

FUNDAMENTALS OF NANOELECTRONICS

B. Quantum Transport

1. Schrodinger Equation
2. Contact-ing Schrodinger
- More Examples**
4. Spin Transport



- 3.1. Introduction
- 3.2. Quantum Point Contact
- 3.3. Self-Energy**
- 3.4. Surface Green's Function
- 3.5. Graphene
- 3.6. Magnetic Field
- 3.7. Golden Rule
- 3.8. Inelastic Scattering
- 3.9. Can NEGF Include Everything?
- 3.10. Summing up ..

3.3a Self-Energy

$$\begin{matrix} \Sigma_1^{in} & & \Sigma_2^{in} \\ \Sigma_1 & H & \Sigma_2 \end{matrix}$$

$$B^2 = f_1(E) \frac{a}{2\pi \hbar v}$$

$$\begin{matrix} \Sigma_1 & & H & & \Sigma_2 \\ \begin{bmatrix} te^{ika} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} & & \begin{bmatrix} \varepsilon & t & 0 \\ t & \varepsilon & t \\ 0 & t & \varepsilon \end{bmatrix} & & \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & te^{ika} \end{bmatrix} \end{matrix}$$

-1 0 .. N N+1

$B e^{+ikna}$ t t ε

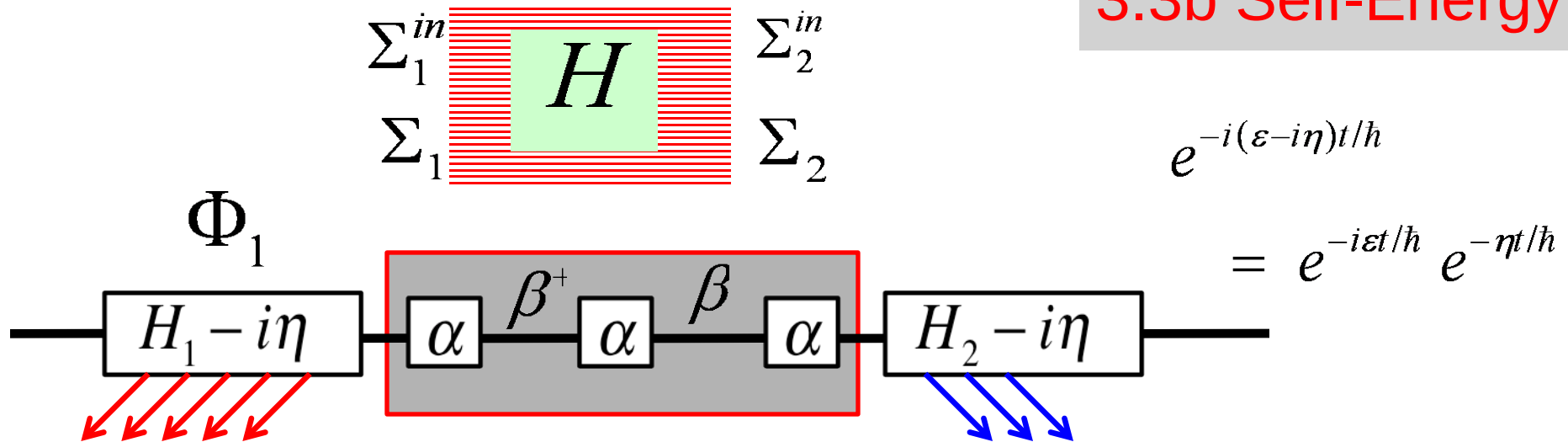
$$s_1 = \begin{Bmatrix} -i \frac{B \hbar v}{a} \\ 0 \\ 0 \end{Bmatrix}$$

$$E\psi = H\psi + (\Sigma_1 + \Sigma_2)\psi + s_1$$

Outflow

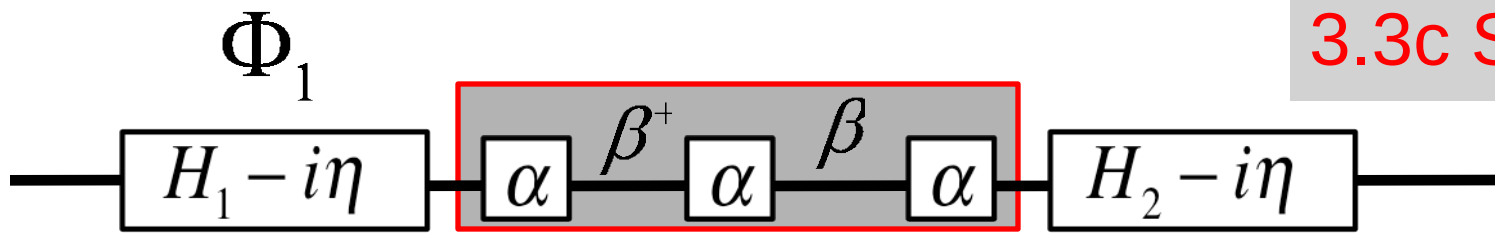
Inflow

3.3b Self-Energy



$$\begin{bmatrix} E + i\eta - H_1 & 0 & 0 \\ 0 & E - H & 0 \\ 0 & 0 & E + i\eta - H_2 \end{bmatrix} \begin{Bmatrix} \Phi_1 \\ 0 \\ 0 \end{Bmatrix} = \begin{Bmatrix} \tilde{s}_1 \\ 0 \\ 0 \end{Bmatrix}$$

$$\begin{bmatrix} E + i\eta - H_1 & -\tau_1^+ & 0 \\ -\tau_1 & E - H & -\tau_2 \\ 0 & -\tau_2^+ & E + i\eta - H_2 \end{bmatrix} \begin{Bmatrix} \Phi_1 + \chi_1 \\ 0 + \psi \\ 0 + \chi_2 \end{Bmatrix} = \begin{Bmatrix} \tilde{s}_1 \\ 0 \\ 0 \end{Bmatrix}$$



$$\chi_1 = [E + i\eta - H_1]^{-1} \tau_1^+ \psi$$

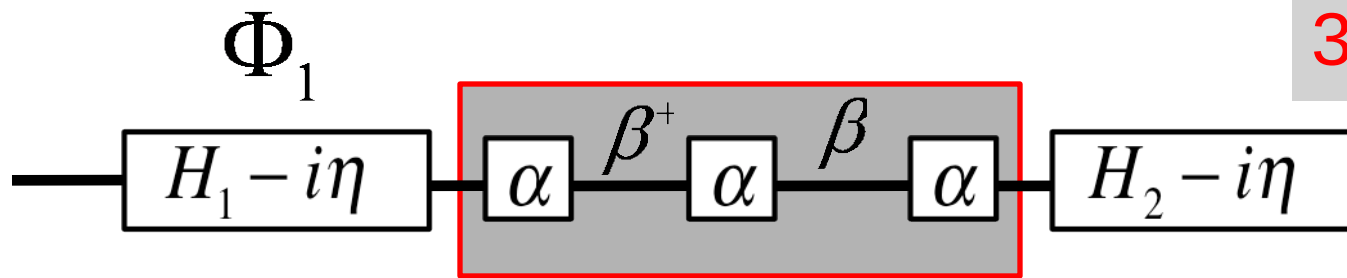
$$\chi_2 = [E + i\eta - H_2]^{-1} \tau_2^+ \psi$$

$$-\tau_1[\Phi_1 + \chi_1] + [E - H]\psi - \tau_2\chi_2 = 0$$

$$\begin{bmatrix} E + i\eta - H_1 & -\tau_1^+ & 0 \\ -\tau_1 & E - H & -\tau_2 \\ 0 & -\tau_2^+ & E + i\eta - H_2 \end{bmatrix} \begin{Bmatrix} \Phi_1 + \chi_1 \\ \psi \\ \chi_2 \end{Bmatrix} = \begin{Bmatrix} \tilde{s}_1 \\ 0 \\ 0 \end{Bmatrix}$$

$$[E + i\eta - H_1]\Phi_1 + [E + i\eta - H_1]\chi_1 - \tau_1^+\psi = \tilde{s}_1$$

$$-\tau_2^+\psi + [E + i\eta - H_2]\chi_2 = 0$$



$$\chi_1 = [E + i\eta - H_1]^{-1} \tau_1^+ \psi$$

$$\chi_2 = [E + i\eta - H_2]^{-1} \tau_2^+ \psi$$

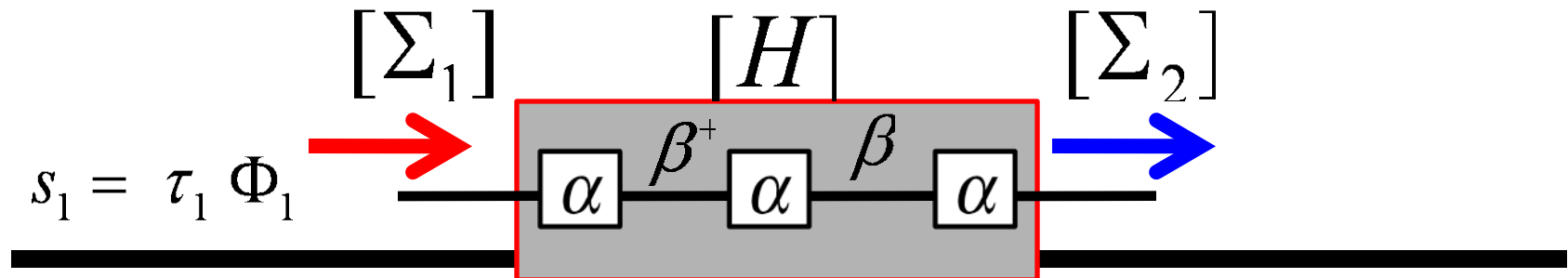
$$-\tau_1[\Phi_1 + \chi_1] + [E - H]\psi - \tau_2\chi_2 = 0$$



$$E\psi = H\psi + (\Sigma_1 + \Sigma_2)\psi + s_1$$

$$= \tau_1 \overbrace{[E + i\eta - H_1]^{-1}}^{g_1} \tau_1^+$$

$$= \tau_2 \overbrace{[E + i\eta - H_2]^{-1}}^{g_2} \tau_2^+$$



$$E\psi = H\psi + (\Sigma_1 + \Sigma_2)\psi + s_1$$

$$\Sigma_1 = \tau_1 \overbrace{[E + i\eta - H_1]^{-1}}^{g_1} \tau_1^+$$

$$s_1 = \tau_1 \Phi_1$$

$$[\Gamma_1] = i[\Sigma_1 - \Sigma_1^+]$$

$$[AB]^+ = B^+ A^+$$

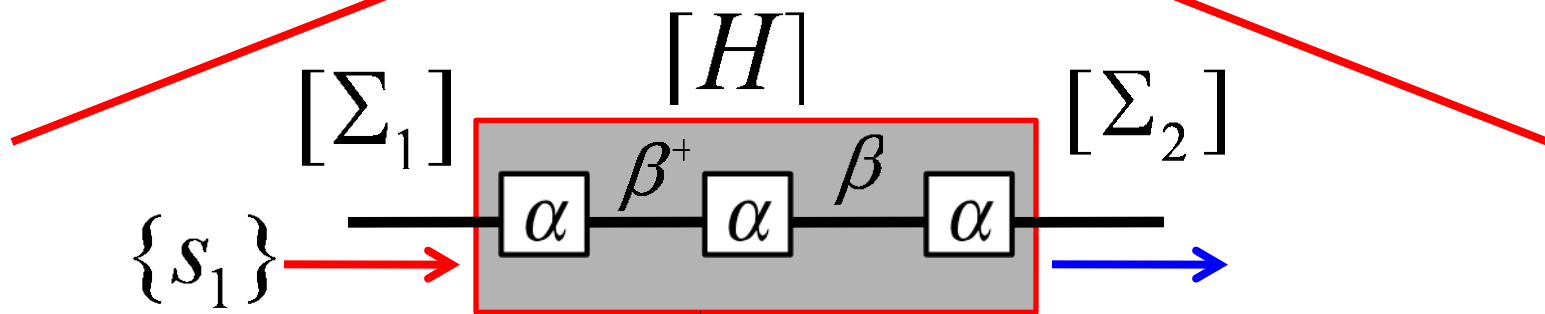
$$[\Sigma_1^{in}] = \{s_1\} \{s_1\}^+$$

$$= \tau_1 \underbrace{\Phi_1 \Phi_1^+}_{g_1^n} \tau_1^+$$

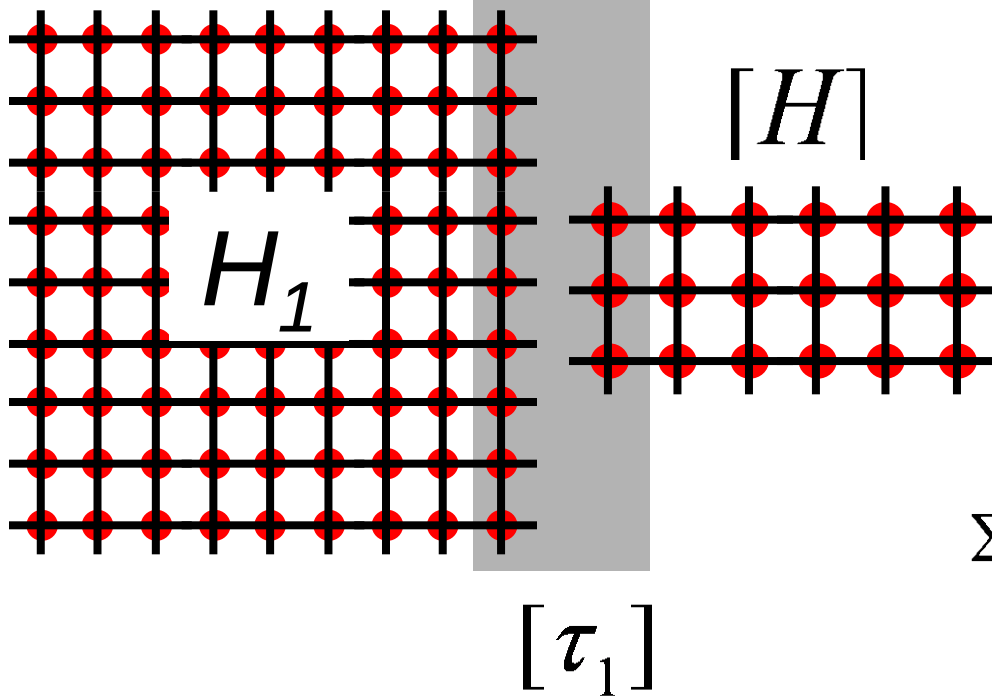
$$= \tau_1 g_1^n \tau_1^+ \rightarrow [\Gamma_1] f_1$$

$$= \tau_1 i[g_1 - g_1^+] \tau_1^+$$

$$= \tau_1 a_1 \tau_1^+ \rightarrow [a_1] f_1$$



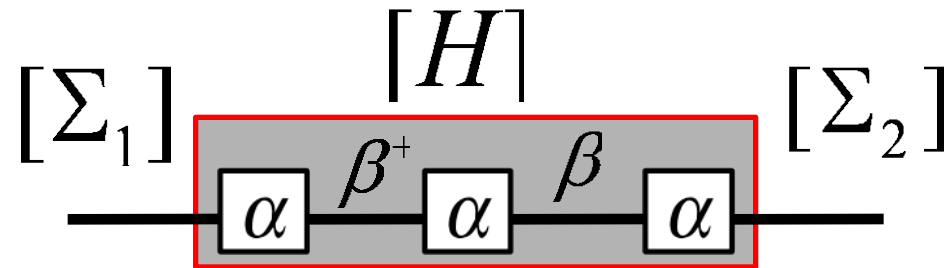
3.3f Self-Energy



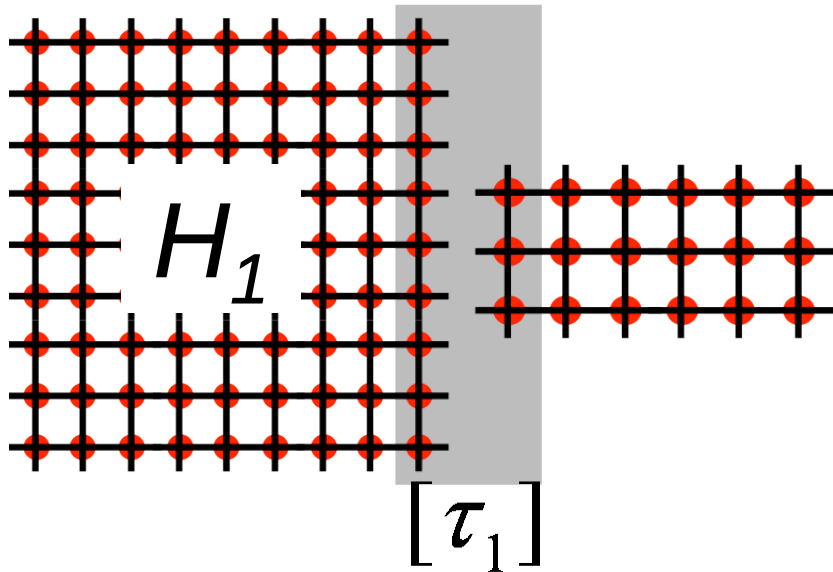
$$\Sigma_1 = \tau_1 \overbrace{[E + i\eta - H_1]^{-1}}^{g_1} \tau_1^+$$

Matrix dimensions: 3×9 (for τ_1), 9×9 (for g_1), and 9×3 (for τ_1^+).

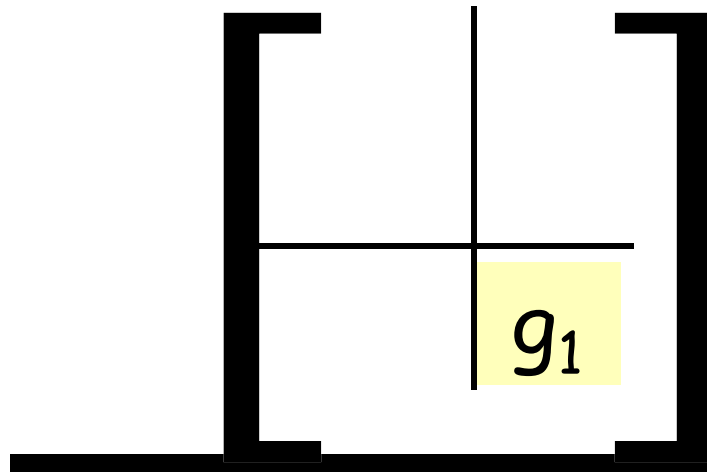
$$\begin{bmatrix} & \\ & g_1 \end{bmatrix}$$



Coming up next ..



$$\Sigma_1 = \tau_1 \overbrace{[E + i\eta - H_1]^{-1}}^{g_1} \tau_1^+$$



3.4. Surface Green's Function

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