

ECE-656: Fall 2011

Lecture 15:

The BTE: Transport Coefficients

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review

BTE:

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

RTA:

$$\hat{C}f = - (f(\vec{p}) - f_0(\vec{p})) / \tau_m$$

Solution:

$$\delta f = \tau_m \left(- \frac{\partial f_0}{\partial E} \right) \vec{v} \bullet \vec{\mathcal{F}}$$

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

coupled current equations

$$J_x = \sigma \mathcal{E}_x - \sigma S dT_L / dx$$

$$J^q = T_L \sigma S \mathcal{E}_x - \kappa_0 dT_L / dx$$

$$\mathcal{E}_x = \rho J_x + S \frac{dT_L}{dx}$$

$$J^q = \pi J_x - \kappa_e \frac{dT}{dx}$$

We know how to compute these parameters with the Landauer approach. How do we do the same with the BTE?

(diffusive transport)

moments

$$n(\vec{r}) = \frac{1}{\Omega} \sum_k f_0(\vec{r}, \vec{k}) + \delta f(\vec{r}, \vec{k}) \approx \frac{1}{\Omega} \sum_k f_0(\vec{r}, \vec{k})$$

$$\vec{J}_n(\vec{r}) = \frac{1}{A} \sum_k (-q) \vec{v}(\vec{k}) \delta f(\vec{r}, \vec{k})$$

$$\vec{J}_w(\vec{r}) = \frac{1}{A} \sum_k E(\vec{k}) \vec{v}(\vec{k}) \delta f(\vec{r}, \vec{k})$$

$$\vec{J}_Q(\vec{r}) = \frac{1}{A} \sum_k (E(k) - F_n) \vec{v}(\vec{k}) \delta f(\vec{r}, \vec{k})$$

To evaluate these quantities, we need to work out sums in k -space.

moments

$$f_0(\vec{p}) = \frac{1}{1 + e^{\frac{[E_C + E(\vec{p}) - E_F]}{k_B T_L}}} \approx e^{\frac{[E_F - E_C - E(\vec{p})]}{k_B T_L}}$$

$$f_0(\vec{p}) = f_0(-\vec{p})$$

even in momentum
“symmetric”

$$f_S(\vec{p}) = \frac{1}{1 + e^{\frac{[E_C + E(\vec{p}) - F_n]}{k_B T_L}}} \approx e^{\frac{[F_n - E_C - E(\vec{p})]}{k_B T_L}}$$

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

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

$$\delta f(\vec{p}) = -\delta f(-\vec{p})$$

odd in momentum
“anti-symmetric”

outline

- 1) Introduction
- 2) Conductivity**
- 3) Drift current
- 4) Diffusion current
- 5) Discussion
- 6) Summary



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moments

$$\vec{J}_n(\vec{r}) = \frac{1}{A} \sum_k (-q) \vec{v}(\vec{k}) \delta f(\vec{r}, \vec{k}) = \sigma_n \vec{\nabla}(F_n/q)$$

electric current in 2D

$$\vec{J}_n(\vec{r}) = \frac{1}{A} \sum_{\vec{k}} (-q) \vec{v} \delta f(\vec{r}, \vec{k}) \quad \delta f = \tau_m \left(-\frac{\partial f_0}{\partial E} \right) \vec{v} \bullet \vec{\mathcal{F}}$$

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

$$\vec{J}_n(\vec{r}) = \frac{(-q)}{A} \sum_{\vec{k}} \tau_m \left(-\frac{\partial f_0}{\partial E} \right) \vec{v} [\vec{v} \bullet \vec{\mathcal{F}}]$$

$$\vec{J}_n(\vec{r}) = \frac{(-q)}{A} \sum_{\vec{k}} \tau_m \left(-\frac{\partial f_0}{\partial E} \right) (\vec{v} \vec{v}) \bullet \vec{\mathcal{F}} \quad \text{tensor}$$

an isotropic, isothermal, 2D conductor

$$\mathcal{F}_x = -\frac{dF_n}{dx}$$

isothermal, spatial variations only in
x-direction

$$\delta f = \tau_m \left(-\frac{\partial f_0}{\partial E} \right) v_x \mathcal{F}_x$$

generalized force in x-direction

$$J_{nx}(\vec{r}) = \frac{1}{A} \sum_{\vec{k}} (-q) v_x \delta f(\vec{r}, \vec{k})$$

current density in x-direction

$$J_{nx} = \frac{(-q)}{A} \sum_k v_x \left[\tau_m \left(-\frac{\partial f_0}{\partial E} \right) v_x \mathcal{F}_x \right] = \left(\frac{1}{A} \sum_{\vec{k}} q v_x^2 \tau_m \left(-\frac{\partial f_0}{\partial E} \right) \right) \times \frac{dF_n}{dx}$$

conductivity

$$J_{nx} = \sigma_s \frac{d(F_n/q)}{dx}$$

$$\sigma_s = \frac{1}{A} \sum_{\vec{k}} q^2 v_x^2 \tau_m \left(-\frac{\partial f_0}{\partial E} \right)$$

To work out this expression, we need to evaluate the sum.

conductivity

$$\sigma_s = \frac{1}{A} \sum_{\vec{k}} q^2 v_x^2 \tau_m \left(-\frac{\partial f_0}{\partial E} \right)$$

$$\frac{1}{A} \sum_{\vec{k}} (\bullet) \rightarrow \frac{1}{A} \int (\bullet) N_k d\vec{k} = \frac{1}{A} g_v \frac{A}{2\pi^2} \int_0^{2\pi} \int_0^\infty (\bullet) k dk d\theta$$

$$\sigma_s = \frac{g_v q^2}{2\pi^2} \int_0^{2\pi} \int_0^\infty v_x^2 \tau_m(k) \left(-\frac{\partial f_0}{\partial E} \right) k dk$$

$$\sigma_s = \frac{g_v q^2}{2\pi^2} \int_0^{2\pi} \cos^2 \theta d\theta \int_0^\infty v^2 \tau_m(k) \left(-\frac{\partial f_0}{\partial E} \right) k dk$$

$v_x = v \cos \theta$
isotropic bands

conductivity

$$\sigma_s = \frac{g_v q^2}{2\pi^2} \int_0^{2\pi} \cos^2 \theta d\theta \int_0^\infty v^2 \tau_m(k) \left(-\frac{\partial f_0}{\partial E} \right) k dk$$

$$\sigma_s = \frac{g_v q^2}{2\pi^2} \pi \int_0^\infty v^2 \tau_m(k) \left(-\frac{\partial f_0}{\partial E} \right) k dk$$

$$\sigma_s = \frac{g_v q^2}{\pi \hbar^2} \int_0^\infty (E - E_c) \tau_m(E) \left(-\frac{\partial f_0}{\partial E} \right) dE$$

$$\tau_m(E) = \tau_0$$

$$E = \frac{\hbar^2 k^2}{2m^*}$$

$$k dk = \frac{m^*}{\hbar^2} dE$$

$$v^2 = \frac{2(E - E_c)}{m^*}$$

parabolic bands

constant scattering time

$$\sigma_s = \frac{g_v q^2 \tau_0}{\pi \hbar^2} \int_0^\infty (E - E_c) \left(-\frac{\partial f_0}{\partial E} \right) dE$$

conductivity

$$\sigma_s = \frac{g_v q^2 \tau_0}{\pi \hbar^2} \int_0^\infty (E - E_c) \left(-\frac{\partial f_0}{\partial E} \right) dE$$

$$\sigma_s = \frac{g_v q^2 \tau_0}{\pi \hbar^2} \left(+\frac{\partial}{\partial E_F} \right) \int_0^\infty (E - E_c) f_0(E) dE$$

$$\sigma_s = \frac{g_v q^2 \tau_0}{\pi \hbar^2} \left(+\frac{\partial}{\partial E_F} \right) \int_0^\infty \frac{(E - E_c) dE}{1 + e^{(E - E_F)/k_B T_L}}$$

$$\sigma_s = \frac{g_v q^2 \tau_0 k_B T_L}{\pi \hbar^2} \left(+\frac{\partial}{\partial \eta_F} \right) \int_0^\infty \frac{\eta d\eta}{1 + e^{\eta - \eta_F}}$$

$$\sigma_s = \frac{g_v q^2 \tau_0 k_B T_L}{\pi \hbar^2} \mathcal{F}_0(\eta_F)$$

$$\eta = \frac{E - E_c}{k_B T_L}$$

$$\eta_F = \frac{E_F - E_c}{k_B T_L}$$

change variables

conductivity

$$\sigma_s = \frac{g_v q^2 \tau_0 k_B T_L}{\pi \hbar^2} \mathcal{F}_0(\eta_F)$$



We have our answer. Why does it look so unfamiliar?

Recall....

$$n_s = N_{2D} \mathcal{F}_0(\eta_F) = \left(\frac{g_v m^*}{\pi \hbar^2} k_B T_L \right) \mathcal{F}_0(\eta_F)$$

$$\sigma_s = n_s q \left(\frac{q \tau_0}{m^*} \right) = n_s q \mu_n$$

For energy-dependent scattering:

$$\tau_0 \rightarrow \langle\langle \tau_m(E) \rangle\rangle$$

conductivity

$$\sigma_s = \frac{g_v q^2 \tau_0 k_B T_L}{\pi \hbar^2} \mathcal{F}_0(\eta_F)$$



We have our answer, but how does it relate to the Landauer approach ?

Let's go back....

$$\sigma_s = \frac{1}{A} \sum_{\vec{k}} q^2 v_x^2 \tau_m \left(-\frac{\partial f_0}{\partial E} \right) = \frac{g_v q^2}{2\pi} \int_0^{\infty} v^2 \tau_m(k) \left(-\frac{\partial f_0}{\partial E} \right) k dk$$

change variables to energy

conductivity

$$\sigma_s = \frac{q^2}{2} \int_0^\infty v^2 \tau_m(E) \left(-\frac{\partial f_0}{\partial E} \right) \left(g_v \frac{m^*}{\pi \hbar^2} \right) dE$$

$$\sigma_s = \frac{q^2}{2} \int_0^\infty (v \tau_m) v D_{2D}(E) \left(-\frac{\partial f_0}{\partial E} \right) dE$$

$$\sigma_s = \frac{q^2}{2} \int_0^\infty \left(\frac{\pi}{2} v \tau_m \right) \left(\frac{2}{\pi} v \right) D_{2D}(E) \left(-\frac{\partial f_0}{\partial E} \right) dE$$

$$\sigma_s = \frac{2q^2}{h} \int_0^\infty M_{2D}(E) \lambda(E) \left(-\frac{\partial f_0}{\partial E} \right) dE \quad \checkmark$$

$$D_{2D}(E) = g_v \frac{m^*}{\pi \hbar^2}$$

$$\langle v_x \rangle = \frac{2}{\pi} v$$

$$M_{2D}(E) = \frac{h}{4} \langle v^+ \rangle D_{2D}(E)$$

$$\lambda(E) = \frac{\pi}{2} v(E) \tau_m(E)$$

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drift current

$$\delta f = \tau_m \left(-\frac{\partial f_0}{\partial E} \right) v_x \mathcal{F}_x$$

generalized force in x -direction

$$J_{nx}(\vec{r}) = \frac{1}{A} \sum_{\vec{k}} (-q) v_x \delta f(\vec{r}, \vec{k})$$

2D current density in x -direction

$$\mathcal{F}_x = -q \mathcal{E}_x$$

(for the drift current)

$$J_{nx}(\vec{r}) = \frac{1}{A} \sum_{\vec{k}} q^2 v_x^2 \tau_m \left(-\frac{\partial f_0}{\partial E} \right) \mathcal{E}_x$$

result

drift current (ii)

$$J_{nx}(\vec{r}) = \frac{1}{A} \sum_{\vec{k}} q^2 v_x^2 \tau_m \left(-\frac{\partial f_0}{\partial E} \right) \mathcal{E}_x$$

$$J_{nx}(\vec{r}) = \left\{ \frac{1}{A} \sum_{\vec{k}} \frac{q^2}{k_B T_L} v_x^2 \tau_m f_0 \right\} \mathcal{E}_x = \sigma_n \mathcal{E}_x$$

$$\sigma_s = \frac{q}{(k_B T_L / q)} \frac{\frac{1}{A} \sum_{\vec{k}} v_x^2 \tau_m f_0}{\frac{1}{A} \sum_{\vec{k}} f_0} \frac{1}{A} \sum_{\vec{k}} f_0$$

$$\sigma_s = n_s q \frac{\langle v_x^2 \tau_m \rangle}{(k_B T_L / q)}$$

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$$f_0(p) = e^{(E_F - E)/k_B T_L}$$

$$\frac{\partial f_0}{\partial E} = -\frac{1}{k_B T_L} f_0$$

$$\langle X \rangle \equiv \frac{\sum_k X(E) f_0(E)}{\sum_k f_0(E)}$$

drift current (iii)

$$\sigma_s = n_s q \frac{\langle v_x^2 \tau_m \rangle}{(k_B T_L / q)} = n_s q \mu_n$$

$$\mu_n = \frac{\langle v_x^2 \tau_m \rangle}{(k_B T_L / q)} = \frac{1}{(k_B T_L / q)} \frac{\langle v_x^2 \tau_m \rangle}{\langle v_x^2 \rangle} \langle v_x^2 \rangle$$

$$\left(\frac{m^* \langle v_x^2 \rangle}{2} \right) = \frac{k_B T_L}{2}$$

$$\mu_n = \frac{q \langle \langle \tau_m \rangle \rangle}{m^*}$$

$$\langle \langle \tau_m \rangle \rangle = \frac{\langle v_x^2 \tau_m \rangle}{\langle v_x^2 \rangle}$$

$$\langle X \rangle \equiv \frac{\sum_k X(E) f_0(E)}{\sum_k f_0(E)}$$

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diffusion current

$$\delta f = \tau_m \left(-\frac{\partial f_0}{\partial E} \right) v_x \mathcal{F}_x$$

generalized force in x -direction

$$J_{nx}(\vec{r}) = \frac{1}{A} \sum_{\vec{k}} (-q) v_x \delta f(\vec{r}, \vec{k})$$

2D current density in x -direction

$$\mathcal{F}_x = -k_B T_L \frac{1}{n_s} \frac{dn_s}{dx}$$

(for the diffusion current)

$$J_{nx}(\vec{r}) = - \left\{ k_B T_L \frac{\frac{1}{A} \sum_{\vec{k}} q^2 v_x^2 \tau_m \left(-\frac{\partial f_0}{\partial E} \right)}{n_s} \right\} \frac{dn_s}{dx} = -D_n \frac{dn_s}{dx}$$

result

drift current (ii)

$$D_n = k_B T_L \frac{\frac{1}{A} \sum_{\vec{k}} q^2 v_x^2 \tau_m \left(-\frac{\partial f_0}{\partial E} \right)}{n_s} = k_B T_L \frac{\frac{1}{A} \sum_{\vec{k}} q^2 v_x^2 \tau_m \left(\frac{f_0}{k_B T_L} \right)}{n_s}$$

$$D_n = \frac{\frac{1}{A} \sum_{\vec{k}} v_x^2 \tau_m f_0}{\frac{1}{A} \sum_{\vec{k}} f_0}$$

$$D_n = \langle v_x^2 \tau_m \rangle$$

drift and diffusion (non-degenerate)

$$\mu_n = \frac{q \langle\langle \tau_m \rangle\rangle}{m^*}$$
$$D_n = \langle v_x^2 \tau_m \rangle$$
$$\langle\langle \tau_m \rangle\rangle = \frac{\langle v_x^2 \tau_m \rangle}{\langle v_x^2 \rangle}$$

$$\frac{D_n}{\mu_n} = \frac{k_B T_L}{q}$$

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energy dependent scattering time

$$\langle\langle \tau_m \rangle\rangle = \frac{\langle v_x^2 \tau_m \rangle}{\langle v_x^2 \rangle}$$
$$(v^2 = v_x^2 + v_y^2 \rightarrow v_x^2 = v^2/2)$$

$$\langle\langle \tau_m \rangle\rangle = \frac{\langle v^2 \tau_m \rangle}{\langle v^2 \rangle}$$

“power law scattering”

$$\langle\langle \tau_m \rangle\rangle = \frac{\langle E \tau_m \rangle}{\langle E \rangle}$$
$$\langle\langle \tau_m \rangle\rangle = \tau_0 \frac{\Gamma(s+2)}{\Gamma(2)}$$

multiple scattering mechanisms

$$\frac{df}{dt} \Big|_{coll} = -\frac{\delta f}{\tau_m} \rightarrow \frac{df}{dt} \Big|_{coll} = -\frac{\delta f}{\tau_1} - \frac{\delta f}{\tau_2} = -\frac{\delta f}{\tau_{tot}}$$

$$\frac{1}{\tau_{tot}} = \frac{1}{\tau_1} + \frac{1}{\tau_2}$$

$$\tau_1 = \tau_{10} (E/k_B T)^{s_1} \quad \tau_2 = \tau_{20} (E/k_B T)^{s_2}$$

$$\begin{aligned}\tau_{tot} &= \frac{\tau_{10} \tau_{20} (E/k_B T)^{s_1 + s_2}}{\tau_{10} (E/k_B T)^{s_1} + \tau_{20} (E/k_B T)^{s_2}} \\ &\neq \tau_0^{tot} (E/k_B T)^{s_{tot}}\end{aligned}$$

$$\mu_n = \frac{q \langle\langle \tau_m \rangle\rangle}{m^*}$$

Mathiessen's Rule

$$s_1 = s_2 = s$$

$$\tau_{tot} = \frac{\tau_{10}\tau_{20}}{\tau_{10} + \tau_{20}} (E/k_B T)^s = \tau_0^{tot} (E/k_B T)^s$$

$$\mu_n = \frac{q \langle\langle \tau_m \rangle\rangle}{m^*}$$

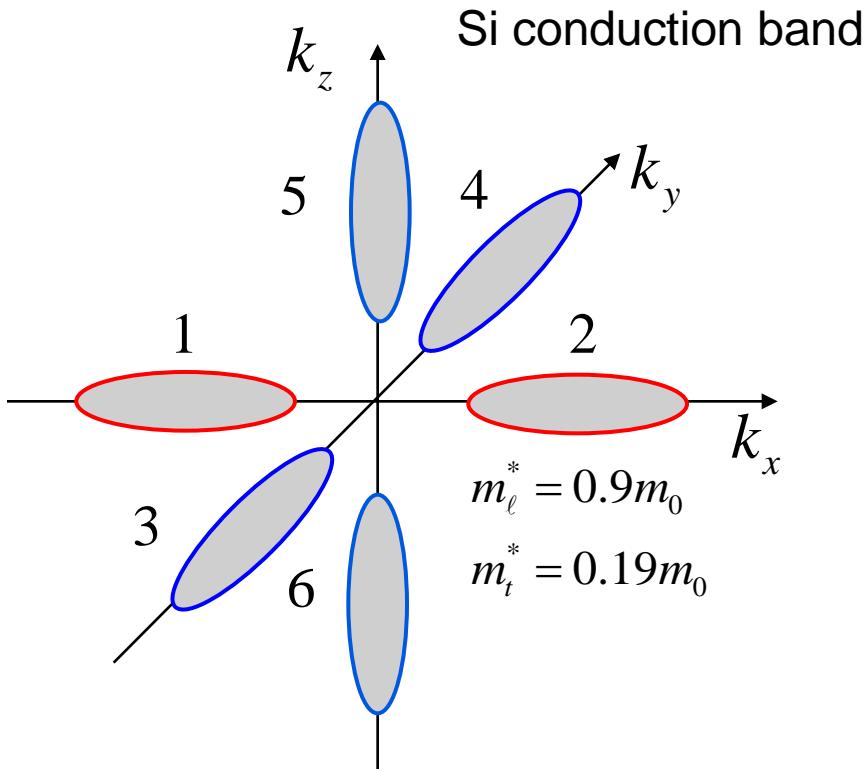
$$\mu_{tot} = \frac{q \tau_0^{tot}}{m^*} \frac{\Gamma(s+2)}{\Gamma(2)}$$

$$\frac{1}{\mu_{tot}} = \frac{1}{\mu_1} + \frac{1}{\mu_2}$$

Mathiessen's Rule

$$\frac{1}{\tau_{tot}(E)} = \frac{1}{\tau_1(E)} + \frac{1}{\tau_2(E)}$$

ellipsoidal bands



$$\sigma_{1,2} = \frac{n}{6} q \frac{q \langle\langle \tau_m \rangle\rangle}{m_\ell^*}$$

$$\sigma_{3-6} = \frac{n}{6} q \frac{q \langle\langle \tau_m \rangle\rangle}{m_t^*}$$

$$\sigma = 2\sigma_1 + 4\sigma_3$$

$$\sigma = \frac{n}{6} q \left[\frac{1}{3m_\ell^*} + \frac{2}{3m_t^*} \right] q \langle\langle \tau_m \rangle\rangle$$

$$\frac{1}{m_c^*} = \frac{1}{3m_\ell^*} + \frac{2}{3m_t^*}$$

“conductivity effective mass”
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transport tensors

$$\delta f = \tau_m \left(-\frac{\partial f_0}{\partial E} \right) \vec{v} \bullet \vec{\mathcal{F}}$$

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

$$\vec{J}_n(\vec{r}) = \frac{1}{\Omega} \sum_k (-q) \vec{v} \delta f(\vec{r}, \vec{k})$$

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

current equation in indicial notation

$$J_i = \frac{1}{\Omega} \sum_k (-q) v_i \delta f \quad \delta f = \tau_m \left(-\frac{\partial f_0}{\partial E} \right) v_j \mathcal{F}_j$$
$$J_i = \frac{(-q)}{\Omega} \sum_k \left(-\frac{\partial f_0}{\partial E} \right) v_i v_j \tau_m \mathcal{F}_j \quad \mathcal{F}_j = -\partial_j F_n - \left[E_C + E(k) - F_n \right] \frac{1}{T_L} \partial_j T_L$$

$$J_i = \frac{(-q)}{\Omega} \sum_k \left(-\frac{\partial f_0}{\partial E} \right) v_i v_j \tau_m \left[-\partial_j F_n - \left[E_C + E(k) - F_n \right] \frac{1}{T_L} \partial_j T_L \right]$$
$$J_i = \frac{1}{\Omega} \sum_k \left\{ q^2 \left(-\frac{\partial f_0}{\partial E} \right) v_i v_j \tau_m \right\} \partial_j \left(F_n / q \right) +$$
$$\frac{1}{\Omega} \sum_k \left\{ q \left(-\frac{\partial f_0}{\partial E} \right) v_i v_j \tau_m \right\} \left[E_C + E(k) - F_n \right] \frac{1}{T_L} \partial_j T_L$$

current equation

$$J_i = \sigma_{ij} \partial_j (F_n/q) + [s_T]_{ij} \partial_j T_L$$

$$\sigma_{ij} = \frac{1}{\Omega} \sum_k q^2 v_i v_j \tau_f \left(-\frac{\partial f_0}{\partial E} \right) \quad \sigma_{ij} = \sigma_0 \delta_{ij} \quad \sigma_0 = nq \frac{q \langle \langle \tau_m \rangle \rangle}{m^*} \quad \langle \langle \tau_m \rangle \rangle = \frac{\langle E \tau_m \rangle}{\langle E \rangle}$$

parabolic $E(k)$, non-degenerate

$$[s_T]_{ij} = \frac{k_B}{\Omega} \sum_k \left(\frac{E_c + E(k) - F_n}{k_B T_L} \right) q v_i v_j \tau_f \left(-\frac{\partial f_0}{\partial E} \right)$$

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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

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