

ECE 495N

Fundamentals of Nanoelectronics

Fall 2008

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**Lecture: 31
Title: Coherent Quantum Transport
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**Video Lectures posted at:
<https://www.nanohub.org/resources/5346/>**

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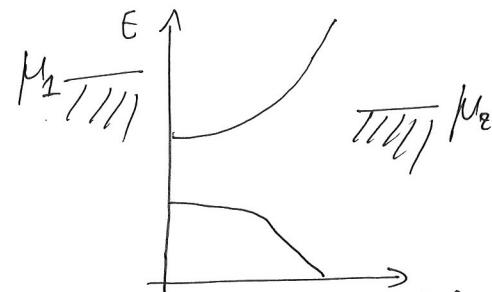
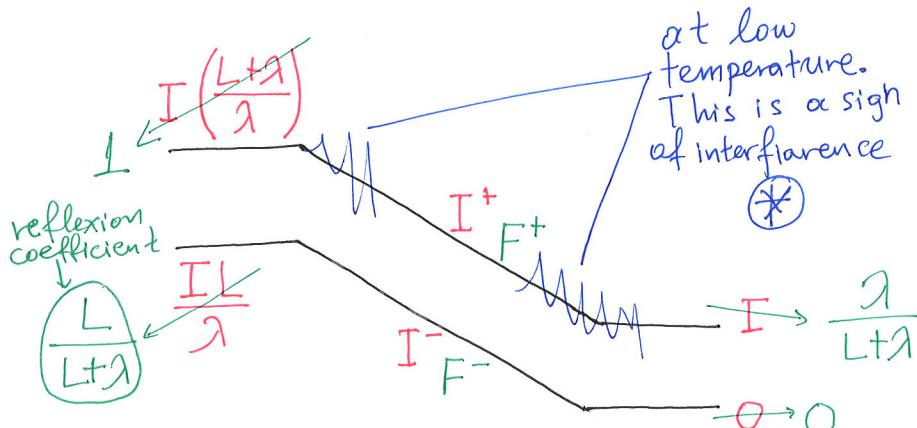
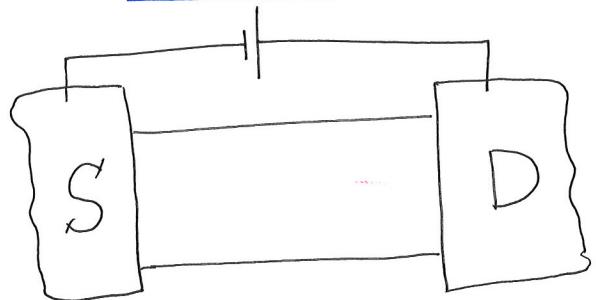
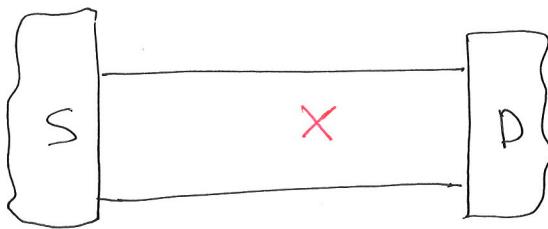


Coherent Quantum Transport

Lecture 31

Nov. 14, 2008

Semiclassical Theory



$$I^+ = \frac{e}{h} M(E) \Delta E \langle F^+ \rangle$$

It says if the state is occupied or not

$$\frac{dI^+}{dx} = \frac{dI^-}{dx} = \frac{-I}{\lambda}$$

mean free path

$$\Rightarrow I = -\lambda \frac{dI^\pm}{dx} = -\lambda \frac{e}{h} M(E) \Delta E \frac{dF^\pm}{dx}$$

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* This interference cannot be explained by the semiclassical theory. So we have to see how we will calculate quantum mechanically these oscillations.

NOTE 1

$$J = qunE + qD \frac{dn}{dx}$$

$$= qun \frac{dF^+}{dx}$$

quasi-Fermi level

NOTE 2

100 states	10 states
100 e ⁻	10 e ⁻
50 e ⁻	5 e ⁻

no current \rightarrow 5 e⁻

current \rightarrow 5 e⁻

The current at the left side is

$$I_1 = \frac{q}{h} \gamma_1 (f_1 - f)$$

at the right side

$$I_2 = \frac{q}{h} \gamma_2 (f - f_2)$$

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

$$I_1 = \frac{q}{h} \gamma_1 (f_1 - f) D(E) \parallel I_2 = \frac{q}{h} \gamma_2 (f - f_2) D(E)$$

$$n = \frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2} D(E)$$

$$\text{So, } I = \frac{q}{h} D(E) - \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} (f_1 - f_2)$$

The significance of Γ_1 and Γ_2 is the same as γ_1 and γ_2 . What we really have is:

antihermitian of Σ_1

$$\Gamma_1 = i [\Sigma_1 - \Sigma_1^+] \quad \text{and}$$

$$\Gamma_2 = i [\Sigma_2 - \Sigma_2^+] \quad \text{and the basic quantity:}$$

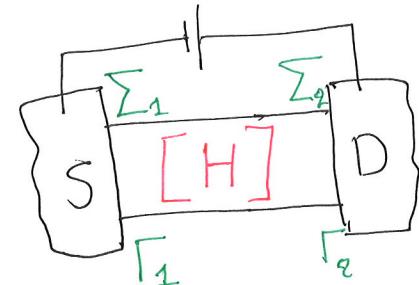
gives the DOS

$$G = \begin{bmatrix} E & I & H & \Sigma_1 & \Sigma_2 \\ \downarrow 10 \times 10 & \downarrow 10 \times 10 & \downarrow 10 \times 10 & \downarrow 10 \times 80 & \downarrow 10 \times 10 \end{bmatrix}^{-1}$$

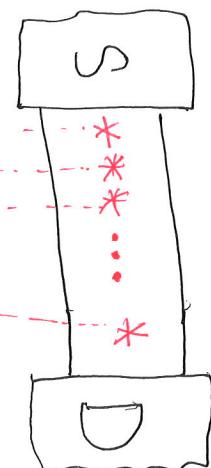
$$A(E) = A = i [G - G^+] = \begin{bmatrix} * & \dots & & & \\ * & \dots & & & \\ * & \dots & & & \\ \vdots & & & & \\ * & \dots & & & \end{bmatrix}$$

spectrum function

Thus finally we are taking not only the total density of states but also the Local Density of states



The new things we need to do current flow is something which will describe the connection of the channel to the contacts.



Similarly if we want to find electron density per energy then:

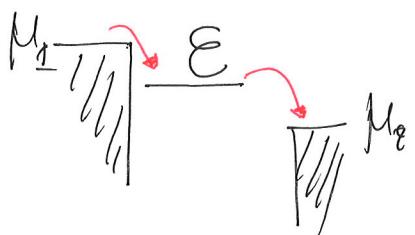
$$G^n = [G \Gamma_1 G^+] f_1 + [G \Gamma_2 G^+] f_2 = G^n(E)$$

if they injected only from the left, that is: $f_1 = 1$ and $f_2 = 0$

then

$$\underbrace{G^n = [G \Gamma_1 G^+]}_{\text{correlation function}}$$

Now we have to see how these equations are coming from. The simplest way to do it is to use a device with only one energy level:



For this device the Hamiltonian is $[H] = [\varepsilon]$

$$\begin{aligned} E\psi &= H\psi \Rightarrow (EI - H)\psi = 0 \\ \xrightarrow{\text{1 level}} (E - \varepsilon)\psi &= 0 \\ \xrightarrow{\substack{\text{non trivial} \\ \text{solution}}} E &= \varepsilon \end{aligned}$$

The time dependent version of this: $i\hbar \frac{d\psi}{dt} = \varepsilon \psi$
 $\Rightarrow \psi(t) = \psi(0) e^{-i\varepsilon t/\hbar}$. If we want electron density that is $\psi^* \psi(t) = \psi^* \psi(0)$. But we have to get in effect of the contacts to the wavefunction when they get in and get out. With the following it could be do it:

$$\left(E - \varepsilon + \frac{i\gamma}{\hbar} \right) \psi = 0 \xrightarrow{S} \psi(t) = \psi(0) e^{-Et/\hbar} e^{-\left(\frac{\gamma}{\hbar}\right)t/\hbar}$$

and hence $\psi^* \psi(t) = \psi^* \psi(0) e^{-\gamma t/\hbar}$