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 ..

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August 2015

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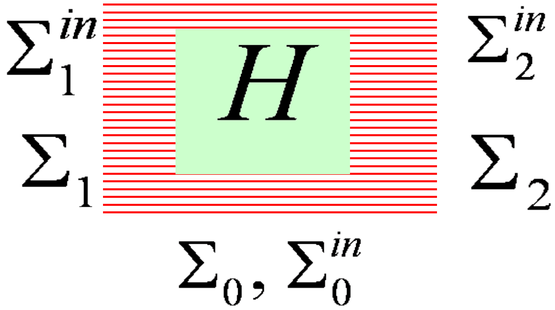

3.9a Can NEGF Include Everything?

One-electron Schrodinger equation

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

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

$$\Sigma_0(E) = -\frac{i}{2}\Gamma_0(E) \otimes \left(\delta(E) + \frac{i}{\pi E}\right)$$

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

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

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

Standard Approach
Many-body Perturbation Theory (MBPT)

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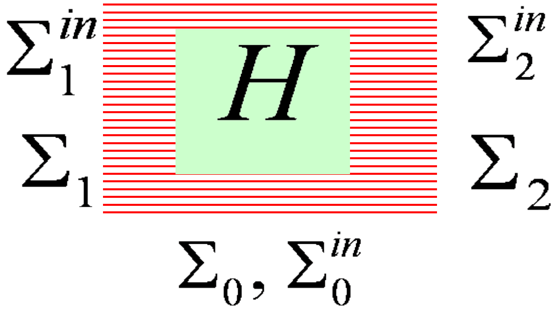
3.9b Can NEGF Include Everything?



Electron-electron Interaction ?

One-electron Schrodinger equation

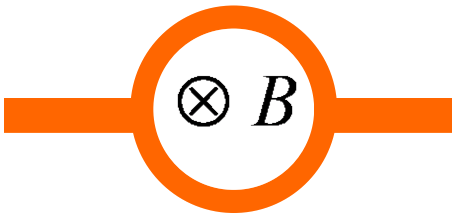
$$i\hbar \frac{\partial \psi}{\partial t} = H\psi + U^R \psi$$

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

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

Conductivity → *Momentum Relaxation Time*

Oscillatory → Magnetoresistance



Conductance *Fluctuations*

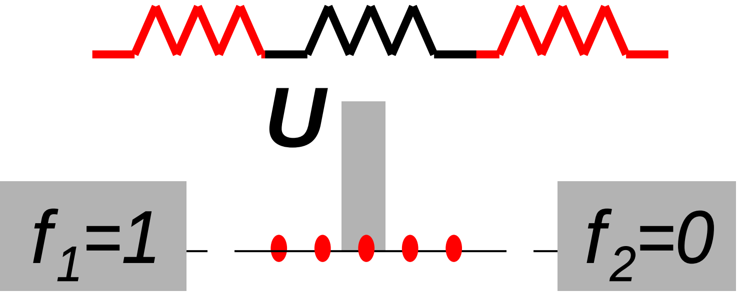
Weak Localization

Phase Relaxation Time

Standard Approach

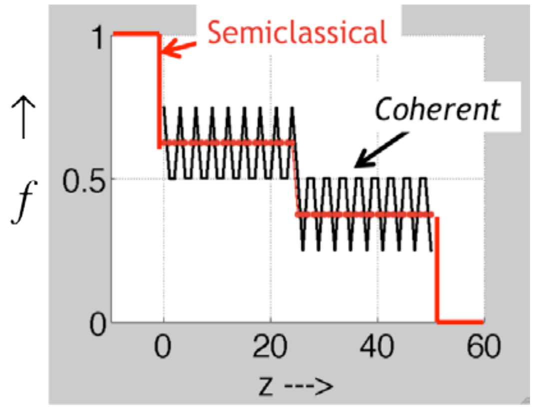
Many-body Perturbation Theory (MBPT)

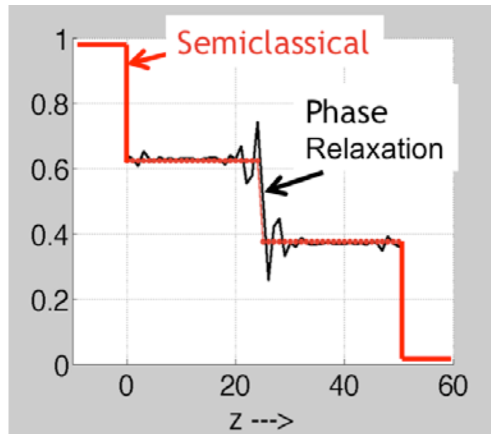
3.9c Can NEGF Include Everything?



One-electron Schrodinger equation

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





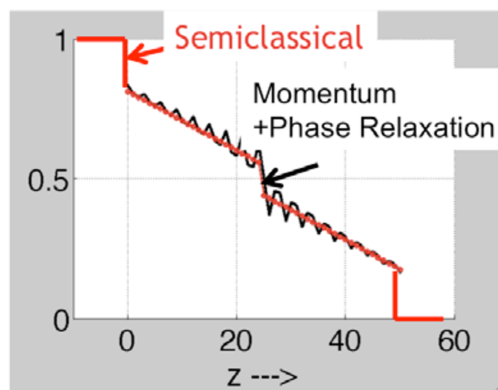
$$i\hbar \frac{\partial \psi}{\partial t} = H\psi + U^R \psi$$

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

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

Part B, Lecture 2.9

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



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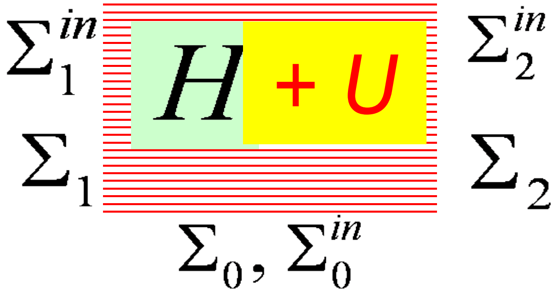


3.9d Can NEGF Include Everything?

Electron-electron Interaction ?

One-electron Schrodinger equation

$$U(\vec{r},\vec{r}\,') = \delta(\vec{r}-\vec{r}\,') \int d\vec{r}\,'' \frac{q^2}{4\pi\varepsilon|\vec{r}-\vec{r}\,''|} \overbrace{\int dE \frac{G^n(\vec{r}\,'',\vec{r}\,'';E)}{2\pi}}^{n(\vec{r}\,'')}$$

$$- \int dE \frac{q^2}{4\pi\varepsilon|\vec{r}-\vec{r}\,'|} G^{ns}(\vec{r},\vec{r}\,';E)$$

Poisson Eq

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

Exchange Correction

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

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

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

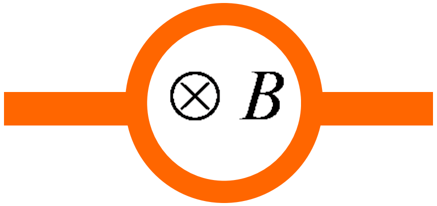
Oscillatory $\rightarrow$

Magnetoresistance

Conductance *Fluctuations*

Weak Localization

Phase Relaxation Time



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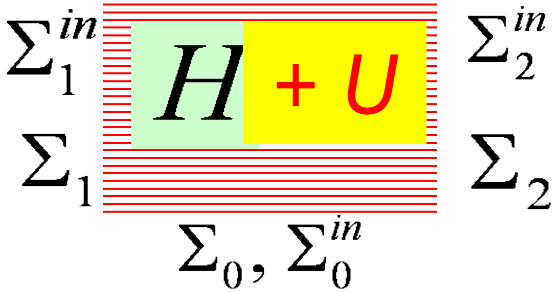
3.9e Can NEGF Include Everything?



Electron-electron Interaction ?

$$U \approx U_0 N$$

Single - electron charging energy

If $U_0 >> kT, \Gamma$

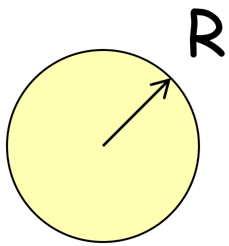
Single - electron charging effects also known as Coulomb blockade

Requires non-perturbative methods

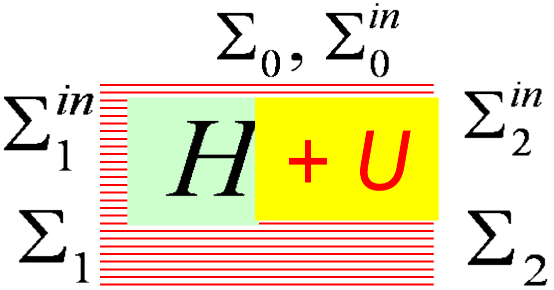
$$\frac{1}{1-x} \approx x + x^2 + \cdots$$

$$U_0 \sim \frac{q^2}{4\pi\varepsilon_0 R}$$

$$\rightarrow \quad 1.6\ eV \ \ for\ R = 1\ nm$$



Standard Approach
Many-body Perturbation Theory (MBPT)



$$\Sigma = \Sigma_1 + \Sigma_2 + \Sigma_0$$

$$\Sigma^{in} = \Sigma_1^{in} + \Sigma_2^{in} + \Sigma_0^{in}$$

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

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

◆ Many applications addressed with one-electron approach

◆ Some applications may require non-perturbative approach

Standard Approach
Many-body Perturbation Theory (MBPT)

Coming up next ..

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