QUANTUM DEVICE MODELING WITH NON-EQUILIBRIUM GREEN FUNCTIONS

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Abstract

I describe the non-equilibrium Green function approach to modeling wide-cross-sectional area quantum devices such as resonant tunneling diodes. Several approximations for treating scattering are discussed: Born, self-consistent Born, and a single-electron multiple sequential scattering algorithm. A generalized treatment of open-system boundaries is presented.

I HAMILTONIAN AND BASIS

The general form of the Hamiltonian is $H = H_o + \underbrace{H_{pop} + H_{ac} + H_{IR}}_{\Sigma}$ where H_o contains the kinetic energy and the effects of the band structure, the applied potential, and the Hartree potential. The three terms to the right represent the potential felt by the electrons due to polar optical phonons, acoustic phonons, and interface roughness, respectively. The underbrace and Σ indicate that these terms are included through self-energies. For numerical reasons, H_o is broken down into three terms, $H_o = H_o^D + \underbrace{H_o^L + H_o^R}_{\Sigma_B}$, which represent the Hamiltonian of the device, the left contact, and the right contact, respectively. The underbrace indicates that the effect of the contacts on the device is also taken into account through a self-energy, Σ_B.

The Hamiltonian matrix will explicitly be written in terms of the basis $\langle \mathbf{r}|\mathbf{k},n\rangle = e^{i\mathbf{k}\cdot\mathbf{r}_t}\phi_i(z)/\sqrt{A}$ where $\mathbf{k}$ is the transverse wavevector and $\phi_i(z)$ is a localized (Wannier) function localized around site 'i'. Keeping only nearest neighbor matrix elements, the matrix elements of H_o are $\langle \mathbf{k},i|H_o|\mathbf{k},j\rangle = (\epsilon_{\mathbf{k}i} + \epsilon_i)\delta_{i,j} - t_{i,j}\delta_{i,j\pm1}$. The site energies and hopping elements can be related to the discretized effective mass Hamiltonian, $H_o = \frac{-\hbar^2}{2}\frac{d}{dz}\frac{1}{m^*(z)}\frac{d}{dz} + V(z)$ in the usual way.

II EQUATION OF MOTION FOR G^R and $G^<$

The non-equilibrium Green function (NEGF) formalism provides a method for calculating the non-equilibrium statistical ensemble average of the single particle correlation operator, ($\hbar = 1$), $G^<_{i,j}(\mathbf{k};t,t') = i\langle c^\dagger_{j,\mathbf{k}}(t')c_{i,\mathbf{k}}(t)\rangle$ where $c_{i,\mathbf{k}}$ is the electron annihilation operator for an electron in localized state 'i' with transverse momentum $\mathbf{k}$. Once the correlation function $G^<$ is known, it immediately provides the electron density, $n_i = \frac{-i}{Aa}\sum_{\mathbf{k}}\int\frac{dE}{2\pi}G^<_{i,i}(\mathbf{k},E)$ and the current density, $J_{i+1/2} = -\frac{1}{A}\sum_{\mathbf{k}}\int\frac{dE}{2\pi}\left[t_{i,i+1}\,G^<_{i+1,i}(\mathbf{k},E) - t_{i+1,i}\,G^<_{i,i+1}(\mathbf{k},E)\right]$.

The two equations of motion that must be solved are (in matrix notation)

$$(E - H_o - \Sigma^R - \Sigma^{RB})\,G^R = 1 \tag{2.1}$$

$$(E - H_o - \Sigma^R - \Sigma^{RB})\,G^< = (\Sigma^< + \Sigma^{<B})G^{R\dagger} \tag{2.2}$$

In Eqs. (2.1) and (2.2), the effects of the scattering are contained in Σ^R and $\Sigma^<$ and the effect of the open boundaries are contained in Σ^{RB} and $\Sigma^{<B}$

III OPEN BOUNDARY SELF ENERGIES

For a device consisting of sites $1,\ldots,N$, I include the coupling to the leads, $t_{0,1}$ and $t_{N,N+1}$ exactly using Dyson's equation to obtain the boundary self energies: $\Sigma^{RB}_{1,1} = g^R_{0,0}|t_{0,1}|^2$, $\Sigma^{RB}_{N,N} = g^R_{N+1,N+1}|t_{N,N+1}|^2$, $\Gamma^B_{1,1} = a_{0,0}|t_{0,1}|^2$, $\Gamma^B_{N,N} = a_{N,N}|t_{N,N+1}|^2$, $\Sigma^{<B}_{1,1} = if_L\Gamma^B_{1,1}$, and $\Sigma^{<B}_{N,N} = if_R\Gamma^B_{N,N}$; where g^R is the Green function of the unconnected lead, a is the corresponding spectral function, and f is the Fermi-factor. The boundary self-energies Σ^{RB} and Γ^B are valid even if the leads have spatially varying potentials, and $\Sigma^{<B}$ is valid if the lead is in equilibrium.

An explicit representation of G^R for a device of 3 sites is

$$\left[G^R\right] = \begin{bmatrix} E-\epsilon_{k,1}-\epsilon_1-\Sigma^R_{1,1}-\Sigma^{RB}_{1,1} & t_{1,2}-\Sigma^R_{1,2} & -\Sigma^R_{1,3} \\ t_{1,2}-\Sigma^R_{1,2} & E-\epsilon_{k,2}-\epsilon_2-\Sigma^R_{2,2} & t_{2,3}-\Sigma^R_{2,3} \\ -\Sigma^R_{3,1} & t_{3,2}-\Sigma^R_{3,2} & E-\epsilon_{k,3}-\epsilon_3-\Sigma^R_{3,3}-\Sigma^{RB}_{3,3} \end{bmatrix}^{-1} \tag{3.3}$$

$\Sigma^B_{0,0}$ is obtained from $g^R_{0,0}$,

$$g^R_{0,0} = \begin{bmatrix} -t_{-2}e^{-i\gamma_{-2}a} & t_{-2,-1} & 0 \\ t_{-1,-2} & E-\epsilon_{k,-1}-\epsilon_{-1} & t_{-1,0} \\ 0 & t_{0,-1} & E-\epsilon_{k,0}-\epsilon_0 \end{bmatrix}^{-1}_{0,0} \tag{3.4}$$

In Eq. (3.4), I have again taken into account the semi-infinite *uniform potential* region to the left by a self energy which can be calculated analytically, $\Sigma^{RB}_{-2,-2} = g^R_{-3,-3}|t_{-3,-2}|^2 = -t_{-3,-2}e^{i\gamma_L a}$, and used the dispersion relation, $E = \epsilon_{k,L} + \epsilon_L - 2t\cos(\gamma_L a)$, to simplify the (-2,-2) element.

Substituting Dyson's equation, $G^<_{0,j} = g^R_{0,0}(-t_{0,1})G^<_{1,j} + g^<_{0,0}(-t_{0,1})G^A_{1,j}$, into the current expression for $J_{1/2}$, using $G^< = G^R(\Sigma^< + \Sigma^{<B})G^{R\dagger}$ and $A = G^R(\Gamma+\Gamma^B)G^{R\dagger}$ gives

$$\begin{aligned} J_{1/2}(k,E) &= ei\Gamma^B_{1,1}\sum_{n,m\in\{1,\ldots,N\}} G^R_{1,n}\left[f_L\Sigma^>_{n,m} + (1-f_L)\Sigma^<_{n,m}\right]G^{R\dagger}_{m,1} \\ &\quad + e\Gamma^B_{1,1}\Gamma^B_{N,N}|G^R_{1,N}|^2(f_L - f_R) \end{aligned} \tag{3.5}$$

The terms in (3.5) are functions of k and E. The first term is the contribution to the current from scattering and the second term is the contribution from direct transitions from the left to right contact. With no scattering, the first term is absent, and the second term is the usual tunneling formula using the Fisher-Lee form of the transmission coefficient [1]. The Γ^B's need not be simply factors of velocity but can account for leads with spatially varying potentials. The boundary conditions may provide a unified treatment within a Tsu-Esaki formulation of current from continuum states and emitter quasi-bound states [2].

IV COMBINING BORN AND SELF-CONSISTENT BORN SELF ENERGIES

The non-local self-energy due to polar-optical phonons couples Eqs. (2.1) and (2.2) in energy, E and momentum, k, necessitating the storage of four four-dimensional functions, $G^<_{i,j}(k,E)$, $G^R_{i,j}(k,E)$, $\Sigma^<_{i,j}(k,E)$, and $\Sigma^R_{i,j}(k,E)$. This is not feasible for any modestly sized device. Therefore, I combine a first Born treatment of the polar optical phonons and a self consistent Born treatment of the elastic scattering mechanisms: interface roughness and high temperature acoustic phonons. The new equations of motion are found from the Dyson equation for the path ordered Green function

$$G^p = g^p + g^p\Sigma^p G^p \tag{4.6}$$

where the matrix notation now denotes both summing over sites and integrating over the Keldysh contour. In a Born or self-consistent Born approximation, Σ has three contributions, one from each scattering process, acoustic phonon, polar optical phonon, and interface roughness: $\Sigma^p = \Sigma^p_{ap} + \Sigma^p_{pop} + \Sigma^p_{IR}$. I iterate once keeping only the first order term in Σ^p_{pop} to obtain $G^p = g^p + g^p[\Sigma^p_{ap} + \Sigma^p_{IR}]G^p + g^p\Sigma^p_{pop}g^p$. Since Σ^p_{pop} is being used in a first Born approximation, it must be calculated in the first Born approximation to conserve current. In keeping with the notation of big G's and little g's, little σ's will be used to denote the self energies due to the polar optical phonons. Breaking up G^p along the two branches of the time path [3], gives

$$G^R = g^R + g^R\Sigma^R G^R + g^R\sigma^R g^R \tag{4.7}$$

and

$$G^< = g^< + g^R\Sigma^R G^< + g^R\Sigma^< G^A + g^<\Sigma^A G^A + g^R\sigma^R g^< + g^R\sigma^< g^A + g^<\sigma^A g^A \tag{4.8}$$

where the large Σ is the sum of the self energies that I treat in the self-consistent Born approximation, ie. $\Sigma \equiv \Sigma_{ap} + \Sigma_{IR}$. Operating on (4.7) and (4.8) from the left with $E - \epsilon_k - H_o - \Sigma^{RB}$ and using the equations of motion for g^R and $g^<$, $(E - \epsilon_k - H_o - \Sigma^{RB})g^R = 1$ and $(E - \epsilon_k - H_o - \Sigma^{RB})g^< = \Sigma^{<B}g^A$ gives the final form of the equations that I need to solve.

$$(E - \epsilon_k - H_o - \Sigma^R - \Sigma^{RB})G^R = 1 + \sigma^R g^R \tag{4.9}$$

and

$$(E - \epsilon_k - H_o - \Sigma^R - \Sigma^{RB})G^< = (\Sigma^< + \Sigma^{<B})G^A + \sigma^R g^< + \sigma^< g^A \tag{4.10}$$

Equations (4.9) and (4.10) conserve current.

Treating the polar optical phonons in the first Born approximation leads to an immense simplification in the numerical solution. Since the self-energies due to high temperature acoustic phonons and interface roughness are elastic, equations (4.9) and (4.10) decouple in energy. Also, Σ^R becomes only a function of G^R so that Eq. (4.9) for G^R is a closed loop in an iterative solution of Σ^R and G^R. Furthermore, $\Sigma^R_{i,j}$ is diagonal $\propto \delta_{i,j}$. Therefore, for a given energy, in the iterative solution of (4.9), I only need to store the diagonal elements $G^R_{i,i}(k)$ and $\Sigma^R_{i,i}(k)$ and invert a tri-diagonal matrix.

V SINGLE-ELECTRON MULTIPLE SEQUENTIAL SCATTERING ALGORITHM

A self-consistent Born approximation (SCBA) requires a converged solution of the Σ's and the G's to conserve current. This can be numerically problematic. The following is an alternative.

The point-of-view which informs the work of Roblin and Liou [4] is used to create a multiple sequential scattering (MSS) algorithm for non-equilibrium Green functions. The point-of-view is as follows. A plane wave, ψ_0, injected from the contact propagates into the device and scatters due to the random potential of phonons and interface roughness. Flux is removed from the incident wave and fed into the scattered wave, ψ_1, which has no phase coherence with ψ_0. ψ_1 now scatters creating ψ_2, etc. The MSS approach is a single electron approach which does not account for the Pauli-exclusion principle, but it provides a means to truncate at any order the infinite expansion leading to the SCBA and still conserve current. In the limit of infinite sequential scattering, MSS is the SCBA for zero electron density.

N sequential scattering events give rise to $N+1$ retarded Green functions, G^R_n, and $N+1$ correlation functions, $G^<_n$, where $n = \{0, ..., N\}$. Here, I consider only elastic processes. For a given

total energy, E, the general form of the retarded self energy is $\Sigma^R(E_z) = \int_{-\infty}^{E} dE_z' D(E_z, E_z') G^R(E_z')$ where E is the total energy, the integral over E_z is the sum over transverse momentum, and $D(E_z, E_z')$ is a known function determined by the type of scattering considered. I have suppressed the position coordinates. The equations defining the propagators G_n^R for the N scattered waves are:

$$\begin{aligned}
\left[E_z^0 - H_o - \Sigma^{RB} - \int_{-\infty}^{E} dE_z^1 D(E_z^0, E_z^1) G_1^R(E_z^1)\right] G_0^R(E_z^0) &= 1 \\
\left[E_z^1 - H_o - \Sigma^{RB} - \int_{-\infty}^{E} dE_z^2 D(E_z^1, E_z^2) G_2^R(E_z^2)\right] G_1^R(E_z^1) &= 1 \\
&\vdots \\
\left[E_z^{N-1} - H_o - \Sigma^{RB} - \int_{-\infty}^{E} dE_z^N D(E_z^{N-1}, E_z^N) G_N^R(E_z^N)\right] G_{N-1}^R(E_z^{N-1}) &= 1 \\
\left[E_z^N - H_o - \Sigma^{RB}\right] G_N^R(E_z) &= 1 \qquad (5.11)
\end{aligned}$$

Since the last wave, by definition, does not scatter, the retarded Green function governing its propagation, G_N^R, is simply the bare Green function, g^R. Starting with the last propagator, $G_N^R = g^R$, and back-substituting into each higher equation, one calculates each G_n^R.

The equations defining $G_n^<$ are

$$\begin{aligned}
(E_z^0 - H_o - \Sigma^{RB} - \Sigma_0^R) G_0^<(E_z^0) &= \Sigma^{<B} G_0^{R\dagger}(E_z^0) \\
(E_z^1 - H_o - \Sigma^{RB} - \Sigma_1^R) G_1^<(E_z^1) &= \int_{-\infty}^{E} dE_z^0 \, D(E_z^1, E_z^0) \, G_0^<(E_z^0) \, G_1^{R\dagger}(E_z^1) \\
&\vdots \\
(E_z^N - H_o - \Sigma^{RB} - \Sigma_N^R) G_N^<(E_z^N) &= \int_{-\infty}^{E} dE_z^{N-1} \, D(E_z^N, E_z^{N-1}) G_{N-1}^<(E_z^{N-1}) G_N^{R\dagger}(E_z^N)
\end{aligned} \qquad (5.12)$$

One solves the set of equations (5.12) by starting at the top, solving for $G_0^<$, substituting that into the second equation, and so on working downward. Notice that the source term, $\Sigma^{<B} G^{R\dagger}$, for $G_0^<$ is due to injection from the contacts while the source terms for the scattered waves ($n = 1, ..., N$) come from the scattering of the previous waves.

The resulting electron density and current density per unit energy are $n_i(E) = -i \sum_{n=0}^{N} \int_{-\infty}^{E} dE_z \, \rho_{2D}(E_z) G_{n_{i,i}}^<(E_z)$ and $J_{i+1/2}(E) = \frac{1}{A} \sum_{n=0}^{N} \int_{-\infty}^{E} dE_z \rho_{2D}(E_z) |t_{i,i+1}|^2 \, 2\mathrm{Re} G_{n_{i,i+1}}^<(E_z)$ where the subscript 'i' is the site index that has been suppressed.

Acknowledgement: I acknowledge a very useful discussion with S. Hershfield.

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