Fundamentals of Nanoelectronics

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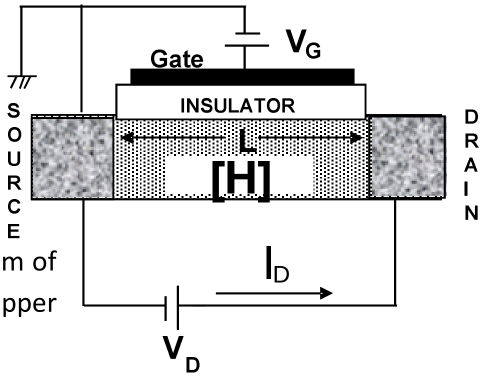
NEGF II

Professor Supriyo Datta

Class notes taken by: Mehdi Salmani



Semi-classical: $I = \frac{q}{h}\int dEM(E)\frac{\lambda}{L+\lambda}(f_1(E) - f_2(E))$

Quantum: $I = \frac{q}{h}\int dETrace(\Gamma_1 G \Gamma_2 G^+)(f_1 - f_2)$

The **trace** of an *n*-by-*n* square matrix *A* is defined to be the sum of the elements on the main diagonal (the diagonal from the upper left to the lower right).

Trace $\begin{bmatrix} 1 & 5 \\ 3 & 0.5 \end{bmatrix} = 1.5$

$$\left[EI - H - \overbrace{\Sigma}^{\Sigma_1+\Sigma_2}\right]\{\Psi\} = \{s\}$$

$\Psi = G\,S$ $\qquad\qquad$ $G^{-1} = EI - H - \Sigma$

$$\frac{[G^n]}{2\pi} = \Psi\Psi^+ = \underbrace{[\mathrm{G}]}_{\mathrm{N\times N}}\ \underbrace{\underbrace{[\mathrm{S}]}_{\mathrm{N\times 1}}\ \underbrace{[\mathrm{S}]^+}_{1\times\mathrm{N}}}_{\substack{\mathrm{N\times N} \\ \frac{[\Gamma]f_1}{2\pi}}}\ \underbrace{[\mathrm{G}]^+}_{\mathrm{N\times N}}$$

$$\frac{[G^n]}{2\pi} = \{\Psi\}\{\Psi\}^+ = \begin{bmatrix} \psi_1\psi_1^* & \psi_1\psi_2^* & \psi_1\psi_3^* & \psi_1\psi_4^* \\ \psi_2\psi_1^* & \psi_2\psi_2^* & . & . \\ . & . & \psi_3\psi_3^* & . \\ . & . & . & \psi_4\psi_4^* \end{bmatrix}$$

Each diagonal element shows electrons density at corresponding point. Trace of G^n will hand in total density of electrons.

$$[G^n] \equiv 2\pi\Psi\Psi^+ = G[\Gamma_1 f_1 + \Gamma_2 f_2]\mathrm{G}^+$$

If we assume f1=f2=1 then we can assume all states are filled and then we would have total number of states.

$$A = G[\Gamma_1 + \Gamma_2]\mathrm{G}^+$$

And as we know $\Gamma_\mathrm{i} = \mathrm{i}[\Sigma_\mathrm{i} - \Sigma_\mathrm{i}^+]$, we can prove $A = \mathrm{i}[\mathrm{G} - \mathrm{G}^+]$.

$[EI - H - \Sigma]\{\Psi\} = \{S\}$

$i\hbar\frac{d}{dt}\{\Psi\} = [H+\Sigma]\{\Psi\} + \{S\} \quad (I)$ This is ***time dependent*** modified Schrodinger Equation.

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

And based on (I) $i\hbar\frac{d}{dt}\{\Psi^+\} = \{\Psi^+\}[H+\Sigma^+] + \{S^+\} \quad (III)$

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

$$i\hbar\frac{dN}{dt} = \underbrace{Trace[H\Psi\Psi^+ - \Psi\Psi^+H]}_{0} + Trace[\Sigma\Psi\Psi^+ - \Psi\Psi^+\Sigma^+] + Trace[S\Psi^+ - \Psi S^+]$$

There is a general rule for trace: $Trace(ABC) = Trace(CAB)$, then:

$$i\hbar\frac{dN}{dt} = Trace[\Sigma-\Sigma^+]\Psi\Psi^+ + Trace[S\Psi^+ - \Psi S^+] = \frac{1}{2\pi}Trace[\Sigma-\Sigma^+]G^n + Trace[S\Psi^+ - \Psi S^+]$$

$$\frac{dN}{dt} = \frac{1}{2\pi\hbar}Trace\frac{[\Sigma-\Sigma^+]}{i}G^n + \frac{1}{i\hbar}Trace[S\Psi^+ - \Psi S^+]$$
$$= \frac{1}{h}(-Trace[\Gamma G^n] - iTrace[SS^+G^+ - GSS^+]$$

$$\frac{1}{i\hbar}\ Trace[SS^+G^+ - GSS^+] = \frac{1}{\hbar}\ Trace\left[\underbrace{SS^+}_{\frac{[\Gamma]f}{2\pi}}\underbrace{\frac{(G^+-G)}{i}}_{A}\right]$$

$$\frac{dN}{dt} = \frac{1}{h}(-Trace[\Gamma \underbrace{G^n}_{n}] + Trace[\Gamma \underbrace{A}_{DOS}]f)$$
$$= \frac{1}{h}(\underbrace{Trace([\Gamma_1 A]f_1 - [\Gamma_1 G^n])}_{I_1} + \underbrace{Trace([\Gamma_2 A]f_2 - [\Gamma_2 G^n])}_{I_2})$$

For I – current – we should multiply the expression by q factor.

As it is in steady state, then qdN/dt = 0 then $I_1=-I_2$.

$$I_1 = \frac{\gamma_1}{\hbar}(Df_1 - n)$$
$$I_2 = \frac{\gamma_2}{\hbar}(Df_2 - n)$$