A determinist method solving the Wigner transport equation for quantum transport in silicon nanowires

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Abstract. A determinist method is presented for solving the steady-state Wigner transport equation in nanoscale MOSFET devices. The three-dimensional quantum transport is computed by solving the coupled 3D Poisson and 2D Schrödinger equations (by a mode-space approach) with the 1D Wigner transport equation along the source-drain direction. Numerical simulations are performed to demonstrate the ability of the Wigner function formalism to correctly reproduce quantum transport properties in gate-all-around silicon nanowire MOSFETs.

1. Introduction
One-dimensional nanostructures such as nanowires are attractive building block to develop novel nanoscale electronic devices. Advances have been made in the fabrication of semiconductor nanowire transistors in which the quantum nature of carrier dynamics cannot longer be neglected [1]. Among the modeling techniques of these devices, the Nonequilibrium Green function (NEGF) formalism is often used [2–4]. Although scattering mechanisms remain a difficult problem to adress, this formalism is especially suitable for quantum transport in mesoscopic devices. Another approach capable of handling quantum coherent propagation and dissipative scattering effects is based on the Wigner function formalism [5, 6]. An advantage of the Wigner equation as compared to NEGF method is the strong analogy with the Boltzmann equation since it is a phase space description similar to the classical Boltzmann distribution function. This analogy will allow to easily highlight the impact of expected quantum effects like tunneling and interference phenomena on performances of nano-scale electronic devices.

In this work, we present a 3D quantum simulation of gate-all-around silicon nanowire using a direct solution of Wigner transport equation (WTE). The 3D ballistic quantum transport is computed by solving the coupled 3D Poisson - 2D Schrödinger equations by a mode-space approach with the 1D Wigner transport equation along the source-drain direction. Our motivation is to demonstrate the possibility to use an alternative to the NEGF method combining both a correct description of quantum transport properties and a strong analogy with the semiclassical Boltzmann transport equation usually used.

2. Wigner’s function formalism for quantum transport
Let us consider the 3D geometry of silicon nanowire shown in figure 1. The x and y axes represent the quantization directions, and z axis represents the transport direction. The length of source/drain (S/D) extensions is 16 nm and the square cross-section is equal to 3 nm × 3 nm. The N-type S/D extensions are doped 5 × 10^25 m^-3 and the silicon channel is assumed undoped.
Figure 1. *Gate-all-around* silicon nanowire simulated in this work. $x$ and $y$ axes represent the quantization direction and $z$ axis represents the transport direction.

The effective mass Hamiltonian of the device satisfies the 3D Schrödinger equation,

$$H^{3D}\Psi(x, y, z) = E\Psi(x, y, z),$$

with the Hamiltonian of the system defined as

$$H^{3D} = -\frac{\hbar^2}{2} \frac{\partial}{\partial x} \left( \frac{1}{m_x^{\text{eff}}} \frac{\partial}{\partial x} \right) - \frac{\hbar^2}{2} \frac{\partial}{\partial y} \left( \frac{1}{m_y^{\text{eff}}} \frac{\partial}{\partial y} \right) - \frac{\hbar^2}{2} \frac{\partial}{\partial z} \left( \frac{1}{m_z^{\text{eff}}} \frac{\partial}{\partial z} \right) + V(x, y, z),$$

where $m_x^{\text{eff}}$, $m_y^{\text{eff}}$ and $m_z^{\text{eff}}$ are the effective masses along the $x$, $y$ and $z$ axes, respectively, and $V(x, y, z)$ is the conduction band-edge profile. In order to significantly reduce the computational burden associated with a full 3D real-space solution, the so-called mode-space approximation is used. Then, the nanowire can be subdivided into a large number of slice along the transport direction $z$. At every discretized real-space point $z$, the energy subbands $E_\nu$ and the corresponding wavefunctions are obtained from 2D Schrödinger’s equation. Then, the Wigner transport equation is solved for each energy subband. By analogy with the Boltzmann transport equation, the Wigner transport equation is computed in order to determine the distribution function dependent on both the position $z$ and the wavevector $k$. Performing the Fourier transformation of the Liouville-von Neumann equation, the Wigner transport equation can be written as [7],

$$\frac{\partial f_w(z, k, t)}{\partial t} + \frac{\hbar k}{m^{\text{eff}}} \frac{\partial f_w(z, k, t)}{\partial z} + \int_{-\infty}^{+\infty} dk' f_w(z, k', t)V_w(z, k - k') = \left( \frac{\partial f_w}{\partial t} \right)_{\text{coll}}$$

Here $f_w(z, k, t)$ is the 1D Wigner function at position $z$, wavevector $k$ and time $t$. The second term of the left-hand side is the kinetic term. It is exactly the same as the corresponding term of the Boltzmann equation. Quantum-interference effects are induced by the non-local potential term represented by the third term of the left-hand side. The non-local Wigner potential $V_w(z, k - k')$ is calculated from the potential energy $E_\nu$. It is defined as [7],

$$V_w(z, k - k') = \frac{2}{\pi\hbar} \int_{0}^{+\infty} dz' \sin[2(k - k')z'] \left[ E_\nu(z + z') - E_\nu(z - z') \right]$$

As can be seen, the Wigner function in $k$ and $z$ depends in a non-local manner on all other momentum points $k'$ and also on the potential at all other locations $z \pm z'$. Due to the non-local potential, we will show in the next section that the steady state Wigner function $f_w(z, k)$ may be negative in some points of the phase space.
The Wigner function being determined, we can readily calculated the 1D carrier density defined as,

\[ n(z) = \int_{-\infty}^{+\infty} \frac{dk}{2\pi} f_w(z, k) \]  

as well as the 3D quantum charge density used for solving the Poisson equation. Then, the potential is updated and 2D Schrödinger’s equation in each slice of the device can be solved again. Once the self-consistency between Poisson-Schrödinger-Wigner equations is obtained, the current density \( j(z) \) can be calculated.

\[ j(z) = \int_{-\infty}^{+\infty} \frac{dk}{2\pi} \frac{\hbar k}{m_{eff}} f_w(z, k) \]  

3. Results and discussion
The validity of our Wigner function-based simulator is evaluated by computing current-voltage electrical characteristics of surround-gated silicon nanowire shown in figure 1.

The two lowest energy subbands of the six ellipsoidal \( \Delta \) valleys of the silicon conduction band are plotted in figure 2. The corresponding 1D electron density calculated for each energy subband is shown in figure 3. It appears that due to the strong confinement in silicon nanowire, most of electrons are located in the first energy subband. The Wigner function corresponding to the first energy subband resulting from \( V_{gs} = 0.2 \) V and \( V_{ds} = 0.4 \) V is shown in figure 4. We can see that oscillations appear at the end of the channel due to quantum interferences. In the highly-doped S/D extensions, the Wigner function is similar to a Maxwell-Boltzmann distribution. However, in the channel, electron’s velocity increases and a peak of ballistic distribution into the positive range of wavevector is observed. Moreover, due to the non-local potential, the Wigner function is negative in some points of the phase-space. Oscillations of Wigner’s function in the channel, not observed for the Boltzmann distribution function, clearly demonstrate the ability of the Wigner function to account for quantum-interference effects.

**Figure 2.** Profile of energy subbands along the transport direction for a gate bias \( V_{gs} = 0.3 \) V and a drain bias \( V_{ds} = 0.4 \) V. The six ellipsoidal \( \Delta \) valleys of silicon conduction band are represented.

**Figure 3.** 1D electron density along the transport direction for a gate bias \( V_{gs} = 0.3 \) V and a drain bias \( V_{ds} = 0.4 \) V. The six ellipsoidal \( \Delta \) valleys of silicon conduction band are represented.

The electrical characteristics \( I_{ds} - V_{gs} \) resulting from solution of Wigner transport equation for \( V_{ds} = 0.4 \) V are plotted on figure 5. In order to validate the Wigner-function based simulator,
the results are compared with the NEGF method. A good agreement is observed between both approaches. Three channel lengths varying from $L_c = 10\, \text{nm}$ down to $L_c = 4\, \text{nm}$ are simulated. For a channel length $L_c = 10\, \text{nm}$, a subthreshold slope of around $60\, \text{mV/dec}$ is recovered. On the other hand, when the channel length is reduced down to $4\, \text{nm}$, a more important degradation of the subthreshold slope is observed. It is the consequence of both drain-induced barrier lowering and tunneling current which is properly accounted for with the Wigner function formalism.

**Figure 4.** Cartography of the Wigner function related to the first energy subband for a gate bias $V_{gs} = 0.2\, \text{V}$ and a drain bias $V_{ds} = 0.4\, \text{V}$. The channel length is $L_c = 10\, \text{nm}$ and the square cross-section is $3\, \text{nm} \times 3\, \text{nm}$.

**Figure 5.** Current-Voltage characteristics of a gate-all-around silicon nanowire calculated using both the NEGF and Wigner function method. Channel lengths varying from $L_c = 10\, \text{nm}$ down to $L_c = 4\, \text{nm}$ are simulated.

4. Conclusion

In summary, we have developed an efficient numerical method to calculate electron transport in semiconductor devices. A direct solution of Wigner transport equation coupled with a Schrödinger/Poisson algorithm is demonstrated. Our simulator is used to calculate electrical characteristics in silicon nanowire with a channel length varying from $10\, \text{nm}$ down to $4\, \text{nm}$. The results clearly demonstrate the presence of expected quantum effects in the transport direction and their impact on electrical performances. Finally, this work shows that alternatively to the NEGF approach, the Wigner function-based formalism is well suited to investigate quantum transport in semiconductor nanostructures using a determinist resolution of transport equation.

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