Lecture 1 - Electrons, Photons and Phonons

September 4, 2002

Contents:

1. Electronic structure of semiconductors
2. Electron statistics
3. Lattice vibrations
4. Thermal equilibrium

Reading assignment:

del Alamo, Ch. 1

Announcements:

Tomorrow's recitation slot will be used as lecture (in exchange for lecture slot in December that will be used as recitation).

Go to http://weblab.mit.edu and register. Put "6.720 student" in the Description field.

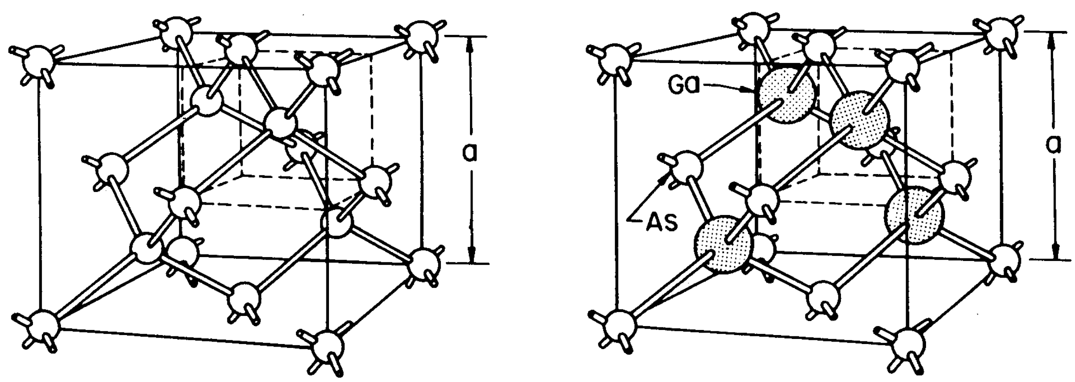
Key questions

- What makes semiconductors so special?
- How do electrons arrange themselves (in energy) in an electronic system?
- Why should we be concerned with the vibrational modes of the lattice of a crystalline solid?
- What is the formal definition of thermal equilibrium? What are some of its consequences?

1. Semiconductors as solids

□ Semiconductors are crystalline solids

Crystalline solid = elemental atomic arrangement, or *unit cell*, repeated ad infinitum in space in three dimensions.



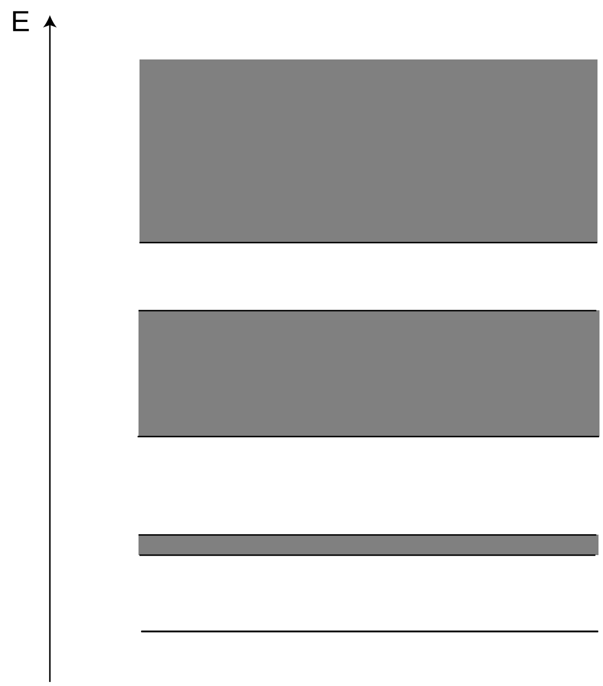
- Si lattice constant: $0.54\ nm$
- Si atomic spacing: $0.24\ nm$
- Si atomic density: $5.0 \times 10^{22}\ cm^{-3}$

Semiconductors held together by *covalent bonding* ⇒ 4 valence electrons shared with 4 neighbours ⇒ low energy situation.

IIB	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
	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

□ Solid is electronic system with *periodic potential*

Fundamental result of solid-state physics: *quantum states cluster in bands leaving bandgaps* (regions without allowed states) *in between.*



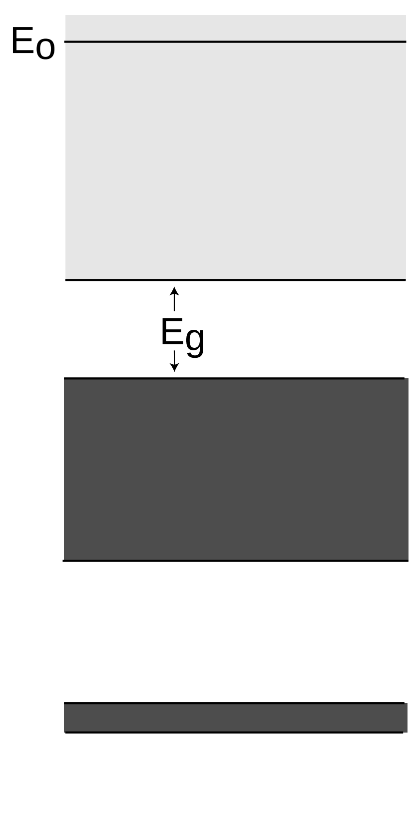
□ Semiconductor band structure

There are many more quantum states than electrons in a solid.

Quantum states filled with one electron per state starting from lowest energy state (*Pauli exclusion principle*).

Distinct feature of semiconductors:

At 0 K, filling ends up with full band separated by $1-3\ eV$ bandgap from next empty band $\Rightarrow$ At around 300 K, some electrons populate next band above bandgap.



2. Electron statistics

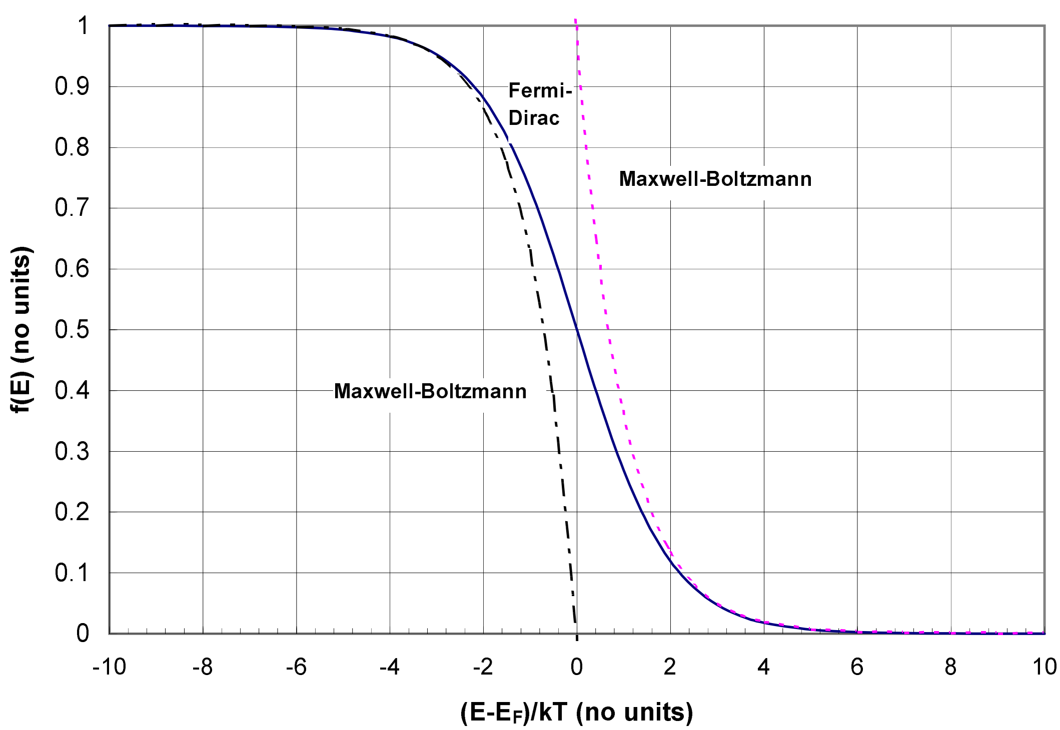
At finite temperature, state occupation probability by electron determined by **Fermi-Dirac distribution function**:

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

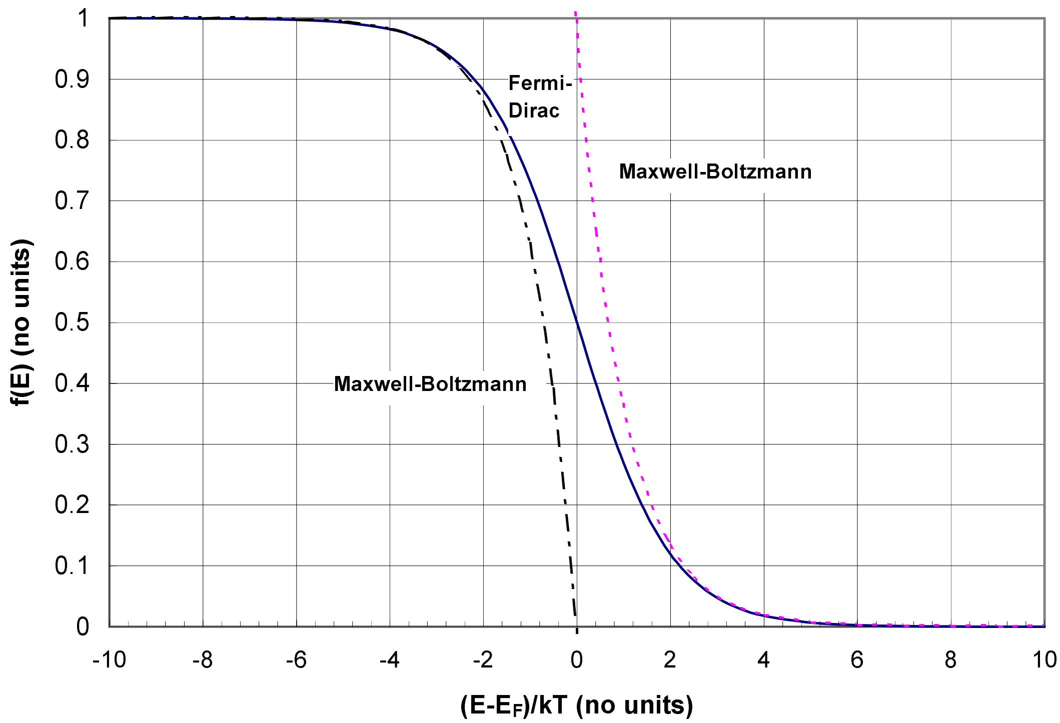
$E_F \equiv$ *Fermi energy* $\equiv$ energy for which occupation probability is 50%

$$k \equiv \textit{Boltzmann constant} \;= 8.62 \times 10^{-5}\ eV/K$$

$$kT \equiv \textit{thermal energy} \;= 25.9\ meV\ @\ 300\ K$$

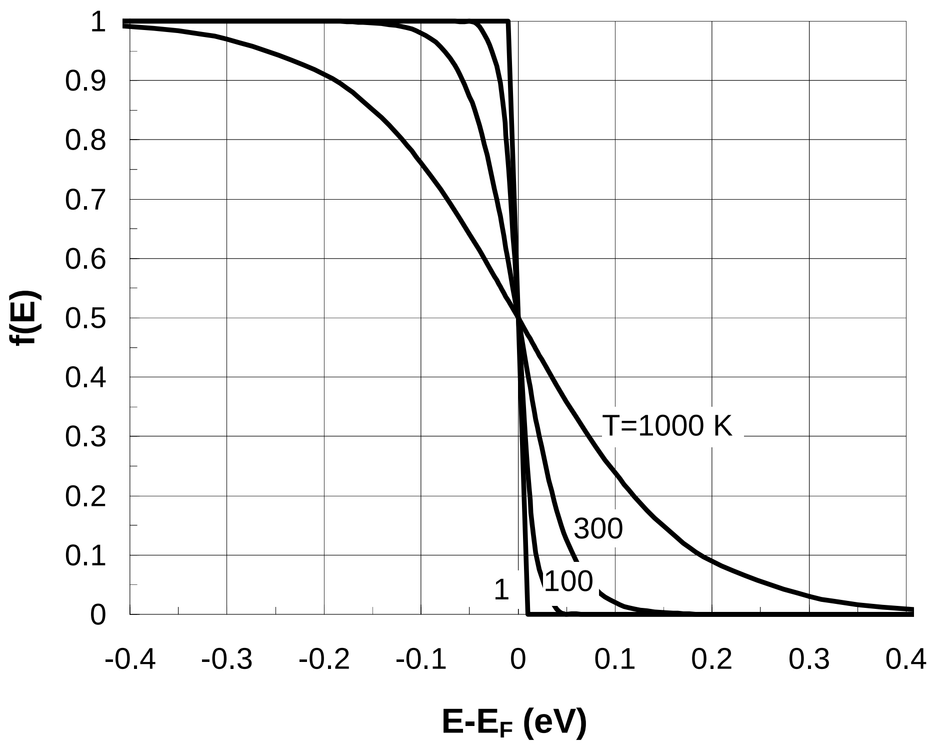


Properties of Fermi-Dirac distribution function:



- for $E \ll E_F$: $f(E) \simeq 1$
- for $E \gg E_F$: $f(E) \simeq 0$
- width of transition around $E_F \simeq\ 3kT$ (20% criterium)
- symmetry: $f(E_F + E_1) = 1 - f(E_F - E_1)$

Temperature dependence of Fermi-Dirac distribution function:



In general, E_F function of T.

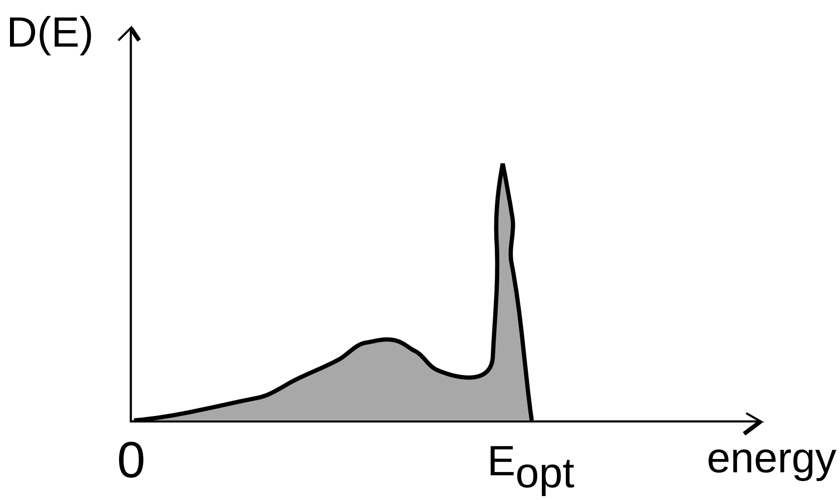
3. Lattice vibrations

At finite T atoms in lattice vibrate.

Solid is large coupled system $\rightarrow$ only certain vibrational modes are possible.

Each vibrational mode is characterized by its mechanical energy.

Define *density of modes*:



- few modes at low energies (*acoustical modes*)
- many modes at a certain energy E_{opt} (*optical modes*)
- no modes beyond E_{opt}

For Si: $E_{opt} = 63\ meV$.

□ Lattice can exchange energy with electrons in the solid:

- an electron can give some energy to the lattice: excites an available vibrational mode
- an electron can acquire energy from lattice: a vibrational mode is extinguished

Easy to think of vibrational modes as particles: **phonons**.

Then talk about:

- phonon emission by an electron
- phonon absorption by an electron

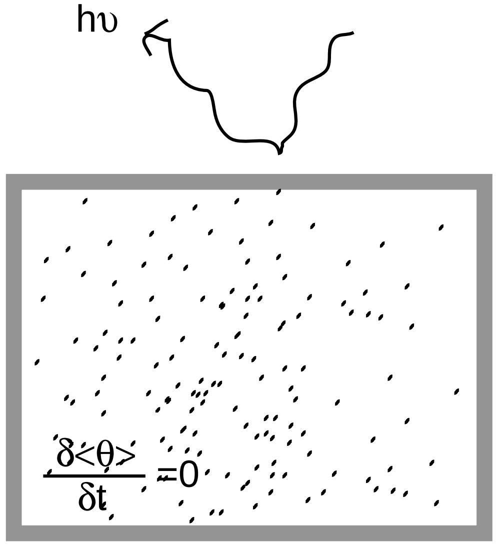
Similarly with **photons** or quanta of light.

Photon and phonon emission and absorption are important energy exchange mechanisms in semiconductors.

4. Thermal equilibrium

A particle system is in thermal equilibrium if:

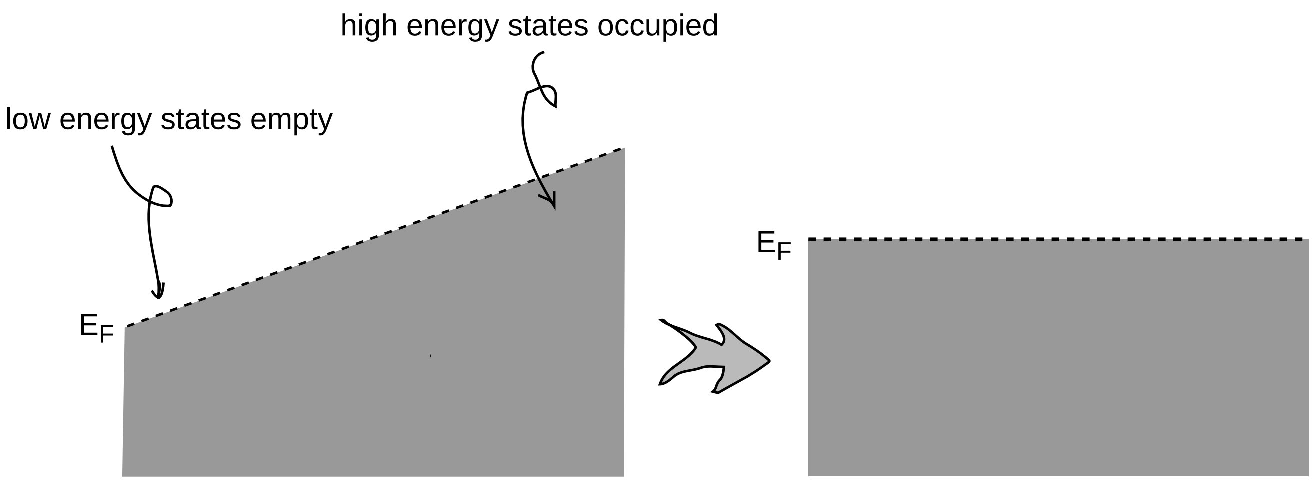
- it is *closed*: no energy flow through boundaries of system
- it is in *steady-state*: time derivatives of all ensemble averages (global and local) are zero



Thermal equilibrium important because all systems evolve towards TE after having been perturbed.

In order to know how a system evolves, it is essential to know where it is going.

□ In thermal equilibrium, E_F constant throughout system



Key conclusions

- In solids, electron states cluster in bands separated by bandgaps.
- Distinct feature of semiconductors: at $0\ K$, quantum state filling ends up with full band separated from next empty band by $1-3\ eV$ bandgap $\Rightarrow$ at around $300\ K$, some electrons populate next band above bandgap.
- Occupation probability of quantum systems in thermal equilibrium governed by *Fermi-Dirac distribution function*:

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

- Electrons can exchange energy with *photons* (quanta of light) and with *phonons* (quanta of vibrational energy of lattice).
- System in *thermal equilibrium*: isolated from outside world + in steady state.
- In thermal equilibrium, E_F is independent of position.
- Order of magnitude of key parameters:
  - atomic density of Si: $N_{Si} \sim 5 \times 10^{22}\ cm^{-3}$
  - bandgap of Si: $E_g \sim 1\ eV$
  - thermal energy: $kT \sim 26\ meV$ @ 300K
  - optical phonon energy of Si: $E_{opt} \sim 60\ meV$

Self-study

- Concept of *blackbody radiation*.
- Concept of *vacuum energy*.
- Concept of *density of states*.
- Understand how can the Fermi energy change with temperature.
- *Maxwell-Boltzmann distribution function*.