Fundamentals of Nanoelectronics

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NEGF I

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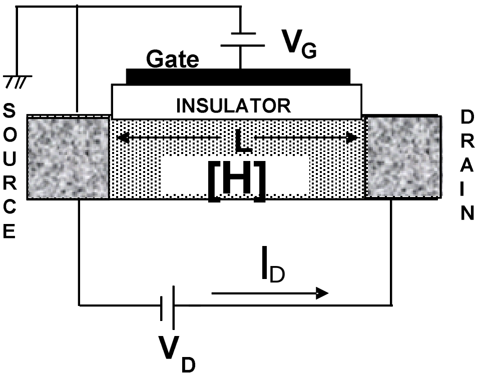
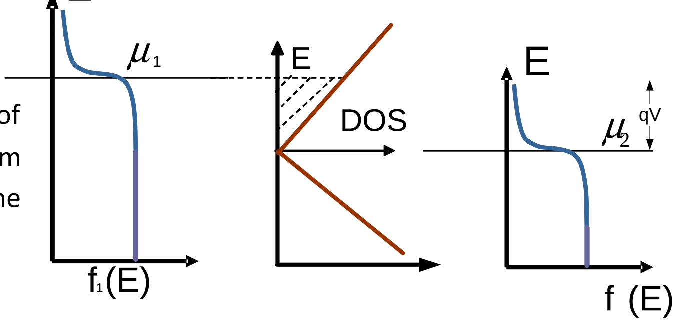


For closed systems the governing equation is:

$$[EI-H]\{\Psi\}=\{0\} \quad (\mathrm{I})$$

the eigenvalues of H give us the energy levels of the device. We are interested in the excitation of the channel due to contact. This change in the problem results in the following change in the Schrödinger equation:

$$[EI-H]\{\Psi\}=\{0\}\rightarrow$$
$$[EI-H-\Sigma]\{\Psi\}=\{S_1\}+\{S_2\} \quad (II)$$



Here, "H" describes the channel. "Σ" is matrix version of γ (which was the escape rate). "S" is the source term which tells us how electrons are getting into the channel.

$$(I)\ \rightarrow E\Psi=-\frac{\hbar}{2m}\nabla^2\Psi \text{ and } \Psi(\mathrm{r})=\sum\psi_{\mathrm{m}}\varphi_{\mathrm{m}}(\mathrm{r})$$

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

$$(II)\ \Rightarrow H\rightarrow H+\Sigma_1+\Sigma_2\xrightarrow{\mathrm{S=0}}\left(\mathrm{E}\begin{bmatrix}1&0\\0&1\end{bmatrix}+\begin{bmatrix}\varepsilon&\mathrm{t}\\\mathrm{t}&0\end{bmatrix}\right)\begin{Bmatrix}\psi_1\\\psi_2\end{Bmatrix}=\begin{Bmatrix}0\\0\end{Bmatrix}\Rightarrow\mathrm{E}\begin{Bmatrix}\psi_1\\\psi_2\end{Bmatrix}=\begin{bmatrix}\varepsilon&\mathrm{t}\\\mathrm{t}&0\end{bmatrix}\begin{Bmatrix}\psi_1\\\psi_2\end{Bmatrix}$$

$$\left(E-\varepsilon+\underbrace{\frac{i\gamma_1}{2}}_{-\Sigma_1}+\underbrace{\frac{i\gamma_2}{2}}_{-\Sigma_2}\right)=0\ \ \textit{and the time dependent version}\quad i\hbar\frac{\partial\Psi}{\partial t}=\left(\varepsilon-i\frac{\gamma}{2}\right)\Psi$$

$$\Rightarrow\begin{matrix}\Psi(t)=\ \psi(0)e^{-i\varepsilon t/\hbar}e^{-\gamma t/2\hbar}\\ \Psi\Psi^*(t)=\ \psi\,\psi^*(0)e^{-\gamma t/\hbar}\end{matrix}\qquad \text{and } \Gamma_1=\mathrm{i}\left[-\frac{\mathrm{i}\gamma_1}{2}-\frac{\mathrm{i}\gamma_2}{2}\right]=\gamma_1$$

$\Gamma_1=\mathrm{i}[\Sigma_1-\Sigma_1^+]$ and $\Gamma_2=\mathrm{i}[\Sigma_2-\Sigma_2^+]$

Green's Function

To show the effect of source in the wave function in the channel we can rewrite equation (I) as:

$$\{\psi\}=[G]\{S\}\quad \textit{where}\quad [G]=[EI-H-\Sigma]^{-1}$$

A nice observation is that, if energy E matches one of the energy levels in H, then the matrix G tends to be large. Since Ψ is given as the matrix product of G and S, there is significant response from the channel and that is reflected in Ψ.

G is called "***Green's function***". Notice that the [H] and [∑] that appear above are of the size of the channel; i.e. in order to describe the channel, you don't have to take the inverse of a matrix that has a huge Hamiltonian describing the whole system; rather you just take the Green's function describing the channel and deal with that which makes things a lot easier computationally. Notice that [∑] (self energy) gives the effect of coupling to the contacts and is important conceptually. For one thing, its imaginary part gives you the lifetime of the electron in the channel.

$$\left(E-\varepsilon+\overbrace{\frac{i\gamma_1}{2}+\frac{i\gamma_2}{2}}^{\gamma=\gamma_1+\gamma_2}\right)\Psi=S_1\Rightarrow\Psi=\frac{S_1}{E-\varepsilon+\frac{i\gamma}{2}}\Rightarrow\Psi\Psi^*=\frac{S_1S_1^*}{(E-\varepsilon)^2+\left(\frac{\gamma}{2}\right)^2}$$

ε is resonant energy of system and E is electron energy.

$$N=\int_{-\infty}^{\infty}dE\Psi\Psi^*=S_1S_1^*\int_{-\infty}^{\infty}dE\frac{1}{(E-\varepsilon)^2+\left(\frac{\gamma}{2}\right)^2}=\frac{S_1S_1^*}{\gamma}\int_{-\infty}^{\infty}dE\frac{\gamma}{(E-\varepsilon)^2+\left(\frac{\gamma}{2}\right)^2}$$

$\Rightarrow N=\frac{S_1S_1^*}{\gamma}.2\pi\Rightarrow N=\frac{S_1S_1^*}{\gamma_1+\gamma_2}.2\pi$ and from the beginning of semester we could remember:

$N=\frac{\gamma_1\overbrace{f_1}^{1}+\gamma_2\overbrace{f_2}^{0}}{\gamma_1+\gamma_2}=\frac{\gamma_1}{\gamma_1+\gamma_2}$ then $\frac{S_1S_1^*}{\gamma_1+\gamma_2}.2\pi=\frac{\gamma_1}{\gamma_1+\gamma_2}\Rightarrow S_1S_1^*=\frac{\gamma_1}{2\pi}$

$S_1S_1^*$, the strength of source, should be proportional to γ_1.

{Ψ} is a column vector and $\{\Psi\}^+$ (psi dagger) is conjugate transpose operator.

Then

$$\{\Psi\}\{\Psi\}^+=\begin{Bmatrix}\psi_1\\\psi_2\\\psi_3\\\psi_4\end{Bmatrix}\{\psi_1^*\quad\psi_2^*\quad\psi_3^*\quad\psi_4^*\}=\begin{bmatrix}\psi_1\psi_1^* & \psi_1\psi_2^* & \psi_1\psi_3^* & \psi_1\psi_4^*\\ \psi_2\psi_1^* & \psi_2\psi_2^* & . & .\\ .\ \cdot & & \psi_3\psi_3^* & .\\ \cdot\ \cdot & & . & \psi_4\psi_4^*\end{bmatrix}$$

All $\psi_i\psi_i^*$ are electron density along the device and other $\psi_i\psi_j^*$ where i≠j, show phase relation between wavefunction i and j.

Non-Equilibrium Green's Function

$\{\Psi\}\{\Psi\}^+\equiv\frac{G^n}{2\pi}$ This is matrix version of ***Density of Electrons.***

$\frac{[G^n]}{2\pi}=\Psi\Psi^+$ and $\underbrace{\Psi^+}_{1\times N}=\underbrace{S_1^+}_{1\times N}\underbrace{G^+}_{N\times N}$ then $\frac{[G^n]}{2\pi}=\Psi\Psi^+=\underbrace{[G]}_{N\times N}\underbrace{\underbrace{[S]}_{N\times 1}\underbrace{[S]^+}_{1\times N}}_{\substack{N\times N\\ \frac{[\Gamma]f_1}{2\pi}}}\underbrace{[G]^+}_{N\times N}$

$$\Rightarrow[G^n]=[G\Gamma_1G^+]f_1\ \overbrace{+[G\Gamma_2G^+]f_2}^{For\ S_2\ if\ we\ have}$$

If we have two sources, it is better to use the last achieved equation instead of the initial equations. They call this equation ***Non-Equilibrium Green's Function (NEGF)***.

$[G]=[EI-H-\Sigma_1-\Sigma_2]^{-1}$ and $[G^n]=[G\Gamma_1G^+]f_1+[G\Gamma_2G^+]f_2$