Compliant energy and momentum conservation in NEGF simulation of electron-phonon scattering in semiconductor nano-wire transistors

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Abstract. The modelling of spatially inhomogeneous silicon nanowire field-effect transistors has benefited from powerful simulation tools built around the Keldysh formulation of non-equilibrium Green function (NEGF) theory. The methodology is highly efficient for situations where the self-energies are diagonal (local) in space coordinates. It has thus been common practice to adopt diagonality (locality) approximations. We demonstrate here that the scattering kernel that controls the self-energies for electron-phonon interactions is generally non-local on the scale of at least a few lattice spacings (and thus within the spatial scale of features in extreme nano-transistors) and for polar optical phonon-electron interactions may be very much longer. It is shown that the diagonality approximation strongly under-estimates the scattering rates for scattering on polar optical phonons. This is an unexpected problem in silicon devices but occurs due to strong polar SO phonon-electron interactions extending into a narrow silicon channel surrounded by high kappa dielectric in wrap-round gate devices. Since dissipative inelastic scattering is already a serious problem for highly confined devices it is concluded that new algorithms need to be forthcoming to provide appropriate and efficient NEGF tools.

1. Introduction

The Keldysh non-equilibrium Green function (NEGF) methodology has been applied successfully to the simulation of silicon nano-wire transistors [1-4]. Its success arises from powerful recursive algorithms coupled with the non-perturbative treatment of impurities and surface/interface roughness [1-4] and the easy incorporation of dissipation through diagonal self-energies [4, 5]. The double space representation is ideal for inhomogeneous systems. For steady state models, it is necessary to solve for the energy-resolved two-point Green function \(G(x_1,x_2;\varepsilon)\) in conjunction with the corresponding self energies. The NEGF formalism is reduced to solving the following system of equations:

\[
G^<(r_1,r_2;\varepsilon) = \int d^3r_3 d^3r_4 G^R(r_1,r_3;\varepsilon) \Sigma^>(r_3,r_4;\varepsilon) G^A(r_4,r_2;\varepsilon)
\]

\[
(\varepsilon 1 - H_0 - V - e\Phi - \Sigma^R)G^R(\varepsilon) = 1
\]

Inelastic modelling of inelastic scattering in short channel silicon nano-transistors was thought to be irrelevant to the simulation of in-channel processes due to quasi-ballistic coherent flows. In practice,
the presence of strong size quantization/confinement, particularly in wrap-round gate structures (fig 1), can enhance energy dissipation within the various sub-band channels[1, 3].

Figure 1: Schematic of a typical silicon nano-wire wrap-round gate transistor

The Green functions then strictly require the inversion of a strongly non-diagonal matrix due to the non-diagonality of the self-energies. For silicon it has been argued that a diagonal approximation is sufficient [5]; however, strict energy and momentum conservation is suspect and has led to poor confidence in estimates of channel mobility. The importance of non-diagonal self energies has been pointed out in studies of quantum cascade lasers [6-7] mainly for polar electron-phonon coupling in III-V devices. Recently, the fabrication of wrap-round gate nano-wire transistors (figure 1) with high-

3. The Scattering Kernel

The scattering kernel gives a measure of the spatial spread or range of the scattering interaction. For inelastic screened polar optical phonon scattering we find:

\[
K = C \int_{-\pi/a}^{\pi/a} dq_z |U(q)|^2 \exp[iq_z(z_1 - z_2)]
\]

\[
C = \frac{\hbar \omega_0}{2 \varepsilon_0} \left( \frac{1}{\varepsilon_{\infty}} - \frac{1}{\varepsilon_s} \right);
\]

\[
|U(q)|^2 = C \frac{q_z^2 + q_{\perp}^2}{(q_z^2 + q_{\perp}^2 + \xi^2)^2}
\]
\[ K = C_1 \int_{-\pi/a}^{\pi/a} dq_1 \exp[iq_1(z_1 - z_2)] = 2aC_1 \frac{\sin[\pi R]}{R} \]  
\[ \text{(8)} \]

in the approximation that \( a \to 0 \) the integration extends to infinity, \( K \) becomes diagonal:
\[ K(R) \to \delta(R) \quad \Rightarrow \Sigma^e(z_1, z_2, k_\perp, \varepsilon) \sim \delta(z_1 - z_2) \]  
\[ \text{(9)} \]

Second, we exhibit the full scattering kernel for weakly screened (\( \xi/a = 8.9 \)) polar optical phonon scattering: figure 2(b) gives the exact result using integration over the first Brillouin zone; figure 2(c) shows the approximation \( a \to 0 \) extending the range of integration; the result closely matches the exact result. Third, the corresponding results for strong screening (shorter screening length \( \xi/a = 1.8 \)) are shown in figures 2(d) (exact), 2(e) (\( a \to 0 \) approximation: a considerably poorer approximation here). Clearly, the effective non-locality (non-diagonality) of \( K \) and hence \( \Sigma \) extends over a range of the order of the screening length. Similar considerations apply to acoustic phonon scattering. Although it is often assumed that the self-energy is diagonal for high temperature acoustic phonon scattering that is only true for the elastic scattering assumption coupled with an extension of integration beyond the first Brillouin zone. If the scattering treated as inelastic we have for high temperatures:
\[ \Sigma^e(z_1, z_2, k_\perp, \varepsilon) = C_2 \int_{-\pi/a}^{\pi/a} dq_1 \int dq_2 \exp[iq_1(z_1 - z_2)] \{G^e(z_1, z_2; k_\perp, \varepsilon - h\omega_q) + G^e(z_1, z_2; k_\perp - q_\perp, \varepsilon + h\omega_q)\} \]
\[ \text{(10)} \]

For \( h\omega_q = hsq \ll \varepsilon \) we may pick out the q-dependence as:
\[ G^e(z_1, z_2; k_\perp - q_\perp, \varepsilon + h\omega_q) = 2G^e(z_1, z_2; k_\perp - q_\perp, \varepsilon) + (hsq)^2 \frac{\partial^2 G^e(z_1, z_2; k_\perp - q_\perp, \varepsilon)}{\partial \varepsilon^2} \]
\[ \text{(11)} \]

The leading term is the elastic approximation; the second term gives rise to a non-diagonal kernel
\[ K^e(1z_1 - z_2 \mid a) = a^3 \int_{-\pi/a}^{\pi/a} dq_1 dq_2 \exp[iq_1(z_1 - z_2)] = \frac{2(\pi R^2 - 2)\sin(\pi R) + 4\pi R \cos[\pi R]}{R^3} \]
\[ \text{(12)} \]

This kernel is plotted in figure 3 where it is compared with the elastic approximation (scaled for comparison). Although many diagonal approximations are used for acoustic phonon scattering including the inelastic case, it is evident the approximation fails at short distances.

**Figure 2:** Exact and approximate Scattering Kernel for inelastic scattering on optical phonons

**Figure 3:** Non-diagonality of the scattering kernel

**4. Scattering rates and non-diagonality of the self-energy**

As a measure of the effects of diagonal/non-diagonality we evaluate the scattering out rate \( \Gamma(k_\perp, k_\perp', \varepsilon = \varepsilon(k_\perp) + \varepsilon(k_\perp')) \) for polar optical phonon scattering using (4) and (5) in the self-consistent Born approximation for the retarded self-energy \( \Sigma^R \) (using iteration on the Born approximation result) in the approximation that level shift terms and \( G^e \) dependence are neglected:
The results are shown in figure 4 for n-GaAs at 300K using the data for figure 2b, for the full-off diagonal self-energy and in the diagonal approximation (in the z-variables). It is clear that diagonality under-estimates the scattering rate and indeed under-estimates the energy and momentum dissipation. Figure 5 shows our recent calculation for the current spectra in a full 3D NEGF simulation of a silicon nanowire transistor with 2.2 nm X 2.2 nm cross section and 6 nm channel length using diagonal self-energies. The current mean energy (red line) shows the hot electron energy relaxation in the drain. The local power dissipation is not equal to the Joule power. The white dashed line represents the first sub-band. The present paper suggests these data under-estimate the energy dissipation in the nanowire.

5. Discussion and Conclusions

The incorporation of full non-diagonal self energies in the 3D-NEGF simulation of nano-transistors presents a major computational challenge as the recursive algorithm is not immediately applicable. We are investigating re-scaling of the self-energy to a quasi-local spatial form to recover a recursive algorithm. Furthermore the approximation must be robust against instabilities arising from commensurability between the mesh spacing and the long-range quasi-periodic non-locality shown in figures 2a, 2d and fig 3b. This work demonstrates that the non-diagonality of the self-energy has a substantial effect on scattering rates and that the simple approximations for scattering kernels are strongly dependent on the value of the screening length. Confining the phonon wave vectors to the first Brillouin zone generates self-energies for which non-locality extends over a few nanometres (and thus within the spatial scale of features in extreme nano-transistors). Although local approximations to SCBA appear to be compatible with the Ward identities it does not follow that they are fully compliant with energy and momentum conservation. Locality is equivalent to isotropic scattering in the corresponding localised dimensions and under-estimates momentum and energy relaxation rates. Recent silicon nanowire devices involve strong polar coupling between channel electrons and interfacial SO phonons excited in the wrap-round dielectric: the self-energies will be highly non-local.

6. References

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