Boltzmann equation & transport properties

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Outline I

Outline II

3. General Transport equation
   - Boltzmann equation
   - Heat
   - General Transport equation
   - Thermal conductivity
   - Compair Electrical and Thermal conduction
4. Thermo-electric effects
   - Seebeck effect
   - Peltier effect
5. references

Introduction

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- 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.

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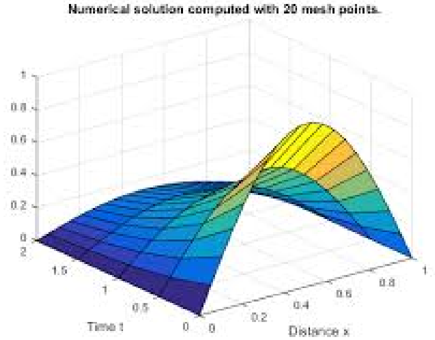

Diffusion

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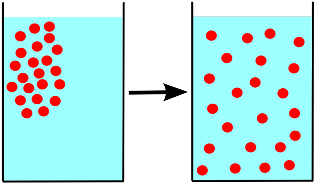

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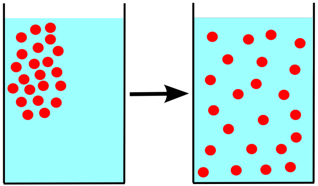

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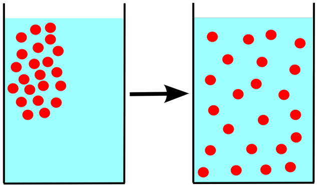

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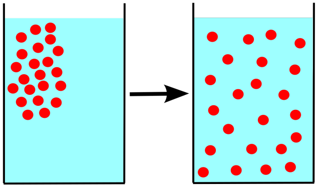

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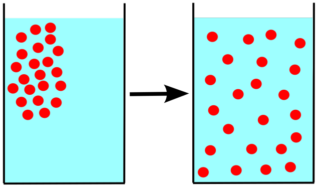

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$$\frac{\partial f}{\partial t}\Big|_{diff} = -\vec{v_k}.\nabla f$$

Electromagnetic field

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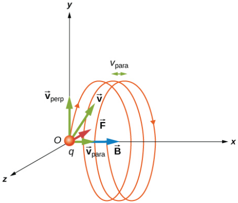

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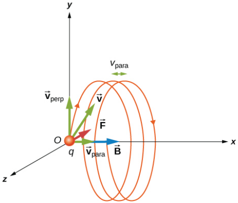

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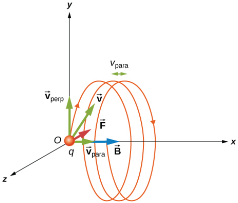

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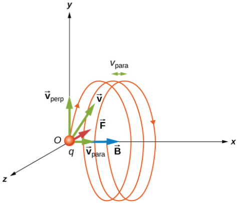

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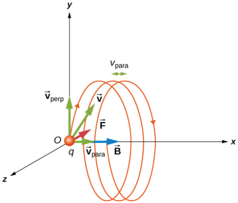

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$$\left.\frac{\partial f}{\partial t}\right|_{field} = -\frac{e}{\hbar}(\vec{E} + \frac{1}{c}\vec{v_k} \times \vec{H}).\nabla_k f$$

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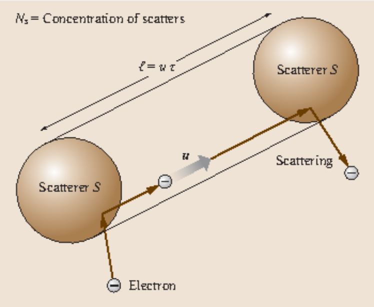
N_s = Concentration of scatters
$\ell = u\tau$
Scatterer S
u
Scattering
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Electron

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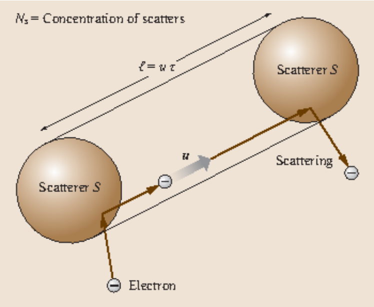

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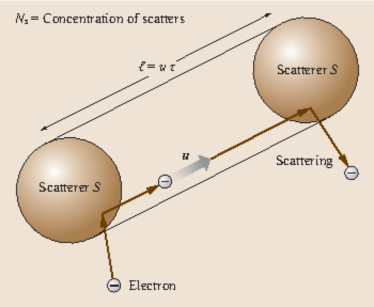

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$$\left.\frac{\partial f}{\partial t}\right|_{scatt} = \int \{f'(1-f) - \quad f(1-f')\}Q(k,k')dk'$$

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

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Theorem

Boltzman equation

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

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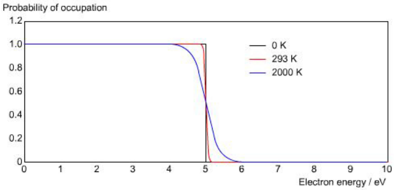

Fermi-Dirac distribution for several temperatures

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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

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

$$= \frac{\partial f}{\partial t}\Big|_{scatt} + \vec{v_k}.\frac{\partial g}{\partial r} + \frac{e}{\hbar c}(\vec{v_k} \times \vec{H}).\frac{\partial g}{\partial k}$$

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

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

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

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

Heat

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

Heat

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

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

General Transport equation

$$\vec{J} = e^2 \overleftrightarrow{K_0}.\vec{E} + \frac{e}{T}\overleftrightarrow{K_1}.(-\nabla T)$$
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$$\overleftrightarrow{K_0} = \frac{\tau}{4\pi^3\hbar}\int \vec{v}\vec{v}\frac{ds_f}{v} \qquad \overleftrightarrow{K_2} = \frac{1}{3}\pi^2(kT)^2 K_0(\zeta)$$
$$\overleftrightarrow{K_1} = \frac{1}{3}\pi^2(kT)^2\frac{\partial}{\partial \varepsilon}K_0(\varepsilon)\Big|_{\varepsilon=\zeta}$$

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

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

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

Seebeck effect

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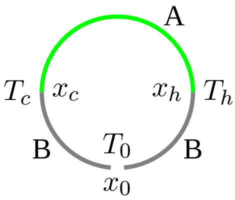

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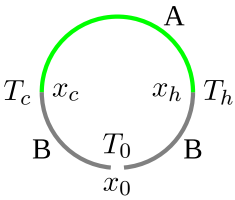

$$V = \int_{x_0}^{x_c} E_B dx + \int_{x_c}^{x_h} E_A dx + \int_{x_h}^{x_0} E_B dx = \int_{T_c}^{T_h} (Q_A - Q_B) dT$$

Peltier effect

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

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

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

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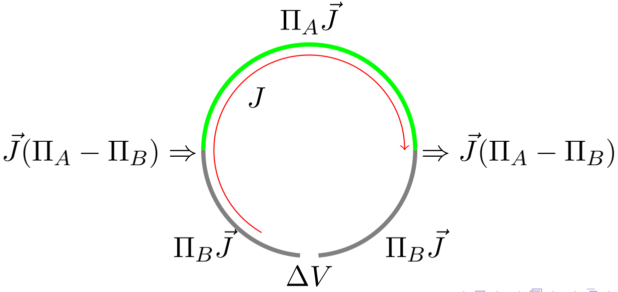

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