

**ECE 495N**

# **Fundamentals of Nanoelectronics**

**Fall 2008**

**Instructor: Supriyo Datta  
Purdue University**

**Lecture: 32**

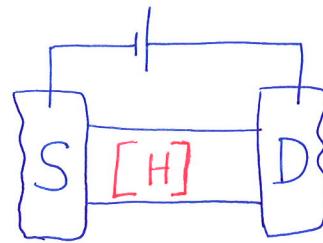
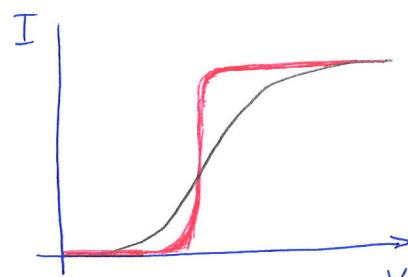
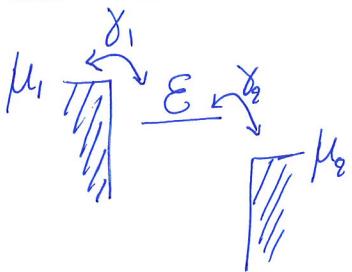
**Title: Correlation and Spectral Functions  
Date: November 17, 2008**

**Video Lectures posted at:  
<https://www.nanohub.org/resources/5346/>**

**Class notes taken by: Panagopoulos Georgios  
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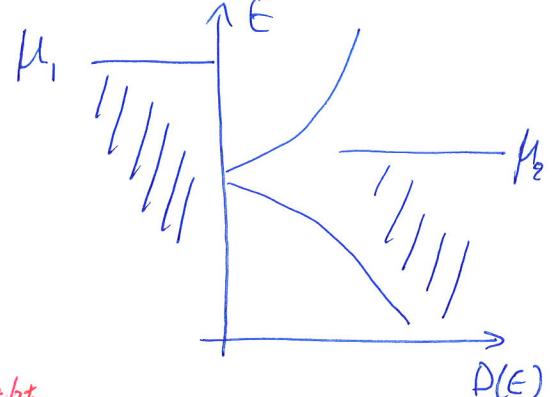
$$\gamma = \gamma_1 + \gamma_2$$



$$E \Phi = E \Phi \quad \text{time independent}$$

$$i\hbar \frac{\partial \Psi}{\partial t} = \epsilon \Psi \quad \text{time dependent}$$

$$\begin{aligned} \Psi(t) &= \Psi(0) e^{-iEt/\hbar} \\ \Psi^* \Psi(t) &= \Psi^* \Psi(0) e^{-iEt/\hbar} \end{aligned}$$



Density of States  
 $D(E)$

Spectral Function  
 $[A(E)]$

$[G''(E)]$

Correlation Function

$$i\hbar \frac{\partial \Psi}{\partial t} = \left( E - \frac{i\gamma_1}{2} - \frac{i\gamma_2}{2} \right) \Psi \quad \downarrow \quad \Psi(t) = \Psi(0) e^{-iEt/\hbar} e^{-\gamma_1 t/2\hbar} e^{-\gamma_2 t/2\hbar}$$

$$\rightarrow E \Phi = \left( E - \frac{i\gamma_1}{2} - \frac{i\gamma_2}{2} \right) \Phi \quad \downarrow \quad \Phi(t) = \Phi(0) e^{-iEt/\hbar} e^{-\gamma_1 t/2\hbar} e^{-\gamma_2 t/2\hbar}$$

$$i\hbar \frac{\partial \Psi}{\partial t} = \left( E - \frac{i\gamma}{2} \right) \Psi \Rightarrow \left( E - E + \frac{i\gamma}{2} \right) \Phi = 0$$

Electron Density  
 $n(E)$

We need to solve the problem of electrons get in from source, that is:

$$\left( E - E + \frac{i\gamma}{2} \right) \Phi = \mathcal{J}_1 \parallel \Phi = \frac{\mathcal{J}_1}{E - E + \frac{i\gamma}{2}}$$

$$\Phi^* \Phi = \frac{\mathcal{J}_1^* \mathcal{J}_1}{(E - \epsilon)^2 + \left(\frac{\gamma}{2}\right)^2}$$

$$N = \int_{-\infty}^{+\infty} dE \Phi^* \Phi = \mathcal{J}_1^* \mathcal{J}_1 \int_{-\infty}^{+\infty} dE \frac{1}{(E - \epsilon)^2 + \left(\frac{\gamma}{2}\right)^2} = \frac{\mathcal{J}_1^* \mathcal{J}_1}{\gamma} \int_{-\infty}^{+\infty} dE \frac{\gamma}{(E - \epsilon)^2 + \left(\frac{\gamma}{2}\right)^2}$$

$$\Rightarrow N = \frac{\mathcal{J}_1^* \mathcal{J}_1}{\gamma} \cdot 2\pi \Rightarrow N = \frac{\mathcal{J}_1^* \mathcal{J}_1}{\gamma_1 + \gamma_2} \cdot 2\pi$$

In the beginning of the semester we argued that

$$N = \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2} = \frac{\gamma_1}{\gamma_1 + \gamma_2}$$

Hence in order to be equal we have:

$$\frac{g_1^* f_1}{\gamma_1 + \gamma_2} \cdot 2\pi = \frac{\gamma_1}{\gamma_1 + \gamma_2} \Rightarrow g_1^* f_1 = \frac{\gamma_1}{2\pi}$$

the strength  
of the source  
should be  
proportional to  $\gamma_1$

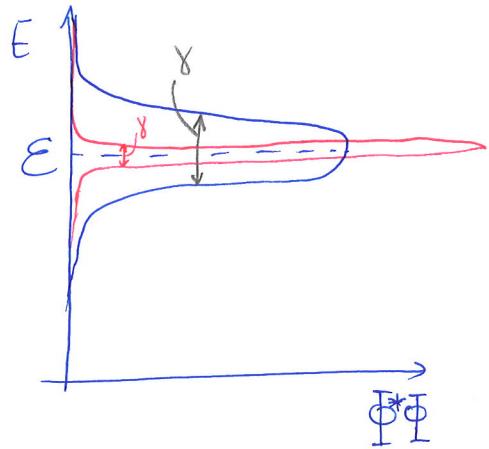
ALSO, electrons come from drain so  
(how we handle this?)

$$(E - \epsilon + \frac{i\gamma}{2}) \Phi = f_1 + f_2$$

$$\Phi = \frac{f_1 + f_2}{E - \epsilon + \frac{i\gamma}{2}}$$

$$\Phi^* \Phi = \frac{g_1^* f_1 + f_2^* f_2 + f_1^* f_2 + f_2^* f_1}{(E - \epsilon)^2 + (\frac{\gamma}{2})^2}$$

interference term  
It's not observed  
from experiment



$$H = \begin{bmatrix} \epsilon_1 & t \\ t & \epsilon_2 \end{bmatrix}$$

$$[EI - H] \{ \Phi \} = 0 \leftarrow \text{Shrodiger Equation for isolated system}$$

"external source frequency"

$$\begin{bmatrix} E - \epsilon_1 + \frac{i\gamma}{2} & -t \\ -t & E - \epsilon_2 + \frac{i\gamma}{2} \end{bmatrix} \begin{Bmatrix} \Phi_1 \\ \Phi_2 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix} = \begin{Bmatrix} f_1 \\ f_2 \end{Bmatrix}$$

or  $[EI - (H) - \sum_1 - \sum_2] \{ \Phi \} = \{ f \}, \quad \sum_1 = \begin{bmatrix} -i\frac{\gamma_1}{2} & 0 \\ 0 & 0 \end{bmatrix}, \quad \sum_2 = \begin{bmatrix} 0 & 0 \\ 0 & -i\frac{\gamma_2}{2} \end{bmatrix}$

$$\{\phi\} = [G] \{f\} *$$

Solution

where  $\{G\} = [E \cdot I - H - \sum_1 - \sum_2]^{-1}$

$\{G\}$  Green function of the system

$\{\phi\}^+ \{\phi\} [I \times I] \leftarrow \underline{1^{st} \text{ Choice}} \quad X$

$$G^n = \{\phi\} \{\phi\}^+ [N \times N] \leftarrow \underline{2^{nd} \text{ Choice}} \quad \checkmark$$

$$= [G] \{f_1\} \cdot \underbrace{\{f_1\}^+ [G]^+}_{[F_1] f_1}$$

↑  
Correlation matrix

if we want to add other sources we will add all of them here  
NOT  
adding  $f$  in the equation  $*$   
in order to find total number of electrons