

The NEGF Method: Capabilities and Challenges

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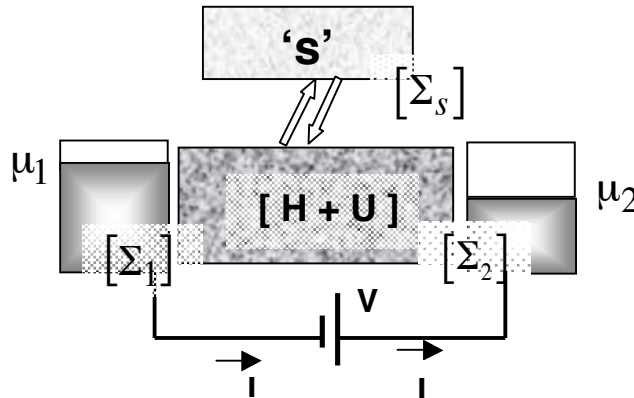
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A fairly versatile model for quantum transport in nanoscale devices is now available based on the Non-equilibrium Green Function (NEGF) method, which originated from the work of Schwinger, Keldysh, Kadanoff and Baym in the 1960's. The inputs to this model are

1. The **Hamiltonian** matrix, $[H]$ describing the active region, which also includes the Laplace potential $[U_L]$ due to the applied voltages on the electrodes,
2. The **contact self-energy matrices**, $[\Sigma_{1,2}(E)]$ describing the effect of the contacts on the active region,
3. The **inscattering** $[\Sigma^{in}(E)]$ ($\equiv [-i\Sigma^<(E)]$) **and outscattering** $[\Sigma^{out}(E)]$ ($\equiv [+i\Sigma^>(E)]$) **matrices**, describing the effect of interactions with the surroundings, and
4. The **potential** matrix $[U]$ describing the effective potential that one electron feels due to the other electrons.

Fig.1. Basic inputs to the NEGF method (adapted from [1]).



Given these inputs, the NEGF method tells us how to calculate the spectral function $[A(E)]$ and the correlation function $[G^n(E)]$ ($\equiv [-iG^<(E)]$) which are analogous to the density of states and the electron density respectively. From these, any one-electron observable quantity like the current can be calculated. Note that items 3 and 4, namely $[\Sigma^{in}(E)]$, $[\Sigma^{out}(E)]$ and $[U]$, depend on the correlation function $[G^n(E)]$, thus requiring an iterative self-consistent solution of the NEGF equations. Note that the size of each of the matrices appearing here is $(N \times N)$, N being the number of basis functions in the active region.

This general model has been applied by different authors to all kinds of devices like semiconductor nanowires, carbon nanotubes, molecular wires having different kinds of contacts, both normal and superconducting. Many issues still need to be clarified such as the best choice of basis functions in different problems, but I think it is safe to say that this approach provides a suitable framework for a wide variety of problems involving nanoscale quantum transport.

The objective of my talk is to present a simple intuitive description of the NEGF method and draw attention to some areas where important conceptual issues remain to be sorted out. An outstanding feature of this approach is the partitioning of the system into a channel described by an Hamiltonian $[H]$ and “contacts” represented by a self-energy $[\Sigma]$. This includes not only the obvious metallurgical contacts, but also phonons and other “contact-like” entities. The basic idea of self-energy is easily appreciated with a simple example: Consider a “molecule” described by a (2x2) Hamiltonian matrix $H = \begin{bmatrix} \varepsilon & \tau \\ \tau^* & \varepsilon_1 \end{bmatrix}$. We could calculate the (2x2) spectral function $[A(E)]$ from the relation

$$[A] = i [G - G^+], \quad \text{where } [G] = [(E + i0^+)I - H]^{-1}$$

and look at its diagonal elements to obtain the local density of states (LDOS) on each of the two sites. For example with $\varepsilon = -0.25$ eV, $\varepsilon_1 = +0.25$ eV, $\tau = 0.5$ eV and $0^+ = 0.01$ eV we obtain



If we are interested primarily in site ‘1’ we could represent the effect of site ‘2’ through a self-energy $\Sigma(E) = |\tau|^2 / (E - \varepsilon_1 + i0^+)$ and calculate the LDOS from a (1x1) spectral function:

$$[a] = i [g - g^+], \quad \text{where } [g] = [E - \varepsilon - \Sigma]^{-1}.$$

The result would be exactly what we obtained earlier from the (2x2) spectral function. On the other hand if we are interested primarily in site ‘2’ we could do the reverse: In short, we could treat site 1 as the channel and site 2 as the contact or vice versa.

In real problems, however, the important question is whether specific “contacts” can be assumed to be in local equilibrium and I will use simple examples to illustrate phenomena where “contacts” get modified in non-trivial ways through their interactions with the channel. As the field of nanoelectronics progresses, we should see more and more examples where traditional “contacts” do not function like well-behaved reservoirs, and some of these phenomena may even be useful!

[1] S. Datta, “Electrical Resistance: An Atomistic View”, *Nanotechnology* **15**, S433 (2004).

[2] For further tutorials including a one-semester course on quantum transport, see <http://nanohub.org> a website hosted by the Network for Computational Nanotechnology.