Solving the BTE:

Semiconductors

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BTE in the Relaxation Time Approximation

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = -\frac{f - f_S}{\tau_m}$$

We will assume steady-state conduction, spatial variation in 1D, and no magnetic fields.

$$\upsilon_x \frac{\partial f}{\partial x} - q\mathcal{E}_x \frac{\partial f}{\partial k_x} = -\frac{f - f_S}{\tau_m}$$

Outline

1) **Equilibrium solution**
2) Small electric fields (the math)
3) Small electric fields (the physics)
4) Small concentration gradients
5) Discussion

Equilibrium solution

$$\hat{C} f_0 = 0$$

$$f_0(E) = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

We already showed that detailed balance in the collision integral tells us something about S(p, p'). Can we learn anything by solving the BTE too?

Equilibrium

$$\vec{\upsilon} \bullet \nabla_r f_0 + \vec{F}_e \bullet \nabla_p f_0 = 0$$

Any function of BTE! total energy satisfies the equilibrium

Assume:

$$f_0 = g\left(E_{TOT}\right) = g\left[E_C(\vec{r}) + E(\vec{k})\right]$$

Then:

$$\vec{\upsilon} \bullet \nabla_r g\left(E_{TOT}\right) + \vec{F}_e \bullet \nabla_p g\left(E_{TOT}\right) = 0$$

$$\vec{\upsilon} \bullet \frac{dg}{dE_{TOT}} \nabla_r E_{TOT} + \vec{F}_e \bullet \frac{dg}{dE_{TOT}} \nabla_p E_{TOT} = 0$$

($\nabla_r E_{TOT} \rightarrow -\vec{F}_e$; $\nabla_p E_{TOT} \rightarrow \vec{\upsilon}$)

Equilibrium

$$\vec{\upsilon} \bullet \nabla_r f_0 + \vec{F}_e \bullet \nabla_p f_0 = \hat{C} f_0 = 0$$

Satisfied by any function of total energy

To ensure detailed balance in equilibrium:

$$f_0 = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

Look more closely at the equilibrium solution

$$\vec{\upsilon} \bullet \nabla_r f_0 + \vec{F}_e \bullet \nabla_p f_0 = 0$$

$$f_0 = \frac{1}{1 + e^{(E - E_F)/k_B T}} = \frac{1}{1 + e^{\Theta}}$$

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

$$\vec{\upsilon} \bullet \frac{df_0}{d\Theta} \nabla_r \Theta + \vec{F}_e \bullet \frac{df_0}{d\Theta} \nabla_p \Theta = 0$$

$$\vec{\upsilon} \bullet \left\{ -\nabla_r E_F + (E - E_F)\left(-\frac{\nabla_r T}{T} \right) \right\} = 0$$

The Fermi level and temperature are constant in equilibrium.

to satisfy this equation for **any** energy, E_{TOT}, $\nabla E_F = \nabla T = 0$

Energy-specific equilibrium

We showed that an equilibrium solution to the BTE demonstrates that to maintain equilibrium at all energies, the Fermi level and temperature must be constant. Nanostructures can be built with a single energy channel for conduction. For an interesting discussion of "energy-specific equilibrium," see:

T. E. Humphrey and H. Linke, "Reversible Thermoelectric Nanomaterials," *Physical Review Letters*, **94**, 096601, 2005.

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Steady-state BTE for small E-fields

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

$n \approx n_0$

$F_n \approx E_F$

Steady-state, 1D, spatially uniform, no B-field:

$$-q\mathcal{E}_x \frac{\partial f}{\partial p_x} = -\frac{f - f_0}{\tau_m}$$

Key assumption: $\frac{\partial f}{\partial p_x} \approx \frac{\partial f_0}{\partial p_x}$ (small E-fields)

Steady-state BTE for small E-fields

$$-q\mathcal{E}_x \frac{\partial f_0}{\partial p_x} = -\frac{f - f_0}{\tau_m}$$

$$f = f_0 + q\tau_m \mathcal{E}_x \frac{\partial f_0}{\partial p_x}$$

Solution of the BTE

$$J_{nx} = \frac{1}{\Omega}\sum_{\vec{k}}(-q)\upsilon_x f$$

$$J_{nx} = \frac{1}{\Omega}\sum_{\vec{k}}(-q)\upsilon_x \left(q\tau_m \mathcal{E}_x \frac{\partial f_0}{\partial p_x} \right)$$

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

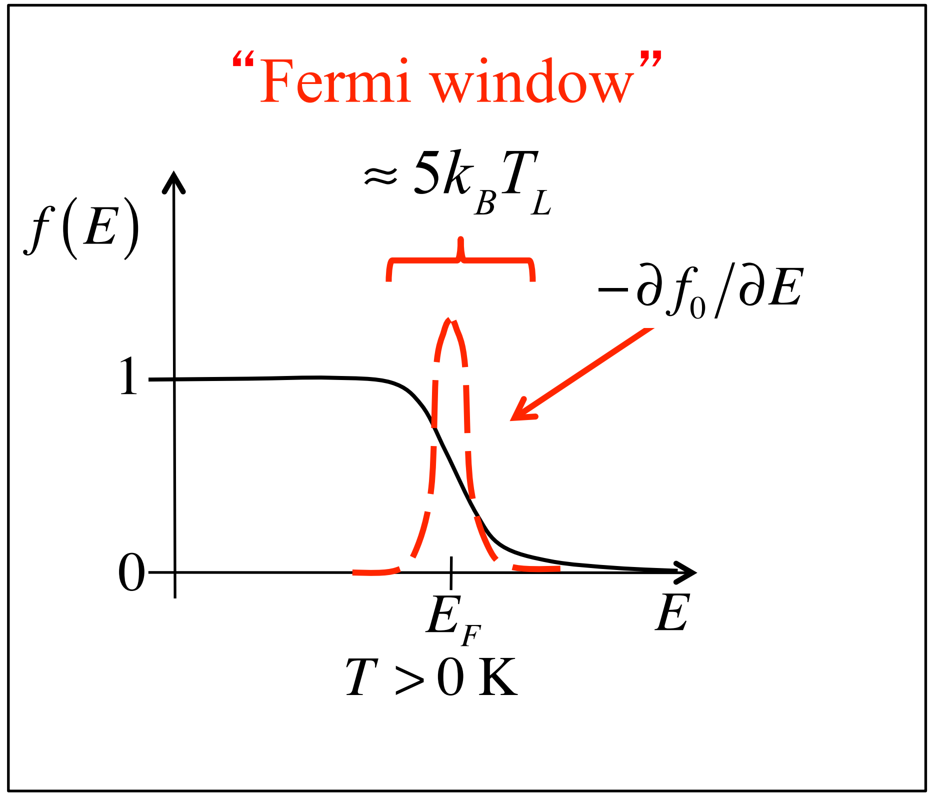
Near-equilibrium current

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

"Fermi window"

$$J_{nx} = \sigma_n \mathcal{E}_x$$

$$\sigma_n = \frac{1}{\Omega}\sum_{\vec{k}} q^2 \upsilon_x^2 \tau_m \left(-\frac{\partial f_0}{\partial E}\right)$$



Conductivity

$$J_{nx} = \sigma_n \mathcal{E}_x$$

$$\sigma_n = \frac{1}{\Omega}\sum_{\vec{k}} q^2 \upsilon_x^2 \tau_m \left(-\frac{\partial f_0}{\partial E}\right)$$

$$\upsilon^2 = \upsilon_x^2 + \upsilon_y^2 + \upsilon_z^2 \qquad \upsilon^2 = 3\upsilon_x^2 \qquad \upsilon_x^2 = \frac{\upsilon^2}{3}$$

$$\upsilon^2 = \frac{2E}{m^*} \qquad \upsilon_x^2 = \frac{2E}{3m^*}$$

$$\sigma_n = \frac{2q^3}{3m^*}\frac{1}{\Omega}\sum_{\vec{k}} E\tau_m \left(-\frac{\partial f_0}{\partial E}\right)$$

Conductivity (non-degenerate)

$$J_{nx} = \sigma_n \mathcal{E}_x$$

$$\sigma_n = \frac{2q^3}{3m^*}\frac{1}{\Omega}\sum_{\vec{k}} E\tau_m\left(-\frac{\partial f_0}{\partial E}\right)$$

$$f_0 = \frac{1}{1+e^{(E-E_F)/k_BT}} \approx e^{(E_F-E)/k_BT}$$

$$E_F << E$$

$$-\frac{\partial f_0}{\partial E} = \frac{1}{k_BT} f_0$$

$$\sigma_n = \frac{2q^3}{3m^* k_BT}\frac{1}{\Omega}\sum_{\vec{k}} E\tau_m f_0$$

Conductivity (non-degenerate)

$$J_{nx} = \sigma_n \mathcal{E}_x$$

$$\sigma_n = \frac{2q^3}{3m^* k_B T} \frac{1}{\Omega} \sum_{\vec{k}} E \tau_m f_0$$

$$\sigma_n = \frac{2q^3}{3m^* k_B T} \times \frac{\frac{1}{\Omega} \sum_{\vec{k}} E \tau_m f_0}{\frac{1}{\Omega} \sum_{\vec{k}} E f_0} \times \frac{1}{\Omega} \sum_{\vec{k}} E f_0$$

$$\frac{1}{\Omega} \sum_{\vec{k}} E f_0 = \langle E \rangle = \frac{3}{2} n k_B T$$

$$\sigma_n = \frac{nq^2}{m^*} \times \frac{\langle E \tau_m \rangle}{\langle E \rangle}$$

Conductivity (non-degenerate)

$$J_{nx} = \sigma_n \mathcal{E}_x$$

$$\sigma_n = \frac{nq^2}{m^*} \times \frac{\langle E\tau_m \rangle}{\langle E \rangle}$$

$$\sigma_n = nq\mu_n$$

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

$$\langle\langle \tau_m \rangle\rangle \equiv \frac{\langle E\tau_m \rangle}{\langle E \rangle}$$

Conductivity (summary)

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

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

$$\tau_m(E) = \tau_0 \left(E/k_B T\right)^s$$

"power law scattering"

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

ADP scattering (3D):

$$\tau_m(E) = \tau_0^{ADP} \left(E/k_B T\right)^{-1/2}$$

FCT eqn. (2.84)

II scattering (3D):

$$\tau_m(E) = \tau_0^{II} \left(E/k_B T\right)^{3/2}$$

FCT eqn. (2.46)

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Displaced Maxwellian

$$f(p_x) = f_0(p_x) + q\tau_0 \mathcal{E}_x \frac{\partial f_0}{\partial p_x}$$

How do we interpret our solution to the BTE?

Recall: Taylor series expansion:

$$f(x + \delta x) = f(x) + \frac{\partial f}{\partial x}\delta x$$

$$\delta x \to q\tau_0 \mathcal{E}_x \qquad f_0(p_x) = f_0(p_x) + \frac{\partial f_0}{\partial p_x} q\tau_0 \mathcal{E}_x = f_0(p_x + q\tau_0 \mathcal{E}_x)$$

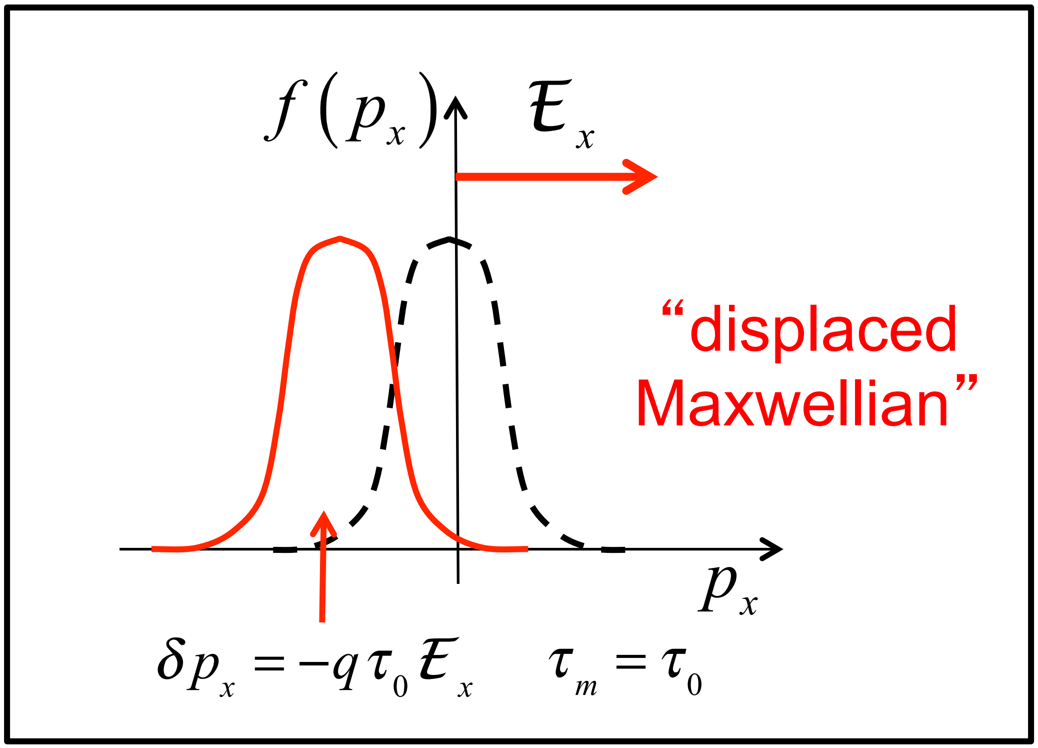
Displaced Maxwellian

$$f = f_0 + q\tau_0 \mathcal{E}_x \frac{\partial f_0}{\partial p_x} \qquad f(p_x) = f_0(p_x + \delta p_x) \qquad \delta p_x = q\tau_0 \mathcal{E}_x$$

$$F_e = \frac{dp_x}{dt}$$

$$F_e = \frac{\Delta p_x}{\tau_0} = -q\mathcal{E}_x$$

$$\Delta p_x = -\tau_0 q \mathcal{E}_x$$



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BTE (like before)

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

Steady-state, 1D, spatially non-uniform, no E- or B-field:

$$\upsilon_x \frac{\partial f}{\partial x} = -\frac{f - f_0}{\tau_m}$$

$$\frac{\partial f}{\partial x} \approx \frac{\partial f_0}{\partial x} = 0$$

f_0 is uniform in equilibrium!

Symmetric and anti-symmetric components

$$f(x, p_x) = f_A(x, p_x) + f_S(x, p_x)$$

$$f_S(x, p_x) = f_S(x, -p_x) \qquad f_A(x, p_x) = -f_A(x, -p_x)$$

$$f_S = \frac{1}{1 + e^{(E - F_n(\vec{r}))/k_B T}} \qquad \left.\frac{\partial f}{\partial t}\right)_{coll} = -\frac{f - f_S}{\tau_m} = -\frac{f_A}{\tau_m}$$

BTE (again)

$$\frac{\partial f}{\partial t} + \upsilon_x \frac{\partial f}{\partial x} + F_{ex} \frac{\partial f}{\partial p_x} = -\frac{f - f_S}{\tau_m}$$

Steady-state, 1D, spatially non-uniform, no E- or B-field:

$$\upsilon_x \frac{\partial f}{\partial x} = -\frac{f - f_S}{\tau_m}$$

$$\frac{\partial f}{\partial x} \approx \frac{\partial f_S}{\partial x}$$

BTE (again)

$$\upsilon_x \frac{\partial f}{\partial x} = -\left(\frac{f - f_S}{\tau_m}\right) \qquad \frac{\partial f}{\partial x} \approx \frac{\partial f_S}{\partial x}$$

$$f = f_S - \tau_m \upsilon_x \frac{\partial f_S}{\partial x}$$

Solution of the BTE

$$J_{nx} = \frac{1}{\Omega}\sum_{\vec{k}}(-q)\upsilon_x f \qquad J_{nx} = \frac{1}{\Omega}\sum_{\vec{k}}(-q)\upsilon_x\left(-\tau_m \upsilon_x \frac{\partial f_S}{\partial x}\right)$$

$$J_{nx} = (q)\frac{\partial}{\partial x}\frac{1}{\Omega}\sum_{\vec{k}}\upsilon_x^2 \tau_m f_S$$

BTE (again)

$$J_{nx} = (q)\frac{\partial}{\partial x}\left\{\frac{1}{\Omega}\sum_{\vec{k}} \upsilon_x^2 \tau_m f_S\right\}$$

$$J_{nx} = (-q)\frac{\partial}{\partial x}\left\{\left(\frac{\sum_{\vec{k}} \upsilon_x^2 \tau_m f_S}{\sum_{\vec{k}} f_S}\right)\frac{1}{\Omega}\sum_{\vec{k}} f_S\right\}$$

$$J_{nx} = qD_n\frac{\partial n}{\partial x} \qquad D_n = \left\langle \upsilon_x^2 \tau_m \right\rangle = \left(\frac{\sum_{\vec{k}} \upsilon_x^2 \tau_m f_S}{\sum_{\vec{k}} f_S}\right)$$

Exercise: Show that D/μ = kT/q.

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Mathiessen's Rule

Two independent scattering mechanisms.

$$\left.\frac{df}{dt}\right|_{coll} = -\frac{\delta f}{\tau_1} - \frac{\delta f}{\tau_2} = -\frac{\delta f}{\tau_{tot}}$$

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

Mathiessen's Rule

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

When is the true?

Mathiessen's Rule

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

$$\frac{1}{\mu_1} = \frac{m^*}{q}\frac{1}{\langle\langle\tau_1\rangle\rangle}$$

$$\frac{1}{\mu_2} = \frac{m^*}{q}\frac{1}{\langle\langle\tau_2\rangle\rangle}$$

$$\frac{1}{\mu_{tot}} = \frac{m^*}{q}\frac{1}{\left\langle\left\langle\left(\frac{\tau_1\tau_2}{\tau_1+\tau_2}\right)\right\rangle\right\rangle}$$

In general:

$$\frac{1}{\langle\langle\tau_1\rangle\rangle} + \frac{1}{\langle\langle\tau_2\rangle\rangle} \neq \frac{1}{\left\langle\left\langle\left(\frac{\tau_1\tau_2}{\tau_1+\tau_2}\right)\right\rangle\right\rangle}$$

Mathiessen's Rule **only holds** when the two scattering processes have the same energy dependence.

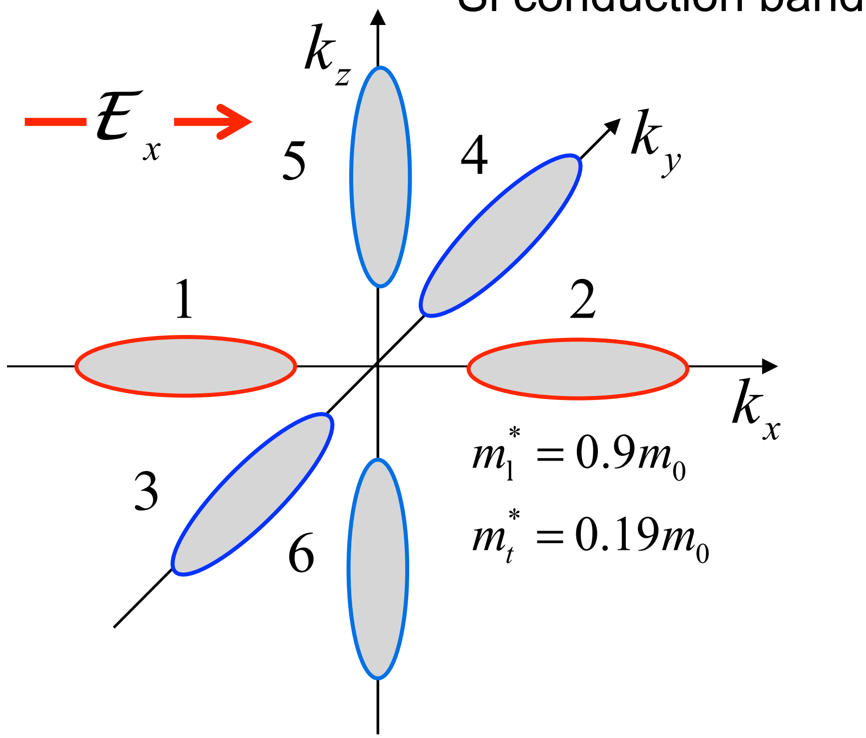
Conductivity effective mass

For complex band structures, we prefer to write the mobility in a simple way:

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

where m_c^* is the "conductivity effective mass". This is analogous to (but different from) the density-of-states effective mass. The idea is to hide the complexity of the band structure in a defined quantity.

Example: Si conduction band



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

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

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

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

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

"conductivity effective mass"

Questions?

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = -\frac{f - f_S}{\tau_m}$$

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