

Week 10 Summary:

Boltzmann Transport Equation

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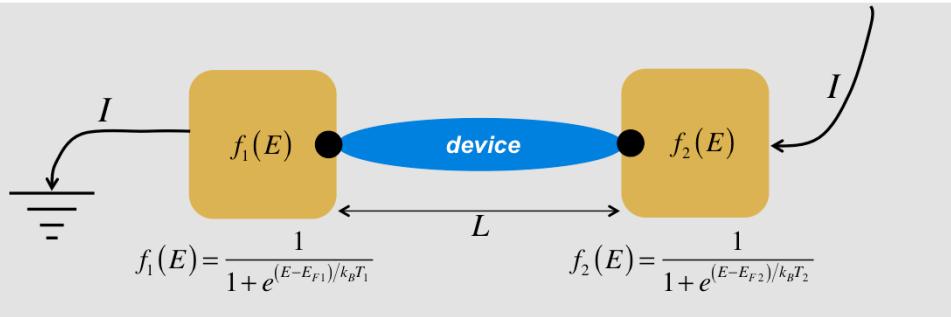


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nano to macro device

$$I = \frac{2q}{h} \int \mathcal{T}(E) M(E) (f_1 - f_2) dE$$



$$f_1(E) = \frac{1}{1 + e^{(E-E_{F1})/k_B T_1}}$$

$$f_2(E) = \frac{1}{1 + e^{(E-E_{F2})/k_B T_2}}$$

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TE coefficients (3D, bulk)

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

$$J_x^q = T \sigma S \mathcal{E}_x - \kappa_0 dT/dx$$

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

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

(diffusive transport)

$$\sigma = \int \sigma'(E) dE$$

$$\sigma'(E) = \frac{2q^2}{h} \lambda(E) \frac{M(E)}{A} \left(-\frac{\partial f_0}{\partial E} \right)$$

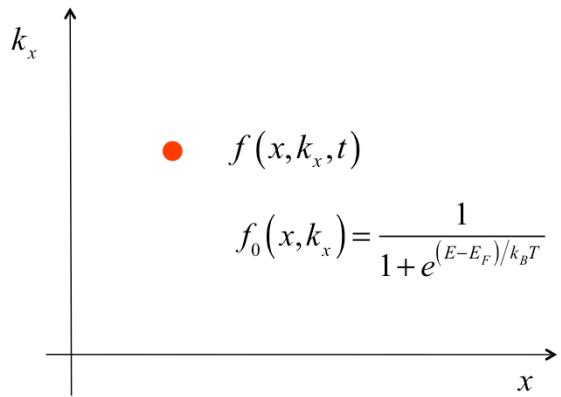
$$S = -\frac{k_B}{q} \int \left(\frac{E - E_F}{k_B T} \right) \sigma'(E) dE / \int \sigma'(E) dE$$

$$\pi = TS$$

$$\kappa_0 = T \left(\frac{k_B}{q} \right)^2 \int \left(\frac{E - E_F}{k_B T} \right)^2 \sigma'(E) dE$$

$$\kappa_e = \kappa_0 - \pi S \sigma$$

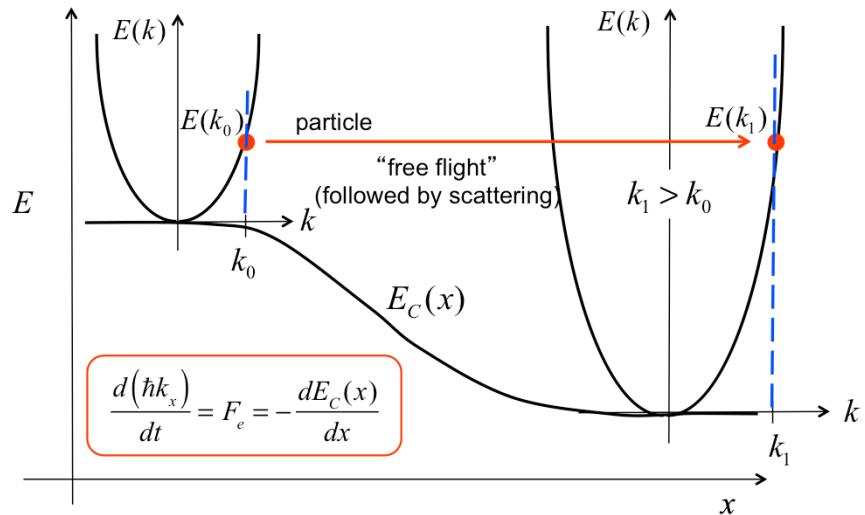
$$f(r, k, t)$$



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

semi-classical transport



$$\frac{d(\hbar k_x)}{dt} = F_e = -\frac{dE_C(x)}{dx}$$

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“semi-classical transport”

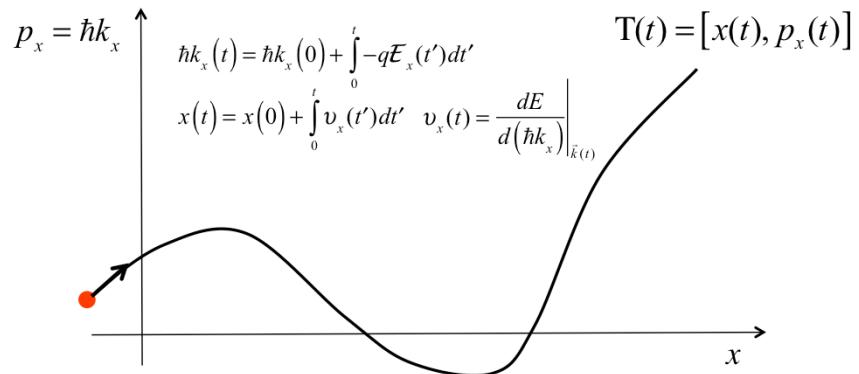
$$\frac{d(\hbar\vec{k})}{dt} = -\nabla_r E_c(\vec{r}) = -q\vec{E}(\vec{r}) \quad \left\{ \frac{d\vec{p}}{dt} = \vec{F}_e \right\}$$

$$\begin{aligned}\hbar\vec{k}(t) &= \hbar\vec{k}(0) + \int_0^t -q\vec{E}(t') dt' \\ \vec{v}_g(t) &= \frac{1}{\hbar} \nabla_k E[\vec{k}(t)] \\ \vec{r}(t) &= \vec{r}(0) + \int_0^t \vec{v}_g(t') dt'\end{aligned}$$

equations of motion for
“semi-classical transport”
 E_C varies slowly on the
scale of the electron’s
wavelength.

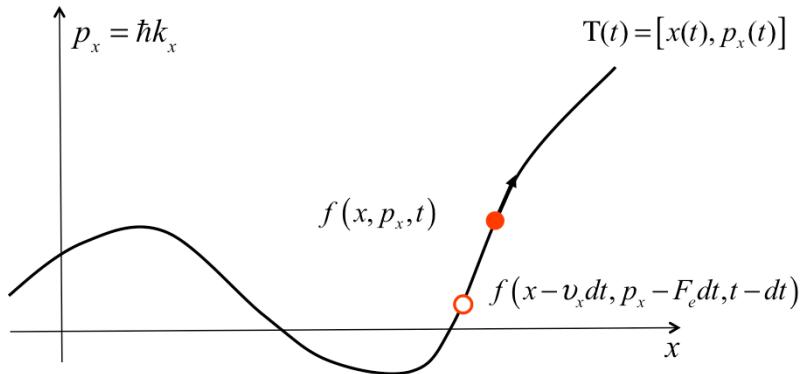
no effective mass!

trajectories in phase space



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Boltzmann Transport Equation (BTE)



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

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

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Boltzmann Transport Equation (BTE)

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

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

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

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

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

in and out-scattering

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

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

nondegenerate scattering operator

$$\hat{C}f(\vec{r}, \vec{p}, t) = \sum_{\vec{p}'} S(\vec{p}' \rightarrow \vec{p}) f(\vec{p}') [1 - f(\vec{p})] - \sum_{\vec{p}'} S(\vec{p} \rightarrow \vec{p}') f(\vec{p}) [1 - f(\vec{p}')] \quad \begin{array}{c} \nearrow \\ \text{probability that the state at } \vec{p}' \text{ is occupied} \end{array} \quad \begin{array}{c} \nwarrow \\ \text{probability that the state at } \vec{p} \text{ is empty} \end{array}$$

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

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

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

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steady-state BTE in 1D

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

RTA

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

$$|f_0(\vec{p})| \gg |\delta f(\vec{p})|$$

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

near-equilibrium

no B-fields for now

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

generalized force

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

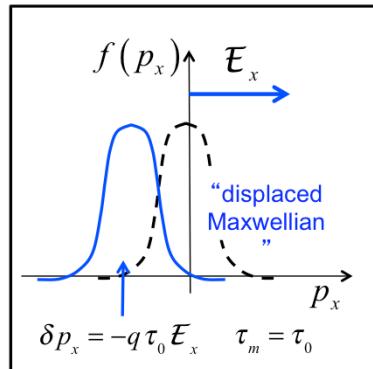
$$\vec{\mathcal{F}} = -\nabla_r F_n + T \left[E_C + E(k) - F_n \right] \nabla_r \left(\frac{1}{T} \right)$$

“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 .

another look at the solution...

$$\delta f = \left(\frac{\partial f_0}{\partial p_x} \right) q \tau_m \mathcal{E}_x \quad f = f_0 + \delta f = f_0 + \left(\frac{\partial f_0}{\partial p_x} \right) q \tau_m \mathcal{E}_x$$



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now what?

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

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

moments

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

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

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

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

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

re-cap

BTE:

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

$$\hat{C}f(\vec{r}, \vec{p}, t) = \sum_{p'} S(\vec{p}', \vec{p}) f(\vec{p}') [1 - f(\vec{p})] - \sum_{p'} S(\vec{p}, \vec{p}') f(\vec{p}) [1 - f(\vec{p}')]$$

RTA:

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

Solution:

$$\delta f = \tau_m \left(-\frac{\partial f_0}{\partial E} \right) \vec{v} \bullet \vec{\mathcal{F}} \quad \vec{\mathcal{F}} = -\nabla_r F_n + T [E_c + E(k) - F_n] \nabla_r \left(\frac{1}{T} \right)$$

current



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

2D 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.

2D 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....

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

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

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 ?

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

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

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

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

drift current

$$\delta f = \tau_m \left(-\frac{\partial f_0}{\partial E} \right) v_x \mathcal{F}_x \quad \text{generalized force in } x\text{-direction}$$

$$J_{nx}(\vec{r}) = \frac{1}{A} \sum_{\vec{k}} (-q) v_x \delta f(\vec{r}, \vec{k}) \quad \text{2D current density in } x\text{-direction}$$

$$\mathcal{F}_x = -q \mathcal{E}_x \quad (\text{for the drift current})$$

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

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drift current (ii)

$$J_{nx}(\vec{r}) = \sigma_n \mathcal{E}_x$$

$$\sigma_s = n_s q \mu_n$$

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

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

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

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diffusion current

$$\delta f = \tau_m \left(-\frac{\partial f_0}{\partial E} \right) v_x \mathcal{F}_x \quad \text{generalized force in } x\text{-direction}$$

$$J_{nx}(\vec{r}) = \frac{1}{A} \sum_{\vec{k}} (-q) v_x \delta f(\vec{r}, \vec{k}) \quad \text{2D current density in } x\text{-direction}$$

$$\mathcal{F}_x = -k_B T \frac{1}{n_S} \frac{dn_S}{dx} \quad \text{(for the diffusion current)}$$

$$J_{nx}(\vec{r}) = -q D_n \frac{dn_S}{dx} \quad \text{result}$$

diffusion current (ii)

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

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

drift and diffusion (non-degenerate)

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

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

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energy dependent scattering time (2D)

$$\tau_0 \rightarrow \langle\langle \tau_m \rangle\rangle = \frac{\langle v_x^2 \tau_m \rangle}{\langle v_x^2 \rangle} \quad (v^2 = v_x^2 + v_y^2 \rightarrow v_x^2 = v^2/2)$$

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

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

“power law scattering”

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

Mathiessen's Rule

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

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

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

Mathiessen's Rule

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

$$s_1 = s_2 = s$$

transport tensors

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

$$\sigma_{ij} = \frac{1}{\Omega} \sum_k q^2 v_i v_j \tau_m \left(-\frac{\partial f_0}{\partial E} \right) \quad [s_T]_{ij} = \frac{k_B q}{\Omega} \sum_k \left(\frac{E_C + E(k) - F_n}{k_B T_L} \right) v_i v_j \tau_m \left(-\frac{\partial f_0}{\partial E} \right)$$

the BTE with a B-field...

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

steady-state with RTA:

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

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

spatially uniform:

$$-q\vec{E} \bullet \nabla_p f - q(\vec{v} \times \vec{B}) \bullet \nabla_p f = -\delta f / \tau_m$$

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

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the current equation...

$$\vec{J}_n = \sigma_s \vec{E} - \sigma_s \mu_H (\vec{E} \times \vec{B})$$

$$\begin{aligned}\sigma_s &= n_s q \mu_n & \mu_H &= \mu_n r_H & \text{Hall mobility} \\ \mu_n &\equiv \frac{q \langle\langle \tau_m \rangle\rangle}{m^*} & r_H &\equiv \frac{\langle\langle \tau_m^2 \rangle\rangle}{\langle\langle \tau_m \rangle\rangle^2} & \text{Hall factor}\end{aligned}$$

the magnetoconductivity tensor...

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

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

$$J_i = \sigma_{ij}(\vec{B}) \mathcal{E}_j$$

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 ($B \neq 0$)

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

$$\vec{J}_\varrho = T_L[s_T(\vec{B})]\vec{\mathcal{E}} - [\kappa_0(\vec{B})]\nabla T_L \quad \vec{J}_\varrho = [\pi(\vec{B})]\vec{J}_n - [\kappa_e(\vec{B})]\nabla T_L$$

(diffusive transport)

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

small B-field criterion

$$\omega_c \tau_m \ll 1$$

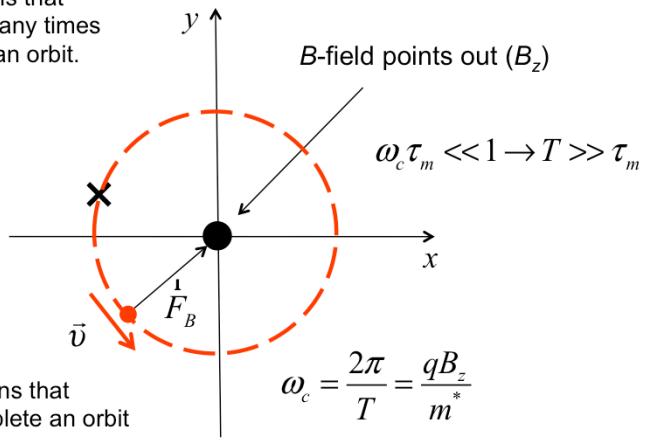
$$\mu_n B_z \ll 1$$

$$\omega_c = \frac{qB}{m^*} \quad \omega_c \tau_m = \frac{q\tau_m B}{m^*} = \mu_n B$$

What does this mean physically?

small B-field: physical meaning

“Low B-field” means that electrons scatter many times before completing an orbit.



“High B-field” means that electrons can complete an orbit without scattering.

some numbers (III-V modulation-doped)

InAlAs/InGaAs

$$T_L = 300\text{K}$$

$$\mu_n \approx 10,000 \text{ cm}^2/\text{V-s}$$

$$B_z = 2,000 \text{ Gauss}$$

$$B_z = 0.2 \text{ Tesla}$$

$$\mu_n B_z \approx 0.2 < 1$$

InAlAs/InGaAs

$$T_L = 77\text{K}$$

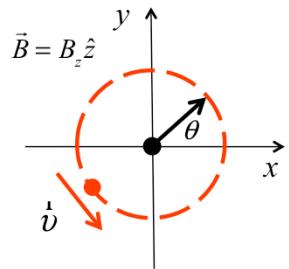
$$\mu_n \approx 100,000 \text{ cm}^2/\text{V-s}$$

$$B_z = 2,000 \text{ Gauss}$$

$$B_z = 0.2 \text{ Tesla}$$

$$\mu_n B_z \approx 2 > 1$$

high B-fields



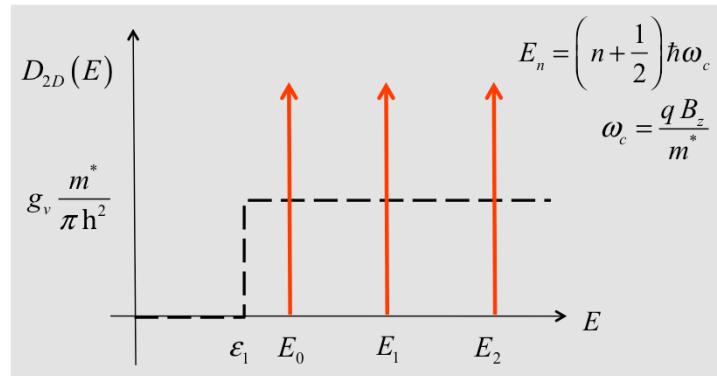
$$\cos \theta(t) = \cos \theta(0) e^{i\omega_c t}$$

harmonic oscillator:

Quantum mechanically:

$$E_n = \left(n + \frac{1}{2} \right) \hbar \omega_c \quad \text{“Landau levels”}$$

effect on DOS

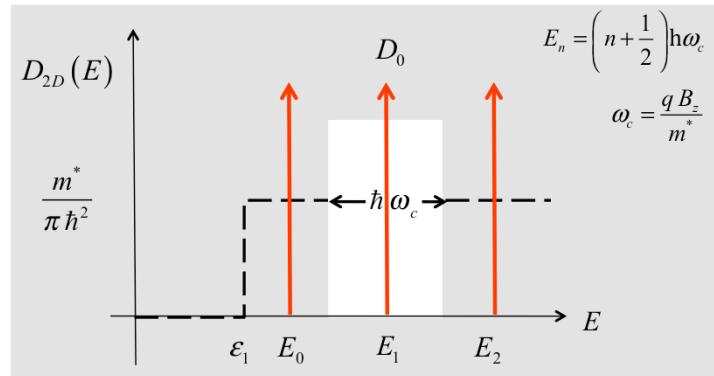


$$D_{2D}(E, B_z) = D_0 \sum_{n=0}^{\infty} \delta \left[E - \epsilon_1 - \left(n + \frac{1}{2} \right) \hbar \omega_c \right]$$

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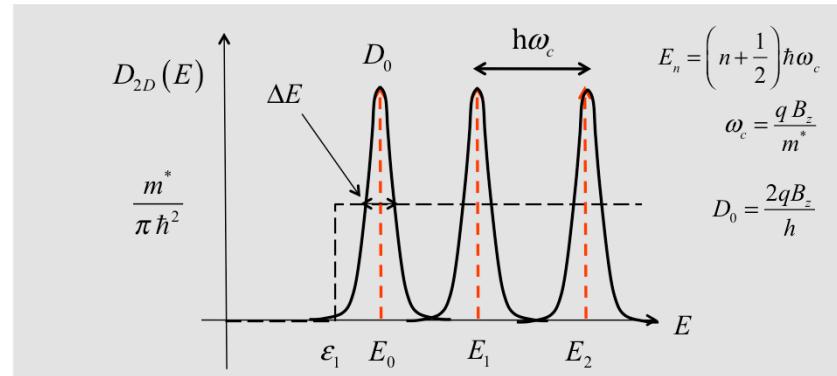
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degeneracy of Landau levels



$$D_0 = \hbar \omega_c \times \frac{m^*}{\pi \hbar^2} = \frac{2qB_z}{h}$$

broadening of Landau levels



$$\Delta E \Delta t = \hbar$$

$$\Delta E = \frac{\hbar}{\tau}$$

to observe Landau levels: $\hbar\omega_c \gg \Delta E \rightarrow \omega_c \tau \gg 1$

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SdH oscillations

Longitudinal
magneto-
resistance

“Shubnikov-deHaas
(SdH) oscillations”

quantized Hall voltage
zero longitudinal resistance, R_{xx}

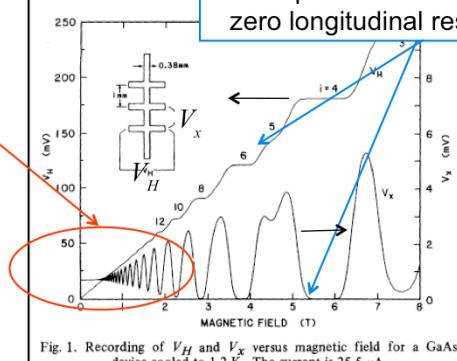


Fig. 1. Recording of V_H and V_x versus magnetic field for a GaAs device cooled to 1.2 K. The current is 25.5 μ A.

M.E. Cage, R.F. Dziuba, and B.F. Field, “A Test of the Quantum Hall Effect as a Resistance Standard,” *IEEE Trans. Instrumentation and Measurement*, Vol. IM-34, pp. 301-303, 1985

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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.

summary

- 5) 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.

about the BTE

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.