Transport Phenomena in Solids

Motions of electrons and transport phenomena
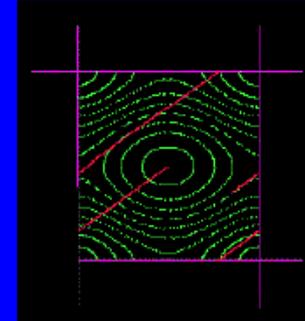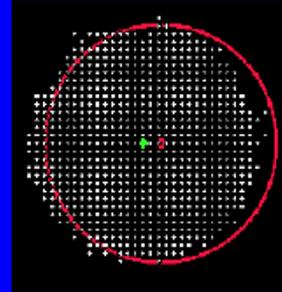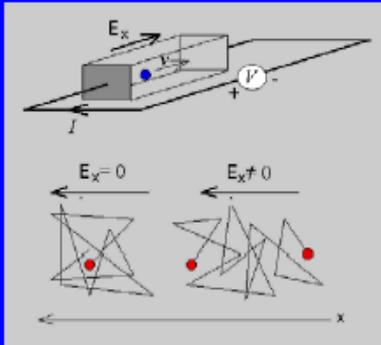
$$\sigma = \frac{ne^2\tau}{m}$$

$$\left(\frac{1}{m*}\right)_{ij} = \frac{1}{\hbar^2}\sum_j \frac{\partial^2 E(\vec{k})}{\partial k_i \partial k_j}$$

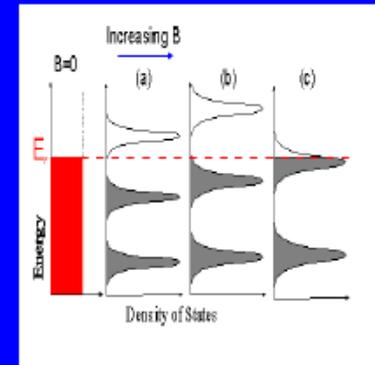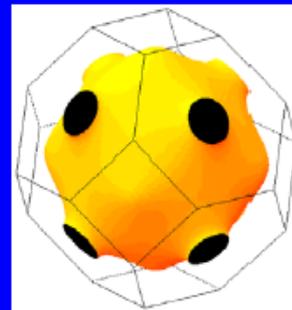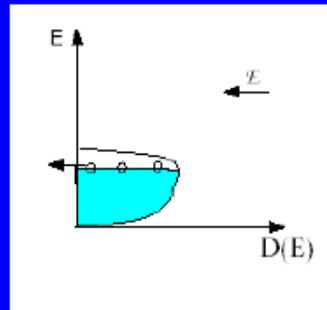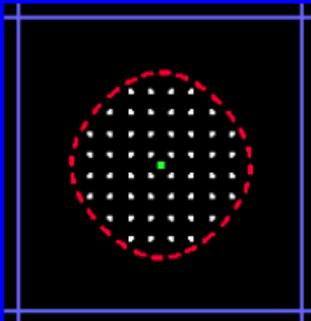the study of **transport phenomena in physics** is related with the exchange of [mass](#), [energy](#), and [momentum](#) studied [systems](#).

- [fluid mechanics](#), [heat transfer](#), and [mass transfer](#)

- in [solid state physics](#), the motion and interaction of electrons, holes and [phonons](#) are studied under "transport phenomena".

Content:

1. Introduction. General. Fick' Law. Boltzmann Eq. Relaxation time.

2. Electronic transport in conductors. Electron-phonon scattering.

3. Electron-imperfection scattering

4. Electrical conductivity. Bloch-Gruneisen

5. Magnetic scattering

6. Thermal conductivity

7. Thermoelectric phenomena

8. Electrical conductivity in magnetic fields.

9. Anomalous Hall effect

10. Magnetoresistance : AMR, CMR

11. Magnetoresistance : GMR TMR.

12. Strongly correlated electron systems

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3. N. W. Ashcroft, N. D. Mermin, *Solid State Physics*, 1976.

4. U. Mizutani, Introduction to the Electron Theory of Metals, Cambridge University Press 2001.

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6. M. Coldea, Magnetorezistenta. Efecte si Aplicatii, Presa Universitara Clujeana, 2009.

7. E. Dagotto, Nanoscale Phase Separation and Colossal Magnetoresistance, Springer-Verlag Berlin Heidelberg 2002.

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9. UvA-VU Master Course: Advanced Solid State Physics

10. H. Ibach and H. Lüth: Solid State Physics 3rd edition (Springer-Verlag, Berlin, 2003) ISBN 3-540-43870-X

11. J. M. ZIMAN, ELECTRONS AND PHONONS ,The Theory of Transport Phenomena in Solids, UNIVERSITY OF CAMBRIDGE , OXFORD AT THE CLARENDON PRESS 1960

Some pictures are taken from the UvA-VU Master Course: Advanced Solid State Physics by Anne de Visser (University of Amsterdam), Solid State Course by Mark Jarrel (Cincinnati University), from Ibach and Lüth, from Ashcroft and Mermin and from several sources on the web.

Introduction. Transport Processes

Nonequilibrium
steady state
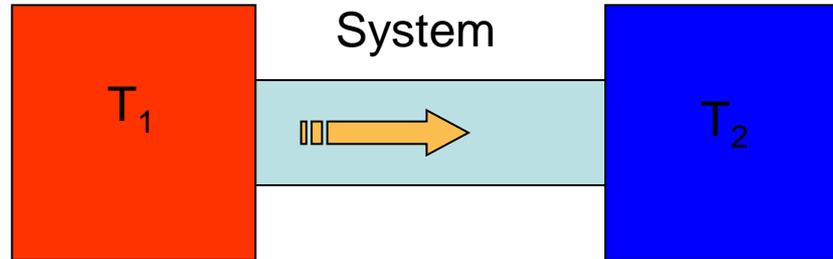
Entropy (reservoir 1+reservoir 2+ System) INCREASES

Driving force=Temperature gradient ⟹ Transport of Energy

Flux = (coeficient) x (driving force)

Linear phenomenological law (if the force is not to large)

e.g. Ohm's law for the conduction of electricity

J_A = flux density of A = net quantity of A transported across area in unit time

Net transport = the transport in one direction – the transport in oposite direction

$$J_A = -D \cdot \text{grad } \rho_A$$

Table 14.2 Summary of phenomenological transport laws

Effect	Flux of particle property	Gradient	Coefficient	Law	Name of law	Approximate expression for coefficient
Diffusion	Number	$\dfrac{dn}{dz}$	Diffusivity D	$\mathbf{J}_n = -D \text{ grad } n$	Fick's law	$D = \frac{1}{3}\bar{c}l$
Viscosity	Transverse momentum	$M\dfrac{dv_x}{dz}$	Viscosity η	$\dfrac{F_x}{A} = J_p{}^x = -\eta \dfrac{dv_x}{dz}$	Newtonian viscosity	$\eta = \frac{1}{3}\rho\bar{c}l$
Thermal conductivity	Energy	$\dfrac{d\rho_u}{dz} = \hat{C}_V \dfrac{dT}{dz}$	Thermal conductivity K	$\mathbf{J}_u = -K \text{ grad } \tau$	Fourier's law	$K = \frac{1}{3}\hat{C}_V\bar{c}l$
Electrical conductivity	Charge	$-\dfrac{d\varphi}{dz} = E_z$	Conductivity σ	$\mathbf{J}_q = \sigma\mathbf{E}$	Ohm's law	$\sigma = \dfrac{nq^2l}{M\bar{c}}$

SYMBOLS: n = number of particles per unit volume
$\bar{c}$ = mean thermal speed = $\langle |v| \rangle$
l = mean free path
$\hat{C}_V$ = heat capacity per unit volume
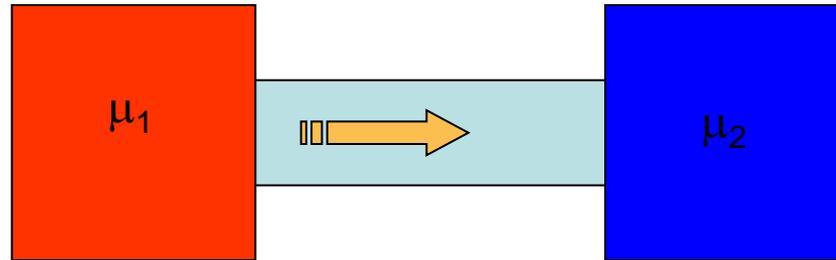ρ_u = thermal energy per unit volume
F_x/A = shear force per unit area

φ = electrostatic potential
$\mathbf{E}$ = electric field intensity
q = electric charge
M = mass of particle
ρ = mass per unit volume
$\mathbf{p}$ = momentum

from Enss

Particle diffusion

T= constant

particle flow

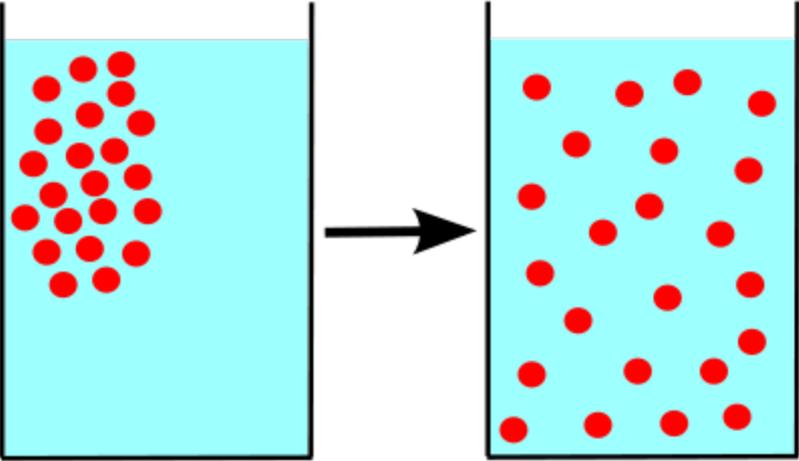Entropy (reservoir 1+reservoir 2+ System) INCREASES

Presume: the difference of chemical potential is caused by a difference in particle concentration

J_n- the number of particels passing through a unit area in unit time
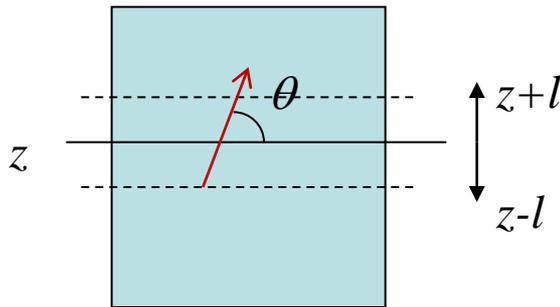
Fick's law:

$$J_n = -D \cdot \text{grad}\, n$$

D – particle diffusion constant - **diffusivity**

l – the mean free path

At position z the particles come into a local equilibrium condition $\mu(z)$ and $n(z)$

$z+l$

$z-l$

$$J_n^z = \frac{1}{2}\left[n(\,z - l_z\,) - n(\,z + l_z\,)\right]\overline{c}_z = -\frac{dn}{dz}\overline{c}_z l_z$$

We express $c_z l_z$ in terms of $\overline{c} \cdot l$

$$l_z = l \cdot cos\,\theta \qquad \overline{c}_z = \overline{c} \cdot cos\,\theta$$

The average is taken over the surface of a hemisphere

The element of surface area is $2\pi \cdot sin\,\theta \cdot d\theta$

$$\langle \overline{c}_z l_z \rangle = \overline{c}l\,\frac{2\pi\displaystyle\int_0^{\frac{\pi}{2}} cos^2\,\theta \cdot sin\,\theta \cdot d\theta}{2\pi} = \frac{1}{3}\overline{c}l$$

So that

$$J_n^z = -\frac{1}{3}\overline{c}\,l\,\frac{dn}{dz}$$

$\Longrightarrow$

$$D = \frac{1}{3}\overline{c}\,l$$

Particle diffusion is the model for other transport probelms

- Particle diffusion → transport of particles
- Thermal conductivity → transport of energy by particles
- Viscosity → transport of momentum by particles
- Electrical conductivity → transport of charge by particles

The linear transport coefficients that describes the processes are proportional to the particles diffusivity D

let

ρ_A – the concentration of the physical quantity A.

-the flux density of A in the z direction is:

$$J_A^z = \rho_A \langle v_z \rangle$$

$\langle v_z \rangle$ is the mean drift velocity of the particles in the z direction

(drift velocity is zero in thermal equilibrium)

If A (e.g. energy, momentum…) depends on the velocity of a molecule:

$$J_A^z = f_A \cdot \rho_A \langle v_z \rangle$$

f_A is a factor with magnitude of the order of unity→ it depends on the velocity dependence of A and may be calculated (e.g. by using the Boltzmann transport equation)
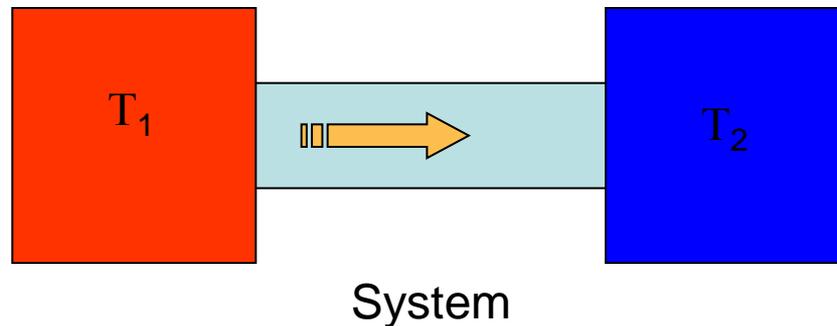
By analogy with
Fick' law

$$J_A = -D \cdot \operatorname{grad} \rho_A$$

Thermal conductivity

Fourier law's

$$J_A = -K \cdot \operatorname{grad} T$$

Describes the energy flux density J_n in terms of the **thermal conductivity K** and the temperature gradient

System

• This form assumes that there is a net transport of energy, but not particles

• Another term must be added if additional energy is transported by means of particle flow (as when electrons flow under the influence of an electric field.)

The energy flux density in the z direction is:

$$J_u^z \cong \rho_u \langle v_z \rangle$$

ρ_u – is the energy density

By analogy with the diffusion equation:

Diffusion of energy

$$-D \cdot d\rho_u / dx = -D(\partial \rho_u / \partial T)(dT / dx)$$

$$\partial \rho_u / \partial T$$

Is the heat capacity per unit volume, C_V.

$$J_u = -D \cdot C_V \cdot \operatorname{grad} T$$

$$K = DC_V = \frac{1}{3} C_V \cdot \bar{c} \cdot l$$

The thermal conductivity of a gas is independent of pressure until very low pressure when the mean free path becomes limited by the dimensions of the apparatus rather then by intermolecular collision.

Q (heat flow)
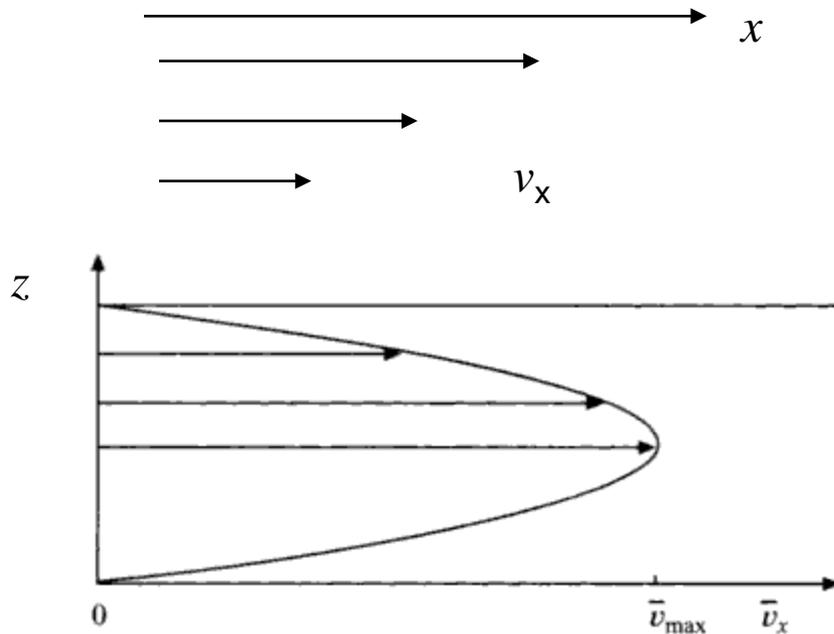
Hot
T_h

Cold
T_c

L
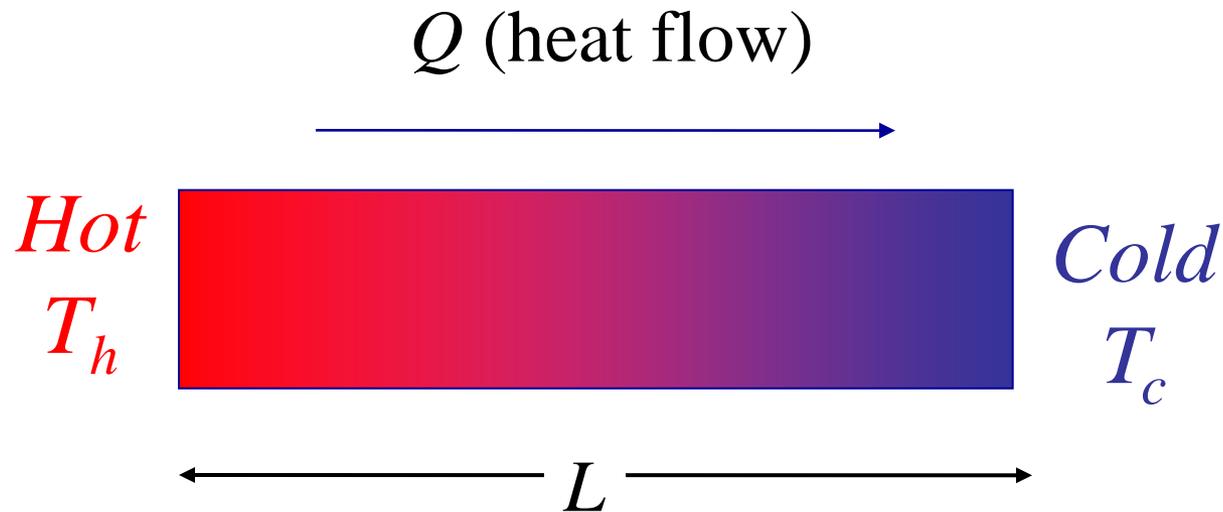
$$Q = kA\frac{T_h - T_c}{L} = kA\frac{dT}{dx}$$

Thermal conductivity

Viscosity

Viscozity is a measure of the diffusion of momentum parallel to the flow velocity and transverse to the gradient of the flow velocity

x

v_x

z

0 $\bar{v}_{max}$ $\bar{v}_x$

Figure 15.6 Velocity profile for slow fluid flow in a pipe. The velocity component $\bar{v}_x$ is the velocity component along the pipe; the overbar denotes an average of molecular velocity components taken over a small volume (that is, small relative to the pipe radius R).

Viscosity coefficient:

$$X_z = -\eta \frac{dv_x}{dz} = J_z(p_x)$$

from Enss

The particle flux density in the z direction: $\quad J_n^z = n\langle v_z \rangle = -D\,dn/dz$

The transverse momentum density: $\quad nMv_x$

Its flux density in the z direction: $\quad (nMv_x)\langle v_z \rangle$

Kittel, Thermal physics

This flux density $\quad -Dd(nMv_x)/dz$

$(\quad \mathbf{J}_A = -\mathbf{D}\cdot\mathrm{grad}\,\rho_A\,)$

Mass density: $\quad \rho = nM$

$$J_z(p_x) = \rho v_x \langle v_x \rangle = -D\rho\,dv_x/dz = -\eta\,dv_x/dz$$

$$\eta = D\rho = \frac{1}{3}\rho\bar{c}l$$

CGS- poise

SI unit: **Pa.s**
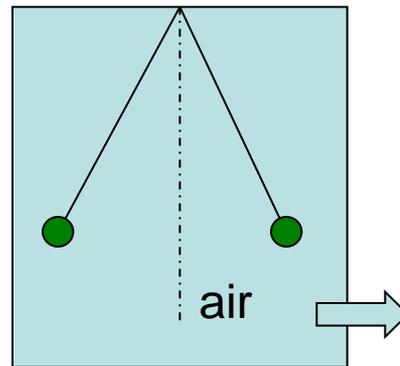
The mean free path: $l = 1/\pi d^2 n$

Viscozity:

$$\eta = M\bar{c}/3\pi d^2$$ independent of gas pressure

The independence fails at **very high pressures** when the molecules are always is contact, or at **very low pressures** when the mean free path is longer than the dimension of the apparatus.

Robert Boyle 1660

air

$$D = \eta/\rho \implies K = \eta C_v / \rho$$

Kinematic viscosity

Generalized Forces

The transfer of entropy from one part of a system to another is a consequence of any transport process.

- We can relate the rate of change of entropy to flux density of particles and of energy

For V= const.

$$dS = \frac{1}{T}dU - \frac{\mu}{T}dN$$

The entropy current density :

$$\vec{J}_s = \frac{1}{T}\vec{J}_u - \frac{\mu}{T}\vec{J}_n \qquad (*)$$

Entropy density $\hat{S}$

The net change of entropy density at a fixed position $\partial\hat{s}/\partial t$ $\Longrightarrow$

$$\boxed{\partial\hat{S}/\partial t = g_S - \operatorname{div}\vec{J}_s}$$

Eq. of continuity

Rate of production of entropy

In a transfer process U and N are conserved

The equations of continuity:

$$\frac{\partial u}{dt} = -\text{div}\vec{J}_u$$

$$\frac{\partial n}{dt} = -\text{div}\vec{J}_n$$

Divergence of $\vec{J}_S$

$$\text{div}\vec{J}_S = \frac{1}{T}\text{div}\vec{J}_u + \vec{J}_u \cdot \text{grad}(1/T) - (\mu/T)\text{div}\vec{J}_n - \vec{J}_n \cdot \text{grad}(\mu/T)$$

(*)

$$\frac{\partial \hat{S}}{\partial t} = \frac{1}{T}\frac{\partial u}{\partial t} - \frac{\mu}{T}\frac{\partial n}{\partial t}$$

$$g_S = \vec{J}_u \cdot \mathrm{grad}(1/T) + \vec{J}_n \cdot \mathrm{grad}(-\mu/T)$$

$$g_S = \vec{J}_u \cdot \vec{F}_u + \vec{J}_n \cdot \vec{F}_n$$

Generalized forces

$$\vec{F}_u \equiv \mathrm{grad}(1/T) \qquad \vec{F}_n \equiv \mathrm{grad}(-\mu/T)$$

Thermodynamics of irreversible processes:

Onsager relation:

Coupled effects

$$\vec{J}_u = L_{11}\vec{F}_u + L_{12}\vec{F}_n$$

$$\vec{J}_n = L_{21}\vec{F}_u + L_{22}\vec{F}_n$$

$$L_{ij}\left(\vec{B}\right) = L_{ji}\left(-\vec{B}\right)$$

In magnetic field

We work in the 6 D (six-dimensional space of Cartesian coordinates *r* and *v*).

The classical distribution function:

$$f(\vec{r}, \vec{v})d\vec{r}d\vec{v} = \text{number of particles in } d\vec{r}d\vec{v}$$

The effect of time displacement dt on the distribution function:

$$f(t + dt, \vec{r} + d\vec{r}, \vec{v} + d\vec{v}) = f(t, \vec{r}, \vec{v})$$

In the absence of collisions

With collisions:

$$f\left(t + dt, \vec{r} + d\vec{r}, \vec{v} + d\vec{v}\right) - f(t, \vec{r}, \vec{v}) = dt(\partial f / \partial t)_{collisions}$$

With a series development:

$$dt(\partial f / \partial t) + d\vec{r} \cdot grad_{\vec{r}} f + d\vec{v} \cdot grad_{\vec{v}} f = dt(\partial f / \partial t)_{collisions}$$

$$\vec{a} \equiv \frac{d\vec{v}}{dt}$$

$$\partial f / \partial t + \vec{v} \cdot grad_{\vec{r}} f + \vec{a} \cdot grad_{\vec{v}} f = (\partial f / \partial t)_{collisions}$$

Boltzmann transport equation

Relaxation time aproximation:

This is based on the assumption that a nonequilibrium distribution $f(t,\vec{r},\vec{v})$ gradually returns to its equilibriun value within a characteristic time, the relaxation time $\tau_c(\vec{r},\vec{v})$, by scattering of particles with the velocity $\vec{v}$ into states $\vec{v}'$, and vice versa.

$$(\partial f / \partial t)_{collisions} = -(f - f_0)/ \tau_c$$

Suppose that a nonequilibrium distribution of velocities is set up by external forces which are suddenly removed.

The decay of the distribution towards equilibrium is then obtained:

$$\frac{\partial(f - f_0)}{\partial t} = -(f - f_0)/ \tau_c$$

$$\partial f_0 / \partial t = 0$$

$$(f - f_0)_t = (f - f_0)_{t=0} \exp(-t / \tau_c)$$

Generally

$$\tau_c = \tau_c\left(\vec{r}, \vec{v}\right)$$

$$\partial f / \partial t + \vec{v} \cdot grad_{\vec{r}} f + \vec{a} \cdot grad_{\vec{v}} f = \frac{f - f_0}{\tau_c}$$

In the steady state:
by definition

$$\partial f / \partial t = 0$$

Particle Diffusion

Consider an isothermal system with a gradient of particle concentration

The steady-state Boltzmann transport equation in the relaxation time approximation:

$$v_x \, df/dx = -(f - f_0)/\tau_c$$

First order approximation

$$f_1 \cong f_0 - v_x \tau_c df_0/dx \qquad \frac{df}{dx} \to \frac{df_0}{dx}$$

Second order approximation

$$f_2 \cong f_0 - v_x \tau_c df_1/dx = f_0 - v_x \tau_c df_0/dx + v_x^2 \tau_c^2 d^2 f_0/dx^2$$

The iteration is necessary for the treatment of nonlinear effects

Classical Distribution

$$f_0 = exp[\,(\,\mu - \varepsilon\,)\,/\,k_B T\,]$$

$$df_0\,/\,dx = (\,df_0\,/\,d\mu\,)(\,d\mu\,/\,dx\,) = (\,f_0\,/\,k_B T\,)(\,d\mu\,/\,dx\,)$$

The first order solution for the nonequilibrium distribution becomes:

$$f = f_0 - (\,v_x \tau_c f_0\,/\,k_B T\,)(\,d\mu\,/\,dx\,)$$

The particle flux density in the x direction:

$$J_n^x = \int v_x f D(\,\varepsilon\,)\,d\varepsilon$$

The density of orbitals per unit volume per unit energy range:

$$D(\,\varepsilon\,) = \frac{1}{4\pi^2}\left(\frac{2M}{\hbar^2}\right)^{3/2}\varepsilon^{1/2}$$

Presume τ_c constant, independent of velocity
$$\int f_0 D(\,\varepsilon\,)d\varepsilon = n$$

finally,

$$J_n^x = -(\,n\tau_c\,/\,M\,)(\,d\mu\,/\,dx\,) = -(\,k_B T\tau_c\,/\,M\,)(\,dn\,/\,dx\,)$$

⇧

because $\quad \mu = k_B T \log n + \text{const.}$

Diffusivity:

$$D = \tau_c k_B T\,/\,M = \frac{1}{3}\langle v^2 \rangle \tau_c$$

If we presume

$$\tau_c = \frac{l}{v} \quad \Longrightarrow \quad D = \frac{1}{3} l \overline{c}$$

Fermi-Dirac distribution

$$f_0 = \frac{1}{exp[(\varepsilon - \mu)/k_B T + 1}$$

$$df_0/d\mu \cong \delta(\varepsilon - \mu)$$

$$\int_{-\infty}^{+\infty} F(\varepsilon)\delta(\varepsilon - \mu)d\varepsilon = F(\mu)$$

$$df_0/dx = \delta(\varepsilon - \mu)d\mu/dx$$

The particle flux density

$$J_n^x = \int v_x f D(\varepsilon)d\varepsilon = -(d\mu/dx)\tau_c \int v_x^2 \delta(\varepsilon - \mu)D(\varepsilon)d\varepsilon$$

We know

$$D(\mu) = 3n/2\varepsilon_F \qquad \mu = (\hbar^2/2m)(3\pi^2 n)^{2/3}$$

$$J_n^x = -(2\tau_c/3m)\varepsilon_F dn/dx = -\frac{1}{3}v_F^2 \tau_c dn/dx$$

$$\boxed{D = \frac{1}{3}v_F^2 \tau_c}$$

$$\frac{1}{3}v_F^2\left(\frac{3n}{2\varepsilon_F}\right) = n/m$$

We multiply the particle flux density by the particle charge q

$$d\mu / dx \implies qd\varphi / dx = -qE_x$$

$$J_q^x = (n\tau_c q / m)(d\mu / dx) = (n\tau_c q^2 / m)E = \sigma E$$

Electrical conductivity

$$\boxed{\sigma = nq^2\tau_c / m}$$

- For a classical gas (Drude)
- For the Fermi-Dirac distribution (Sommerfeld)

We will discuss this in more detail, later.