Perturbative vs Non-Perturbative impurity scattering in a narrow Si Nanowire GAA transistor: A NEGF study

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Abstract. In this paper we study the effect of impurity scattering on the performance of a Si gate-all-around nanowire transistors. The non-equilibrium Green function formalism is used in order to describe the carrier transport. Impurity scattering is introduced using two different formalisms, one that considers the impurity potential as a small perturbation by introducing self energies and the other in which the impurity potential is described exactly by included the impurity potential through the Poisson equation. The non-perturbative method does not use a fitting parameter but the perturbative one uses a phenomenological constant that can be calibrated to match the result of the non-perturbative method. We confirm Ohms-law-type behaviour by using the perturbative approach for larger channel lengths.

1. Introduction
The revolution in device miniaturisation has led to nanometre-dimension transistors. Short channel effects plague the bulk MOSFET architecture, which is at the core of the current Silicon VLSI technology. These effects degrade the transistor performance, making it impossible to continue the scaling of devices. SOI, and 3D architectures such as FinFETs and nanowires, offer a realistic alternative solution. These devices are not affected by short channel effects and possess a better electrostatic integrity compared to bulk MOSFET architectures. At nanometre dimensions, quantum mechanical effects play an important role; volume inversion, threshold voltage shift and increased leakage are some of the consequences at the device level of the underlying quantum rules. Those effects are linked to the wave structure of the electron, which appears when the dimensions of the system became of the order as the de Broglie wavelength. The interaction of the electron with the device becomes more like a wave interaction or scattering with the electrostatic potential.

Groups of dopants in enclosed domains can not be considered as continuous doping when the average number of them in the device is on the order of a hundred or less, and when their location has a direct impact on the $I_D$-$V_G$ characteristics. Work [1] on the description of random discrete dopants has been carried out using different levels of sophistication and approaches. Classical and semi-classical simulation techniques have been deployed from the micrometre scale to tens-of-nanometres. Recently, non-perturbative quantum mechanical simulations of nanowire transistors [2, 3, 4] based on the Non-Equilibrium Green’s function (NEGF) formalism have been carried out. The discrete dopants are introduced as an electronic charge associated to a volume. The advantage of this technique is the straightforward incorporation of decoherence, which could be used to treat all types of perturbative scattering mechanisms such as phonon and impurity scattering. Recently [5] a perturbative approach using the self-consistent Born approximation has been used in order to estimate the effect of impurity
scattering in a Si nanowire transistor. This model uses an empirical parameter. In this work we calibrated this parameter from our non-perturbative calculations. In section 2 we describe the different approaches used to treat scattering using the NEGF formalism. The simulated results for a thin Si nanowire transistor are presented in section 3. The last section reviews the conclusions of this work.

2. Impurity scattering in the NEGF formalism

The NEGF formalism was developed to treat many particle systems under external field at finite temperature. In the sixties, with the success of the perturbative quantum field theory based on the propagators or Green function, Schwinger [6] wrote a set of functional equations for the full Green function at zero temperature. These equations could be solved with the use of approximations and partial summation of terms. The extension of this formalism to finite temperature and non-equilibrium problems was pioneer by Schwinger, Kadanov, Baym and Keldysh [7, 8, 9]. The single particle Green function allows the calculation of the macroscopic physical magnitudes of interest such as the electron and current density without the hazard of calculating the many-particle wave function. In the finite temperature case the Green function becomes a 2x2 matrix [7, 9] where the four elements split into two types: two that have pure dynamical information (the retarded $G^R$ and the advanced $G^A$ Green function), and two that have statistical information (the less-than $G^<$ and the greater-than $G^>$ green function). All are called Green functions but the former two are the only Green functions from a mathematical point-of-view. The steady state versions of the equations for $G^R$ and $G^<$ are:

$$\left(E - T - U - \Sigma_c^R(E) - \Sigma_S^R(G^>,G^>)\right)G^R(E) = I$$

(1)

$$G^>(E) = G^R(E)\left[\Sigma_c^>(E) + \Sigma_S^>(G^>)\right]G^A(E)$$

(2)

where $E$, $T$ and $U$ are the total, kinetic and potential energies of the carrier and the retarded self energies for the contact and scattering are denoted by $\Sigma_c^R$, $\Sigma_S^R$ respectively (the structure of $\Sigma_S^R$ includes the Pauli exclusion principle [8]) $\Sigma^<$ stands for the less-than self energy. Eqs 1 and 2 are matrix equations in the spatial indices, which are implicit. The $I$ on the right hand side of Eq. 1 is the identity matrix, which indicates that the $G^R$ is truly a Green function in the mathematical sense. Eqs 1 and 2 are solved for the relevant energy interval, which usually consist in 600 to 1000 energy points. When scattering is considered the equations became a coupled set of non-linear matrix equations, which are very computational demanding. The non-linearity appears in the dependence on $G^>$ and $G^<$ of the self-energies. The electron and current densities are calculated by the diagonal and the first off-diagonal block of $G^>$. A recursive algorithm [10] is deployed in order to calculate just the diagonal and off-diagonal elements, dramatically reducing the computation time. Eqs. 1 and 2 are supplemented with boundary conditions. In the case of Eq. 1, open boundary conditions are imposed through the contact self-energies. Note that these equations are now matrix equations in the spatial indices (not shown), therefore matrix $G^R$ could be solved by inversion. This boundary condition allows injection of electrons into the system and makes the contacts less reflective. The boundary condition for $G^<$ or $G^>$ at the contact is called the equilibrium condition or KMS (Kubo-Martin-Schwinger) [11] which guarantees that, in the contacts, $G^<$ and $G^>$ reduce to the corresponding equilibrium values i.e $G^< = \text{Imaginary}(G^R)f_c(E)$, where $f_c(E)$ is the Fermi-Dirac distribution function at the corresponding contact. This means that the electron density in the reservoirs is the local density-of-states multiplied by the equilibrium probability (Fermi-Dirac) of finding an electron there. In the presence of decoherent processes such as phonon and impurity scattering, which are accounted for through self-energies, the energy distribution of an electron inside the simulated region is no longer a simple addition of the Fermi-Dirac distributions of the contacts, and we are in the presence of a genuinely non-equilibrium distribution like those considered in high-field Monte Carlo simulations. One advantage of considering the impurity scattering as self-energies is that it can account for the
broadening in the density states, which is not possible in the non-perturbative case. In the perturbative approach we follow the approach of [5], in which the less-than self-energy is written as:

\[ \Sigma_{\text{imp}}^{c}(E) = C \ G^{\Delta}(E) \]  

(3)

where \( C \) is a constant which depends on the doping concentration in the source and drain and the strength of the interaction, a formal description of which can be found in [5]. In this work the \( C \) parameter is varied to produce the non-perturbative results, which have no fitting parameter. The impurity scattering is assumed to be elastic (energy conserved). In the non-perturbative case the impurities are introduced as a charge homogeneously distributed in a discretisation volume (0.2×0.2×0.2 nm\(^3\)). It is important to mention that the static dielectric constant is approximately valid at a distance larger than two Angstroms away from the impurity location.

3. Simulation results

A very narrow gate-all-around (GAA) nanowire with 2.2×2.2 nm\(^2\) cross-section and a channel length of 6nm has been used in the simulation. The source/drain doping is 10\(^{20}\) cm\(^{-3}\) and the channel is undoped. First we have simulated the impurity scattering through a non-perturbative approach, i.e. we have introduced the impurity scattering through discrete dopants, which are randomly distributed through the source/drain (S/D) extension regions as is shown in Fig. 1.

![Figure 1. Schematic of the simulated nanowire.](image)

Thirty nanowire transistors, which differ in the random locations of the discrete dopants, have been simulated at a low drain bias (1mV) in order to ensure the device is working in the linear response region. Fig. 2 shows the \( I_{D}\text{-}V_{G} \) characteristics of the simulated transistors, and the corresponding average characteristic. At high gate bias the effective resistance of the source/drain extensions have been extracted by using the ballistic \( I_{D}\text{-}V_{G} \) device characteristic. This resistance is 1.68×10\(^4\) Ω.

The perturbative approach [5], which includes density-of-states broadening and decoherence has also been used to study the effect of impurity scattering. This model has been applied to include scattering through self-energies in 4nm regions of the source and drain. The \( I_{D}\text{-}V_{G} \) characteristic of the transistor with incoherent scattering is shown in Fig. 3 as well as the curves for the atomistic average and ballistic transistor.

The \( I_{D}\text{-}V_{G} \) of the transistor with incoherent scattering (short S/D) gives similar results to the atomistic average \( I_{D}\text{-}V_{G} \). The perturbative approach is able to reproduce the atomistic average \( I_{D}\text{-}V_{G} \) characteristic by varying the \( C \) parameter at all the gate voltages. We have also calculated the \( I_{D}\text{-}V_{G} \) characteristic for a device in which scattering is included in a 10 nm region of the source and drain (long S/D) using the calibrated \( C \) parameter. The on-current for this device reduces to 1/3 of the ballistic current, compared to 2/3 for the shorter channel, as can be seen in Fig. 3. This should be expected if a linear dependence of the resistance as function of the wire length is assumed. For the
large S/D device, the scattering reduces the on-current to 30% of the current in the smooth device. Note that the effect is mainly in the on-state.

4. Conclusions
In this work we have employed the NEGF formalism to simulate the impurity scattering for a GAA Si nanowire transistor using two very different models. One model is non-perturbative (atomistic) and introduces the impurity scattering through discrete charges and the other is perturbative and introduces the impurity scattering through the imaginary part of the self-energy. From the atomistic simulation, by averaging all the $I_D-V_G$ curves we have extracted the series resistance associated with the impurity scattering. The perturbative method has been calibrated to the atomistic method and used to simulate impurity scattering in a large S/D region, producing Ohmic-type behaviour. The perturbative method can be used to include the series resistances in the heavily doped source/drain regions using a mode-space approach, which is less computationally expensive than the fully-3D real-space approach.

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