ECE 656: Electronic Transport in Semiconductors Fall 2017

Coupled Current Equations

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Outline

1) **Different forms of the equations**
2) Properties of coupled flows
3) Transport tensors
4) Effects of a B-field
5) Summary

Coupled Current Equations

$$J = \sigma \mathcal{E} - \sigma S \, dT/dx$$

$$J_Q = T\sigma S \mathcal{E} - \kappa_0 \, dT/dx$$

$$\mathcal{E} = \rho J + S \frac{dT}{dx}$$

$$J_Q = \pi J - \kappa_e \frac{dT}{dx}$$

(diffusive transport)

$$\sigma = \int \sigma'(E) \, dE$$

$$\sigma'(E) = \frac{2q^2}{h} \lambda(E) \frac{M(E)}{A} \left(-\frac{\partial f_0}{\partial E} \right)$$

$$S = -\frac{k_B}{q} \int \left(\frac{E - E_F}{k_B T} \right) \sigma'(E) \, dE \Big/ \int \sigma'(E) \, dE$$

$$\pi = TS$$

$$\kappa_0 = T \left(\frac{k_B}{q} \right)^2 \int \left(\frac{E - E_F}{k_B T} \right)^2 \sigma'(E) \, dE$$

$$\kappa_e = \kappa_0 - \pi S \sigma$$

Coupled Current Equations

$$\sigma = \frac{1}{\rho} = L_{11}$$

$$S = \frac{L_{12}}{L_{11}}$$

$$\pi = T\frac{L_{12}}{L_{11}}$$

$$\kappa_e = L_{22} - \frac{L_{12}L_{21}}{L_{11}}$$

$$L_{11} = \frac{q^2}{3}\int \upsilon^2 \tau D(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$

$$L_{12} = \frac{q}{3T}\int \upsilon^2 \tau (E - E_F) D(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$

$$L_{21} = TL_{12}$$

$$L_{22} = \frac{1}{3T}\int \upsilon^2 \tau (E - E_F)^2 D(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$

Gang Chen, *Nanoscale Energy Transport and Conversion*, Oxford, 2005, pp. 254-258.

Coupled Current Equations

$$\sigma = q^2 \int \left(-\frac{\partial f_0}{\partial E} \right) \Sigma(E)\, dE$$

$$\Sigma(E) = \frac{1}{\Omega} \sum_{\vec{k}} \upsilon_x \left(\vec{k}\right)^2 \tau\left(\vec{k}\right) \delta\left(E - E\left(\vec{k}\right)\right)$$

"transport function"

$$S = \frac{q}{T\sigma} \int \left(E - E_F\right) \left(-\frac{\partial f_0}{\partial E} \right) \Sigma(E)\, dE$$

$$\Sigma(E) = \frac{2}{h} \left(M(E)/A \right) \lambda(E)$$

$$\pi = TS$$

$$\kappa_0 = \frac{1}{T} \int \left(E - E_F\right)^2 \left(-\frac{\partial f_0}{\partial E} \right) \Sigma(E)\, dE$$

$$\kappa_e = \kappa_0 - T\sigma S^2$$

G.D. Mahan and J.O. Sofo, "The Best Thermoelectric," *Proc. Nat. Acad. Sci.*, **93**, pp. 7436-7439, 1996.

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Properties of coupled flows

$$\pi_n = TS_n(T)$$ "Kelvin relation"

"Onsager relations" for coupled flows

$$\mathcal{E}_x = \rho_n J_{nx} + S_n \frac{dT}{dx}$$

$$J_{Qx} = \pi_n J_{nx} - \kappa_n \frac{dT}{dx}$$

WF "law"

Onsaeger relations

$$J_x = L_{11}\frac{dF_n}{dx} + L_{12}\frac{d}{dx}\left(\frac{1}{T}\right)$$

$$J_q^x = L_{21}\frac{dF_n}{dx} + L_{22}\frac{d}{dx}\left(\frac{1}{T}\right)$$

$$J_1 = L_{11}\left(\vec{B}\right)F_1 + L_{12}\left(\vec{B}\right)F_2$$

$$J_2 = L_{21}\left(\vec{B}\right)F_1 + L_{22}\left(\vec{B}\right)F_2$$

J_1, J_2 "generalized fluxes"

F_1, F_2 "generalized forces"

$L_{12} = L_{21}$ Onsager relation

Onsaeger relations

1) temperature differences produce heat currents

2) pressure differences produce matter currents

→

3) heat flow per pressure difference = matter flow per temperature difference

Lars Onsaeger, Nobel Prize in Chemistry, 1968.

http.en.wikipedia.org/wiki/Onsaeger_reciprocal_relations

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Basic equations of thermoelectricity

$$\mathcal{E}_x = \rho_n J_x + S_n \frac{dT}{dx}$$

$$J_x^q = \pi_n J_{nx} - \kappa_n \frac{dT}{dx}$$

We can write these equations in **vector notation** as:

$$\vec{\mathcal{E}} = \rho_n \vec{J} + S_n \vec{\nabla} T$$

$$\vec{J}_q = \pi_n \vec{J} - \kappa_n \vec{\nabla} T$$

or in **indicial notation** as:

$$\mathcal{E}_i = \rho_n J_i + S_n \partial_i T$$

$$J_i^q = \pi_n J_i - \kappa_n \partial_i T \qquad i = x, y, z$$

Transport tensors

$$\vec{\mathcal{E}} = \rho \vec{J} + S\vec{\nabla}T$$

$$\vec{J}_q = \pi \vec{J} - \kappa_n \vec{\nabla}T$$

$$\vec{\mathcal{E}} = [\rho]\vec{J} + [S]\vec{\nabla}T$$

$$\vec{J}_q = [\pi]\vec{J} - [\kappa_n]\vec{\nabla}T$$

$$\begin{bmatrix} \mathcal{E}_x \\ \mathcal{E}_y \\ \mathcal{E}_z \end{bmatrix} = \begin{bmatrix} \rho_{11} & \rho_{12} & \rho_{13} \\ \rho_{21} & \rho_{22} & \rho_{23} \\ \rho_{31} & \rho_{32} & \rho_{33} \end{bmatrix} \begin{bmatrix} J_x \\ J_y \\ J_z \end{bmatrix}$$

$$\mathcal{E}_i = \sum_{j=1}^{3} \rho_{ij} J_j$$

$$\mathcal{E}_i \equiv \rho_{ij} J_j$$ "summation convention"

Coupled current equations in indicial notation

$$\vec{\mathcal{E}} = [\rho]\vec{J} + [S]\vec{\nabla}T$$

$$\vec{J}_q = [\pi]\vec{J} - [\kappa_n]\vec{\nabla}T$$

$$\mathcal{E}_i = \rho_{ij}J_j + S_{ij}\partial_j T$$

$$J_i^Q = \pi_{ij}J_j - \kappa_{ij}^n \partial_j T$$

Isotropic materials → diagonal tensors

$$\mathcal{E}_i = \rho_0 J_j + S_0 \partial_j T$$

$$J_i^q = \pi_0 J_j - K_0^e \partial_j T$$

$$[\rho] = \rho_0 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

"Kronecker delta"

$$\rho_{ij} = \rho_0 \delta_{ij}$$

$$\delta_{ij} = 1 \quad (i = j)$$

$$= 0 \quad (i \neq j)$$

Coupled current equations in indicial notation

$$\mathcal{E}_i = \rho_{ij} J_j + S_{ij} \partial_j T$$

$$J_i^q = \pi_{ij} J_j - \kappa_{ij}^e \partial_j T$$

For isotropic materials, such as common, cubic semiconductors, the tensors are diagonal (under low-fields).

For a given crystal structure, the form of the tensors (i.e. which elements are zero and which are non-zero) can be deduced from symmetry arguments. (See Smith, Janak, and Adler, Chapter 4.)

The transport tensors can be readily computed by solving the Boltzmann Transport Equation (BTE).

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Magnetoconductivity tensor

$$\begin{pmatrix} J_{nx} \\ J_{ny} \end{pmatrix} = \begin{pmatrix} \sigma_S & -\sigma_S \mu_H B_z \\ +\sigma_S \mu_H B_z & \sigma_S \end{pmatrix} \begin{pmatrix} \mathcal{E}_x \\ \mathcal{E}_y \end{pmatrix}$$

$$J_{ni} = \sum_j \sigma_{ij}\left(B_z\right)\mathcal{E}_j \qquad \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} = \begin{pmatrix} \sigma_S & -\sigma_S \mu_H B_z \\ +\sigma_S \mu_H B_z & \sigma_S \end{pmatrix}$$

$$J_{ni} = \sigma_{ij}\left(B_z\right)\mathcal{E}_j$$ (summation convention)

$$J_i = \sigma_S \mathcal{E}_i - \sigma_S \mu_H \varepsilon_{ijk} \mathcal{E}_j B_k$$

$$\begin{aligned} \varepsilon_{ijk} &= +1\left(i, j, k \ \text{ cyclic}\right) \\ &= -1\left(i, j, k \ \text{ anti-cyclic}\right) \\ &= 0\left(\text{otherwise}\right) \end{aligned}$$

Coupled current equations

$$\mathcal{E}_i = \rho_{ij}\left(\vec{B}\right) J_j + S_{ij}\left(\vec{B}\right) \partial_j T$$

$$J_i^Q = \pi_{ij}\left(\vec{B}\right) J_j - \kappa_{ij}^e\left(\vec{B}\right) \partial_j T$$

$$\rho_{ij}\left(\vec{B}\right) = \rho_0 + \rho_0 \mu_H \varepsilon_{ijk} B_k + \ldots$$

$$S_{ij}\left(\vec{B}\right) = S_0 + S_1 \varepsilon_{ijk} B_k + \ldots$$

$$\pi_{ij}\left(\vec{B}\right) = \pi_0 + \pi_1 \varepsilon_{ijk} B_k + \ldots$$

$$\kappa_{ij}^e\left(\vec{B}\right) = \kappa_0^e + \kappa_1 \varepsilon_{ijk} B_k + \ldots$$

Nearnst effect

Assume that there is a temperature gradient in the *x*-direction. How is the electric field (Hall voltage) affected?)

$$\mathcal{E}_i = \rho_{ij}\left(\vec{B}\right)J_j + S_{ij}\left(\vec{B}\right)\partial_j T$$

$$\rho_{ij}\left(\vec{B}\right) = \rho_0 + \rho_0\mu_H\varepsilon_{ijk}B_k + \ldots$$

$$S_{ij}\left(\vec{B}\right) = S_0 + S_1\varepsilon_{ijk}B_k + \ldots$$

$$\mathcal{E}_y = \rho_0 J_y + \rho_0\mu_H\varepsilon_{yjz}B_z J_j + S_0\partial_y T + S_1\varepsilon_{yjz}B_z\partial_j T$$

$$\mathcal{E}_y = +\rho_0\mu_H\varepsilon_{yxz}B_z J_x + S_1\varepsilon_{yxz}B_z\partial_x T$$

$$\mathcal{E}_y = -\rho_0\mu_H B_z J_x - S_1 B_z\partial_x T$$

Nernst voltage
Reverse direction of B_z and J_x and average results to eliminate.

Other effects

Other "thermomagnetic effects" such as the Ettingshaussen and Righi-Leduc effects also occur and affect the measured Hall voltage. See Lundstrom, Chapter 4, Sec. 4.6.2 for a discussion.

For more about this topic

A.C. Smith, J.F. Janak, and R.B. Adler, *Electronic Conduction in Solids*, McGraw-Hill, New York, 1967.

Irreversible thermodynamics: Chapter 2

Onsager relations: Chapter 3

Questions?

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