ECE-656: Fall 2009

Lecture 15: Solving the BTE: General Solution for *B* = 0

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the BTE

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

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = -\frac{(f - f_0)}{\tau_f}$$

1) 1, 2, and 3D with arbitrary bandstructures

2) Concentration and temperature gradients and electric fields

from lecture 14

You should now:

1) Be able to write down the BTE in the RTA

2) Be able to solve it for small electric fields

3) Be able to solve it for small concentration gradients

4) Understand how to treat energy-dependent scattering, multiple scattering processes, ellipsoidal energy bands

outline

1) **General solution**

2) Current equation

3) Coupled current equations

4) The RTA

5) Summary

BTE

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = \left. \frac{df}{dt} \right|_{coll}$$

1) steady-state transport: $\partial f / \partial t = 0$

2) electric field (magnetic fields later): $\vec{F}_e = -q\vec{\mathcal{E}} = 0$

3) near-equilibrium and RTA:

$$f(\vec{p}) = f_S(\vec{p}) + f_A(\vec{p}) \quad \left| f_S(\vec{p}) \right| >> \left| f_A(\vec{p}) \right| \quad df/dt\big|_{coll} \approx -f_A/\tau_f$$

symmetric and anti-symmetric components

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

$$f_S(\vec{p}) = f_S(-\vec{p})$$

even in momentum
"symmetric"

$$f_A(\vec{p}) = -f_A(-\vec{p})$$

odd in momentum
"anti-symmetric"

$$f_S(\vec{p}) = \frac{1}{1 + e^{\left[E_C + E(\vec{p}) - F_n\right]/k_B T}}$$

near eq., s.s BTE

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

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

$$\vec{\upsilon} \bullet \nabla_r f_S - q\vec{\mathcal{E}} \bullet \nabla_p f_S = -\frac{f_A(\vec{p})}{\tau_f}$$

$$f_A(\vec{p}) = -\tau_f \vec{\upsilon} \bullet \nabla_r f_S + q\tau_f \vec{\mathcal{E}} \bullet \nabla_p f_S$$

moments

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

$$n(\vec{r}) = \frac{1}{\Omega}\sum_{k} f_S(\vec{r},\vec{k})$$

$$W(\vec{r}) = \frac{1}{\Omega}\sum_{k} E(k) f_S(\vec{r},\vec{k}) = n(\vec{r})u(\vec{r})$$

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

$$\vec{J}_E(\vec{r}) = \frac{1}{\Omega}\sum_{k} E(k)\vec{\upsilon} f_A(\vec{r},\vec{k})$$

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

$$n_\phi(\vec{r}) = \frac{1}{\Omega}\sum_{k} \phi(\vec{k}) f(\vec{r},\vec{k})$$

BTE solution

$$f_A = -\tau_f \vec{\upsilon} \bullet \nabla_r f_S + q\tau \vec{\mathcal{E}} \bullet \nabla_p f_S$$

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

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

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

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

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

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

BTE solution

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

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

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

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

BTE solution

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

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

$$f_A = \tau_f \left(-\frac{\partial f_S}{\partial E} \right) \vec{\upsilon} \bullet \left\{ \left(\left[\nabla_r E_C - \nabla_r F_n \right] + k_B T \left[E_C + E(k) - F_n \right] \nabla_r \left(\frac{1}{k_B T} \right) \right) - q\vec{\mathcal{E}} \right\}$$

generalized force

$$f_A = \tau_f\left(-\frac{\partial f_S}{\partial E}\right)\vec{\upsilon}\bullet\left\{-\nabla_r F_n + T\left[E_C + E(k) - F_n\right]\nabla_r\left(\frac{1}{T}\right)\right\}$$

$$f_A = \tau_f\left(-\frac{\partial f_S}{\partial E}\right)\vec{\upsilon}\bullet\vec{\mathcal{F}}$$

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

“generalized force”

from lecture 14

$$-q\mathcal{E}_x \frac{\partial f_0}{\partial p_x} = -\frac{f_A}{\tau_f} \qquad f_A(\vec{p}) = \tau_f\left(-\frac{\partial f_0}{\partial E}\right)\upsilon_x\left(-q\mathcal{E}_x\right)$$

$$f_A = \tau_f\left(-\frac{\partial f_S}{\partial E}\right)\vec{\upsilon}\bullet\vec{\mathcal{F}}$$

real force → generalized force

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

outline

1) General solution

2) Current equation

3) Coupled current equations

4) The RTA

5) Summary

electric current

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

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

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

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

tensor

indicial notation

$$\vec{\upsilon} \bullet \vec{\mathcal{F}} = \sum_{j=1}^{3} \upsilon_j \mathcal{F}_j \equiv \upsilon_j \mathcal{F}_j$$ "summation convention"

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

$$J_i = \frac{1}{\Omega}\sum_k (-q)\upsilon_i f_A$$

$$J_i = \frac{(-q)}{\Omega}\sum_k \upsilon_i\left[\tau_f\left(-\frac{\partial f_S}{\partial E}\right)\upsilon_j \mathcal{F}_j\right]$$

$$f_A = \tau_f\left(-\frac{\partial f_S}{\partial E}\right)\upsilon_j \mathcal{F}_j$$

$$\mathcal{F}_j = \partial_j F_n$$ (temperature constant)

conductivity tensor

$$J_i = \frac{(-q)}{\Omega} \sum_k \upsilon_i \left[\tau_f \left(-\frac{\partial f_S}{\partial E} \right) \upsilon_j \mathcal{F}_j \right] \qquad \mathcal{F}_j = \partial_j F_n$$

$$J_i = \sigma_{ij} \partial_j \left(F_n / q \right)$$

$$\sigma_{ij} = \frac{q^2}{\Omega} \sum_k \upsilon_i \upsilon_j \tau_f \left(-\frac{\partial f_S}{\partial E} \right)$$

This expression is valid in 1D, 2D, or 3D for a general *E*(*k*) and for degenerate or non-degenerate conditions.

spherical bands

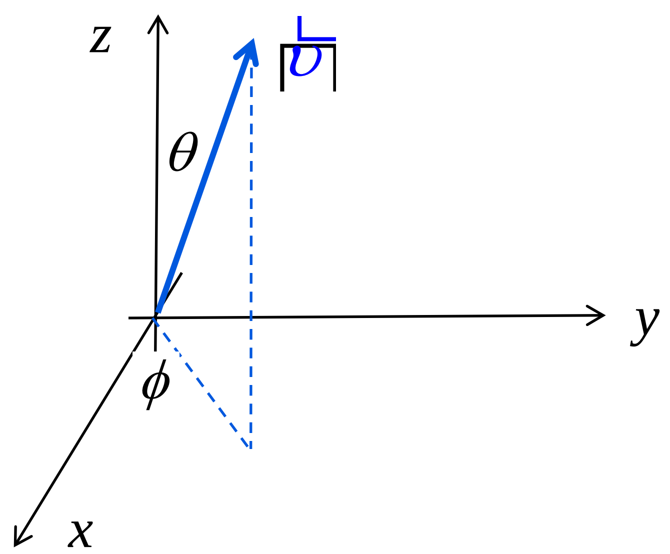
$$\sigma_{ij} = \frac{q^2}{\Omega}\sum_k \upsilon_i \upsilon_j \tau_f \left(-\frac{\partial f_S}{\partial E}\right)$$

Assume τ is a function of energy but not direction.

$$\sum_k \upsilon_i \upsilon_j \tau_f(E)\left(-\frac{\partial f_S}{\partial E}\right) = \frac{1}{4\pi^3}\int_0^\infty k\,dk\,\tau_f(E)\left(-\frac{\partial f_S}{\partial E}\right)\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\, \upsilon_i \upsilon_j$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\, \upsilon_i \upsilon_j = \frac{4\pi}{3}\upsilon^2 \delta_{ij}$$

$$\sigma_{ij} = \sigma_0 \delta_{ij}$$



conductivity tensor

$$J_i = \sigma_{ij}\partial_j\left(F_n/q\right) \qquad \left(\mathcal{F}_j = \partial_j F_n\right)$$

$$\sigma_{ij} = \frac{q^2}{\Omega}\sum_k \upsilon_i \upsilon_j \tau_f \left(-\frac{\partial f_S}{\partial E}\right) \qquad \left(-\frac{\partial f_S}{\partial E}\right) = \frac{1}{k_B T} f_S$$

(non-degenerate)

$$\sigma_{ij} = \frac{q^2}{k_B T}\frac{1}{\Omega}\sum_k \upsilon_i \upsilon_j \tau_f f_S$$

$$\sigma_{xx} = \frac{q^2}{k_B T}\frac{1}{\Omega}\sum_k \upsilon_x^2 \tau_f f_S = \frac{q^2}{k_B T}\frac{1}{\Omega}\sum_k \frac{\upsilon^2}{3}\tau_f f_S = \frac{q^2}{m^*\left(3k_B T/2\right)}\frac{1}{\Omega}\sum_k \frac{m^*\upsilon^2}{2}\tau_f f_S$$

$$\sigma_{xx} = nq\frac{q}{m^*}\frac{\langle E\tau_f\rangle}{\langle E\rangle} \qquad \upsilon^2 = \upsilon_x^2 + \upsilon_y^2 + \upsilon_z^2$$

electric current

$$J_i = \sigma_{ij}\partial_j\left(F_n/q\right)$$

$$\sigma_{ij} = nq\frac{q\langle\langle\tau_f\rangle\rangle}{m^*}\delta_{ij}$$

$$\langle\langle\tau_f\rangle\rangle = \frac{\langle E\tau_f\rangle}{\langle E\rangle}$$

1) non-degenerate conditions

2) spherical, parabolic energy bands

3) near-equilibrium

4) RTA (power law scattering)

$$\tau_f\left(E\right) = \tau_0\left(E/k_BT\right)^s \rightarrow \langle\langle\tau_f\rangle\rangle = \tau_0\frac{\Gamma\left(s+5/2\right)}{\Gamma\left(5/2\right)}$$

outline

1) General solution

2) Current equation

3) Coupled current equations

4) The RTA

5) Summary

electric current with temperature gradients

$$f_A = \tau_f \left(-\frac{\partial f_S}{\partial E} \right) \vec{\upsilon} \bullet \vec{\mathcal{F}}$$

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

$$\vec{J}_n(\vec{r}) = \frac{1}{\Omega} \sum_k (-q) \vec{\upsilon} f_A(\vec{r}, \vec{k})$$

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

current equation in indicial notation

$$J_i = \frac{1}{\Omega}\sum_k (-q)\upsilon_i f_A \qquad f_A = \tau_f\left(-\frac{\partial f_S}{\partial E}\right)\upsilon_j \mathcal{F}_j$$

$$J_i = \frac{(-q)}{\Omega}\sum_k \left(-\frac{\partial f_S}{\partial E}\right)\upsilon_i\upsilon_j\tau_f\mathcal{F}_j \qquad \mathcal{F}_j = -\partial_j F_n - \left[E_C + E(k) - F_n\right]\frac{1}{T}\partial_j T$$

$$J_i = \frac{(-q)}{\Omega}\sum_k \left(-\frac{\partial f_S}{\partial E}\right)\upsilon_i\upsilon_j\tau_f\left[-\partial_j F_n - \left[E_C + E(k) - F_n\right]\frac{1}{T}\partial_j T\right]$$

$$J_i = \frac{1}{\Omega}\sum_k \left\{q^2\left(-\frac{\partial f_S}{\partial E}\right)\upsilon_i\upsilon_j\tau_f\right\}\partial_j\left(F_n/q\right) +$$

$$\frac{1}{\Omega}\sum_k \left\{q\left(-\frac{\partial f_S}{\partial E}\right)\upsilon_i\upsilon_j\tau_f\right\}\left[E_C + E(k) - F_n\right]\frac{1}{T}\partial_j T$$

current equation

$$J_i = \sigma_{ij}\,\partial_j\left(F_n/q\right) + \left[sg\right]_{ij}\,\partial_j T$$

$$\sigma_{ij} = \frac{1}{\Omega}\sum_k q^2 \upsilon_i \upsilon_j \tau_f\left(-\frac{\partial f_S}{\partial E}\right) \qquad \sigma_{ij} = \sigma_0 \delta_{ij} \qquad \sigma_0 = nq\frac{q\left\langle\left\langle \tau_f \right\rangle\right\rangle}{m^*} \qquad \left\langle\left\langle \tau_f \right\rangle\right\rangle = \frac{\left\langle E\tau_f \right\rangle}{\left\langle E \right\rangle}$$

parabolic <u>*E*</u>(*k*), non-degenerate

$$\left[sg\right]_{ij} = \frac{k_B}{\Omega}\sum_k \left(\frac{E_C + E(k) - F_n}{k_B T}\right) q\,\upsilon_i \upsilon_j \tau_f\left(-\frac{\partial f_S}{\partial E}\right)$$

current equation

$$[sg]_{ij} = \frac{k_B}{\Omega}\sum_k \left(\frac{E_C + E(k) - F_n}{k_B T}\right) q\,\upsilon_i \upsilon_j \tau_f \left(-\frac{\partial f_S}{\partial E}\right)$$

parabolic energy bands, non-degenerate conditions:

$$[sg]_{ij} = [sg]_0\,\delta_{ij}$$

$$[sg]_0 = \frac{k_B}{\Omega}\sum_k \left(\frac{E_C + E(k) - F_n}{k_B T}\right) q\frac{\upsilon^2}{3}\tau_f \frac{f_S}{k_B T}$$

$$[sg]_0 = \frac{k_B}{q}\left\{\left(\frac{E_C - F_n}{k_B T}\right) + \frac{3\langle E^2 \tau\rangle}{2\langle E\rangle\langle E\tau\rangle}\right\}\sigma_0$$

current equation

$$J_i = \sigma_0 \mathcal{E}_i + [sg]_0 \partial_i T$$

$$\sigma_0 = nq \frac{q\langle\langle \tau_f \rangle\rangle}{m^*}$$

$$\langle\langle \tau_f \rangle\rangle = \langle E \tau_f \rangle / \langle E \rangle$$

$$[sg]_0 = \frac{k_B}{q}\left\{\left(\frac{E_C - F_n}{k_B T}\right) + \frac{3\langle E^2 \tau \rangle}{2\langle E \rangle \langle E \tau \rangle}\right\}\sigma_0$$

$$\mathcal{E}_i = \rho_0 J_i + S_0 \partial_i T$$

$$\rho_0 = 1/\sigma_0$$

$$S_0 = [sg]_0/\sigma_0 = \frac{k_B}{(-q)}\left\{\left(\frac{E_C - F_n}{k_B T}\right) + \frac{3\langle E^2 \tau \rangle}{2\langle E \rangle \langle E \tau \rangle}\right\}$$

To keep things simple, we have assumed that $\partial_i (F_n/q) = \mathcal{E}_i$

Seebeck coefficient

$$\mathcal{E}_i = \rho_0 J_i + S_0 \partial_i T$$

$$S_0 = \frac{k_B}{(-q)}\left\{\left(\frac{E_C - F_n}{k_B T}\right) + \frac{3\langle E^2\tau\rangle}{2\langle E\rangle\langle E\tau\rangle}\right\}$$

$$\tau_f(E) = \tau_0 (E/k_B T)^s \rightarrow \frac{3\langle E^2\tau\rangle}{2\langle E\rangle\langle E\tau\rangle} = s + 5/2$$

$$S_0 = \frac{k_B}{(-q)}\left\{\ln(N_C/n) + (s + 5/2)\right\}$$

heat current

$$f_A = \tau_f\left(-\frac{\partial f_S}{\partial E}\right)\vec{\upsilon}\bullet\vec{\mathcal{F}} \qquad \vec{\mathcal{F}} = -\nabla_r F_n + \left[E_C + E(k) - F_n\right]\frac{1}{T}\left(-\nabla_r T\right)$$

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

$$\vec{J}_Q(\vec{r}) = \frac{1}{\Omega}\sum_k \left(E_C + E(k) - F_n\right)\vec{\upsilon} f_A\left(\vec{r},\vec{k}\right)$$

coupled current equations

$$J_i = \sigma_0 \mathcal{E}_i + [sg]_0 \partial_i T$$

$$J_i^Q = T [sg]_0 \mathcal{E}_i - K_0 \partial_i T$$

$$\mathcal{E}_i = \rho_0 J_i + S_0 \partial_i T$$

$$J_i^Q = \pi_0 J_i - \kappa_0^e \partial_i T$$

$$\pi_0 = T S_0 \qquad S_0 = \frac{k_B}{(-q)} \left\{ \ln\left(N_C/n\right) + \left(s + 5/2\right) \right\}$$

$$\kappa_0 = T \left(k_B/q\right)^2 \left(s + 5/2\right) \sigma_0 \qquad \rho_0 = 1/\left(nq\mu_n\right)$$

Wiedeman Franz / Lorenz

$$\kappa_0 = T\left(k_B/q\right)^2\left(s+5/2\right)\sigma_0$$

thermal conductivity (electrons)

$$\sigma_0 = nq\mu_n$$

electrical conductivity (electrons)

$$\frac{\kappa_0}{\sigma_0} = T\left(\frac{k_B}{q}\right)^2\left(s+5/2\right)$$

"Wiedeman Franz Law"

$$L = \frac{\kappa_0}{T\sigma_0} = \left(\frac{k_B}{q}\right)^2\left(s+5/2\right)$$

"Lorenz number"

outline

1) **General solution**

2) Current equation

3) Coupled current equations

4) **The RTA**

5) Summary

collision integral and RTA

$$\hat{C}f \approx -\frac{f_S - f_A}{\tau_f}$$

The RTA can be rigorously justified for:

a) non-degenerate semiconductors near-equilibrium

b) isotropic scattering

c) elastic scattering

in which case, the characteristic time is the “momentum relaxation time.”

RTA: comments

See Lundstrom, Chapter 3, Sec. 5, pp. 139-141 for a derivation of the RTA from the scattering integral.

But, the RTA is commonly used – even when it is hard to justify rigorously – because it is a reasonable approximation that produces reasonable results.

outline

1) General solution

2) Current equation

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5) Summary

summary

We have discussed the formal procedure for solving the BTE in the presence of small gradients in electrostatic potential, concentration, and temperature.

The same procedure can be used in 1D, 2D, and 3D and for semiconductors with different $E(k)$ and scattering processes.

In the diffusive limit, the results are the same as those we obtain from the Landauer approach.

questions

1) General solution
2) Current equation
3) Coupled current equations
4) The RTA
5) Discussion
6) Summary