Non-Equilibrium Green's Function (NEGF) Method: A Different Perspective

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INTRODUCTION

The NEGF method was established in the 1960's through the classic work of Keldysh [1] and others using the methods of many-body perturbation theory (MBPT) and this apporach is widely used. By contrast I have introduced a different approach starting with the one-electron Schrodinger equation [2] and in this talk I will try to answer the quaestions I often get regarding the relation between them.

NEGF EQUATIONS

Our central equations

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

$$G^n = G^R \, \Sigma^{in} \, G^A \quad (2)$$

are essentially the same as Eqs.(75)-(77) of [1] which is one of the seminal founding papers on the NEGF method.

We obtain Eqs.(1) and (2) directly from a one-electron Schrodinger Equation using elementary arguments and use them to discuss many problems of great interest like quantized conductance, (integer) quantum Hall effect, Anderson localization, resonant tunneling and spin transport.

All these problems involve quantum transport but do not require a systematic treatment of many-body effects. On the other hand it goes beyond purely coherent transport allowing us to include phase-breaking interactions (both momentum-relaxing and momentum-conserving) within a self-consistent Born approximation (see Figure 2 for an illustrative example).

SHOULD WE CALL THIS NEGF?

* The answer is NO, if we associate NEGF with the MBPT used to obtain the sigma's appearing in Eqs.(1) and (2).
* The answer is YES, if we associate NEGF with Eqs.(1) and (2) ***irrespective*** of how the sigma's are obtained.

The second viewpoint seems more in keeping with the Boltzmann approach identified with the equation:

$$\frac{\partial f}{\partial t} + \vec{v}.\vec{\nabla} f + \vec{F}.\vec{\nabla}_p f = S_{op} f \quad (3)$$

and NOT with the evaluation of the scattering operator S_{op} which is analogous to the sigma's in (1) and (2). Indeed Boltzmann himself was unaware of the Fermi's golden rule commonly used nowadays to evaluate the S_{op} appearing *in the equation bearing his name*.

Similarly, totally new approaches for evaluating the sigma's have been and will be developed as we apply NEGF to newer problems like Coulomb blockade.

CONTACT-ING SCHRODINGER

In other words, we feel that the scope and utility of Eqs.(1) and (2) transcends the MBPT-based approach originally used to derive it. It teaches us how to combine quantum dynamics with "contacts", much as Boltzmann taught us how to combine classical dynamics with "contacts", using the word "contacts" in a broad figurative sense to denote all kinds of irreversible processes.

We feel that this should be a part of the training of all science and engineering students so that they can apply it effectively to a wide variety of basic and applied problems that require "***connecting contacts to the Schrodinger equation***".

REFERENCES

[1] Keldysh L.V. (1965) Diagram Technique for non-equilibrium processes. *Sov.Phys. JETP* 20, 1018. We have changed the notation somewhat, writing Σ for Σ^R, G^n *for* $-iG^<$ and Σ^{in} *for* $-i\Sigma^<$
[2] S. Datta, *Electron Transport in Mesoscopic Systems*, Chapter 8, Cambridge (1995); *Quantum Transport, Atom to Transistor,* Cambridge (2005); *Lessons from Nanoelectronics,* World Scientific (2012)

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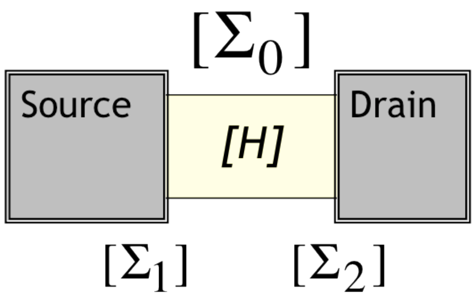
Fig.1. The NEGF-based quantum transport model allows us to model current flow given the Hamiltonian matrix *[H]* describing the channel, the self-energy matrices $[\Sigma_{1,2}]$ describing the connection of the channel to the contacts, and $[\Sigma_0]$ describing interactions within the channel.



The NEGF equations can be obtained from a one-electron Schrodinger equation modified to include the effect of contacts through the terms of Σ and s.

Modified Schrodinger Equation

$$E\psi = H\psi + \Sigma\psi + s$$

$$G^R = [EI - H - \Sigma]^{-1}$$

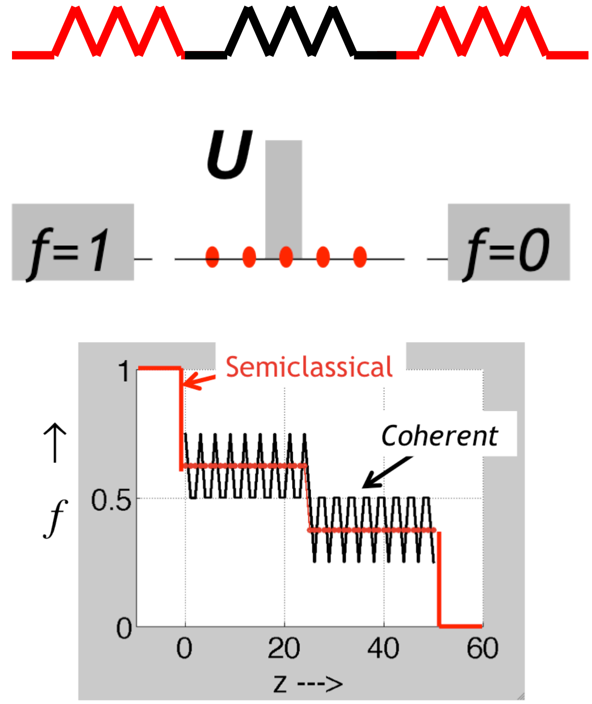
$$G^n = G^R \Sigma^{in} G^A$$

NEGF Equations

$$I^{op} = \frac{\Sigma G^n - G^n \Sigma^+}{i\hbar} + \frac{\Sigma^{in} G^R - G^A \Sigma^{in}}{i\hbar}$$

Current Operator

Fig.2. A simple example involving the transmission through a scatterer. The occupation factor f (proportional to the electrochemical potential) calculated from a coherent NEGF model shows oscillations around the semiclassical result.



An NEGF model that includes phase relaxation smooths out the oscillations while a model with momentum relaxation adds a slope to the potential as expected for a distributed resistance. All models assume elastic scattering.