

¹ Department of Electrical Engineering, ² Department of Mathematics , Arizona State University, Tempe, AZ 85287, E-Mail:sahmed@asu.edu,ringhofer@ asu.edu,vasileska@asu.edu

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Abstract

We present a thermodynamic approach to introducing quantum corrections to the classical transport picture in semiconductor device simulation. This approach leads to a modified Boltzmann equation with an effective quantum potential. We study the quantum interaction of electrons with a gate oxide barrier potential in a 25 nm MOSFET.

KEYWORDS: Quantum thermodynamics, effective potentials.

Introduction.

For quite some time, the dimensions of semiconductor devices have been scaled aggressively in order to meet the demands of reduced cost per function on a chip used in modern integrated circuits. There are some problems associated with device scaling, however. Critical dimensions, such as transistor gate length and oxide thickness, are reaching physical limitations. In addition to the processing issues, there are also some fundamental device issues. As the oxide thickness becomes very thin, the gate leakage current due to tunneling increases drastically. This significantly affects the power requirements of the chip and the oxide reliability. Yet another issue that becomes prominent in nano-scale MOSFET devices is the quantum-mechanical nature of the charge description which, in turn, gives rise to inversion layer capacitance comparable to the oxide capacitance. This, in turn, degrades the total gate capacitance and, therefore, the device transconductance. In this paper we introduce an effective potential formalism, based on thermodynamic considerations, to include space quantization effects into the classical transport picture. This approach has been applied to modelling transport in nano-scale MOSFETs with gate length of 25 nm that are of both industrial and scientific interest. We find that the inclusion of the barrier potential into a classical Monte Carlo particle-based simulation scheme gives rise to on-state current reduction of about 20 % due to the displacement of the charge from the interface and that the introduction of the inversion layer capacitance that degrades the oxide capacitance and, therefore, the MOSFET transconductance. The approach proposed here is compared to a similar approach by Ferry et al. [1], in which the effective potential is calculated as a convolution of a Gaussian function and the Hartree potential obtained from solving the two-dimensional or three-dimensional Poisson equation.

Quantum Transport and Effective Potentials.

The quantum mechanical description of electron transport in a semiconductor, assuming mean field theories and effective mass approximations, is given by the quantum Boltzmann equation

$$\partial_t f + [\mathcal{E}, f]_{\mathcal{W}} = (\partial_t f)_{coll}, \quad \mathcal{E} := \frac{|p|^2}{2m_*} + eV(x, t), \quad (1)$$

for the Wigner function $f(x, p, t)$. We denote the momentum vector by $p = \hbar k$ and assume an effective mass m_* . The potential $V := V_H + V_B$ will in general be given by the superposition of a Hartree potential $V_H(x, t)$ (computed from Poisson's equation) and a barrier potential $V_B(x)$ accounting for $Si - SiO_2$ interfaces. The symbol $[\mathcal{E}, f]_{\mathcal{W}}$ in (1) denotes the quantum mechanical commutator in the Wigner picture, i.e. the Wigner transform of the usual commutator with the Hamiltonian

$$[\mathcal{E}, f]_{\mathcal{W}} = \frac{i}{\hbar} \mathcal{W}[H, \rho], \quad \mathcal{E} = \mathcal{W}H, \quad f = \mathcal{W}\rho$$

holds where symbols and Wigner functions are related to operators and density matrices via the Weyl quantization

$$f(x, p, t) = \mathcal{W}\rho(x, p, t) = \int_{\mathbb{R}^3} \rho(x - \frac{\hbar}{2}\eta, x + \frac{\hbar}{2}\eta, t) e^{i\eta \cdot p} d\eta, \quad (2)$$

which yields for the Wigner commutator $[\mathcal{E}, f]_{\mathcal{W}}$

$$[\mathcal{E}, f]_{\mathcal{W}} = \frac{i}{\hbar} \sum_{\nu=\pm 1} \nu \mathcal{E}(x + \frac{i\nu\hbar}{2}\nabla_p, p - \frac{i\nu\hbar}{2}\nabla_x) f(x, p, t) = \nabla_x \cdot (\frac{p}{m_*} f) + \frac{i}{\hbar} \sum_{\nu=\pm 1} \nu V(x + \frac{i\nu\hbar}{2}\nabla_p) f.$$

A rigorous treatment of the collision operator $(\partial_t f)_{coll}$ on the right hand side of (1) can be done by an actual quantum mechanical description of the creation / destruction processes of phonons, but is too complicated to be used on the time scales necessary for device simulation [2].

In an effective potential approach, one replaces the quantum Boltzmann equation (1) by a corresponding semiclassical equation with a modified potential. So, the Wigner commutator $[\mathcal{E}, f]_{\mathcal{W}}$ is replaced by the classical commutator $[\mathcal{E}^{eff}, f]_{\mathcal{C}} = \nabla_p \mathcal{E}^{eff} \cdot \nabla_x f - \nabla_x \mathcal{E}^{eff} \cdot \nabla_p f$, $\mathcal{E}^{eff} = \frac{|p|^2}{2m_*} + eV^{eff}$, and the collision operator $(\partial_t f)_{coll}$ is taken to be the usual semiclassical operator using Fermi's Golden Rule [6]. Thus all the quantum effects in the system are modelled solely through the forces acting on the electron. For this reason the same form of numerical simulations tools can be used as for the Boltzmann transport equation, i.e. only the acceleration terms in the free flight phase of a Monte Carlo method have to be modified. An effective potential approach, using Gaussian smoothing based on the original work in [3], has been used to model quantization effects in 50nm MOSFETS in [1] and [8]. In this approach electrons are represented by Gaussian wave packets with a certain coherence length, which results in the effective potential V^{eff} being obtained from the Hartree potential V_H through a spatial convolution with this Gaussian.

Approximations to the Thermodynamic Equilibrium State.

The approach presented in this paper consists essentially of a perturbation theory around thermal equilibrium. The basic problem in using a particle model is that particles, i.e. simultaneous δ - functions in space and momentum, cannot be a solution of the quantum Boltzmann equation (1), since they contradict the Heisenberg principle. We therefore seek an effective potential V^{eff} which, when applied to the effective particle system, produces the same observables as the actual potential when applied to the quantum system. This should be true at least close to the thermal equilibrium state. In particular, the classical commutator with the effective potential $[\mathcal{E}^{eff}, f]_{\mathcal{C}}$ should produce the same equilibrium as the Wigner commutator $[\mathcal{E}, f]_{\mathcal{W}}$, using the actual potential. In the quantum mechanical setting the thermal equilibrium state is given, as a density matrix, by $\rho^{eq} = e^{-\beta H}$ [9], where H is the Hamiltonian for a given potential and β denotes the inverse thermal energy. The classical commutator with the effective potential will have thermal equilibria of the form $f^{eq} = \hbar^{-3} \exp(-\beta \mathcal{E}^{eff})$. Thus the effective potential can be derived by approximately expressing the Weyl quantization of $e^{-\beta H}$ as $\exp(-\beta \mathcal{E}^{eff})$. Note, that, in one case we are dealing with the exponential of a matrix and in the other case with the usual exponential function. The matrix exponential $\rho^{eq} = e^{-\beta H}$ is defined by

$$\rho^{eq}(r, s) = \sum_{\lambda} \psi_{\lambda}(r) e^{-\beta \lambda} \psi_{\lambda}(s)^*, \quad H\psi_{\lambda} = \lambda\psi_{\lambda} \quad (3)$$

and the ψ_{λ} denote the complete orthonormal eigensystem of the self adjoint operator H . The solution of the eigenvalue problem in (3) is not very amenable to asymptotic approximations, and it is preferable to express the equilibrium state via the semigroup generated by the Hamiltonian. Introducing an artificial non-dimensional parameter γ , we define $\rho(\gamma, r, s) = \sum_{\lambda} \psi_{\lambda}(r) e^{-\gamma \beta \lambda} \psi_{\lambda}(s)^*$. Differentiating ρ w.r.t. γ and using the eigenfunction property of the ψ_{λ} gives

$$\partial_{\gamma} \rho = -\frac{\beta}{2} (H \cdot \rho + \rho \cdot H), \quad \rho|_{\gamma=0} = \delta(r - s), \quad \rho^{eq} = \rho|_{\gamma=1}. \quad (4)$$

(4) is usually referred to as the Bloch equation and has been used in a similar context to derive quantum fluid models for semiconductor transport [4],[5]. In the Wigner picture the Bloch equation (4) reads, using

the Weyl quantization formula (2)

$$\partial_\gamma f = \frac{\beta\hbar^2}{8m} \Delta_x f - \frac{\beta|p|^2}{2m_*} f - \frac{\beta}{2} \sum_{\nu=\pm 1} V(x + \frac{i\nu\hbar}{2} \nabla_p) f, \quad f|_{\gamma=0} = \hbar^{-3}, \quad f^{eq} = f|_{\gamma=1}. \quad (5)$$

To obtain the effective Hamiltonian \mathcal{E}^{eff} , one takes the logarithm of the Wigner - Bloch equation (5), i.e. sets $f = \hbar^{-3} e^{-\beta u}$ and obtains

$$\partial_\gamma u = \frac{\hbar^2}{8m_*} (\beta \Delta_x u - \beta^2 |\nabla_x u|^2) + \frac{|p|^2}{2m_*} + \frac{1}{2} e^{\beta u} \sum_{\nu=\pm 1} V(x + \frac{i\nu\hbar}{2} \nabla_p) e^{-\beta u}, \quad u|_{\gamma=0} = 0, \quad \mathcal{E}^{eff} = u|_{\gamma=1}. \quad (6)$$

The approximate effective Hamiltonian (or effective potential) is now obtained by solving the logarithmic Bloch equation (6) asymptotically. Clearly, setting $\hbar = 0$ in (6) yields $\mathcal{E}^{eff} = \mathcal{E}$. However, computing first order corrections in \hbar would involve differentiating the potential V . In the presence of barriers, $V = V_H + V_B$ is discontinuous and this is not possible. In this case we refer to the resulting model as the QBF (Quantum Barrier Field) model. Instead, we use the Born approximation, i.e. we solve (6) iteratively taking the highest order differential operator (the Laplacian) implicitly. This gives in first order (see [7] for details)

$$u(\gamma) = \frac{\gamma|p|^2}{2m_*} + \frac{2m_*}{i\beta\hbar p \cdot \nabla_x} \sinh\left(\frac{i\beta\gamma\hbar p \cdot \nabla_x}{2m_*}\right) \exp\left(\frac{\gamma\beta\hbar^2 \Delta_x}{8m_*}\right) V, \quad \mathcal{E}^{eff} = \frac{|p|^2}{2m_*} + V^{eff},$$

with the effective potential $V^{eff}(x, p)$ given by

$$(a) \quad V^{eff}(x, p) = \frac{2m_*}{i\beta\hbar p \cdot \nabla_x} \sinh\left(\frac{i\beta\hbar p \cdot \nabla_x}{2m_*}\right) \exp\left(\frac{\beta\hbar^2 \Delta_x}{8m_*}\right) V(x) = \int_{\mathbb{R}^3} \Gamma(x - y, p) V(y) dy \quad (7)$$

$$(b) \quad \Gamma(z, p) = (2\pi)^{-3} \int_{\mathbb{R}^3} \frac{2m_*}{\beta\hbar p \cdot \xi} \sinh\left(\frac{\beta\hbar p \cdot \xi}{2m_*}\right) \exp\left(-\frac{\beta\hbar^2 |\xi|^2}{8m_*} + i\xi \cdot z\right) d\xi.$$

Note, that without the presence of the hyperbolic sine term, the smoother Γ in (7)(b) reduces to the Gaussian smoothing in [1], and the effective potential becomes independent of the momentum vector p . Thus the thermal equilibrium approximation has the effect of making the 'size' of the electron dependent on its kinetic energy. Moreover, in the classical limit (for $\hbar \rightarrow 0$ formally) the effective potential reduces to the classical potential term.

Simulation Results.

To capture the role of the quantum-mechanical size-quantization effects, we have applied the effective potential approach in conjunction with a Monte Carlo particle-based simulation scheme. Although a simple effective mass approximation has been used for the derivation of the QBF model, the Monte Carlo model, used in the transport portion of the simulator, is based on the usual Si band-structure for three-dimensional electrons in a set of non-parabolic D-valleys with energy-dependent effective masses. We simulate a 25 nm MOSFET device with an oxide thickness of 1.2 nm. The substrate doping is $N_A = 10^{19} \text{ cm}^{-3}$ and the doping of the source and drain regions equals $N_D = 10^{19} \text{ cm}^{-3}$. The junction depth is 30 nm and the source/drain extensions are 50 nm. Figure 1 shows the electron distribution in the triangular potential well. The top panel corresponds to the case when there is no quantization, the middle panel corresponds to the case when quantization is included in the model via the QBF (quantum barrier field) presented in this paper approach and the bottom panel corresponds to the case with quantization included in the model using approach by Ferry et al [1]. We use $V_g = 1.2 \text{ V}$ and $V_d = 1 \text{ V}$ in these simulations. The results are consistent with the results that show the position of the electrons in the triangular potential well due to the finite band-bending. Both the QBF and the Ferry approach lead to larger average displacement of the low-energy electrons for which the quantum-mechanical effects are most pronounced. From the results shown, we see that there is no carrier heating as the maximum electron energy is below 0.8 eV. Figure 2 shows the output characteristics. We observe that the slope of Id-Vd curve is lowered down in the linear region, when including the quantization, and infer that the threshold voltage increases with quantization. We also observe some transconductance degradation when we include quantization.

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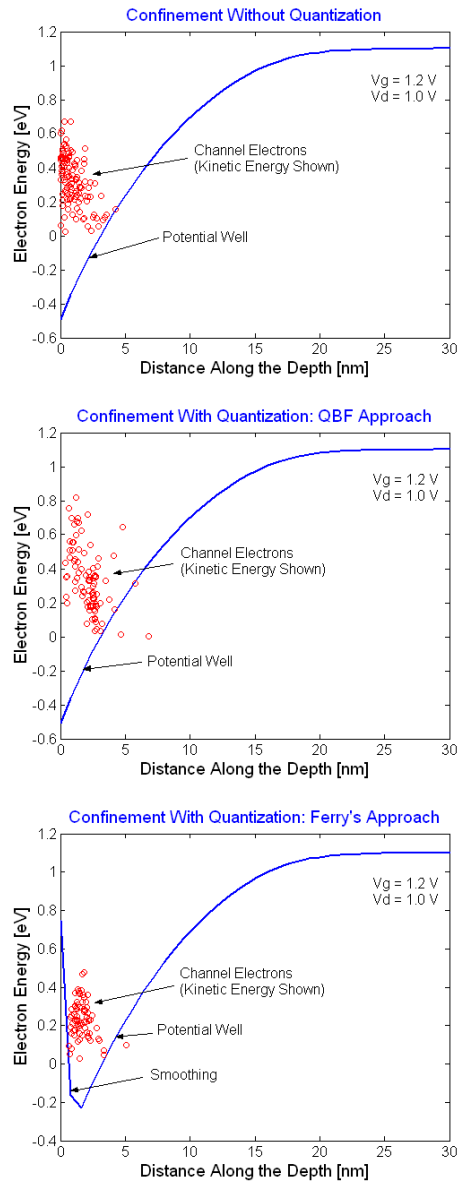


Figure 1: Electron distribution in the potential well.

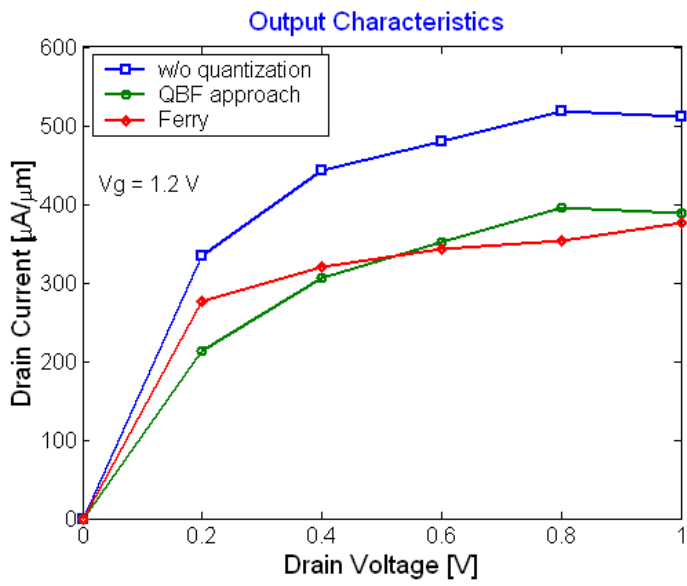


Figure 2: Output characteristics.