ECE 656: Electronic Transport in Semiconductors Fall 2017

The BTE Revisited

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The BTE

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = \hat{C}f$$

$$\left.\frac{df}{dt}\right|_{coll} = \hat{C}f = \text{in-scattering - out-scattering}$$

$$\hat{C}f = -\frac{\delta f(\vec{p})}{\tau_m} \qquad \delta f = f(\vec{p}) - f_S(\vec{p})$$

Relaxation Time Approximation

Outline

1. **Solution without B-field**
2. Transport tensors
3. B-fields
4. Example
5. Summary

Steady-state BTE with no B-fields

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = \hat{C}f \rightarrow \vec{\upsilon} \bullet \nabla_r f - q\vec{\mathcal{E}} \bullet \nabla_p f = \hat{C}f$$

We have previously solved this equation for no spatial gradients and found an expression for the **mobility**.

We also previously solved this equation for no electric field and found an expression for the **diffusion coefficient.**

What if there is both an electric field and a spatial gradient (and a temperature gradient)?

Steady-state BTE with no B-fields

$$\vec{\upsilon} \bullet \nabla_r f - q\vec{\mathcal{E}} \bullet \nabla_p f = -\frac{\delta f}{\tau_m}$$

RTA

no B-fields for now

$$\vec{F}_e = -q\vec{\mathcal{E}}$$

$$f(\vec{p}) = f_S(\vec{p}) + \delta f(\vec{p})$$

$$f_S(\vec{p}) >> \left|\delta f(\vec{p})\right|$$

"near-equilibrium"

Solving the near eq., s.s BTE

$$\vec{\upsilon} \bullet \nabla_r f - q\vec{\mathcal{E}} \bullet \nabla_p f = -\frac{\delta f(\vec{p})}{\tau_m}$$

$$\nabla_r f \approx \nabla_r f_S \qquad \nabla_p f \approx \nabla_p f_S$$

$$\vec{\upsilon} \bullet \nabla_r f_S - q\vec{\mathcal{E}} \bullet \nabla_p f_S = -\frac{\delta f(\vec{p})}{\tau_m}$$

$$\delta f(\vec{p}) = -\tau_m \vec{\upsilon} \bullet \nabla_r f_S + q\tau_m \vec{\mathcal{E}} \bullet \nabla_p f_S$$

BTE solution

$$\delta f = -\tau_m \vec{\upsilon} \bullet \nabla_r f_S + q\tau_m \vec{\mathcal{E}} \bullet \nabla_p f_S$$

$$f_S(\vec{p}) = \frac{1}{1+e^{\Theta}}$$

$$\Theta(\vec{r},\vec{p}) = \left[E(\vec{r},\vec{p}) - F_n(\vec{r})\right]/k_B T$$
$$= \left[E_C(\vec{r}) + E(\vec{p}) - F_n(\vec{r})\right]/k_B T$$

$$\nabla_r f_S = \frac{\partial f_S}{\partial \Theta} \nabla_r \Theta$$

$$\nabla_p f_S = \frac{\partial f_S}{\partial \Theta} \nabla_p \Theta$$

$$\frac{\partial f_S}{\partial \Theta} = k_B T \frac{\partial f_S}{\partial E}$$

$$\delta f = \tau_m k_B T \left(-\frac{\partial f_S}{\partial E}\right)\left[\vec{\upsilon} \bullet \nabla_r \Theta - q\vec{\mathcal{E}} \bullet \nabla_p \Theta\right]$$

BTE solution

$$\delta f = \tau_m k_B T\left(-\frac{\partial f_S}{\partial E}\right)\left[\vec{\upsilon}\bullet\nabla_r\Theta - q\vec{\mathcal{E}}\bullet\nabla_p\Theta\right]$$

$$\Theta(\vec{r},\vec{p}) = \left[E_C(\vec{r}) + E(\vec{p}) - F_n(\vec{r})\right]/k_B T$$

$$\nabla_r\Theta = \frac{1}{k_B T}\left[\nabla_r E_C - \nabla_r F_n\right] + \left[E_C + E(\vec{p}) - F_n\right]\nabla_r\left(\frac{1}{k_B T}\right) \qquad \nabla_p\Theta = \frac{\vec{\upsilon}(\vec{p})}{k_B T}$$

$$\delta f = \tau_m\left(-\frac{\partial f_S}{\partial E}\right)\vec{\upsilon}\bullet\left\{-\nabla_r F_n + T\left[E_C + E(\vec{p}) - F_n\right]\nabla_r\left(\frac{1}{T}\right)\right\}$$

Generalized force

$$\delta f = \tau_m \left(-\frac{\partial f_S}{\partial E} \right) \vec{\upsilon} \bullet \vec{\mathcal{F}}$$

$$\vec{\mathcal{F}} = -\nabla_r F_n + T\left[E_C + E(k) - F_n \right] \nabla_r \left(\frac{1}{T} \right)$$

The two forces driving currents are:

1) gradients in the QFL
2) gradients in (inverse) temperature.

According to the Landauer Approach ($f_1 - f_2$) produces currents. Differences in Fermi level and temperature cause differences in f.

What next?

$$\delta f = \tau_m \left(-\frac{\partial f_S}{\partial E} \right) \vec{\upsilon} \bullet \vec{\mathcal{F}}$$

Moments

$$f\left(\vec{r},\vec{k}\right) = f_S\left(\vec{r},\vec{k}\right) + \delta f\left(\vec{r},\vec{k}\right)$$

$$n\left(\vec{r}\right) = \frac{1}{\Omega}\sum_{\vec{k}} f_S\left(\vec{r},\vec{k}\right) + \delta f\left(\vec{r},\vec{k}\right) \approx \frac{1}{\Omega}\sum_{\vec{k}} f_S\left(\vec{r},\vec{k}\right)$$

$$\vec{J}_n\left(\vec{r}\right) = \frac{1}{\Omega}\sum_{\vec{k}} (-q)\vec{\upsilon}\left(\vec{k}\right)\delta f\left(\vec{r},\vec{k}\right)$$

$$\vec{J}_Q\left(\vec{r}\right) = \frac{1}{\Omega}\sum_{\vec{k}} \left(E - F_n\right)\vec{\upsilon}\left(\vec{k}\right)\delta f\left(\vec{r},\vec{k}\right)$$

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Current (symbolic notation)

$$\vec{J}_n(\vec{r}) = \frac{1}{\Omega}\sum_{\vec{k}}(-q)\vec{\upsilon}\,\delta f\left(\vec{r},\vec{k}\right) \qquad \delta f = \tau_m\left(-\frac{\partial f_S}{\partial E}\right)\vec{\upsilon}\bullet\vec{\mathcal{F}}$$

$$\vec{\mathcal{F}} = -\nabla_r F_n + T\left[E_C + E(k) - F_n\right]\nabla_r\left(\frac{1}{T}\right)$$

$$\vec{J}_n(\vec{r}) = \frac{(-q)}{\Omega}\sum_{\vec{k}}\tau_m\left(-\frac{\partial f_S}{\partial E}\right)\vec{\upsilon}\left[\vec{\upsilon}\bullet\vec{\mathcal{F}}\right]$$

$$\vec{J}_n(\vec{r}) = \frac{(-q)}{\Omega}\sum_{\vec{k}}\tau_m\left(-\frac{\partial f_S}{\partial E}\right)(\vec{\upsilon}\vec{\upsilon})\bullet\vec{\mathcal{F}}$$

tensor

Current (indicial notation)

$$\vec{J}_n(\vec{r}) = \frac{1}{\Omega}\sum_{\vec{k}}(-q)\vec{\upsilon}\,\delta f\left(\vec{r},\vec{k}\right)$$

$$J_i(\vec{r}) = \frac{1}{\Omega}\sum_{\vec{k}}(-q)\upsilon_i\delta f\left(\vec{r},\vec{k}\right)$$

$$\delta f = \tau_m\left(-\frac{\partial f_S}{\partial E}\right)\vec{\upsilon}\bullet\vec{\mathcal{F}}$$

$$\vec{\mathcal{F}} = -\nabla_r F_n + T\left[E_C + E(k) - F_n\right]\nabla_r\left(\frac{1}{T}\right)$$

$$\delta f = \tau_m\left(-\frac{\partial f_S}{\partial E}\right)\upsilon_j\mathcal{F}_j$$

$$\mathcal{F}_i = -\partial_i F_n + T\left[E_C + E(k) - F_n\right]\partial_i\left(\frac{1}{T}\right)$$

Current (indicial notation)

$$\vec{J}_i(\vec{r}) = \frac{1}{\Omega}\sum_{\vec{k}}(-q)\upsilon_i \delta f(\vec{r},\vec{k}) \qquad \delta f = \tau_m\left(-\frac{\partial f_0}{\partial E}\right)\upsilon_j \mathcal{F}_j \qquad \boxed{\mathcal{F}_i = -\partial_i F_n}$$

$$J_i(\vec{r}) = \frac{1}{\Omega}\sum_{\vec{k}}(-q)\upsilon_i \tau_m\left(-\frac{\partial f_0}{\partial E}\right)\upsilon_j \mathcal{F}_j$$

$$J_i(\vec{r}) = \frac{1}{\Omega}\sum_{\vec{k}}(-q)\upsilon_i \tau_m\left(-\frac{\partial f_0}{\partial E}\right)\upsilon_j \partial_j F_n$$

$$J_i(\vec{r}) = \left\{\frac{1}{\Omega}\sum_{\vec{k}}(-q)\upsilon_i \tau_m\left(-\frac{\partial f_0}{\partial E}\right)\upsilon_j\right\}\partial_j F_n \qquad \boxed{J_i(\vec{r}) = \sigma_{ij}\,\partial_j F_n}$$

Conductivity tensor

$$J_i(\vec{r}) = \sigma_{ij}\,\partial_j F_n$$

$$\sigma_{ij} = \frac{1}{\Omega}\sum_{\vec{k}}(-q)\upsilon_i\upsilon_j\tau_m\left(-\frac{\partial f_S}{\partial E}\right)$$

Coupled charge and heat current equations

electrical current:

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

$$\mathcal{E}_i = \rho_{ij} J_j + S_{ij}\frac{\partial T}{\partial x_j}$$

heat current (electronic):

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

$$J_{Qi} = \pi_{ij} J_j - \kappa_{ij}^{e}\frac{\partial T}{\partial x_j}$$

heat current (lattice):

$$q_x = -\kappa_L\left(\frac{dT}{dx}\right)$$

$$q_i = -\kappa_{ij}^{L}\left(\frac{\partial T}{\partial x_j}\right)$$

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B-field dependent transport

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

$$J_{Qi} = \pi_{ij}\left(\vec{B}\right)J_j - \kappa_{ij}^{e}\left(\vec{B}\right)\frac{\partial T}{\partial x_j}$$

$$\rho_{ij}\left(\vec{B}\right) = \rho_{ij}\left(\vec{B}=0\right) + \frac{\partial \rho_{ij}\left(\vec{B}\right)}{\partial B_k}B_k +$$

$$\rho_{ij}\left(\vec{B}\right) = \rho_{ij}\left(\vec{B}=0\right) + \rho_{ijk}B_k +$$

Cubic semiconductors:

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

Form of the tensors (cubic semiconductors)

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

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

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

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

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

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

See Smith, Janek, and Adler, Chapter 9, for expressions for the B-field dependent transport tensors.

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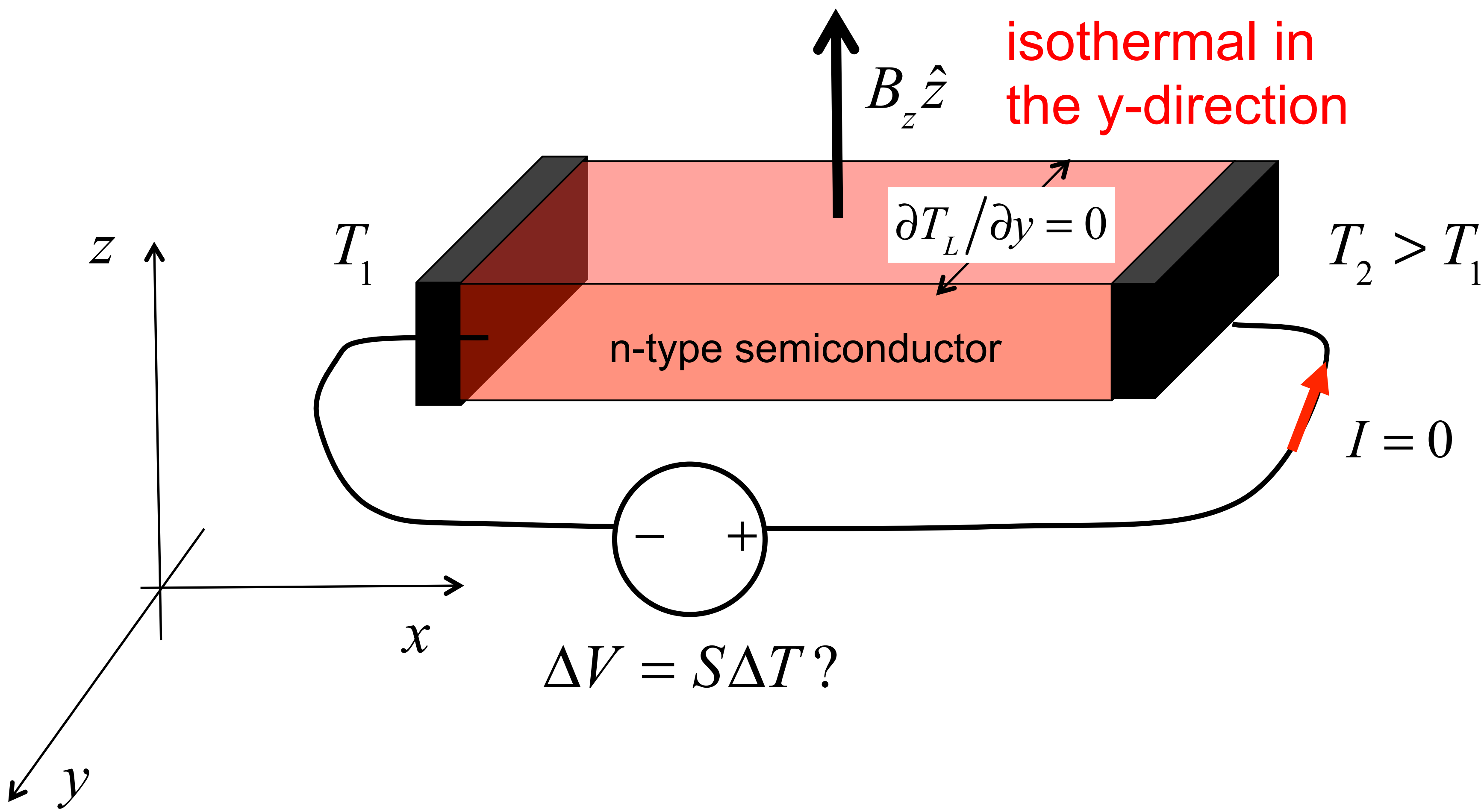
B-field dependent Seebeck coefficient



Magneto-Seebeck effect (isothermal in y)

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

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

$$\mathcal{E}_x = S_0 \partial_x T$$

B-field has no effect (to first order)

$$\mathcal{E}_x = \rho_{ij}\left(\vec{B}\right)J_j + S_{xx}\left(\vec{B}\right)\partial_x T$$

$$\mathcal{E}_x = S_{xx}\left(\vec{B}\right)\partial_x T$$

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

$$S_{xx}\left(\vec{B}\right) = S_0 + S_1\varepsilon_{xxz}B_z$$

$$S_{xx}\left(\vec{B}\right) = S_0$$

Magneto-Seebeck effect (adiabatic in y)

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

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

$$J_y^Q = 0 = -\kappa_{yj}^e\left(\vec{B}\right)\partial_j T$$

$$\kappa_{ij}^e = \kappa_0^e\delta_{ij} + \kappa_1^e\varepsilon_{ijk}B_k$$

$$0 = -\kappa_0^e\,\partial_y T - \kappa_1^e\varepsilon_{yxz}\,\partial_x T\,B_z$$

$$\partial_y T = \frac{\kappa_1^e}{\kappa_0^e}B_z\partial_x T$$

$$\mathcal{E}_x = S_{xj}\left(\vec{B}\right)\partial_j T$$

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

$$\mathcal{E}_x = S_0\partial_x T + S_1 B_z\partial_y T$$

$$\mathcal{E}_x = \left(S_0 + \frac{S_1\kappa_1^e}{\kappa_0^e}B_z^2\right)\partial_x T$$

$$\mathcal{E}_x = S_{app}\partial_x T$$

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Comments

See Lundstrom, p. 179 for table listing other effects involving a transverse B-field.

(Also includes effects to second order in B-field)

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Summary

1) Under near-equilibrium conditions with the RTA, the BTE can be solved to find the probability that states in the device are occupied.

2) From the solution, we can determine the electric and heat currents. For diffusive transport, the results are equivalent to the Landauer approach.

3) The BTE is convenient for anisotropic transport, for including B-fields, for resolving transport in space, and for off-equilibrium transport, but ballistic transport is hard.

Summary

4) When the RTA cannot be used, the near-equilibrium transport equations still have the same form, but to evaluate the transport coefficients, numerical methods are necessary.

   See:

   D.L. Rode, "Low-field electron transport," in *Semiconductors and Semimetals*, Vol. 10, pp. 1-89, ed. by R.K. Willardson and A.C. Beer, Academic Press, NY, 1975.

Summary

$f\left(\vec{r},\vec{p},t\right)$

$$\frac{\partial f}{\partial t}+\vec{\upsilon}\bullet\nabla_r f+\vec{F}_e\bullet\nabla_p f=\hat{C}f$$

This is a six-dimensional integro-differential equation for *f*(*r*, *p*, *t*).

For near-equilibrium conditions in bulk semiconductors, analytical solutions are (sometimes) possible.

Summary

$$f\left(\vec{r},\vec{p},t\right) \qquad \frac{\partial f}{\partial t}+\vec{\upsilon}\bullet\nabla_r f+\vec{F}_e\bullet\nabla_p f=\hat{C}f$$

Far from equilibrium, solving the BTE becomes even more difficult. The RTA cannot be used, and devices have complicated structures with rapidly varying fields.

Some problems can be solved by special techniques (e.g. Monte Carlo simulation), but solving the BTE in 3D (or even 2D) is usually not possible.

Is there a better way?

Questions

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