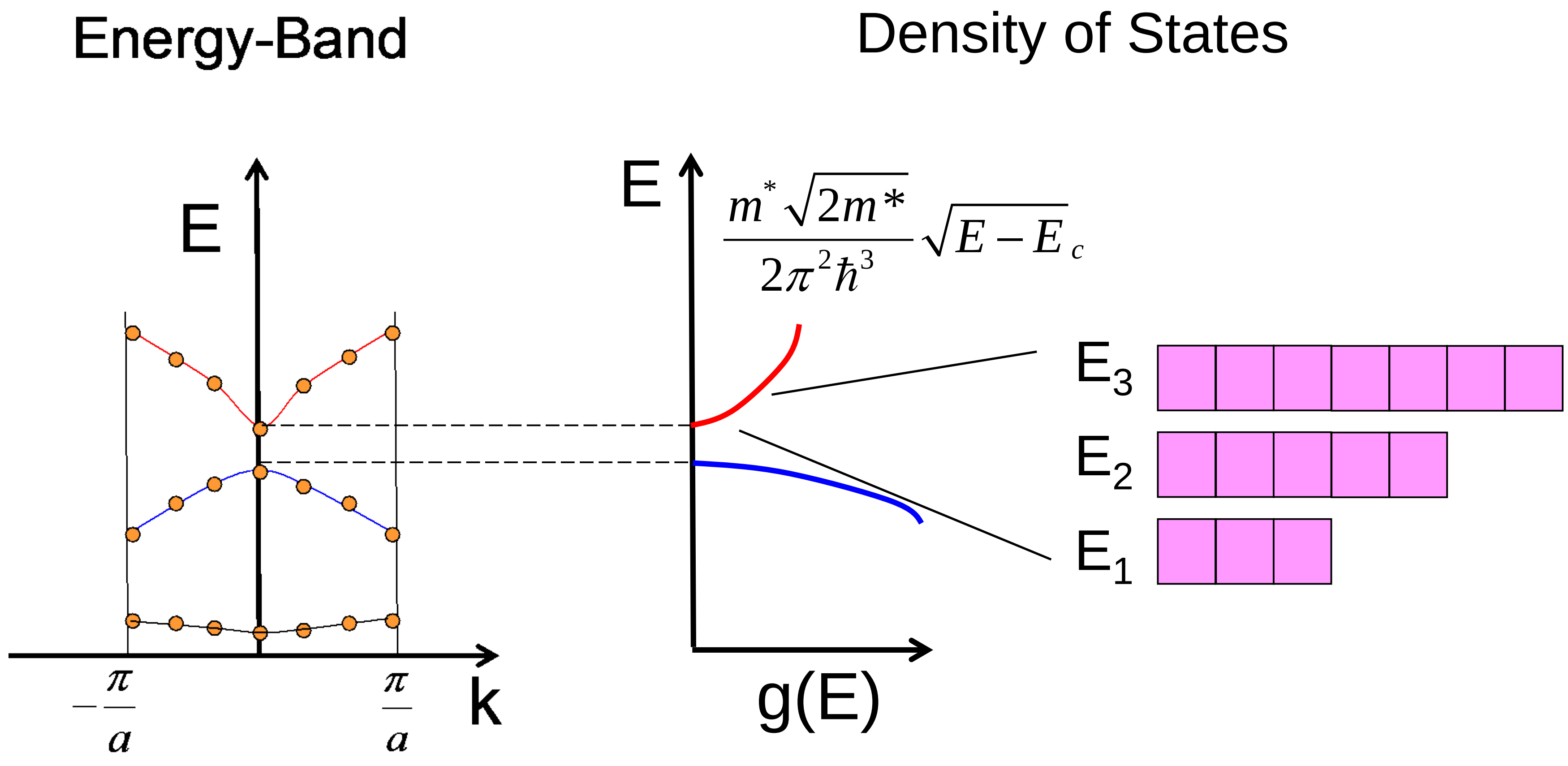
$\Rightarrow$ **Equilibrium Statistical Mechanics**
- Occupation factors



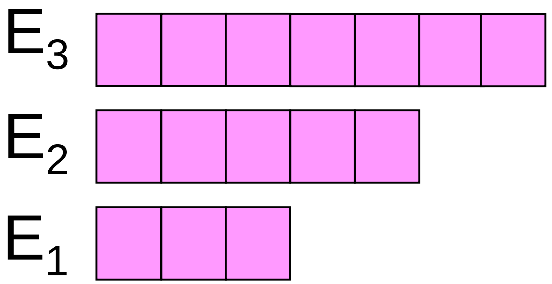
Carrier number =
Number of states x ***filling factor***

12.1 Rules of filling electronic states
12.2 Three Derivations of Fermi-Dirac Statistics
12.3 Intrinsic carrier concentration

E-k diagram and Electronic States



Rules for filling up the States



- Pauli Principle: Only one electron per state
- Total number of electrons is conserved $N_T = \sum_i N_i$
- Total energy of the system is conserved $E_T = \sum_i E_i N_i$

Section 12
Occupation of States

One Video Segment

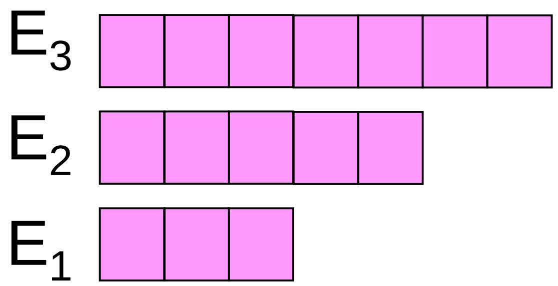
- 12.1 Rules of filling electronic states
  - » Pauli exclusion
  - » Total particle conservation
  - » Total energy conservation

Carrier number =
Number of states x ***filling factor***

status

One Video Segment

- 12.2 Derivation of Fermi-Dirac Statistics: three techniques



One Video Segment

- 12.3 Intrinsic carrier concentration

Reference: Vol. 6, Ch. 4

One Video Segment

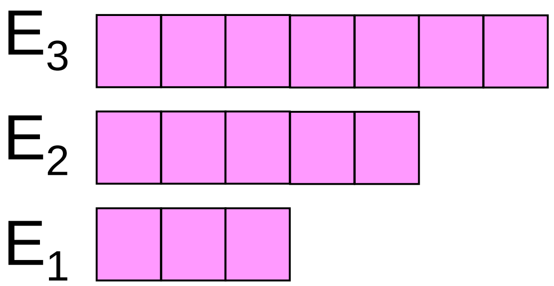
- 12.1 Rules of filling electronic states
  - » Pauli exclusion
  - » Total particle conservation
  - » Total energy conservation

Carrier number =
Number of states x ***filling factor***

One Video Segment

- 12.2 Derivation of Fermi-Dirac Statistics: three techniques
  - » Microcanonical ensemble - statistics
  - » Detailed Balance – thermal equilibrium & Pauli exclusion
  - » Partition Function – statistical mechanics

status



One Video Segment

- 12.3 Intrinsic carrier concentration

Reference: Vol. 6, Ch. 4