

FUNDAMENTALS OF NANO ELECTRONICS

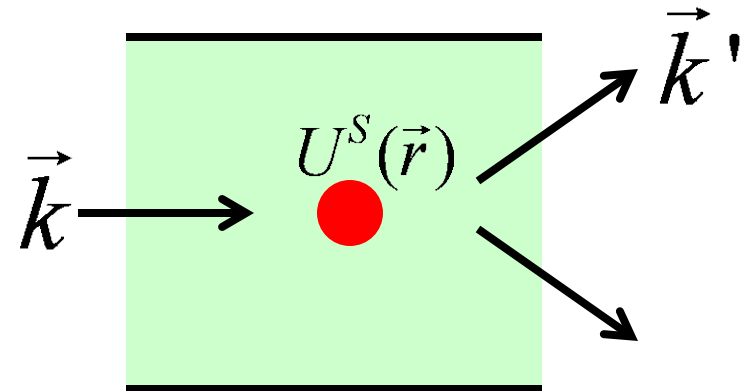
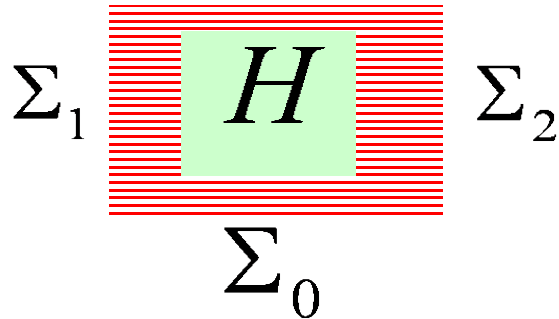
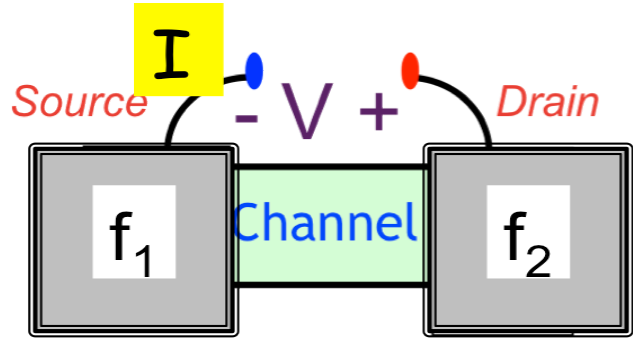
B. Quantum Transport

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 ..

3.7a Fermi's golden rule



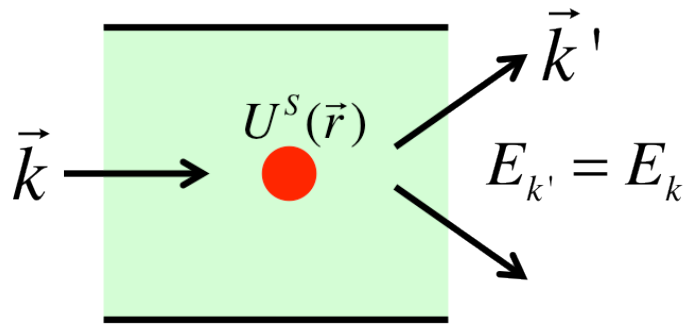
$$\Sigma = \tau g \tau^+$$

$$\begin{aligned} \Gamma &= i \left[\Sigma - \Sigma^+ \right] \rightarrow \frac{\hbar}{\text{"lifetime"}} \\ &= \tau i \left[g - g^+ \right] \tau^+ \\ &= \tau a \tau^+ \end{aligned}$$

$$S_{k,k'} = \frac{2\pi}{\hbar} |\tau_{k,k'}|^2 \delta(E_k - E_{k'})$$

$$\tau_{k,k'} = \int d\vec{r} \phi_{\vec{k}}^*(\vec{r}) U^S(\vec{r}) \phi_{\vec{k}'}(\vec{r})$$

3.7b Fermi's golden rule

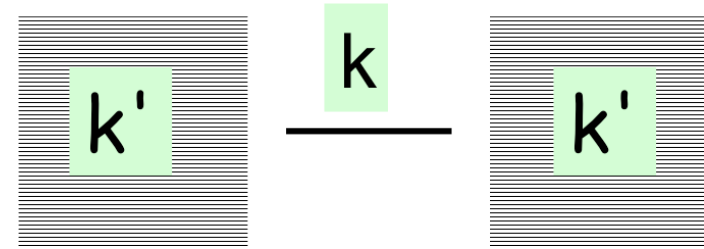


$$\vec{\beta} \equiv \vec{k} - \vec{k}'$$

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

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

$$\rightarrow \frac{\hbar}{\text{"lifetime"}}$$

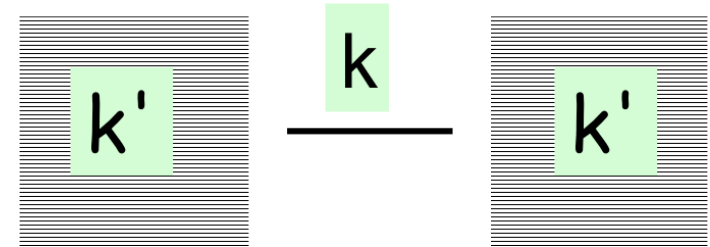
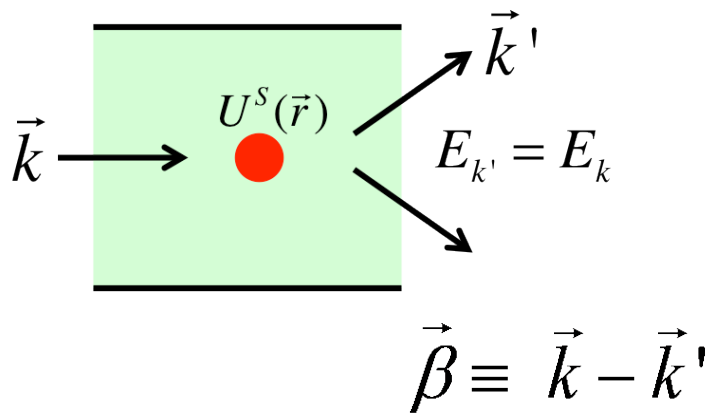


$$\begin{aligned} \Gamma_{k,k}(E) &= \sum_{k'} \tau_{k,k'} a_{k',k'}(E) \tau_{k',k}^+ \\ &= \sum_{k'} \tau_{k,k'} \tau_{k,k'}^* \underbrace{a_{k',k'}(E)} \end{aligned}$$

$$= \hbar \sum_{k'} \frac{1}{\hbar} |\tau_{k,k'}|^2 2\pi \delta(E_k - E_{k'})$$

$$S_{k,k'}$$

3.7c Fermi's golden rule



$$\frac{\Gamma_{k,k}(E)}{\hbar} = \sum_{k'} S_{k,k'}$$

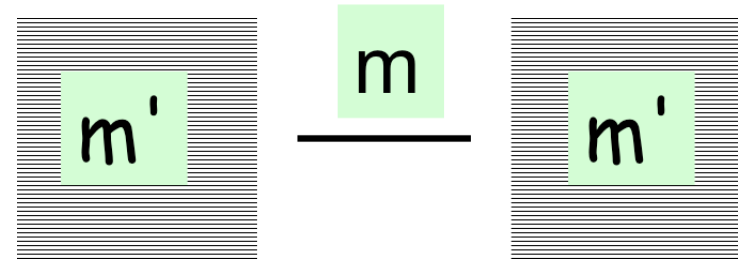
$$S_{k,k'} = \frac{2\pi}{\hbar} |\tau_{k,k'}|^2 \delta(E_k - E_{k'})$$

Part B,
Lecture 1.3

$$\begin{aligned} \tau_{k,k'} &= \int d\vec{r} \phi_{\vec{k}}^*(\vec{r}) U^S(\vec{r}) \phi_{\vec{k}'}(\vec{r}) \\ &= \frac{e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{V}} U^S(\vec{r}) \frac{e^{i\vec{k}'\cdot\vec{r}}}{\sqrt{V}} \\ &= \frac{1}{V} \int d\vec{r} U^S(\vec{r}) e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}} \\ &\rightarrow \tilde{U}^S(\vec{\beta}) \end{aligned}$$

$$\bullet U^S(\vec{r}) \cos \omega t$$

3.7d Fermi's golden rule



Absorption: $E_m + \hbar\omega = E_{m'}$

$$S_{m,m'} = \frac{2\pi}{\hbar} |\tau_{m,m'}|^2 N_\omega \times \delta(E_m - E_{m'} + \hbar\omega) + \frac{2\pi}{\hbar} |\tau_{m,m'}|^2 (N_\omega + 1) \times \delta(E_m - E_{m'} - \hbar\omega)$$

$$\frac{\Gamma_{m,m}(E)}{\hbar} = \sum_{m'} S_{m,m'}$$

$$S_{m,m'} = \frac{2\pi}{\hbar} |\tau_{m,m'}|^2 \delta(E_m - E_{m'})$$

$$\tau_{m,m'} = \int d\vec{r} \phi_m^*(\vec{r}) U^S(\vec{r}) \phi_{m'}(\vec{r})$$

Emission: $E_m - \hbar\omega = E_{m'}$

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

$$\bullet U^S(\vec{r}) \cos \omega t$$

Absorption

$$E_m + \hbar\omega = E_{m'}$$

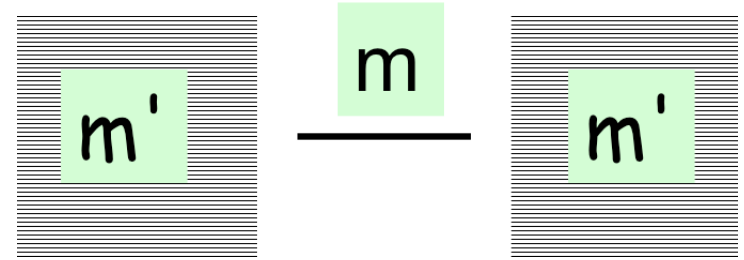
$$S_{m,m'} = \frac{2\pi}{\hbar} |\tau_{m,m'}|^2 N_\omega \times \delta(E_m - E_{m'} + \hbar\omega)$$

$$+ \frac{2\pi}{\hbar} |\tau_{m,m'}|^2 (N_\omega + 1) \times \delta(E_m - E_{m'} - \hbar\omega)$$

Emission

$$E_m - \hbar\omega = E_{m'}$$

3.7e Fermi's golden rule



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

$\phi_m(\vec{r}) e^{-iE_m t/\hbar}$

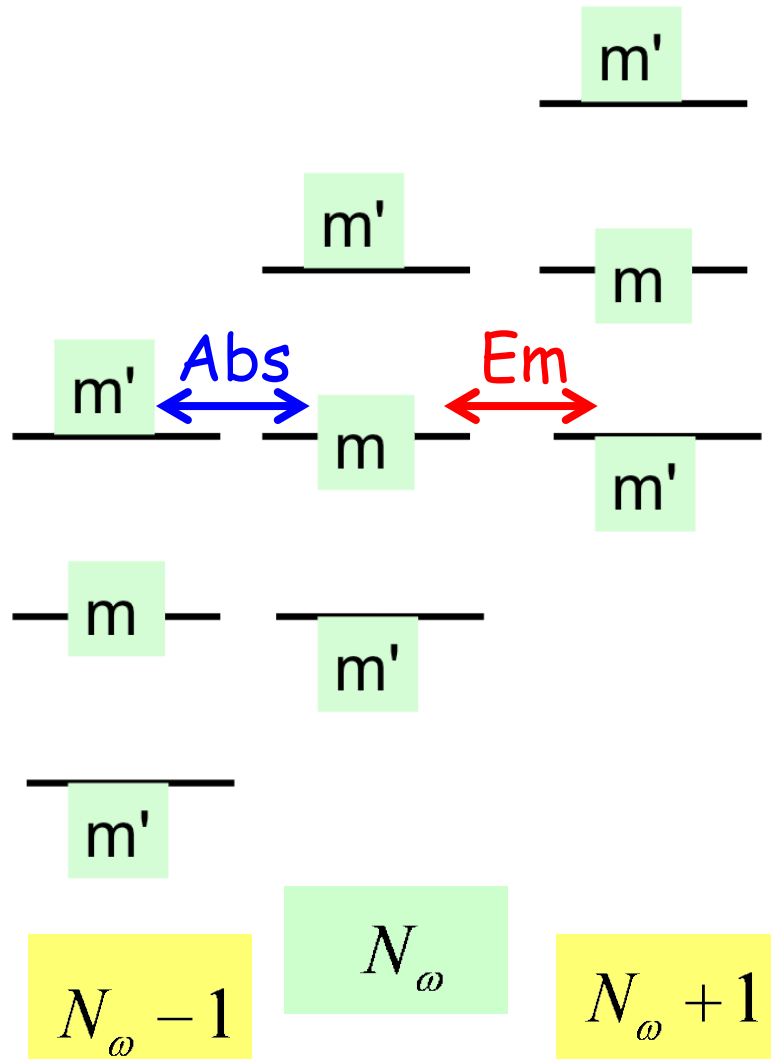
$e^{+i\omega t} + e^{-i\omega t}$

$\sim e^{-i(E_m - \hbar\omega)t/\hbar}$

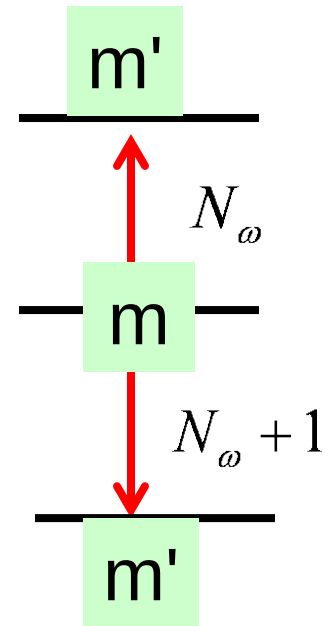
$\sim e^{-i(E_m + \hbar\omega)t/\hbar}$

Emission **Absorption**

$$S_{m,m'} = \frac{2\pi}{\hbar} |\tau_{m,m'}|^2 \delta(E_m - E_{m'})$$



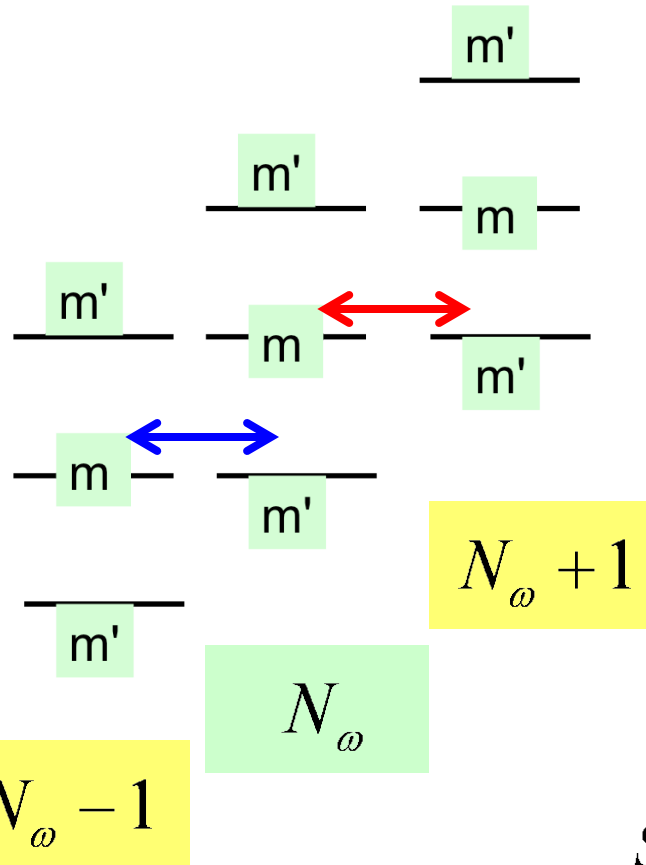
3.7f Fermi's golden rule



$$S_{m,m'} = \frac{2\pi}{\hbar} |\tau_{m,m'}|^2 \times \left[(N+1) \delta(E_m - E_{m'} - \hbar\omega) + N \delta(E_m - E_{m'} + \hbar\omega) \right]$$

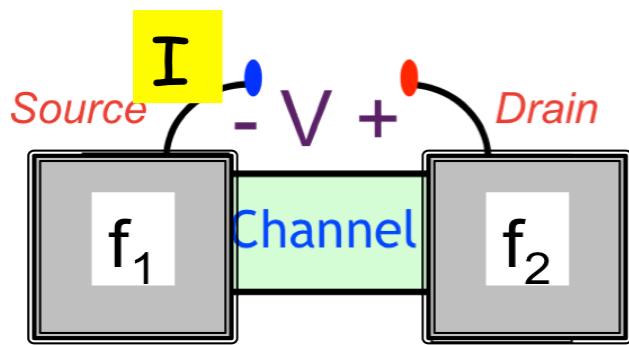
3.7g Fermi's golden rule

$$S_{m,m'} = \frac{2\pi}{\hbar} |\tau_{m,m'}|^2 \delta(E_m - E_{m'})$$



$$S_{m,m'} = \frac{2\pi}{\hbar} |\tau_{m,m'}|^2 |\tau_{N,N+1}|^2 \times \delta(E_m + N\hbar\omega - E_{m'} - \overline{N+1}\hbar\omega) + \frac{2\pi}{\hbar} |\tau_{m,m'}|^2 |\tau_{N,N-1}|^2 \times \delta(E_m + N\hbar\omega - E_{m'} - \overline{N-1}\hbar\omega)$$

$$S_{m,m'} = \frac{2\pi}{\hbar} |\tau_{m,m'}|^2 \times \left((N+1) \delta(E_m - E_{m'} - \hbar\omega) + N \delta(E_m - E_{m'} + \hbar\omega) \right)$$



The diagram shows a central green square labeled H . It is surrounded by three red hatched rectangular regions. The region on the left is labeled Σ_1 , the region on the right is labeled Σ_2 , and the region below is labeled Σ_0 . This represents a quantum system H interacting with three reservoirs Σ_0 , Σ_1 , and Σ_2 .

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

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

$$S_{m,m'} = \frac{2\pi}{\hbar} |\tau_{m,m'}|^2 \delta(E_m - E_{m'})$$

$$S_{m,m'} = \frac{2\pi}{\hbar} |\tau_{m,m'}|^2 \times$$

$$\begin{pmatrix} (N+1) \delta(E_m - E_{m'} - \hbar\omega) \\ + N \delta(E_m - E_{m'} + \hbar\omega) \end{pmatrix}$$

Coming up next ..

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 ..