# An Approach to Quantum Correction in Monte Carlo Device Simulation

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## ABSTRACT

A particle-based approach coupled with quantum potential corrections is very attractive for practical simulation of nanoscale semiconductor devices. We present here a quantum correction approach derived from a simplification of the Wigner function transport equation, which is applied to Monte Carlo particle simulation of semiconductor devices. The quantum potential is obtained from a first order truncation of the expansion form of the Wigner equation, resembling the semi-classical Boltzmann transport equation with additional terms for the driving forces, appearing as differentials of the quantum potential correction. We present here several recent applications, that illustrate the capabilities and the limitations of quantum corrected Monte Carlo simulation. The method is applied to 1-D MOS capacitor structures and results are compared with the solution of a coupled Schrödinger/Poisson solver. Tunneling through single barriers in III-V compound structures is also analyzed.

***Keywords***: Monte Carlo device simulation, quantum correction, Wigner function, tunneling.

## 1 INTRODUCTION

In usual quantum approaches, the physical state of an individual system is specified by a wave function obtained from the solution of Schrödinger equation. For simulation of practical devices at normal temperatures, the use of a full quantum method is still problematic because of the difficulty of including realistic scattering models. In alternative, a particle description of quantum theory is possible, in terms of a quantum potential correction. In this case, the notion of a well-defined particle trajectory is retained, while the quantum potential correction modifies the potential energy profile to account for quantum effects, like size quantization and tunneling.

A particle-based approach coupled with quantum potential corrections is very attractive for practical simulation of nanoscale semiconductor devices. We apply to Monte Carlo particle simulation a quantum correction approach derived from a simplification of the Wigner function transport equation. The form of the quantum potential is obtained by considering a truncation to first order of the expansion form of the Wigner function equation, which resembles the semi-classical Boltzmann transport equation with additional terms for the driving forces, appearing as differentials of the quantum potential correction. For a practical implementation, it is convenient to transform the correction terms to be a function of local density. Different levels of approximation for the model can be formulated, by making the force correction a function of energy or actual momentum components.

This paper reports on recent applications for MOS devices and III-V compound structures. The results illustrate capabilities and limitations of this approach to quantum correction. One of our main interests is in the simulation of MOSFETs. In order to calibrate the effect of quantum corrections in these systems, the approach is applied to resolve size quantization in a 1-D MOS capacitor structure and results are compared with the solution of a coupled Schrödinger/Poisson solver. Tunneling through single barriers in III-V compound structures is also analyzed, with specific examples that underline the difference between quantum corrections solely based on energy or on the momentum components.

## 2 QUANTUM CORRECTION MODEL

The model starts from a form of the Wigner transport equation [1], given as

$$\frac{\partial f}{\partial t} + \mathrm{v}\cdot\nabla_{\mathrm{r}} f - \frac{1}{\hbar}\nabla_{\mathrm{r}} U\cdot\nabla_{\mathrm{k}} f + \sum_{\alpha=1}^{\infty} \frac{(-1)^{\alpha+1}}{\hbar 4^{\alpha}(2\alpha+1)!}\left(\nabla_{\mathrm{r}} U\cdot\nabla_{\mathrm{k}} f\right)^{2\alpha+1} = \left(\frac{\partial f}{\partial t}\right)_c$$

Here, $U$ is the classical potential distribution and the term on the right-hand side represents the effects of collisions. The third term on the left-hand side contains the non-local effects on the distribution due to quantum effects. In the limit of slow spatial variations, the non-local terms disappear and we recover the standard Boltzmann Transport equation (BTE). The approach taken here is to start by using only the lowest order term with $\alpha = 1$ in the summation. Following this approximation, one obtains an equation that resembles in structure the BTE, with the

addition of a term that contains the quantum correction. The quantum corrected BTE then takes the form

$$\frac{\partial f}{\partial t}+\vec{\mathrm{v}}\cdot\nabla_{\mathrm{r}} f-\frac{1}{\hbar}F^{qc}\cdot\nabla_{k} f=(\frac{\partial f}{\partial t})_{c}$$

where the term $F^{qc}$ contains the quantum correction. This term can be derived analytically if one assumes a distribution function and a dispersion relation for the energy. We have also derived a momentum-dependent quantum corrected force [2]. Assuming a 2-D domain, this is given below for the x-component

$$F_x^{qc}=-\frac{\partial}{\partial x}\left(U-\frac{k_B T}{24}\left\{\left[\gamma_x^2\left(k_x-\bar{k}_x\right)^2-3\gamma_x\right]\frac{\partial^2 \ln n}{\partial x^2}\right.\right.$$

$$\left.\left.+3\left[\gamma_y^2\left(k_y-\bar{k}_y\right)^2-\gamma_y\right]\frac{\partial^2 \ln n)}{\partial y^2}\right\}\right)$$

$$\gamma_x=\frac{\hbar^2}{m_x k_B T};\quad \gamma_y=\frac{\hbar^2}{m_y k_B T}$$

This result has been obtained, in order to have smooth potential variations, using an approximate relation obtained by integrating the displaced Maxwellian distribution with the momentum as

$$\frac{\partial^2 U}{\partial x^2}\simeq -k_B T\,\frac{\partial^2(\ln n)}{\partial x^2}$$

where *n* is the density. The right-hand –side substitutes the second order derivatives of the potential *U* that would appear in the correction, causing problems at potential interface discontinuities, where typically quantum effects are most interesting. A simpler models uses the quantum corrected forces as functions of energy [3], rather than momentum, replacing momentum term with the thermal energy, as

$$\frac{\hbar^2\left(k_i-\bar{k}_i\right)^2}{2m_i}=\frac{k_B T}{2}$$

## 3 RESULTS

The quantum correction illustrated above was applied first to the case of a 1-D MOS capacitor structure. Due to the complexity and cost of the Monte Carlo simulations in this case, we only applied the simple energy-dependent correction model. The MOS capacitor is the basic building block of MOSFET devices, where size quantization takes place in the quantum well created by the gate potential at the silicon dioxide interface. A classical solution of the MOS capacitor in inversion results in a maximum of the charge concentration at the oxide interface.

The quantum correction applied to a semi-classical simulation modifies the potential energy, so that on the average the particles are not as close to the interface. In addition, the bottom of the potential energy is lifted by the correction, to account for quantization sub-bands. This is illustrated by the plot in Fig. 1, which shows a snapshot from a Monte Carlo simulation, for a capacitor with oxide thickness $T_{ox}$ = 3 nm, gate bias $V_g$ = 1.0 V and substrate acceptor doping $N_A = 2 \times 10^{17}$ cm$^{-3}$. The continuous line indicates the potential solved by the classical Poisson equation, and it defines the quasi-triangular well at the oxide interface. The simulated particles are plotted as dots, according to position and energy. One can clearly see that the quantum correction prevents the otherwise classical particles from falling to energy states forbidden by the quantization, thus reshaping the potential energy so that the particle ensemble mimic the overall quantum behavior. The maximum of the charge density is now shifted from the interface.

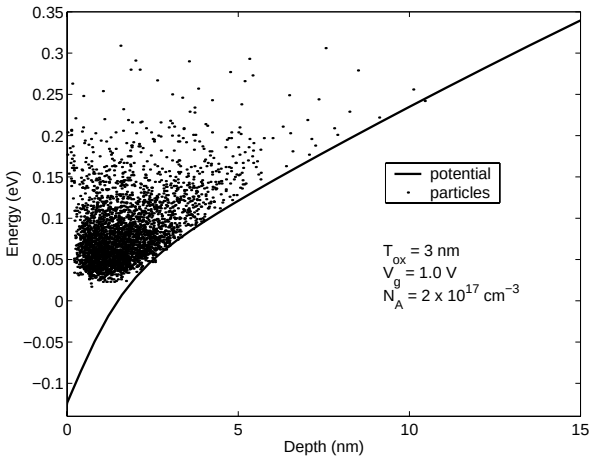


Fig. 1 – Example of quantum-corrected Monte Carlo simulation for MOS capacitor.

A set of simulations was carried on to characterize the capacitor structures under different gate bias conditions. Figure 2 shows the electron concentration in the direction normal to the interface for the same structure in Fig.1, using gate bias from 0.25 V to 3.0 V. The figure shows Monte Carlo results indicated by open circles. These are compared with results from a 1-D self-consistent Schrödinger/Poisson solver. The very good agreement indicates that the quantum correction is able to capture the most important quantum features in this system.

Although we are looking at a 1-D structure, the simulations are carried out with the 2-D simulator MOCA developed at the University of Illinois. In order to resolve completely the dynamics of semi-classical particles under the strong interface fields, we used a very small time-step of $2.0 \times 10^{-18}$ s. Simulation runs were typically over several picoseconds. In order to achieve a good match with the quantum solution, one also needs to ensure that the charge

density at the surface, as used in the Poisson equation coupled to the Monte Carlo simulator, matches as much as possible the quantum density. This is difficult to achieve when solving a particle system, since hardly any particle ends up reaching the oxide interface when the quantum correction is applied. Observing that the quantum solution lets some wave function leak into the oxide, we have solved this problem by assigning a small charge layer inside the oxide region (~$10^{-15}$cm$^{-3}$). This choice seems to allow for a proper adjustment of the interface density condition in the wide range of biases used here. Similar simulations were conducted for a capacitor in accumulation regime, with the same geometry and substrate donor doping $N_D = 2 \times 10^{17}$ cm$^{-3}$. The results are shown in Fig. 3.

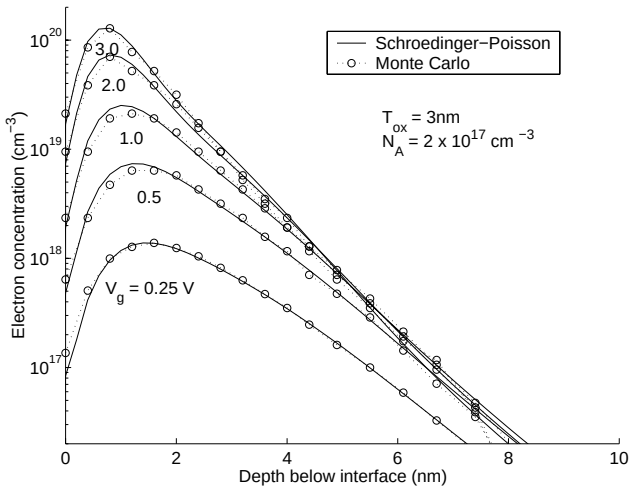


Fig. 2 – Electron concentration in the inversion region of the simulated MOS capacitor.

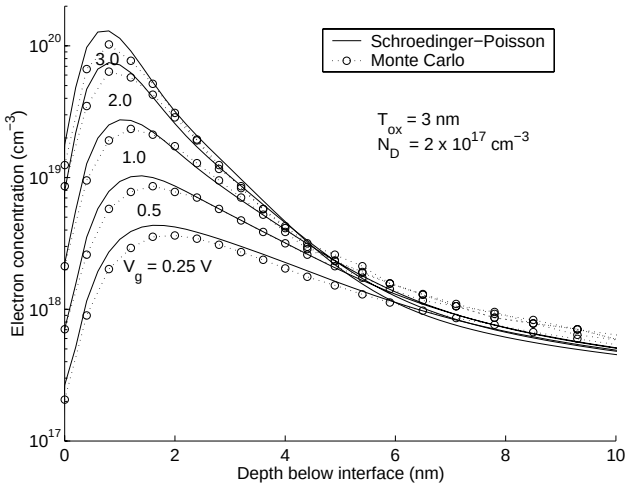


Fig. 3 – Electron concentration in the accumulation region of the simulated MOS capacitor.

The quantum correction scheme has also been applied to the simulation of MOSFETs, implementing very small structures with channel length well below 0.1 μm. We use as prototype the so-called "well-tempered" MOSFET structures, developed as reference test structures by Prof. Antoniadis of MIT. Complete data for these devices are posted at http://www-mtl.mit.edu/Well/. In Fig. 4, we show a simulation example of the electron density in a 25 nm channel MOSFET, obtained by applying the quantum correction scheme. The main feature differentiating this result from standard semi-classical simulation is the displacement of the maximum channel density from the interface, as expected from size quantization effects.

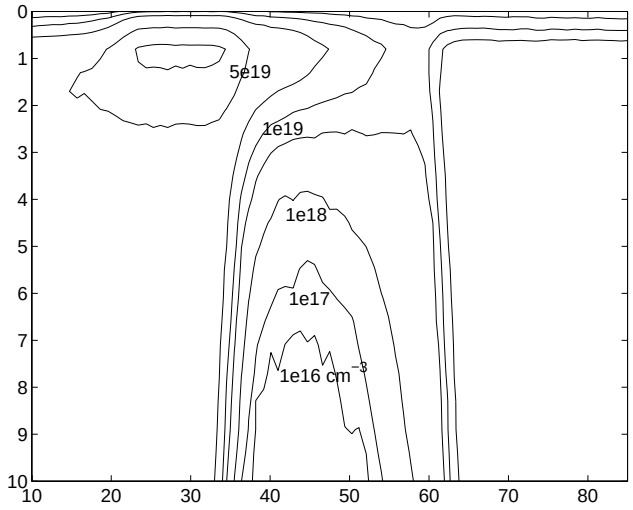


Fig. 4 – Contours of electron density from simulation of a 25 nm channel n-MOSFET,

The quantum corrections can also be applied to tunneling phenomena. These are best explored by simulation in III-V compound heterojunction structures, because one create relatively small and narrow barriers. In these system one can also explore better the effect of the momentum-dependence in the quantum correction, since tunneling is quite sensitive to the actual direction of the momentum vector. To generate suitable reference results, we have examined simple AlGaAs barriers embedded in a GaAs system. Figure 5 shows the result of Monte Carlo simulation for the quantum correction applied to carriers impinging against a 0.22 eV barrier of 2.5 nm thickness, in ideal conditions of flat band equilibrium. The effective barrier is rounded at the top, indicating the effective potential lowering due to the tunneling, while the potential skirts on the side indicate the effect of quantum repulsion. When the correction forces are taken to be function of momentum, rather than energy, the system better represents the quantum repulsion, while the barrier lowering by tunneling is very similar in magnitude.

We show in Fig. 6 snapshots of the Monte Carlo simulation under bias conditions. The result in Fig 6(a) is only for semi-classical simulation, while in Fig. 6(b) the momentum-dependent quantum correction has been included. Tunneling through the barrier can be clearly

seen, along with size quantization effects in the small well formed before the barrier.

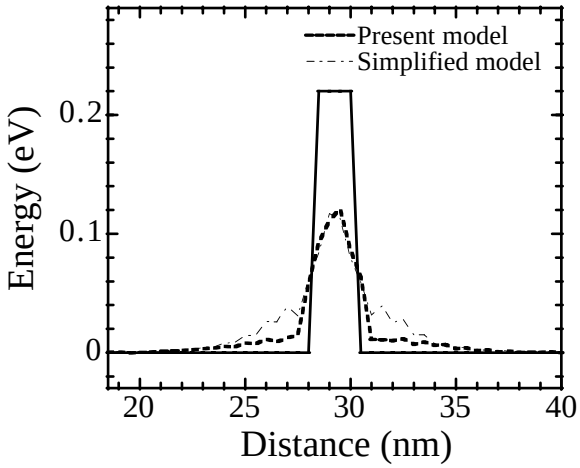


Figure 5 – Quantum potential corrections for a single GaAs/AlGaAs/GaAs barrier.

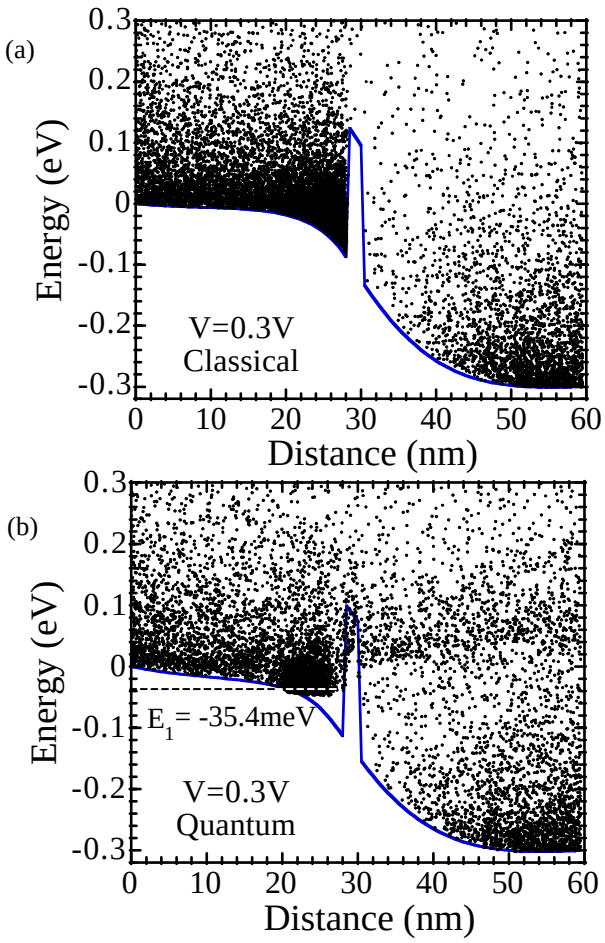


Fig. 6 – Monte Carlo simulation results for a single GaAs/AlGaAs/GaAs barrier under bias conditions for semi-classical (a) and quantum corrected (b) simulation .

## 4 CONCLUSIONS

We have developed quantum corrections based on a truncated expansion of the Wigner transport equation, and we have applied them to Monte Carlo simulation of semiconductor devices. For simulations of MOS structures we used simpler corrections based on energy, while a more complete momentum-dependent correction was used to look at tunneling in GaAs/AlGaAs/GaAs barriers. Our results indicated that it is practical to extend the applicability of semi-classical Monte Carlo simulation to nanoscale by including quantum corrections. The cost of simulation increases considerably when near rapidly varying potentials very small time steps are required to resolve the particle dynamics. This is the case for quantum wells at oxide interfaces in MOS systems. The method as presented here does not have the ability to account for coherent effects, since the quantum corrections are still applied to particles simulated semi-classically. However, we are working on an extension of the approach that could treat resonant tunneling, thus capturing some of the coherent effects at the basis of this phenomenon.

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