

*“Complementi di Fisica”*  
*Lectures 20, 21*



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Trieste, 15-12-04

# Course Outline - Reminder

- The physics of semiconductor devices: an introduction
- Quantum Mechanics: an introduction
- (slightly more) Advanced semiconductor fundamentals
  - Energy bands, effective mass
  - Equilibrium Carrier Statistics: density of states, Fermi function
  - **Non-equilibrium: transport of charge carriers**
  
- no time left for:
  - An example of device simulation; revisiting the Shockley experiment and its interpretation; discussing a device as an application



# Lectures 20, 21 - outline

- Electrons in a “perfectly periodic crystal” (reminder)
  - Effect of external forces: “Semi-classical Model”
  - Motion of electrons in bands and “effective mass”
  - Currents in bands: electrons and “holes”
- Electrons in a real crystal
  - Scattering of electrons by:
    - “defects” (elastic)
    - “phonons” (inelastic)
    - electrons ?
  - Boltzmann equation and the “relaxation time” approximation
  - Electrical conductivity in metals and in semiconductors
  - Integrals of the Boltzmann equation and drift-diffusion equation for the current density  $J$
- Conclusions



# Electrons and holes in a perfect crystal (reminder)

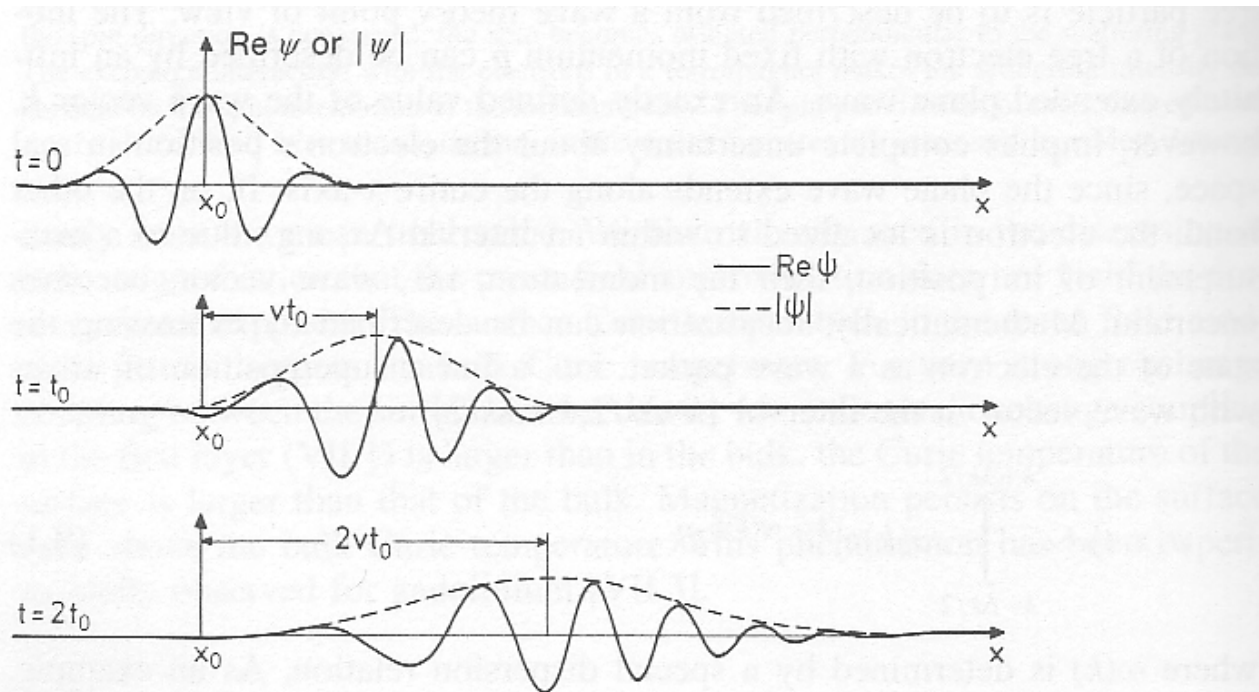
Semi-classical model

“Effective mass”

Electrons and “holes”

# Bloch Wave Packets in crystals

A packet of Bloch waves with a spread  $\Delta k$  in wave vector  $k$ , that is small on the scale of the Brillouin zone ( $2\pi/d$ ), must be spread in space over several primitive cells ( $d$ ), since (as we already saw) for wave packets  $\Delta x \approx 1/\Delta k$



**Fig. 9.1.** Real space representation of the wave packet describing the motion of a spatially localized free electron at times  $t=0, t_0, 2t_0 \dots$  ( $\text{Re}\{\psi$ : —;  $|\psi|$ : - - -). The center of the wave packet, i.e., in the particle picture the electron itself, moves with the group velocity  $v = \partial\omega/\partial k$ . The halfwidth of the envelope increases with time. As the wave packet spreads, the wavelength of the oscillations of  $\text{Re}\{\psi$  becomes smaller at the front and larger at the rear

Group velocity

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

$$\vec{v}_g = \frac{1}{\hbar} \vec{\nabla}_k E$$

# The “Semi-Classical Model”

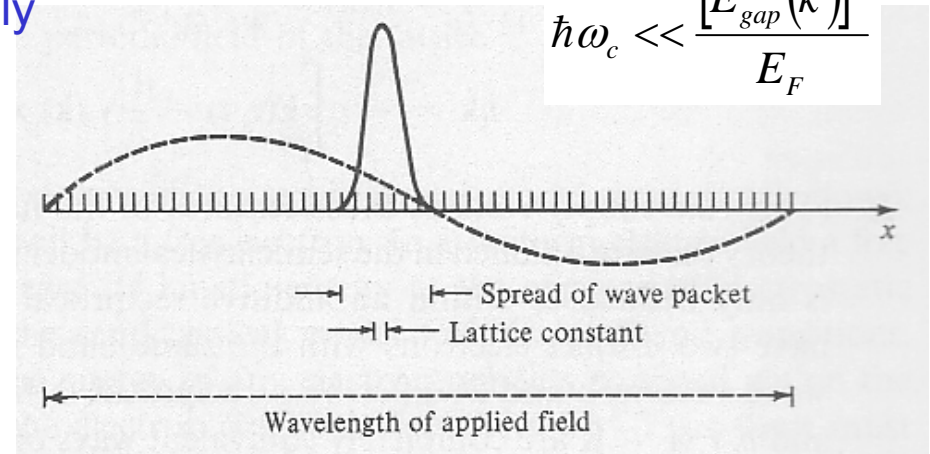
... treats the response of electrons to electric and magnetic fields, that vary slowly over the dimensions of a Bloch wave packet and therefore exceedingly slowly over a few primitive cells.

The external field is treated classically, the periodic field of the ions quantistically (Bloch packet, “crystal” vector  $k$ : all distinct wave vectors lie in a single Brillouin zone, since  $k + 2n\pi/d$  describes the same state ).

Evolution of position  $r$  and wave vector  $k$  in the presence of external fields is entirely dependent on the band structure, as expressed by  $E(k)$  in the band

$$eEd \ll \frac{[E_{gap}(\vec{k})]^2}{E_F}$$

$$\hbar\omega_c \ll \frac{[E_{gap}(\vec{k})]^2}{E_F}$$



$$\dot{\vec{r}} = \vec{v}_g(\vec{k}) = \frac{1}{\hbar} \vec{\nabla}_k E$$

$$\hbar \dot{\vec{k}} = -e \left[ \vec{E}(\vec{r}, t) + \frac{1}{c} \vec{v}_g(\vec{k}) \times \vec{H}(\vec{r}, t) \right]$$

# Group velocity variations: effective mass

- What happens if an “external” force is applied, for instance an external electric field ? (the lattice forces are already included in the Bloch wave functions!)
  - “force”  $\Rightarrow$  “change in particle energy” or absorbed power  $\Rightarrow$  “changes in group velocity”  $\Rightarrow$  “acceleration”  $\Rightarrow$  “effective mass”:

$$dE = Fdx = Fv_g dt, \quad v_g = \frac{1}{\hbar} \frac{dE}{dk} \Rightarrow$$

$$\Rightarrow F = \frac{1}{v_g} \frac{dE}{dt} = \frac{1}{v_g} \frac{dE}{dk} \frac{dk}{dt} = \hbar \frac{dk}{dt} = \frac{d(\hbar k)}{dt}$$

$$\Rightarrow \frac{dv_g}{dt} = \frac{1}{\hbar} \frac{d}{dt} \left( \frac{dE}{dk} \right) = \frac{1}{\hbar} \frac{d}{dk} \left( \frac{dE}{dk} \right) \frac{dk}{dt} = \frac{1}{\hbar^2} \frac{d^2 E}{dk^2} \frac{d(\hbar k)}{dt}$$

Formally similar to Newton's law, if...

$$a_g = \frac{dv_g}{dt} = \frac{F}{m^*}$$

$$m^* = \frac{1}{\frac{1}{\hbar^2} \frac{d^2 E}{dk^2}}$$

... if this coefficient is interpreted as an “effective mass”

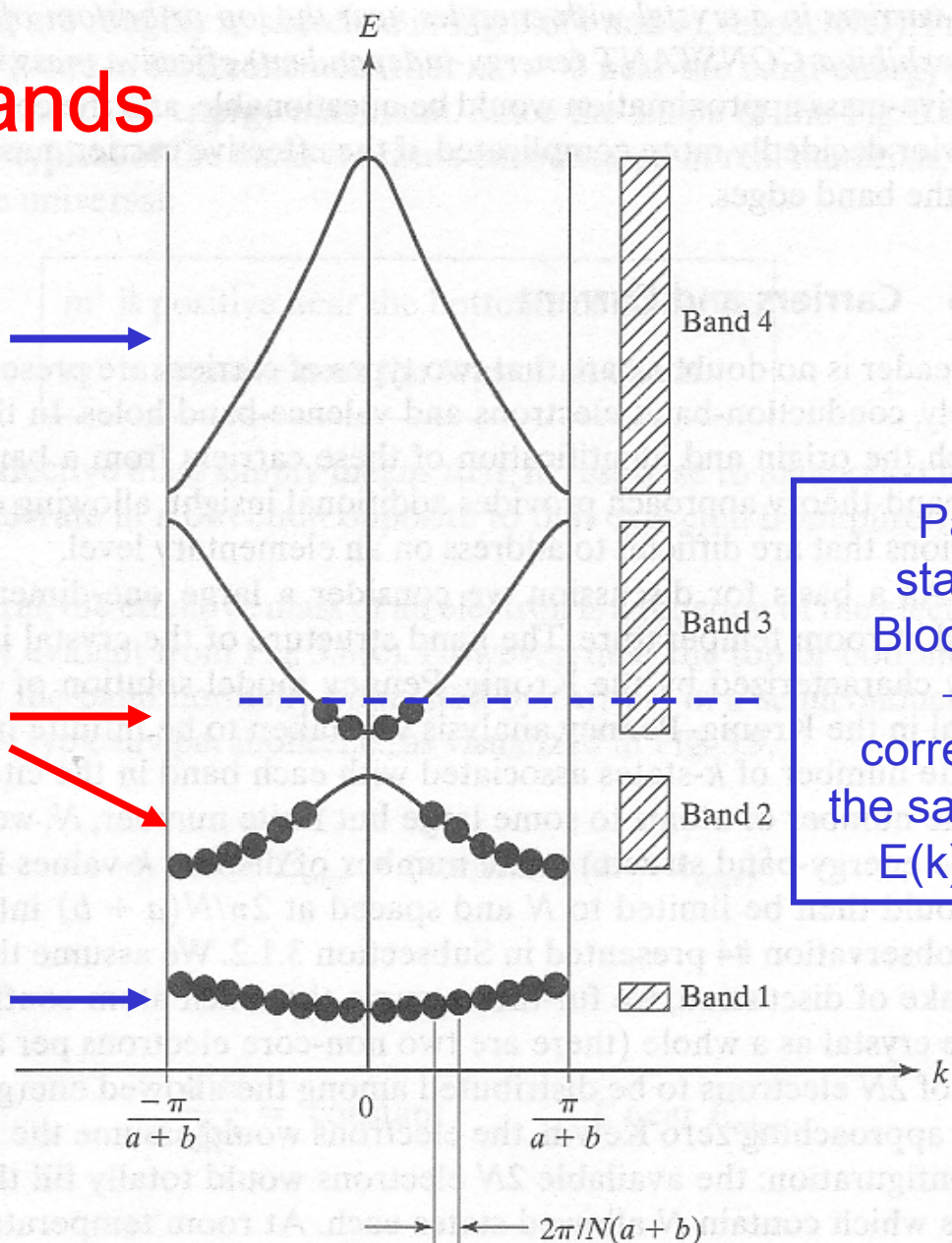


# Currents in bands

Empty band: no current →

Partially filled bands contribute to current →

Full band: no current →



Pairs of stationary Bloch waves  $-k, +k$  correspond to the same energy  $E(k) = E(-k)$





# Currents in full and in partially filled bands

More detailed explanation in terms of group velocities:  
contribution of a k-volume element to the electron current density  
and total electrical current density from a full band:

$$d \vec{j}_n = \vec{v}(\vec{k}) \frac{d\vec{k}}{8\pi^3} = \frac{1}{8\pi^3 \hbar} \vec{\nabla}_k E(\vec{k}) d\vec{k}$$

$$\vec{j} = \frac{-e}{8\pi^3 \hbar} \int_{\text{1st.Br.z.}} \vec{\nabla}_k E(\vec{k}) d\vec{k}$$

A fully occupied band  
cannot conduct current!  
(insulators)

$$E(\vec{k}) = E(-\vec{k}) \Rightarrow \vec{v}(-\vec{k}) = \frac{1}{\hbar} \vec{\nabla}_{-\vec{k}} E(-\vec{k}) d\vec{k} = -\frac{1}{\hbar} \vec{\nabla}_k E(\vec{k}) d\vec{k} = -\vec{v}(\vec{k})$$

$\Rightarrow \vec{j}(\text{full band}) \equiv 0$  A full band has a symmetric distribution  
of k about k=0 and of electron velocities

$\Rightarrow \vec{j}(\text{partially filled band}) \neq 0$  In a partially filled band electrons  
can be shifted by external fields  
to states that are no longer symmetric



# “Holes interpretation” of partially filled bands

For partially filled bands, the integral for the current density is no longer zero and extends over the occupied states:

$$\begin{aligned}\vec{j} &= \frac{-|e|\hbar}{8\pi^3} \int_{(\text{k occupied})} \vec{v}(\vec{k}) d\vec{k} = \\ &= \frac{-|e|\hbar}{8\pi^3} \int_{1\text{st.Br.z.}} \vec{v}(\vec{k}) d\vec{k} - \frac{-|e|\hbar}{8\pi^3} \int_{(\text{k empty})} \vec{v}(\vec{k}) d\vec{k} = \\ &= \frac{|e|\hbar}{8\pi^3} \int_{(\text{k empty})} \vec{v}(\vec{k}) d\vec{k}\end{aligned}$$

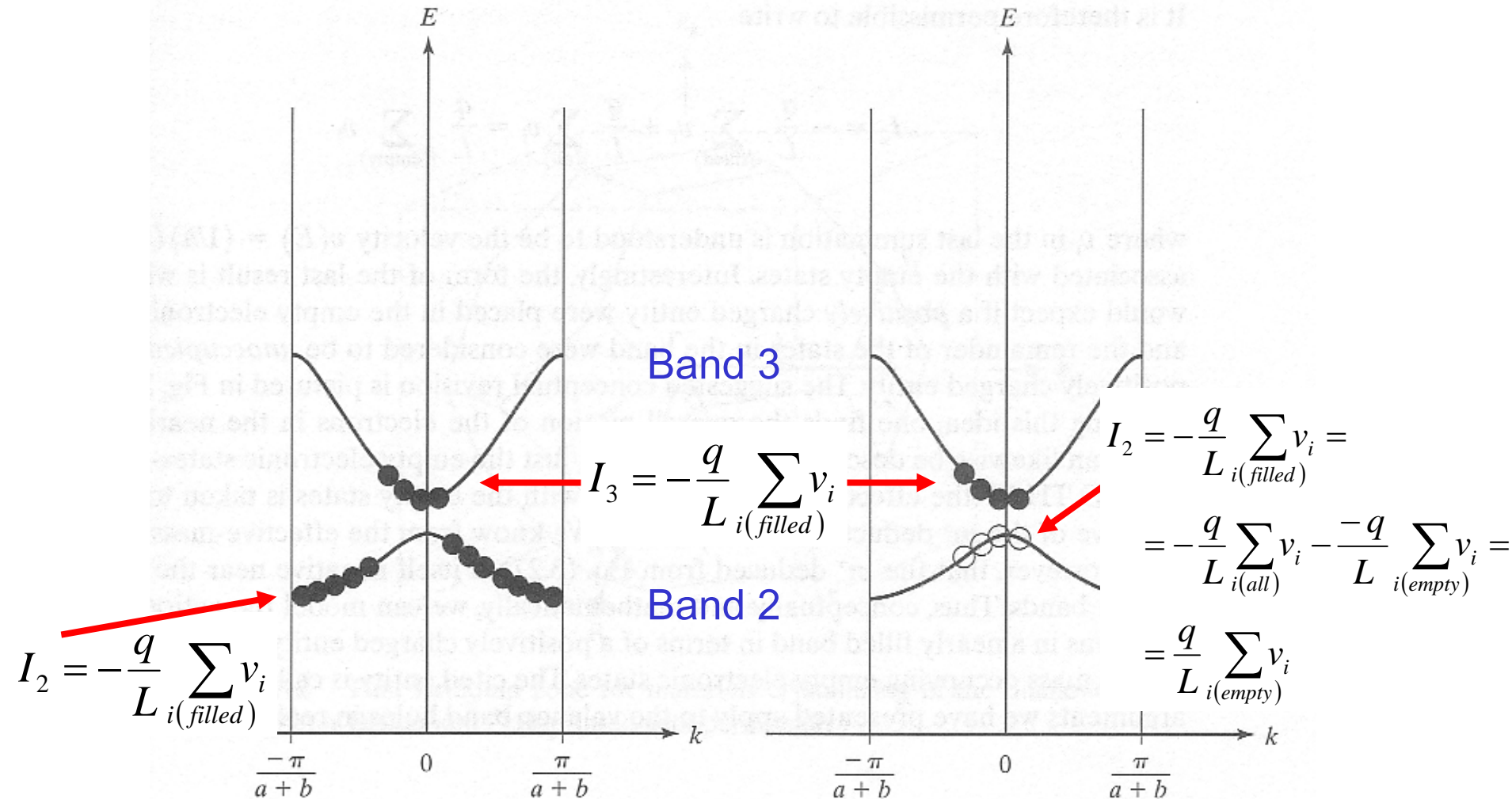
$\vec{j}(\text{full band}) \equiv 0$

Formally:

Total current density = integral over *occupied* states (*electrons*) =  
= integral over *all* states in the 1<sup>st</sup> Brillouin zone (*electrons*: **zero**, due to the symmetry in  $v(k)$ ) – integral over *empty* states (*electrons*) =  
= current of positive “quasi-particles” (“*holes*”) assigned to the *unoccupied* states of the band (“empty k”)

# Currents in bands and holes

An example: band 2 partially filled: “holes” interpretation



# Holes: effective mass

Electrons adopt the lowest energy states, so that holes are found at the upper edge of the band, where the parabolic approx. for  $E(k)$  applies, and *electrons would have negative effective mass*:

$$m^* = -|m^*| < 0 \quad \Rightarrow \quad E(\vec{k}) = E_0 - \frac{\hbar^2 k^2}{2|m^*|} \quad \begin{array}{l} \text{quadratic approx.} \\ \text{for } E(k) \end{array}$$

$$\Rightarrow \dot{\vec{v}} = \frac{1}{\hbar} \frac{d}{dt} \left[ \vec{\nabla}_k E(\vec{k}) \right] = -\frac{1}{|m^*|} \hbar \dot{\vec{k}} = -\frac{1}{|m^*|} (-|e| \vec{E}) = \frac{|e|}{|m^*|} \vec{E}$$

acceleration

group  
velocity

see  
slide #7

external force  
effective mass

The resulting equation of the motion in an external electric field is that of *positively charged particles with a positive effective mass*:  
*holes at the top of a band have positive effective mass!*



# Electrons in real crystals

Scattering on  
defects, phonons, other electrons

Boltzmann equation

Relaxation time approximation

Electrical conductivity

Drift-diffusion equation

# Scattering of electrons

- Classical theory (Drude, 1900):
  - Scattering expected from positive ions in the lattice
  - Predicted mean free path (1-5 Å) ...
  - Mean free path from data: 2 orders of magnitude higher!
- Bloch waves or Bloch packets:
  - Stationary solutions, describe unperturbed electron propagation if the periodicity is perfect
  - Possible origin of perturbations of stationary Bloch waves:
    - One-electron approximation (non-interacting electrons):
      - *Lattice defects*, fixed in time and space
      - Time-dependent deviations from periodicity: *lattice vibrations*
    - Electron-electron collisions
      - Usually much less probable!
- We will give a qualitative picture of these processes
  - Quantitative treatment: beyond our scope...!



# Scattering: transition probabilities

- ingredients of the general method to compute “transition probabilities” from “perturbation theory”:
  - Potential  $H'$  representing the additional interaction as a small perturbation of the periodic potential (Hamiltonian  $H$ )
  - Initial ( $k$ ) and final ( $k'$ ) stationary Bloch states for electrons
  - Recipe to compute the probability  $w_{k'k}$  that the initial state ( $k$ ) is scattered into the final state ( $k'$ ), from perturbation theory:

$$w_{k'k} \approx \left| \int d\vec{r} u_{k'}^* e^{-i\vec{k}' \cdot \vec{r}} H' u_k e^{-i\vec{k} \cdot \vec{r}} \right|^2$$

- These probabilities can be entered in a statistical description of how the population of electrons in available states is influenced by the scattering process, moving electrons between stationary states according to probability  $w_{k'k}$



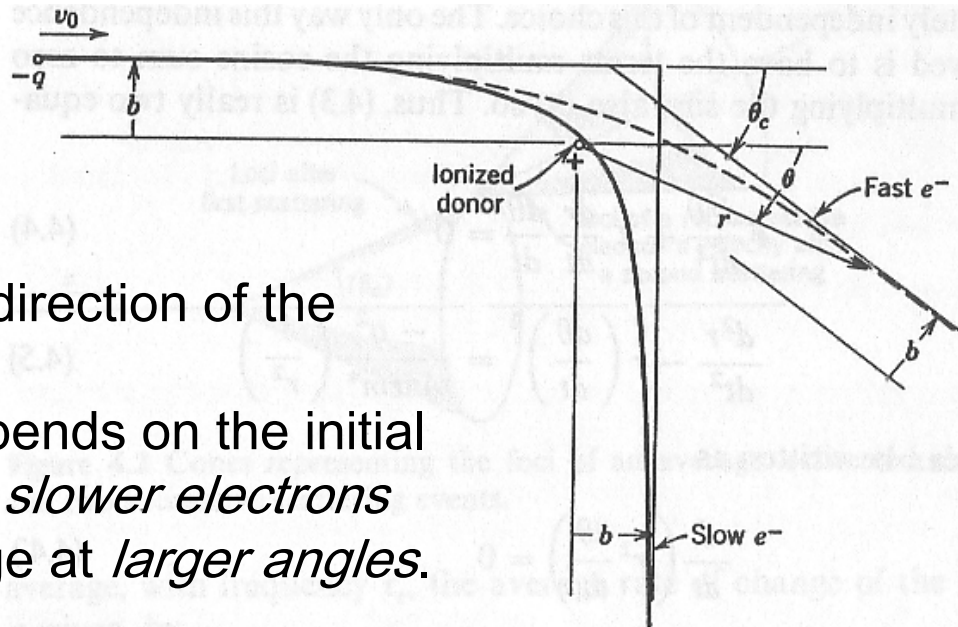
# Scattering on lattice defects



# Scattering of electrons on lattice defects - 1

- Qualitatively:

- Impurities and defects are fixed. For charged impurities:
- The electron mass is much smaller than the ion's mass
- Elastic scattering is expected, with electrons retaining their initial energy



Only the velocity (or  $k$ ) direction of the electron changes:  
the scattering angle depends on the initial velocity of the electron: *slower electrons* are scattered on average at *larger angles*.

Figure 4.1 Electron scattering by an ionized donor. Trajectories for fast and slow electrons are shown.

# Scattering of electrons on lattice defects - 2

- Quantitative result: scattering angle
  - From energy and angular momentum conservation (...):  
for a given “impact parameter  $b$ ” and “initial speed  $v_0$ ” of the incident particle (*see FELD p.157-162, WANG p.214*):

$$\tan\left(\frac{\theta_c}{2}\right) = \frac{q^2}{4\pi\epsilon m^*} \frac{1}{v_0^2 b}$$

- The scattering angle is inversely proportional to the *square* of the incident particle’s initial speed  $v_0$ , at a given impact parameter  $b$ , and increases with decreasing  $b$



# Scattering of electrons on lattice defects - 3

- Quantitative result: randomization or “relaxation” time:
  - After a large number of scattering events:
    - the *speed* (energy) distribution of the electron population does not change, but
    - the direction is randomized, for example:
      - Switch on an external electric field  $E_x \Rightarrow$  average  $v_{0x} \neq 0$
      - After switching off  $E_x \Rightarrow$  average  $v_x$  is brought back to 0
      - Exponential law: average  $v_x = v_{0x} \exp(-t / \tau_R)$
  - Randomization or “relaxation time” (*see FELD p.157-162*):

$$\tau_R \propto \frac{v_0^3}{\log\left(1 + v_0^4 b_m^2 / a^2\right)}$$

$$b_m \approx (1/2)N^{-1/3}$$

$$a = \frac{q^2}{4\pi\epsilon m^*}$$

$b_m$ : max. impact parameter  
 $N$ : defects concentration

- Fast* electrons are redistributed *slowly* (larger  $\tau_R$ ) and vice-versa
- Speed* (scalar): absolute value of *velocity* (vector)



# Scattering on phonons

# Scattering of electrons on “phonons” - 1

- What is a “phonon”? qualitatively:
  - A “phonon” is a *quantum of energy associated to a lattice vibration mode*, equivalent in many respects to the “photon” as a quantum of “electromagnetic vibrations”:
  - both photons and phonons are bosons, and share similar wave properties (Planck and DeBroglie relations)

$$E = \hbar\omega = h\nu \qquad p = \hbar k = \frac{h}{\lambda}$$

- Electron (fast) and atom (slow) dynamics:
  - Some physical properties of crystals are determined mainly by the *relatively slow* movement of atoms about their equilibrium position (for example: sound velocity and thermal properties like specific heat, thermal expansion, thermal conductivity)
  - Electrical conductivity in metals and semiconductors requires an understanding of the interaction between atom dynamics and electron dynamics, via “electron scattering on phonons”



# Scattering of electrons on “phonons” - 2

- To compute the electron-phonon scattering probability:
  - (1) From the analysis of vibrations of atomic chains:
    - derive E-k dispersion relations for phonons, and represent them in Brillouin zones (similar to what we have done for electrons!);
    - classify phonons (higher energy: “optical”; lower energy: “acoustic”; polarization: “longitudinal”, “transverse”)
  - (2) Find the number (or density) of phonons as a function of temperature, using Bose statistics (phonons = bosons)
  - (3) Understand the conditions that must be satisfied for electron-phonon scattering to take place
  - (4) Evaluate the scattering probability by counting the number of ways each scattering event could take place
    - Since the potential representing the interaction of electrons and phonons is time-dependent, their scattering is expected to be eminently *inelastic*: the electron changes energy.



# (1) E(k) for phonons - 1

Simplest model:

1-d lattice of equal atoms (mass M) interacting only with nearest neighbours by linear springs of strength K.

In this model: dispersion relation E(k):

$$\omega^2 = 2 \frac{K}{M} (1 - \cos kd)$$

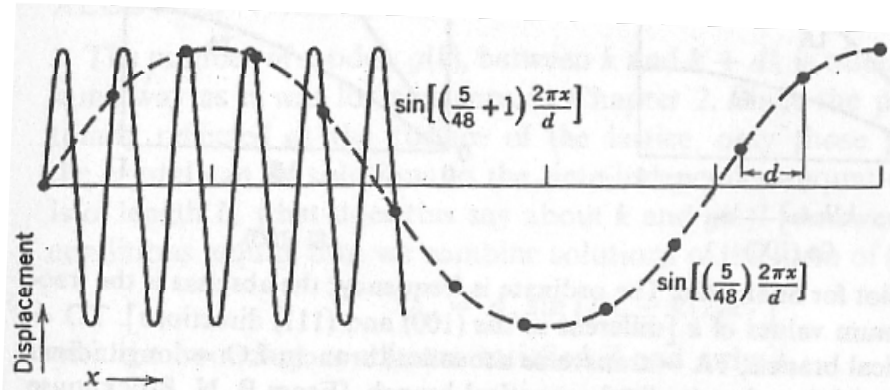


Figure 4.3 Two waves that correspond to the same sinusoidal displacement of the atoms. Since there is no way to observe the wavelength directly, and since both yield the same physically observable effect, the two waves are equivalent.

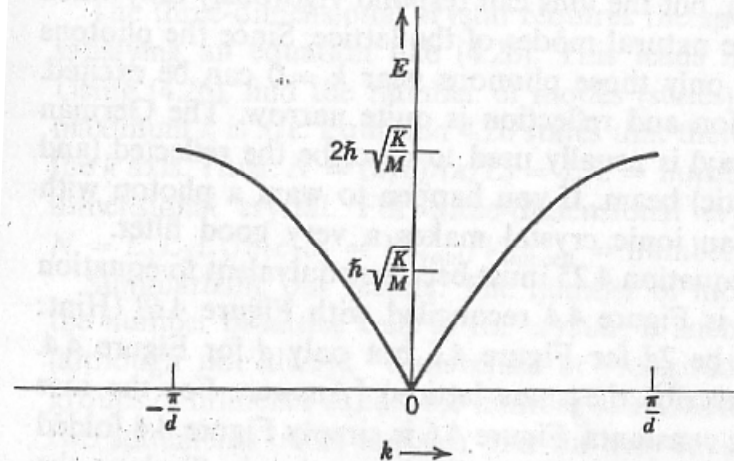


Figure 4.4 The E:k plot (also called a dispersion diagram) for one mode of a monoatomic lattice.



# (1) Lattice model for Ge, Si

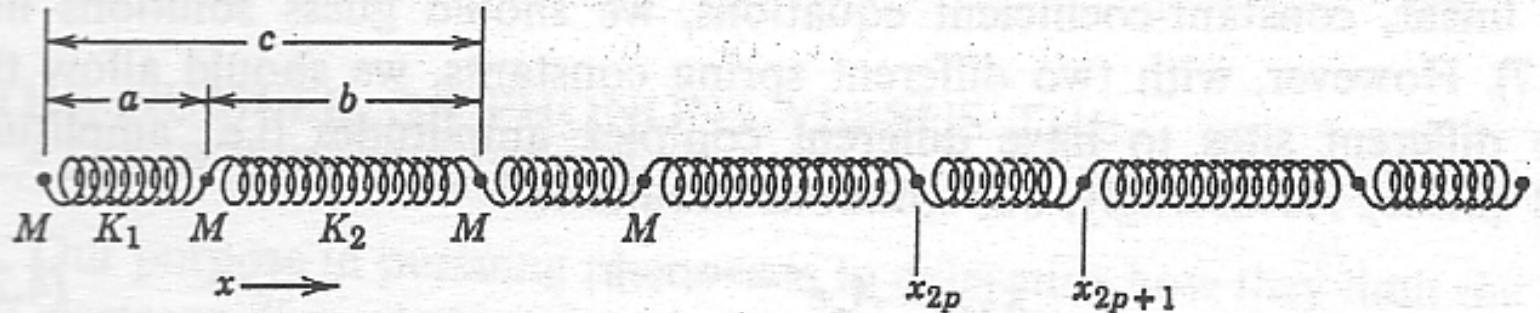


Figure 4.5 A one-dimensional monoatomic lattice with two inequivalent sites. This is a one-dimensional analog of germanium and silicon.

More realistic model,  
approaching the properties  
of Ge, Si

⇒ two relations for  $E(k)$ :  
+ “optical branch” (higher energy)  
– “acoustic branch” (lower energy)

$$\omega^2 = \frac{K_1 + K_2}{M} \pm \sqrt{\frac{K_1^2 + K_2^2}{M^2} + \frac{2K_1K_2}{M^2} \cos kc}$$



# (1) Phonon classification

“real life” for Ge, Si:  
 Transverse (T) and  
 Longitudinal (L)  
 oscillation modes for  
 Acoustic branch (A) and  
 Optical branch (O)

at small  $k$ :

*Acoustic phonons* have  
 frequencies characteristic  
 of *sound waves*

*Optical phonons* can  
 couple via ion dipole  
 moments to *infrared*  
*photons*:

$$h\nu \approx (36 \times 10^{-16} \times 10^{13}) \text{ eV} \\ \approx 4 \text{ meV}$$

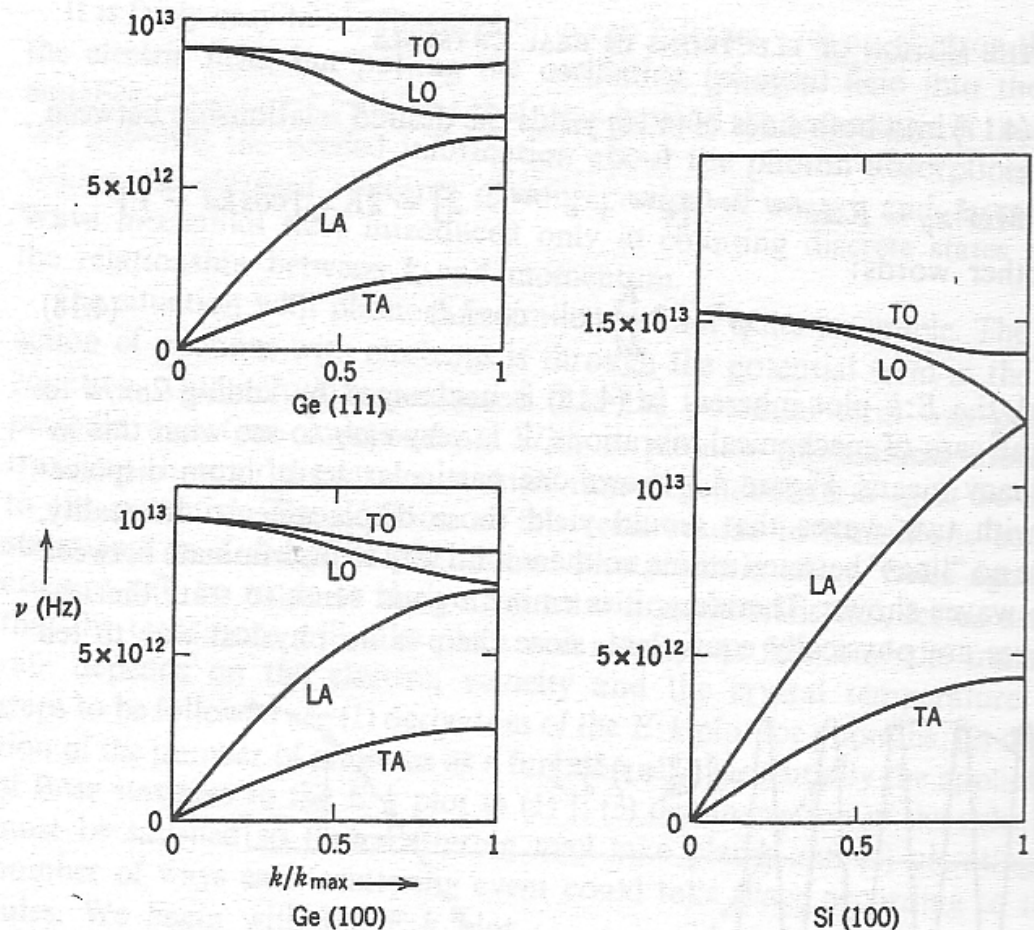


Figure 4.6  $E:k$  plot for Si and Ge. The ordinate is frequency; the abscissa is the fraction of the maximum values of  $k$  [different in the (100) and (111) directions]. TO = transverse optical branch; TA = transverse acoustical branch; LO = longitudinal optical branch; and LA = longitudinal acoustical branch. [From B. N. Brockhouse and P. K. Iyengar, *Phys. Rev.* 111, 747 (1958).]



## (2) Number of phonons and (3) scattering regimes

- Number of phonons = (number of “modes”)  $\times$  (number of phonons in each mode)
  - Number of “modes” = number of lattice cells in the crystal (computation similar to number of “states” for electrons)
  - Number of phonons in each mode at temperature  $T$ : Bose-Einstein probability distribution function (phonons=bosons!)
- From an analysis of energy ( $E$ ) and momentum ( $k$ ) conservation in electron-phonon scattering:
  - *At moderate  $T$  and low electric field:* scattering rate dominated by *low-energy acoustic phonons*
  - Larger  $T$  and/or electric field: also electrons jumping between band minima (“valleys”) contribute (with large change in  $k$ )
  - *Large electric fields:* electron drift velocity saturation due to *spontaneous emission of (higher energy) optical phonons*



# (4) electron-phonon scattering rate

- From a detailed analysis (FELD p.181, WANG p.216)

- Dominant contribution from acoustic phonons:  
rate = 1/("mean free time" between collisions):

$$R = \frac{1}{\tau_c} \propto kT v_e$$

- The electron-phonon scattering rate is proportional to the temperature  $T$  and to the electron speed  $v_e$
- Comparing with the rate for electron-impurity scattering (we found smaller rate for faster electrons):
  - *Impurity scattering* is dominant at *low* temperature  $T$
  - *Phonon scattering* is dominant at *high* temperature  $T$



# Electron-electron scattering

# Electron-electron scattering

- Naively one would expect it to be important, but:
  - It is elastic, does not change the energy and total momentum
  - Despite their high density, electrons are partially screened by the lattice, and
  - The Pauli principle allows electrons to scatter only if they can find appropriate empty final states !!!
- As a result:
  - Many orders of magnitude less probable than scattering on defects and phonons
  - To a good approximation, in most conditions electron-electron scattering can be neglected!



# The Boltzmann Equation

# Basic idea

- In the statistical approach, all properties of a system (i.e.: electrons in a semiconductor crystal) can be deduced, once the probability density function  $f$  of its components (electrons) in the appropriate “phase-space” (position and momentum or wave number) is known:
  - For instance, drift velocity of electrons in a semiconductor: computed as the average of the (group) velocities of individual electrons, weighted by the pdf  $f$ ;

$$\vec{u}(\vec{r}, t) = \frac{\frac{1}{4\pi^3} \int \vec{v}_g(\vec{r}, \vec{k}) f(\vec{r}, \vec{k}, t) d^3\vec{k}}{n(\vec{r}, t)}$$

- Electrical current density: similar method... (see later)
- The first common task is to find the pdf, on- and off-(thermal) equilibrium

# Carriers distribution off-equilibrium ?

- What happens when...
  - ... the distribution of carriers, originally in thermal equilibrium, is altered by the presence of *external forces* and by *scattering processes* ?

Thermal equilibrium:  
Fermi distribution

$$f_0 \left[ E(\vec{k}) \right] = \frac{1}{e^{\left[ E(\vec{k}) - E_F \right] / kT} + 1}$$

Away from equilibrium:

Boltzmann distribution function =  
= probability of finding an electron  
in a small phase space volume

$(dx \, dy \, dz \, dk_x \, dk_y \, dk_z)$

at position  $r$ , momentum  $k$  and time  $t$ :

$$f(\vec{r}, \vec{k}, t)$$

⇒ Set up a differential continuity equation (Boltzmann equation, describing in general all transport phenomena) for the pdf  $f$

⇒ Book-keeping of all possible changes with time of the number of electrons in a given phase space  $(d^3r \, d^3k)$  volume





# The Boltzmann Equation - 1

In the absence of scattering:

Time evolution in phase space

$$t: \quad \vec{r}, \quad \vec{k}$$

$$t' = t + dt: \quad \vec{r}' = \vec{r} + \vec{v}dt, \quad \vec{k}' = \vec{k} + (-e)\vec{E} dt/\hbar$$

Example of  $k$  changing because of an external field:  $d(\hbar k) = (-eE)dt$

$r$  changing because of velocity:  $dr = vdt$

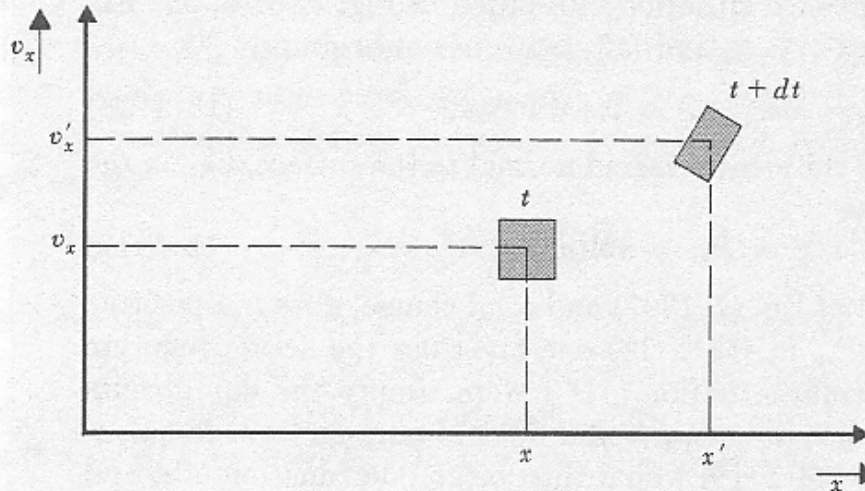


Fig. 13·2·1 Figure illustrating the motion of a particle in one dimension in a two-dimensional phase space specified by the particle position  $x$  and its velocity  $v_x$ .

# The Boltzmann Equation - 2

Conservation of the number of particles (electrons):

$$f(\vec{r}', \vec{k}', t') d^3\vec{r}' d^3\vec{k}' = f(\vec{r}, \vec{k}, t) d^3\vec{r} d^3\vec{k}$$

$$d^3\vec{r}' d^3\vec{k}' = d^3\vec{r} d^3\vec{k} \Rightarrow f(\vec{r}', \vec{k}', t') - f(\vec{r}, \vec{k}, t) = 0$$



Phase-space volume-element: it can be distorted in shape, but (it can be shown that) its volume remains constant !

$$\Rightarrow \left[ \left( \frac{\partial f}{\partial x} \dot{x} + \frac{\partial f}{\partial y} \dot{y} + \frac{\partial f}{\partial z} \dot{z} \right) + \left( \frac{\partial f}{\partial k_x} \dot{k}_x + \frac{\partial f}{\partial k_y} \dot{k}_y + \frac{\partial f}{\partial k_z} \dot{k}_z \right) + \frac{\partial f}{\partial t} \right] = 0$$

$$\frac{\partial f}{\partial t} + \vec{\nabla}_{\vec{r}} f \cdot \dot{\vec{r}} + \vec{\nabla}_{\vec{k}} f \cdot \dot{\vec{k}} = 0$$

Boltzmann Equation  
in compact (gradient) notation  
in the absence of scattering



# The Boltzmann Equation - 3

With the additional scattering contribution:

$$\frac{\partial f}{\partial t} + \vec{\nabla}_{\vec{r}} f \cdot \dot{\vec{r}} + \vec{\nabla}_{\vec{k}} f \cdot \dot{\vec{k}} = \left( \frac{\partial f}{\partial t} \right)_S$$

$$\dot{\vec{r}} = \vec{v} \quad \dot{\vec{k}} = -e\vec{E}/\hbar$$

$$\frac{\partial f}{\partial t} = -\vec{v} \cdot \vec{\nabla}_{\vec{r}} f + \frac{e}{\hbar} \vec{E} \cdot \vec{\nabla}_{\vec{k}} f + \left( \frac{\partial f}{\partial t} \right)_S$$

Net particle flux in-out  
phase-space element  
due to velocity  
(change in position)

Net particle flux in-out  
phase-space element  
due to acceleration  
(change in velocity or  $k$ )

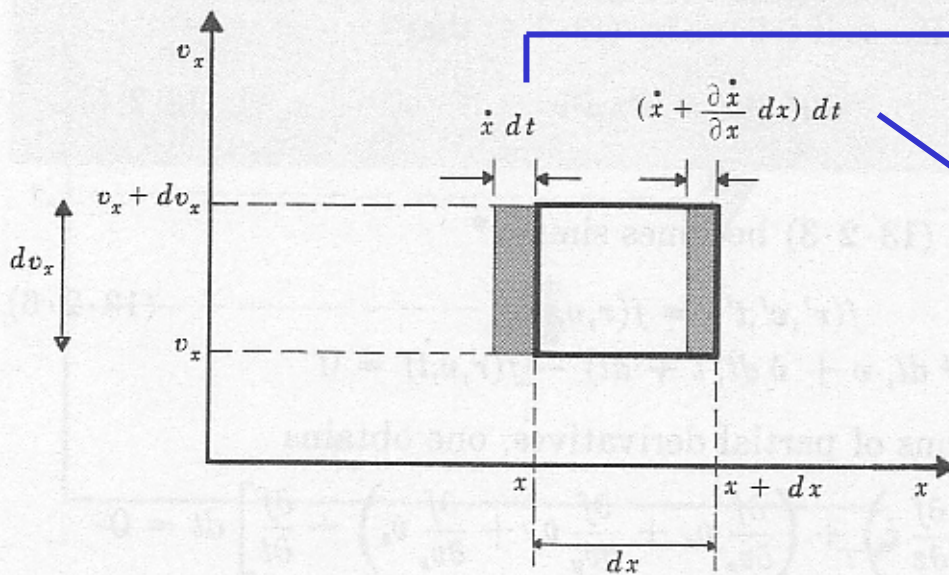
Net particle flux in-out  
phase-space element  
due to scattering  
(change in velocity or  $k$ )

# Boltzmann Equation: interpretation

What is the meaning of the terms containing gradients, for instance:

$$-\vec{v} \cdot \vec{\nabla}_{\vec{r}} f = \boxed{-v_x \frac{\partial f}{\partial x}} - v_y \frac{\partial f}{\partial y} - v_z \frac{\partial f}{\partial z}$$

Net particle flux (in-out) a phase-space element: consider for example the x-projection, for the position part:



Incoming electrons:

$$f(x, y, z, \vec{k}, t) dy dz d^3 \vec{k} v_x dt$$

Outgoing electrons:

$$f(x + dx, y, z, \vec{k}, t) dy dz d^3 \vec{k} v_x dt$$

Net flux (in-out):

$$v_x [f(x, y, z, \vec{k}, t) - f(x + dx, y, z, \vec{k}, t)] dy dz d^3 \vec{k} dt = \boxed{-v_x \frac{\partial f}{\partial x}} dx dy dz d^3 \vec{k} dt$$

Similar for the other projections of position and  $k$ !

Fig. 13·2·2 Figure illustrating a fixed element of volume of phase space for a particle moving in one dimension and specified by its position  $x$  and velocity  $v_x$ .

# Scattering term & relaxation-time approx.

Scattering term: in principle computed from scattering probability  $w_{kk'}$  and from the pdf  $f$ ; the net effect is in general:

$$\left( \frac{\partial f(\vec{k})}{\partial t} \right)_s = \frac{V}{(2\pi)^3} \int d\vec{k}' \left\{ \overbrace{\left(1 - f(\vec{k})\right) w_{kk'}}^{k \rightarrow k'} f(\vec{k}') - \left(1 - f(\vec{k}')\right) w_{k'k} f(\vec{k}) \right\}$$

For the scattering to take place (Pauli Principle):  
initial state must be filled ( $f$ ), final state must be empty ( $1-f$ )

“relaxation time approximation”

$$\left( \frac{\partial f(\vec{k})}{\partial t} \right)_s = - \frac{f(\vec{k}) - f_0(\vec{k})}{\tau(\vec{k})}$$

Assumptions on the effect of collisions:  
restore the local equilibrium described by  $f_0$ ,  
changing  $f$  back to  $f_0$  exponentially,  
with a relaxation time of the order  
of the time between collisions

# Boltzmann Equation solutions

# Boltzmann Equation solutions

- To understand how this equation works, and the meaning of the “relaxation time”, let us consider a “simple” case with no dependence on the position in the crystal, and let us find the solutions for the non-equilibrium pdf  $f$  in two interesting cases:
  - 1) An applied electric field brings the system to a non-equilibrium *stationary* condition (steady current)
  - 2) The electric field is switched off and the system “*relaxes back*” to the equilibrium state, in a characteristic time.



# Stationary non-equilibrium solution (1)

Under the influence of an external field, a stationary non-equilibrium condition can be reached: in a simple case with  $f$  not dependent on position:

$$\vec{\nabla}_{\vec{r}} f = 0 \quad (\text{not dep. on position}) \qquad \frac{\partial f}{\partial t} = 0 \quad (\text{stationary})$$

The Boltzmann equation is reduced to:

$$-\frac{e}{\hbar} \vec{E} \cdot \vec{\nabla}_{\vec{k}} f = -\frac{f(\vec{k}) - f_0(\vec{k})}{\tau(\vec{k})}$$

$$f(\vec{k}) = f_0(\vec{k}) + \frac{e}{\hbar} \vec{E} \cdot \vec{\nabla}_{\vec{k}} f(\vec{k})$$

Approximate solution:  
the normal Fermi  
function, computed at  
shifted values of  $k$   
(see next slide)

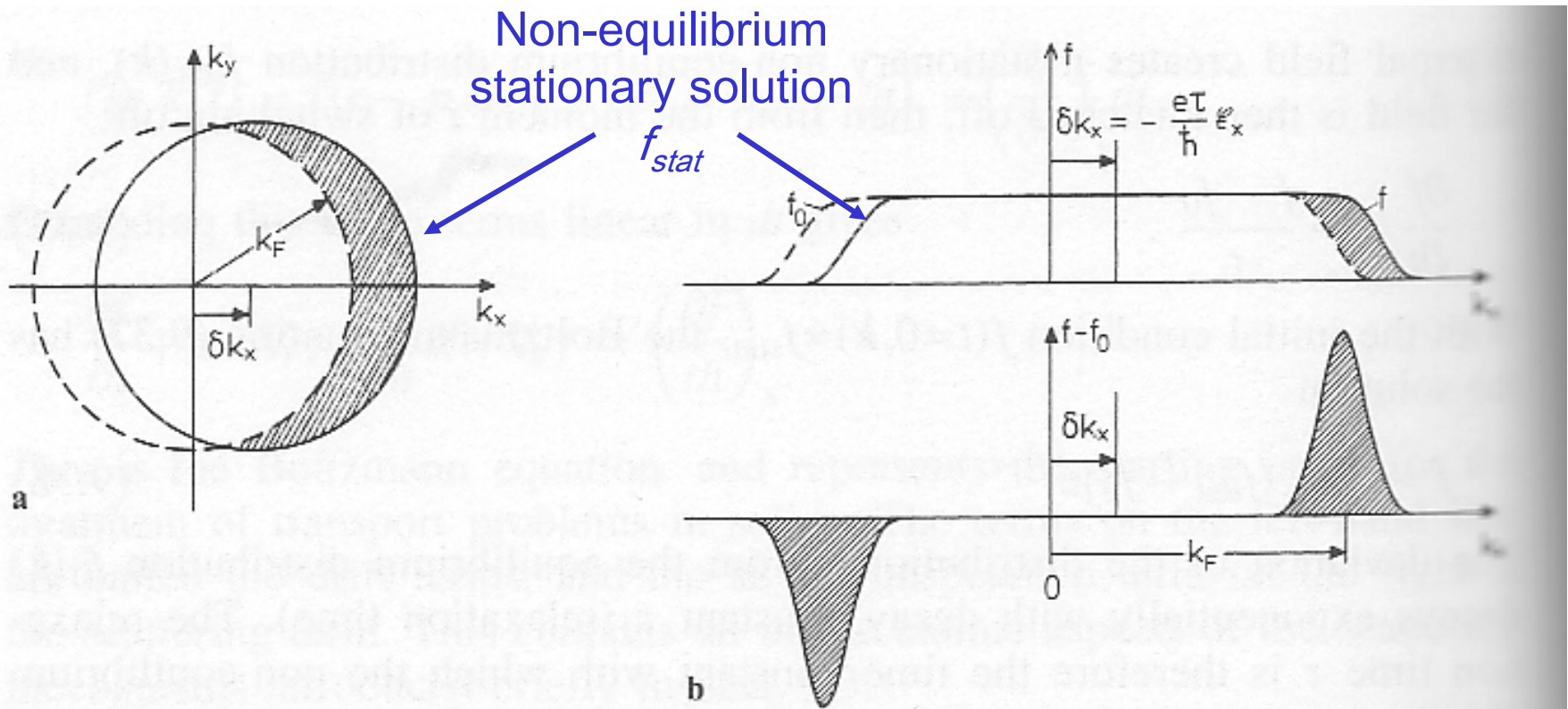
Approximate linearized solution for small fields:

$$f(\vec{k}) \cong f_0\left(\vec{k} + \frac{e}{\hbar} \tau(\vec{k}) \vec{E}\right)$$

Results from the action of the external field  $E$   
and includes the effects of scattering ( $\tau$ )



# Non-equilibrium stationary solution



**Fig. 9.4 a, b.** The effect of a constant electric field  $\mathcal{E}_x$  on the  $k$ -space distribution of quasi-free electrons: (a) The Fermi sphere of the equilibrium distribution [---, centered at  $(0,0,0)$ ] is displaced in the stationary state by an amount  $\delta k_x = -e\tau \mathcal{E}_x / \hbar$ . (b) The new Fermi distribution  $f(E(k))$  only differs significantly from the equilibrium distribution  $f_0$  (---) in the vicinity of the Fermi energy (Fermi radius)

# Relaxation to the equilibrium distribution (2)

At  $t=0$ , when the system is in the stationary non-equilibrium condition  $f_{stat}$  the external field is switched off (initial condition).

The Boltzmann equation in the “relaxation approximation” is then reduced to, for  $t > 0$ :

$$\frac{\partial f}{\partial t} = -\frac{f - f_0}{\tau}$$
$$f(t = 0) = f_{stat}$$

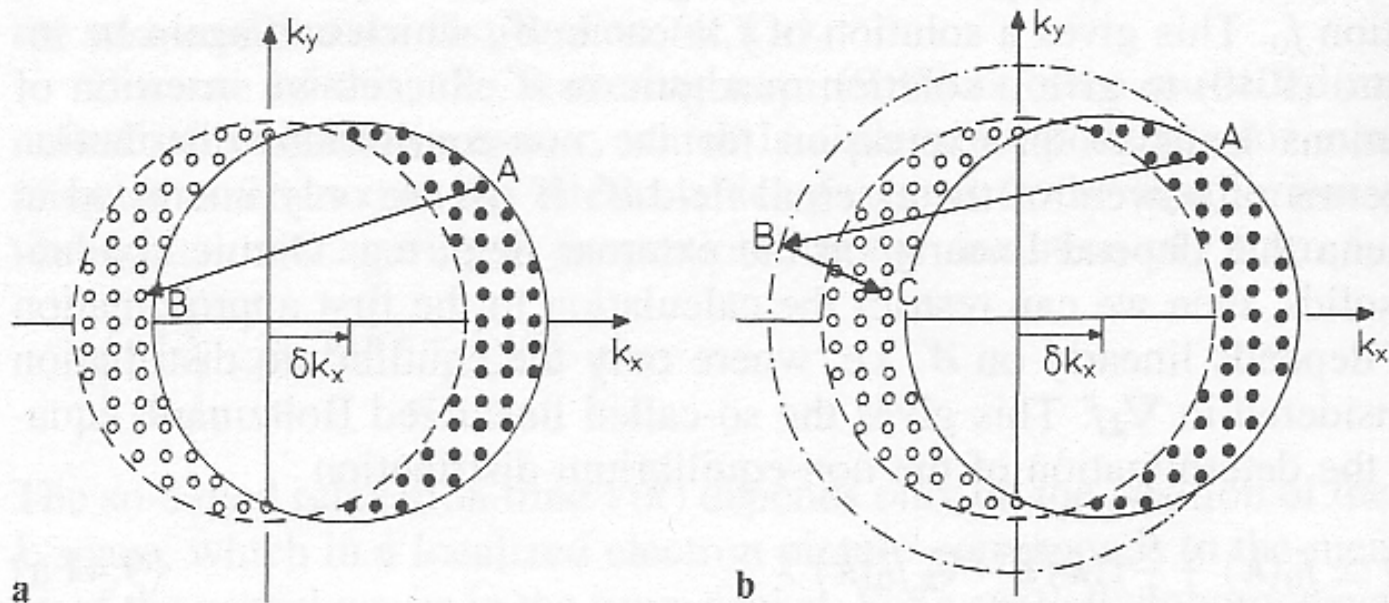
Solution:

$$f - f_0 = (f_{stat} - f_0)e^{-t/\tau}$$

The meaning of  $\tau$  is now clear: it is the time needed by the system to “relax back” to the equilibrium state, under the action of the scattering processes



# Relaxation to equilibrium



**Fig. 9.5 a, b.** Electron scattering processes in  $k$ -space. The dashed circle represents the Fermi surface in thermodynamic equilibrium ( $\mathcal{E} = 0$ ). Under the influence of an electric field  $\mathcal{E}_x$  and for a constant current, the Fermi surface is displaced as shown by the full circle. (a) When the electric field is switched off, the displaced Fermi surface relaxes back to the equilibrium distribution by means of electron scattering from occupied states ( $\bullet$ ) to unoccupied states ( $\circ$ ). Since the states  $A$  and  $B$  are at different distances from the  $k$ -space origin (i.e., have different energies), the relaxation back to equilibrium must involve inelastic scattering events (e.g., phonon scattering). (b) For purely elastic scattering (from states  $A$  to  $B$ ), the Fermi sphere would simply expand. When the field is switched off, equilibrium can only be achieved by inelastic scattering into states  $C$  within the dashed (equilibrium) Fermi sphere

# Conductivity in metals and semiconductors

# Electrical conductivity - old

- In the first part of the course:
  - we wrote down a relation between carrier drift velocity and external electric field, introducing conductivity and mobility
  - It was based on simple assumptions about not well identified scattering processes for electrons
  - The original model (Drude, 1900) assumed an ideal electron gas with all free electrons contributing to conduction (This point of view is in contradiction with the Pauli principle!)

$$m\dot{v} + \frac{m}{\tau}v_D = -eE$$

$$\dot{v} = 0 \Rightarrow v_D = -\frac{e\tau}{m}E \Rightarrow j = -env_D = ne\mu E = \frac{e^2 n \tau}{m}E$$

Drude  
model:

$$\sigma = \frac{j}{E} = \frac{e^2 n \tau}{m}$$

$$\mu = \left| \frac{v_D}{E} \right| = \frac{e\tau}{m}$$



# Electrical conductivity - new

- Let us consider the implications of the new concepts:
  - Electrons in crystals are a Fermi gas: due to the Pauli principle only the electrons close to the Fermi surface can contribute!
  - The current density can be computed summing the contributions of all states in the first Brillouin zone, and assuming for small fields the approximate linearized solution to the Boltzmann equation just discussed (assume  $E=E_x$ )

$$\vec{j}_n = \frac{1}{8\pi^3} \int_{1st.Br.z.} \vec{v}(\vec{k}) f(\vec{k}) d\vec{k} \quad \text{Particle current density}$$

$$\vec{j} = -\frac{e}{8\pi^3} \int_{1st.Br.z.} \vec{v}(\vec{k}) f(\vec{k}) d\vec{k} = \quad \text{electrical current density}$$

$$= -\frac{e}{8\pi^3} \int_{1st.Br.z.} d\vec{k} \vec{v}(\vec{k}) \left[ f_0(\vec{k}) + \frac{e\tau(\vec{k})}{\hbar} E_x \frac{\partial f_0}{\partial k_x} \right]$$

# Electrical conductivity in metals - 1

- Developing these expressions:
  - The integral becomes a surface integral at the Fermi surface in k-space
  - Only the properties at the Fermi surface are important
    - Electron velocity, Relaxation time, Effective mass
  - The result is (explicit derivation beyond our scope, see Ibach p.245-249)

$$\sigma = \frac{j_x}{E_x} \cong \frac{e^2 \tau(E_F)}{m^*} n, \quad \mu \cong \frac{e \tau(E_F)}{m^*}$$

- Formally equivalent to the Drude model, but now:
  - Well defined relaxation time (electrons at the Fermi level)
  - Effective mass instead of free electron mass
  - $n$  = total concentration of electrons in the “conduction band”





# Electrical conductivity in metals - 2

- From these expressions:

$$\sigma = \frac{j_x}{E_x} \cong \frac{e^2 \tau(E_F)}{m^*} n, \quad \mu \cong \frac{e \tau(E_F)}{m^*}$$

- Correct orders of magnitude!
- Correct temperature-dependence of conductivity
  - Concentration  $n$  of carriers: not dependent on  $T$
  - $T$ -dependence entirely from the relaxation time, evaluated at the Fermi energy  $E_F$

$$\rho \equiv \frac{1}{\sigma} \propto \frac{1}{\tau} = \frac{1}{\tau_{\text{phonons}}} + \frac{1}{\tau_{\text{defects}}} \Rightarrow \rho = \rho_{\text{ph}}(T) + \rho_{\text{def}}$$

phonons contribution:  
approx. linear in  $T$

defects contribution:  
approx. constant in  $T$

At "high"  $T$





# Electrical conductivity in metals - 3

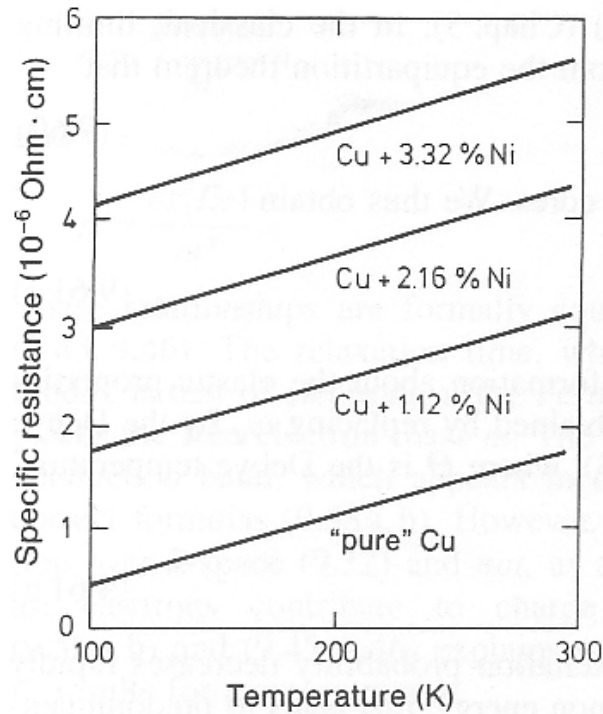


Fig. 9.7. Resistivity  $\rho$  of pure copper and of copper-nickel alloys of various compositions. (After [9.4])

$$\rho \equiv \frac{1}{\sigma} \propto \frac{1}{\tau} = \frac{1}{\tau_{\text{phonons}}} + \frac{1}{\tau_{\text{defects}}} \Rightarrow \rho = \rho_{\text{ph}}(T) + \rho_{\text{def}}$$

phonons contribution:  
approx. linear in  $T$

defects contribution:  
approx. constant in  $T$

At "high"  $T$



# Electrical conductivity in semiconductors - 1

- Both electrons in lower conduction band and holes in upper valence band contribute:

$$\vec{j} = e(n\mu_n + p\mu_p)\vec{E} \quad \mu = \frac{e}{m^*} \frac{\langle \tau(\vec{k})v^2(\vec{k}) \rangle}{\langle v^2(\vec{k}) \rangle}$$

The expression for the mobility is obtained (...) averaging over the appropriate states at the edges of the conduction (electrons) or valence (holes) band

Qualitatively: continuing this computation one obtains:

$$\mu \propto \tau \quad \frac{1}{\tau} \propto \langle v \rangle \Sigma$$

Average velocity  $\nearrow$  scattering "cross-section"  $\uparrow$

phonons:  $\langle v \rangle \propto \sqrt{T}$ ,  $\Sigma_{\text{ph}} \propto T$   
 defects:  $\langle v \rangle \propto \sqrt{T}$ ,  $\Sigma_{\text{def}} \propto \langle v \rangle^{-4} \propto T^{-2}$

$\Rightarrow$

phonons:  $\mu_{\text{ph}} \propto T^{-3/2}$   
 defects:  $\mu_{\text{def}} \propto T^{3/2}$

# T – dependence of mobility in semiconductors

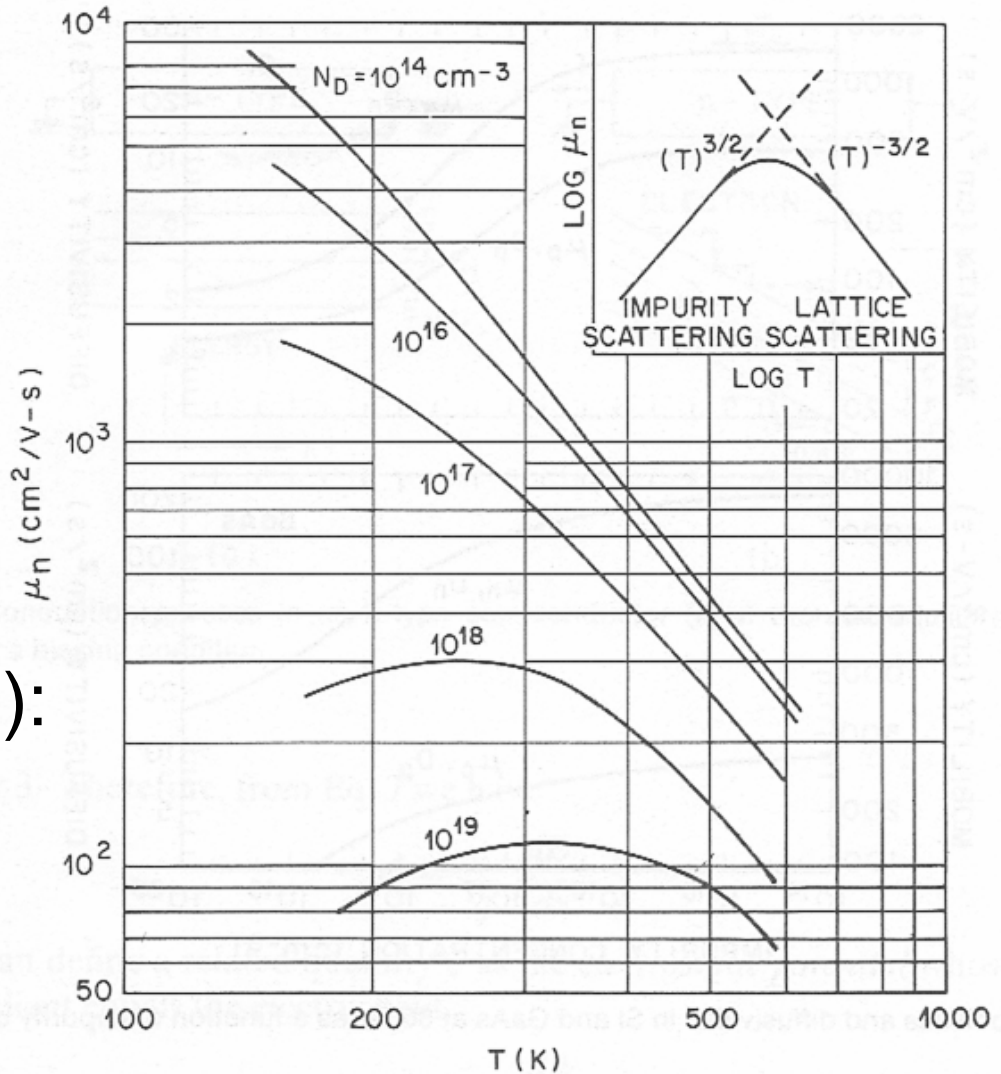
(See also Lecture 4)

Scattering on phonons (lattice):

$$\mu_{\text{ph}} \propto \tau_{\text{ph}} \propto T^{-3/2}$$

Scattering on defects (impurities):

$$\mu_{\text{def}} \propto \tau_{\text{def}} \propto T^{3/2}$$



# Drift-Diffusion Continuity Equation

# From the Boltzmann Equation...

- The continuity equations for the electrical current density in semiconductors can be obtained from the Boltzmann equation:

$$\frac{\partial f}{\partial t} = -\vec{v}_g \cdot \vec{\nabla}_{\vec{r}} f - \frac{\vec{F}}{\hbar} \cdot \vec{\nabla}_{\vec{k}} f - \frac{f - f_0}{\tau} \quad \vec{F} = -e\vec{E}$$

Force on electrons

- Multiplying by the group velocity and integrating over the momentum space  $dk_x dk_y dk_z$ :

$$\int \vec{v}_g \frac{\partial f}{\partial t} d^3\vec{k} = - \int \vec{v}_g (\vec{v}_g \cdot \vec{\nabla}_{\vec{r}} f) d^3\vec{k} - \int \vec{v}_g \left( \frac{\vec{F}}{\hbar} \cdot \vec{\nabla}_{\vec{k}} f \right) d^3\vec{k} - \int \vec{v}_g \frac{f - f_0}{\tau} d^3\vec{k}$$

- One obtains the continuity equation discussed in Lectures 6-8...  
(detailed derivation: see FELD p.187-194, MOUT p.100-104)

# ...integrals (1, 2)...

Do not depend on time

First term:

$$\int \vec{v}_g \frac{\partial f}{\partial t} d^3\vec{k} = \frac{\partial}{\partial t} \int \vec{v}_g f d^3\vec{k} = \frac{\partial}{\partial t} (4\pi^3 \vec{u}n) = 4\pi^3 \frac{\partial(\vec{u}n)}{\partial t} = 0$$

$$\vec{u}(\vec{r}, t) = \frac{1}{4\pi^3} \frac{\int \vec{v}_g(\vec{r}, \vec{k}) f(\vec{r}, \vec{k}, t) d^3\vec{k}}{n(\vec{r}, t)}$$

Second term:

$$\int \vec{v}_g (\vec{v}_g \cdot \vec{\nabla}_{\vec{r}} f) d^3\vec{k} = \vec{\nabla}_{\vec{r}} \int \vec{v}_g (\vec{v}_g f) d^3\vec{k} = \dots = \frac{4\pi^3}{m} \vec{\nabla}_{\vec{r}} (nk_B T)$$

Kinetic energy, equipartition theorem:

# ...integrals (3, 4)...

Third term:

Integrating  
by parts

$$\int \vec{v}_g \left( \frac{\vec{F}}{\hbar} \cdot \vec{\nabla}_{\vec{k}} f \right) d^3 \vec{k} = \frac{\vec{F}}{\hbar} \int \vec{v}_g (\vec{\nabla}_{\vec{k}} f) d^3 \vec{k} = \frac{\vec{F}}{\hbar} \int \frac{\hbar \vec{k}}{m} (\vec{\nabla}_{\vec{k}} f) d^3 \vec{k} =$$

$$= \frac{\vec{F}}{m} \int (\vec{\nabla}_{\vec{k}} (\cancel{\vec{k}f}) - f \vec{\nabla}_{\vec{k}} \vec{k}) d^3 \vec{k} = -\frac{\vec{F}}{m} \int f d^3 \vec{k} = -4\pi^3 n \frac{\vec{F}}{m}$$

$\left[ \vec{k}f \right]_{-\infty}^{+\infty} = 0$ 
 $\int f d^3 \vec{k} = 4\pi^3 n$

Fourth term:

$$\int \vec{v}_g \frac{f - f_0}{\tau} d^3 \vec{k} = \frac{1}{\tau} \left( \int \vec{v}_g f d^3 \vec{k} - \int \vec{v}_g \cancel{f_0} d^3 \vec{k} \right) = \frac{4\pi^3 n \vec{u}}{\tau}$$

average velocity = 0  
at equilibrium



# ...continuity equation!

Substituting in:

$$\int \vec{v}_g \frac{\partial f}{\partial t} d^3\vec{k} = - \int \vec{v}_g (\vec{v}_g \cdot \vec{\nabla}_{\vec{r}} f) d^3\vec{k} - \int \vec{v}_g \left( \frac{\vec{F}}{\hbar} \cdot \vec{\nabla}_{\vec{k}} f \right) d^3\vec{k} - \int \vec{v}_g \frac{f - f_0}{\tau} d^3\vec{k}$$

$$\frac{\partial(n\vec{u})}{\partial t} + \frac{1}{m} \vec{\nabla}_{\vec{r}}(nk_B T) - n \frac{\vec{F}}{m} = - \frac{n\vec{u}}{\tau}$$

introducing:

$$\begin{aligned} \vec{F}_n &= -q\vec{E} & \vec{F}_p &= q\vec{E} \\ \vec{J}_n &= -qn\vec{u}_n & \vec{J}_p &= -qp\vec{u}_p \\ \mu_n &= q\tau_n/m & \mu_p &= q\tau_p/m \end{aligned}$$

and multiplying by  $q\tau$ :

$$\tau_n \frac{\partial \vec{J}_n}{\partial t} + \vec{J}_n = qn\mu_n \left( \vec{E} + \frac{1}{n} \frac{k_B T}{q} \vec{\nabla}_{\vec{r}} n + \frac{k_B}{q} \vec{\nabla}_{\vec{r}} T \right)$$

For electrons (similar for holes):



# Drift-diffusion continuity equation

For electrons (similar for holes):

$$\tau_n \frac{\partial \vec{J}_n}{\partial t} + \vec{J}_n = qn\mu_n \left( \vec{E} + \frac{1}{n} \frac{k_B T}{q} \vec{\nabla}_{\vec{r}} n + \frac{k_B}{q} \vec{\nabla}_{\vec{r}} T \right)$$

Drift

Diffusion

The two familiar terms

relaxation time  $\tau$  is small:  
This new term can be neglected  
if frequency is not too high  
(few hundred MHz)

Temperature gradient:  
We did not discuss this before!  
Also a temperature gradient  
can drive an electric current

# Lectures 20, 21 – summary - 1

- We revisited the properties of electrons, treated as Bloch waves, and holes, in a “perfect crystal”: effective mass, currents
- The description of electrons in “real” crystals has to take into account scattering processes on impurities or defects and on phonons (lattice deformations corresponding to vibration modes)
- The Boltzmann equation governs the probability distribution function for electrons in “phase-space” (position and momentum), when the system is brought away from thermal equilibrium (Fermi pdf)
- We considered two typical non-equilibrium solutions: steady-state and relaxation towards equilibrium, in the relaxation-time approximation



# Lectures 20, 21 – summary - 2

- The qualitative and quantitative features of electrical conductivity in metals and semiconductors (for instance: conductivity, mobility, temperature dependence) are well described by considering electrons as Bloch waves and computing the relevant average quantities (drift velocity, current density etc) over k-space.
- Formally, the expressions found for conductivity and mobility are similar to those of the classical Drude model; crucial differences are the properties of relaxation time and the effective mass.
- Finally, averaging over k-space the Boltzmann transport equation, also for Bloch waves or packets one obtains the “drift-diffusion equation” for electric current densities: a detailed derivation predicts additional terms with respect to those we already discussed, for instance a diffusion term depending on temperature gradient; this treatment can be further extended.



# Lectures 20, 21 – summary - 3

- The drift-diffusion continuity equation obtained from the Boltzmann equation explicitly contains the “Einstein relation” between drift and diffusion coefficients, that we had already discussed in previous lectures
- The Boltzmann transport equation is the basis for simulations, both in the “averaged mode” (continuity equation for current densities), and in a “Monte Carlo” mode (tracing individual wave packets).
- This second mode is relevant for simulating very small devices, where carriers undergo a small number of collisions.



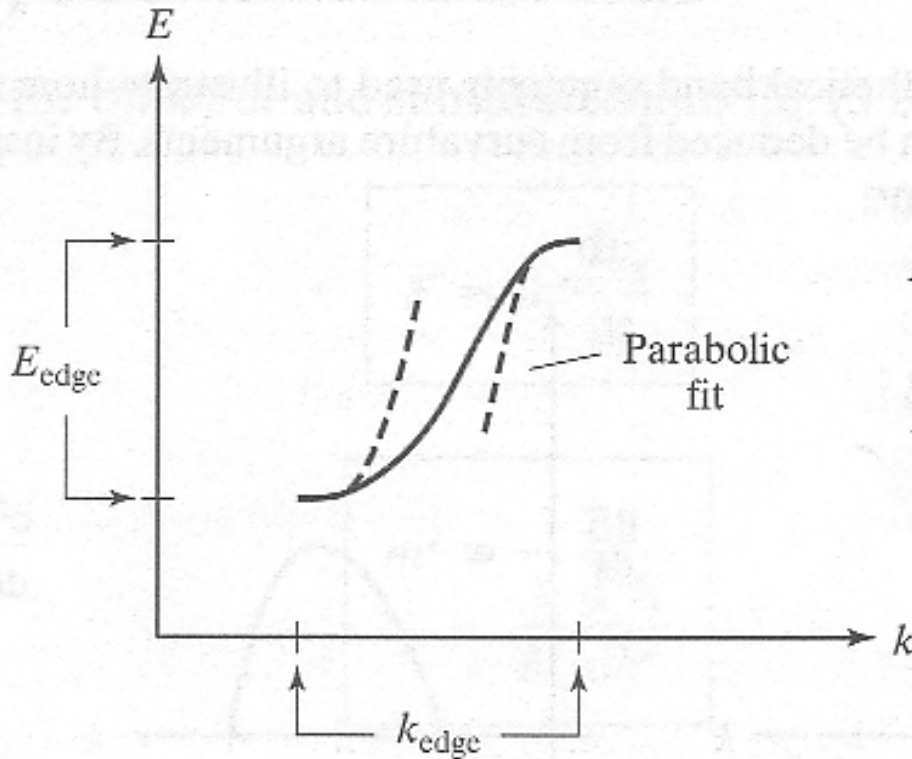
# Lectures 20, 21 - exercises

- **Exercise 20.1:** From slide 25, figure 4.6: determine the order of magnitude of phonon energies in Silicon in the different branches, at  $k=k_{\max}$ . What is the order of magnitude for  $k_{\max}$  in Silicon (1<sup>st</sup> Brillouin zone)?
- **Exercise 21.1:** Write down the expression of conductivity and mobility in the classical Drude model. What changes in these expressions in the quantum theory of conductivity for metals? And for semiconductors?
- **Exercise 20.2:** Write down the Boltzmann transport equation and the drift-diffusion continuity equation. Discuss qualitatively the meaning of each term.



**Back-up slides**

# Effective mass and E-k near band edges



near the band edges:

$$E - E_{\text{edge}} \simeq (\text{constant}) (k - k_{\text{edge}})^2$$

$$\frac{d^2E}{dk^2} \simeq \text{constant} \quad \dots E \text{ near } E_{\text{edge}}$$

... the effective mass is approximately constant (energy-independent)!

$$m^* = \frac{1}{\frac{1}{\hbar^2} \frac{d^2E}{dk^2}}$$