FUNDAMENTALS OF NANOELECTRONICS

B. Quantum Transport

1. Schrodinger Equation

Contact-ing Schrodinger →

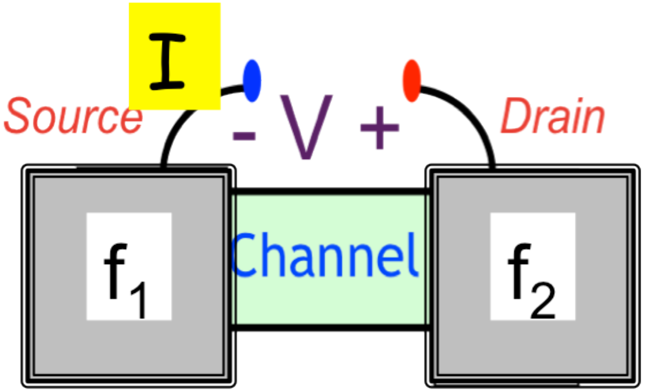
3. Advanced Examples

4. Spin Transport

Supriyo Datta

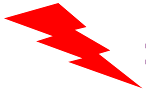
May 2015

http://nanohub.org/groups/lnebook



$$E\{\psi\} = [H]\{\psi\}$$

$$E\{\psi\} = [H]\{\psi\}$$

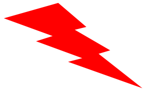
Schrodinger +  = NEGF

Quantum Transport

Part B

Semiclassical Transport

Part A

Newton +  = 

Entropy-driven processes

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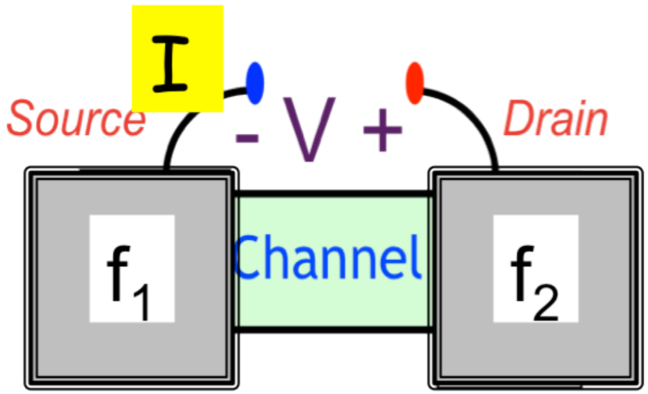
2.1b Introduction

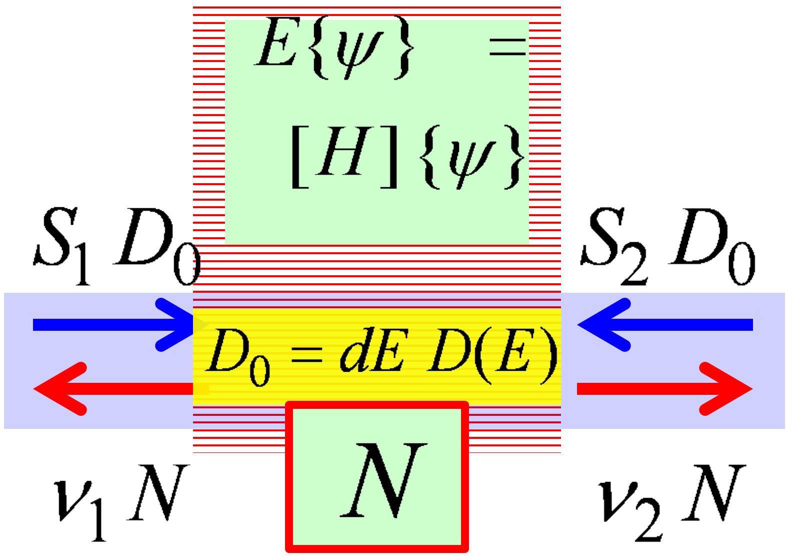


$$E\{\psi\} = [H]\{\psi\}$$

Schrodinger + = NEGF

Quantum Transport

Part B



$$\frac{dN}{dt} = -(\nu_1+\nu_2)\,N \qquad \text{Outflow}$$

$$+\ (S_1+S_2)\,D_0 \qquad \text{Inflow}$$

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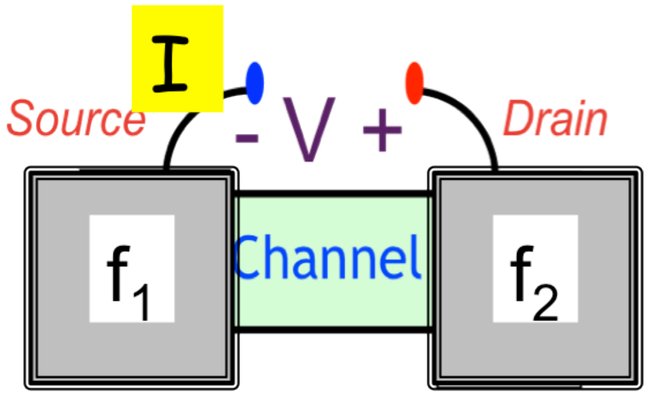


$$i\hbar \frac{d}{dt}\{\tilde{\psi}\} = [H]\{\tilde{\psi}\}$$

$$\{\tilde{\psi}\} = \{\psi\}\, e^{-iEt/\hbar}$$

$$i\hbar \times -\frac{iE}{\hbar} = E$$

From boundary conditions

$$E\{\psi\} = [H]\{\psi\} + [\Sigma_1 + \Sigma_2]\{\psi\} + \{s_1\} + \{s_2\}$$

?

Outflow

Inflow

$$E\{\psi\} = [H]\{\psi\}$$

$S_1 D_0$ $\quad$ $S_2 D_0$

$$D_0 = dE\; D(E)$$

$\nu_1 N$ $\quad$ $\nu_2 N$

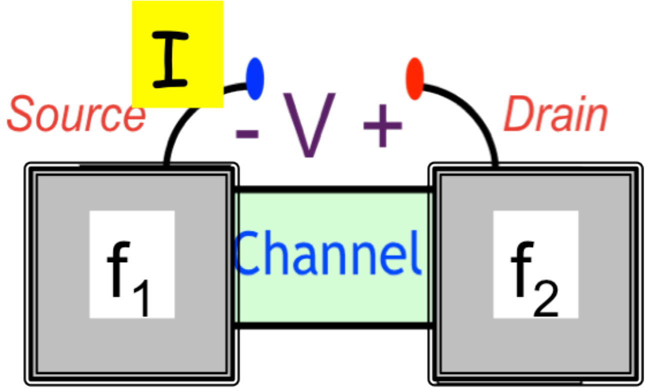
$$N = \tilde{\psi}^+ \tilde{\psi} = \psi^+ \psi$$

$$\frac{dN}{dt} = -(\nu_1 + \nu_2)\, N + (S_1 + S_2)\, D_0$$

Outflow

Inflow

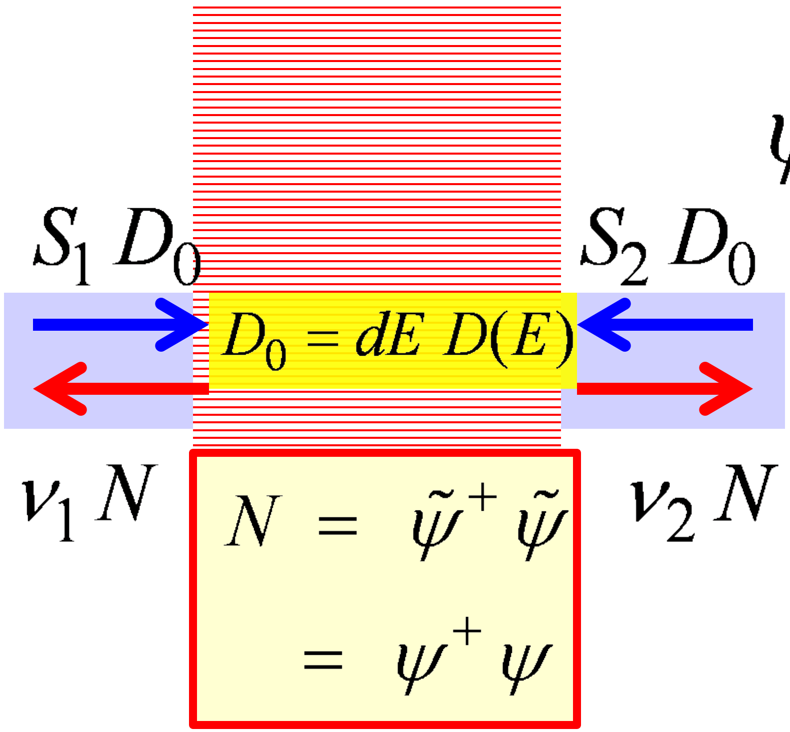
2.1d Introduction



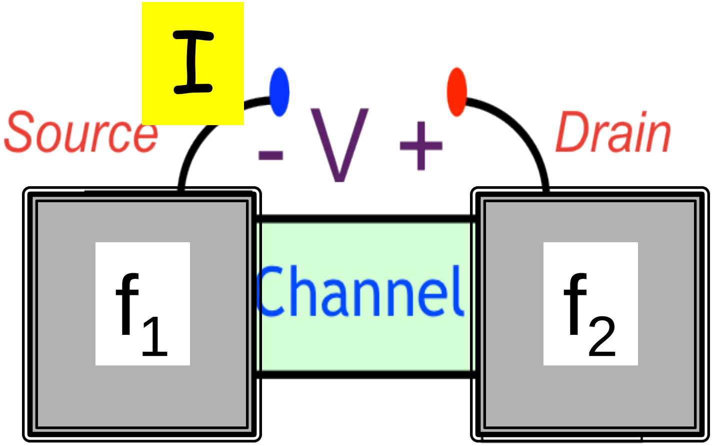
$$E\psi = H\psi$$
$$+ \; (\Sigma_1 + \Sigma_2)\psi$$
Outflow
$$+ \; (s_1 + s_2)$$
? Inflow ?

$$\psi \sim (s_1 + s_2)$$

$$\psi^+ \psi \sim (s_1 + s_2)^+ \times (s_1 + s_2)$$
$$= s_1^+ s_1 + s_2^+ s_2 \quad + \cancel{s_1^+} s_2 + \cancel{s_2^+} s_1$$



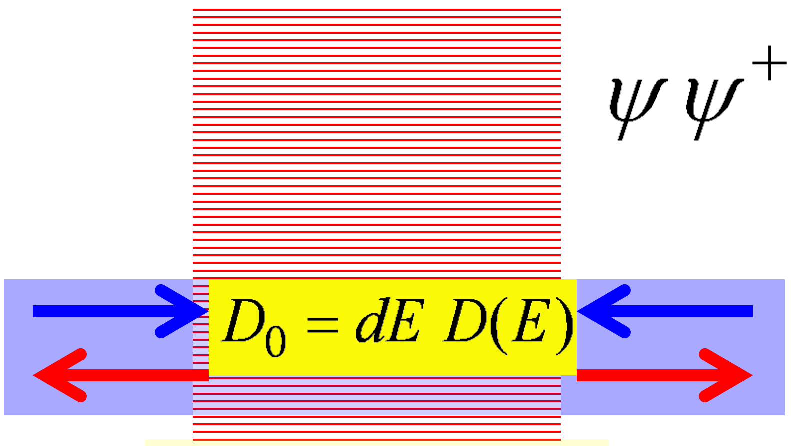
$$\frac{dN}{dt} = -(\nu_1 + \nu_2)\, N$$
Outflow
$$+ \; (S_1 + S_2)\, D_0$$
Inflow



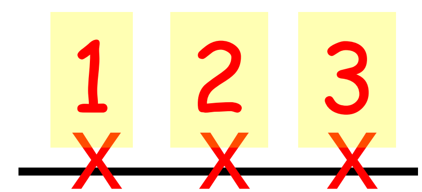
$$E\psi = H\psi + (\Sigma_1 + \Sigma_2)\psi + s$$

$$s\,s^+ \sim [\Sigma^{in}]$$

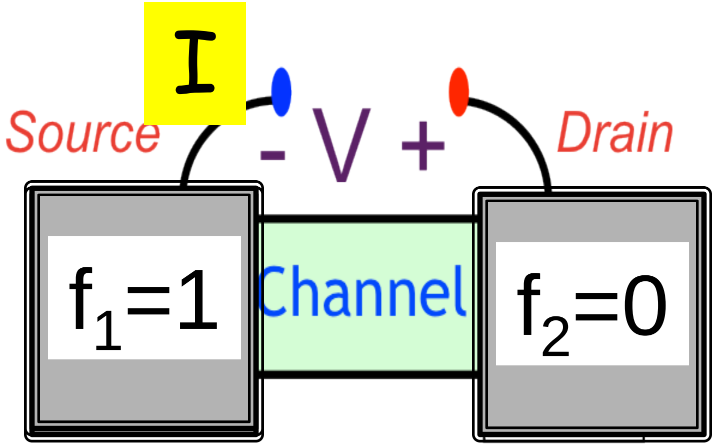
$$\psi\,\psi^+ = \begin{Bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{Bmatrix} \begin{Bmatrix} \psi_1^* & \psi_2^* & \psi_3^* \end{Bmatrix} = \begin{bmatrix} 1,1 & 1,2 & 1,3 \\ 2 & \sim [G^n] & ,3 \\ 3,1 & 3,2 & 3,3 \end{bmatrix}$$



$$N = \tilde{\psi}^+ \tilde{\psi} = \psi^+ \psi = \begin{Bmatrix} \psi_1^* & \psi_2^* & \psi_3^* \end{Bmatrix} \begin{Bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{Bmatrix}$$



2.1f Introduction



$$E\psi = H\psi + \Sigma\psi + s$$

$$[EI - H - \Sigma]\ \psi = s$$

$$\psi = G^R \{s\}$$

$$\psi^+ = \{s\}^+ G^A$$

$$s_1 + E\psi = \Sigma_1\psi + H\psi + \Sigma_2\psi$$

$$G^< = G\ \Sigma^<\ G^+$$

$$\boxed{G^R = [EI - H - \Sigma]^{-1}}$$

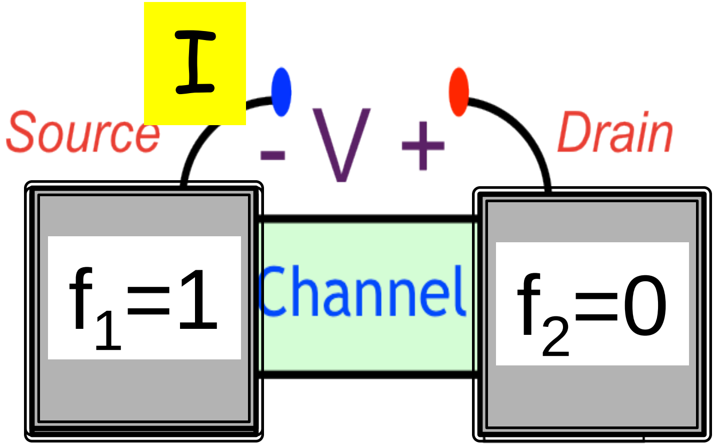
$$\boxed{G^n = G^R\, \Sigma^{in}\, G^A}$$

$$G^A = [G^R]^+$$

$$\underbrace{\psi\psi^+} = G^R\ \underbrace{s\,s^+}\ G^A$$

$$-iG^< \equiv G^n \qquad -i\Sigma^< \equiv \Sigma^{in}$$

2.1g Introduction



$$s_1 + \Sigma_1\psi + E\psi = H\psi + \Sigma_2\psi$$

Elastic Processes

$$E\psi = H\psi + \Sigma\psi + s$$

$$\boxed{G^R = [EI - H - \Sigma]^{-1}}$$

$$\boxed{G^n = G^R\,\Sigma^{in}\,G^A}$$

$$G^< = G\,\Sigma^<\,G^+$$

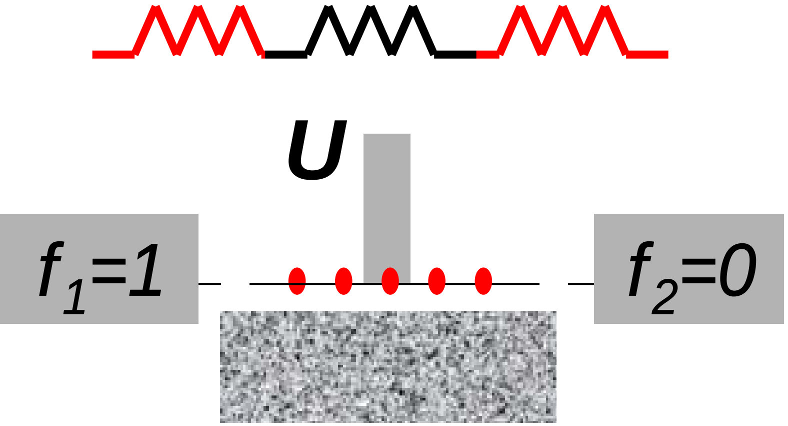
Datta
Cambridge (1995, 2005)

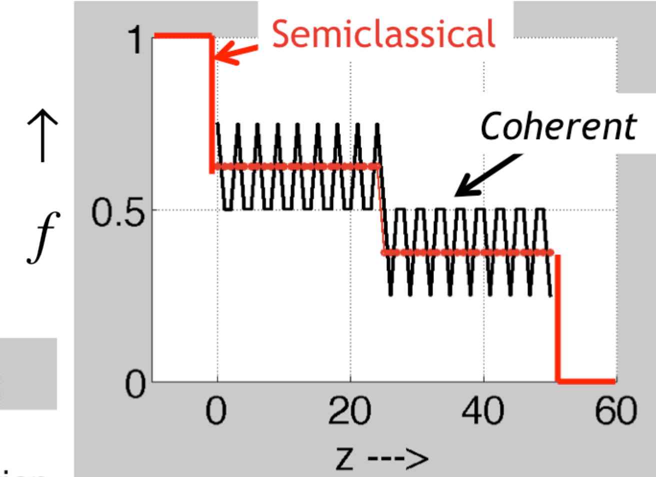
$$\Sigma = \Sigma_1 + \Sigma_2 + \Sigma_0 + \left(\Sigma_0\right)_{diss}$$

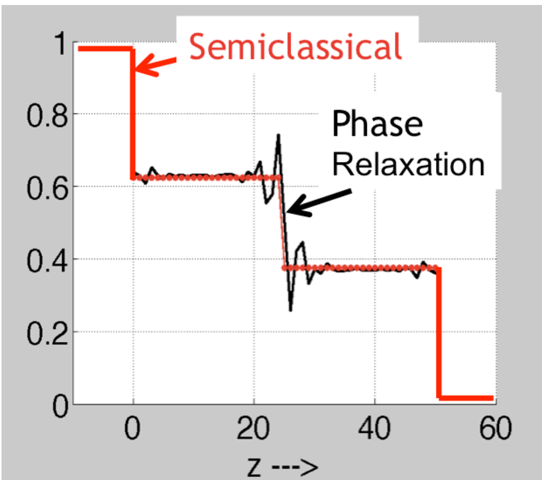
$$\Sigma^{in} = \Sigma_1^{in} + \Sigma_2^{in} + \Sigma_0^{in} + \left(\Sigma_0^{in}\right)_{diss}$$

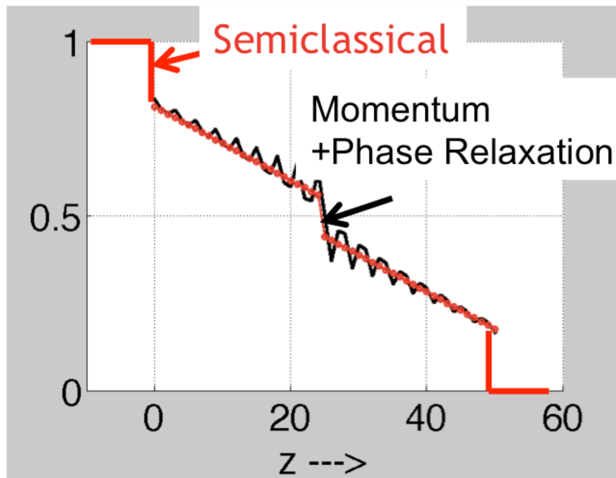
Keldysh (1965):
Diagram technique for non-equilibrium processes

2.1h An Example



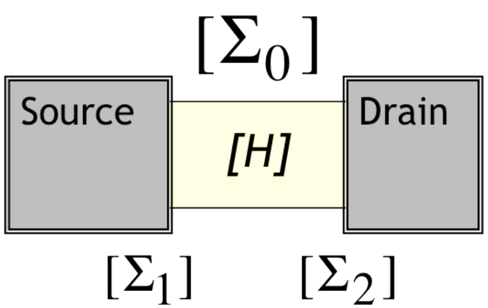






$$\Sigma = \Sigma_1 + \Sigma_2 + \Sigma_0 \cancel{+ \left(\Sigma_0\right)_{diss}}$$

$$\Sigma^{in} = \Sigma_1^{in} + \Sigma_2^{in} + \Sigma_0^{in} \cancel{+ \left(\Sigma_0^{in}\right)_{diss}}$$



$$E\psi = H\psi + \Sigma\psi + s$$

$$G^R = [EI - H - \Sigma]^{-1}$$

$$G^n = G^R \Sigma^{in} G^A$$

NEGF Equations

$$I^{op} = \frac{\Sigma G^n - G^n \Sigma^+}{i\hbar} + \frac{\Sigma^{in} G^R - G^A \Sigma^{in}}{i\hbar}$$

Current Operator

Coming up next ..

1D Examples

UNIT 3

More advanced examples