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Near-equilibrium Transport:
Fundamentals and Applications

Lecture 7: Boltzmann Transport Equation

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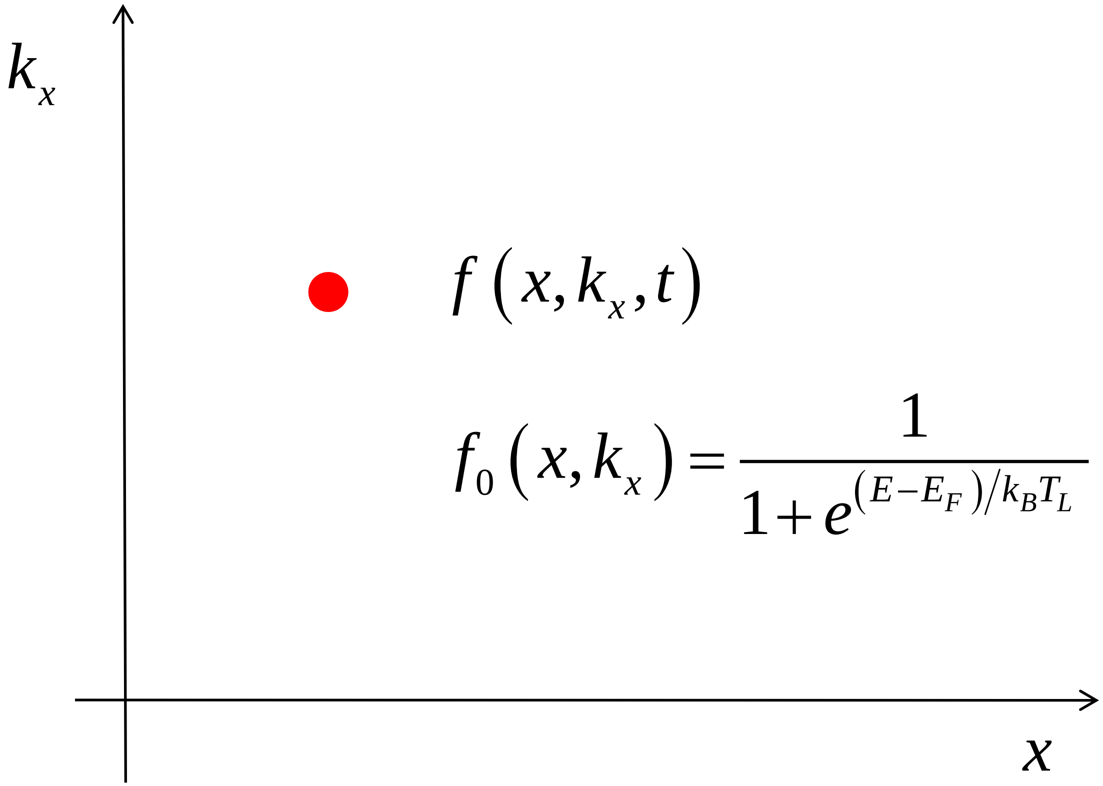
outline

f(*r*, *k*, *t*)



$$f\left(x, k_x, t\right)$$

$$f_0\left(x, k_x\right) = \frac{1}{1 + e^{\left(E - E_F\right)/k_B T_L}}$$

goals

1) Find an equation for $f(r, p, t)$ out of equilibrium

2) Learn how to solve it near equilibrium

3) Relate the results to our Landauer approach results – *in the diffusive limit*

4) Add a B-field and show how transport changes

For much more about the BTE, see
Lundstrom, *Fundamentals of Carrier Transport*, Cambridge, 2000.
ECE 656: L12-17 http://nanohub.org/resources/7281

outline

1) Introduction
2) **The BTE**
3) Solving the s.s. BTE
4) Transport coefficients
5) Magnetic fields
6) Discussion
7) Summary

semi-classical transport

$$\frac{d\left(\hbar\vec{k}\right)}{dt} = -\nabla_r E_C(\vec{r}) = -q\vec{\mathcal{E}}(\vec{r}) \qquad \left\{ \frac{d\vec{p}}{dt} = \vec{F}_e \right\}$$

$$\hbar\vec{k}(t) = \hbar\vec{k}(0) + \int_0^t -q\vec{\mathcal{E}}(t')dt'$$

$$\vec{\upsilon}_g(t) = \frac{1}{\hbar}\nabla_k E\left[\vec{k}(t)\right]$$

$$\vec{r}(t) = \vec{r}(0) + \int_0^t \vec{\upsilon}_g(t')dt'$$

equations of motion for "semi-classical transport"

E_C varies slowly on the scale of the electron's wavelength.

no effective mass!

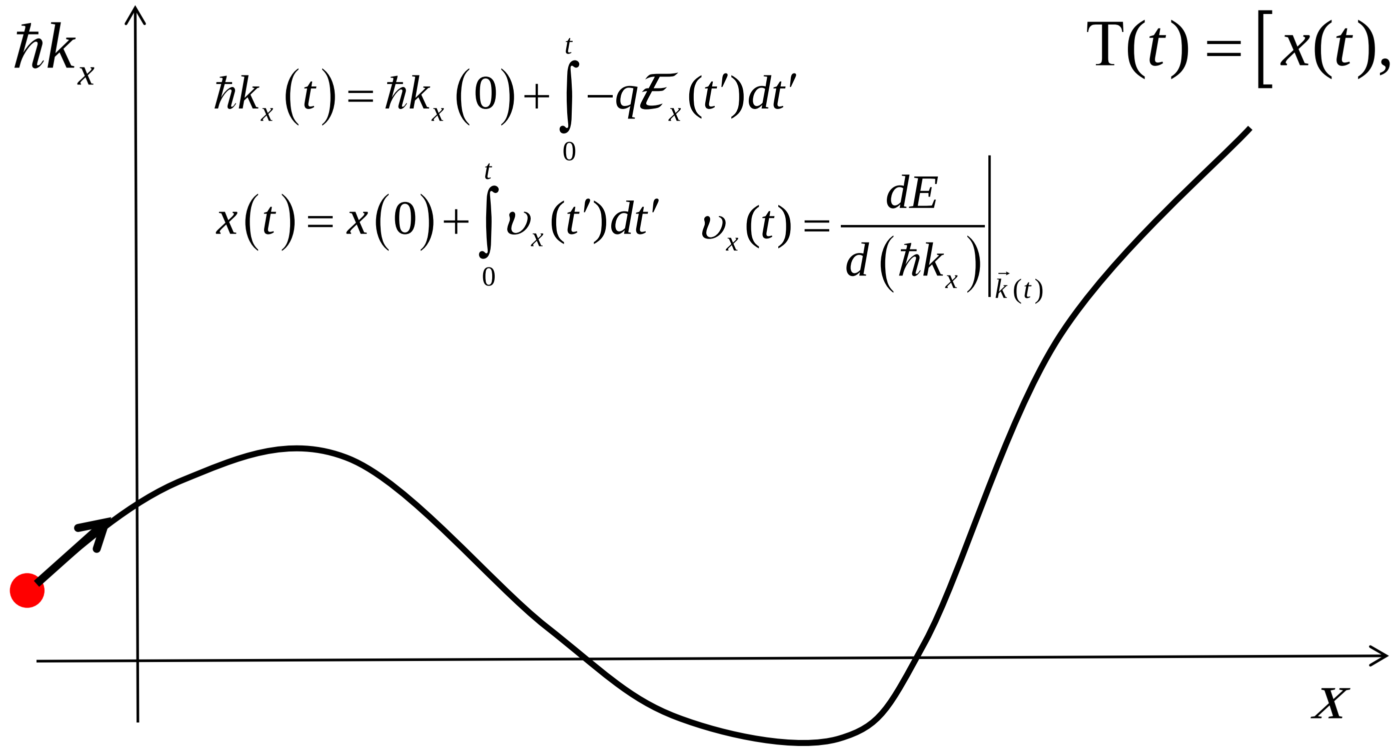
trajectories in phase space

$$p_x = \hbar k_x$$

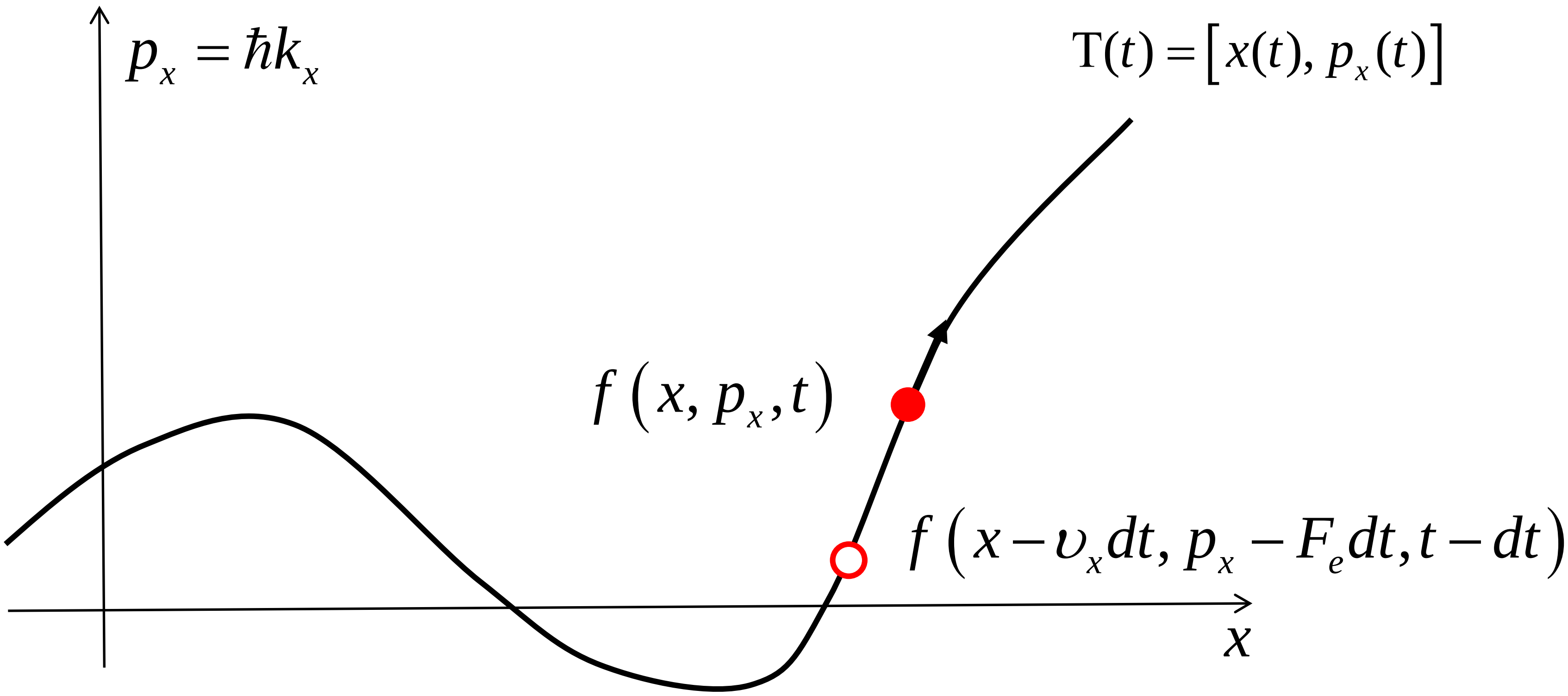
$$\mathrm{T}(t) = \left[x(t), p_x(t) \right]$$

$$\hbar k_x(t) = \hbar k_x(0) + \int_0^t -q\mathcal{E}_x(t')dt'$$

$$x(t) = x(0) + \int_0^t \upsilon_x(t')dt' \qquad \upsilon_x(t) = \left. \frac{dE}{d(\hbar k_x)} \right|_{\vec{k}(t)}$$



Boltzmann Transport Equation (BTE)



$$f(x, p_x, t) = f(x - \upsilon_x dt, p_x - F_e dt, t - dt)$$

$$\frac{df}{dt} = 0$$

Boltzmann Transport Equation (BTE)

$$f\left(x, p_x, t\right) \qquad \frac{df}{dt} = 0$$

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial p_x}\frac{dp_x}{dt} = 0$$

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\upsilon_x + \frac{\partial f}{\partial p_x}F_x = 0$$

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = 0$$

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

$$\nabla_r f = \frac{\partial f}{\partial x}\hat{x} + \frac{\partial f}{\partial y}\hat{y} + \frac{\partial f}{\partial z}\hat{z}$$

$$\nabla_p f = \frac{\partial f}{\partial p_x}\hat{p}_x + \frac{\partial f}{\partial p_y}\hat{p}_y + \frac{\partial f}{\partial p_z}\hat{p}_z$$

$$\vec{p} = \hbar\vec{k}$$

result

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

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

optical absorption, impact ionization, etc.
and carrier scattering

Boltzmann Transport Equation (BTE)

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

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = 0$$

neglected scattering!

assumptions:

1) semi-classical treatment of electrons in a crystal with *E*(*k*)

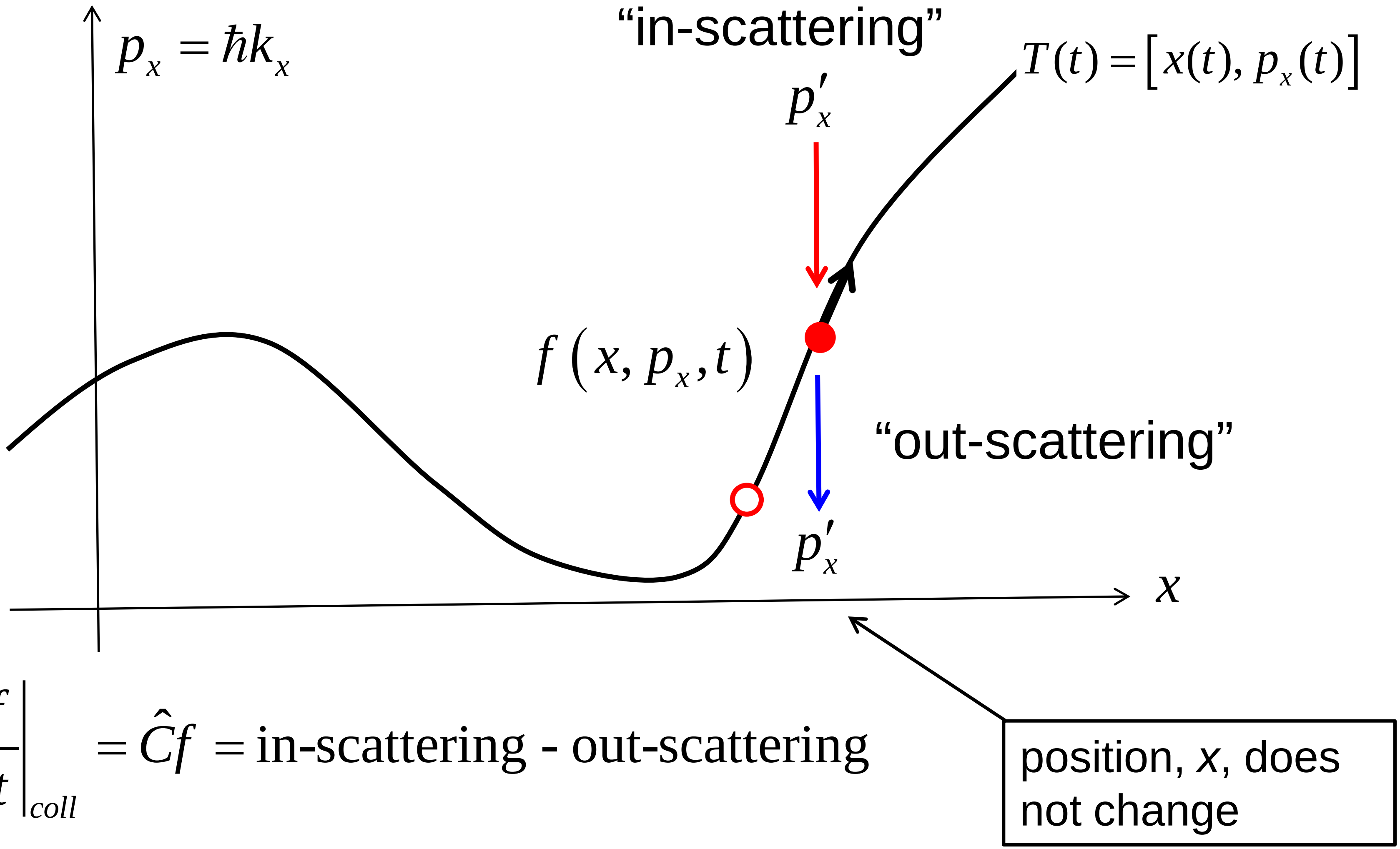
$$\frac{d\left(\hbar \vec{k}\right)}{dt} = -\nabla E_C(\vec{r}) = -q\vec{\mathcal{E}}(\vec{r}) \qquad E = E_C(\vec{r}) + E\left(\vec{k}\right)$$

$$\upsilon_g\left(t\right) = \frac{1}{\hbar}\nabla_k E\left[k\left(t\right)\right] \qquad \Delta p_x \Delta x \geq \hbar$$

2) neglected generation-recombination

3) neglected e-e correlations (mean-field-approximation)

in and out-scattering



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

Relaxation Time Approximation (RTA)

$$\hat{C}f = -\left(\frac{f(\vec{p}) - f_0(\vec{p})}{\tau_m}\right)$$

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

in-scattering – out-scattering

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

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

See Lundstrom: pp. 139-141. The RTA can be justified when the scattering is **isotropic and/or elastic** in which case the proper time to use is the "momentum relaxation time."

meaning of the RTA

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = 0$$

Assume spatial uniformity, no *E*-field.

$$\frac{\partial f}{\partial t} = -\frac{\delta f}{\tau_m}$$

$$\delta f = f - f_0$$

$$\frac{\partial (\delta f)}{\partial t} = -\frac{\delta f}{\tau_m}$$

$$\delta f(t) = \delta f(0) e^{-t/\tau_m}$$

Perturbations decay away exponentially with a characteristic time, τ_m

steady-state BTE in 1D

$$\upsilon_x \frac{\partial f}{\partial x} + F_x \frac{\partial f}{\partial p_x} = -\frac{\delta f}{\tau_m}$$

RTA

no B-fields for now

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

$$f(\vec{p}) = f_0(\vec{p}) + \delta f(\vec{p})$$

$$\left|f_0(\vec{p})\right| >> \left|\delta f(\vec{p})\right|$$

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

near-equilibrium

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near eq., s.s BTE

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

$$\nabla_r f \approx \nabla_r f_0 \qquad \nabla_p f \approx \nabla_p f_0$$

$$\vec{\upsilon} \bullet \nabla_r f_0 - q\vec{\mathcal{E}} \bullet \nabla_p f_0 = -\frac{\delta f(\vec{p})}{\tau_m}$$

$$\delta f(\vec{p}) = -\tau_m \vec{\upsilon} \bullet \nabla_r f_0 + q\tau_m \vec{\mathcal{E}} \bullet \nabla_p f_0$$

BTE solution

$$\delta f = -\tau_m \vec{\upsilon} \bullet \nabla_r f_0 + q\tau_m \vec{\mathcal{E}} \bullet \nabla_p f_0$$

$$f_0(\vec{p}) = \frac{1}{1+e^{\Theta}} \qquad \Theta(\vec{r},\vec{p}) = \left[E(\vec{r},\vec{p}) - F_n(\vec{r})\right]/k_B T_L$$

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

$$\nabla_r f_0 = \frac{\partial f_0}{\partial \Theta} \nabla_r \Theta$$

$$\nabla_p f_0 = \frac{\partial f_0}{\partial \Theta} \nabla_p \Theta$$

$$\frac{\partial f_0}{\partial \Theta} = k_B T_L \frac{\partial f_0}{\partial E}$$

$$\delta f = \tau_m k_B T_L \left(-\frac{\partial f_0}{\partial E}\right)\left[\vec{\upsilon} \bullet \nabla_r \Theta - q\vec{\mathcal{E}} \bullet \nabla_p \Theta\right]$$

BTE solution

$$\delta f = \tau_m k_B T_L \left(-\frac{\partial f_0}{\partial E}\right)\left[\vec{\upsilon} \bullet \nabla_r \Theta - q\vec{\mathcal{E}} \bullet \nabla_p \Theta\right]$$

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

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

$$\delta f = \tau_m \left(-\frac{\partial f_0}{\partial E}\right)\vec{\upsilon} \bullet \left\{-\nabla_r F_n + T_L\left[E_C + E(\vec{p}) - F_n\right]\nabla_r\left(\frac{1}{T_L}\right)\right\}$$

Lundstrom 2011

generalized force

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

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

"generalized force"

The two forces driving current flow are gradients in QFL and gradients in (inverse) temperature. In Lecture 4, we saw that ($f_1 - f_2$) produces current flow and that differences in Fermi level and temperature cause differences in *f*.

now what?

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

We have solved the BTE,
now what do we do with the solution?

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moments

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

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

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

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

recall lecture 4

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

sums and integrals in *k*-space

$$\sum_{\vec{k}} (\bullet) \rightarrow \int (\bullet) N_k d\vec{k}$$

N_k is the density of states in *k*-space. Note that it is independent of bandstructure.

1D $\quad N_k = 2 \times \left(\frac{L}{2\pi} \right) = \frac{L}{\pi} \qquad d\vec{k} = dk$

2D $\quad N_k = 2 \times \left(\frac{A}{4\pi^2} \right) = \frac{A}{2\pi^2} \qquad d\vec{k} = dk_x dk_y$

3D $\quad N_k = 2 \times \left(\frac{\Omega}{8\pi^2} \right) = \frac{\Omega}{4\pi^3} \qquad d\vec{k} = dk_x dk_y dk_z$

See:
Lundstrom, Ch. 1, *Fundamentals of Carrier Transport*, Cambridge, 2000.
ECE 656: L2 http://nanohub.org/resources/7281

electric current in 2D

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

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

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

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

an isotropic, isothermal, 2D conductor

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

isothermal, spatial variations only in *x*-direction

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

generalized force in *x*-direction

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

current density in *x*-direction

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

conductivity

$$J_{nx} = \sigma_S \frac{d\left(F_n/q\right)}{dx}$$

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

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

conductivity

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

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

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

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

$$\upsilon_x = \upsilon\cos\theta$$

isotropic bands

conductivity

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

$$\sigma_S = \frac{g_v q^2}{2\pi} \pi \int_0^{\infty} \upsilon^2 \tau_m(k) \left(-\frac{\partial f_0}{\partial E}\right) kdk$$

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

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

$$kdk = \frac{m^*}{\pi\hbar^2} dE$$

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

parabolic bands

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

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….

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

$$\sigma_S = n_S q \left(\frac{q \tau_0}{m^*} \right) = n q \mu_n$$

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….

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

change variables to energy

conductivity

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

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

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

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

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

$$\langle \upsilon_x \rangle = \frac{2}{\pi}\upsilon$$

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

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

finally

$$\sigma_S = \frac{2q^2}{h}\int_0^{\infty} M(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$

$$\sigma_S = \frac{2q^2}{h}\left\langle M_{2D}(E)\right\rangle\left\langle\left\langle \lambda(E)\right\rangle\right\rangle$$

So the result from solving the BTE is equivalent to the result from the Landauer approach in the diffusive limit.

Similarly, it is easy to show that the BTE gives the same answers for the Seebeck coefficient and electronic heat conductivity.

for more about the BTE

For more on the BTE, see:

Lundstrom, Chapters 3, 4, *Fundamentals of Carrier Transport*, Cambridge, 2000.

ECE 656: L12-15 http://nanohub.org/resources/7281

For more on the connection of the Landauer and BTE approaches, see:

Changwook Jeong, et al. "On Landauer vs. Boltzmann and Full Band vs. Effective Mass Evaluation of Thermoelectric Trans-port Coefficients," J. Appl. Phys., **107**, 023707, 2010.

ECE-656 Lecture 17. http://nanohub.org/resources/7281.

summary

Landauer approach:

- clear physical insight
- works in ballistic limit as well as quasi-ballistic and diffusive regimes

BTE approach:

- "easy" to add magnetic field
- anisotropic materials (transport tensors) straight-forward
- can resolve transport spatially
- "off-equilibrium" easy to handle
- ballistic transport can be handled, but not easily
- not as physically transparent

Bottom line: should know both approaches.

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the BTE with a B-field…

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

steady-state with RTA:

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

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

spatially uniform:

$$-q\vec{\mathcal{E}} \bullet \nabla_p f - q\left(\vec{\upsilon} \times \vec{B}\right) \bullet \nabla_p f = -\delta f / \tau_m$$

$$\nabla_p f \rightarrow \nabla_p f_0 \ ?$$

the BTE with a B-field…

$$-q\vec{\mathcal{E}} \bullet \nabla_p f_0 - q\left(\vec{\upsilon} \times \vec{B}\right) \bullet \nabla_p f_0 = -\delta f / \tau_m$$

OK here:

But not here:

$$\nabla_p f = \frac{\partial f_0}{\partial E} \nabla_p E = \frac{\partial f_0}{\partial E} \vec{\upsilon} \qquad \left(\vec{\upsilon} \times \vec{B}\right) \bullet \vec{\upsilon} = 0\,!$$

$$-q\vec{\mathcal{E}} \bullet \nabla_p f_0 - q\left(\vec{\upsilon} \times \vec{B}\right) \bullet \nabla_p \left(\delta f\right) = -\delta f / \tau_m$$

a much more difficult equation to solve

solving the BTE with a B-field…

Recall that without the B-field: $-q\vec{\mathcal{E}} \bullet \nabla_p f_0 = -\delta f / \tau_m$

The solution was: $\delta f = \tau_m \left(-\dfrac{\partial f_0}{\partial E} \right) \vec{\upsilon} \bullet \vec{\mathcal{F}}$

So with a B-field: $-q\vec{\mathcal{E}} \bullet \nabla_p f_0 - q\left(\vec{\upsilon} \times \vec{B}\right) \bullet \nabla_p \left(\delta f\right) = -\delta f / \tau_m$

Assume a solution of the form: $\delta f = \tau_m \left(-\dfrac{\partial f_0}{\partial E} \right) \vec{\upsilon} \bullet \vec{G}$

And find the unknown vector, $\vec{G}$

the solution with a B-field…

$$\vec{G} = \frac{-q\vec{\mathcal{E}} - \left(q^2\tau_m/m^*\right)\left(\vec{B}\times\vec{\mathcal{E}}\right) - q\left(q\tau_m/m^*\right)^2\left(\vec{\mathcal{E}}\bullet\vec{B}\right)\vec{B}}{1+\left(\omega_c\tau_m\right)^2}$$

cyclotron frequency: $\omega_c = \dfrac{qB}{m^*}$ low B-field: $\omega_c\tau_m << 1$

(An electron gets only a little way along its orbit, and then it scatters.)

Assume a planar geometry with the electric field in the *x*-*y* plane and a z-directed, **small B-field** normal to the plane.

$$\vec{G} = -q\vec{\mathcal{E}} - \left(q^2\tau_m/m^*\right)\left(\vec{B}\times\vec{\mathcal{E}}\right)$$

G lies in the *x*-*y* plane.

the current equation…

$$\vec{J}_n = \frac{1}{A}\sum_{\vec{k}}(-q)\vec{\upsilon}\left(f_0 + \delta f\right) = \frac{1}{A}\sum_{\vec{k}}(-q)\vec{\upsilon}\left(\delta f\right) \qquad \delta f = \tau_m\left(-\frac{\partial f_0}{\partial E}\right)\vec{\upsilon} \bullet \vec{G}$$

$$\vec{J}_n = \sigma_S \vec{\mathcal{E}} - \sigma_S \mu_H \left(\vec{\mathcal{E}} \times \vec{B}\right)$$

$$\sigma_S = n_S q \mu_n \qquad \mu_H = \mu_n r_H$$

Hall mobility

$$\mu_n \equiv \frac{q\langle\langle\tau_m\rangle\rangle}{m^*} \qquad r_H \equiv \frac{\langle\langle\tau_m^2\rangle\rangle}{\langle\langle\tau_m\rangle\rangle^2}$$

Hall factor

the magnetoconductivity tensor…

$$\vec{J}_n = \sigma_S \vec{\mathcal{E}} - \sigma_S \mu_H \left(\vec{\mathcal{E}} \times \vec{B} \right)$$

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

the coupled current equations (B = 0)

From Lecture 5:

$$\vec{J} = \sigma\vec{\mathcal{E}} - s_T \nabla T_L$$

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

$$\vec{J}_Q = T_L s_T \vec{\mathcal{E}} - \kappa\nabla T_L$$

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

(diffusive transport)

Transport tensors were ***diagonal*** for parabolic energy bands.

the coupled current equations ($B \neq 0$)

$$\vec{J} = \left[\sigma\left(\vec{B}\right)\right]\vec{\mathcal{E}} - \left[s_T\left(\vec{B}\right)\right]\nabla T_L \qquad \vec{\mathcal{E}} = \left[\rho\left(\vec{B}\right)\right]\vec{J}_n + \left[S\left(\vec{B}\right)\right]\nabla T_L$$

$$\vec{J}_Q = T_L\left[s_T\left(\vec{B}\right)\right]\vec{\mathcal{E}} - \left[\kappa_0\left(\vec{B}\right)\right]\nabla T_L \qquad \vec{J}_Q = \left[\pi\left(\vec{B}\right)\right]\vec{J}_n - \left[\kappa_e\left(\vec{B}\right)\right]\nabla T_L$$

(diffusive transport)

Transport tensors now depend on the B-field and have off-diagonal terms.

outline

1) Introduction
2) The BTE
3) Solving the s.s. BTE
4) Transport coefficients
5) Magnetic fields
6) **Discussion**
7) Summary

matrix and vector notation

$$J_{nx} = \sigma_S \mathcal{E}_x - \sigma_S \mu_H B_z \mathcal{E}_y$$

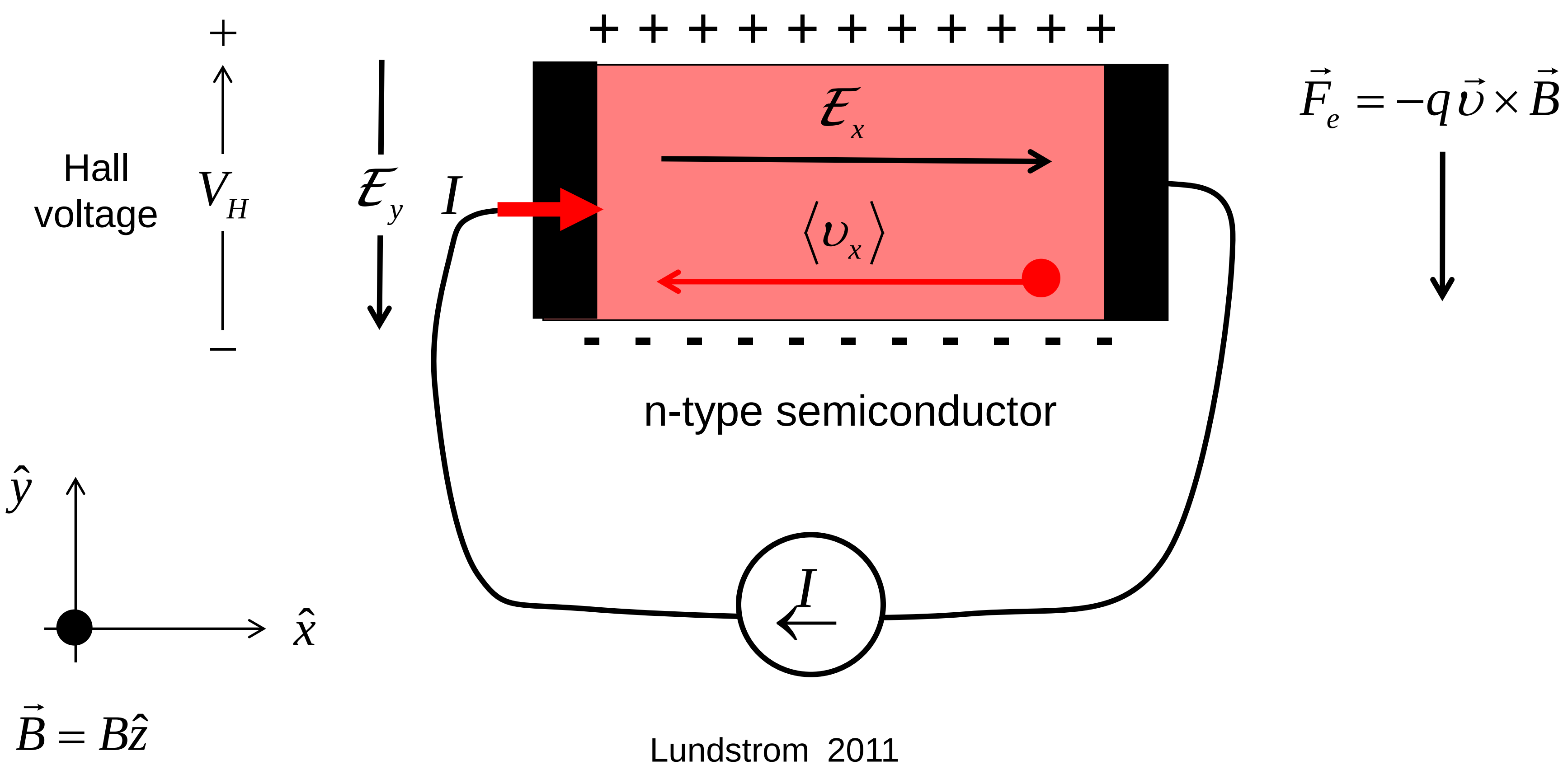
$$J_{ny} = \sigma_S \mathcal{E}_y + \sigma_S \mu_H B_z \mathcal{E}_x$$

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

$$\vec{J}_n = \sigma_S \vec{\mathcal{E}} - \sigma_S \mu_H \vec{\mathcal{E}} \times \vec{B}$$

physical picture

$$\vec{J}_n = \sigma_0 \vec{\mathcal{E}} - \sigma_0 \mu_H \vec{\mathcal{E}} \times \vec{B}$$



Lundstrom 2011

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the BTE

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

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

Six-dimensional integro-differential equation for *f*(*r*, *p*, *t*).

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

summary

1) Semi-classical transport assumes a bulk bandstructure with a slowly varying applied potential, so that quantum reflections can be ignored and position and momentum can both be precisely specified.

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

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

4) 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.

questions

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