NEGF Notes

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1 Self-Energy

In order to describe transport, one has to calculate the retarded Green's function of a system. It is defined as

$$G^R = [(E + i\eta)\mathbb{1} - H]^{-1}$$

where H is the Hamiltonian of the entire system. η is some infinitesimal matrix so as to ensure the proper inverse.

In practice, one only needs the part of the G^R in the device region.

In principle. G^R is infinite dimensional and hence can't be calculated numerically. Considera system consisting of an infinite contact connected to a conductor.

We can write,

$$G^R = \begin{pmatrix} (E + i\eta)\mathbb{1} - H_C & \tau \\ \tau^\dagger & (E + i\eta)\mathbb{1} - H_D \end{pmatrix}^{-1}$$

$$\begin{pmatrix} G_C & G_{DC} \\ G_{DC}^\dagger & G_D \end{pmatrix} = \begin{pmatrix} (E + i\eta)\mathbb{1} - H_C & \tau \\ \tau^\dagger & (E + i\eta)\mathbb{1} - H_D \end{pmatrix}^{-1}$$

We ideally want to find the G_D term.

From the above defintion, we have the following equations that must hold among the G elements.

$$\begin{pmatrix} (E + i\eta)\mathbb{1} - H_C & \tau \\ \tau^\dagger & (E + i\eta)\mathbb{1} - H_D \end{pmatrix} \begin{pmatrix} G_C & G_{DC} \\ G_{DC}^\dagger & G_D \end{pmatrix} = \mathbb{1}$$

$$((E + i\eta)\mathbb{1} - H_C)G_C + \tau G_{DC}^\dagger = \mathbb{1}$$

$$((E + i\eta)\mathbb{1} - H_C)G_{DC} + \tau G_D = 0$$

$$\tau^\dagger G_C + ((E + i\eta)\mathbb{1} - H_D)G_{DC}^\dagger = 0$$

$$\tau^\dagger G_{DC} + ((E + i\eta)\mathbb{1} - H_D)G_D = \mathbb{1}$$

Consider the two equations involving G_D, namely the second the fourth. From the second one, we have,

$$G_{DC} = -((E + i\eta)\mathbb{1} - H_C)^{-1}\tau G_D$$

Using this in the fourth equation

$$-\tau^\dagger((E + i\eta)\mathbb{1} - H_C)^{-1}\tau G_D + ((E + i\eta)\mathbb{1} - H_D)G_D = \mathbb{1}$$

$$\boxed{\mathrm{G}_D = \left[(E + i\eta)\mathbb{1} - H_D - \tau^\dagger((E + i\eta)\mathbb{1} - H_C)^{-1}\tau\right]^{-1}}$$

Note that G_D has dimensions equal to those in the device region and hence is finite dimensional. One can rewrite the above equation as

$$G_D = [E + i\eta - H_D - \Sigma]^{-1}$$

where Σ is called the self-energy matrix. For a given contact, it has to be determined once and can be calculated analytically or using a iterative procedure since the contact is infinite.