Green function study of quantum transport in ultra-small devices with embedded atomistic clusters

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Transport in limiting scale MOSFET transistors will be strongly influenced by quantum effects and the presence of atomistic scattering centres either intentionally or un-intentionally present in the channel and the device environs. The scattering in such systems is non-asymptotic and the self-averaging conditions of the Kohn-Luttinger theorem fail so that a self-energy for impurity scattering does not exist. Atomistic scattering must therefore be treated non-perturbatively. Previously it has been shown that quantized micro-vortices may occur at definite energies in the current flow contributing to both the blocking effect and to effective mobility. The present study uses the Glasgow and NASA NEGF simulators to study vortex formation and tunnelling through small clusters of atomistic impurities arranged with various configurations within the 5 nm wide by 12 nm long channel of a Double Gate MOSFET. The I-V characteristics and the threshold voltage are severely affected by the distribution of the charges in the channel. A variety of different geometry atomistic clusters have been studied. Examination of the energy dependent current density allows an evaluation of the admixture of strong quantum flows such as micro-vortices to the net current. It is found that the threshold voltage and conductance are strongly dependent on the impurity configuration. The I-V characteristics are monotonic in most cases due to the strong thermal smoothing that prevents resolution of the mode structure.

1. Introduction
The need to model ultra-small silicon MOSFET devices in the hypothesised quasi-ballistic regime has focussed attention on schemes based on quantum transport methodology. The deepest advances have been made by the application of the non-equilibrium Green function (NEGF) formalism to semiconductor devices\textsuperscript{1-5}. The NEGF formalism as applied to devices\textsuperscript{2} is based on infinite-order perturbation theory that leads to a set of coupled integro-differential equations for the various Green functions determined by the appropriate self-energy functions. The open system problem is circumvented by selecting the Green function for the finite device region by folding the coupling to the contacts into a boundary-controlled self-energy. Although this makes the problem just tractable, the existence of the standard equations, in particular the collisional self-energies, depends especially on the assumption that the scattering perturbations are self-averaging. This is reasonable for coupling to the large phonon bath but the conventional structure of the self-energy for impurity scattering only exists if the self-averaging ansatz of Kohn and Luttinger\textsuperscript{6}, Luttinger\textsuperscript{7}, holds true. Unfortunately, for finite small devices the microscopic discrete distributions of impurities in the channel and source and drain regions are non-self-averaging random variables\textsuperscript{8-15}. Classical studies have shown that these are important for contributing strong fluctuations in...
the device parameters such as threshold voltage and effective channel mobility \cite{16-17}. In the present paper we discuss the consequences of non-self-averaged scattering on finite atomistic clusters of impurities using the NEGF formalism adapted to treat impurity scattering non-perturbatively. In a companion paper we present an extension of the formalism to interface roughness scattering in ultra-small MOSFETs.

2. Break-down of the Kohn-Luttinger ansatz
Consider the total scattering potential for a randomly distributed system of $N_I$ identical discrete impurities (typically fixed screened Coulomb centres) as:

$$V_{\text{total}}(\mathbf{r}) = \sum_{j=1}^{N_I} V(\mathbf{r} - \mathbf{r}_j) \quad (1)$$

The Fourier transform of eqn. (1) yields a convenient extraction of the Fourier transform of the particle density of the impurities $\rho_I(\mathbf{q})$:

$$V_{\text{total}}(\mathbf{q}) = \rho_I(\mathbf{q})V(\mathbf{q}) \quad (2)$$

$$\rho_I(\mathbf{q}) = \sum_{j=1}^{N_I} e^{-i\mathbf{q} \cdot \mathbf{r}_j} \quad (3)$$

The crucial self-averaging property of large numbers of such randomly distributed impurity potentials was established by Kohn and Luttinger \cite{6}, Luttinger \cite{7} for uniform random distributions. An extension to more general distributions is discussed in Elliot et al \cite{18}. The standard perturbation expansion \cite{7} of the Green functions for electrons interacting with the random impurity array involves products of the form

$$F_I(\mathbf{q}_1,\mathbf{q}_2,...,\mathbf{q}_n) = \rho_I(\mathbf{q}_1)\rho_I(\mathbf{q}_2)...\rho_I(\mathbf{q}_n) \quad (4)$$

In conventional Green function theory the structure factors $F_I(\mathbf{q}_1,\mathbf{q}_2,...,\mathbf{q}_n)$ are averaged over a random ensemble. As an example, for large numbers of impurities, $N_I>>1$, the Kohn-Luttinger ansatz asserts that we may replace expression (3) by

$$\langle F_I(\mathbf{q}_i) \rangle = \langle \rho_I(\mathbf{q}_i) \rangle = \langle e^{-i\mathbf{q}_i \cdot \mathbf{r}_j} \rangle = N_I \delta_{\mathbf{q}_i \mathbf{0}} \quad (5)$$

i.e the sum over random impurities is zero unless $\mathbf{q}=0$, when the generally complex sum becomes a real number equal to the number of impurities $N_I$. In a recent study one of us \cite{9,11} examined over 100 sequences of uniform random distributions of impurities at different doping densities. It is found that condition (5) only holds for $N_I>1000$ impurities. For smaller numbers the structure factor is complex; the imaginary part is non-zero for most values of $\mathbf{q}$. In particular for $qd>1$, where $d$ is the mean separation between impurities, there will be interference between the scattering from the individual impurity potentials. Figure 1 shows the function $K(\mathbf{q}) = \left| \sum_{j=1}^{N_I} e^{-i\mathbf{q} \cdot \mathbf{r}_j} / N_I \right|$ for 10, 100, and 1000 impurities randomly distributed in a
50 nm side box. The function is plotted in the $q_z = 0$ plane. The wave vector limits are at $\pm \pi/10 \text{ nm}^{-1}$. Self-averaging occurs approximately for $N_I > 1000$, when $K(q) \to \delta_{q,0}$.

Figure 1: Structure factor spectrum $K(q)$ in $q_z = 0$ plane for random dopant distributions in 50 nm side box. Positions are projected into the central plane
(a) 10 impurities (b) 100 impurities (c) 1000 impurities. Adapted from reference 11.

Similar conclusions are found for the second-order structure factor

$$< F_j(q_1, q_2) >= < \prod_{j=1}^{N_I} e^{-i q_{j} \cdot r_{j}} e^{-i q_{2} \cdot r_{j}} > \to \sum_{N_I > 1000} N_I \delta_{q_{1},+q_{2},0} + N_I (N_I - 1) \delta_{q_{1},0} \delta_{q_{2},0}$$

(6)

For atomistic devices, where $N_I < 1000$, the Kohn-Luttinger ansatz and standard infinite-order perturbation theory fail: the Green function expansion $G$ in Figure 2 is not equivalent to the ensemble average $\langle G \rangle$ and a self-energy cannot be defined. As a consequence the standard gain-loss NEGF transport equations are not valid for impurity scattering which must instead be treated non-perturbatively.

The nature of the scattering for non-self-averaging configurations may be seen by using the $T$-matrix expansion of the Green function (retarded):

$$G = G_0 + G_0 T G_0$$

(7)

Where the full $T$-matrix may be expanded in terms of the individual $t$-matrices for the $j=1 \ldots N_I$ impurities.

$$T = \sum_{j=1}^{N_I} t_j + \prod_{j=1}^{N_I} t_j G_0 t_j + ...$$

(8)
The leading term in (8) describes the scattering off each impurity; in non-self-averaging systems it produces interference effects due to the final superposition of each scattered wave. The second term describes scattering on one impurity followed by propagation and scattering off a second impurity; pair-wise multiple scattering. Both terms are significant in atomistic devices. Indeed, the leading term gives rise to strong interference effects; the matrix element for $T$ for example becomes:

$$\langle k | T | k' \rangle^2 = N_f \langle k | t | k' \rangle^2 \{1 + \frac{2}{N_f} \sum_{j \neq j'} \cos q (r_j - r_{j'})\}$$

(9)

It is clear that if the interference term did not occur the scattering cross section would be just $N_f$ times the cross section for single impurity scattering. For $qd << 1$, the interference term sums to $N_f - 1$, yielding a cross section that is $N_f^2$ bigger than the single impurity case. For $qd >> 1$, the interference term oscillates very rapidly and approximately cancels out when the number of impurities is very large. We then obtain the self-averaging limit: the cross section is then $N_f$ times larger than the individual impurity case, which is the assumption used in deriving quantum relaxive transport (self-energy exists) or Boltzmann-Bloch transport.

3. Double gate device model

For finite open coherent atomistic systems the long sequences of incoherently repeated collisions encountered in the limit of large numbers of impurities cannot occur. The dominant effect on transport will come from the simple coherent superposition of scattered waves from each impurity and also the incident waves entering from the source and any reflected waves at the drain. Previously, approximate analytical models were developed for the scattering Green function in an open finite atomistic device using hard sphere scattering models. It was shown that the net flow in a steady pure state of constant energy is a meandering open flow from source to drain, enclosing the few impurities and several localised micro-vortex flows. The latter arise particularly from the leading interference terms in (8). In the following we show that this result is quite general.
Here, we investigate, the self-consistent current density in a realistic short channel double gate silicon MOSFET device (figure 3) containing just 3 unintentional discrete dopants in the channel. The spatial configuration is varied to investigate the dependence of both the flows and the device performance on the spatial geometry.

The layout of the simulated double gate MOSFET device is shown in figure 3. The device has metal gate contacts and 1nm oxide thickness. The channel length is 12 nm that allows a ballistic approach; the channel body thickness is 5nm; the doping in the source and drain regions, $N_{D}$, is $10^{20}$ cm$^{-3}$, and the channel doping, $N_{A}$, is $10^{14}$ cm$^{-3}$. The reservoir alignment was varied from well-matched (source and drain cross section = channel cross-section) to wide reservoir. The device is simulated at 300K.

![Figure 3: layout of model silicon double gate device.](image)

### 4. Modelling

The results are presented for NEGF modelling of the device assuming an anisotropic effective mass Hamiltonian $H_{b}$ for each of $N_{b}$ independent valleys:

$$H_{b} = -\frac{\hbar^{2}}{2}\left\{ \frac{\partial}{\partial x} \frac{1}{m_{x}^{b}} \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \frac{1}{m_{y}^{b}} \frac{\partial}{\partial y} + \frac{\partial}{\partial z} \frac{1}{m_{z}^{b}} \frac{\partial}{\partial z} + e\phi(R) \right\}$$

![Figure 4: energy iso-surfaces for the electron valleys in silicon.](image)
The anisotropic effective mass ratios (silicon) are: 0.19 and 0.98. The silicon effective mass ratio in the isotropic model is taken as 0.3283. Other data correspond to reference 3.

In (10), \( \phi(R) = \phi(r,z) \) is the local electrostatic potential obtained self-consistently from Poisson’s equation applied to the full device geometry and continuous doping distributions including the fields of the three unintentionally discrete dopant (Coulombic) impurities. The impurity and electrostatic potentials are treated non-perturbatively. The simulation is very compute-intensive for 3D models. Instead, we assume the double gate device is very wide in the z-direction, rendering the computation effectively two-dimensional. As a consequence the 3D description of the atomistic impurities corresponds to long line charges perpendicular to the x-y plane. The limitations of the 2D simulation are discussed further in the final section.

The simulation is based on the self-consistent recursive thermodynamic Green function method, outlined elsewhere\(^3\), using a suitable discrete spatial grid. The computations yield the total charge density \( n(r) \) and total current density \( j(r) \). The energy resolved charge density \( n(r; E) \) and current density \( j(r; E) \) are also computed at interesting energies \( E \). The ratios \( v(r) = j(r)/n(r) \), \( v(r; E) = j(r; E)/n(r; E) \), define the total velocity field and energy-resolved velocity field that are useful for examining the quantum hydrodynamics of the flows. As an example, the valley-resolved electron density is determined from the valley Green functions as:

\[
n_b(E,r) = -iG^<(r,r;E) (11)
\]

Poisson’s equation is

\[
\nabla^2 \phi = \frac{e}{\epsilon}(n - p - N_D + N_A) (12)
\]

Equation (12) augmented for the point impurities is solved self-consistently with the Green functions.

5. **Atomistic configurations**

The simulations are based on four configurations of three (repulsive Coulombic) atomistic dopants as shown in figure 5.

![Figure 5: qualitative spatial configurations of three atomistic dopants used in the simulation](image)

Configuration H is a horizontal strongly localised configuration that acts to divide the channel; the configuration V is a vertical configuration that acts to strongly block the channel; the configuration S is axially symmetric that classically would allow current flow between the forward impurities; finally, T is an asymmetric arrangement that blocks the flow on the lower
region of the channel. Figure 6 shows the calculated potential distribution for the four different configurations (H, V, S, T) of three dopants for gate voltage $V_G=1.5$ V and drain voltage $V_D=0.6$ V. The source and drain are located at the left and right of every panel. The two gates are located at the top and the bottom of the panels. The spatial scale is stretched in the x-direction leading to some apparent distortion of the distributions. Figure 6 also shows the impurity potential peaks and the effective barriers presented to electrons incident from the source.

Figure 6: The potential landscape (at $V_G = 1.5$ V) for the four arrangements of the three charges in the channel: upper left panel (V), upper right panel (H), lower left panel (S), and lower right panel (T). A landscape plot of the potential distribution in the S-configuration.

The three pronounced peaks in the potential mark a region where current may form circulatory flows and where diffraction, interference and tunnelling may occur in the ballistic current due to the triangular configuration of impurities. The strong confinement couples with scattering on the discrete charges to create macroscopic quantum interference patterns that produce regions of low electron concentration where, classically, a high electron concentration is expected. At any given energy, an electron moves coherently through the channel and may tunnel through the potential barrier created by the charge configuration. This tunnelling current can produce significant differences in the current-voltage characteristics compared with semi-classical derivations (such as the density-gradient – drift diffusion method).
6. Current – voltage characteristics

Figure 7 shows the computed current-voltage characteristics corresponding to the four configurations (H, V, S, T) at $V_D = 0.6$ V. Results are shown for the isotropic (full lines) and anisotropic (dashed lines) effective mass models. At sub-threshold the conductances $dI/dV$ are very similar for the anisotropic mass model and the weaker isotropic model. However, the use of the realistic anisotropic mass model leads to a 200 mV shift in threshold voltage from the predictions of the isotropic model.

![Figure 7: The I_D-V_G characteristics of the four devices (see fig. 5) using the isotropic (I) and the anisotropic (A) mass models at V_D = 0.6 V.](image)

The I-V characteristics and the threshold voltage are severely affected by the distribution of the charges in the channel. Conductances and threshold voltages show significant statistical spread.

7. The spatial distribution of current

The current density reveals interesting structure. The current density profile $J_y(x,y)$ at low gate voltage ($V_G=1.5$ V) is shown in figure 8 for the S-configuration in the anisotropic mass model. It shows the majority of the current flow is between the two foremost impurities followed by bifurcation of the flow around the rear impurity. At very high gate voltage, $V_G=2.4$ V, the current flow concentrates close to the gates in two parallel streams that avoid the dopants.
The high voltage behaviour, shown in figure 9, does not occur for the isotropic mass model. There is significant tunnelling present that is enhanced by the low mass components. The full current density vector field $J(x,y)$ is also shown in figure 8.

8. Macro-vortices
The related velocity fields, $v(r)$, and $v(r;E)$ are useful for a quantum hydrodynamic picture of the flow. For steady flows it is simple to demonstrate that for pure or mixed states the
streamlines do not cross and the topology of the flow is determined by hyperbolic and vortex centre singularities of the autonomous equation

\[
\frac{dx}{dy} = v_x(x,y) \quad \frac{dy}{dx} = v_y(x,y) \quad (13)
\]

For pure states, the velocity field \( \mathbf{v}(\mathbf{r}; E) \) may contain quantised vortices at the strong nodes of the electron density \( n(\mathbf{r}; E) \^{8-15,19} \). The energy-resolved velocity fields that underlie the data for figure 8 show micro-vortices located within a meandering current. The vortices act to turn the current flow in space: they are essentially localised centres with well-defined angular momentum states. In closed systems, the localised centres may still occur but they are degenerate with clockwise and anti-clockwise circulation corresponding to the usual degenerate angular momentum states. The full velocity field \( \mathbf{v}(\mathbf{r}) \) shows a meandering flow very like the classical flow predicted for atomistic landscapes \^{16-17} \ but with additional structure following from the energy resolved vortices which are generally hidden in the total flow by the thermal superposition of states.

Figure 9: Current densities for the S-configuration at gate voltage \( V_G = 2.4 \) V.
Interestingly, despite the strong thermal suppression, it is easy to find atomistic configurations that display vortex flows in the total electron velocity field (classical-like idealised vortex) and indeed, the current density vector field (Rankine-like vortex). However, defining these macro-vortices are mixed state flows that show non-zero but not necessarily quantised circulation. Figure 10 illustrates a case-in-point: a double gate device with four unintentional dopants. For this particular (artificial) configuration the impurities form an effective offset cavity in the channel. The current density and velocity field show a strong macro-vortex in the flow.

Figure 10. Total electron density, total current density $J_y$ and total current density vector field for four atomistic impurities embedded in a double gate device at 300 K.

9. Transmission function profiles

The quantisation of the transverse states in the channel of the double-gate device gives rise to a transmission function $T(E)$ that has a characteristic stepped structure as a function of energy. This is a consequence of opening new Landauer channels as the energy is increased. The NEGF simulations predict very different behaviour for $T$ depending on the reservoir geometry (figure 11) and the presence of atomistic impurities. Figure 12 show the various transmission functions corresponding to different contributing valleys (see figure 5) for no atomistic impurities and for wide and matched reservoir geometries. At low gate bias there is more reflection at the wide reservoir-channel junction. At high gate bias resonances appear in the wide reservoir transmission as noted elsewhere.\textsuperscript{20}
Figure 11. Matched and wide reservoir geometries for double gate device.

Figure 12. Transmission curves for different valleys at low gate bias (0.6 V) and high gate bias (1.0 V). Full curves: matched reservoir; dashed curves: wide reservoir.

Figure 13 shows the effect of adding three atomistic impurities to the simulation using configuration S of figure 5. The transmission function loses the sharp step structure as interference scattering from the impurities adds or subtracts to the number of Landauer channels in the system.
At low bias the transmission is similar for the wide and matched reservoirs. At high bias, large differences occur between the wide and matched reservoir devices. The complex patterns are associated with tunnelling and resonances as the bare impurity potentials emerge from the potential landscape.

10. Conclusions
We have found that the predicted threshold voltage and conductance for a short channel double gate MOSFET are strongly dependent on the impurity configuration. The underlying energy-resolved transport shows complex flows typified by meandering streamlines enclosing localised vortex flows. The consequent transmission functions are very random. However, the current-voltage characteristics are monotonic in all cases due to the strong thermal smoothing that prevents resolution of the mode structure. Some configurations may nevertheless generate macro-vortices in the flow. The overall processes predicted for atomistic scattering are in accord with the break-down of the Kohn-Luttinger ansatz for small numbers of impurities. Results of a parallel study suggest that de-coherence processes do not seriously impair these quantum processes provided the coherence lengths are long compared to the 12 nm channel. This situation may not be true for devices with high κ gate stacks for which a plasmon-enhanced SO phonon scattering extends into the channel from the interfaces.

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