Fundamentals of Nanoelectronics

ECE495 - Session 31, Nov 11, 2009

Non-Equilibrium Green's Function (NEGF) Method

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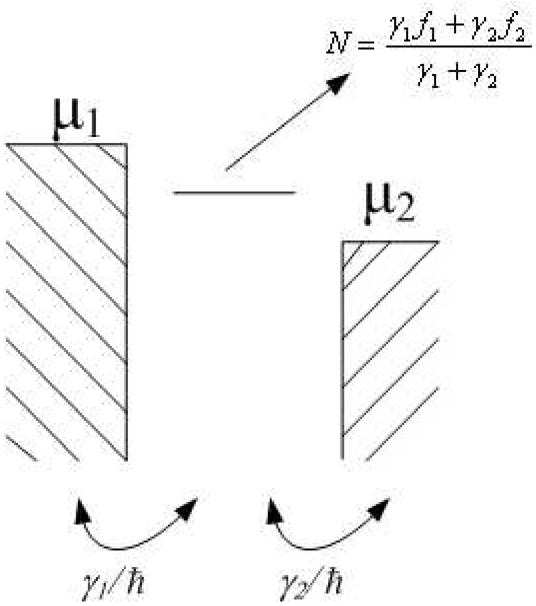
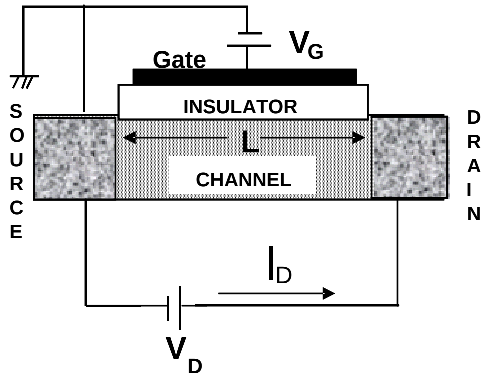
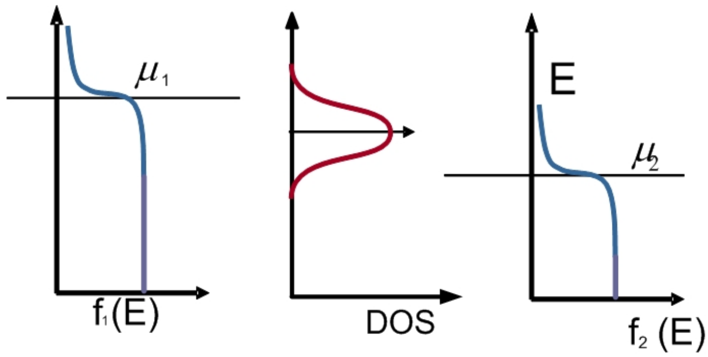
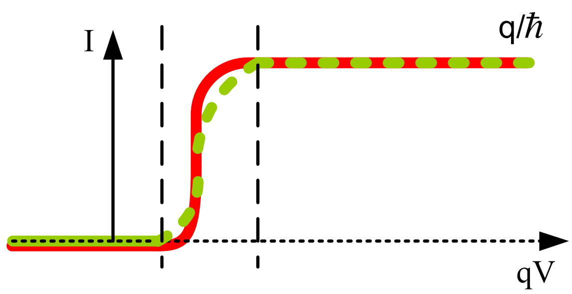
Review







$$I = \frac{q}{h}\int dE D(E)\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}(f_1 - f_2)$$



Schrodinger Eq. and Modified Schrodinger Eq.

$$E\{\Psi\} = [H]\{\Psi\}$$

$$E\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix} - \begin{bmatrix}\varepsilon & t\\t & \varepsilon\end{bmatrix} = \begin{bmatrix}E-\varepsilon & -t\\-t & E-\varepsilon\end{bmatrix}\begin{Bmatrix}\Psi_1\\\Psi_2\end{Bmatrix} = \begin{Bmatrix}0\\0\end{Bmatrix}$$

$$[\mathrm{EI} - \underbrace{\mathrm{H}}_{[\varepsilon]}]\{\Psi\} = \{0\}$$

$$\left(E - \varepsilon + \overbrace{\frac{i\gamma_1}{2} + \frac{i\gamma_2}{2}}^{\frac{i\gamma}{2}}\right)\{\Psi\} = \overbrace{0}^{S_1+S_2}$$ Modified Schrödinger Equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \left(\varepsilon - i\frac{\gamma}{2}\right)\Psi \qquad \textit{the time dependent version}$$

If we assume γ=0 then ⇒ $\begin{matrix}\Psi(t) = \psi(0)e^{-i\varepsilon t/\hbar} \\ \Psi\Psi^*(t) = \psi\,\psi^*(0)\end{matrix}$

$$\Rightarrow \begin{matrix}\Psi(t) = \psi(0)e^{-i\varepsilon t/\hbar}e^{-\gamma t/2\hbar} \\ \Psi\Psi^*(t) = \psi\,\psi^*(0)e^{-\gamma t/\hbar}\end{matrix}$$

If we assume $S_1 \neq 0$ then $\left(E - \varepsilon + \frac{i\gamma}{2}\right)\{\Psi\} = S_1$ then

$$\Psi = \frac{S_1}{E - \varepsilon + \frac{i\gamma}{2}} \Rightarrow \Psi\Psi^* = \frac{S_1 S_1^*}{(E-\varepsilon)^2 + \left(\frac{\gamma}{2}\right)^2}$$

$$N = \frac{S_1 S_1^*}{\gamma/2\pi}\underbrace{\int_{-\infty}^{\infty} dE \frac{1}{(E-\varepsilon)^2 + \left(\frac{\gamma}{2}\right)^2}}_{1} = \frac{\overbrace{S_1 S_1^*}^{\gamma_1/2\pi}}{\gamma/2\pi} = \frac{\gamma_1}{\gamma}$$

$$[EI - H - \Sigma_1 - \Sigma_2]\{\Psi\} = \{\mathrm{S}\}$$

Σ is a matrix in size of H and describes connect to contact.

$$\left(E - \varepsilon + \frac{i\gamma}{2}\right)\{\Psi\} = S_1 + S_2 \Rightarrow \Psi = \frac{S_1 + S_2}{E - \varepsilon + \frac{i\gamma}{2}} \Rightarrow \Psi\Psi^* = \frac{\overbrace{S_1 S_1^*}^{f_1} + \overbrace{S_2 S_2^*}^{f_2} + \overbrace{S_2 S_1^*}^{0} + \overbrace{S_1 S_2^*}^{0}}{(E-\varepsilon)^2 + \left(\frac{\gamma}{2}\right)^2}$$