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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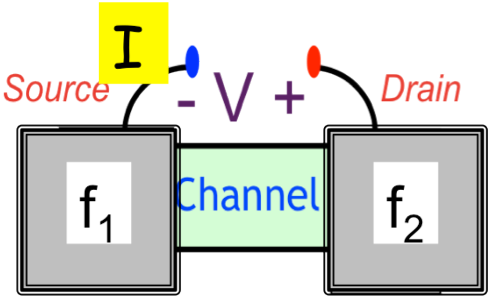
3.8a Inelastic Scattering



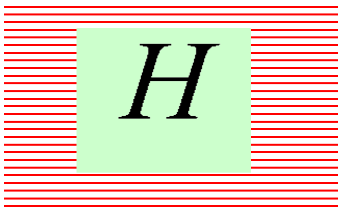
$$\Sigma = \tau g \tau^{+}$$

Part B, Lecture 3.3

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

$$\Gamma = \tau\, a\, \tau^{+} \rightarrow \frac{\hbar}{\text{"}lifetime\text{"}}$$

Σ_1^{in} Σ_2^{in}



Σ_1 Σ_2

Σ_0, Σ_0^{in}

$$[\Sigma_0^{in}]_{ij} = \sum_{m,n} \tau_{im}\, [G^n]_{mn}\, \tau_{nj}^{+}$$

$$= \sum_{m,n} \underbrace{\tau_{im}\, \tau_{jn}^{*}}\, [G^n]_{mn}$$

$$= \sum_{m,n} D_{im;\, jn}\, [G^n]_{mn}$$

$$= D_{ii;\, jj}\, [G^n]_{ij}$$

Part B, Lecture 2.9

$$\tau_{im} \rightarrow \tau_{ii}$$

$$[\Sigma_0^{in}(E)]_{ij} = D_{ij}\, [G^n(E)]_{ij}$$

$$[\Gamma_0(E)]_{ij} = D_{ij}\, [A(E)]_{ij}$$

$$U^S(\vec{r}, \vec{r}\,')$$

$$\rightarrow U^S(\vec{r})$$

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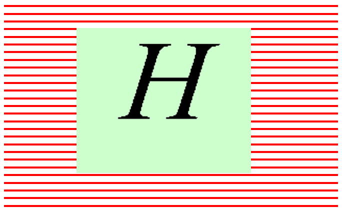
3.8b Inelastic Scattering

Σ_1^{in} Σ_2^{in}

Σ_1 Σ_2



Σ_0, Σ_0^{in}

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

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

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

$$\Sigma_0^{in}(E) = \quad D\, G^n(E)$$

$$[\Gamma_0(E)]_{ij} = \sum_{m,n} D_{im;jn}\, [G^n(E)]_{mn}$$

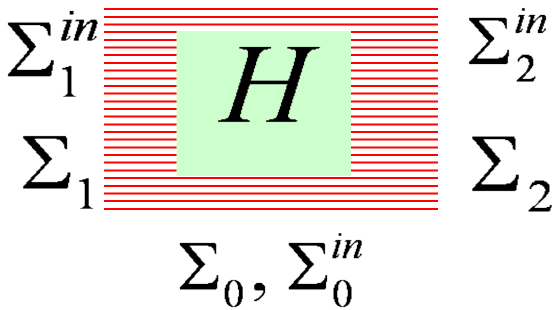
$$\Gamma_0(E) = \quad D\, A(E)$$

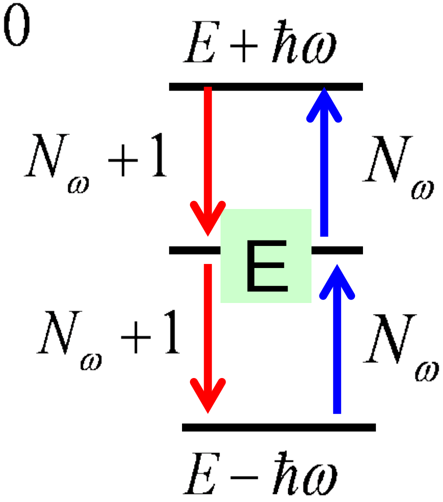
$$D_{im;jn} = \left\langle \tau_{im}\;\tau^*_{jn} \right\rangle \xrightarrow{?} \left\langle \tau_{ii}\;\tau^*_{jj} \right\rangle \delta_{im}\delta_{jn}$$

3.8c Inelastic Scattering

Emission $\hbar\omega > 0$

Absorption $\hbar\omega < 0$





Scatterers in Equilibrium

$$\frac{N_\omega + 1}{N_\omega} = e^{\hbar\omega/kT}$$

$$\Sigma_0^{in}(E) = D\,G^n(E) \rightarrow \Sigma_0^{in}(E) = \int_{-\infty}^{+\infty} \frac{d(\hbar\omega)}{2\pi} D(\hbar\omega)\, G^n(E+\hbar\omega)$$

$$\Gamma_0(E) = D\,A(E) \rightarrow \Gamma_0(E) = \int_{-\infty}^{+\infty} \frac{d(\hbar\omega)}{2\pi} D(\hbar\omega) \times \left[G^p(E-\hbar\omega) + G^n(E+\hbar\omega)\right]$$

$$A(E) \downarrow G^p(E) + G^n(E)$$

3.8d Inelastic Scattering

Inflow

$$D\, n(E+\hbar\omega)\, p(E)$$

$$+$$

$$D\, n(E+\hbar\omega)\, n(E)$$

$$\downarrow$$

$$\frac{D}{2\pi} G^n(E+\hbar\omega)\, A(E)$$

Outflow

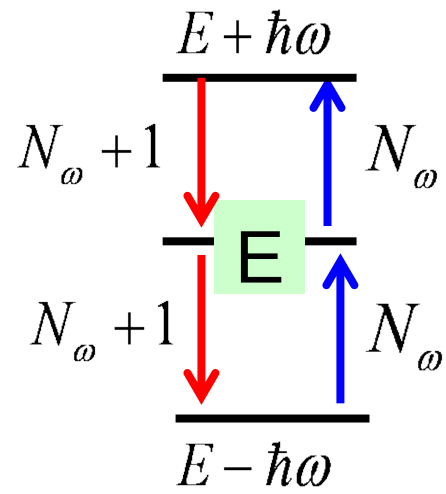
$$D\, n(E)\, p(E-\hbar\omega)$$

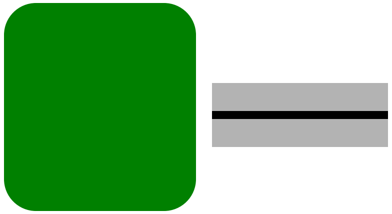
$$+$$

$$D\, n(E+\hbar\omega)\, n(E)$$

$$\downarrow$$

$$\frac{D}{2\pi}\begin{pmatrix} G^n(E+\hbar\omega)+ \\ G^p(E-\hbar\omega) \end{pmatrix} \times G^n(E)$$





Emission $\hbar\omega > 0$

Absorption $\hbar\omega < 0$

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3.8e Inelastic Scattering

Inflow

$$D\, n(E+\hbar\omega)p(E)$$

$$+$$

$$D\, n(E+\hbar\omega)n(E)$$

$$\underbrace{\frac{D}{2\pi} G^n(E+\hbar\omega)\, A(E)}_{\Sigma_0^{in}(E)}$$

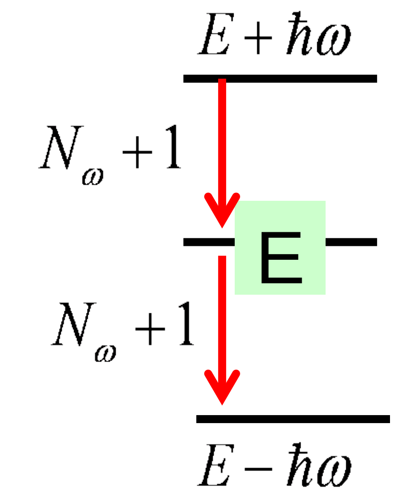
Outflow

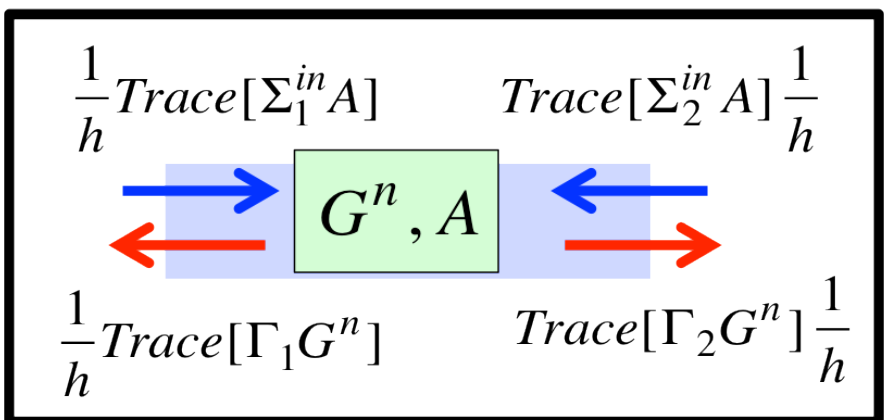
$$D\, n(E)p(E-\hbar\omega)$$

$$+$$

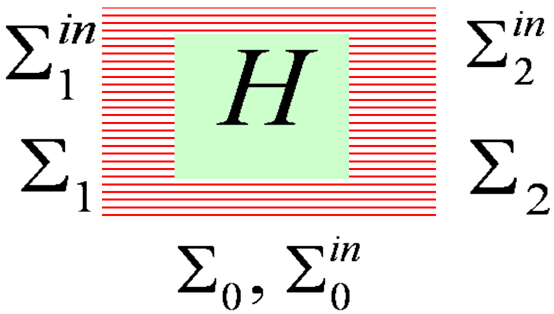
$$D\, n(E+\hbar\omega)n(E)$$

$$\underbrace{\frac{D}{2\pi}\begin{pmatrix} G^n(E+\hbar\omega)+ \\ G^p(E-\hbar\omega) \end{pmatrix}}_{\Gamma_0(E)} \times G^n(E)$$



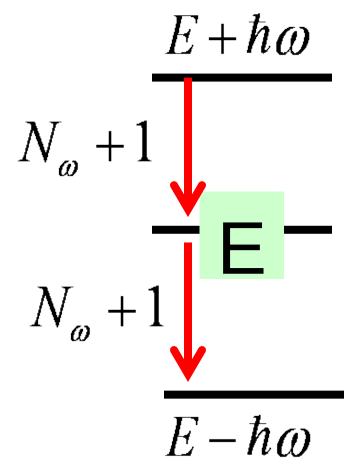


3.8f Inelastic Scattering



$$\underbrace{\frac{D}{2\pi} G^n(E+\hbar\omega)\, A(E)}_{\Sigma_0^{in}(E)}$$

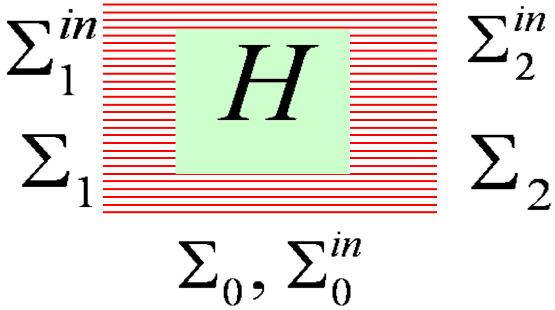
$$[\Sigma_0^{in}(E)]_{ij} = \int_{-\infty}^{+\infty} \frac{d(\hbar\omega)}{2\pi} \sum_{m,n} D_{im;jn}(\hbar\omega)\, [G^n(E+\hbar\omega)]_{mn}$$



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

$$\underbrace{\frac{D}{2\pi} \begin{pmatrix} G^n(E+\hbar\omega) + \\ G^p(E-\hbar\omega) \end{pmatrix}}_{\Gamma_0(E)} \times G^n(E)$$

3.8g Inelastic Scattering



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

$$\Gamma = i\left[\Sigma - \Sigma^+\right]$$

$$= \tau\, i\left[g - g^+\right]\, \tau^+$$

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

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

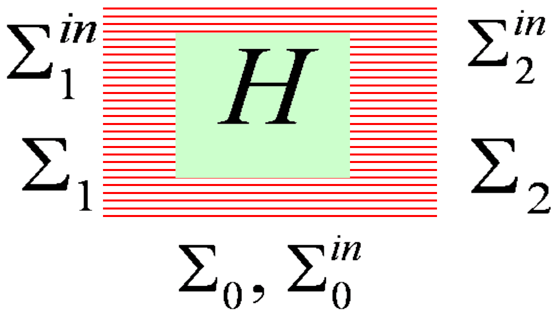
$$\Gamma_0(E) = D\, A(E)$$

$$G^p(E) + G^n(E)$$

$$[\Sigma_0(E)] = [h_0(E)] - \frac{i}{2}[\Gamma_0(E)]$$

$$2i\,[\Sigma_0(E)] = \Gamma_0(E) + 2i\,h_0(E) = \Gamma_0(E) \otimes \left(\delta(E) + \frac{i}{\pi E}\right)$$

$$\tilde{\Gamma}_0(t) \times \vartheta(t)$$



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

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

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

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

Scatterers in Equilibrium $\rightarrow \dfrac{D_{im;jn}(+\hbar\omega)}{D_{nj;mi}(-\hbar\omega)} = e^{\hbar\omega/kT_s}$

Coming up next ..

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