# Boltzmann equation & transport properties

MR Torkamani

Kharazmi university

Spring 2019

# Outline I

# Outline II

# Introduction

- The carriers in a metal can be affected by external fields and temperature gradians.

# Introduction

- The carriers in a metal can be affected by external fields and temperature gradians.
- We want to calculate ordinary transport properties when constant fields are applied.

# Introduction

- The carriers in a metal can be affected by external fields and temperature gradians.
- We want to calculate ordinary transport properties when constant fields are applied.
- Simplest approach to do this porblem is to set up the transport equation or Boltzmann equation.

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

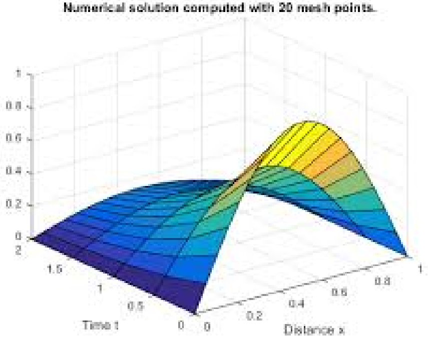
- $f(\vec{r}, \vec{k}, t)$: local concentration of carrier in the state $k$ in the neighborhood of the point $r$ in space.

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

- $f(\vec{r}, \vec{k}, t)$: local concentration of carrier in the state $k$ in the neighburhood of the point $r$ in space.
- Boltzmann's equation study $f(\vec{r}, \vec{k}, t)$ changes over time.

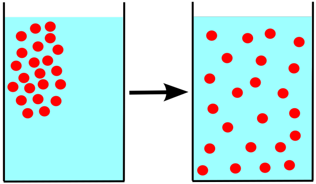
# What is $f(\vec{r}, \vec{k}, t)$

- $f(\vec{r}, \vec{k}, t)$: local concentration of carrier in the state $k$ in the neighburhood of the point $r$ in space.
- Boltzmann's equation study $f(\vec{r}, \vec{k}, t)$ changes over time.

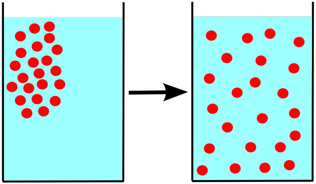


# Diffusion

# Diffusion

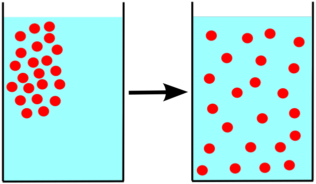


# Diffusion



- $\vec{v_k}$ is the velocity of a carrier in state $k$ .

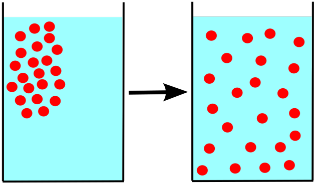
# Diffusion



- $\vec{v_k}$ is the velocity of a carrier in state $k$ .

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

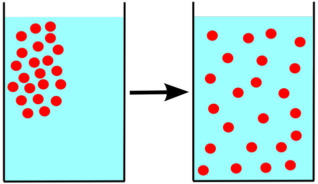
# Diffusion



- $\vec{v_k}$ is the velocity of a carrier in state $k$ .

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

$$\frac{\partial f}{\partial t} = \frac{f(\vec{r},\vec{k},\Delta t) - f(\vec{r},\vec{k},0)}{\Delta t}$$



- $\vec{v_k}$ is the velocity of a carrier in state $k$ .

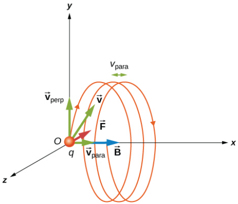
$$f(\vec{r},\vec{k},\Delta t) = f(\vec{r} - \vec{v_k}\Delta t, k, 0)$$

$$\frac{\partial f}{\partial t} = \frac{f(\vec{r},\vec{k},\Delta t) - f(\vec{r},\vec{k},0)}{\Delta t}$$

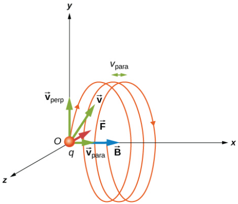
$$\frac{\partial f}{\partial t}\Big|_{diff} = -\vec{v_k}.\nabla f$$

# Electromagnetic field

# Electromagnetic field

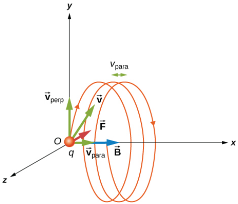


# Electromagnetic field




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

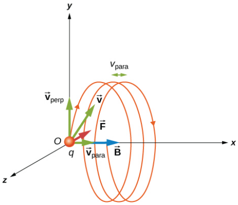
# Electromagnetic field




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

$$\dot{\vec{k}} = \frac{e}{\hbar}(\vec{E} + \frac{1}{c}\vec{v_k} \times \vec{H})$$

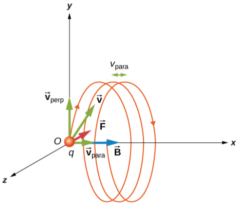
# Electromagnetic field




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

$$\dot{\vec{k}} = \frac{e}{\hbar}(\vec{E} + \frac{1}{c}\vec{v_k} \times \vec{H})$$

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




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

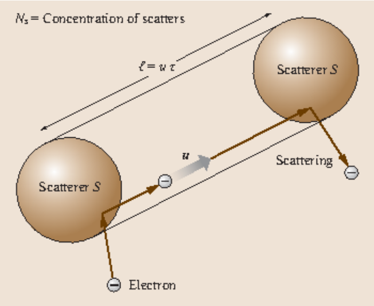
$$\dot{\vec{k}} = \frac{e}{\hbar}(\vec{E} + \frac{1}{c}\vec{v_k} \times \vec{H})$$

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

$$\frac{\partial f}{\partial t}\bigg|_{field} = -\frac{e}{\hbar}(\vec{E} + \frac{1}{c}\vec{v_k} \times \vec{H}).\nabla_k f$$

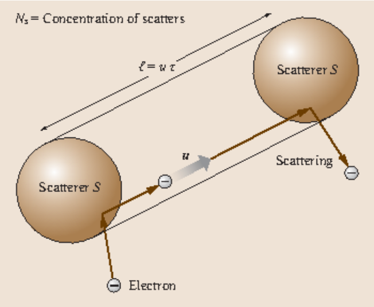
# Scattering

# Scattering



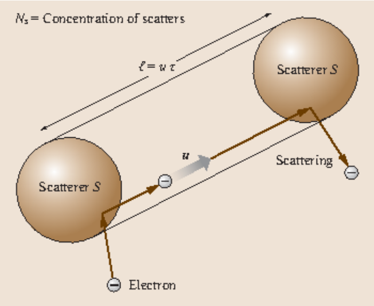
$N_s$ = Concentration of scatters
$\ell = u\tau$
Scatterer $S$
Scatterer $S$
$u$
Scattering
Electron

# Scattering




- the effect of scattering is more complicated.

# Scattering




- the effect of scattering is more complicated.

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

# 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

# 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

**Theorem**

*Boltzman equation*

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

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

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

- $f^0$ : equilibrium distribution

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

- $f^0$ : equilibrium distribution

$$f^0 = \frac{1}{e^{(\varepsilon_k - \zeta)/KT}} = f^0(\varepsilon_k)$$

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

- $f^0$ : equilibrium distribution

$$f^0 = \frac{1}{e^{(\varepsilon_k - \zeta)/KT}} = f^0(\varepsilon_k)$$

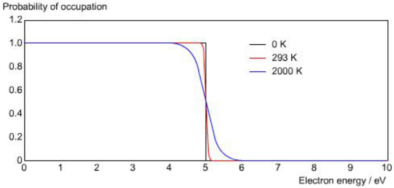
$$g(\vec{r}, \vec{k}, t) = f(\vec{r}, \vec{k}, t) - f^0$$

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

- $f^0$ : equilibrium distribution

$$f^0 = \frac{1}{e^{(\varepsilon_k - \zeta)/KT}} = f^0(\varepsilon_k)$$

$$g(\vec{r}, \vec{k}, t) = f(\vec{r}, \vec{k}, t) - f^0$$




Fermi-Dirac distribution for several temperatures

# Velocity of an electron!

# Velocity of an electron!

- the velocity of an electron in the state $|k>$ is just the gradient of $\varepsilon(k)$ in k-space.

# Velocity of an electron!

- the velocity of an electron in the state $|k>$ is just the gradient of $\varepsilon(k)$ in k-space.

$$\vec{v} = \frac{1}{\hbar} \nabla_k \varepsilon(k)$$

# Velocity of an electron!

- the velocity of an electron in the state $|k>$ is just the gradient of $\varepsilon(k)$ in k-space.

$$\vec{v} = \frac{1}{\hbar}\nabla_k \varepsilon(k)$$

for free electron

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

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

# Boltzmann equation

$$(-\frac{\partial f^0}{\partial \varepsilon})\vec{v_k}.(-\frac{\varepsilon(k)-\zeta}{T})\nabla T + e(\vec{E} - 1/c\nabla\zeta)$$
$$= \frac{\partial f}{\partial t}\Big|_{scatt} + \vec{v_k}.\frac{\partial g}{\partial r} + \frac{e}{\hbar c}(\vec{v_k} \times \vec{H}).\frac{\partial g}{\partial k}$$

# Boltzmann equation

suppose we have only an electic field $\vec{E}$

# Boltzmann equation

suppose we have only an electic field $\vec{E}$

$$(-\frac{\partial f^0}{\partial \varepsilon})\vec{v_k}.e\vec{E} = -\frac{\partial f}{\partial t}\Big|_{scatt}$$

# Boltzmann equation

suppose we have only an electic field $\vec{E}$

$$(-\frac{\partial f^0}{\partial \varepsilon})\vec{v_k}.e\vec{E} = -\frac{\partial f}{\partial t}|_{scatt}$$

$$-\frac{\partial f}{\partial t}|_{scatt} = \frac{g}{\tau} \quad \text{assumption}$$

suppose we have only an electic field $\vec{E}$

$$(-\frac{\partial f^0}{\partial \varepsilon})\vec{v_k}.e\vec{E} = -\frac{\partial f}{\partial t}|_{scatt}$$

$$-\frac{\partial f}{\partial t}|_{scatt} = \frac{g}{\tau} \quad \text{assumption}$$

$$g(t) = g(0)e^{-\frac{t}{\tau}}$$

suppose we have only an electic field $\vec{E}$

$$(-\frac{\partial f^0}{\partial \varepsilon})\vec{v_k}.e\vec{E} = -\frac{\partial f}{\partial t}\Big|_{scatt}$$

$$-\frac{\partial f}{\partial t}\Big|_{scatt} = \frac{g}{\tau} \quad \text{assumption}$$

$$g(t) = g(0)e^{-\frac{t}{\tau}}$$

$$\boxed{g = (-\frac{\partial f^0}{\partial \varepsilon})\vec{v_k}.e\tau\vec{E}}$$

# Current density

# Current density

$$\vec{J} = 2\int ev_k f(\vec{r}, \vec{k}, t)dk$$

# Current density

$$\vec{J} = 2\int ev_k f(\vec{r}, \vec{k}, t)dk$$

$$\vec{J} = 2\int e\vec{v_k} g(r, k, t)dk \quad (\text{since} \int \vec{v_k} f^0 dk \equiv 0)$$

# Current density

$$\vec{J} = 2\int ev_k f(\vec{r},\vec{k},t)dk$$

$$\vec{J} = 2\int e\vec{v_k} g(r,k,t)dk \quad (\text{since} \int \vec{v_k} f^0 dk \equiv 0)$$

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

# Current density

$$\vec{J} = 2\int e v_k f(\vec{r},\vec{k},t)dk$$

$$\vec{J} = 2\int e\vec{v_k} g(r,k,t)dk \quad (\text{since} \int \vec{v_k} f^0 dk \equiv 0)$$

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

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

# conducting scalar

- we usually deal with crystals having cubic symmetry in which case the conductivity tensor reduce to an scalar.

# conducting scalar

- we usually deal with crystals having cubic symmetry in which case the conductivity tensor reduce to an scalar.
- thinking of the case where $\vec{E}$ and $\vec{J}$ both in x-direction.

- we usually deal with crystals having cubic symmetry in which case the conductivity tensor reduce to an scalar.
- thinking of the case where $\vec{E}$ and $\vec{J}$ both in x-direction.

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

# conducting scalar

- we usually deal with crystals having cubic symmetry in which case the conductivity tensor reduce to an scalar.
- thinking of the case where $\vec{E}$ and $\vec{J}$ both in x-direction.

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

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

# conducting scalar

# conducting scalar

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

# conducting scalar

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

$$f = f^0(k - \frac{e\tau}{\hbar}\vec{E}) \qquad \text{in k-space}$$

# conducting scalar

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

$$f = f^0(k - \frac{e\tau}{\hbar}\vec{E}) \qquad \text{in k-space}$$

$$f = f^0(\varepsilon_k - e\tau\vec{v_k}.\vec{E}) \qquad \delta\varepsilon_k = e\tau\vec{v_k}.\vec{E}$$

# conducting scalar

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

$$f = f^0(k - \frac{e\tau}{\hbar}\vec{E}) \qquad \text{in k-space}$$

$$f = f^0(\varepsilon_k - e\tau\vec{v_k}.\vec{E}) \qquad \delta\varepsilon_k = e\tau\vec{v_k}.\vec{E}$$

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

# conducting scalar

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

$$f = f^0(k - \frac{e\tau}{\hbar}\vec{E}) \qquad \text{in k-space}$$

$$f = f^0(\varepsilon_k - e\tau\vec{v_k}.\vec{E}) \qquad \delta\varepsilon_k = e\tau\vec{v_k}.\vec{E}$$

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

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

# Boltzmann equation

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

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

$$(-\frac{\partial f^0}{\partial \varepsilon})\vec{v_k}.(-\frac{\varepsilon(k)-\zeta}{T})\nabla T + e(\vec{E} - 1/c\nabla\zeta) = \frac{\partial f}{\partial t}|_{scatt}$$

# Boltzmann equation

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

$$(-\frac{\partial f^0}{\partial \varepsilon})\vec{v_k}.(-\frac{\varepsilon(k)-\zeta}{T})\nabla T + e(\vec{E} - 1/c\nabla\zeta) = \frac{\partial f}{\partial t}|_{scatt}$$

$$\vec{J} = \frac{1}{4\pi^3}\frac{e^2\tau}{\hbar}\int\int \vec{v_k}\vec{v_k}(-\frac{\partial f^0}{\partial \varepsilon})\frac{ds}{v_k}d\varepsilon.(\vec{E} - \frac{1}{e}\nabla\zeta)$$
$$+\frac{1}{4\pi^3}\frac{e^2\tau}{\hbar}\int\int \vec{v_k}\vec{v_k}(\frac{\varepsilon-\zeta}{T})(-\frac{\partial f^0}{\partial \varepsilon})\frac{ds}{v_k}d\varepsilon.(-\nabla T)$$

# Heat

- heat $=$ internal energy $-$ free energy

# Heat

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

$$U = 2\int f(\varepsilon - \zeta)v_k dk$$

# General Transport equation

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

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

# General Transport equation

$$\vec{J} = e^2\vec{K}_0.\vec{E} + \frac{e}{T}\vec{K}_1.(-\nabla T)$$
$$\vec{U} = e\vec{K}_1.\vec{E} + \frac{1}{T}\vec{K}_2.(-\nabla T)$$

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

# General Transport equation

$$\vec{J} = e^2\vec{K}_0.\vec{E} + \frac{e}{T}\vec{K}_1.(-\nabla T)$$
$$\vec{U} = e\vec{K}_1.\vec{E} + \frac{1}{T}\vec{K}_2.(-\nabla T)$$

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

$$K_0 = \frac{\tau}{4\pi^3\hbar}\int \vec{v}\vec{v}\frac{ds_f}{v}$$
$$K_2 = \frac{1}{3}\pi^2(kT)^2K_0(\zeta)$$
$$K_1 = \frac{1}{3}\pi^2(kT)^2\frac{\partial}{\partial\varepsilon}K_0(\varepsilon)\Big|_{\varepsilon=\zeta}$$

# Thermal conductivity

# Thermal conductivity

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

# Thermal conductivity

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

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

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

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

# Thermal conductivity

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

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

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

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

# Wiedemann-Franz law

# Wiedemann-Franz law

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

$$\sigma = e^2 K_0$$

# Wiedemann-Franz law

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

$$\sigma = e^2 K_0$$

$$K_2 = \frac{1}{3}\pi^2 (kT)^2 K_0(\zeta)$$

# Wiedemann-Franz law

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

$$\sigma = e^2 K_0$$

$$K_2 = \frac{1}{3}\pi^2 (kT)^2 K_0(\zeta)$$

$$\boxed{\kappa = \frac{\pi^2}{3}\frac{k^2}{e^2} T\sigma}$$

# Compair Electrical and Thermal conduction

| electircal conduction | thermal conduction |
|---|---|
| each electorn 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 $kT$ its 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 $= \dfrac{k^2T}{e^2}$

# Seebeck effect

# Seebeck effect

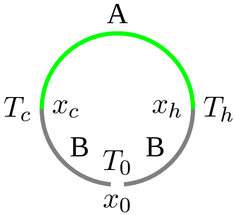
in open circuit with thermal gradient we have:

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

# Seebeck effect

in open circuit with thermal gradient we have:

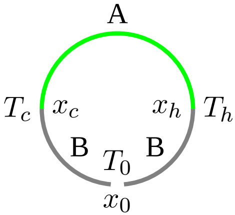
$$\vec{E} = \frac{1}{eT} K_0^{-1} K_1 (\nabla T) = Q \nabla T$$



# Seebeck effect

in open circuit with thermal gradient we have:

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




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

# Peltier effect

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

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

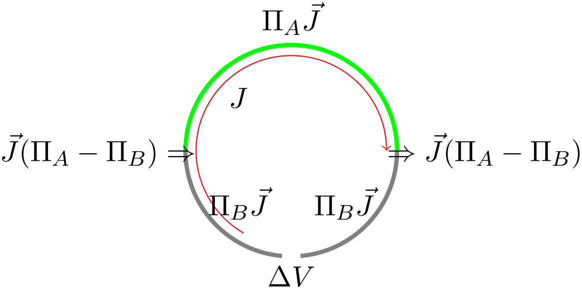
$$\vec{U} = \frac{1}{e}K_0^{-1}K_1\vec{J} = \Pi\vec{J}$$

# Peltier effect

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

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

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



# 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