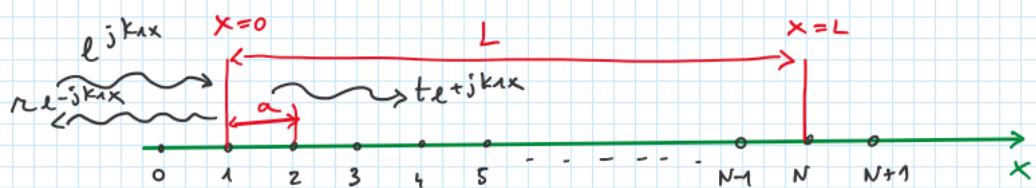
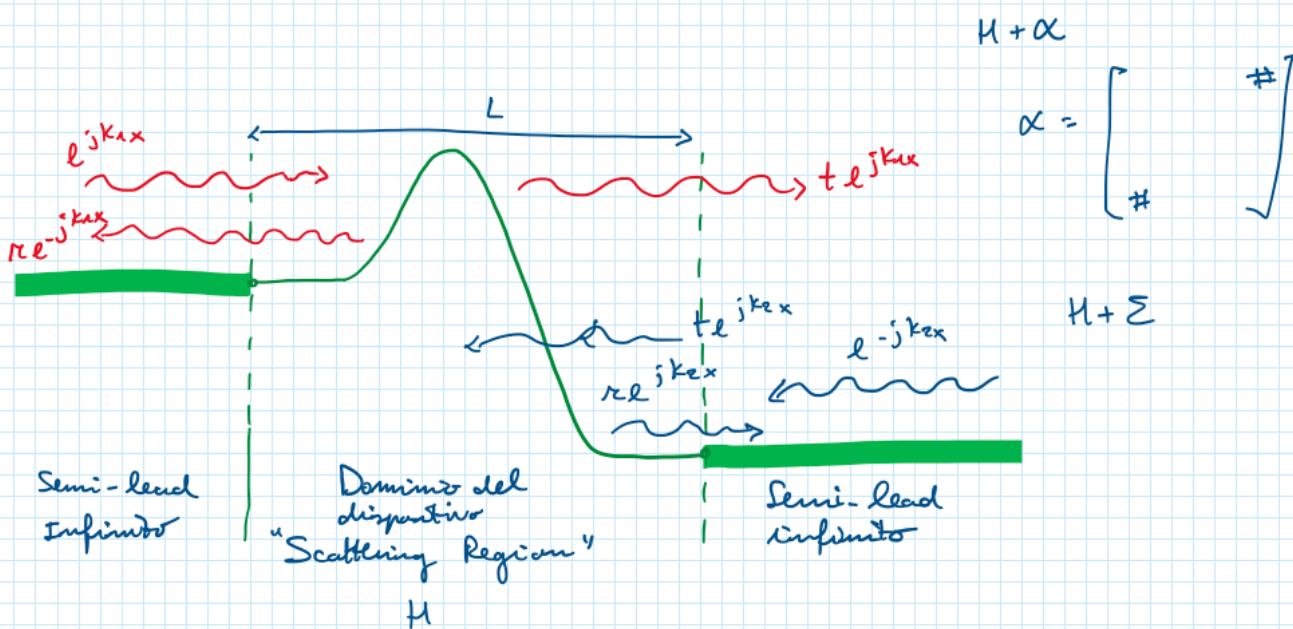
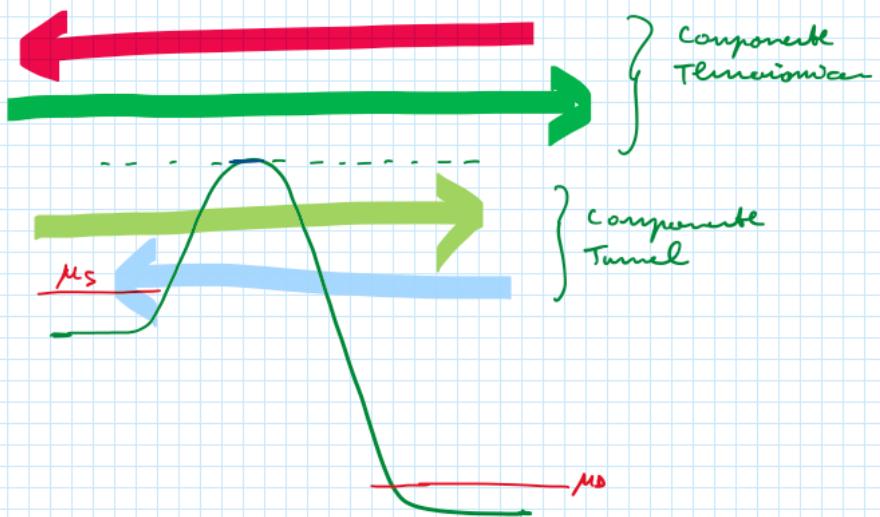


OPEN BOUNDARY CONDITIONS

Monday, 6 May 2019 09:35



$$x \leq 0 \quad \varphi(x) = 1 \cdot e^{j k x} + r e^{-j k x}$$

$$\varphi(x=0) = \varphi(0) = 1 + r = \varphi_1$$

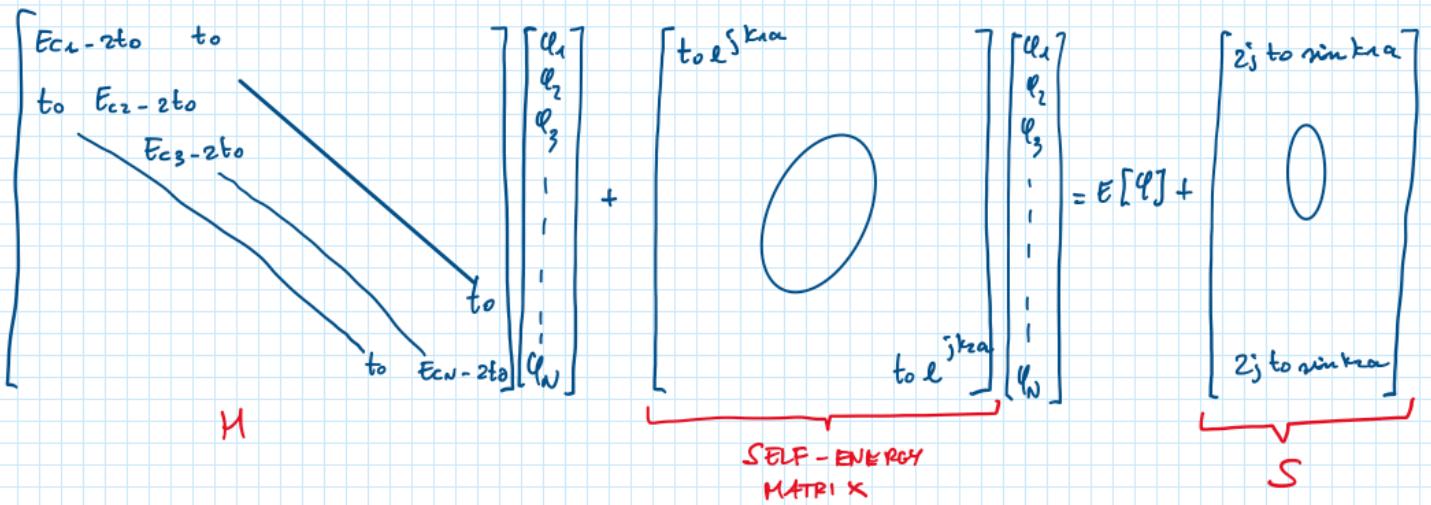
$$\begin{aligned} \varphi(x=-a) &= \varphi_0 = e^{-j k a} + r e^{j k a} = e^{-j k a} + r e^{j k a} + e^{j k a} - e^{j k a} = \\ &= e^{-j k a} - e^{j k a} + e^{j k a} [r + 1] = \\ &= e^{-j k a} - e^{j k a} + e^{j k a} \varphi_1 = \varphi_0 \end{aligned}$$

$x = -a$
 punto del lead
 semi-infinito

$$t_0 \varphi_0 + (E_{C1} - 2t_0) \varphi_1 + t_0 \varphi_2 = E \varphi_1$$

$$t_o \begin{bmatrix} e^{-jk\alpha} & -e^{jk\alpha} \end{bmatrix} + t_o e^{jk\alpha} \varphi_1 + (E_1 - 2t_o) \varphi_1 + t_o \varphi_2 = E \varphi_1$$

$$\left[E_1 - 2t_o + t_o e^{jk\alpha} \right] \varphi_1 + t_o \varphi_2 = E \varphi_1 + 2j t_o \sin(k\alpha)$$



$$(EI - H - \Sigma) \varphi = S$$

$$\Sigma = \Sigma_1 + \Sigma_2$$

$$\Sigma_1 = \begin{bmatrix} t_o e^{jk\alpha} & & \\ & \textcircled{1} & \\ & & t_o e^{jk\alpha} \end{bmatrix} ; \quad \Sigma_2 = \begin{bmatrix} & & \\ & \textcircled{2} & \\ & & t_o e^{jk\alpha} \end{bmatrix}$$

$$\varphi = \underbrace{\begin{bmatrix} EI - H - \Sigma \end{bmatrix}}_{G(E)}^{-1} S$$

GREEN'S
FUNCTION

H, Σ Ingredients

$$G(\mathbf{r}) = [E_I - H - \Sigma_1 - \Sigma_2]^{-1} \quad \text{Green's function}$$

$$\begin{aligned} \Gamma_1 &= i [\Sigma_1 - \Sigma_1^+] \\ \Gamma_2 &= i [\Sigma_2 - \Sigma_2^+] \end{aligned} \quad \left. \begin{array}{l} \text{Spectral} \\ \text{Matrix} \end{array} \right\}$$

$$LDOS_1 = \frac{1}{2\pi} \text{diag} \{ G \Gamma_1 G^+ \}$$

$$LDOS_2 = \frac{1}{2\pi} \text{diag} \{ G \Gamma_2 G^+ \}$$

$$LDOS = LDOS_1 + LDOS_2$$

$$T = \text{tr} \left\{ \Gamma_2 G \Gamma_1 G^+ \right\} = \text{tr} \left\{ \Gamma_1 G \Gamma_2 G^+ \right\}$$

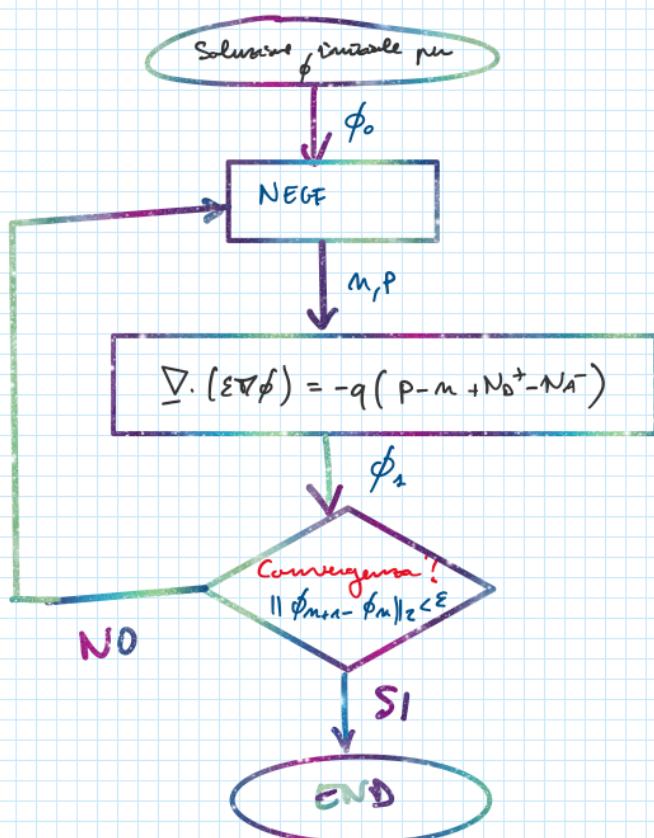
S. Datta "From Atoms to Transistors", Ed. Cambridge Univ. Press (Chapt. 8, 9, 10)

S. Datta, Superlattices & Microstructures, Vol. 28, No. 4, p. 253, 2000.

$$m = ② \int_{E_C}^{+\infty} dE \left\{ LDOS_1 f(E-E_{F1}) + LDOS_2 f(E-E_{F2}) \right\}$$

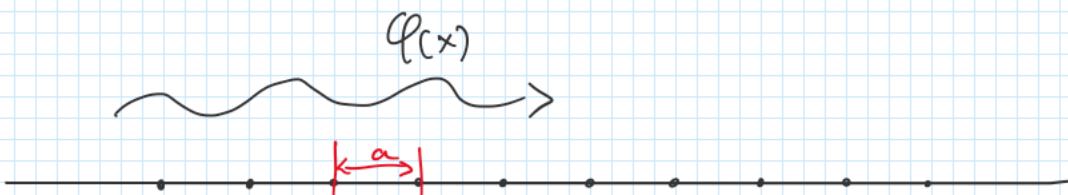
$$P = 2 \int_{-\infty}^{E_V} dE \left\{ LDOS_1 [1 - f(E-E_{F1})] + LDOS_2 [1 - f(E-E_{F2})] \right\}$$

$$J = \frac{2e}{n} \int_{-\infty}^{+\infty} T(E) [f(E-E_{F1}) - f(E-E_{F2})] dE$$



RELATI~~O~~NE DISPERSIONE EMA DISCRETIZZATA

Monday, 6 May 2019 10:45



$$-\frac{\pi^2}{2m\omega} \frac{\delta^2 \phi}{\delta x^2} + E_c \phi = E \phi$$

$$-t_0 [\phi_{m+1} - 2\phi_m + \phi_{m-1}] = (E - E_c) \phi_m$$

$$\phi(x) = e^{j k x} \xrightarrow{x=m a} \phi(m a) = e^{j k m a}$$

$$-t_0 [e^{j k(m+1)a} - 2e^{j k m a} + e^{j k(m-1)a}] = (E - E_c) e^{j k m a}$$

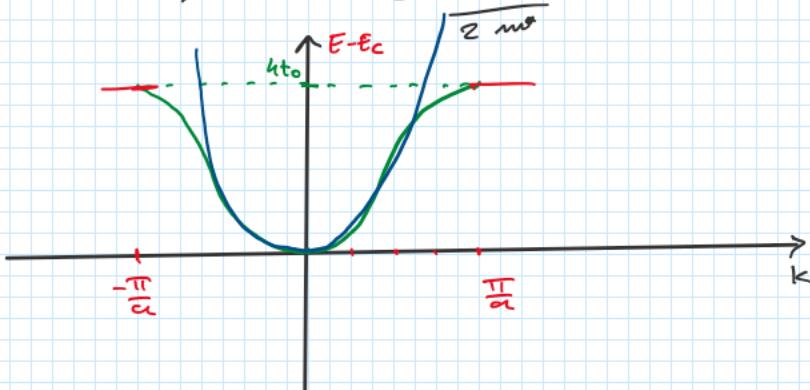
Se dividere per $e^{j k m a}$

$$-t_0 [e^{j k a} - 2 + e^{-j k a}] = (E - E_c)$$

$$E = E_c - t_0 [2 \cos(k a) - 2] = E_c + 2t_0 [1 - \cos k a]$$

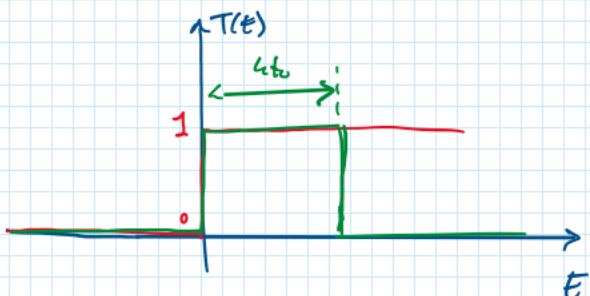
$$ka \ll 1 \Rightarrow 1 - \cos ka \approx 1 - \left[1 - \frac{k^2 a^2}{2} \right] \approx \frac{k^2 a^2}{2}$$

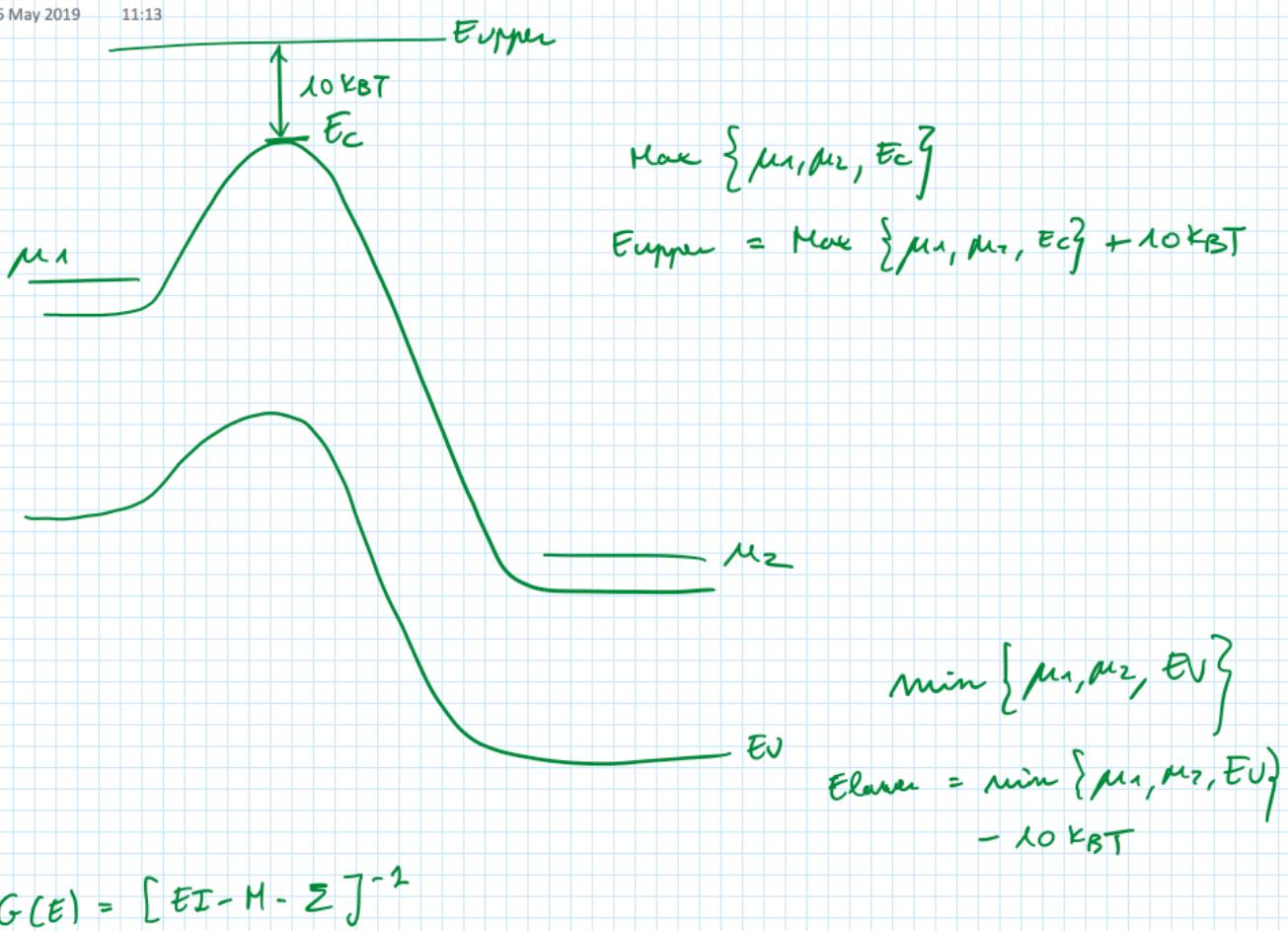
$$ka \ll 1 \Rightarrow E \approx E_c + \frac{\pi^2 k^2}{2 m \omega}$$



$$E = 0$$

$$E \ll \underline{u_{t_0}}$$





$$G(E) = [EI - H - \Sigma]^{-1}$$

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} & H_{23} \\ & H_{32} & H_{33} & H_{34} \\ & H_{43} & H_{44} & H_{45} \end{bmatrix}$$

N_c # di matrici sulla diagonale

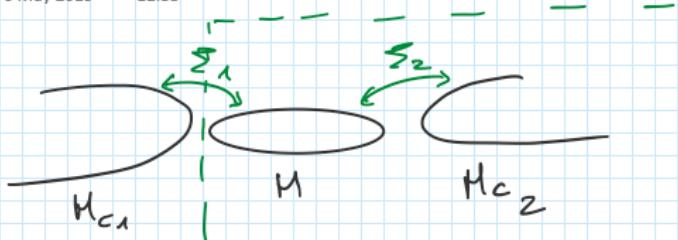
n è l'ordine della matrice

ordine di $H = n \cdot N_c$

$$\Theta[(n \cdot N_c)^3]$$

RGF Recursive Green's Function

$$\Theta [N_c \cdot (n)^3]$$



$$\boldsymbol{M}_{\text{TOT}} = \begin{bmatrix} M & \beta \\ \beta^+ & M_c \end{bmatrix}$$

$$G = [EI - M]^{-1}$$

$$\boldsymbol{M} = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \quad \boldsymbol{M}^{-1} = \begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}$$

$$\boldsymbol{M}_M = [A - BD^{-1}C]^{-1}$$

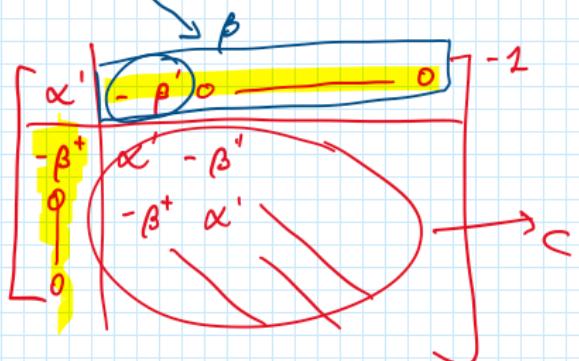
$$G = \begin{bmatrix} EI - M & -\beta \\ -\beta^+ & EI - M_c \end{bmatrix}^{-1}$$

$$EI - M = \alpha$$

$$G = \begin{bmatrix} \alpha & -\beta \\ -\beta^+ & EI - M_c \end{bmatrix}^{-1} = \begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix}$$

$$G = [EI - M - \beta(EI - M_c)^{-1}\beta^+]^{-1}$$

$$[EI - M_c]^{-1} = C^{-1} =$$



$$C^{-1} = \begin{bmatrix} \alpha' & -\beta \\ -\beta^+ & C \end{bmatrix}^{-1}$$

$$C^{-1} = \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix}$$

$$\sum = \beta(EI - M_c)^{-1}\beta^+ = \beta' g_{11} \beta'^+$$

$$g_{11} = [\alpha' - \beta' g_{11} \beta'^+]^{-1}$$