Effective Bohm Quantum Potential for device simulators based on drift-diffusion and energy transport

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Abstract

In this paper we present a derivation of a very convenient approach to include quantum confinement effects in drift-diffusion or hydrodynamic device simulators, without explicitly solving the Schrödinger equation. With respect to similar methods recently proposed in the literature, the presented approach has a few advantages: it does not depend on the transport model (drift-diffusion or hydrodynamic); it can straightforwardly include Fermi-Dirac statistics; it provides an additional degree of freedom for calibration, which is particularly useful for considering non planar device structures; finally, it can be discretized in such a way to exhibit very stable convergence properties.

1 Introduction

The theoretical basis for the definition of an effective quantum potential is Bohm's interpretation of quantum mechanics, which dates back to 1952 [1], and is at the origin of other more recent derivations based on a first order expansion of the Wigner equation [2], or on the so-called density gradient approach [3].

The great advantage of such a method consists in the possibility to correctly model quantum effects without the explicit solution of the Schrödinger equation and, more importantly, to be easy integrable in widespread simulation approaches based on drift-diffusion or hydrodynamic equations. Therefore, the capability of commercial device simulators, generally based on the approximate solution of the semiclassical Boltzmann equation, can be conveniently extended also to the quantum regime which is relevant in recent nanoscale semiconductor technology.

2 Model

According to Bohm's interpretation of quantum mechanics, if we write the wave function in a polar representation, i.e., $\Psi = R \exp\left(i\frac{S}{\hbar}\right)$ where R, a probability density per unit volume, is the modulus of Ψ and S has the dimension of an "action" (energy $\times$ time) and represents the phase of Ψ multiplied by $\hbar$, the Schrödinger equation can be written as:

$$-\frac{\hbar^2}{2}\nabla\left\{M^{-1}\nabla\left[R\exp\left(i\frac{S}{\hbar}\right)\right]\right\} + VR\exp\left(i\frac{S}{\hbar}\right) = ER\exp\left(i\frac{S}{\hbar}\right). \qquad (1)$$

Since $M^{-1}\nabla S$ is the local velocity of the probability density flux i.e. the local velocity of the particle associated to the wave function, the real part of (1) may be interpreted

as a continuity equation of the probability density while the imaginary part states that the total energy E is conserved and equal to the sum of the potential energy V, of the kinetic energy $\frac{1}{2}\nabla S \cdot M^{-1} \cdot \nabla S$, and of the term $Q = -\frac{\hbar^2}{2}\frac{\nabla(M^{-1}\nabla R)}{R}$ which is interpreted as the "quantum potential".

According to the previous derivation, the Schrödinger equation has been transformed into two coupled continuity and energy conservation equations, in which quantum mechanics manifests itself only in the quantum potential term. It is worth noticing that if the term Q is forced to zero, a complete classical system is recovered. Since the quantum term Q is obtained by the single particle Schrödinger equation, in our model we use a sort of "mean field approximation" and consider an "effective quantum Bohm potential", defined as the weighted average potential for all the carriers constrained in the confining potential. The weights are represented by the probability density of all states in the considered position. In particular, after weighting, for a quantum system of electrons (the electron density can be written as $n = \sum_i f_i R_i^2$), we obtain for the effective potential the following expression:

$$Q_{\text{eff}} = -\frac{\hbar^2}{2}\gamma \left[\frac{\nabla(M^{-1}\nabla n)}{2n} - \frac{\eta}{4}\frac{\nabla n \cdot M^{-1} \cdot \nabla n}{n^2} \right] = -\frac{\hbar^2}{2}\gamma \frac{\nabla[M^{-1}\nabla(n^\alpha)]}{n^\alpha}. \quad (2)$$

where we have defined the two parameters

$$\gamma \equiv = \frac{\sum_i \nabla[M^{-1}\nabla(f_i R_i^2)]}{\nabla[M^{-1}\nabla(\sum_i f_i R_i^2)]}, \text{ and} \quad (3)$$

$$\alpha \equiv 1 - \frac{1}{2}\frac{\sum_i f_i R_i^2}{\sum_i f_i \nabla R_i^2 \cdot \sum_i f_i \nabla[M^{-1}(R_i^2)]} \sum_i \frac{f_i \nabla(R_i^2) M^{-1}\nabla(R_i^2)}{R_i^2}. \quad (4)$$

Parameters γ and α depend on the device structure and on the applied bias. In our approximation, we consider them as constant parameters obtained from a fitting procedure, greatly simplifying the computation of the quantum potential and eliminating the need for a direct solution of the Schrödinger equation.

Moreover, it must be mentioned that two different parameters, instead of one [4], provide an additional degree of freedom during the calibration procedure since they can be used differently to tune the model in regions where confining potential is strong and in regions where carriers are only weakly confined.

Out of equilibrium, the occupation factor f_i of state i may depend on position, and the above equations are not directly applicable. Therefore, we cannot assume, as we do in equilibrium, that $\nabla n = \sum_i f_i \nabla(R_i^2)$. In that case we have to simply define a special partial differentiation operator $\tilde{\nabla}$ as $\tilde{\nabla} n \equiv \sum_i f_i \nabla(R_i^2)$. If, for example, a transport model such as the hydrodynamic model is used, the occupation factor of an electron state depends on the quasi-Fermi level E_{fn} and the carrier temperature T_e, which are both a function of position, i.e., $f_i = f_i[E_{fn}(\mathbf{r}), T_e(\mathbf{r})]$, then the relationship between $\tilde{\nabla}$ and ∇ is simply

$$\nabla n = \tilde{\nabla} n + \left(\frac{\partial n}{\partial E_{fn}}\nabla E_{fn} + \frac{\partial n}{\partial T_e}\nabla T_e \right). \quad (5)$$

In plain language, $\tilde{\nabla}n$ is a partial gradient of n, that does not take into account temperature and quasi-fermi level gradients. Out of equilibrium, *independently of* the transport model used, equation (2) becomes:

$$Q_{\text{eff}} = -\frac{\hbar^2}{2}\gamma\frac{\tilde{\nabla}\left[M^{-1}\tilde{\nabla}\left(n^\alpha\right)\right]}{n^\alpha}. \tag{6}$$

3 Results

In the following we will focus on structures where quantum confinement is strong in one and two directions and the results obtained with the quantum potential approach are compared with those obtained from a fully quantum calculation. In particular, the first considered structure is a MOS capacitor with oxide thickness of 2 nm and acceptor concentration in the bulk $N_A = 1 \times 10^{18}$ cm^{-3}. In our simulations we have included a metal gate, in order to study only the confinement of electrons in the channel, and have neglected quantization and depletion of the polysilicon. In Figure 1 (top) we show a comparison between the electron density profiles computed by coupling the Poisson equation both with the one-dimensional Schrödinger equation and those obtained with the effective Bohm quantum potential equation. Also shown on the left are the C-V curves obtained with the two different methods. The fitting parameters using for such device are $\gamma = 1.089, \alpha = 0.5$ (Fig 2(c)). The second device considered has the structure depicted in Figure 2(a). The oxide thickness is 2 nm and the acceptor concentration is $N_A = 10^{18}$ cm^{-3}. Quantum confinement is strong in both the x and y directions, so a complete solution of the Schrödinger equation in two dimensions is required. As can be observed in Figure 2(b), the effective quantum potential method is capable to get both the height and the shape of the carrier density profile as the applied voltage is varied. The method is also capable to well reproduce the carrier density per unit area obtained with the direct solution of the Schrödinger equation.

4 Conclusion

In summary, we have proposed an expression for an effective quantum potential, an appropriate algorithm and a discretization scheme. The model has been implemented into the ATLAS device simulator by SILVACO, both for drift-diffusion and energy transport models. With respect to previously published density gradient methods the main advantages of our proposal are represented by the possibility of including both Maxwell-Boltzmann and Fermi-Dirac statistics, by its independence of the transport model adopted, and by the presence of an additional degree of freedom, which may provide better fit and improved calibration. The authors gratefully acknowledge support from SILVACO GRECE (Grenoble REsearch CEnter).

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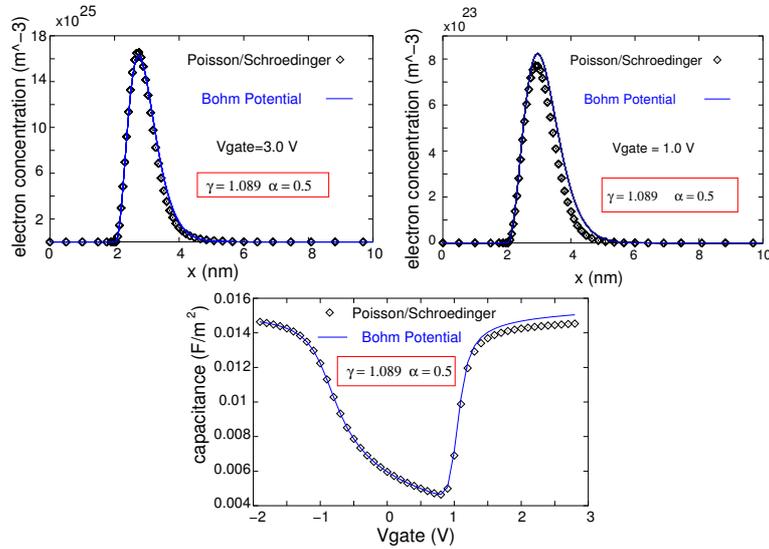
Figure 1: Top: electron density along the growth direction for a voltage applied to the gate of V_G=3 V and $V_G = 1$ V obtained with the EBQP (Effective Bohm Quantum Potential) approach and with the PS approach. Bottom: C-V characteristics obtained with the EBQP approach and with a fully quantum approach.
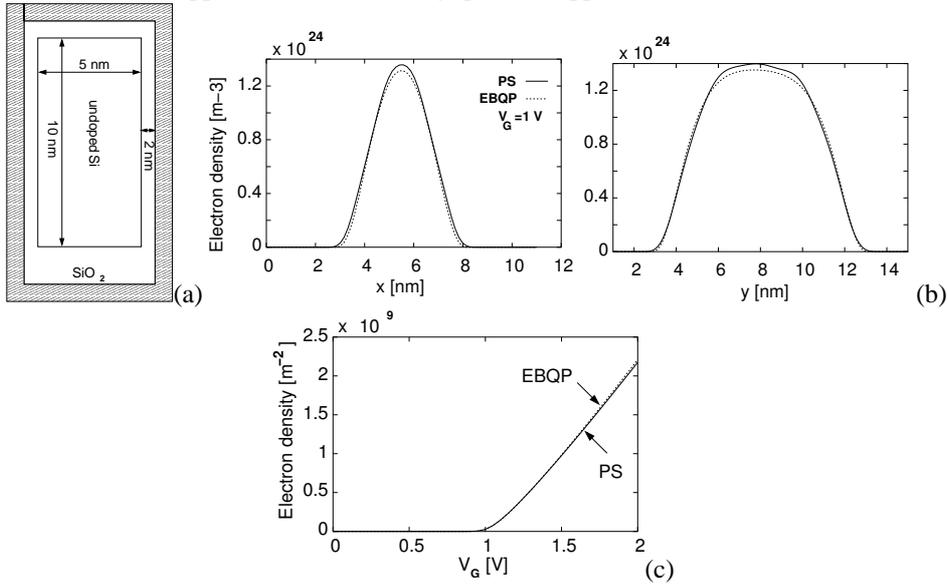

Figure 2: (a)Schematic representation of the wire composed by a silicon layer embedded in a SiO$_2$ layer. (b) Electron density along the growth direction (left) and along the longitudinal direction (right) for a voltage applied to the gate of V$_G$=1 V obtained with the EBQP approach and with the PS approach. (c) Electron density per unit area obtained with the EBQP approach and with a fully quantum approach.