ECE-656: Fall 2009

Lecture 10: The drift-diffusion equation

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outline

1) **Transport in the bulk**

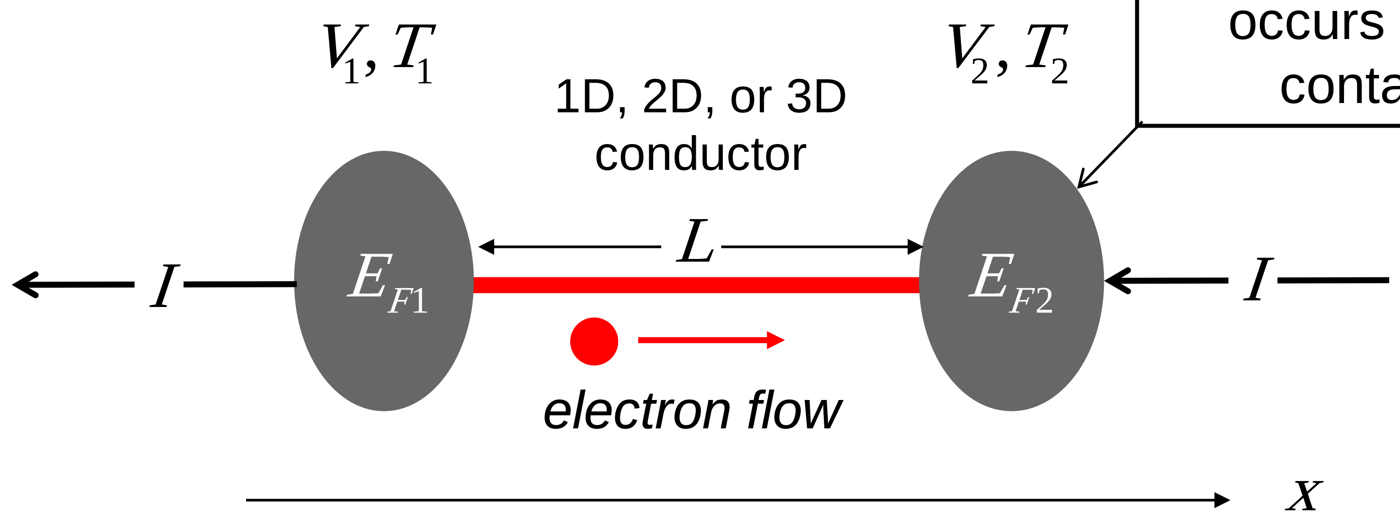
2) The DD equation

3) Indicial notation

4) DD equation with B-field

current flow in a nanoresistor

inelastic scattering occurs in the contacts



$$I_x = -\frac{2q}{h}\int_{\varepsilon_1}^{\infty} T(E)M(E)\left(f_1 - f_2\right)dE$$

$$T(E) = \frac{\lambda(E)}{\lambda(E) + L}$$ (elastic scattering)

$$\left\{ f_1 = f_2 = f_0 \right\}$$

transport regimes and driving forces

1) Ballistic: $\lambda >> L,\ T \approx 1$

2) Quasi-Ballistic: $\lambda \approx L,\ T < 1$

3) Diffusive: $\lambda << L,\ T << 1$

bulk transport

Driving "forces" for current

$$\Delta E_F = -q\Delta V = -q\left(V_2 - V_1\right)$$

$$\Delta T = T_2 - T_1$$

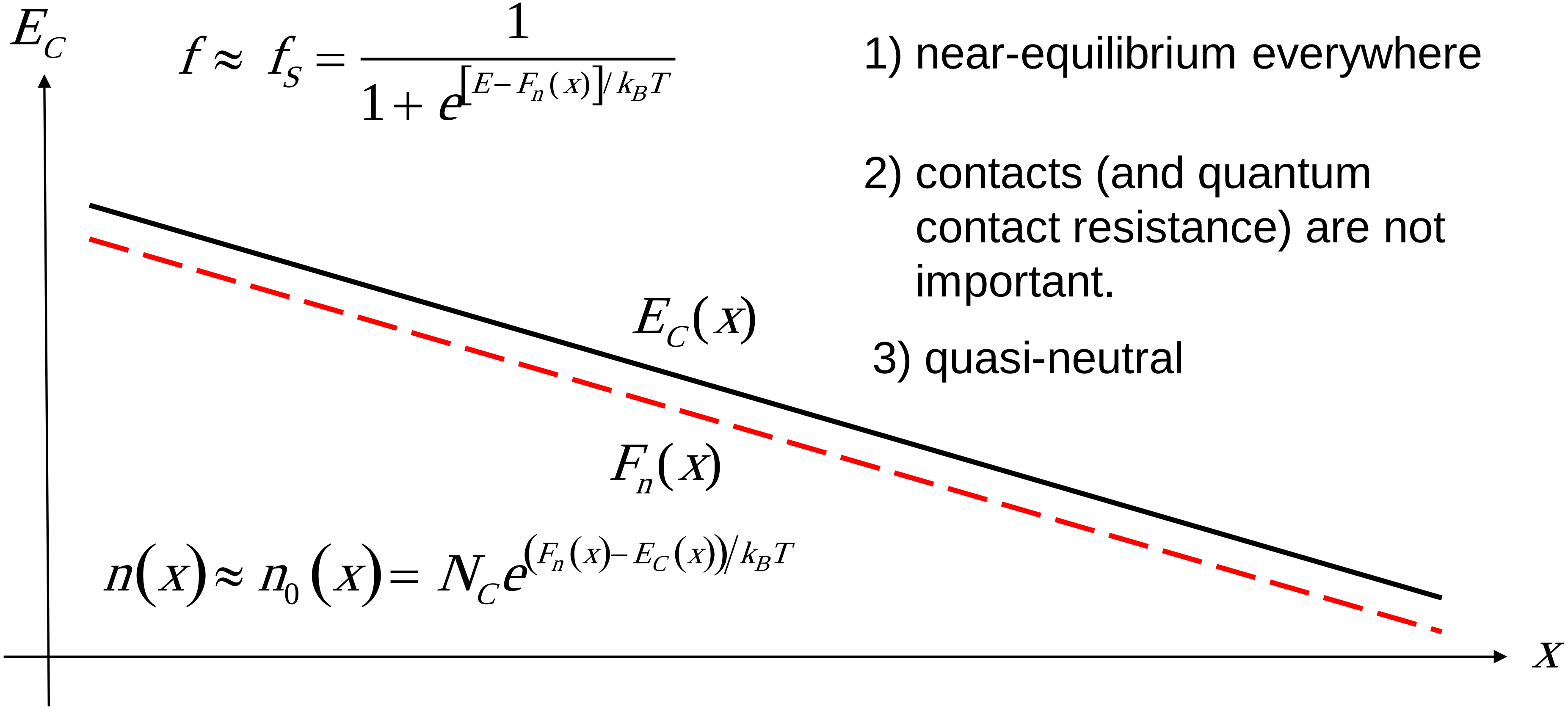
bulk transport

$$f \approx f_S = \frac{1}{1 + e^{\left[E - F_n(x)\right]/k_B T}}$$

1) near-equilibrium everywhere

2) contacts (and quantum contact resistance) are not important.

3) quasi-neutral



$$n(x) \approx n_0(x) = N_C e^{\left(F_n(x) - E_C(x)\right)/k_B T}$$

bulk transport

$$I_x = \left\{ -\frac{2q^2}{h} \int T(E)\left(-\frac{\partial f_0}{\partial E}\right) M(E)\, dE \right\} V \qquad T(E) = \frac{\lambda(E)}{\lambda(E)+L} \approx \frac{\lambda(E)}{L}$$

$$I_x = \left\{ -\frac{2q^2}{h} \int \lambda(E)\left(-\frac{\partial f_0}{\partial E}\right) M(E)\, dE \right\} \frac{V}{L}$$

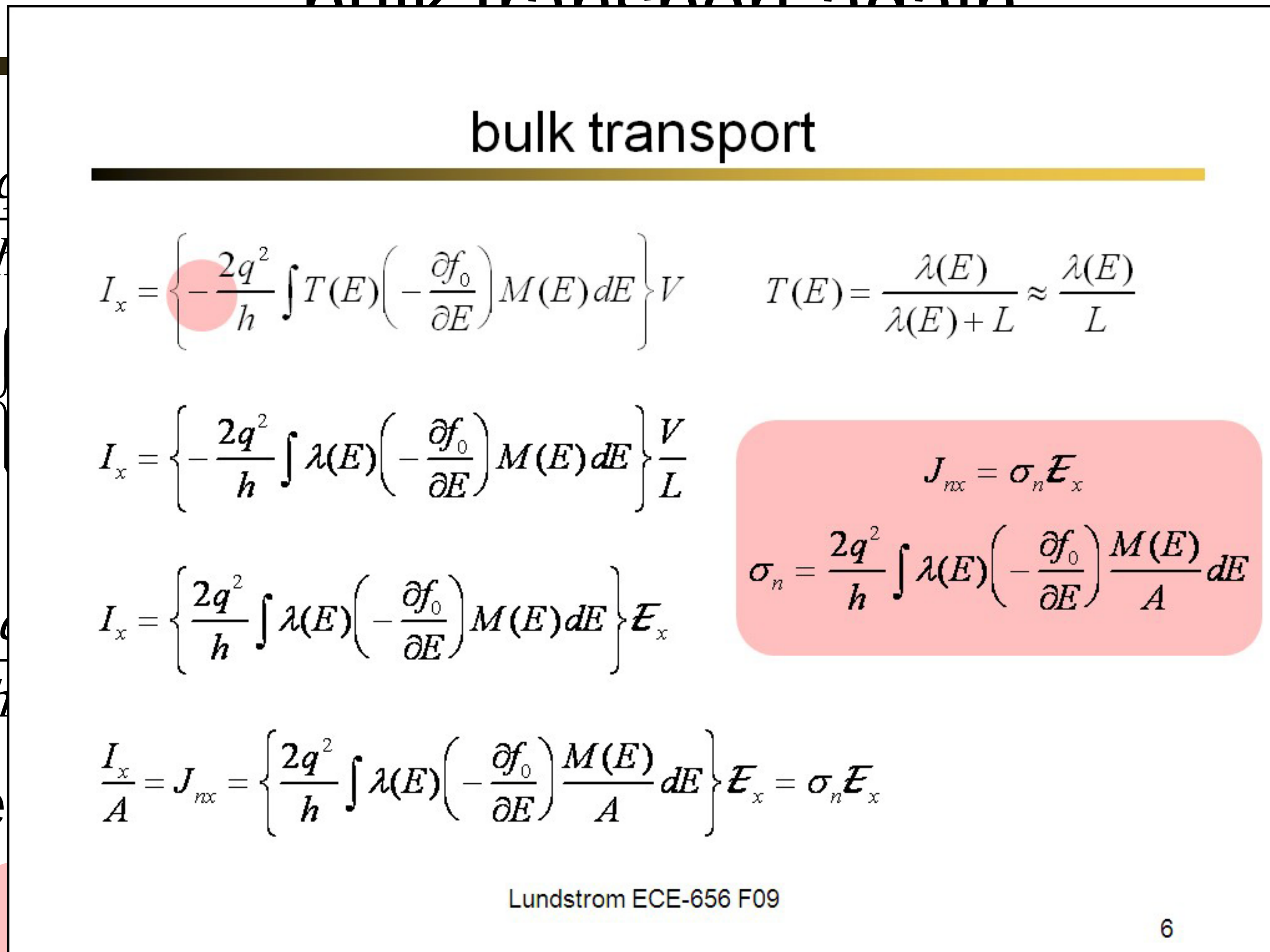
$$I_x = \left\{ \frac{2q^2}{h} \int \lambda(E)\left(-\frac{\partial f_0}{\partial E}\right) M(E)\, dE \right\} \mathcal{E}_x$$

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

$$\sigma_n = \frac{2q^2}{h} \int \lambda(E)\left(-\frac{\partial f_0}{\partial E}\right) \frac{M(E)}{A}\, dE$$

$$\frac{I_x}{A} = J_{nx} = \left\{ \frac{2q^2}{h} \int \lambda(E)\left(-\frac{\partial f_0}{\partial E}\right) \frac{M(E)}{A}\, dE \right\} \mathcal{E}_x = \sigma_n \mathcal{E}_x$$

bulk transport again



bulk transport

$$I_x = \left\{ -\frac{2q^2}{h} \int T(E) \left(-\frac{\partial f_0}{\partial E} \right) M(E)\, dE \right\} V \qquad T(E) = \frac{\lambda(E)}{\lambda(E)+L} \approx \frac{\lambda(E)}{L}$$

$$I_x = \left\{ -\frac{2q^2}{h} \int \lambda(E) \left(-\frac{\partial f_0}{\partial E} \right) M(E)\, dE \right\} \frac{V}{L}$$

$$I_x = \left\{ \frac{2q^2}{h} \int \lambda(E) \left(-\frac{\partial f_0}{\partial E} \right) M(E)\, dE \right\} \mathcal{E}_x$$

$$\frac{I_x}{A} = J_{nx} = \left\{ \frac{2q^2}{h} \int \lambda(E) \left(-\frac{\partial f_0}{\partial E} \right) \frac{M(E)}{A}\, dE \right\} \mathcal{E}_x = \sigma_n \mathcal{E}_x$$

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

$$\sigma_n = \frac{2q^2}{h} \int \lambda(E) \left(-\frac{\partial f_0}{\partial E} \right) \frac{M(E)}{A}\, dE$$

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$I_x = -\frac{2q}{h}$ … of the

$= \frac{2q}{h}$ …

$I_x = \frac{2q}{h}$ …

We … ow bias:

$J_{nx} = \sigma_n \frac{\quad}{dx}$ … $\sigma_n = \frac{\quad}{h} \int \lambda(E) \left(\frac{\quad}{\partial E} \right) \frac{\quad}{A}\, dE$

gradients in F_n and T

$$I_x(E) = -\frac{2q}{h}T(E)M(E)\left(f_1 - f_2\right) \qquad I_x = \int I_x(E)\,dE$$

$$\left(f_1 - f_2\right) \approx \left(-\frac{\partial f_0}{\partial E}\right)\left(-\Delta F_n\right) - \left(-\frac{\partial f_0}{\partial E}\right)\frac{\left(E - E_F\right)}{T}\Delta T$$

$$I_x(E) = -\frac{2q}{h}\frac{\lambda(E)}{dx}M(E)\left(-\frac{\partial f_0}{\partial E}\right)\left\{\left(-\Delta F_n\right) - \frac{\left(E - E_F\right)}{T}\Delta T\right\}$$

$$J_{nx}(E) = \frac{2q}{h}\lambda(E)\frac{M(E)}{A}\left(-\frac{\partial f_0}{\partial E}\right)\left\{\frac{dF_n}{dx} + \frac{\left(E - E_F\right)}{T}\frac{dT}{dx}\right\}$$

gradients in F_n and T

$$J_{nx}(E) = \frac{2q}{h}\lambda(E)\frac{M(E)}{A}\left(-\frac{\partial f_0}{\partial E}\right)\left\{\frac{dF_n}{dx} + \frac{(E-E_F)}{T}\frac{dT}{dx}\right\}$$

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

$$\frac{2q}{h}\lambda(E)\frac{M(E)}{A}\left(-\frac{\partial f_0}{\partial E}\right)\left\{\frac{(E-E_F)}{T}\right\} = \left(\frac{k_B}{q}\right)\sigma_n(E)\left\{\frac{(E-E_F)}{k_B T}\right\}$$

$$J_{nx}(E) = \sigma_n(E)\frac{d(F_n/q)}{dx} + \left(\frac{k_B}{q}\right)\sigma_n(E)\left(\frac{E-E_F}{k_B T}\right)\frac{dT}{dx} \qquad J_{nx} = \int J_{nx}(E)\,dE$$

$$J_{nx} = \sigma_n\frac{d(F_n/q)}{dx} + [SG]\frac{dT}{dx}$$

gradients in F_n and T

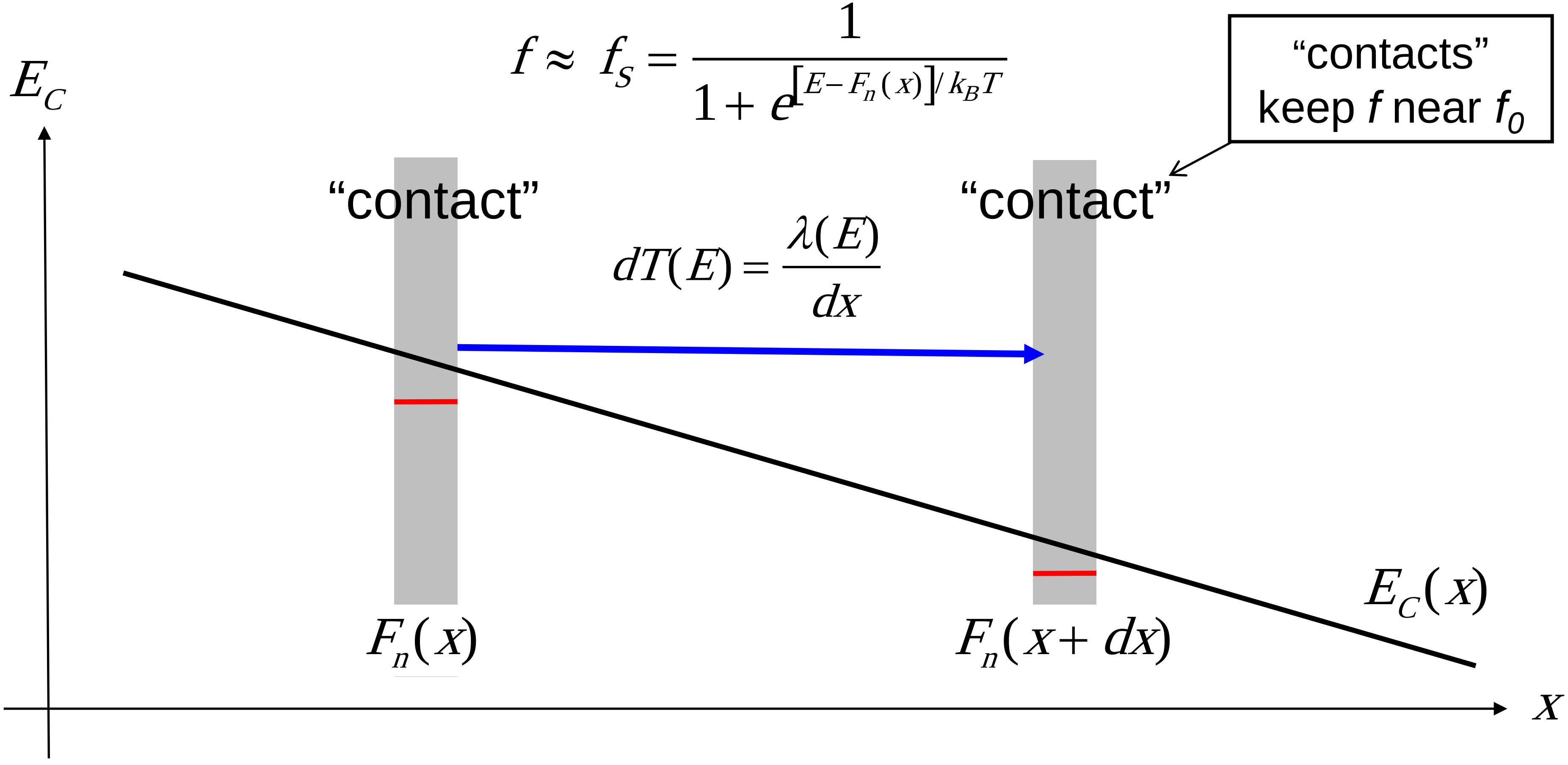
$$J_{nx} = \sigma_n \frac{d\left(F_n/q\right)}{dx} + [SG]\frac{dT}{dx}$$

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

$$[SG] = +\left(\frac{k_B}{q}\right)\int \sigma_n(E)\left(\frac{E-E_F}{k_B T}\right) dE$$

the Landauer picture for bulk transport

$$f \approx f_S = \frac{1}{1 + e^{[E - F_n(x)]/k_B T}}$$



outline

1) Transport in the bulk

2) The DD equation

3) Indicial notation

4) DD equation with B-field

gradients in F_n and T

$\sigma_n(E) = \frac{2}{\ }$

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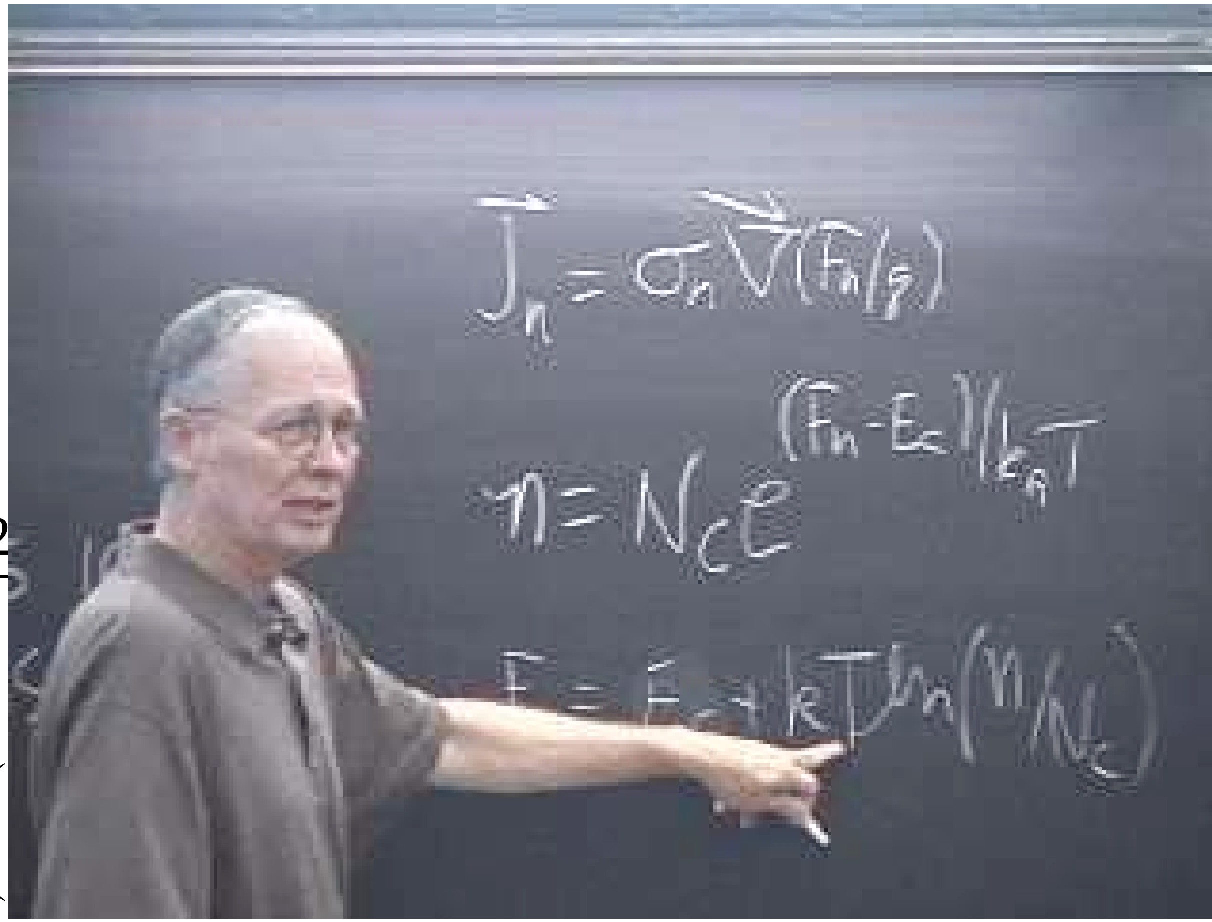
$[SG] = +\Big($



constant temperature

$$J_{nx} = \sigma_n \frac{d(F_n/q)}{dx} = \sigma_n \mathcal{E}_x + \sigma_n \frac{k_B T}{q} \frac{1}{n} \frac{dn}{dx}$$

$$n(x) = N_C \, e^{(F_n(x) - E_C(x))/k_B T}$$ (Boltzmann statistics)

$$F_n(x) = E_C(x) + k_B T \ln\left[n(x)/N_C \right]$$

$$\frac{dF_n(x)}{dx} = \frac{dE_C(x)}{dx} + k_B T \frac{N_C}{n(x)} \frac{dn(x)/dx}{N_C} = q\mathcal{E}_x + \frac{1}{n} \frac{dn}{dx}$$

DD equation

$$J_{nx} = \sigma_n \mathcal{E}_x + \sigma_n \frac{k_B T}{q} \frac{1}{n} \frac{dn}{dx}$$

$$\sigma_n = n(x) q \mu_n$$

$$J_{nx} = n(x) q \mu_n \mathcal{E}_x + k_B T \mu_n \frac{dn}{dx}$$

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

$$J_{nx} = n(x) q \mu_n \mathcal{E}_x + q D_n \frac{dn}{dx}$$

-diffusive ($\lambda \ll L$)

-constant temperature

-non-degenerate

DD equation: questions

1) What do the DD equation and Einstein relation look like in the degenerate limit?

2) What is the general DD equation (and Einstein relation) in terms of FD integrals?

3) How does dimensionality affect the result? (i.e. what does the DD equation look like in 1D?)

4) How does bandstructure affect the result? (i.e. what is the DD equation for graphene?)

$$J_{nx} = n(x) q \mu_n \mathcal{E}_x + q D_n \frac{dn}{dx}$$

-diffusive ($\lambda \ll L$)

-constant temperature

-non-degenerate

DD equation with temperature gradients

$$J_{nx} = \sigma_n \frac{d(F_n/q)}{dx} + [SG]\frac{dT}{dx}$$

$$J_{nx} = n(x) q \mu_n \mathcal{E}_x + qD_n \frac{dn}{dx}$$

$$[SG] = \left(\frac{k_B}{q}\right) \int \sigma_n(E) \left(\frac{E - E_F}{k_B T}\right) dE$$

non-degenerate:

$$[SG] = \sigma_0 \left(\frac{k_B}{q}\right) \left[\ln(N_C/n) + 2\right]$$

(All signs assume electron transport)

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the equations

$$J_x = \sigma \frac{d(F_n/q)}{dx} + [SG]\frac{dT}{dx}$$

$$J_x^Q = -T[SG]\frac{d(F_n/q)}{dx} - \kappa_0 \frac{dT}{dx}$$

If the carrier density is uniform, then: $\frac{d(F_n/q)}{dx} = \mathcal{E}_x$

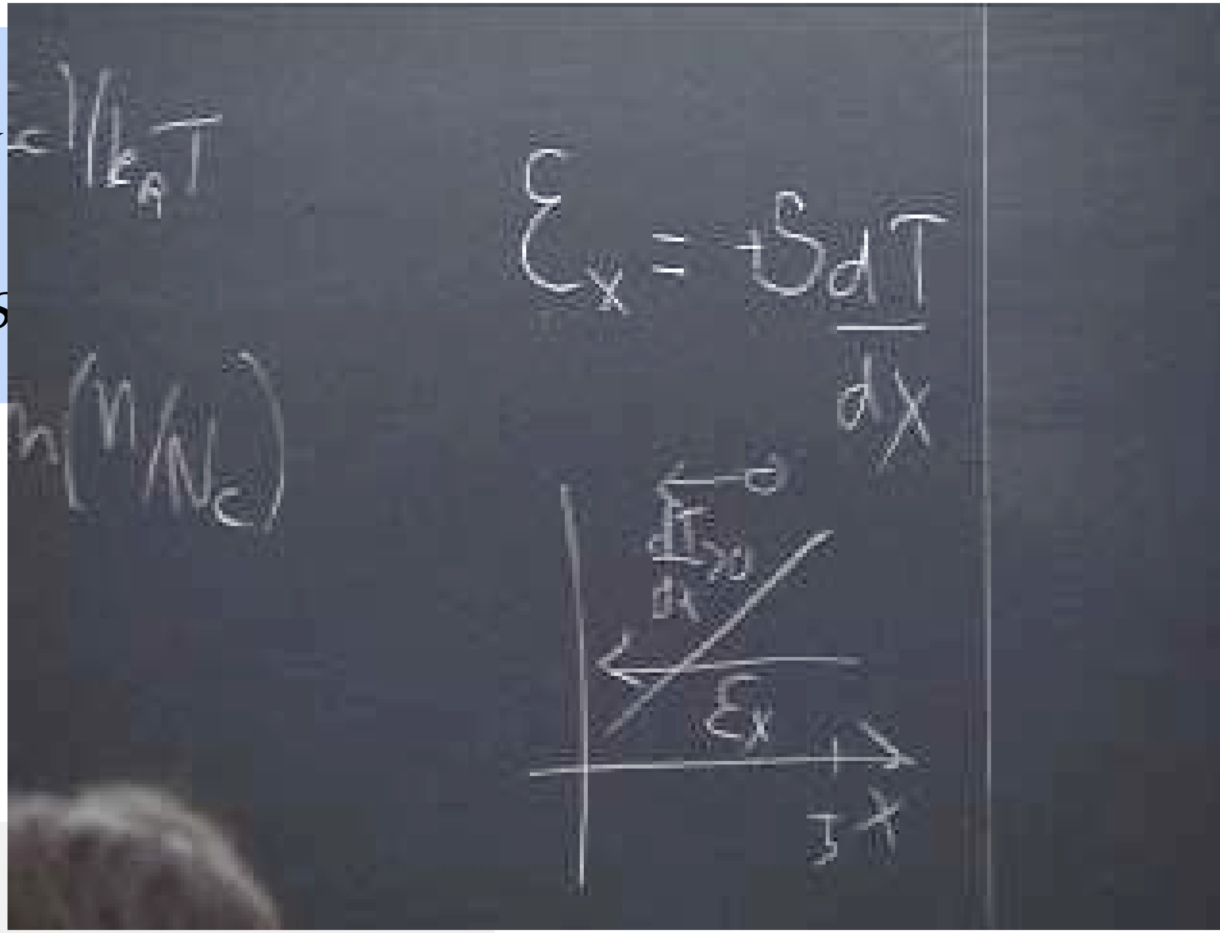
$$J_x = \sigma_n \mathcal{E}_x + [SG]\frac{dT}{dx}$$

$$J_x^Q = -T[SG]\mathcal{E}_x - \kappa_0 \frac{dT}{dx}$$

the inverted equations

$J_x = \sigma \mathcal{E}_x$ ...

$J_x^Q = -T[S$ ...



... $\vec{\nabla} T$

... $\vec{\nabla} T$

$\mathcal{E}_x = \rho J_x$ ...

$J_x^Q = \pi J_x$ ...

...sport

...ors,

$\rho = 1/\sigma$ ...

$\pi = TS \qquad \kappa_e = \left(\kappa_0 - T\frac{[SG]}{\sigma} \right)$

tensors

$$\vec{J} = [\sigma]\vec{\mathcal{E}}$$

$$\begin{bmatrix} J_x \\ J_y \\ J_z \end{bmatrix} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} \begin{bmatrix} \mathcal{E}_x \\ \mathcal{E}_y \\ \mathcal{E}_z \end{bmatrix}$$

$$J_i = \sum_{j=1}^{3} \sigma_{ij}\mathcal{E}_j$$ “indicial notation”

$$J_i = \sum_{j=1}^{j=3} \sigma_{ij}\mathcal{E}_j \equiv \sigma_{ij}\mathcal{E}_j$$ “summation convention”

coupled current equations

$$\vec{\mathcal{E}} = [\rho]\vec{J} + [S]\vec{\nabla}T$$

$$\vec{J}_Q = [\pi]\vec{J} - [\kappa_e]\vec{\nabla}T$$

$$\mathcal{E}_i = \rho_{ij}J_j + S_{ij}\partial_j T$$

$$J_i^Q = \pi_{ij}J_j - \kappa_{ij}^e\partial_j T$$

For isotropic materials, the tensors are diagonal.

$$\mathcal{E}_i = \rho_0 J_j + S_0\partial_j T$$

$$J_i^Q = \pi_0 J_j - K_0^e\partial_j T$$

$$[\rho] = \rho_0\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

"Kronecker delta"

$$\rho_{ij} = \rho_0\delta_{ij}$$

$$\delta_{ij} = 1 \quad (i = j)$$

$$= 0 \quad (i \neq j)$$

form of the tensors

$$\mathcal{E}_i = \rho_0 J_j + S_0 \partial_j T$$

$$J_i^Q = \pi_0 J_j - \kappa_0^e \partial_j T$$

For isotropic materials, such as common, cubic semiconductors, the tensors are diagonal (under low-fields).

For a given crystal structure, the form of the tensors (i.e. which elements are zero and which are non-zero) can be deduced from symmetry arguments. (See Smith, Janak, and Adler, Chapter 4.)

The transport tensors can be readily computed by solving the Boltzmann Transport Equation (BTE).

magnetic fields

$$\mathcal{E}_i = \rho_{ij}\left(\vec{B}\right)J_j + S_{ij}\left(\vec{B}\right)\partial_j T$$

$$J_i^Q = \pi_{ij}\left(\vec{B}\right)J_j - \kappa_{ij}^e\left(\vec{B}\right)\partial_j T$$

Magnetic fields introduce off-diagonal elements, which lead to effects like the Hall effect.

The B-field transport tensors can be computed by solving the Boltzmann Transport Equation (BTE).

dealing with small magnetic fields

$$\mathcal{E}_i = \rho_{ij}\left(\vec{B}\right) J_j$$

$$\rho_{ij}\left(\vec{B}\right) = \rho_{ij}\left(\vec{B}=0\right) + \frac{\partial \rho_{ij}}{\partial B_k} B_k + \frac{1}{2}\frac{\partial^2 \rho_{ij}}{\partial B_k \partial B_l} B_k B_l + \ldots$$

$$\rho_{ij}\left(\vec{B}\right) = \rho_{ij} + \rho_{ijk} B_k + \rho_{ijkl} B_k B_l + \ldots$$

cubic semiconductors

$$\rho_{ij} = \rho_0 \delta_{ij}$$

$$\rho_{ijkl} \quad \left(\rho_{\alpha\alpha\alpha\alpha} \quad \rho_{\alpha\alpha\beta\beta} \quad \rho_{\alpha\beta\alpha\beta} \quad \rho_{\alpha\beta\beta\alpha}\right)$$

$$\rho_{ijk} = \rho_1 \varepsilon_{ijk} = \rho_0 \mu_H \varepsilon_{ijk}$$

(alternating unit tensor)

alternating unit tensor

$$\rho_{ijk} = \rho_1 \varepsilon_{ijk} = \rho_0 \mu_H \varepsilon_{ijk}$$

$$\vec{C} = \vec{E} \times \vec{B}$$

$$\vec{C} = \begin{bmatrix} \hat{x} & \hat{y} & \hat{z} \\ \mathcal{E}_x & \mathcal{E}_y & \mathcal{E}_z \\ B_x & B_y & B_z \end{bmatrix} = \hat{x}\left(\mathcal{E}_y B_z - \mathcal{E}_z B_y\right) + \ldots$$

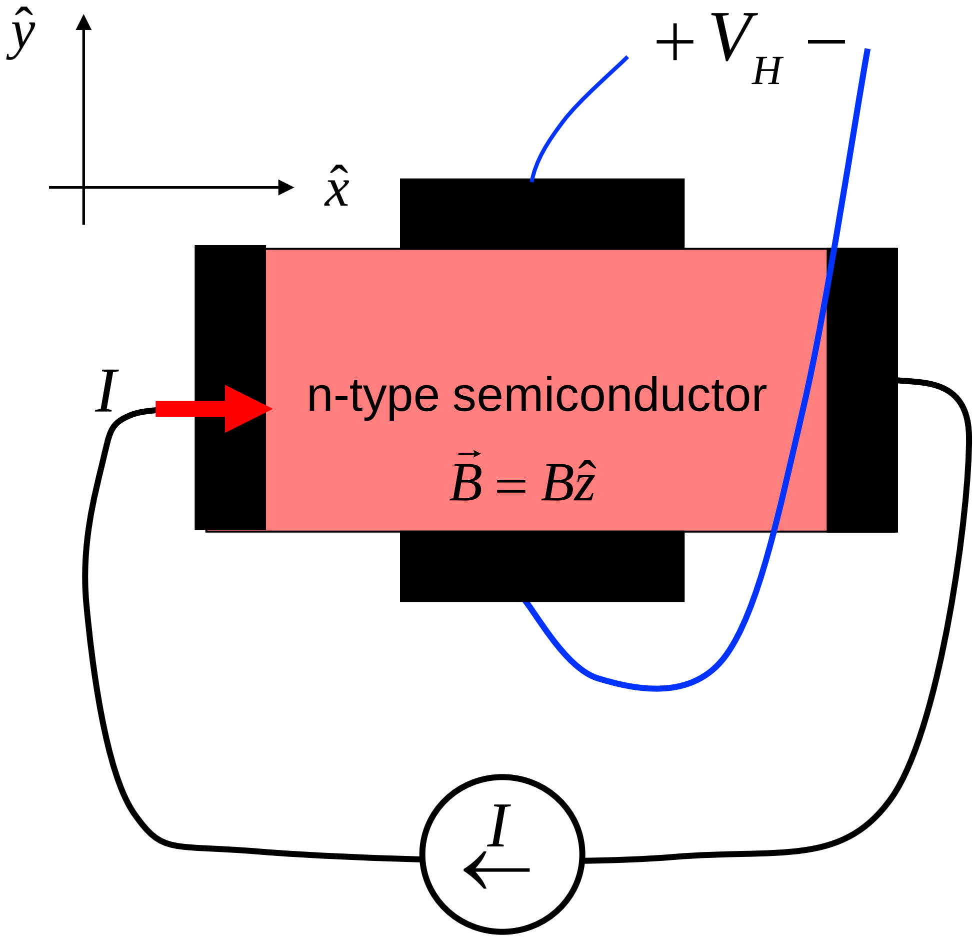
$$C_i = \varepsilon_{ijk} \mathcal{E}_j B_k$$

$$\begin{aligned} C_x &= \varepsilon_{xjk} \mathcal{E}_j B_k \\ &= \varepsilon_{xyz} \mathcal{E}_y B_z + \varepsilon_{xzy} \mathcal{E}_z B_y \\ &= \mathcal{E}_y B_z - \mathcal{E}_z B_y \end{aligned}$$

✓

$$\begin{aligned} \varepsilon_{ijk} &= +1\left(i, j, k \text{ cyclic}\right) \\ &= -1\left(i, j, k \text{ anti-cyclic}\right) \\ &= 0\left(\text{otherwise}\right) \end{aligned}$$

Example: "Hall effect"



current in x-direction:

$$I_x$$

B-field in z-direction:

$$\vec{B} = B\hat{z}$$

Hall voltage measured in the y-direction:

$$V_H < 0 \quad (\text{n-type})$$

The Hall effect was discovered by Edwin Hall in 1879 and is widely used to characterize electronic materials. It also finds use magnetic field sensors.

Example: Hall effect

$$\mathcal{E}_i = \rho_{ij} J_j + \rho_{ijk} J_i B_k + \ldots + S_{ij} \partial_j T \qquad \partial_j T = 0 \quad \text{(isothermal)}$$

$$\mathcal{E}_i = \rho_0 J_i + \rho_1 \varepsilon_{ijk} J_j B_k$$

(cubic semiconductor)

$$\mathcal{E}_y = \rho_0 J_y + \rho_1 \varepsilon_{yxz} J_x B_z$$

"measures" the carrier density

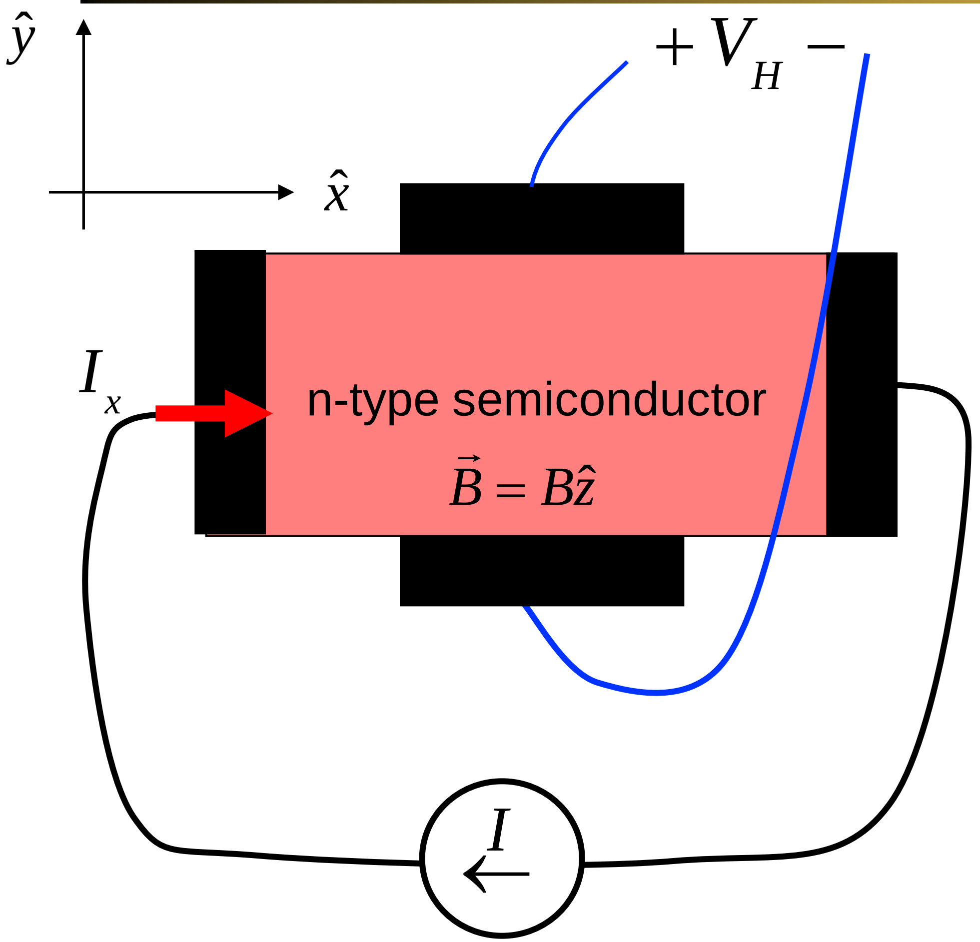
$$\mathcal{E}_y = 0 - \rho_1 J_x B_z$$

$$\frac{\mathcal{E}_y}{J_x B_z} \equiv R_H = -\rho_1 = -\rho_0 \mu_H = -\frac{\mu_H}{nq\mu_n} = \frac{r_H}{(-q)n}$$

(R_H: Hall coefficient)

(Hall factor, $1 < r_H < 2$)

Hall effect



$$R_H \equiv \frac{\mathcal{E}_y}{J_x B_z} = \frac{r_H}{(-q)n}$$

$$1 < r_H < 2$$

(depends on the energy dependence of the dominant scattering processes)

The Hall effect was discovered by Edwin Hall in 1879 and is widely used to characterize electronic materials. It also finds use magnetic field sensors.

integer quantum Hall effect

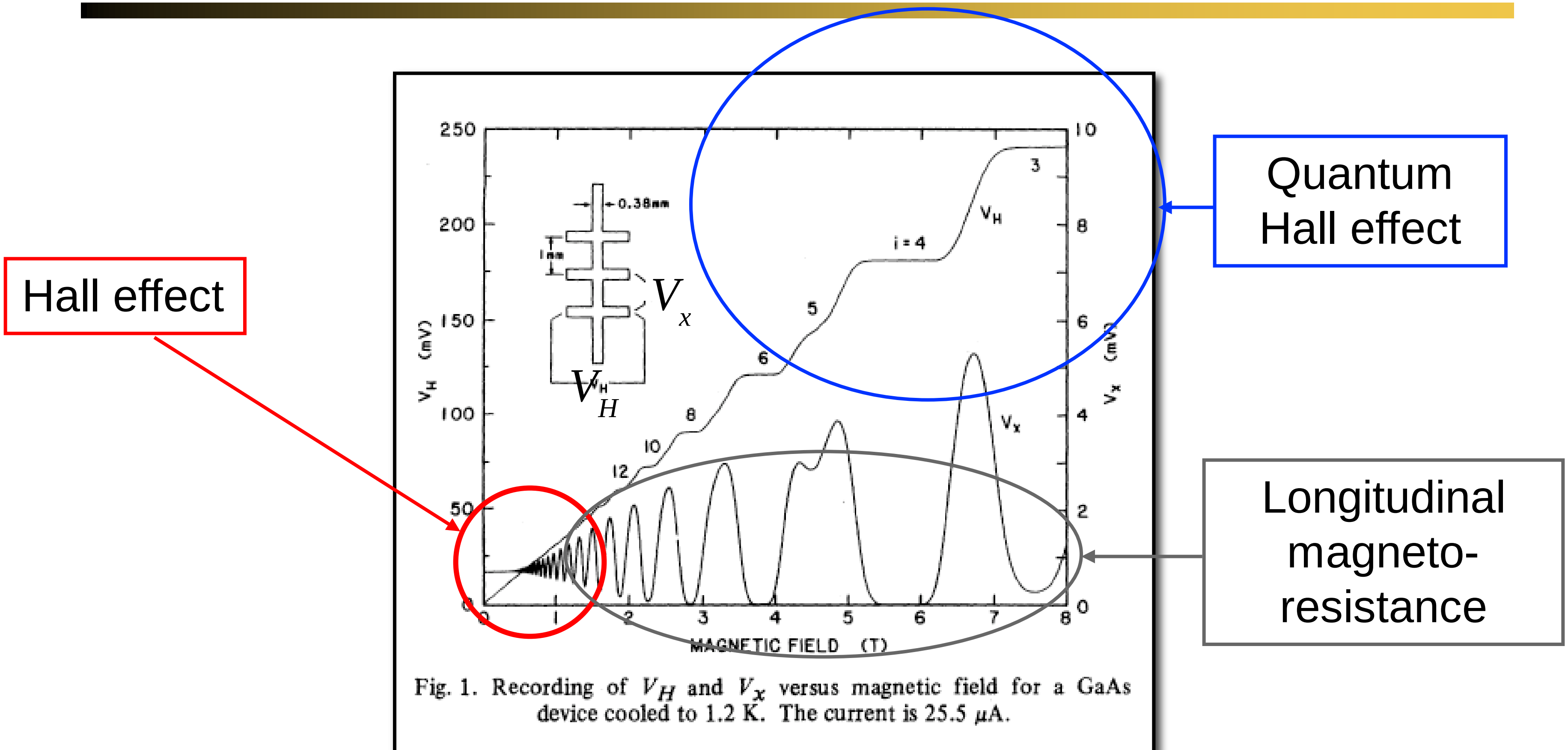


Fig. 1. Recording of V_H and V_x versus magnetic field for a GaAs device cooled to 1.2 K. The current is 25.5 μA.

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

for more information

1) Lundstrom, *Fundamentals of Carrier Transport*, 2nd Ed. Cambridge Univ. Press, 2000, Ch. 4

2) A.C. Smith, J.F. Janak, and R.B. Adler, *Electronic Conduction in Solids,* McGraw-Hill, New York, 1967

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