QUANTUM DEVICE SIMULATION INCLUDING INTERACTIONS

S.Datta, G.Klimeck[*], R.Lake[**], Y.Lee[+] and M.J.McLennan[++]
*School of Electrical Engineering, Purdue University,
West Lafayette, IN 47907-1285.*
*Present Address : *University of Texas at Dallas, **Texas Instruments,*
+Hiroshima University, ++AT&T Bell Laboratories.

Abstract

Electron-phonon and electron-electron interactions are commonly included in semiclassical device simulation programs. However, such interactions are often neglected in the simulation of quantum devices. In this talk we will describe a general approach to quantum device simulation based on the non-equilibrium Green's function (NEGF) formalism that allows us to include these interactions.

I. INTRODUCTION

The cornerstone of semiclassical transport theory is the Boltzmann equation

$$v.\bar{\nabla}f + (e\bar{E}/\hbar).\bar{\nabla}_k f + S^{out}f = S^{in}(1-f) \qquad (1.1)$$

which describes the behavior of the distribution function f(r,k). This description is based on a physical picture which views electrons as particles that move in the external electric field according to "Newton's laws" (the quotes are used as a reminder that bandstructure effects are included) and are scattered by the random microscopic fields arising from impurities, phonons or other electrons (described by the functions $S^{in}(r,k)$ and $S^{out}(r,k)$). The Boltzmann equation effectively combines semiclassical dynamics with a stochastic description of the scattering processes:

Boltzmann $\Rightarrow$ "Newton's laws" + Random scattering

This approach works quite well for most devices under most conditions. However, there are quantum devices like resonant tunneling diodes which cannot be described at all within this semiclassical framework. Their operation is based on quantum interference effects arising from the wave nature of electrons. Moreover, as devices shrink to smaller dimensions, it is expected that quantum interference effects will become increasingly significant even in the operation of conventional devices. In order to include these effects we need a quantum version of the Boltzmann equation which combines quantum dynamics with a stochastic description of the scattering processes. The non-equilibrium Green's function (NEGF) formalism (also referred to as the Keldysh formalism) provides us with just that:

NEGF $\Rightarrow$ "Schrodinger equation"+ Random scattering

In this talk we will briefly summarize this formalism. For more details we refer the reader to the cited references and the references therein.

II. BASIC CONCEPTS

Before we can introduce the NEGF formalism we need to discuss a few basic concepts. Consider a homogeneous conductor. In the semiclassical picture we can describe the electrons by specifying the distribution function f(k) which tells us the number of electrons occupying a particular state 'k'. But in the quantum mechanical picture this is not enough. We also need to specify the phase-relationship among the different states. One way to do this is to define a density matrix $\rho(k,k')$. The distribution function f(k) only gives us the diagonal elements of this matrix:

$$f(k) = \left[\rho(k,k')\right]_{k'=k}$$

The rest of the story is contained in the off-diagonal elements which cannot be neglected unless the phase-relaxation length is much shorter than the other length scales.

It will be noted that although we have used a representation in terms of k-states to define the correlation function, we can always transform to other representations using an appropriate unitary transformation. For example we could transform to a real space representation as follows:

$$\rho(r,r') = \langle r|\rho|r' \rangle = \sum_{k,k'} \langle r|k \rangle \langle k|\rho|k' \rangle \langle k'|r' \rangle$$

$$= \frac{1}{V} \sum_{k,k'} \rho(k,k') \exp[i(kr - k'r')] \qquad (V \equiv \text{normalization volume})$$

In principle it is possible to find a representation that diagonalizes the correlation function. In such a representation there are no phase-correlations to worry about and we could use semiclassical reasoning. In practice it may not always be convenient to find this special representation or to use it.

To include the time coordinate into this description, in general we need a two-time correlation function of the form $G^n(k,k';t,t')$. In steady-state problems, the correlation function depends only on the *difference* between the two times and can be Fourier transformed to yield

$$G^n(k,k';E) \equiv \int d\tau\, G^n(k,k';\tau) e^{-iE\tau/\hbar} \qquad (\tau \equiv t - t') \qquad \text{(II.1)}$$

One way to understand the Fourier transform relationship between the energy 'E' and the difference time coordinate (t-t') is to note that the wavefunction of a particle with energy E evolves in time with a phase factor of exp $[-iEt / \hbar]$. Consequently

$$\psi(t)\psi^*(t') \sim \exp[-iE(t-t')/\hbar]$$

This suggests that the Fourier transform of the correlation function with respect to (t-t') should yield the energy spectrum.

Some treatments of quantum transport are based on the equal time correlation function obtained from $G^n(k,k';t,t')$ by setting $t' = t$. It is straightforward to show that this is equivalent to integrating $G^n(k,k'; E)$ over all energy:

$$\left[G^n(k,k';t,t')\right]_{t=t'} = \int \frac{dE}{2\pi} G^n(k,k';E)$$

As a result the energy-resolved information is lost making it difficult to describe scattering processes which transfer electrons from one energy to another. In general we need to use the full two-time correlation function. Since our interest is confined to steady-state transport, the correlation function depends only on the time difference (t - t') and can be Fourier transformed to obtain $G^n(k,k'; E)$ as described above. This energy-dependent correlation function is what we will use in this talk.

In the semiclassical picture we can define a function $S^{out}(k,t)$ that tells us the rate at which electrons are scattered out of a state 'k' assuming it is initially full. In a quantum mechanical description we have to generalize this concept, too, to include phase-correlations:

$$S^{out}(k,t) \rightarrow \Sigma^{out}(k,k';t,t')$$

Once again for steady-state problems the outscattering function depends only on the difference time coordinate and can be Fourier transformed yield an energy-dependent outscattering function $\Sigma^{out}(k,k'; E)$.

In deriving semiclassical kinetic equations we usually balance the outflow of electrons against the inflow of electrons. The inflow of electrons can alternatively be viewed as an outflow of 'holes' (whose number is given by (1-f)). We use the quotes as a reminder that we are talking about holes in the conduction band itself (we are considering only one band) and not in some other valence band. To describe the outflow of holes in the quantum formalism we define a *hole correlation function* G^P and an *inscattering function* Σ^{in} (which is a hole outscattering function) using exactly the same argument as we used above for electrons.

Before proceeding further we should point out that we are using a notation that is slightly different from the standard notation in the literature. We have deliberately chosen the notation to reflect the physical meaning of these functions. The correspondence, however, is quite straightforward:

$$G^n, G^P, \Sigma^{in}, \Sigma^{out} \quad \rightarrow \quad -iG^<, +iG^>, -i\Sigma^<, +i\Sigma^>$$

This set of four functions G^n, G^P, Σ^{in} and Σ^{out} (which are the quantum analogs of the semiclassical concepts f, (1-f), S^{in} and S^{out}) provide us with the language needed to include phase-correlations into a transport theory. If we represent our device by a set of 'N' nodes (in real space or in momentum space or in some other representation), then each of these quantities is a matrix of dimensions (NxN) at a given energy 'E". From hereon we will not write the energy coordinate 'E' explicitly for clarity.

III. KINETIC EQUATION

The correlation function is related to the scattering function by the relation

$$G^n = G^R \Sigma^{in} G^A \tag{III.1}$$

This equation is written in matrix notation and could be applied in any convenient representation. The Green's function G^R is calculated from a Schrodinger-like equation

$$\left[EI - H_0 - \Sigma^R \right] G^R = I \tag{III.2}$$

where H_0 is the Hamiltonian operator describing the device and I is the identity matrix (the other new function G^A is just the Hermitian conjugate of G^R).

To understand the physical meaning of the Green's function we note that in ordinary quantum mechanics the wavefunction of an electron is described by a Schrodinger equation $\left[EI - H_0 \right] \Psi = 0$. Comparing with Eq.(III.2) for G^R we note two differences. Firstly there is a delta function source term (I) on the right hand side of Eq.(III.2) suggesting that the function $G^R(r,r')$ be interpreted as the wavefunction at 'r' due to a delta function source at r' in the position representation. Similar interpretations are of course possible in other representations as well. Secondly there is an extra term Σ^R known as the *self-energy*. It represents the effective potential that an electron feels due to its interactions with phonons, other electrons etc (which are not included in H_0).

It is interesting that we can rewrite the Boltzmann equation (Eq.(I.1)) in a form that looks a lot like Eqs.(III.1) and (III.2). We could define a Green's function g^R as follows

$$v.\vec{\nabla} g^R + (e\vec{E}/\hbar).\vec{\nabla}_k g^R + (S^{out} + S^{in}) g^R(r,k;r',k') = \delta(r-r')\,\delta(k-k') \tag{III.3a}$$

and express the distribution function in terms of this Green's function:

$$f(r,k) = \int dr'\, dk'\, g^R(r,k;r',k')\, S^{in}(r',k') \tag{III.3b}$$

IV. SELF-ENERGY FUNCTIONS

In order to perform any concrete calculations based on the Boltzmann equation we need a recipe for calculating the functions S^{in} and S^{out}. These functions describe the physics of the interactions and the precise recipe depends on what interaction we want to describe and what approximation we wish to use. In the quantum formalism the same is true of the functions Σ^{in}, Σ^{out} and Σ^{R}. For a detailed description of different types of interactions we refer the reader to [2]. Here we will simply summarize the results for electron-phonon interactions in the self-consistent Born approximation (SCBA) and for electron-electron interactions in the Hartree-Fock approximation.

Phonon scattering in lowest order perturbation theory is described by

$$\Sigma^{in}(\vec{r},\vec{r}';E) = \int d(\hbar\omega)\, D(\vec{r},\vec{r}';\hbar\omega)\, G^{n}(\vec{r},\vec{r}';E-\hbar\omega) \tag{IV.1a}$$

$$\Sigma^{out}(\vec{r},\vec{r}';E) = \int d(\hbar\omega)\, D(\vec{r},\vec{r}';\hbar\omega)\, G^{p}(\vec{r},\vec{r}';E+\hbar\omega) \tag{IV.1b}$$

where the function D describes the spatial correlation and energy spectrum of the phonons ($\hbar\omega > 0$ corresponds to absorption and $\hbar\omega < 0$ to emission).

$$D(\vec{r},\vec{r}';\hbar\omega) = \sum_{q}|U_{q}|^{2}\left\{\begin{array}{l}\exp[-iq.(\vec{r}-\vec{r}')]\, N_{q}\delta(\omega-\omega_{q})\\[2mm] +\exp[+iq.(\vec{r}-\vec{r}')]\,(N_{q}+1)\delta(\omega+\omega_{q})\end{array}\right\} \tag{IV.2}$$

where N_{q} is the number of phonons with wavevector q and frequency ω_{q} and U_{q} is the potential felt by an electron due to a single phonon with wavevector q. Assuming that the bath of phonons is always maintained in thermal equilibrium N_{q} is given by the Bose-Einstein function. The self-energy function is given by

$$\Sigma^{R}(E) = \Gamma^{H}(E) + \frac{i}{2}\Gamma(E) \qquad \text{where} \quad \Gamma(E) = \Sigma^{in}(E) + \Sigma^{out}(E) \tag{IV.3}$$

and $\Gamma^{H}(E)$ is the Hilbert transform of $\Gamma(E)$.

Electron-electron interactions in the Hartree-Fock approximation, do not give rise to any Σ^{in}, Σ^{out}. It only contributes to Σ^{R}:

$$\Sigma^{R}(\vec{r},\vec{r}';E) = U_{H}(\vec{r})\,\delta(\vec{r}-\vec{r}') + \Sigma_{F}(\vec{r},\vec{r}') \tag{IV.4}$$

The first term is the Hartree potential:

$$U_{H}(\vec{r}) = \int d\vec{r}' \int \frac{dE}{2\pi} G^{n}(\vec{r}',\vec{r}';E) \frac{e^{2}}{4\pi\varepsilon|\vec{r}-\vec{r}'|} \tag{IV.5}$$

The second term is the exchange potential:

$$\Sigma_{F}^{s}(\vec{r},\vec{r}') = -\int dE\, G^{ns}(\vec{r},\vec{r}';E) \frac{e^{2}}{4\pi\varepsilon|\vec{r}-\vec{r}'|} \tag{IV.7}$$

The superscript 's' is added as a reminder that an electron only feels an exchange potential due to other electrons of the same spin.

V. TERMINAL CURRENT

In general we are interested in calculating the current that flows when a conductor is connected by to two (or more) contacts across which a potential difference is maintained by an external source. So far we have not worried about the leads connected to the conductor. One way to treat the leads is to impose an appropriate boundary condition on $G^n(r,r';E)$ and $G^R(r,r';E)$ when solving Eqs.(III.1) and (III.2), in the same way that we impose boundary conditions on the distribution function $f(r,k)$ in semiclassical theory. Once we have solved for $G^n(r,r';E)$, we can calculate the current density $J(r;E)$ throughout the conductor and then integrate over the cross-section to obtain the current in the contact [6,7].

An alternative approach that is often very convenient is to introduce the effect of the leads through functions Σ_m^{in}, Σ_m^{out} and Σ_m^R (defined for each lead 'm') and add it to the functions Σ_ϕ^{in}, Σ_ϕ^{out} and Σ_ϕ^R describing the interactions.

$$\Sigma^{in,out,R} = \Sigma_\phi^{in,out,R} + \sum_m \Sigma_m^{in,out,R} \qquad (V.1)$$

Using a discrete lattice, or what is often referred to as the 'tight-binding' model, the self-energy function due to the leads can be written as [5]

$$\Sigma_m^R(i,j;E) = -t\,\phi_m(i)\,e^{ik_m a}\,\phi_m^*(j) \qquad (V.2)$$

where $\qquad E = U_m + 2t(1 - \cos(k_m a))$

Here 'i' and 'j' are points on a discretized lattice with spacing 'a' and $t = \hbar^2/2ma^2$. The self-energy is non-zero only for lattice sites that are adjacent to the lead with mode 'm' and ϕ_m represents the transverse wavefunction corresponding to mode 'm'. U_m is the potential energy in lead 'm'.

The inscattering and outscattering functions corresponding to the leads are given by

$$\Sigma_m^{in}(i,j;E) = f_m(E)\,\Gamma_m(i,j;E) \qquad (V.3a)$$

$$\Sigma_m^{out}(i,j;E) = (1 - f_m(E))\,\Gamma_m(i,j;E) \qquad (V.3b)$$

where $\qquad \Gamma_m(i,j;E) = \phi_m(i)\dfrac{\hbar v_m}{a}\phi_m^*(j) \qquad$ and $\qquad \hbar v_m = \partial E/\partial k_m = 2at\,\sin(k_m a)$

Here we have assumed that each mode 'm' in the leads is maintained in local equilibrium with some Fermi distribution $f_m(E)$.

It seems feasible to do something similar in semiclassical theory as well, namely, define functions $S_m^{in}(k)$ and $S_m^{out}(k)$ corresponding to each contact 'm'. The current in lead 'm' can then be calculated from the relation

$$I_m \sim \sum_k S_m^{in}(k)(1 - f(k)) - S_m^{out}(k)f(k) \qquad (V.5)$$

We are not aware of anyone using this approach in semiclassical theory, but it has been used successfully in the quantum version. The quantum analog of Eq.(V.5) is given by

$$I_m = \frac{2e}{h}\int dE \, \mathrm{Tr}\left[\Sigma_m^{in} G^p - \Sigma_m^{out} G^n\right] \qquad (V.6)$$

VI. EXAMPLES

To apply Eqs.(III.1a,b) to a specific conductor we could discretize the spatial coordinate into a discrete lattice with N points. All the matrices like G^n, G^R, Σ^{in} etc. are then of order (NxN). the energy coordinate 'E' too has to be discretized into a convenient number of nodes. At each energy node, we have to invert (NxN) matrices. The functions Σ^{in}, Σ^{out} and Σ^R then have to be recomputed and the calculation repeated till the process converges.At low temperature and bias a single energy node is adequate allowing us to handle conductors with many spatial nodes. So far we have applied this formalism to (1) two -dimensional conductors at low temperature and bias. This includes the study of the Hall effect (low and high magnetic fields) in ballistic as well as disordered conductors [6] and (2) one-dimensional conductors at room temperature and large bias. This involves the study of current flow and energy dissipation in single barrier and double barrier structures [7].

VII. FUTURE DIRECTIONS

The NEGF formalism provides a general framework for quantum transport comparable to that provided by the Boltzmann formalism for semiclassical transport. In this talk we have described how this formalism can be used to describe steady-state transport in mesoscopic devices. Although the basic ideas seem clear, much remains to be done in terms of incorporating realistic scattering models and bandstructure effects.

There are two areas where the basic concepts are not fully clear. One is the area of transient or ac response. The other is the area of transport in strongly interacting systems. The Coulomb blockade regime which has attracted much attention lately belongs to this category. The calculation of self-energy and scattering functions describing the interactions (Section IV) is based on perturbation theory which is not valid for strong interactions. Under these conditions we cannot use Eqs.(III.1) and (III.2) to calculate G^n, G^R etc. Alternative non-perturbative techniques are needed [8,9]. Interestingly the Boltzmann formalism too runs into similar difficulties when applied to strongly interacting systems. We then have to worry about higher order (two-particle, three-particle) distribution functions.

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