Analytical Model for Nanowire and Nanotube Transistors covering both dissipative and ballistic transport

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Abstract:

We present an analytical model for silicon nanowire and carbon nanotube transistors that allows us to seamless cover the whole range of transport regimes from drift-diffusion to ballistic, taking into account the one-dimensional electron or hole gas in the channel. We propose an analytical description of the transition from drift-diffusion to ballistic transport based on the Büttiker approach to dissipative transport. We start from the derivation of an analytical expression for ballistic nanowire transistors and show that a generic transistor with finite scattering length can be described as a chain of elementary ballistic transistors. Then, we are able to compact the behavior of an arbitrary ballistic chain in a simple analytical model, suitable for circuit simulators. In the derivation of the model, we find a relation between the mobility and the mean free path, that has deep consequences on the understanding of transport in nanoscale devices.

1. Introduction

The reduction of short-channel effects is a very important issue in the progressive scaling of field-effect-transistors. Multiple gate architectures such as gate-all-around (GAA) MOSFETs are emerging as promising candidates in order to control the short channel effects. In addition, multiple gate architectures are expected to have improved mobility given by the reduced surface scattering due to the lower vertical fields and by the reduced Coulomb scattering in the lightly doped channel.
In recent years, much attention has been placed on the analytical and numerical modeling of far-from-equilibrium transport, that is expected to be important in such device architectures, but no proposed treatment of far-from-equilibrium transport describes the transition from drift-diffusion to ballistic transport regime.
The aim of the present paper is the development of a compact model of far-from-equilibrium transport, following the Büttiker probes approach to inelastic scattering [1]. For such a purpose, we will use the method exposed in [2] for planar MOSFETs.

2. Modeling nanowires and nanotubes

In the following discussion, we will consider a quantum wire channel with generic geometry, as in Fig.1. The effective gate capacitance is: $C_g = C_{ox} \parallel C_d$ where C_{ox}

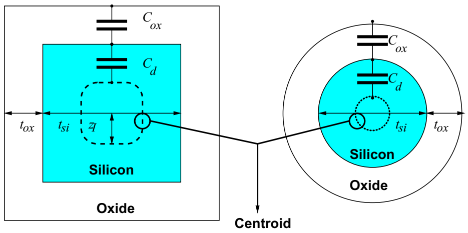

Figure 1: Schematic capacitance diagram for a wire with square and circular section. In the square shape the interface between the silicon and the insulator is considered approximately isopotential and the mobile charge layer (the centroid) is approximated with a square contour.

is the oxide capacitance and C_d includes the effects of the carrier centroid [3] z_I. Because of quantum confinement, we have a series of 1D subbands with associated eigenvalues in the v-th minimum: $E_n^v = q\phi_c + \varepsilon_n^v$ (n integer), where ϕ_c is the electrostatic potential in the center of the cross section, and the ε_n^v can be estimated from the well-known analytical solution of Schröedinger equation [4], or from numerical simulations. Well separated subbands will be considered so that intersubband mixing is not present.

2.1 Ballistic transport: case $L = \lambda$

In the case of ballistic transport, there is no local equilibrium so that no quasi-Fermi level can be locally defined, because two different carrier populations exist, originating from source and drain, that can be considered at equilibrium with the injecting electrode:

$$C_g\left(V_g' - \phi_c\right) = q\sum_{v,n} g_v \frac{\sqrt{2kTm_d^v}}{2\pi\hbar}\left[\Im_{-\frac{1}{2}}\left(\frac{\phi_c - V_s - \varepsilon_n^v}{\phi_t}\right) + \Im_{-\frac{1}{2}}\left(\frac{\phi_c - V_d - \varepsilon_n^v}{\phi_t}\right)\right] \quad (1)$$

where $V_g' = V_g - (\phi_m - \chi)$
Notwithstanding the simple structure, the model has been compared with a 2D Schrödinger- Poisson simulator giving a good agreement, as we can see in Fig.2, where rectangular confinement has been considered.

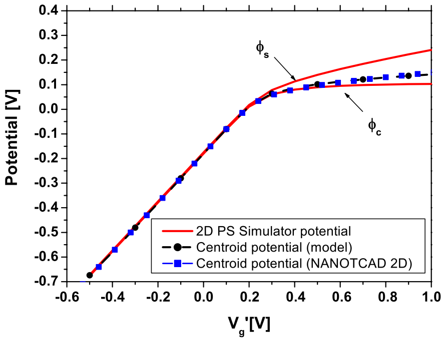

Figure 2: Surface, central and centroid potentials obtained a 2D Poisson-Schröedinger simulator and the centroid potential obtained with the compact model for an undoped wire with square cross section, $t_{si} = 10$nm, $t_{ox} = 2$nm, $z_I = 2.5$nm, $T = 300$K.

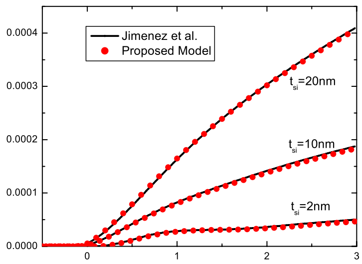

Figure 3: Ballistic nanowire transistor. Comparison between our model and the model [4].

For the current, from the Landauer formula, we have [4]:

$$I_{ds} = \sum_{v,n} g_v \frac{qkT}{\pi\hbar} \left[\Im_0 \left(\frac{\phi_c - V_s - \varepsilon_n^v}{\phi_t} \right) - \Im_0 \left(\frac{\phi_c - V_d - \varepsilon_n^v}{\phi_t} \right) \right] \quad (2)$$

where $\Im_n$ is the Fermi-Dirac integral of order n. It can be interesting to compare the behavior of the proposed ballistic model with the similar model presented in [4] in Fig. 3, where a good agreement can be observed, but we want remark that the proposed model has a lower computational burden, because only one transcendental equation for the vertical electrostatics must be solved, as opposed to the model in [4], where two equations are needed for the vertical electrostatics. In addition, the model [4] suffers of the problems characteristics of intrinsic asymmetry between the drain and source, as we can see in Figure 4, where the behaviors of the proposed model and the model in [4] are compared through the Gummel symmetry test [5], that consists in biasing the FET with $-V_s = V_d = V_x$, and then varying V_x and V_g. If the model is fully symmetrical, as it must be from a physical point of view, the current must satisfy: $I_{ds}(-V_x) = -I_{ds}(V_x)$ and $\left.\frac{d^2 I_{ds}(V_x)}{dV_x^2}\right|_{V_x=0} = 0$.

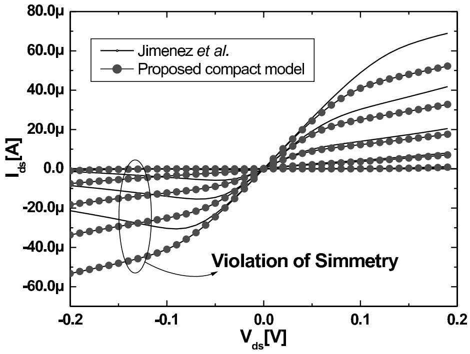

Figure 4: Ballistic nanowire transistor. Gummel test for the proposed model and the model [4]. $t_{ox} = 1.5$nm, $t_{si} = 3$nm.

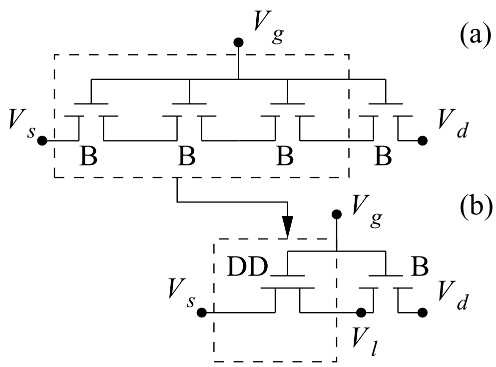

Figure 5: (a)Chain of ballistic MOSFETs. Contacts act as virtual reservoir. (b)Approximate aggregation of first $N-1$ ballistic transistors in an equivalent Drift-Diffusion transistor. The global circuit can be seen as a macromodel for a device in intermediate transport.

2.2 Drift-diffusion transport; case $L >> \lambda$

We recall that within the Büttiker probes approach, inelastic scattering is localized in special points (the "virtual" contacts) that are spaced by a "mean-free path" λ. When carriers enter in virtual contacts, they are re-emitted with thermal equilibrium distribution, so that current continuity is preserved. A generic transistor can be seen as a chain of $N = L/\lambda$ ballistic transistors as shown in Fig.5(a). At the internal contact (placed at $x_k = k\lambda$, we can define the Fermi potential V_k. Since the current in any MOSFET is I_{ds}, we have $N+1$ equations determining the local Fermi potentials:

$$I_{ds} = q \sum_{v,n} g_v \frac{kT}{\pi\hbar} \left[\Im_0 \left(\frac{\phi_{c,k+\frac{1}{2}} - V_k - \varepsilon_n^v}{\phi_t} \right) - -\Im_0 \left(\frac{\phi_{c,k+\frac{1}{2}} - V_{k+1} - \varepsilon_n^v}{\phi_t} \right) \right] \quad (3)$$

where $k = 0, \ldots, N$, and we have placed for the k-th transistor: $\phi_{c,k+\frac{1}{2}}$ is the electrostatics potential in the peak of the barrier, V_k and V_{k+1} are the source and drain Fermi levels respectively, therefore $V_k = V_s$ and $V_k + 1 = V_d$ for $k = 0$ and $k = N$, respectively. We can show that for $N >> 1$, we recover a drift-diffusion equation for the nanowire transistor. We suppose that every ballistic

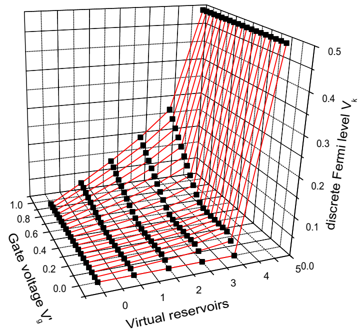

Figure 6: Discrete quasi-Fermi potential with $N = 5$ at fixed $V_{ds} = 0.5$V Fermi-Levels are defined only at points $x = k \times \lambda$ with k integer.$t_{ox} = 2.5$ nm.

transistor works in the linear region i.e. that:

$$V_{k+1} - V_k << 2\phi_t \quad (4)$$

We can define a continuous quasi-Fermi level V_{Fn} subject to these conditions:

$$V_{Fn}\left(x_{k+1/2}\right) \equiv \frac{V_k + V_{k+1}}{2} \quad (5)$$

$$\frac{dV_{Fn}}{dx}\left(x_{k+1/2}\right) \equiv \frac{V_{k+1} - V_k}{\lambda} \quad (6)$$

Then, substituting (5,6) in (3), expanding in Taylor series, truncating to the first order in λ, we have for the drift-diffusion current:

$$I_{ds} = \frac{q^2}{\pi\hbar}\sum_{v,n} g_v \Im_{-1}\left(\frac{\phi_c - V_{Fn} - \varepsilon_n^v}{\phi_t}\right)\lambda\frac{dV_{Fn}}{dx} \quad (7)$$

where we have used the property of Fermi-Dirac integrals:$\frac{d\Im_0(x)}{dx} = \Im_{-1}(x)$and, consistently the vertical electrostatics (1) becomes:

$$C_g\left(V_g' - \phi_c\right) = q\sum_{v,n} g_v \frac{\sqrt{2kTm_d^v}}{\pi\hbar}\Im_{-\frac{1}{2}}\left(\frac{\phi_c - V_{Fn} - \varepsilon_n^v}{\phi_t}\right) \quad (8)$$

If we integrate along the channel, we obtain:

$$I_{ds} = \int_0^L q\sum_{v,n} g_v \frac{kT}{\pi\hbar}\Im_{-1}\left(\frac{\phi_c - V_{Fn} - \varepsilon_n^v}{\phi_t}\right)\frac{dV_{Fn}}{dx}\frac{\lambda}{L}dx \quad (9)$$

The integral in (9) can not be placed in a simple analytical closed-form, because of the dependence of $\phi_c(V_{fn})$ by V_{Fn} given by (8), but can be approximated with a simple expression adopting the symmetrical linearization technique [5]. Indeed if we define: $\phi_{cm} = \frac{\phi_{cs}+\phi_{cd}}{2}$ where $\phi_{cd,s}$ are the electrostatic potential at source and drain, and then substitute the integration variable $V_{Fn} \longrightarrow \phi_c$, we obtain:

$$I \simeq q\frac{kT}{\pi\hbar}n_q\frac{\lambda}{L}\sum_{v,n} g_v \Im_{-1}\left(\frac{\phi_{c,m} - V_{Fn} - \varepsilon_n^v}{\phi_t}\right)(\phi_{cd} - \phi_{cs}) \quad (10)$$

where we have defined the "quantum factor"n_q:

$$n_q \equiv 1 + \frac{Q_n}{q\frac{\sqrt{2kT}}{2\pi\hbar}\sum_{v,n} g_v\sqrt{m_d^v}\Im_{-\frac{3}{2}}\left(\frac{\phi_{c,m} - V_{Fn,m} - \varepsilon_n^v}{\phi_t}\right)} \quad (11)$$

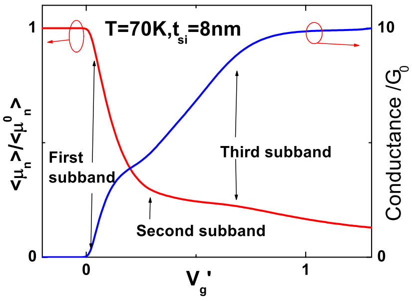

Figure 7: Influence of the Fermi-Dirac statistics on the low-field mobility.

An important aspect of the expressions (7) and (8) is that the current I_n^v in the generic subband can be written in terms of the mobile charge density qN_n and of a mobility $\mu_{deg,n}$ as:

$$I_n^v = \mu_{deg,n} q N_n^v \frac{dV_{Fn}}{dx} \quad (12)$$

and then we have that the generic subband contributes to the conduction with the mobility $\mu_{deg,n}$ that is given by:

$$\mu_{deg,n}^v = \frac{v_{th}\lambda}{2\phi_t}\frac{\Im_{-1}\left(\frac{\phi_c - V_{Fn} - \varepsilon_n^v}{\phi_t}\right)}{\Im_{-\frac{1}{2}}\left(\frac{\phi_c - V_{Fn} - \varepsilon_n^v}{\phi_t}\right)} \quad (13)$$

where $\frac{v_{th}\lambda}{2\phi_t}$ is the non-degenerate low-field mobility of the generic subband and $v_{th} = \sqrt{\frac{kT}{2m_d^v}}$.

We highlight that since a constant mean free path λ is considered, (13) determines a degradation on the mobility for high vertical biases, caused by Fermi-Dirac statistics, as we can see in Fig.7. Indeed an analogous degradation of the mobility caused by degeneracy has been recently observed in a Monte-Carlo study [6].

2.3 Compact model for $L \gtrsim \lambda$

Now we are interested in the development of a compact model that will be valid in the case of intermediate transport. It is evident that in the general case of intermediate transport regime, the simplifying hypothesis (4), that enforces each transistor of the ballistic chain to operate in linear region, does not hold, and then we can expect that some elementary transistor can work near or in the saturation region. The behavior of a transistor operating in such intermediate transport regime, can be obtained solving the complete ballistic chain (3). In order to build a model that can be handled more easily, we can observe in the example in Fig. 6 that when the saturating behavior of the elementary ballistic transistor emerges, it manifests its effects approximately only on the last ballistic transistor of the chain. This fact suggests that we can aggregate the first $N-1$ ballistic transistors in an approximate equivalent drift-diffusion transistor with ratio $L/\lambda = N-1$, as it is represented in Fig.5(b), similarly to what we have seen in [2]. Therefore we can state that a transistor in intermediate transport regime, that can be described by a suitable ballistic chain, can be approximated by the DD+B series, because it is verified the first $N-1$ transistors work near

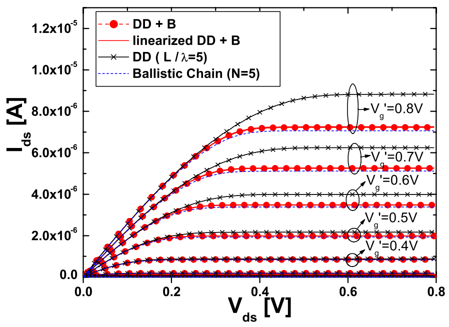

Figure 8: Comparison of the output characteristics of the compact model, the ballistic chain for $L/\lambda = 5$.

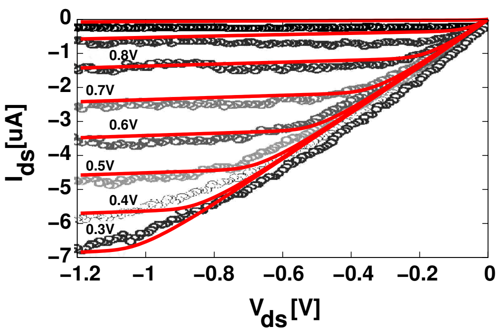

Figure 9: Comparison between the experimental output characteristics of a carbon nanotube transistor [7] (symbols) and the compact model (solid line). $T = 300$K, $C_g = 500$pF/m, $R_s = R_d = 65k\Omega$, $L/\lambda = 2$..

their linear region and then they can be substituted with an equivalent Drift-Diffusion transistor, described by (10).
A comparison between the output current characteristics when $N = 5$ is provided in Fig.8, where we have also reported the curves obtained with a DD+B model with simplified drift-diffusion current (10), and we can see that such model is in a good agreement with the DD+B model with drift-diffusion current obtained by (9). Moreover, we can verify that the series of a simple DD and a ballistic transistor has a small error with respect the complete ballistic chain, given by the linearization of transport in first $N - 1$ mean free paths. A corrected model is currently under development for the degenerate case and it was obtained in the non-degenerate limit [2].

2.4 Carbon nanotubes

The aboveseen compact model can be adapted to a Carbon Nanotube Transistors (CNTFET) with doped source and drain, that is a promising device for the future development of nanoelectronics.
An important issue is that the effective mass approximation is rigorously good only at low bias. Concerning quantum confinement, we can adopt the approximate expression [8]:$\epsilon_n = \epsilon_1 \frac{6n-3-1(-1)^n}{4}$ where $\epsilon_1 = .45/t_{cnt}$ is the bandgap and t_{cnt} is the diameter of the nanotube. Here we want to compare the model with the experimental characteristics of a CNTFET [7], with $t_{cnt} = 2$nm, from which we obtain an effective mass $0.06m_0$. The comparison is shown in Fig.9, where we have used to obtain a good fitting two series resistances $R_s = R_d = 65k\Omega$, and $L/\lambda = 2$, meaning that transport is strongly quasi-ballistic. The effective gate capacitance $C_g = 500$pF/m, provided in [7], has been used. Such effective capacitance includes the effects of the high-κ insulator and the carbon nanowire geometry.

3. Conclusions

We have presented a physics-based macromodel that can describe nanowire field effect transistor subject to far-from equilibrium transport, that extends the results obtained for planar transistors [2]. Starting from a model for ballistic one-dimensional FET model, and adopting the Büttiker probes interpretation of inelastic scattering, we have shown that the case of intermediate transport between fully ballistic transport and drift-diffusion transport can be described by the series of an equivalent drift-diffusion transistor with a ballistic transistor, consistently with the results in [2]. Therefore this compact macromodel can be considered an adequate description of transport in ultrascaled nanowire FETs.

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