FUNDAMENTALS OF NANOELECTRONICS

B. Quantum Transport

1. Schrodinger Equation
2. Contact-ing Schrodinger

More Examples

4. Spin Transport

3.1. Introduction

3.2. Quantum Point Contact

3.3. Self-Energy

3.4. Surface Green's Function

3.5. Graphene

3.6. Magnetic Field

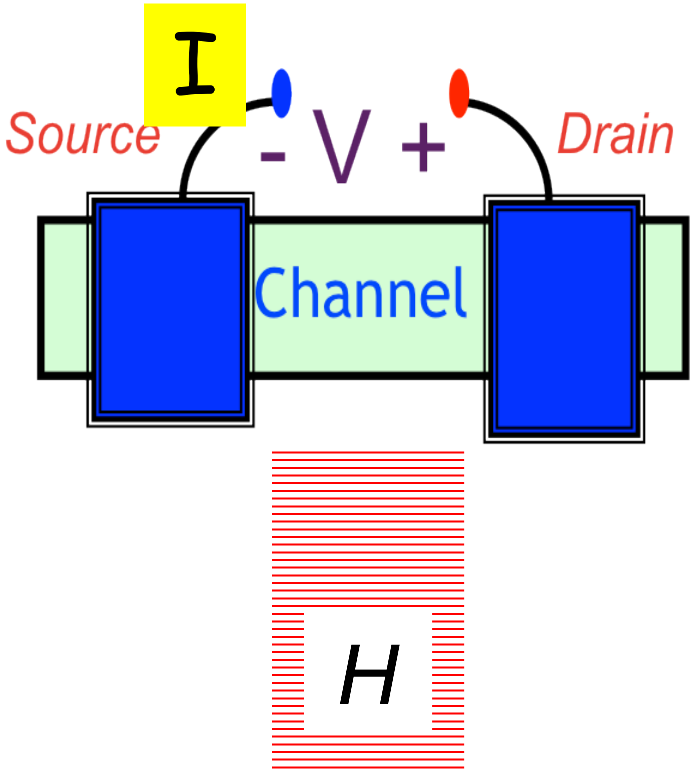
3.7. Golden Rule

3.8. Inelastic Scattering

3.9. Can NEGF Include Everything?

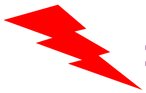
3.10. Summing up ..

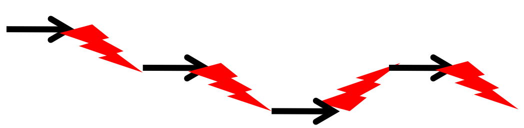
Supriyo Datta



$$E\psi = H\psi$$

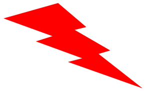
Part B: Quantum Transport

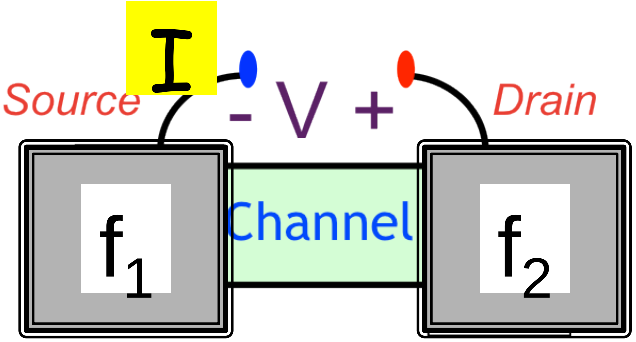
Schrodinger +  = NEGF



Entropy driven *Force driven*

Part A: Semiclassical Transport

Newton +  = 



3.10b Summing up ..

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

$$\Sigma = \Sigma_1 + \Sigma_2$$

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

B 2.2-2.5 NEGF Equations

$$\boxed{\begin{aligned} G^R &= [EI - H - \Sigma]^{-1} \\ G^n &= G^R \Sigma^{in} G^A \end{aligned}}$$

$$\psi\psi^+ \qquad ss^+$$

$$\Sigma^{in} = \Sigma_1^{in} + \Sigma_2^{in}$$

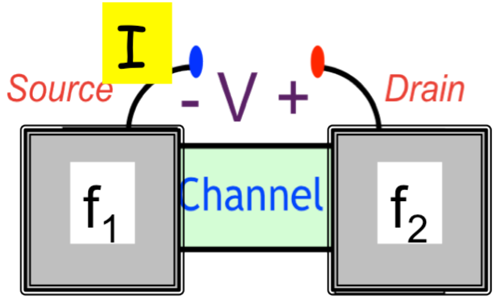
Current Operator

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

$$I_1 = \frac{q}{h} Trace\,[\Sigma_1^{in} A - \Gamma_1 G^n]$$

$$\cancel{\rightarrow} \frac{q}{h} \; Trace\,[\Gamma_1 G^R \Gamma_2 G^A]\;(f_1 - f_2)$$

3.10c Summing up ..



$$\Sigma = \Sigma_1 + \Sigma_2$$

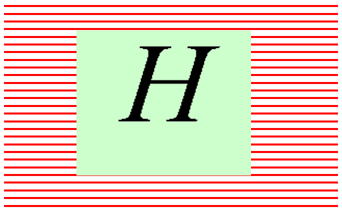
$$\Sigma^{in} = \Sigma_1^{in} + \Sigma_2^{in}$$

$$\Gamma \equiv i(\Sigma - \Sigma^+)$$

$$A = i\,[G^R - G^A]$$

Σ_1^{in} Σ_2^{in}

Σ_1 Σ_2



$$\Sigma = \tau g \tau^+$$

B 3.3-3.4

$$\Sigma \rightarrow t e^{ika}$$

B 2.6-2.7

B 2.2-2.5

$\frac{A}{2\pi} \leftrightarrow D$	$\frac{G^n}{2\pi} \leftrightarrow N$
$\frac{\Sigma^{in}}{\hbar} \leftrightarrow S$	$\frac{\Gamma}{\hbar} \leftrightarrow \nu$

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

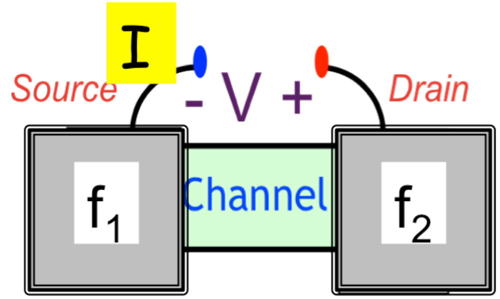
$$G^n = G^R \Sigma^{in} G^A$$

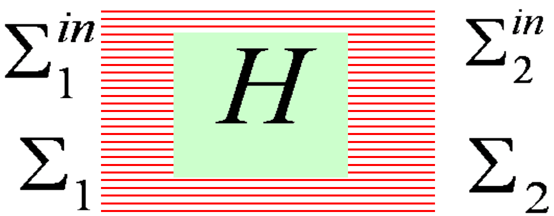
NEGF Equations

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

Current Operator

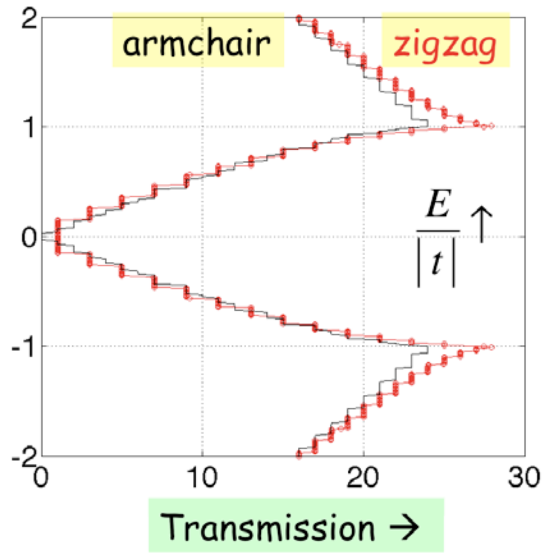
3.10d Summing up ..





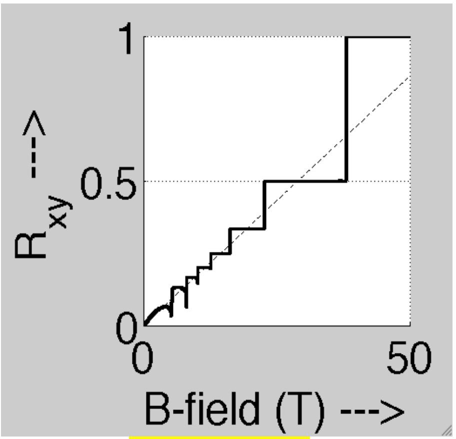
$$\Sigma = \tau g \tau^{+}$$

B 3.3-3.4



B 3.5

◆ Graphene CNT



B 3.6

◆ (Quantum) Hall Effect

$$\Sigma \rightarrow te^{ika}$$

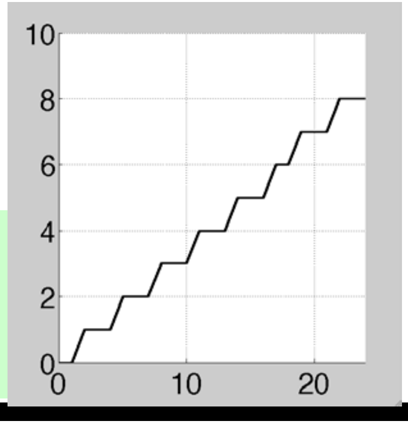
B 2.6-2.7

B 2.8

◆ Resonant Tunneling

B 3.2

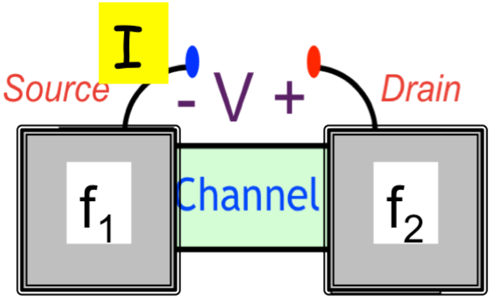
◆ Quantum Point Contact

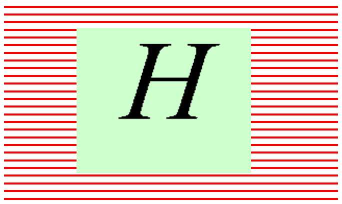


↑ $\bar{T}(E = t_0)$

Number of points along width

3.10e Summing up ..





Σ_1^{in} Σ_2^{in}

Σ_1 Σ_2

Σ_0, Σ_0^{in}

$$[\Sigma_0^{in}(E)]_{ij} = \int_{-\infty}^{+\infty} \frac{d(\hbar\omega)}{2\pi} \sum_{m,n} D_{im;jn}(\hbar\omega)[G^n(E+\hbar\omega)]_{mn}$$

B 3.7-3.8

$$[\Gamma_0(E)]_{ij} = \int_{-\infty}^{+\infty} \frac{d(\hbar\omega)}{2\pi} \sum_{m,n} D_{im;jn}(\hbar\omega)\times \left[G^p(E-\hbar\omega)+G^n(E+\hbar\omega)\right]_{mn}$$

$$D_{im;jn} = \left\langle \tau_{im}\, \tau^*_{jn} \right\rangle$$

$$\Sigma = \tau g \tau^+$$

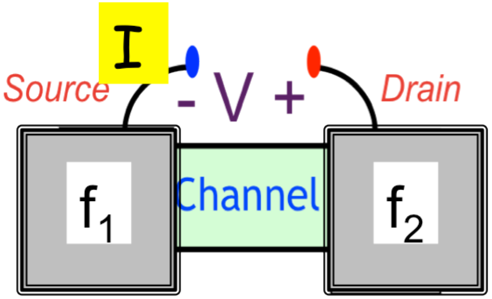
B 3.3-3.4

$$\Gamma = \tau\, a\, \tau^+ \quad \rightarrow \quad [\Gamma_0(E)]_{ij} = \sum_{m,n} D_{im;jn}\,[A(E)]_{mn}$$

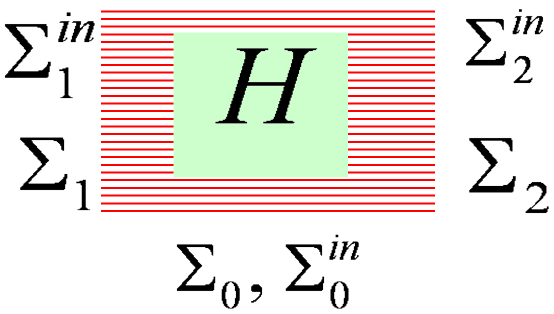
$$\left\langle \tau_{im}\, \tau^*_{jn} \right\rangle$$

$$\Sigma^{in} = \tau\, g^n\, \tau^+ \quad \longrightarrow \quad [\Sigma_0^{in}(E)]_{ij} = \sum_{m,n} D_{im;jn}\,[G^n(E)]_{mn}$$

3.10f Summing up ..



$$[\Sigma_0^{in}(E)]_{ij} = \int_{-\infty}^{+\infty} \frac{d(\hbar\omega)}{2\pi} \sum_{m,n} D_{im;jn}(\hbar\omega)[G^n(E+\hbar\omega)]_{mn}$$



B 3.7-3.8

$$[\Gamma_0(E)]_{ij} = \int_{-\infty}^{+\infty} \frac{d(\hbar\omega)}{2\pi} \sum_{m,n} D_{im;jn}(\hbar\omega) \times$$

$$\left[G^p(E-\hbar\omega) + G^n(E+\hbar\omega)\right]_{mn}$$

$$D_{im;jn} = \left\langle \tau_{im}\, \tau_{jn}^* \right\rangle$$

$$\Sigma = \tau g \tau^+$$

B 3.3-3.4

$$\Gamma = \tau\, a\, \tau^+$$

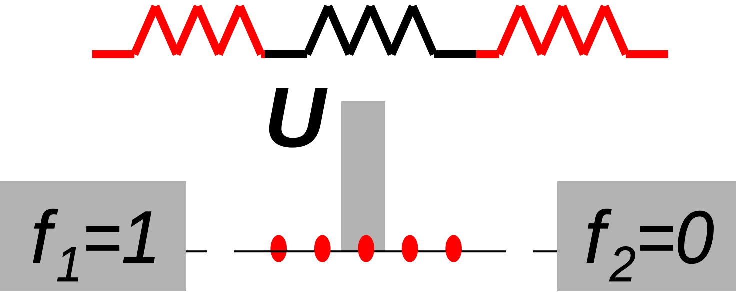
$$\Sigma^{in} = \tau\, g^n\, \tau^+$$

Our approach
One-electron Schrodinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi + U^R \psi$$

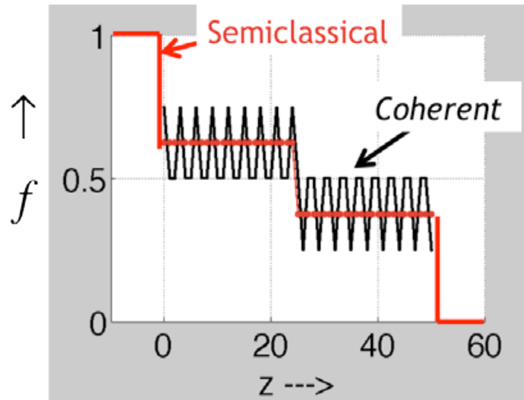
Standard Approach
Many-body Perturbation Theory (MBPT)

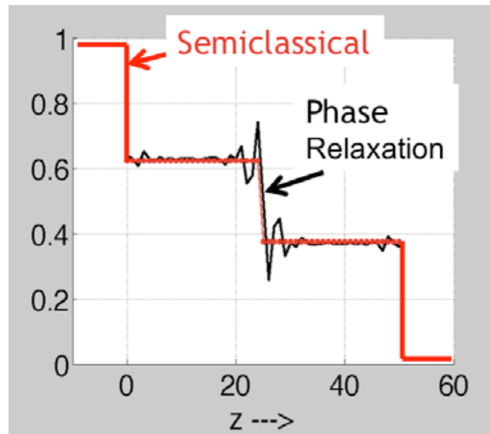
3.10g Summing up ..



$$D = d_0 \begin{bmatrix} 1 & 1 & 1 & \cdots \\ 1 & 1 & 1 & \cdots \\ 1 & 1 & 1 & \cdots \\ & \cdots & \cdots & \end{bmatrix}$$

Our approach
One-electron Schrodinger equation





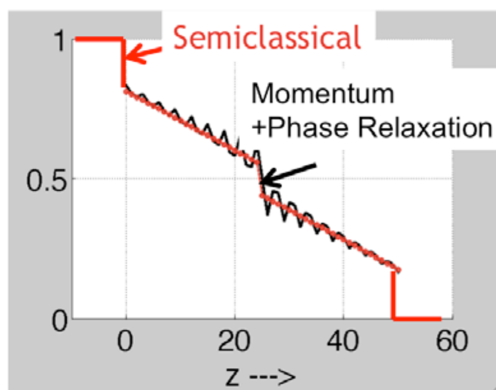
$$i\hbar \frac{\partial \psi}{\partial t} = H\psi + U^R \psi$$

$$D_{im;jn} = \left\langle \tau_{im} \, \tau^*_{jn} \right\rangle$$

$$\rightarrow \left\langle \tau_{ii} \, \tau^*_{jj} \right\rangle \delta_{im} \delta_{jn}$$

B 2.9

$$D = d_0 \begin{bmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ & \cdots & \cdots & \end{bmatrix}$$



Standard Approach
Many-body Perturbation Theory (MBPT)

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3.10h Summing up ..

$$\Sigma_1^{in} \quad H + U \quad \Sigma_2^{in}$$

$$\Sigma_1 \qquad\qquad \Sigma_2$$

$$\Sigma_0 , \Sigma_0^{in}$$

One-electron Schrodinger equation

Poisson Eq

$$\nabla^2 U = \frac{q^2}{\varepsilon} n$$

Minus corrections for "exchange" and "correlation"

$$U \approx U_0 N$$

Single - electron charging energy

If $U_0 >> kT , \Gamma$

Single - electron charging effects

Requires non-perturbative methods

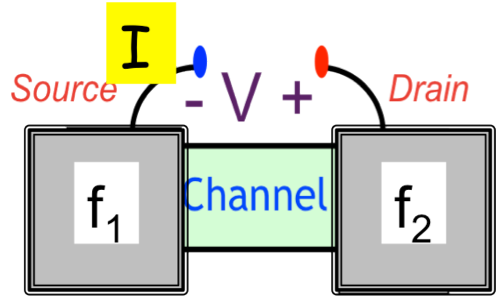
$$i\hbar \frac{\partial \psi}{\partial t} = H\psi + U^R \psi$$

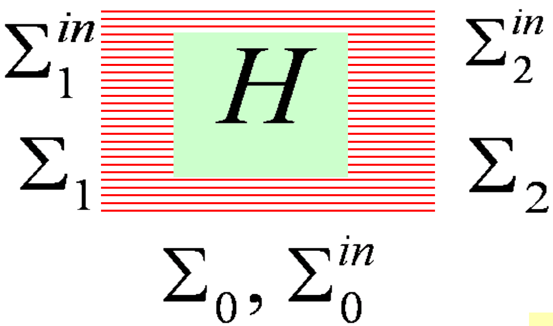
$$D_{im;jn} = \left\langle \tau_{im} \, \tau^*_{jn} \right\rangle$$

$$\tau_{im} = \int d\vec{r} \, \phi_i^* \; U^R \, \phi_m$$

Standard Approach
Many-body Perturbation Theory (MBPT)

3.10i Summing up ..





H, Σ_1, Σ_2

μ_1, μ_2

NEGF Equations + Current Operator

I

$U, \Sigma_0, \Sigma_0^{in}$

G^R, G^n

Self-energy Equations

May need non-perturbative techniques

Our approach
One-electron Schrodinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi + U^R \psi$$

Standard Approach
Many-body Perturbation Theory (MBPT)

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

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

NEGF Equations

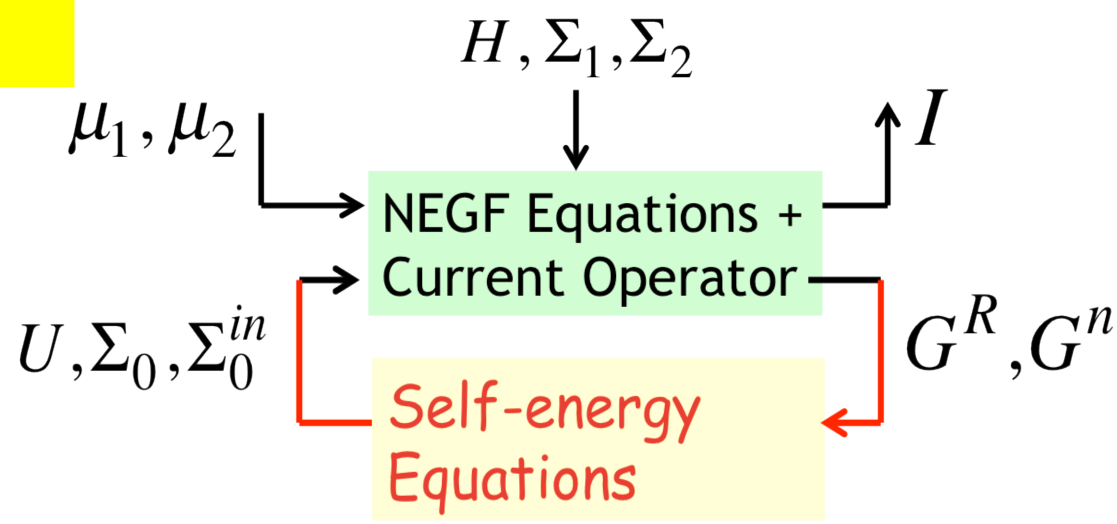
$$I^{op} = \frac{\Sigma G^n - G^n \Sigma^+}{i\hbar} + \frac{\Sigma^{in} G^A - G^R \Sigma^{in}}{i\hbar}$$

Current Operator

NEGF viewed as esoteric tool accessible to those well-versed in many-body perturbation theory

3.10j Summing up ..

Should be part of grad / undergrad curriculum



Our approach
One-electron Schrodinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi + U^R \psi$$

Standard Approach
Many-body Perturbation Theory (MBPT)

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

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

NEGF Equations

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

Current Operator

Coming up next ..

B. Quantum Transport

1. Schrodinger Equation
2. Contact-ing Schrodinger
3. More Examples
4. Spin Transport →

4.1. Introduction
4.2. One-level spin valve
4.3. Rotating contacts
4.4. Spin density
4.5. Vectors and Spinors
4.6. Pauli spin matrices
4.7. Spin-orbit coupling
4.8. Spin precession
4.9. Spin circuits
4.10. Summing up ..