

# Elements of the conductivity matrix

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$$\vec{j}_{elec} = -e \int \vec{v}(\vec{k}) D(\vec{k}) f(\vec{k}) d\vec{k}$$

$$\vec{j}_{elec} = \frac{-e}{4\pi^3} \int \vec{v}(\vec{k}) \left( \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left( -\frac{e}{\hbar} (\vec{v}(\vec{k}) \times \vec{B} + \vec{E}) \cdot \nabla_k E(\vec{k}) + \vec{v}(\vec{k}) \cdot \left( \frac{E(\vec{k}) - \mu}{T} \nabla T + \nabla \mu \right) \right) \right) d^3k$$

$$\vec{B} = 0, \quad \nabla T = 0, \quad \nabla \mu = 0$$

$$\vec{j}_{elec} = \frac{e^2}{4\pi^3 \hbar} \int \vec{v}(\vec{k}) \left( \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} (\vec{E} \cdot \nabla_k E(\vec{k})) \right) d^3k$$

$j$  is not necessarily parallel to  $E$

$$j_{elec\ n} = \sigma_{nm} E_m$$

set  $\vec{E} = \hat{x}$  to calculate  $\sigma_{xx}$ ,  $\sigma_{xy}$ , and  $\sigma_{xz}$

# Free electrons

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$$\vec{j}_{elec} = -e \int \vec{v}(\vec{k}) D(\vec{k}) f(\vec{k}) d\vec{k}$$

$$\vec{v}(\vec{k}) = \frac{\hbar \vec{k}}{m}$$

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

$$D(\vec{k}) = \frac{2}{(2\pi)^3} \leftarrow \text{spin}$$

$$\nabla_{\vec{k}} E(\vec{k}) = \frac{\hbar^2}{m} \vec{k}$$

$$\vec{j}_{elec} = \frac{-e\hbar}{4\pi^3 m} \int \vec{k} f(\vec{k}) d^3 k$$

probability that the states  
are occupied

# Ohm's law (free electrons)

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$$\vec{j}_{elec} = \frac{-e\hbar}{4\pi^3 m} \int \vec{k} \left( \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left( -\frac{e}{\hbar} \left( \frac{\hbar \vec{k}}{m} \times \vec{B} + \vec{E} \right) \cdot \frac{\hbar^2 \vec{k}}{m} + \frac{\hbar \vec{k}}{m} \cdot \left( \frac{\hbar^2 k^2 / 2m - \mu}{T} \nabla T + \nabla \mu \right) \right) \right) d^3 k$$

$$\vec{B} = 0, \quad \nabla T = 0, \quad \nabla \mu = 0$$

$$\vec{j}_{elec} = \frac{e^2}{4\pi^3 m} \int \vec{k} \left( \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \vec{E} \cdot \frac{\hbar^2 \vec{k}}{m} \right) d^3 k$$

Choose  $E$  to be in the  $z$ -direction

$$\vec{j}_{elec} = \frac{\hbar^2 e^2 \tau E}{4\pi^3 (m^*)^2} \int \vec{k} \frac{\partial f_0}{\partial \mu} |k| \cos \theta d^3 k$$

# A useful integral

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$$\int \vec{k} \frac{\partial f_0}{\partial \mu} |k| \cos \theta d^3 k \approx \frac{4\pi m k_F^3}{3\hbar^2}$$
$$= \int \frac{\partial f_0}{\partial \mu} |k| \cos \theta (k_x \hat{x} + k_y \hat{y} + k_z \hat{z}) d^3 k$$

The  $x$  and  $y$  components are zero: odd functions over even intervals.

$$d^3 k = k^2 \sin \theta d\varphi d\theta dk \qquad k_z = |k| \cos \theta$$

$$= \int \frac{\partial f_0}{\partial \mu} k^2 \cos^2 \theta k^2 \sin \theta d\varphi d\theta dk$$

The  $\varphi$  integration contributes a factor of  $2\pi$ .

$$= 2\pi \int \frac{\partial f_0}{\partial \mu} k^4 \cos^2 \theta \sin \theta d\theta dk$$

## A useful integral (2)

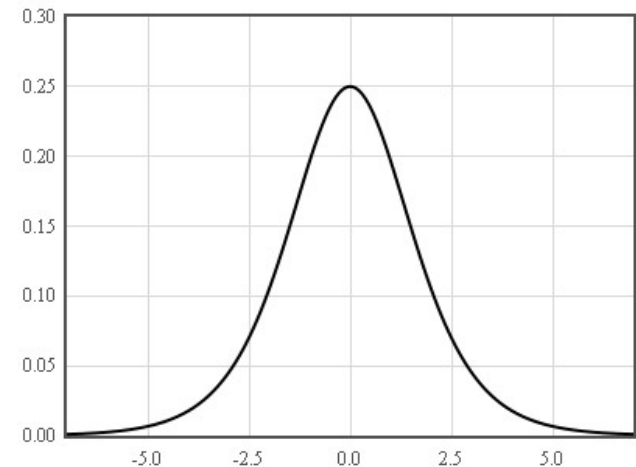
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$$= 2\pi \int \frac{\partial f_0}{\partial \mu} k^4 \cos^2 \theta \sin \theta d\theta dk$$

The  $\theta$  integration contributes a factor of  $2/3$ .

$$= \frac{4\pi}{3} \int \frac{\partial f_0}{\partial \mu} k^4 dk$$

$$\frac{\partial f_0}{\partial \mu} \approx \frac{m^*}{\hbar^2 k_F} \delta(k - k_F)$$



$$\int \vec{k} \frac{\partial f_0}{\partial \mu} k \cos \theta d^3 k \approx \frac{4\pi m k_F^3}{3\hbar^2}$$

# Ohm's law (free electrons)

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$$j_z \approx \frac{\hbar^2 e^2 \tau E}{3\pi^2 (m^*)^2} \int \vec{k} \frac{\partial f_0}{\partial \mu} k \cos \theta d^3 k = \frac{e^2 \tau E k_F^3}{3\pi^2 m^*}$$

$\nearrow$   
 $\frac{4\pi m k_F^3}{3\hbar^2}$

For free electrons:  $n = \frac{k_F^3}{3\pi^2}$

Drude result:  $j_z \approx \frac{ne^2 \tau E_z}{m^*} = ne\mu_{mob} E_z$

Project: Write a program that will calculate the integral over  $k$ .

# Boltzmann equation

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The general form of the electrical current density is:

$$\vec{j}_{elec} = -e \int \vec{v}(\vec{k}) D(\vec{k}) f(\vec{k}) d\vec{k}$$

$$\vec{j}_{elec} = \frac{-e}{4\pi^3} \int \vec{v}(\vec{k}) \left( \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left( -\frac{e}{\hbar} (\vec{v}(\vec{k}) \times \vec{B} + \vec{E}) \cdot \nabla_k E(\vec{k}) + \vec{v}(\vec{k}) \cdot \left( \frac{E(\vec{k}) - \mu}{T} \nabla T + \nabla \mu \right) \right) \right) d^3k$$

# Thermoelectric current (free electrons)

$$\vec{j}_{elec} = \frac{-e\hbar}{4\pi^3 m} \int \vec{k} \left( \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left( -\frac{e}{\hbar} \left( \frac{\hbar \vec{k}}{m} \times \vec{B} + \vec{E} \right) \cdot \nabla_k E(\vec{k}) + \frac{\hbar \vec{k}}{m} \cdot \left( \frac{E(\vec{k}) - \mu}{T} \nabla T + \nabla \mu \right) \right) \right) d^3 k$$

$$\vec{B} = 0, \quad \vec{E} = 0, \quad \nabla \mu = 0, \quad E(\vec{k}) = \frac{\hbar^2 k^2}{2m}$$

$$\vec{j}_{elec} = \frac{-e\hbar}{4\pi^3 m} \int \vec{k} \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \frac{\hbar \vec{k}}{m} \cdot \frac{E(\vec{k}) - \mu}{T} \nabla T d^3 k$$

$$\vec{j}_{elec} = -\frac{e\hbar^4 \tau \nabla T}{4\pi^3 m^3 T} \int \vec{k} \frac{\partial f_0}{\partial \mu} k^3 \cos \theta d^3 k + \frac{e\hbar^2 \tau \nabla T \mu}{4\pi^3 m^2 T} \int \vec{k} \frac{\partial f_0}{\partial \mu} k \cos \theta d^3 k$$

Similar to the  
useful integral

Useful integral



# Thermoelectric current

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$$\vec{j}_{elec} = -\frac{e\hbar^4\tau\nabla T}{4\pi^3 m^{*3}T} \frac{4\pi m k_F^5}{3\hbar^2} + \frac{e\hbar^2\tau\nabla T\mu}{4\pi^3 m^{*2}T} \frac{4\pi m k_F^3}{3\hbar^2}$$

$$\vec{j}_{elec} = \frac{k_F^3 e\tau}{3\pi^2 m^* T} \left( \frac{\hbar^2 k_F^2}{m^*} - \mu \right) \nabla T$$

$\approx (2E_F - E_F)$

$$\vec{j}_{elec} = \frac{k_F^3 e\tau}{3\pi^2 m^* T} E_F \nabla T$$

For free electrons:  $n = \frac{k_F^3}{3\pi^2}$

$$\vec{j}_{elec} = \frac{ne\tau}{m^* T} E_F \nabla T = n\mu_{mob} \frac{E_F}{T} \nabla T$$

# Diffusion current (free electrons)

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$$\vec{j}_{elec} = \frac{-e\hbar}{4\pi^3 m} \int \vec{k} \left( \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left( -\frac{e}{\hbar} \left( \frac{\hbar \vec{k}}{m} \times \vec{B} + \vec{E} \right) \cdot \nabla_k E(\vec{k}) + \frac{\hbar \vec{k}}{m} \cdot \left( \frac{E(\vec{k}) - \mu}{T} \nabla T + \nabla \mu \right) \right) \right) d^3 k$$

$$\vec{B} = 0, \quad \nabla T = 0, \quad \vec{E} = 0$$

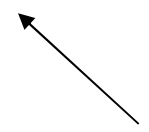
$$\vec{j}_{elec} = \frac{-e\hbar}{4\pi^3 m} \int \vec{k} \left( \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \frac{\hbar \vec{k}}{m} \cdot \nabla \mu \right) d^3 k$$

Choose  $\nabla \mu$  in the  $z$  direction

$$\vec{j}_{elec} = \frac{-e\hbar^2 |\nabla \mu| \tau}{4\pi^3 m^2} \int \vec{k} \frac{\partial f_0}{\partial \mu} k \cos \theta d^3 k$$

$$\vec{j}_{elec} = \frac{-e\tau n}{m} \nabla \mu = -n \mu_{mob} \nabla \mu$$

Useful integral



# Seebeck effect

$$\vec{j}_{elec} = \frac{-e}{4\pi^3} \int \vec{v}_{\vec{k}} \left( \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left( -\frac{e}{\hbar} (\vec{v}(\vec{k}) \times \vec{B} + \vec{E}) \cdot \nabla_k E(\vec{k}) + \vec{v}(\vec{k}) \cdot \left( \frac{E(\vec{k}) - \mu}{T} \nabla T + \nabla \mu \right) \right) \right) d^3 k$$

$$\vec{B} = 0, \quad \vec{j}_{elec} = 0, \quad \vec{E} \neq 0 \quad \nabla \mu \neq 0$$

The electric current due to an electromotive force is cancelled by the electric current due to a thermal gradient

$$0 = \int \vec{v}_{\vec{k}} \left( \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left( -\frac{e}{\hbar} \vec{E} \cdot \nabla_k E(\vec{k}) + \vec{v}(\vec{k}) \cdot \left( \frac{E(\vec{k}) - \mu}{T} \nabla T + \nabla \mu \right) \right) \right) d^3 k$$

Thermopower (Seebeck effect):

$$Q_{mn} = \frac{\int (\vec{E} - \nabla \mu / e) \cdot d\vec{x}_m}{\nabla T_n}$$



# Thermoelectric effects

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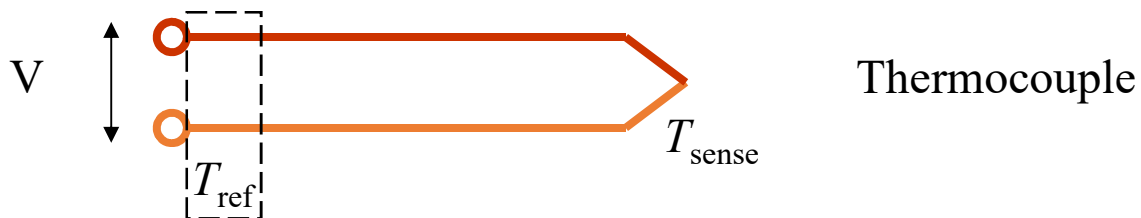
## Seebeck effect:

A thermal gradient causes a thermal current to flow. This results in a voltage which sends the low entropy charge carriers back to the hot end.

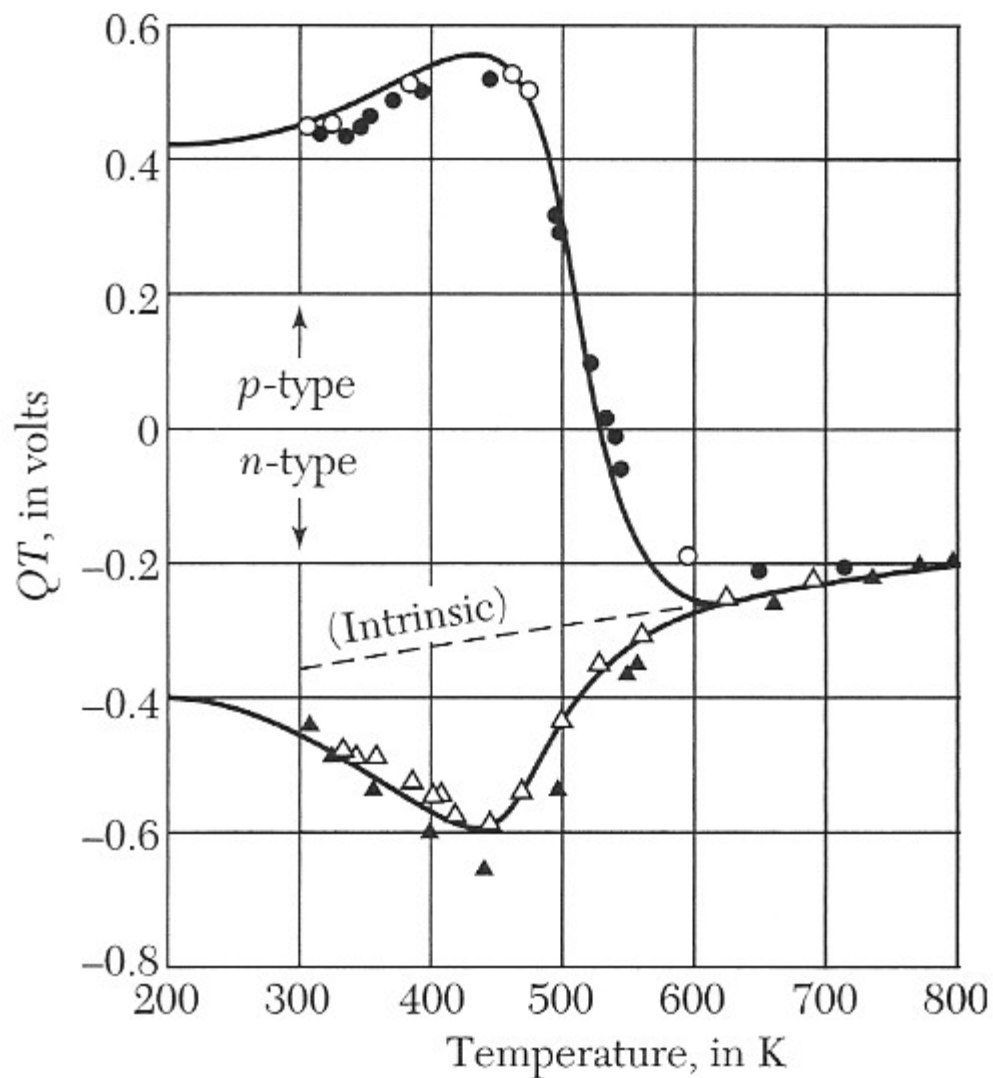
$$\nabla V_{\text{electrochemical}} = Q \nabla T$$

$Q$  is the absolute thermal power. The sign of the voltage (electrochemical potential, electromotive force) is the same as the sign of the charge carriers.

The Seebeck effect can be used to make a thermometer. The gradient of the temperature is the same along both wires but the gradient in electrochemical potential differs.



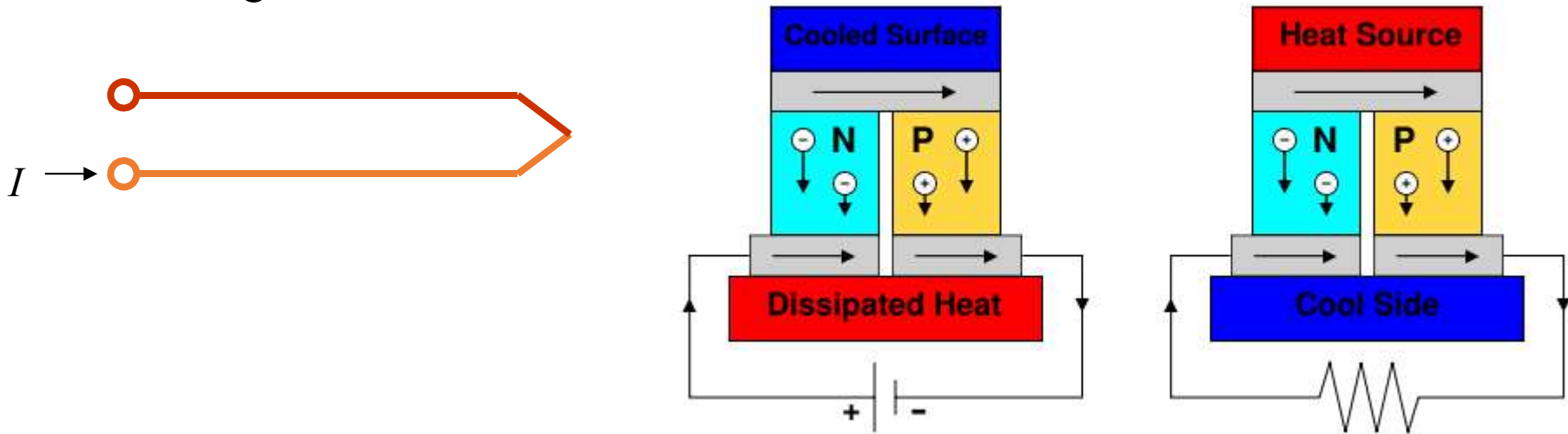
# Thermoelectric effects



Intrinsic  $Q$  is negative because electrons have a higher mobility.

# Thermoelectric effects

**Peltier effect:** driving a through a bimetallic junction causes heating or cooling.



Cooling takes place when the electrons make a transition from low entropy to high entropy at the junction.

# Hall effect

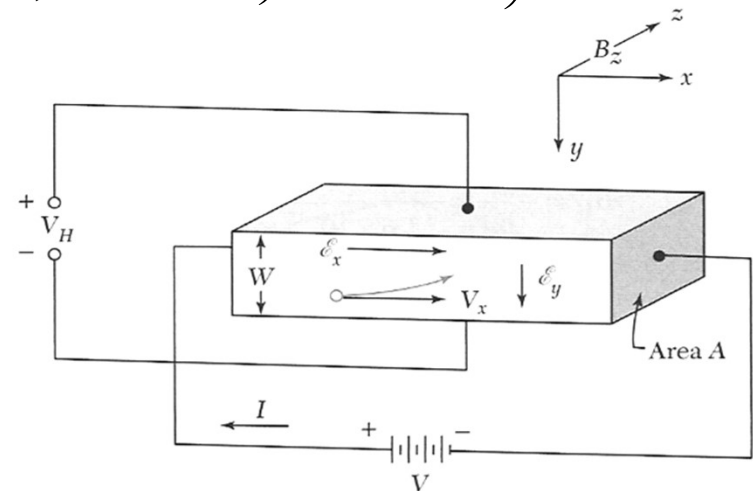
$$\vec{j}_{elec} = \frac{-e\hbar}{4\pi^3 m} \int \vec{k} \left( \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left( -\frac{e}{\hbar} \left( \frac{\hbar \vec{k}}{m} \times \vec{B} + \vec{E} \right) \cdot \nabla_k E(\vec{k}) + \frac{\hbar \vec{k}}{m} \cdot \left( \frac{E(\vec{k}) - \mu}{T} \nabla T + \nabla \mu \right) \right) \right) d^3 k$$

$$\vec{B} = \vec{B}_z, \quad \vec{j}_x = \frac{I_x}{A}, \quad \vec{j}_y = 0, \quad \vec{j}_z = 0, \quad \nabla T = 0$$

$$\vec{j}_{elec} = \frac{-e\hbar}{4\pi^3 m} \int \vec{k} \left( \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left( -\frac{e}{\hbar} \left( \frac{\hbar \vec{k}}{m} \times \vec{B} + \vec{E} \right) \cdot \nabla_k E(\vec{k}) \right) + \frac{\hbar \vec{k}}{m} \cdot \nabla \mu \right) d^3 k$$

Hall coefficient:  $R_{lmn} = \frac{E_l}{j_{em} B_n}$

diffusive metals:  $R_H = \frac{-1}{ne}$



# Nernst effect

$$\vec{j}_{elec} = \frac{-e\hbar}{4\pi^3 m} \int \vec{k} \left( \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left( -\frac{e}{\hbar} \left( \frac{\hbar \vec{k}}{m} \times \vec{B} + \vec{E} \right) \cdot \nabla_k E(\vec{k}) + \frac{\hbar \vec{k}}{m} \cdot \left( \frac{E(\vec{k}) - \mu}{T} \nabla T + \nabla \mu \right) \right) \right) d^3 k$$

$$\vec{B} = \vec{B}_z, \quad \nabla T$$

$$0 = \frac{-e\hbar}{4\pi^3 m} \int \vec{k} \left( \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left( -\frac{e}{\hbar} \left( \frac{\hbar \vec{k}}{m} \times \vec{B} + \vec{E} \right) \cdot \nabla_k E(\vec{k}) + \frac{\hbar \vec{k}}{m} \cdot \frac{E(\vec{k}) - \mu}{T} \nabla T \right) \right) d^3 k$$

Nernst coefficient:  $N_{lmn} = \frac{E_l}{B_m \nabla T_n}$

Open circuit and measure voltage



# Etingshausen effect

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$$\vec{j}_{elec} = \frac{-e\hbar}{4\pi^3 m} \int \vec{k} \left( \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left( -\frac{e}{\hbar} \left( \frac{\hbar \vec{k}}{m} \times \vec{B} + \vec{E} \right) \cdot \nabla_k E(\vec{k}) + \frac{\hbar \vec{k}}{m} \cdot \left( \frac{E(\vec{k}) - \mu}{T} \nabla T + \nabla \mu \right) \right) \right) d^3 k$$

$$\vec{B} = \vec{B}_z, \quad \vec{E} = 0, \quad \nabla T$$

$$\vec{j}_{elec} = \frac{-e\hbar}{4\pi^3 m} \int \vec{k} \left( \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left( \frac{-e\vec{k}}{m} \times \vec{B} \cdot \nabla_k E(\vec{k}) + \frac{\hbar \vec{k}}{m} \cdot \frac{E(\vec{k}) - \mu}{T} \nabla T \right) \right) d^3 k$$

Etingshausen coefficient: 
$$P_{lmn} = \frac{-1}{j_{el} B_m \nabla T_n}$$

short circuit and measure current

# Boltzmann Group

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Albert von Ettingshausen,  
Prof. at TU  
Graz.



Nernst was a student of Boltzmann and von Ettingshausen. He won the 1920 Nobel prize in Chemistry.

(Standing, from the left) Walther Nernst, Heinrich Streintz, Svante Arrhenius, Hiecke, (sitting, from the left) Aulinger, Albert von Ettingshausen, Ludwig Boltzmann, Ignacij Klemencic, Hausmanninger (1887).

Annalen der Physik, vol. 265, pp. 343–347, 1886

**IX. Ueber das Auftreten electromotorischer Kräfte  
in Metallplatten, welche von einem Wärmestrome  
durchflossen werden und sich im magnetischen  
Felde befinden;**

**von A. v. Ettingshausen und stud. W. Nernst.**

(Aus d. Anz. d. k. Acad. d. Wiss. in Wien, mitgetheilt von den Herren Verf.)

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Bei Gelegenheit der Beobachtung des Hall'schen Phänomens im Wismuth wurden wir durch gewisse Unregelmässigkeiten veranlasst, folgenden Versuch anzustellen.

Eine rechteckige Wismuthplatte, etwa 5 cm lang, 4 cm breit, 2 mm dick, mit zwei an den längeren Seiten einander gegenüber liegenden Electroden versehen, ist in das Feld eines Electromagnets gebracht, sodass die Kraftlinien die Ebene der Platte senkrecht schneiden; dieselbe wird durch federnde Kupferbleche getragen, in welche sie an den kürzeren Seiten eingeklemmt ist, jedoch geschützt vor directer metallischer Berührung mit dem Kupfer durch zwischengelegte Glimmerblätter.

# Thermoelectric effects

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$$f(\vec{k}) \approx f_0(\vec{k}) + \frac{\tau(\vec{k})e(\vec{v} \times \vec{B} + \vec{E}) \cdot \nabla_{\vec{k}} f_0}{\hbar} + \tau(\vec{k})\vec{v} \cdot \left( \frac{\partial f_0}{\partial T} \nabla T + \frac{\partial f_0}{\partial \mu} \nabla \mu \right)$$

Electrical current:  $\vec{j}_{elec} = \frac{-e}{4\pi^3} \int \vec{v}(\vec{k}) f(\vec{k}) d^3 k$

Particle current:  $\vec{j}_n = \frac{1}{4\pi^3} \int \vec{v}(\vec{k}) f(\vec{k}) d^3 k$

Energy current:  $\vec{j}_E = \frac{1}{4\pi^3} \int \vec{v}(\vec{k}) E(\vec{k}) f(\vec{k}) d^3 k$

Heat current:  $\vec{j}_Q = \frac{1}{4\pi^3} \int \vec{v}(\vec{k}) (E(\vec{k}) - \mu) f(\vec{k}) d^3 k$

# Thermal conductivity

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$$\vec{j}_Q = \frac{\hbar}{4\pi^3 m} \int (E(\vec{k}) - \mu) \vec{k} \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \left( -\frac{e}{\hbar} \left( \frac{\hbar \vec{k}}{m} \times \vec{B} + \vec{E} \right) \cdot \nabla_{\vec{k}} E(\vec{k}) + \frac{\hbar \vec{k}}{m} \cdot \left( \frac{E(\vec{k}) - \mu}{T} \nabla T + \nabla \mu \right) \right) d^3 k$$

$$\vec{B} = 0, \quad \vec{j}_{elec} = 0$$

$$\vec{j}_Q = \frac{\hbar}{4\pi^3 m} \int (E(\vec{k}) - \mu) \vec{k} \tau(\vec{k}) \frac{\partial f_0}{\partial \mu} \frac{\hbar \vec{k}}{m} \cdot \frac{E(\vec{k}) - \mu}{T} \nabla T d^3 k$$

$$\kappa_{mn} = \frac{-j_{Qm}}{\nabla T_n}$$