

# ECE 659 Quantum Transport: Atom to Transistor

Lecture 19: Self Energy

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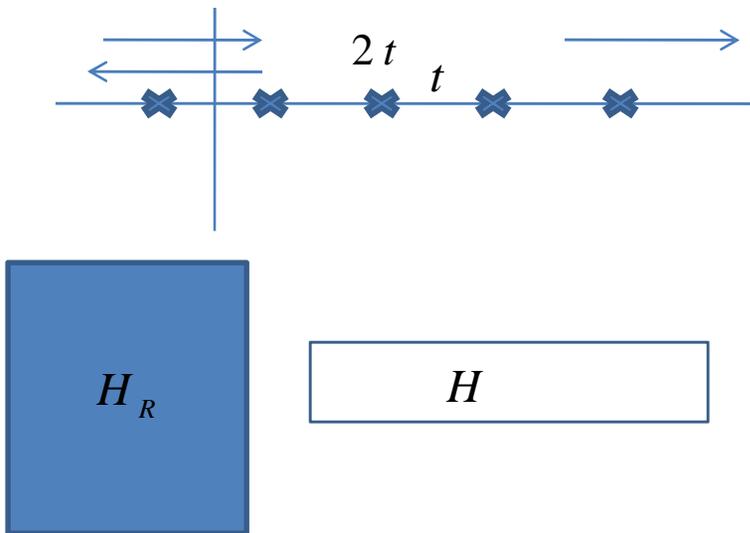
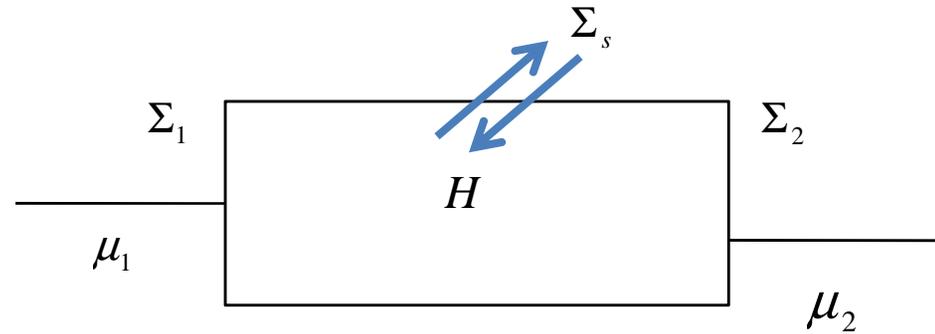
$$\Gamma_j = i[\Sigma_j - \Sigma_j^+]$$

$$\Sigma_j^{in} = \Gamma_j f_j$$

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

$$G^n = 2\pi\psi\psi^+$$

$$\Sigma^{in} = 2\pi s s^+$$



When reservoir and channel are disconnected

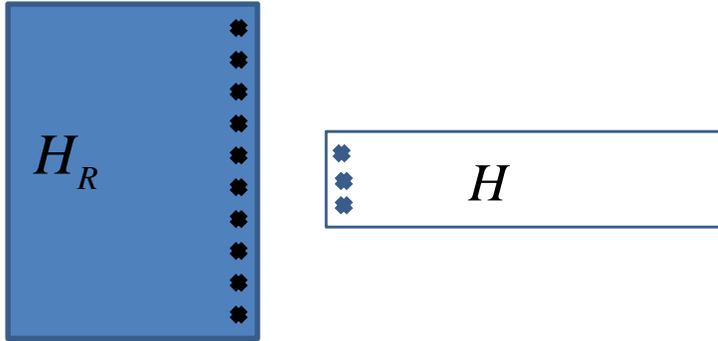
$$[EI - H]\psi = 0$$

$$[EI_R - H_R]\Phi_R = 0$$

To connect a battery to the reservoir:

$$[(E + i\eta)I_R - H_R]\Phi_R = s_R$$

$\eta$  allows an electron to go out of the reservoir



$$\begin{bmatrix} EI - H & -\tau \\ -\tau^+ & (E + i\eta)I_R - H_R \end{bmatrix} \begin{Bmatrix} \psi \\ \Phi_R \end{Bmatrix} = \begin{Bmatrix} 0 \\ s_R \end{Bmatrix}$$

$-\tau$  gives the coupling between reservoir and channel

$\Phi_R$  is changed due to that

$$\begin{bmatrix} EI - H & -\tau \\ -\tau^+ & (E + i\eta)I_R - H_R \end{bmatrix} \begin{Bmatrix} \psi \\ \Phi_R + \chi \end{Bmatrix} = \begin{Bmatrix} 0 \\ s_R \end{Bmatrix}$$

$$((E + i\eta)I_R - H_R)\Phi_R$$

$$+ ((E + i\eta)I_R - H_R)\chi$$

$$-\tau^+\psi = s_R$$

$$\chi = G_R \tau^+ \psi$$

where

$$G_R = [(E + i\eta)I_R - H_R]^{-1}$$

now

$$(EI - H) - \tau\chi = \tau\Phi_R$$

gives

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

$$\Sigma = \tau G_R \tau^+$$

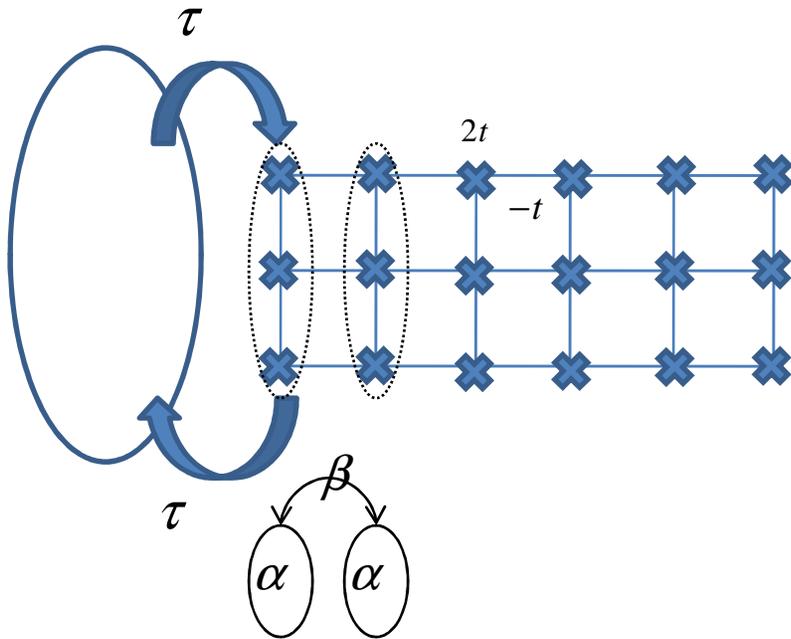
$$s = \tau\Phi_R$$

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

$$\Gamma = i\tau[G_R - G_R^+]\tau^+$$

$$= \tau A_R \tau^+$$

$$\Sigma^{in} \sim \tau\Phi_R\Phi_R^+\tau^+ \rightarrow \tau A_R \tau^+ f \rightarrow \Gamma f$$

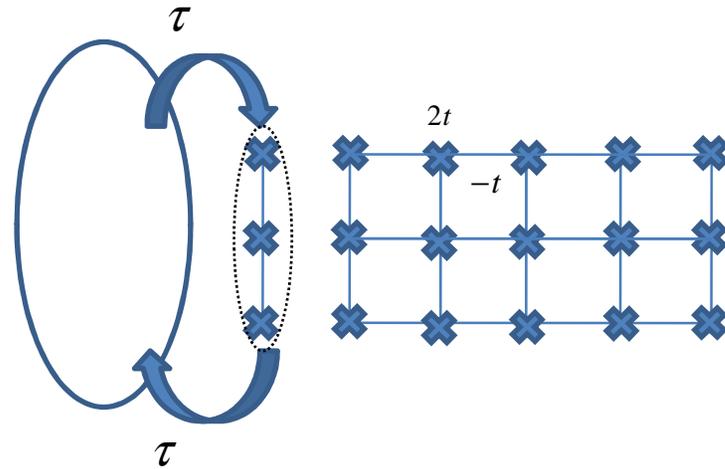


$$H = \begin{bmatrix} \alpha & \beta & & & \\ \beta^* & \alpha & \beta & & \\ & \beta^* & \alpha & \ddots & \\ & & & \ddots & \ddots \end{bmatrix}$$

We need top 3x3 elements of:

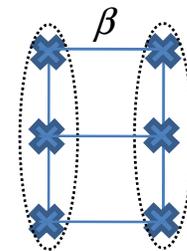
$$\left[ (E + i\eta)I_R - H_R \right]^{-1}$$

For 1 column:



$$g_1 = \left[ (E + i\eta)I - \alpha \right]^{-1}$$

For 2 columns:



$$g_2 = \left[ (E + i\eta)I - \alpha - \beta g_1 \beta^+ \right]^{-1}$$

In general: 
$$g_{n+1} = \left[ (E + i\eta)I - \alpha - \beta g_n \beta^+ \right]^{-1}$$

This can be solved recursively till  $g_{n+1}$  and  $g_n$  converge

In 1-D wire:

$$\Sigma = -te^{ika} = t^2 \left( -\frac{1}{t} e^{ika} \right)$$

with

$$\alpha = 2t$$

$$\beta = -t$$

Gives the same result with

$$\tau G_R \tau^+$$