Electron Transport based on the Non-Equilibrium Green's Function (NEGF) Method

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Electron density of states (DOS)

“Straightforward” approach:

$$\mathbf{HC} = \mathbf{ESC}$$

$$\mathrm{DOS}(\omega) = \frac{dN/d\omega}{\Omega}$$

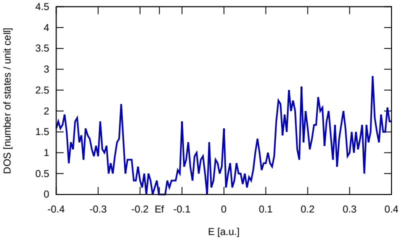
ω – energy variable

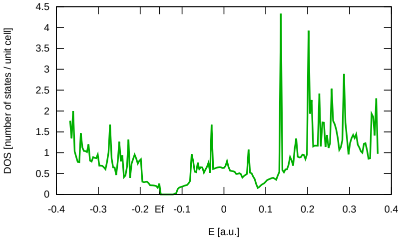
Green’s function method:

$$\mathbf{G}^{\mathrm{r}}(\omega) = (\omega \mathbf{S} - \mathbf{H})^{-1}$$

$$\mathrm{DOS}(\omega) = -\frac{1}{\pi} \lim_{\eta \to 0^+} \mathrm{Tr}\left\{ \mathrm{Im}\left[\mathbf{G}^{\mathrm{r}}(\omega + i\eta)\mathbf{S}\right]\right\}$$

Zigzag carbon nanotube (16,0)

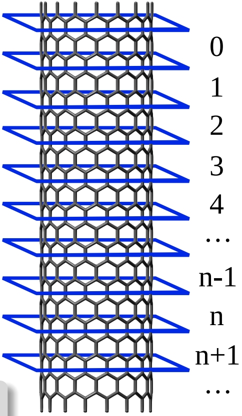




Calculation of a Retarded Surface Green's Function

- ✓ Semi-infinite stack of identical layers;
- ✓ Nearest-neighbour interaction

$$\mathbf{H}_{\mathrm{L(R)}} = \begin{pmatrix} \mathrm{H}_{00} & \mathrm{H}_{01} & 0 & 0 \\ \mathrm{H}_{01}^{\dagger} & \mathrm{H}_{00} & \mathrm{H}_{01} & 0 \\ 0 & \mathrm{H}_{01}^{\dagger} & \mathrm{H}_{00} & \ddots \\ 0 & 0 & \ddots & \ddots \end{pmatrix};$$



- ✓ Iterative method

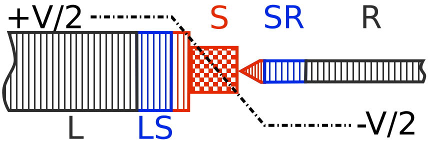
$$\epsilon_0 = \omega \mathrm{S}_{00} - \mathrm{H}_{00}, \quad \alpha_0 = \omega \mathrm{S}_{01} - \mathrm{H}_{01}, \quad \beta_0 = \alpha_0^{\dagger}.$$

$$g_i = \epsilon_i^{-1}, \quad \alpha_{i+1} = \alpha_i g_i \alpha_i, \quad \beta_{i+1} = \beta_i g_i \beta_i, \quad \epsilon_{i+1} = \epsilon_i - \alpha_i g_i \beta_i - \beta_i g_i \alpha_i$$

$$\mathrm{G}^{\mathrm{r}}_{\mathrm{L(R)}}(\omega) = \epsilon_n^{-1}$$

M.P. López Sancho et al., *J. Phys. F* 15 (1985), 851.

Model system



- ✓ Contact region connected by two semi-infinite electrodes;
- ✓ Nearest-neighbour interaction:

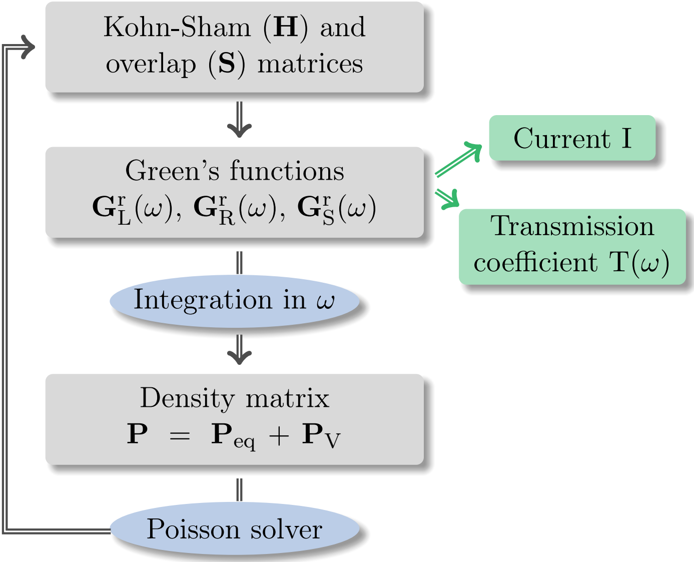
$$\mathbf{H} = \begin{pmatrix} \mathbf{H}_L & \mathbf{H}_{\mathrm{LS}} & 0 \\ \mathbf{H}_{\mathrm{LS}}^{\dagger} & \mathbf{H}_{\mathrm{S}} & \mathbf{H}_{\mathrm{SR}} \\ 0 & \mathbf{H}_{\mathrm{SR}}^{\dagger} & \mathbf{H}_{\mathrm{R}} \end{pmatrix};$$

- ✓ To calculate the steady state current flow (I) we need to know the retarded Green's function of the scattering region:

$$\mathbf{G}_{\mathrm{S}}^{\mathrm{r}}(\omega) = \lim_{\eta\to 0} \left[(\omega + i\eta)\mathbf{S}_{\mathrm{S}} - \mathbf{H}_{\mathrm{S}} - \Sigma_{\mathrm{L}}(\omega) - \Sigma_{\mathrm{R}}(\omega)\right]^{-1};$$

$$\text{self-energy} : \Sigma_{\mathrm{R}}(\omega) = \left[(\omega\mathbf{S}_{\mathrm{SR}} - \mathbf{H}_{\mathrm{SR}}) G_{\mathrm{R}}^{\mathrm{r}}(\omega)(\omega\mathbf{S}_{\mathrm{SR}} - \mathbf{H}_{\mathrm{SR}})^{\dagger}\right]^{-1}$$

Algorithm



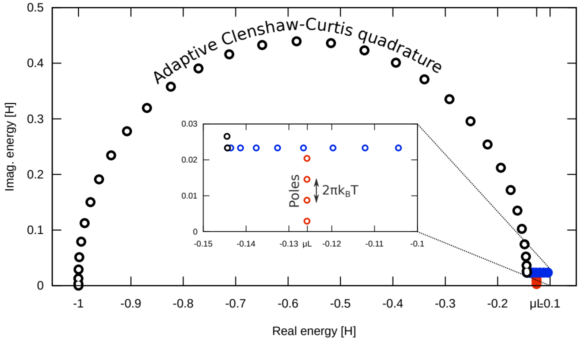
M. Brandbyde et al., *Phys. Rev. B* 65 (2002), 165401.

Integration in energy space

$$\mathbf{P}_{\mathrm{eq}} = -\frac{1}{\pi}\mathrm{Im}\left(\int_{-\infty}^{\infty} \mathrm{d}\omega \mathbf{G}_{\mathrm{S}}^{\mathrm{r}}(\omega) n_{\mathrm{F}}(\omega - \mu_L)\right);$$

$$n_{\mathrm{F}}(z) = \left[e^{z/(k_{\mathrm{B}}T)} + 1\right]^{-1} \qquad \mu_L = E_{\mathrm{F}} + V/2$$

Integration along complex contour



Integration in energy space

$$\mathbf{P}_{\mathrm{V}} = -\frac{1}{2\pi}\mathrm{Im}\left(\int_{-\infty}^{\infty} \mathrm{d}\omega \mathbf{G}_{\mathrm{S}}^{\mathrm{r}}(\omega)(\Sigma_{\mathrm{R}}(\omega) - \Sigma_{\mathrm{R}}^{\dagger}(\omega))\mathbf{G}_{\mathrm{S}}^{\mathrm{r},\dagger}(\omega)\times \right.$$
$$\left. [n_{\mathrm{F}}(\omega - E_{\mathrm{F}} - V/2) - n_{\mathrm{F}}(\omega - E_{\mathrm{F}} + V/2)]\right)$$

Fine-grained numerical integration along real axis