

“Complementi di Fisica”

Lectures 22-23

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In these lectures: contents

- **After completing the discussions of charge-carrier concentrations in semiconductors at equilibrium, now:**
- **Introduction to drift and diffusion**
- **Electrons in a real crystal**
 - **Scattering of electrons by:**
 - “defects” (elastic)
 - “phonons” (inelastic)
 - electrons ?
 - **Boltzmann transport 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**

Textbooks: references

- **Simplified approach to transport phenomena (drift and diffusion):**
 - D.A. Neamen, *Semiconductor Physics and Devices*, McGraw-Hill, 3rd ed., 2003, p.154-180 (5.1 Carrier drift, 5.2 Carrier diffusion, 5.3 Graded impurity distribution)
 - R.F.Pierret, *Advanced Semiconductor Fundamentals*, Prentice Hall, 2003, 2nd ed., p. 175-210 (6.1 Drift, 6.2 Diffusion).
 - S.M.Sze, *Semiconductor Devices - Physics and Technology*, J.Wiley & Sons, 2nd ed., 1985, p. 30-43 (2.1 Drift, 2.2 Diffusion).
- **Transport phenomena including the Boltzmann transport equation:**
 - H.Ibach, H.Luth, *Solid State Physics*, 3rd ed., Springer, p.241-250 (9.4 The Boltzmann Equation and Relaxation Time, 9.5 The Electrical Conductivity of Metals), p.409-415 (12.5 Conductivity of Semiconductors)
 - J.M.Feldman, *The Physics and Circuit Properties of Transistors*, J.Wiley&Sons, 1972, p.152-194 (4 The Motion of electrons in Real Crystals)

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Introduction

Transport of charge carriers:
Drude Model (simplified)
Drift and Diffusion

Drude Model

- **Conduction electrons:**
 - Ideal classical gas, confined in the crystal
 - Collisions with the walls and with crystal imperfections
 - Characteristic mean time τ between collisions taken as a constant
- **Why should it be at least partially OK?**
 - Response of electrons to external forces: classical dynamics, provided effective mass is used
 - Occupation probability of conduction band states for non-degenerate s.c.: Fermi-Dirac pdf approximated by the classical Boltzmann pdf
- **Weak points**
 - Quantum approach needed for collision probabilities
 - Mean time: complicated function of energy $\tau(E)$

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Drift

Drift current density (Drude model)

Random thermal motion
Statistical mechanics:
equipartition theorem
for electrons

$$\frac{1}{2} m_n^* \langle v_{th}^2 \rangle = \frac{3}{2} kT$$

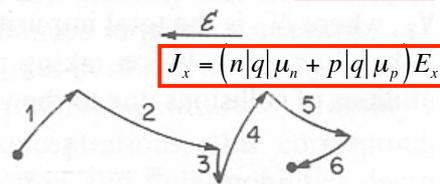
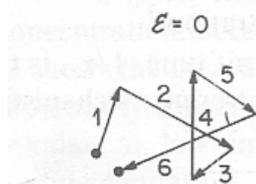
$$T = 300 \text{ K} \Rightarrow \sqrt{\langle v_{th}^2 \rangle} \approx 10^7 \text{ cm/s}$$

Drift combined with thermal motion
“classical electron”:
charge $-|q|$
effective mass m_n^*

$$-|q| E_x \tau_C = m_n^* v_n \quad E_x = \text{electric field}$$

$$v_n = - \left(\frac{|q| \tau_C}{m_n^*} \right) E_x = -\mu_n E_x \quad \mu_n \equiv \frac{|q| \tau_C}{m_n^*}$$

$$v_p = \left(\frac{|q| \tau_C}{m_p^*} \right) E_x = \mu_p E_x \quad \mu_p \equiv \frac{|q| \tau_C}{m_p^*}$$



$$J_x = (n|q|\mu_n + p|q|\mu_p) E_x$$

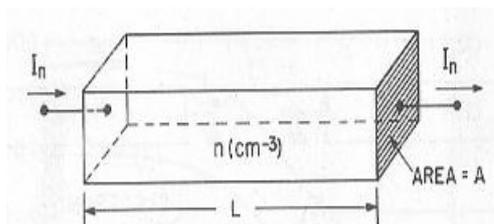
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Drift current density and conductivity

- “average” behaviour of individual carriers in an external electrical field: **drift velocity, mobility**
- collective behaviour: **current density (electrons and holes)**



$$J_x = J_{x,n} + J_{x,p} = \underbrace{(|q|n\mu_n)}_{\text{electrons}} + \underbrace{(|q|p\mu_p)}_{\text{holes}} \epsilon_x = \sigma \epsilon_x$$

Resistivity and conductivity:

$$\rho \equiv \frac{1}{\sigma} = \frac{1}{qn\mu_n + qp\mu_p} = \frac{1}{q(n\mu_n + p\mu_p)} \quad \sigma = \frac{nq^2\tau}{m_n^*} + \frac{pq^2\tau}{m_p^*}$$

Electric field

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Diffusion

Diffusion process

- **Qualitatively:**
 - *If* there is a space variation of carrier concentration in the semiconductor material: *then* carriers tend to move predominantly from a region of high concentration to a region of low concentration

Microscopic scale: in each section,

- equal out-flow to $+x$ and $-x$
- different in-flow from right and left

Net effect:
carrier concentrations tend to level out

(a)

Macroscopic scale:
current densities

$J_{n,diff}$
 $J_{p,diff}$

(b)

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Diffusion process (simplified)

Quantitative flux, for electrons:

Left to right through plane at $x = 0$

$$F_1 = \frac{1}{2} \frac{n(-l)l}{\tau_c} = \frac{1}{2} n(-l)v_{th}$$

Right to left through the same plane

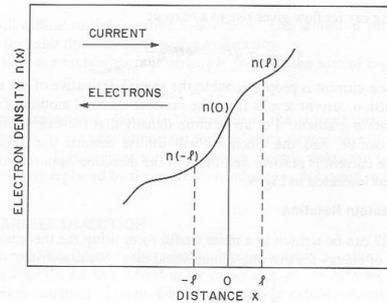
$$F_2 = \frac{1}{2} n(l)v_{th}$$

Net rate of carrier flow at $x = 0$

$$F = F_1 - F_2 = \frac{1}{2} v_{th} [n(-l) - n(l)] = -v_{th} l \frac{dn}{dx} \equiv -D_n \frac{dn}{dx}$$

$$l = v_{th} \tau_c$$

Thermal motion:
mean free path = thermal velocity \times mean free time



Taylor series expansion:

$$n(-l) = n(0) - l \left(\frac{dn}{dx} \right)_{x=0}$$

$$n(l) = n(0) + l \left(\frac{dn}{dx} \right)_{x=0}$$

Diffusion equations

- **Diffusion current, electrons (1-dimensional case):**

$$J_{n,x} = -|q|F = |q|D_n \frac{dn}{dx}$$

if positive gradient $dn/dx > 0$
then: positive current $J_{n,x} > 0$

- **Similarly, holes:**

$$J_{p,x} = |q|F = -|q|D_p \frac{dp}{dx}$$

if positive gradient $dp/dx > 0$
then: negative current $J_{p,x} < 0$

- **Diffusivity:**

$$D_n \equiv v_{th,n} l_n = v_{th,n}^2 \tau$$

$$D_p \equiv v_{th,p} l_p = v_{th,p}^2 \tau$$

Dimensionally OK;
a more complete 3-d analysis gives a numerical coefficient (1/3)

Drift and Diffusion

Drift and diffusion are correlated:
Einstein's relation

Mobility and Diffusivity

• **Mobility:**
$$\mu = \frac{|q|\tau}{m^*} \quad \text{(For electrons, holes)}$$

• **Diffusivity:**
$$D = \frac{1}{3} v_{th}^2 \tau$$

• **Einstein's relations** (from equipartition theorem)

$$\langle v_x^2 \rangle = \langle v_y^2 \rangle = \langle v_z^2 \rangle = \frac{\langle v_{th}^2 \rangle}{3} = \frac{k_B T}{m}$$

Mobility and diffusivity
are correlated !

$$D = \frac{k_B T}{m} \tau = \frac{k_B T}{|q|} \frac{|q|}{m} \tau = \frac{k_B T}{|q|} \mu \Rightarrow D/\mu = \frac{k_B T}{|q|}$$

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:**
 - Separable 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! (Pauli principle at work)
- **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:

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

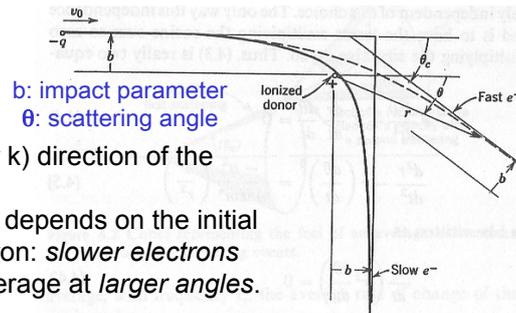
- These probabilities can be entered in a statistical description of how the population of electrons in available states is influenced by the scattering process, moving electrons between stationary states according to probability $w_{k'k}$

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 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.

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Scattering of electrons on lattice defects - 2

- **Results (semi-quantitative):**

- **scattering angle θ**

- inversely proportional to:
 - v_0^2 (squared speed)
 - b (impact parameter)

- **“relaxation” time τ_R**

- After a large number of scattering events:
 - the *speed* (energy) distribution of electrons does not change, but
 - the *direction* is randomized
- *Fast* electrons: redistributed *slowly* (larger τ_R)
- *Slow* electrons: redistributed *quickly* (smaller τ_R)

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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.

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(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):

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

$$E = \hbar \omega$$

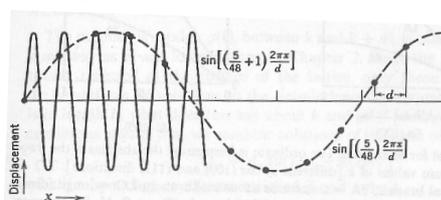


Figure 4.3 Two waves that correspond to the same sinusoidal displacement of the atoms. Since there is no way to observe the wavelength directly, and since both yield the same physically observable effect, the two waves are equivalent.

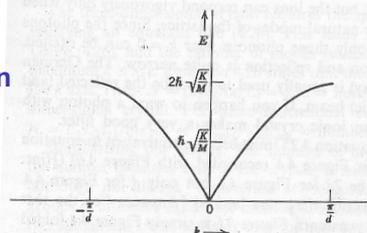


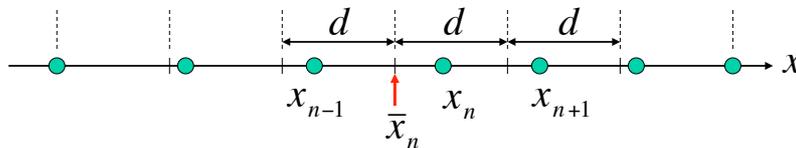
Figure 4.4 The E:k plot (also called a dispersion diagram) for one mode of a monoatomic lattice.

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(1) E(k) for phonons - 2



Classical equation for the position of the n-th atom (elastic forces)

$$M \frac{d^2 x_n}{dt^2} = -K[(x_n - x_{n+1}) - (x_{n-1} - x_n)]$$

$$x_n(t) = Ae^{i(\omega t - k \cdot nd)} \quad , \quad \text{where } \bar{x}_n = nd \text{ is the average position}$$

$$\Rightarrow -M\omega^2 x_n = KAe^{i(\omega t - k \cdot nd)} [e^{ikd} + e^{-ikd} - 2] = 2Kx_n [\cos kd - 1]$$

In this model: $\omega^2 = 2 \frac{K}{M} (1 - \cos kd)$
dispersion relation E(k): $E = \hbar\omega$

(1) Lattice model for Ge, Si

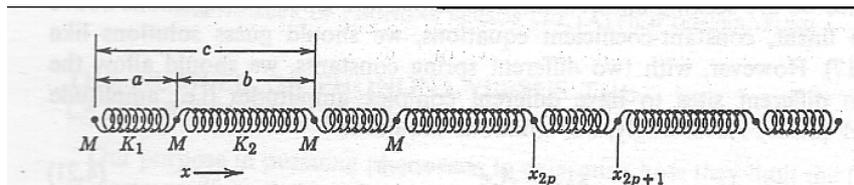


Figure 4.5 A one-dimensional monoatomic lattice with two inequivalent sites. This is a one-dimensional analog of germanium and silicon.

More realistic model, approaching the properties of Ge, Si \Rightarrow **two relations for E(k):**
 + "optical branch" (higher energy)
 - "acoustic branch" (lower energy)

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

(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:

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

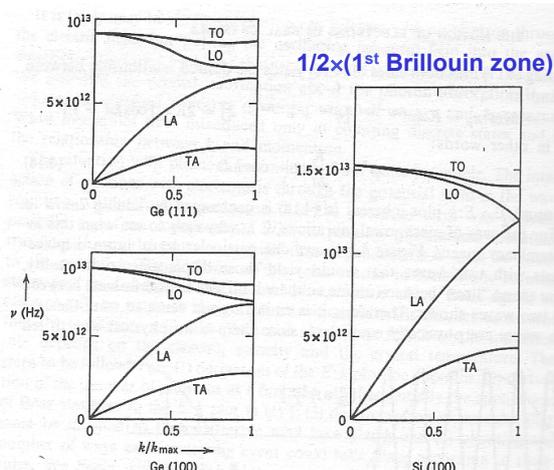


Figure 4.6 $E:k$ plot for Si and Ge. The ordinate is frequency; the abscissa is the fraction of the maximum values of k [different in the (100) and (111) directions]. TO = transverse optical branch; TA = transverse acoustical branch; LO = longitudinal optical branch; and LA = longitudinal acoustical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

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

- **Number of phonons = (number of “modes”) × (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*

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(4) electron-phonon scattering rate

- From a more 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

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Conclusion

- Comparing the rates at different temperatures

- *Impurity scattering* is dominant at *low T*
- *Phonon scattering* is dominant at *high T*

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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 ;

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

- 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**

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

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

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The Boltzmann Equation - 1d version

With the additional scattering contribution, for electrons in an external electric field:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x} \dot{x} + \frac{\partial f}{\partial k_x} \dot{k}_x = \left(\frac{\partial f}{\partial t} \right)_S$$

$$\dot{x} \equiv \frac{dx}{dt} = v_x \quad \dot{k}_x \equiv \frac{dk_x}{dt} = -eE_x/\hbar$$

$$\frac{\partial f}{\partial t} = -v_x \frac{\partial f}{\partial x} + \frac{e}{\hbar} E_x \frac{\partial f}{\partial k_x} + \left(\frac{\partial f}{\partial t} \right)_S$$

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)

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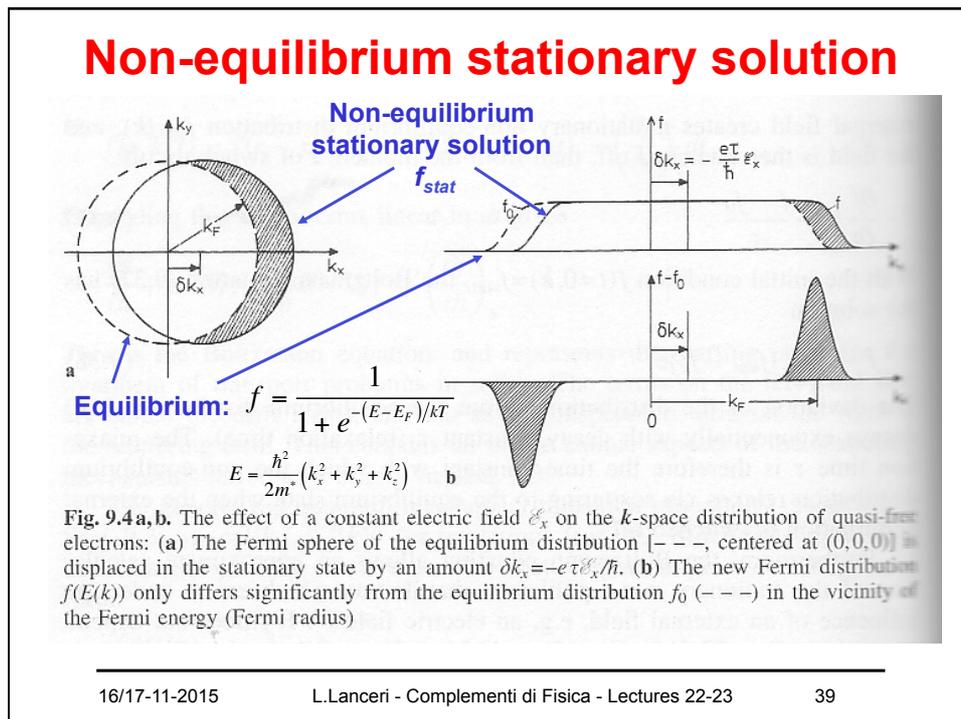
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Boltzmann Equation solutions

Boltzmann Equation solutions

- To understand how this equation works, and the meaning of “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.



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 τ is now clear: it is the characteristic time needed by the system to “relax back” from the *stationary non-equilibrium* state to the *equilibrium* state, under the action of all the different scattering processes

Relaxation to equilibrium

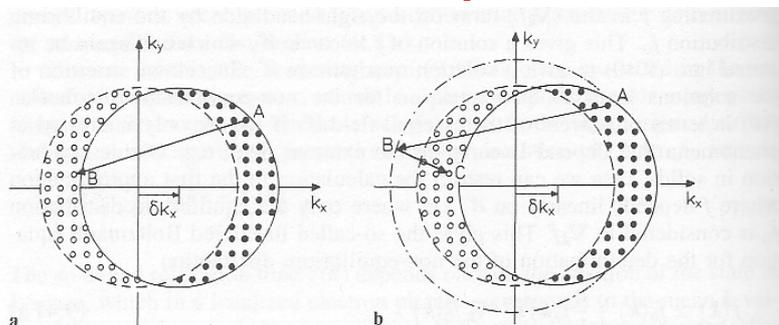


Fig. 9.5a,b. Electron scattering processes in k -space. The dashed circle represents the Fermi surface in thermodynamic equilibrium ($\mathcal{E} = 0$). Under the influence of an electric field \mathcal{E}_x and for a constant current, the Fermi surface is displaced as shown by the full circle. (a) When 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

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Conductivity in metals and semiconductors

Electrical conductivity - old

- In a previous lecture:

- 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, every τ seconds
- 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!), in the presence of a "frictional" force leading to a constant average drift velocity:

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

acceleration → "friction" ← external field

average velocity: $\dot{v}_x = 0 \Rightarrow v_D = -\frac{e\tau}{m}E_x \Rightarrow j_x = -env_D = ne\mu E_x = \frac{e^2 n\tau}{m}E_x$

Drude model:

$$\sigma = \frac{j_x}{E_x} = \frac{e^2 n\tau}{m}$$

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

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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 electric field $E = E_x$)

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

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

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

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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”**

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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 in metals: not dependent on *T*
 - *T*-dependence entirely from the relaxation time, evaluated at the Fermi energy E_F

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

phonons contribution:
approx. linear in *T*

defects contribution:
approx. constant in *T*

At “high” *T*

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Electrical conductivity in metals - 3

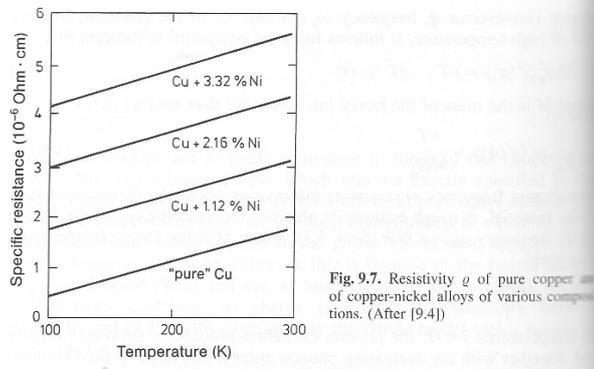


Fig. 9.7. Resistivity ρ of pure copper and of copper-nickel alloys of various compositions. (After [9.4])

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

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: performing this computation (...) one obtains:

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

Average velocity
↑
scattering "cross-section"
↑
⇒

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

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

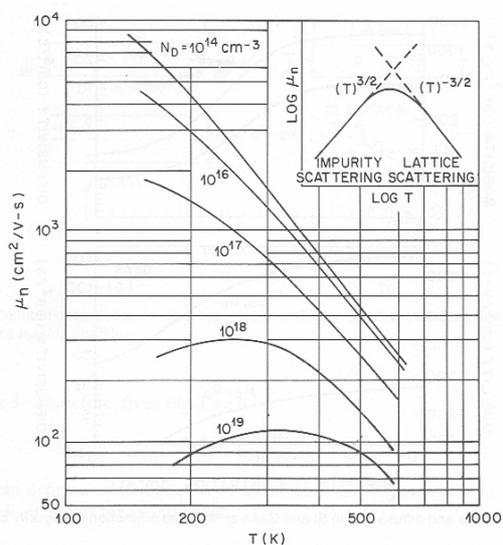
T – dependence of mobility in semiconductors

Scattering on phonons (lattice):

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

Scattering on defects (impurities):

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



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Lectures 22-23 – 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

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Lectures 22-23 – 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** (for conductors: computed at the Fermi surface!), 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.

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Lectures 22-23 – summary - 3

- The drift-diffusion continuity equation obtained from the Boltzmann equation explicitly contains the **“Einstein relation” between drift and diffusion coefficients**, that can be also justified in simpler terms
- 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.

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Lectures 28-30 - exercises

- **Exercise 1:** From slide 19, 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 (1st Brillouin zone)?
- **Exercise 2:** 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 3:** Write down the Boltzmann transport equation and the drift-diffusion continuity equation. Discuss qualitatively the meaning of each term.

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Back-up slides

More details
on the Boltzmann equation
and the
drift-diffusion continuity equation

Drift-Diffusion Continuity Equation

From the Boltzmann Equation...

- The Boltzmann equation tells us how the *density f of electrons in phase space* (position, momentum) evolves as a function of *time*:

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

External force on electrons

- But we are mainly interested in the electrical current density in real space, related to the drift velocity distribution in position-space: how do we get it? Remember that if the pdf f is known, the drift velocity should be computed as an average over k -space of the group velocity v_g :

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

- The recipe is then clear: multiply each term of the Boltzmann eq. by v_g and integrate over all k -space, to obtain the "continuity equation" for electrical current densities

...continuity equation!

Some rather lengthy calculations:

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

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

introducing:

$$\vec{F}_n = -q\vec{E} \quad \vec{F}_p = q\vec{E}$$

$$\vec{J}_n = -qn\vec{u}_n \quad \vec{J}_p = -qp\vec{u}_p$$

$$\mu_n = q\tau_n/m \quad \mu_p = q\tau_p/m$$

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):

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Drift-diffusion continuity equation

For electrons (similar for holes), if T is uniform:

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

Drift

↑

Diffusion

↑

“Mobility” and “Diffusivity” go together...!

“Diffusion coefficient”:

$$D_n = \mu_n \frac{k_B T}{q}$$

Drift

$$J_x^{drift} = J_{x,n}^{drift} + J_{x,p}^{drift} = qn\mu_n E_x + qp\mu_p E_x$$

Diffusion

$$J_x^{diff} = J_{x,n}^{diff} + J_{x,p}^{diff} = qD_n \frac{\partial n}{\partial x} - qD_p \frac{\partial p}{\partial x}$$

here :

$$q = |q_e|$$

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Boltzmann equation

General, 3-d

The Boltzmann Equation - 1

In the absence of scattering:

Time evolution in phase space

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

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

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

x changing because of velocity: $dx = v_x dt$

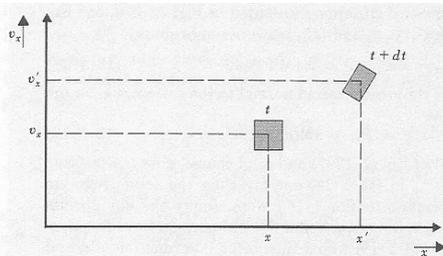


Fig. 13·2·1 Figure illustrating the motion of a particle in one dimension in a two-dimensional phase space specified by the particle position x and its velocity v_x .

The Boltzmann Equation - 2

Conservation of the number of particles (electrons):

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

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

↓
Phase-space volume-element: it can be distorted in shape, but (Liouville theorem) its volume remains constant in time!

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

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

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

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The Boltzmann Equation - 3

**With the additional scattering contribution,
for electrons in an external electric field:**

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

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

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

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)

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Boltzmann Equation: interpretation

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

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

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

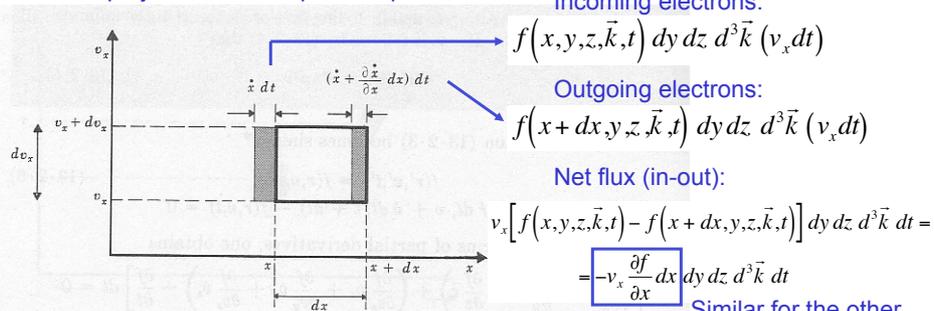


Fig. 13.2.2 Figure illustrating a fixed element of volume of phase space for a particle moving in one dimension and specified by its position x and velocity v_x .

Similar for the other projections of position and k !

Drift-diffusion continuity equation

Derivation
from the Boltzmann 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” (detailed derivation: see FELD p. 187-194, MOUT p.100-104)

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...integrals...

Boltzmann equation for the pdf f:

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

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

Multiplying by v_g , integrating over k -space, and expressing the results in terms of the average velocities u and of the concentrations n (if you are really interested, hints about integral computations are given in the back-up slides) one obtains (next slide)...

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

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

First term:

Do not depend on time

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

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

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:

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

Third term:

Integrating by parts

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

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

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

Fourth term:

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

average velocity = 0 at equilibrium

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...continuity equation!

Substituting in:

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

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

introducing:

$$\vec{F}_n = -q\vec{E} \quad \vec{F}_p = q\vec{E}$$

$$\vec{J}_n = -qn\bar{u}_n \quad \vec{J}_p = -qp\bar{u}_p$$

$$\mu_n = q\tau_n/m \quad \mu_p = q\tau_p/m$$

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):

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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 τ 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!

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Backup slides

Other details

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):

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

$$b_m \approx (1/2)N^{-1/3} \quad \begin{matrix} b_m: \text{max. impact parameter} \\ N: \text{defects concentration} \end{matrix}$$

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

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

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_x changing because of an external field: $d(\hbar k_x) = (-eE_x)dt$

x changing because of velocity: $dx = v_x dt$

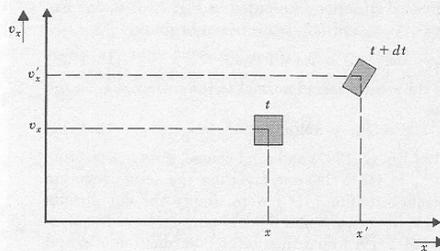


Fig. 13.2.1 Figure illustrating the motion of a particle in one dimension in a two-dimensional phase space specified by the particle position x and its velocity v_x .

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:

$$\left(\frac{\partial f(\vec{k})}{\partial t} \right)_S = \frac{V}{(2\pi)^3} \int d\vec{k}' \left\{ \overset{\boxed{k \rightarrow k'}}{\underbrace{(1-f(\vec{k})) w_{kk'} f(\vec{k}')}_{\text{in}}}} - \overset{\boxed{k' \rightarrow k}}{\underbrace{(1-f(\vec{k}')) w_{k'k} f(\vec{k})}_{\text{out}}}} \right\}$$

For the scattering to take place (Pauli Principle):
the initial state must be filled (f), the 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

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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:

$$\frac{\partial f}{\partial x} = 0 \quad (\text{not dep. on position}) \quad \frac{\partial f}{\partial t} = 0 \quad (\text{stationary})$$

The Boltzmann equation (1-d version for simplicity) is reduced to:

$$-\frac{e}{\hbar} E_x \frac{\partial f}{\partial k_x} = - \frac{f(\vec{k}) - f_0(\vec{k})}{\tau(\vec{k})}$$

$$f(\vec{k}) = f_0(\vec{k}) + \frac{e}{\hbar} E_x \tau(\vec{k})$$

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

Approximate linearized solution for small fields:

$$f(\vec{k}) \cong f_0\left(\vec{k} + \frac{e}{\hbar} \tau(\vec{k}) \vec{E}\right) \quad \text{Results from the action of the external field } E \text{ and includes the effects of scattering } (\tau)$$

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