ECE 495N

Fundamentals of Nanoelectronics

Fall 2008

Instructor: Supriyo Datta
Purdue University

Lecture: 35
Title: NEGF II
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Video Lectures posted at:
https://www.nanohub.org/resources/5346/

Class notes taken by: Panagopoulos Georgios
Purdue University

PURDUE UNIVERSITY

NEGF continued II

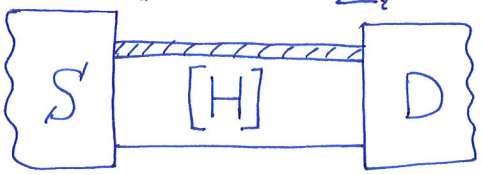
Lecture 35

Nov. 24, 2008

$$G = \left[EI - H - \Sigma\right]^{-1}$$

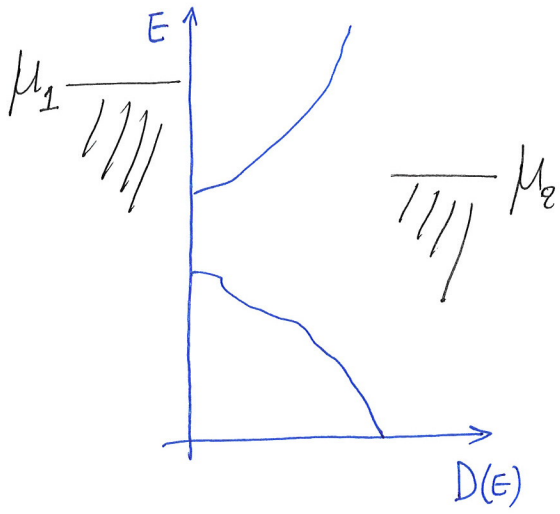
$$\Gamma = i\left[\Sigma - \Sigma^{+}\right]$$

$$\Sigma = \Sigma_1 + \Sigma_2$$



$$A = i\left[G - G^{+}\right] = G\left[\Gamma_1 + \Gamma_2\right]G^{+}$$

$$G^{n} = G\left[\underbrace{\Gamma_1 f_1}_{\Sigma_1^{in}} + \underbrace{\Gamma_2 f_2}_{\Sigma_2^{in}}\right]G^{+}$$



$$I_i = \frac{q}{h}\,\mathrm{Trace}\left[\Sigma_i^{in} A - \Gamma_i G^{n}\right]$$

$$i\hbar\frac{d\Psi}{dt} = H\Psi + \Sigma\Psi + S$$

$$\underset{1\times n}{\Psi^{*}}\;\underset{n\times 1}{\Psi^{+}} = G^{n}$$

$$i\hbar\frac{d}{dt}\left(\Psi\Psi^{+}\right) = \left(i\hbar\frac{d\Psi}{dt}\right)\Psi^{+} + \Psi\left(i\hbar\frac{d\Psi^{+}}{dt}\right)$$

$$\Rightarrow i\hbar\frac{d}{dt}\left(\Psi\Psi^{+}\right) = \left[H\Psi + \Sigma\Psi + S\right]\Psi^{+} + \Psi\left(i\hbar\frac{d\Psi^{+}}{dt}\right)$$

$$\rightarrow -i\hbar\frac{d\Psi^{+}}{dt} = \Psi^{+}H^{+} + \Psi^{+}\Sigma^{+} + S^{+}$$

$$\left[\Sigma - \Sigma^{+}\right]\left[\Psi\Psi^{+}\right]\cdot G^{n} = -i\Gamma\cdot G^{n}$$

$$\Rightarrow i\hbar\frac{d}{dt}\left(\Psi\Psi^{+}\right) = \left[H\Psi + \Sigma\Psi + S\right]\Psi^{+} - \Psi\left[\Psi^{+}H^{+} + \Psi^{+}\Sigma^{+} + S^{+}\right]$$

(because we apply trace: trace(ABC) = trace(CAB))

$$\Rightarrow \boxed{i\hbar\frac{d}{dt}\left(\Psi\Psi^{+}\right) = -i\Gamma G^{n} + S\Psi^{+} - \Psi S^{+}}$$

NOTE

$$\Psi = G S \Rightarrow \Psi^{+} = S^{+} G^{+}$$

$$\Rightarrow i\hbar \frac{d}{dt}\left(\Psi\Psi^{+}\right) = -i\Gamma G^{n} + S S^{+} G^{+} - S^{+} G S$$

due to traces $\Longrightarrow$

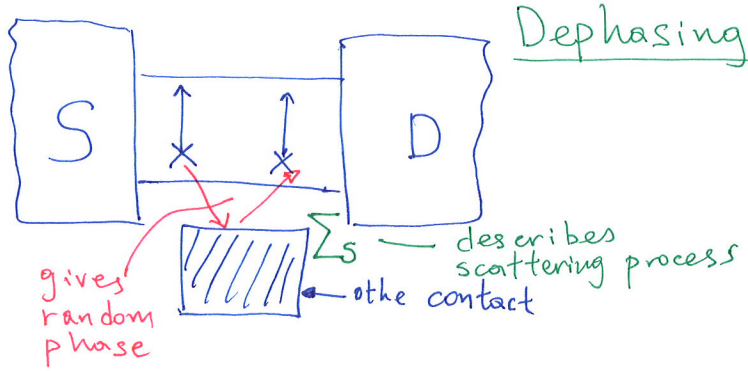
$$i\hbar \frac{d}{dt}\left(\Psi\Psi^{+}\right) = -i\Gamma G^{n} + \underbrace{S S^{+}}_{\Sigma^{in}} \underbrace{\left[G^{+} - G\right]}_{iA}$$

$$\Rightarrow \frac{d}{dt}\left(\Psi\Psi^{+}\right) = -\frac{\Gamma G^{n}}{\hbar} + \frac{\Sigma^{in} A}{\hbar} \xrightarrow{\text{at steady state}} 0$$

$\Gamma = \Gamma_1 + \Gamma_2$ — contribution to current I_1

$\Sigma^{in} = \Sigma_1^{in} + \Sigma_2^{in}$ — contribution to current I_2

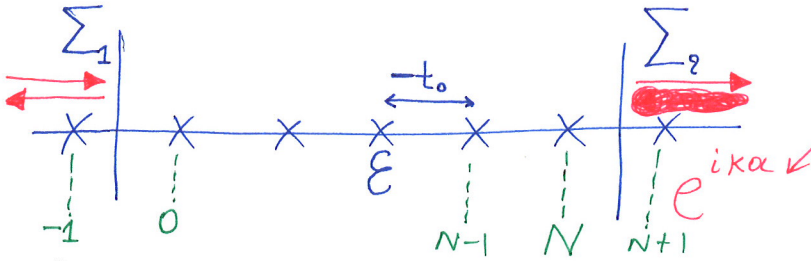
Dephasing



$$\begin{bmatrix} \varepsilon & t \\ t & \varepsilon \end{bmatrix}$$

$$-\frac{i}{2}\begin{bmatrix} \gamma_1(E) & 0 \\ 0 & 0 \end{bmatrix}$$

$$-\frac{i}{2}\begin{bmatrix} 0 & 0 \\ 0 & \gamma_2(E) \end{bmatrix}$$



we are supposing that the wavefunction at the end will have this form. This is just a boundary condition.

We know from previous lectures that the $E(k)$ relationship is:

$$E(k) = \varepsilon + 2t_0 \cos ka$$

$$\Sigma_1(E) = \left[\begin{array}{c|c} -t_0 e^{ika} & 0 \\ \hline 0 & 0 \end{array}\right]$$

$$\Sigma_2(E) = \left[\begin{array}{c|c} 0 & 0 \\ \hline 0 & -t_0 e^{ika} \end{array}\right]$$

For the last point (N)

$$E\psi_N = \varepsilon\psi_N - t_0\psi_{N-1} - t_0\psi_{N+1}$$

$$\psi_{N-1} = \sim e^{ik(N-1)a} = e^{ika}\psi_N$$

boundary condition that we are trying to impose

and $\psi_N = \sim e^{ikNa}$

$$\Rightarrow E\psi_N = \varepsilon\psi_N - t_0\psi_{N-1} - t_0 e^{ika}\psi_N$$

$$\Rightarrow E\psi_N = \left(\varepsilon - t_0 e^{ika}\right)\psi_N - t_0\psi_{N-1}$$

For the first point (0)

$$\Psi_n = e^{ikna} + re^{-ikna}$$

$n=0$: $\Psi_0 = 1 + r$

$n=-1$: $\Psi_{-1} = e^{-ika} + re^{ika} = (1+r)e^{ika} + (e^{-ika} - e^{ika})$

$$E\Psi_0 = \varepsilon\Psi_0 - t_0\Psi_{-1} - t_0\Psi_{+1} \quad \| \quad \Psi_{-1} = \Psi_0 e^{ika} + (e^{-ika} - e^{ika})$$

$$\Rightarrow E\Psi_0 = \varepsilon\Psi_0 - t_0\Psi_0 e^{ika} - t_0(e^{-ika} - e^{ika}) - t_0\Psi_{+1}$$

$$\Rightarrow E\Psi_0 = (\varepsilon - t_0 e^{ika})\Psi_0 - t_0\Psi_{+1} - t_0(e^{-ika} - e^{ika})$$

So, $\Sigma = -t_0 e^{ika}$

$$\Gamma = i(\Sigma - \Sigma^+) = -it_0(e^{ika} - e^{-ika})$$