

G5: NEGF simulation of graphene-based devices

Supriyo Datta



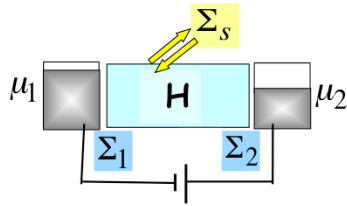
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Supriyo Datta



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G5.1. NEGF equations with elastic scatterers in equilibrium



$$\Gamma = i[\Sigma - \Sigma^*]$$

$$\varepsilon \rightarrow [H]$$

$$\gamma \rightarrow [\Gamma], [\Sigma]$$

$$n(E) \rightarrow [G^n(E)]$$

$$D(E) \rightarrow [A(E)]$$

Green function $[G] = [EI - H - \Sigma_1 - \Sigma_2 - \Sigma_s]^{-1}$

"Density of states" $A = i[G - G^*]$

"Electron density"

$$G^n = G\Gamma_2G^* f_2 + G\Gamma_1G^* f_1 + G\Sigma_s^{in}G^*$$

Current $\frac{I_1}{q/\hbar} = \text{Trace}([[\Gamma_1A] f_1 - [\Gamma_1G^n])$

Dephasing $[\Sigma_s^{in}] = D[G^n]$

$$[\Sigma_s] = D[G]$$



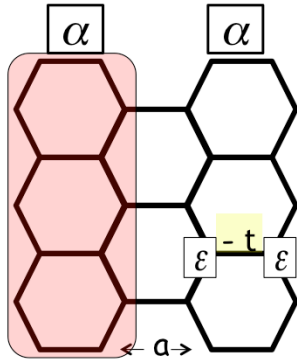
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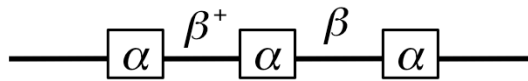
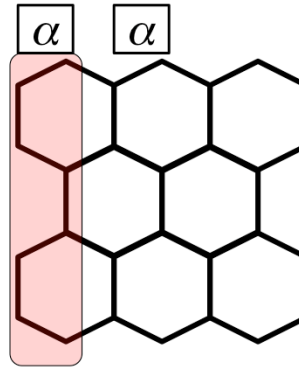


G5.2. Tight-binding model

Armchair



Zigzag

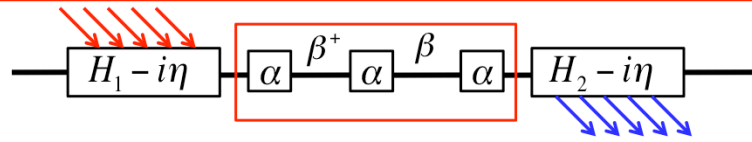


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Supriyo Datta

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G5.3. Contact self-energy



$$\begin{bmatrix} E + i\eta - H_1 & -\beta & 0 \\ -\beta^+ & E - H & -\beta \\ 0 & -\beta^+ & E + i\eta - H_2 \end{bmatrix} \begin{Bmatrix} \Phi_1 + \chi_1 \\ \psi \\ \chi_2 \end{Bmatrix} = \begin{Bmatrix} s_1 \\ 0 \\ 0 \end{Bmatrix}$$

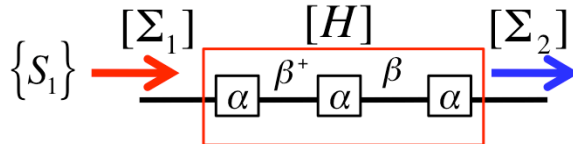
$$\Sigma_2 = \beta g_2 \beta^+$$

$$[E - H - \Sigma_1 - \Sigma_2] \{\psi\} = \{S_1\}$$

Iterative solution of

$$[g_2]^{-1} = EI - \alpha - \beta^+ g_2 \beta$$

yields g_2



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