21. Transport

Dec. 13, 2018

Boltzmann equation: relaxation time approx.

The relaxation time approximation:

$$\frac{\partial f}{\partial t} = -\frac{\vec{F}_{ext}\cdot\nabla_k f}{\hbar} - \vec{v}\cdot\nabla f + \frac{f_0(\vec{k}) - f(\vec{k})}{\tau(\vec{k})}$$

in a stationary state $\frac{\partial f}{\partial t} = 0$

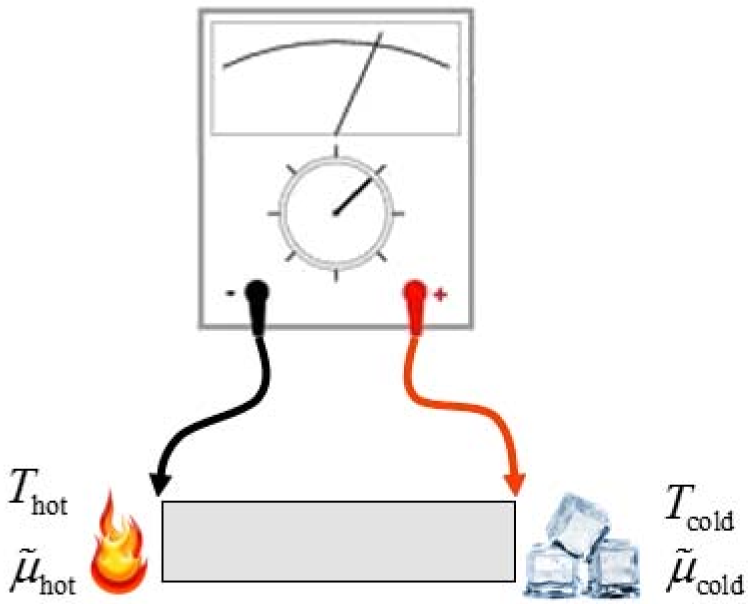
If the system is not far from equilibrium, $f \approx f_0$, and we can substitute f_0 for f on the right

$$f(\vec{k}) = f_0(\vec{k}) - \tau(\vec{k})\left(\frac{\vec{F}_{ext}\cdot\nabla_k f_0}{\hbar} + \vec{v}\cdot\nabla f_0\right)$$

$$f_0(\vec{k}) = \frac{1}{\exp\left(\frac{E(\vec{k})-\mu}{k_B T}\right)+1}$$

Seebeck effect

$$\nabla_{\vec{r}}\tilde{\mu} = -S\nabla_{\vec{r}}T$$



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

$\vec{j}_{\text{elec}} = 0$ $\qquad\qquad$ $\vec{B} = 0$

Thermoelectric effects

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.

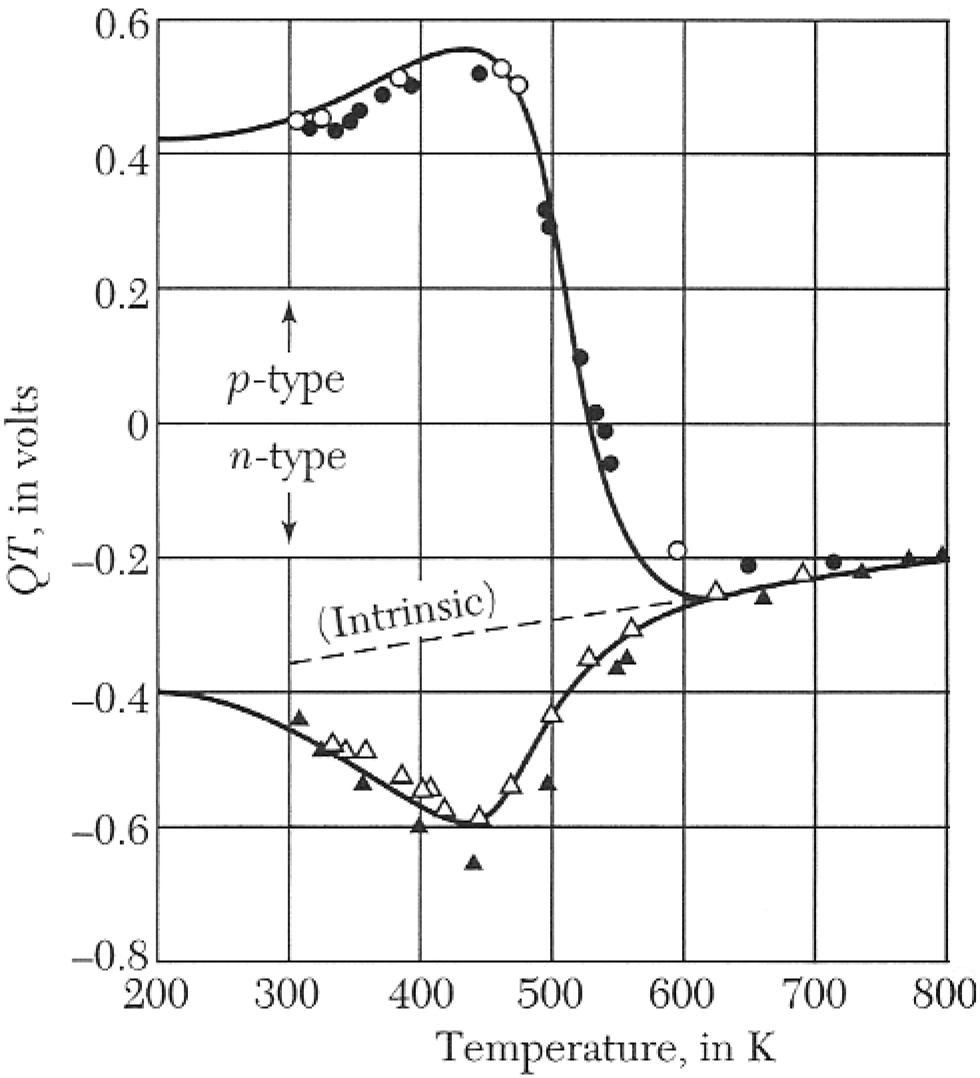
$$\nabla \tilde{\mu} = -S \nabla T$$

S is the absolute thermal power (often also called *Q*). 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.

Thermocouple

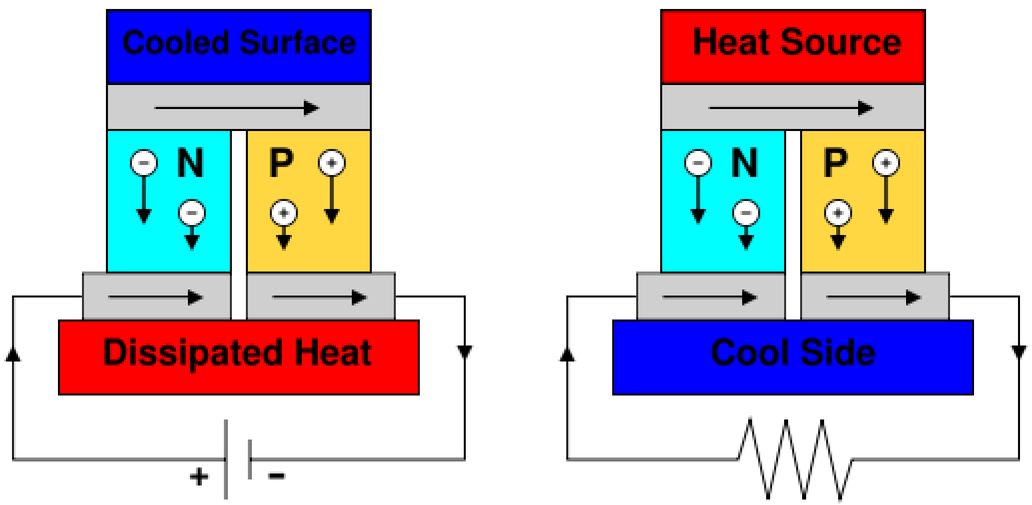
Thermoelectric effects



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.

Bismuth chalcogenides Bi_2Te_3 and Bi_2Se_3

http://en.wikipedia.org/wiki/Peltier_effect#Peltier_effect

Hall effect

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

$$\nabla_{\vec{r}}T = 0$$

$$\vec{j}_{\text{elec}} = \frac{e}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial\mu}\nabla_{\vec{k}}E(\vec{k})\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\nabla_{\vec{r}}\tilde{\mu} + \frac{e}{\hbar}\nabla_{\vec{k}}E(\vec{k})\times\vec{B}\right)\right)d^3k$$

$$R_{lmn} = \frac{\nabla_{\vec{r}}\tilde{\mu}_l}{ej_mB_n}.$$

$$R_{lmn} = \left[\frac{e^2}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial\mu}\nabla_{\vec{k}}E(\vec{k})\cdot\hat{e}_m\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\hat{e}_l + \frac{e}{\hbar}\nabla_{\vec{k}}E(\vec{k})\times\hat{e}_n\right)\right)d^3k\right]^{-1}$$

Nerst effect

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

$$\vec{j}_{\text{elec}} = 0$$

$$0 = \frac{e}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial \mu}\nabla_{\vec{k}}E(\vec{k})\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\nabla_{\vec{r}}\tilde{\mu}+\frac{E(\vec{k})-\mu}{T}\nabla_{\vec{r}}T+\frac{e}{\hbar}\nabla_{\vec{k}}E(\vec{k})\times\vec{B}\right)\right)d^3k.$$

$$N_{lmn} = \frac{\nabla\tilde{\mu}_l}{e\nabla T_m B_n}$$

$$0 = \frac{e}{4\pi^3\hbar^2}\int \tau(\vec{k})\frac{\partial f_0}{\partial \mu}\nabla_{\vec{k}}E(\vec{k})\cdot\hat{e}_i\left(\nabla_{\vec{k}}E(\vec{k})\cdot\left(\begin{pmatrix}eN_{xyz}\\ eN_{yyz}\\ eN_{zzz}\end{pmatrix}+\frac{E(\vec{k})-\mu}{T}\hat{y}+\frac{e}{\hbar}\nabla_{\vec{k}}E(\vec{k})\times\hat{z}\right)\right)d^3k.$$

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

http://dx.doi.org/10.1002/andp.18862651010

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.)

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.

Ettingshausen effect

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

The sample is electrically grounded so $\nabla_{\vec{r}}\tilde{\mu} = 0$.

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

Boltzmann Group

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).

Thermoelectric effects

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

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

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

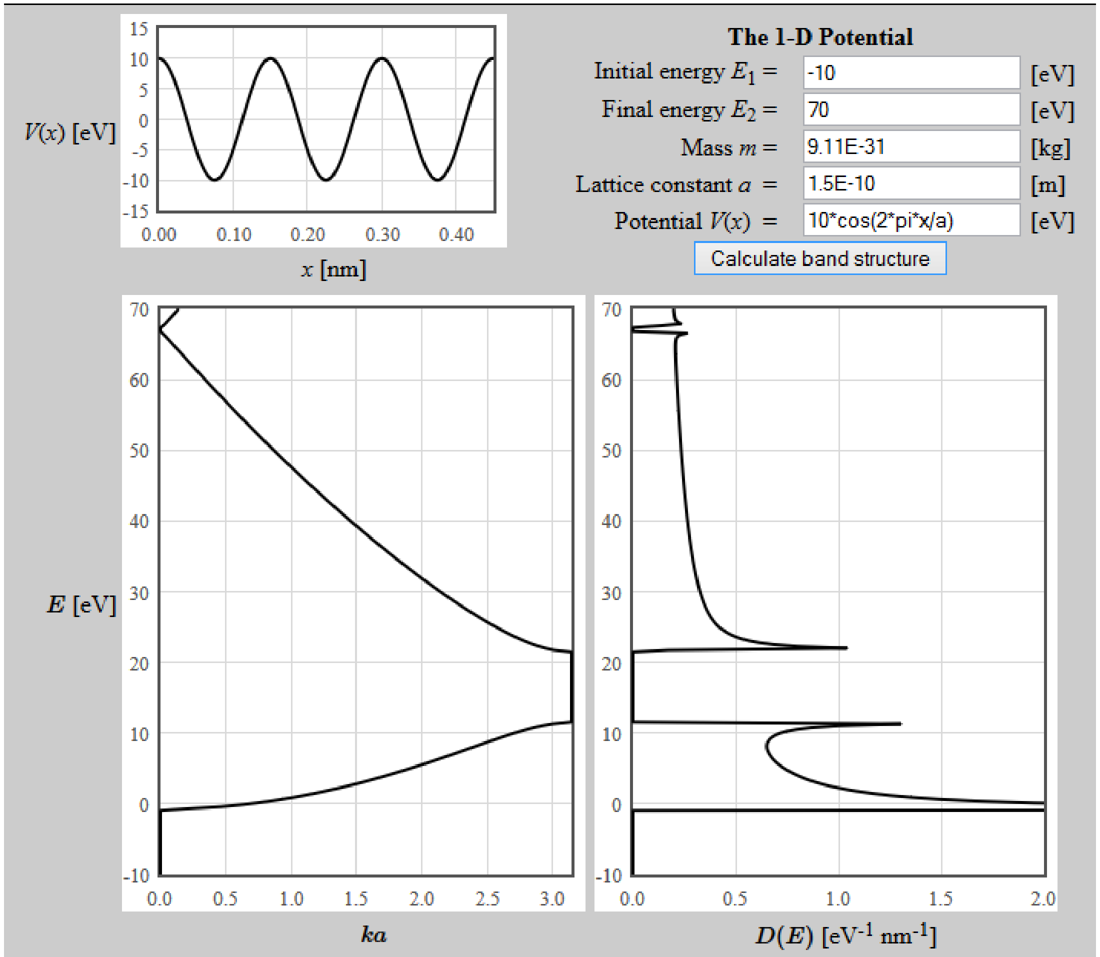
Energy current: $\vec{j}_E = \frac{1}{4\pi^3}\int v(\vec{k})E(\vec{k})f(\vec{k})d^3k$

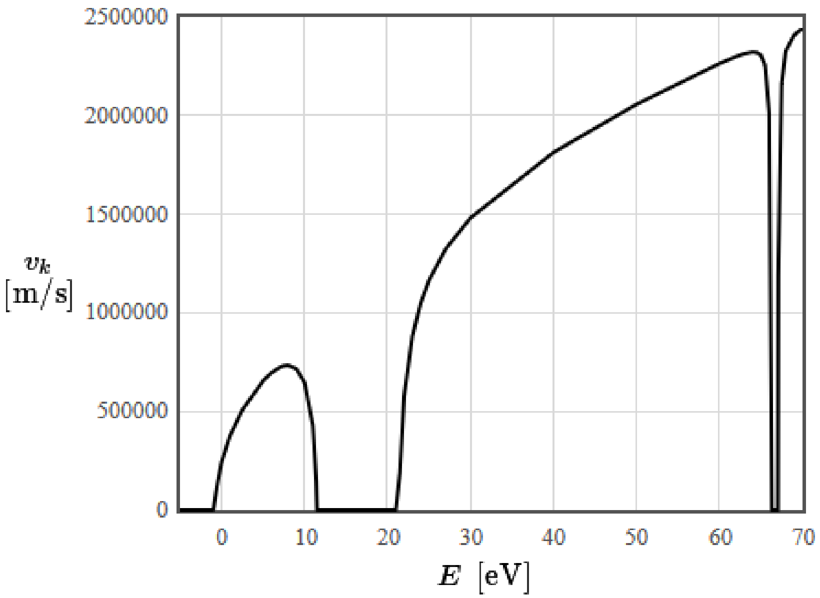
Heat current: $\vec{j}_Q = \frac{1}{4\pi^3}\int v(\vec{k})\left(E(\vec{k})-\mu\right)f(\vec{k})d^3k$

Thermoelectric effects

Electrical conductivity:	$\sigma_{mn} = \frac{j_{em}}{E_n}$	$\nabla T = 0, \vec{B} = 0$
Thermal conductivity:	$\kappa_{mn} = \frac{-j_{Qm}}{\nabla T_n}$	$\vec{B} = 0$
Peltier coefficient:	$\Pi_{mn} = \frac{j_{Qm}}{j_{en}}$	$\nabla T = 0, \vec{B} = 0$
Thermopower (Seebeck effect):	$S_{mn} = \frac{-\nabla \tilde{\mu}_m}{\nabla T_n}$	$\vec{j}_e = 0, \vec{B} = 0$
Hall effect:	$R_{lmn} = \frac{E_l}{j_{em} B_n}$	$\nabla T = 0, j_{el} = 0$
Nerst effect:	$N_{lmn} = \frac{E_l}{B_m \nabla T_n}$	$j_{elec} = 0$

Velocity of k-states





$$v = \frac{1}{\hbar}\frac{dE}{dk}$$

Student Projects

Calculate some transport property for a free electron gas or for a semiconductor.

Numerically calculate a transport property for a one dimensional material.

Prove that my two expressions for probability current are the same.

Probability current in 1-D

The normalized probability current density:

$$S = \frac{-i\hbar}{2m} \frac{\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}}{\int_0^L \psi^* \psi \, dx}$$

$$j = -eS = -nev$$

$$n = \frac{1}{Na}$$

$$v = NaS$$

$$v_k = -v_{-k} = \frac{-i\hbar a}{2m} \frac{\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}}{\int_0^a \psi^* \psi \, dx}$$

The properties of solids

$$H = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_A \frac{\hbar^2}{2m_A}\nabla_A^2 - \sum_{i,A}\frac{Z_A e^2}{4\pi\varepsilon_0 r_{iA}} + \sum_{i<j}\frac{e^2}{4\pi\varepsilon_0 r_{ij}} + \sum_{A<B}\frac{Z_A Z_B e^2}{4\pi\varepsilon_0 r_{AB}}$$

electronic band structure E vs. k

structure
bond potentials

phonon band structure ω vs. k

density of states

density of states

equilibrium properties
c_v, free energies, bulk modulus,...

Boltzmann transport

optical
absorption

optical properties