

Boltzmann equation & transport properties

MR Torkamani & M Afkani

Kharazmi university

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Outline I

1 Boltzmann equation

- What is $f(\vec{r}, \vec{k}, t)$
- Changing $f(\vec{r}, \vec{k}, t)$ with time
- Boltzmann equation
- What is $g(\vec{r}, \vec{k}, t)$
- Velocity of an electron!

2 Electrical conductivity

- Boltzmann equation
- Current density
- Conducting scalar I
- Conducting scalar II

Outline II

3 General Transport equation

- Boltzmann equation
- Heat
- General Transport equation
- Thermal conductivity
- Compare Electrical and Thermal conduction

4 Thermo-electric effects

- Seebeck effect
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5 references

Introduction

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- We want to calculate ordinary transport properties when constant fields are applied.
- Simplest approach to do this problem is to set up the transport equation or Boltzmann equation.

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

- $f(\vec{r}, \vec{k}, t)$: local concentration of carrier in the state k in the neighbourhood of the point r in space.

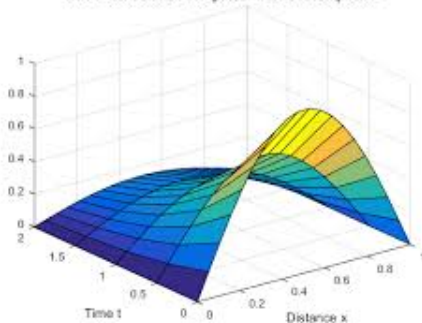
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Numerical solution computed with 20 mesh points.



Boltzmann equation

Electrical conductivity

General Transport equation

Thermo-electric effects

references

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

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Velocity of an electron!

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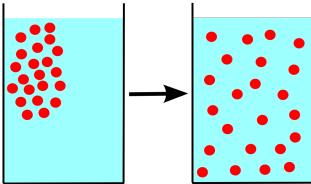
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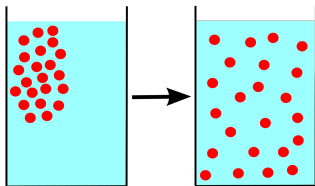
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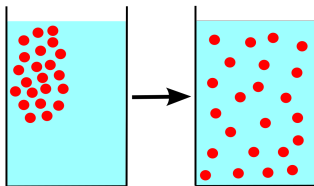
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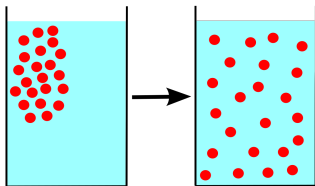
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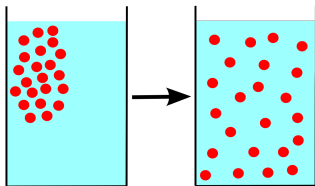
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$$\left. \frac{\partial f}{\partial t} \right|_{diff} = -\vec{v}_k \cdot \nabla f$$



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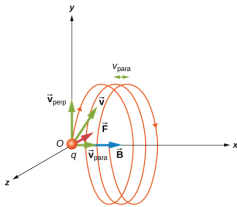
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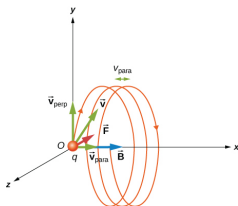
Electromagnetic field

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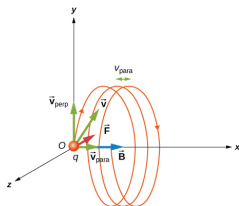
Electromagnetic field

- external fields will change the k-vector of each carrier.



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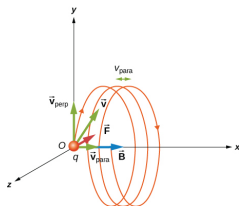
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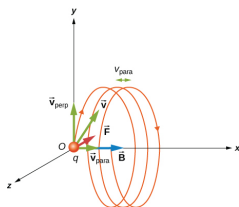


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- thus :
 $f(\vec{r}, \vec{k}, \Delta t) = f(\vec{r}, \vec{k} - \vec{k}\Delta t, 0)$ in k -space.

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 $f(\vec{r}, \vec{k}, \Delta t) = f(\vec{r}, \vec{k} - \vec{k}\Delta t, 0)$ in k -space.

$$\left. \frac{\partial f}{\partial t} \right|_{field} = -\frac{e}{\hbar}(\vec{E} + \frac{1}{c}\vec{v}_k \times \vec{H}) \cdot \nabla_k f$$

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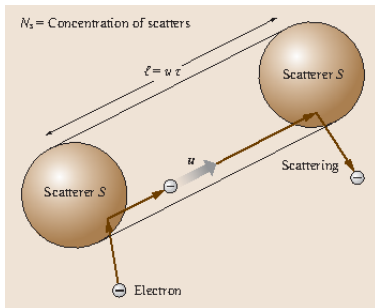
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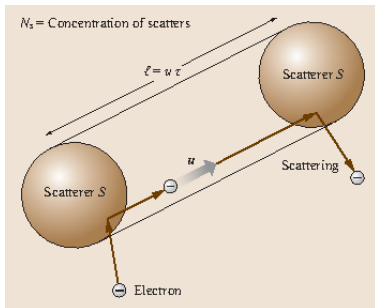
Velocity of an electron!

Scattering

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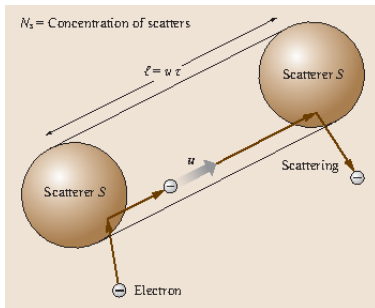


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$$\left. \frac{\partial f}{\partial t} \right|_{\text{scatt}} = \int \{f'(1-f) - f(1-f')\} Q(k, k') dk'$$

Boltzmann equation

The Boltzmann transport equation is a statement that in the steady state, there is no net change in the distribution function $f(\vec{r}, \vec{k}, t)$ which determines the probability of finding an electron at position \vec{r} , crystal momentum \vec{k} and time t . Therefore we get a zero sum for the changes in $f(\vec{r}, \vec{k}, t)$ due to the 3 processes of diffusion, the effect of forces and fields, and collisions

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Theorem

Boltzman equation

$$\frac{df}{dt} = \frac{\partial f}{\partial t}|_{diff} + \frac{\partial f}{\partial t}|_{field} + \frac{\partial f}{\partial t}|_{scatt} = 0$$

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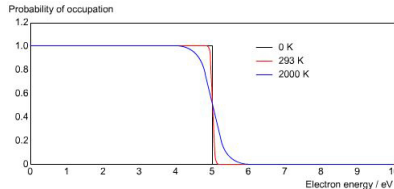
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Fermi-Dirac distribution for several temperatures

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for free electron

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m}$$

$$\vec{v} = \frac{\hbar \vec{k}}{m} = \frac{\vec{p}}{m}$$

Boltzmann equation

$$\begin{aligned} & \left(-\frac{\partial f^0}{\partial \varepsilon}\right) \vec{v}_k \cdot \left(-\frac{\varepsilon(k) - \zeta}{T}\right) \nabla T + e(\vec{E} - 1/c \nabla \zeta) \\ &= \frac{\partial f}{\partial t} \Big|_{scatt} + \vec{v}_k \cdot \frac{\partial g}{\partial \vec{r}} + \frac{e}{\hbar c} (\vec{v}_k \times \vec{H}) \cdot \frac{\partial g}{\partial \vec{k}} \end{aligned}$$

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$$\vec{J} = \frac{1}{4\pi^3} \int \int e^2 \tau \vec{v}_k \cdot \vec{E} \left(-\frac{\partial f^0}{\partial \varepsilon} \right) \frac{ds}{\hbar v_k} d\varepsilon$$

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$$\vec{J} = \frac{1}{4\pi^3} \frac{e^2 \tau}{\hbar} \int \frac{\vec{v}_k \vec{v}_k}{v_k} ds_f \cdot \vec{E}$$

conducting scalar

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$$(\vec{v}_k \vec{v}_k \cdot \vec{E})_x = v_x^2 E = \frac{1}{3} v^2 E$$

$$\sigma = \frac{1}{4\pi^3} \frac{e^2}{3\hbar} \int \Lambda ds_f \quad \Lambda = \tau v$$

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$$g = f - f^0(k) = -\frac{\partial f^0}{\partial \varepsilon} \frac{\partial \varepsilon}{\partial k} \cdot \frac{e\tau}{\hbar} \vec{E}$$

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$$\delta \vec{v} \frac{\partial \varepsilon}{\partial v} = e\tau \vec{v}_k \cdot \vec{E} \Rightarrow \delta \vec{v} = \frac{ev\tau}{mv} \vec{E}$$

$$\vec{J} = ne\delta \vec{v} = \frac{ne^2\tau}{m} \vec{E}$$

Boltzmann equation

suppose now that we have a temperature gradient in the specimen as well as an electric field. ignoring size and shape effects.

Boltzmann equation

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$$\left(-\frac{\partial f^0}{\partial \varepsilon}\right) \vec{v}_k \cdot \left(-\frac{\varepsilon(k) - \zeta}{T}\right) \nabla T + e(\vec{E} - 1/c \nabla \zeta) = \frac{\partial f}{\partial t} \Big|_{scatt}$$

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$$\begin{aligned} \vec{J} = & \frac{1}{4\pi^3} \frac{e^2 \tau}{\hbar} \int \int \vec{v}_k \vec{v}_k \left(-\frac{\partial f^0}{\partial \varepsilon}\right) \frac{ds}{v_k} d\varepsilon \cdot \left(\vec{E} - \frac{1}{e} \nabla \zeta\right) \\ & + \frac{1}{4\pi^3} \frac{e^2 \tau}{\hbar} \int \int \vec{v}_k \vec{v}_k \left(\frac{\varepsilon - \zeta}{T}\right) \left(-\frac{\partial f^0}{\partial \varepsilon}\right) \frac{ds}{v_k} d\varepsilon \cdot (-\nabla T) \end{aligned}$$

Heat

- $\text{heat} = \text{internal energy} - \text{free energy}$

Heat

- heat = internal energy – free energy
- the total flux of heat (per unit volume) is:

$$\vec{U} = 2 \int (\varepsilon - \zeta) f(\vec{r}, \vec{k}, t) v_k d^3k$$

General Transport equation

$$\vec{J} = e^2 \overleftrightarrow{K}_0 \cdot \vec{E} + \frac{e}{T} \overleftrightarrow{K}_1 \cdot (-\nabla T)$$

$$\vec{U} = e \overleftrightarrow{K}_1 \cdot \vec{E} + \frac{1}{T} \overleftrightarrow{K}_2 \cdot (-\nabla T)$$

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$$\overleftrightarrow{k}_n \equiv \frac{1}{4\pi^3} \frac{\tau}{\hbar} \int \int \vec{v} \vec{v} (\varepsilon - \zeta)^n \left(-\frac{\partial f^0}{\partial \varepsilon} \right) \frac{ds}{v} d\varepsilon$$

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$$\overleftrightarrow{K}_0 = \frac{\tau}{4\pi^3 \hbar} \int \vec{v} \vec{v} \frac{ds f}{v} \quad \overleftrightarrow{K}_2 = \frac{1}{3} \pi^2 (kT)^2 K_0(\zeta)$$

$$\overleftrightarrow{K}_1 = \frac{1}{3} \pi^2 (kT)^2 \frac{\partial}{\partial \varepsilon} K_0(\varepsilon) \Big|_{\varepsilon=\zeta}$$

Thermal conductivity

Thermal conductivity

$$\vec{E} = \frac{1}{e^2} K_0^{-1} K_1 \frac{e}{T} (-\nabla T)$$

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$$\vec{U} = \frac{1}{T} K_1 K_0^{-1} K_1 \cdot \nabla T - \frac{1}{T} K_2 \cdot \nabla T$$

$$\vec{U} = \frac{1}{T} (-K_1 K_0^{-1} K_1 + K_2) \cdot (-\nabla T)$$

$$\vec{U} = \kappa \cdot (-\nabla T)$$

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But for metal, we can ignore the $K_1 K_0^{-1} K_1$

$$\kappa = \frac{1}{T} K_2$$

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Compare Electrical and Thermal conduction

Wiedemann-Franz law

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the coefficient of \vec{E} in \vec{J} equation is σ

$$\sigma = e^2 K_0$$

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Compar Electrical and Thermal conduction

| electrical conduction | thermal conduction |
|--|--|
| each electron carries its charge e , and is acted on by the field $e\vec{E}$ the current per unit field is proportional to e^2 | each electron carries thermal energy kT it is acted by a thermal force $k\nabla T$ the heat current per unit thermal gradient is proportional to k^2T |

the ratio of these two transport coefficients = $\frac{k^2T}{e^2}$

Seebeck effect

Seebeck effect

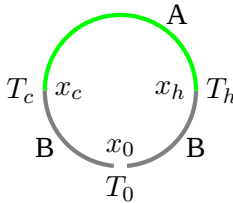
in open circuit with thermal gradient we have:

$$\vec{E} = \frac{1}{eT} K_0^{-1} K_1(\nabla T) = Q \nabla T$$

Seebeck effect

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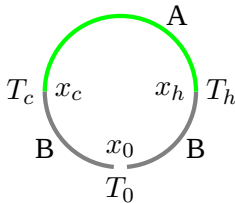
$$\vec{E} = \frac{1}{eT} K_0^{-1} K_1(\nabla T) = Q \nabla T$$



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$$V = \int_{x_0}^{x_c} E_B dx + \int_{x_c}^{x_h} E_A dx + \int_{x_h}^{x_0} E_B dx = \int_{T_c}^{T_h} (Q_A - Q_B) dT$$

Peltier effect

suppose we keep $\nabla T = 0$ round the same circuit

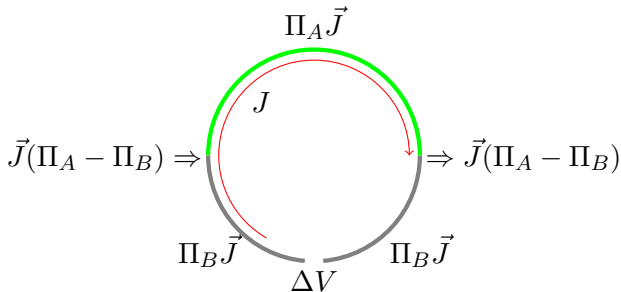
$$\vec{U} = eK_1\vec{E} \quad \vec{J} = e^2K_0\vec{E}$$

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$$\vec{U} = \frac{1}{e} K_0^{-1} K_1 \vec{J} = \Pi \vec{J}$$



references

- Ziman, Principles of the Theory of Solids, Cambridge Univ. Press, 1972, Chapter 7
- M. S. Dresselhaus, Transport Properties of Solids, MIT Univ. press, 2001, Chapters 4 and 5