Non-Equilibrium Green's Function (NEGF)

Friday, 14 December 2018 09:07

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

S. Datta, "From atoms to transistors", Ed. Cambridge University Press (Capt. 8, 9, 10)

Nanohub.org : lecture

To solve transport problem, you need these ingredients:

$$\boxed{H, \Sigma \text{ (you can have multiple leads, so } \Sigma_1, \Sigma_2, \dots, \Sigma_n)}$$

Ingredients

The "recipe":

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

$$\Gamma_1 = j[\Sigma_1 - \Sigma_1^+]$$ Spectral Matrix

$$\Gamma_2 = j[\Sigma_2 - \Sigma_2^+]$$

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

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

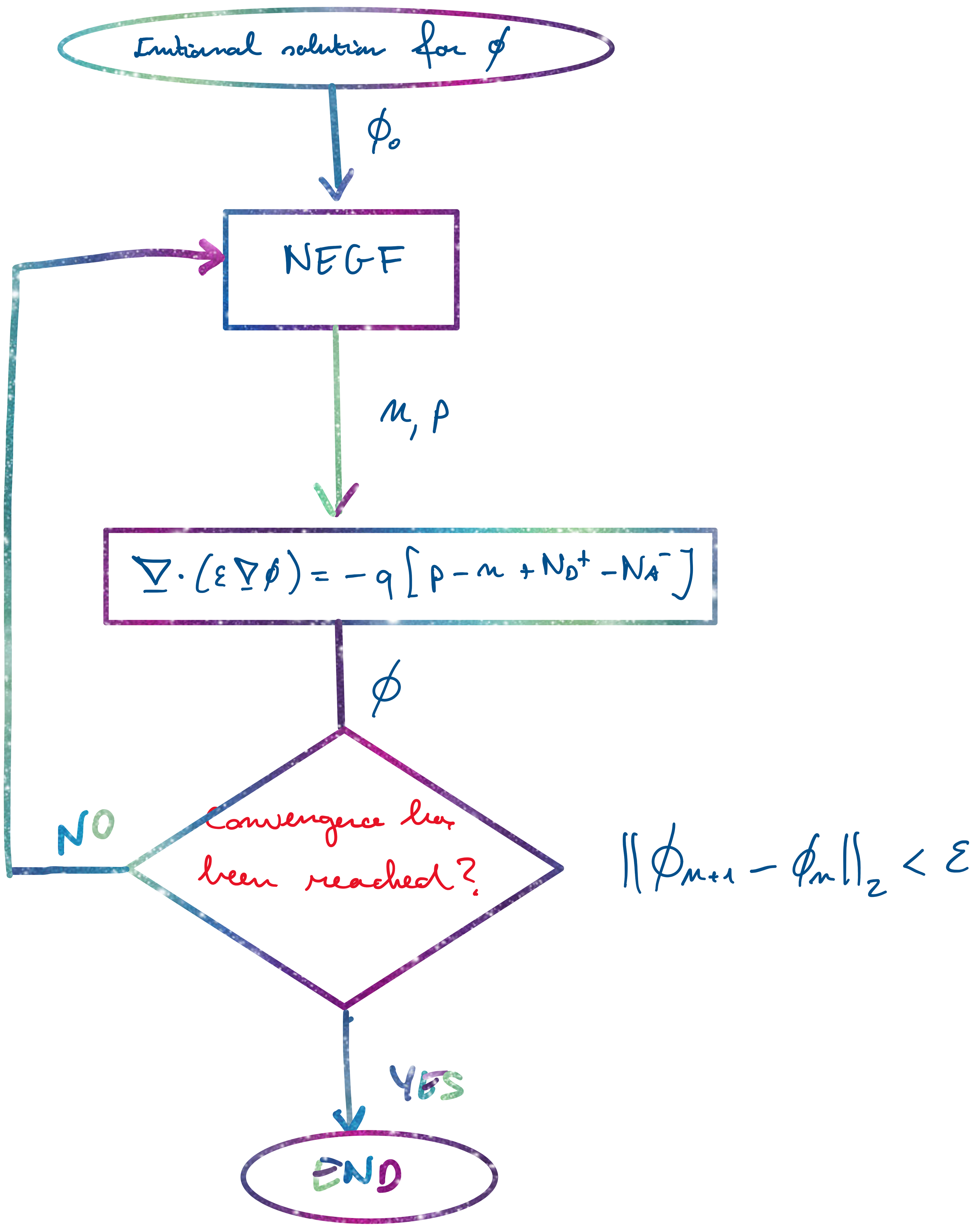
$$T = \operatorname{tr}\{\Gamma_2 G \Gamma_1 G^+\} = \operatorname{tr}\{\Gamma_1 G \Gamma_2 G^+\}$$

RECIPE OF NEGF

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

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

Self-consistent solution



$$\|\phi_{n+1} - \phi_n\|_2 < \varepsilon$$

LANDAUER'S FORMULA

$$\boxed{I = \frac{2q}{h} \int_{-\infty}^{+\infty} dE\, T(E) [f(E-E_{F1}) - f(E-E_{F2})]}$$