Incorporation of Quantum Corrections to Semiclassical 2-Dimensional Device Modeling with the Boltzmann/Wigner Equation

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Abstract: A new method for accounting for quantum effects in semiclassical device simulation is presented. The approach is based on the solution to the Boltzmann/Wigner equation, which is derived from the Schrodinger equation. The Boltzmann/Wigner equation is truncated to order $\bar{h}^2$, and then formulated using spherical harmonics. This facilitates analytical evaluation of the collision integral, and allows for reduction of dimensionality. The Boltzmann/Wigner equation is solved self-consistently with the Poisson and hole-current continuity equations for a BJT and a MOSFET. The results show that the carrier concentrations predicted by the Boltzmann/Wigner equation near the base-emitter junction and the MOSFET channel are less than that predicted by the semiclassical Boltzmann model. Calculations show terminal currents to be 2% and 7% lower for the quantum simulations than the semiclassical results for the BJT and MOSFET, respectively.
1 Introduction

Now that the critical dimensions in many semiconductor devices are on the nanometer scale, quantum effects are becoming increasingly noticeable. Researchers are introducing various methods to include quantum effects in device simulation. These methods range from using 1-dimensional (1-D) quantum corrections in the moment equations used for modeling semiconductor devices, to the solution of the Boltzmann/Wigner equation. These various approaches have their respective strengths as well as their limitations. For example, the moment approaches can give quantum corrections to macroscopic quantities such as carrier concentration. However, they employ many of the same approximations as their classical analogues, and they do not provide a quantum distribution function. On the other hand, methods that employ the Wigner formalism can provide the quantum distribution function, but they usually rely on simplified phenomenological scattering terms to make their equations tractable for numerical solution. In general, the various approaches share a common challenge which is that inclusion of quantum effects in device simulation almost always makes the modeling effort considerably more complicated, especially for 2-dimensional (2-D) applications.

In this paper, we introduce a new method for incorporating quantum effects in device modeling using the Wigner formalism. The method is suitable for both 1-D and 2-D applications, and it accounts in detail for quantum corrections to semiclassical transport in both real and momentum space. We start with the Boltzmann/Wigner transport equation, which is derived directly from the Schrodinger equation. To this equation we add the collision integral, allowing for the incorporation of elastic and inelastic scattering, including optical, acoustic phonon and ionized impurity scattering. These scattering mechanisms are critical to determining electron transport in semiconductors. The direct mathematical formulation of the Boltzmann/Wigner formalism gives rise to a virtually intractable seven-dimensional, high order integral-differential equation. To help solve the equation we express it in spherical coordinates, and employ a spherical harmonic expansion. This reduces the dimensionality of the Boltzmann/Wigner transport equation and allows for analytical evaluation of the collision integrals. As a result, the Boltzmann/Wigner transport equation is reduced to a differential-difference equation that is tractable using numerical methods. We solve the Boltzmann/Wigner equation for electrons, self-consistently with the Poisson equation and the hole-current continuity equation. The results give the quantum corrected distribution
function, as well as the potential and hole concentration throughout a semiconductor device. From the quantum corrected distribution function we can calculate virtually all important device characteristics.

We apply our method to solving the Boltzmann/Wigner transport equation to a BJT and a MOSFET. We find that including quantum corrections has the effects of reducing carrier concentration near potential barriers, including those which exist in PN junctions, and in the MOSFET channel near the oxide interface. Our calculations further predict that quantum corrections also give rise to reduced magnitudes for terminal currents. We also find that including quantum effects predicts reduced high-energy electron density in the quantum corrected distribution function.

## 2 Device Quantum Model

To analyze semiconductor devices on the nanometer scale, while including the detailed effects of electronic interactions, we employ a device model which includes the Poisson equation (1), the Boltzmann/Wigner equation (2), and the hole-current continuity equation (3). The Boltzmann/Wigner equation describes electron transport on the quantum mechanical level. Formally it may be desirable to solve a Boltzmann/Wigner equation for holes as well. However, for devices where carrier transport is dominated by electrons, we solve the hole-current continuity equation to reduce complexity without significant sacrifice in accuracy.

\[
\nabla^2 V(\vec{r}) = \frac{q}{\epsilon_s} \left[ \int w(\vec{k}, \vec{r}, t) d\vec{k} - p(\vec{r}, t) + N_A(\vec{r}) - N_D(\vec{r}) \right]
\]

(1)

\[
\frac{\partial w}{\partial t} + \frac{\nabla \varepsilon}{\hbar} \cdot \nabla w - \frac{q}{\hbar} \sum_{n=0}^{\infty} (-1)^{2n} \frac{4^n (2n + 1) \hbar}{(2n + 1)} \left( \nabla \vec{k} \cdot \nabla \vec{r} \right)^{2n+1} V(\vec{r}) w = 0
\]

(2)

\[
\frac{\partial p(\vec{r}, t)}{\partial t} + \nabla \cdot \left[ \mu_p p(\vec{r}) \nabla V(\vec{r}) + \mu_p V_t \nabla \cdot \nabla p(\vec{r}) \right] = R(V, n, p) - G_{ii}(n, p)
\]

(3)

\(V(\vec{r})\) is the potential; \(p(\vec{r}, t)\) is the hole concentration; \(N_A(\vec{r})\) and \(N_D(\vec{r})\) are the doping concentration for acceptors and donors respectively; \(w(\vec{r}, \vec{k}, t)\) is the electron Wigner or quantum distribution function; \(\varepsilon\) is the energy; \(\vec{k}\) is the electron wave-vector; \(\vec{r}\) is the position vector; \(\hbar\) is Planck’s constant; \(\epsilon_s\) is the silicon dielectric constant; \(\mu_p\) is the hole mobility; \(R(n, p)\) is the recombination rate; \(G_{ii}(n, p)\) is the hole generation rate from impact ionization. For
the band structure we use two spherically symmetrical bands, which represent k-space angular averages of the dispersion relation. This averaged band structure, which was originally developed for Monte Carlo simulations\([?, ?]\), gives rise to accurate values for the density of states and drift velocity.

### 2.1 Formulation of Boltzmann/Wigner Equation

The quantum-corrected model is very difficult to evaluate for numerous reasons. The most obvious is due to the complexity of the Boltzmann/Wigner equation, which is 7-dimensional and contains an infinite expansion of higher order mixed derivatives in both real and momentum space. In addition, care must be taken to solve the hole-current continuity equation to resolve the exponential variation in the hole concentration. Of course, the coupling between equations in the device model gives rise to a nonlinear system. This requires an iterative solution scheme so attention must be paid to convergence. While these are all critical issues, the greatest challenge is to adapt the Boltzmann/Wigner equation to a form which is suitable for device simulation, and then to develop the numerical techniques to solve it.

The Boltzmann/Wigner equation can be considered to be a modified semiclassical Boltzmann equation, which has been extended to contain quantum mechanical corrections. The Boltzmann/Wigner equation is a transport equation whose solution is the Wigner function. The Wigner function can be considered to be a quantum mechanical analogue to the semiclassical distribution function. The Wigner function is defined as the Fourier transformation of the product of wave functions over nonlocal coordinates\([?]\):

\[
w(\vec{r}, \vec{k}, t) = \frac{1}{\pi^3} \int e^{2i\vec{r} \cdot \vec{k}} \psi^* (\vec{r} + \vec{r}', t) \psi (\vec{r} - \vec{r}', t) d\vec{r}'
\]

(4)

Where \(\psi\) is the wave equation which is the solution of Schrödinger equation at the point \(\vec{r} \pm \vec{r}'\). By differentiating the Wigner function with respect to time, and employing the Schrödinger equation, transport equation (2) for the Wigner function can be derived \([?]\).

It is important to keep in mind that in equation (2), \(\nabla_{\vec{k}}\) only operates on \(w\), and \(\nabla_{\vec{r}}\) only operates on the potential \(V(\vec{r})\). We separate the potential into two basic terms: one resulting from fields and barriers, and one due to scattering. The time variation of \(w\) due to scattering is then given by the collision integral in the semiclassical Boltzmann equation for semiconductors. This gives rise to the following Boltzmann/Wigner transport equation:
\[
\frac{\partial w}{\partial t} + \frac{\nabla \bar{\epsilon}}{\hbar} \cdot \nabla_{\vec{r}} w - \frac{q}{\hbar} \sum_{n=0}^{\infty} \frac{(-1)^{2n}}{4^n(2n+1)!} (\nabla_{\vec{k}} \cdot \nabla_{\vec{r}})^{2n+1} V(\vec{r}) w = \left( \frac{\partial w}{\partial t} \right)_{\text{coll}}
\] (5)

where

\[
\left( \frac{\partial w}{\partial t} \right)_{\text{coll}} = \frac{1}{(2\pi)^3} \sum_{j} \int \left[ w(\vec{r}, \vec{k}) S_j(\vec{k}', \vec{k}) - w(\vec{r}, \vec{k}) S_j(\vec{k}, \vec{k}') \right] d^3\vec{k}'
\] (6)

Where the functions \( S_j(\vec{k}', \vec{k}) \) refer to the matrix element for \( j' \)th type of scattering obtained from Fermi’s golden rule. In general, the \( S_j \) correspond to the important semiconductor processes. We include optical and acoustic phonons, surface scattering, ionized impurity scattering and impact ionization.

It is interesting to note that if we keep only the first order expansion of potential, the Boltzmann/Wigner transport equation reduces to the Boltzmann transport equation given by

\[
\frac{\partial w}{\partial t} + \frac{\nabla \bar{\epsilon}}{\hbar} \cdot \nabla_{\vec{r}} w - \frac{q}{\hbar} \nabla_{\vec{r}} V(\vec{r}) \cdot \nabla_{\vec{k}} w = \left( \frac{\partial w}{\partial t} \right)_{\text{coll}}
\] (7)

It can therefore be interpreted that the high order terms of the potential expansion give the quantum correction to the BTE. Furthermore, if the independent variable \( p = \hbar k \) is used in the Wigner equation, the higher order terms explicitly contain the factor \( \hbar^{2n} \), which quickly decrease in magnitude. We therefore retain the first two terms of the potential expansion, which yields an order \( \hbar^2 \) truncation. Such a truncation seems to be appropriate for application in devices where semiclassical transport is dominant. Keeping the first and second two terms of the potential expansion the steady-state Boltzmann/Wigner equation is obtained:

\[
\frac{\nabla \bar{\epsilon}}{\hbar} \cdot \nabla_{\vec{r}} w - \frac{q}{\hbar} \nabla_{\vec{r}} V(\vec{r}) \nabla_{\vec{k}} w - \frac{q}{24\hbar^3} (\nabla_{\vec{k}} \cdot \nabla_{\vec{r}})^3 V(\vec{r}) w = \left( \frac{\partial w}{\partial t} \right)_{\text{coll}}
\] (8)

### 2.2 Spherical Harmonic Formulation

The difficulties that are usually associated with solving the Boltzmann equation are even further complicated when quantum effects are included, which requires solving the Boltzmann/Wigner equation. The main difference between the two equations is the quantum
correction term in the Boltzmann/Wigner equation. As shown in equation (8), this correction contains a product of third order derivatives. Since the Spherical Harmonic method has been applied extensively to solving the BTE, where it has been shown to be a powerful method for overcoming obstacles [?, ?, ?, ?, ?, ?, ?, ?, ?, ?], we extend the approach to the Boltzmann/Wigner equation. The spherical harmonics expansion of the distribution function allows for analytical evaluation of the collision integral and reduction of dimensionality making the Boltzmann/Wigner equation tractable for numerical solution. Below we outline the derivation of the Spherical Harmonic Boltzmann/Wigner equation for the 1-D case.

1-Dimensional Spherical Harmonic Boltzmann/Wigner Equation

For 1-D applications the Boltzmann/Wigner equation (8) becomes:

\[
 v_\parallel(\vec{k}) \frac{\partial w}{\partial x} - \frac{q}{\hbar} \frac{\partial V}{\partial x} \frac{\partial w}{\partial k_\parallel} - \frac{q^2}{24\hbar} \frac{\partial^3 V}{\partial^3 x} \frac{\partial^3 w}{\partial^3 k_\parallel} = \left( \frac{\partial w}{\partial t} \right)_{\text{coll}}
\]  

(9)

where the terms \(v_\parallel\) and \(k_\parallel\) indicate components that are parallel to the electric field.

It is interesting to note that the first two terms on the left hand side (LHS) of equation (9) are the same as in the semiclassical Boltzmann equation. The inclusion of the third term on the LHS provides the quantum correction. We now express the solution of this equation, which is the Wigner function \(w(x, \vec{k})\), using the following spherical harmonic expansion in momentum space:

\[
 w(x, \vec{k}) = \sum_{l=0}^{\infty} w_l(x, k) P_l(\cos \theta_k)
\]  

(10)

\(P_l(\cos \theta_k)\) are the 1-D spherical harmonics and \(\theta\) is the angle between momentum and the electric field. (For 1-D applications \(P_l\) are equivalent to the Legendre polynomials.) \(w_l(x, k)\) are the expansion coefficients, which have to be determined. It is important to note that the expansion coefficients are functions of momentum magnitude only \(k\), and thus have no angular dependence in momentum space.

To determine the coefficients, this expansion is substituted into the Boltzmann/Wigner equation. By using the spherical harmonics recurrence relations, the Boltzmann/Wigner equation is then expressed in a form which facilitates projection onto the spherical harmonic basis. Once this projection is achieved, a set of equations for the unknown coefficients is derived. Authors typically truncate this expansion after \(l=1\), this corresponds to the
first two spherical harmonics for 1-D calculations, and inclusion of the first four spherical
harmonics for 2-D calculations \([?, ?, ?, ?, ?, ?]\). This follows physically since these
components represent the symmetrical and antisymmetrical parts of the distribution function
with respect to the electric field direction, and helps to explain why this approach provides
agreement with Monte Carlo simulations and experiment\([?, ?, ?, ?, ?, ?]\). Following previous
works we truncate the expansion, and solve the system numerically to find the distribution
function throughout the device. The details of this formulation as applied to the Boltzmann
equation are given in references \([?, ?, ?, ?, ?, ?]\). Instead of rederiving the entire spherical harmonic
formulation for the Boltzmann/Wigner equation, we start by restating previous results.
These earlier works show that the steady state part of the semiclassical Boltzmann equation
\((7)\) can be transformed into the following spherical harmonic expression\([?, ?, ?, ?]\):

\[
v \left( \frac{\partial}{\partial x} + \frac{\partial \gamma}{\partial x} \right) \left( \sqrt{\frac{1}{3}} w_1 \right) P_0 + v \left( \frac{\partial}{\partial x} \sqrt{\frac{1}{3}} w_0 \right) P_1 = \left[ \frac{\partial w_0}{\partial t} \right]_{\text{coll}} P_0 - \frac{w_1}{\tau} P_1
\]

where \(w_0\) and \(w_1(\cos \theta_k)\) can be taken to be the symmetrical and antisymmetrical components
of the semiclassical distribution function, \(P_0\) and \(P_1\) are the first two spherical harmonics,
\(\frac{1}{\tau(\epsilon)}\) is the total scattering rate, and \(\gamma(\epsilon) = \frac{k^2 k^2}{2m} \) is the dispersion relation for nonparabolic
bands. Explicit expressions for \(\frac{1}{\tau(\epsilon)}\) and \(\gamma(\epsilon)\) can be found in \([?, ?, ?]\), and \(w_0\) and \(w_1\) are found
by solving \((11)\) along with the Poisson and hole continuity equations.

To obtain the Boltzmann/Wigner equation, we add the quantum correction term to equation \((11)\). This term is \(-\frac{q}{24} \frac{\partial^3 V}{\partial x^3} \frac{\partial^3 w}{\partial k^3}\), which we have to re-express using spherical harmonics:

\[
-\frac{q}{24} \frac{\partial^3 V}{\partial x^3} \frac{\partial^3 w}{\partial k^3} \approx [QM]_0 P_0 + [QM]_1 P_1
\]

\([QM]_0\) and \([QM]_1\) represent the operators that are obtained when we re-express \(-\frac{q}{24} \frac{\partial^3 V}{\partial x^3} \frac{\partial^3 w}{\partial k^3}\)
with spherical harmonics. Adding the quantum correction term into equation \((11)\), gives the
following form for the Boltzmann/Wigner equation:

\[
v \left( \frac{\partial}{\partial x} + \frac{\partial \gamma}{\partial x} \right) \left( \sqrt{\frac{1}{3}} w_1 \right) P_0 + v \left( \frac{\partial}{\partial x} \sqrt{\frac{1}{3}} w_0 \right) P_1 + \frac{w_1}{\tau} P_1 + [QM]_0 P_0 + [QM]_1 P_1 = \left[ \frac{\partial w_0}{\partial t} \right]_{\text{coll}} P_0
\]
Now, we must formulate the quantum correction terms using spherical harmonics to obtain explicit expressions for the operators \([QM]_0\) and \([QM]_1\). We begin by restating the result from [1], where it is shown that \(\partial w(x, \vec{k})/\partial k_{||}\) can be expressed using spherical harmonics:

\[
\frac{\partial w(x, \vec{k})}{\partial k_{||}} = \sum_l \left[ \left( \frac{\partial}{\partial k} - \frac{l - 1}{k} \right) \alpha_{l-1} w_{l-1} \right. \\
\left. + \left( \frac{l + 1}{l + 2} \frac{\partial}{\partial k} + \frac{l + 1}{k} \right) \alpha_{l+1} w_{l+1} \right] P_l
\]  

(14)

where

\[
\alpha = \frac{l + 1}{2l + 1} \quad (15)
\]

While equation (14) appears complicated, it represents a simplification since the angular dependence in \(w(x, \vec{k})\) is transferred algebraically to the basis functions \(P_l\). We now use equation (14) as a starting point for deriving the quantum correction term, which contains a third order derivative. First we define a new operator \(\hat{A}\):

\[
\hat{A}w_l = \left( \frac{\partial}{\partial k} - \frac{l - 1}{k} \right) \alpha_{l-1} w_{l-1} + \left( \frac{l + 1}{l + 2} \frac{\partial}{\partial k} + \frac{l + 1}{k} \right) \alpha_{l+1} w_{l+1}
\]  

(16)

To obtain a third derivative, we apply this operator three times:

\[
\left( \frac{\partial}{\partial k_{||}} \right)^3 w(x, \vec{k}) = \sum_l (\hat{A} \hat{A} \hat{A} w_l) P_l
\]  

(17)

After a considerable amount of mathematical manipulation involving the spherical harmonics recurrence relations and truncation, it can be shown that the third derivative term is given by the following expression. (For complete details see reference [2]).

\[
\left( \frac{\partial}{\partial k_{||}} \right)^3 w(x, \vec{k}) = \sum_l \left( \frac{\partial}{\partial k_{||}} \right)^3 w_l(t, x, k) P_l(\cos \theta)
\]

\[
\approx \left[ \hat{K}_0 \left( \frac{3}{5} \sqrt{\frac{2}{3}} w_1 \right) \right] P_0 + \left[ \hat{K}_1 \left( \frac{3}{10} \sqrt{\frac{2}{3}} w_0 \right) \right] P_1
\]  

(18)
where

\[ \hat{K}_0 = \frac{\partial^3}{(h\partial k)^3} + \frac{2}{h^3 k} \frac{\partial^2}{\partial k^2} - \frac{2}{h^3 k^2} \frac{\partial}{\partial k} \]  

(19)

and

\[ \hat{K}_1 = \frac{\partial^3}{(h\partial k)^3} + \frac{4}{h^3 k} \frac{\partial^2}{\partial k^2} \]  

(20)

Up until this point we have been using the wave-vector \( k \) as our independent variable. However, in our previous work we found that using electron energy as the independent variable facilitated was preferable, mainly because intervalley phonon scattering rates could be expressed in terms of electron energy. In addition, this enables direct calculation of the energy distribution function, which gives insight into nonequilibrium behavior. Thus we transfer our independent variable from \( k \) to energy and express the operator \( \hat{K}_0 \) and \( \hat{K}_1 \) in terms of \( \varepsilon \). Using the chain rule we use the following substitution

\[ \frac{\partial}{h\partial k} = \frac{\partial\varepsilon}{\partial\varepsilon} \]  

(21)

Using the above expression to obtain the second and third derivatives with respect to \( k \) as well, we obtain the following expressions for the operators \( \hat{K}_0 \) and \( \hat{K}_1 \) in terms of energy.

\[ \hat{K}_0 = \left( \frac{\partial\varepsilon}{h\partial k} \right)^3 \frac{\partial^3}{\partial\varepsilon^3} + \left[ 3 \frac{\partial\varepsilon}{h\partial k} \frac{\partial^2\varepsilon}{h^2\partial k^2} + \frac{4}{(2m^*\gamma)^{\frac{1}{2}}} \left( \frac{\partial\varepsilon}{h\partial k} \right)^2 \right] \frac{\partial^2}{\partial\varepsilon^2} \]

\[ + \left[ \frac{\partial^3\varepsilon}{h^3\partial k^3} \right] + \frac{2}{(2m^*\gamma)^{\frac{1}{2}}} \frac{\partial^2\varepsilon}{h^2\partial k^2} \left( \frac{\partial\varepsilon}{h\partial k} \right)^2 \frac{\partial}{\partial\varepsilon} \]  

(22)

\[ \hat{K}_1 = \left( \frac{\partial\varepsilon}{h\partial k} \right)^3 \frac{\partial^3}{\partial\varepsilon^3} + \left[ 3 \frac{\partial\varepsilon}{h\partial k} \frac{\partial^2\varepsilon}{h^2\partial k^2} + \frac{2}{(2m^*\gamma)^{\frac{1}{2}}} \left( \frac{\partial\varepsilon}{h\partial k} \right)^2 \right] \frac{\partial^2}{\partial\varepsilon^2} \]

\[ + \left[ \frac{\partial^3\varepsilon}{h^3\partial k^3} \right] + \frac{2}{(2m^*\gamma)^{\frac{1}{2}}} \frac{\partial^2\varepsilon}{h^2\partial k^2} - \frac{1}{m^*\gamma h\partial k} \left( \frac{\partial\varepsilon}{h\partial k} \right) \frac{\partial}{\partial\varepsilon} \]  

(23)

Where derivatives of the form \( \frac{\partial\varepsilon}{h\partial k} \) in equations 23 and ?? are evaluated directly from the dispersion relation described above.

To formulate the potential energy component of this term \( \frac{\partial V^3}{\partial\varepsilon^3} \), we invoke the Poisson equation:
\[
\frac{\partial V^3}{\partial x^3} = \frac{\partial}{\partial x} \left( \nabla^2 V \right) = -\frac{1}{\epsilon} \frac{\partial \rho}{\partial x}
\]  
\text{(24)}

where \( \rho = q(p - n + D) \) represents the charge density. Combining (24) and (18) we obtain

\[
\frac{\partial V^3}{\partial x^3} \left( \frac{\partial}{\partial k} \right) w(x, \vec{k}) = -\frac{\hbar^3}{\epsilon} \left\{ \frac{\partial \rho}{\partial x} \left[ \hat{K}_0 \left( \frac{3}{5} \sqrt{\frac{1}{3} w_1} \right) \right] \right\} P_0
\]

\[-\frac{\hbar^3}{\epsilon} \left\{ \frac{\partial \rho}{\partial x} \left[ \hat{K}_1 \left( \frac{3}{5} \sqrt{\frac{1}{3} w_0} \right) \right] \right\} P_1
\]  
\text{(25)}

Now, if we substitute (25) for the quantum terms \([QM]_0 P_0 + [QM]_1 P_1 \) in equation (13), project onto the spherical harmonic basis, transform our independent variable from momentum magnitude to energy, we obtain equations for the symmetrical \( w_0 \) and antisymmetrical \( w_1 \) coefficients of the quantum distribution function, respectively.

\[
v \left( \frac{\partial}{\partial x} + \frac{\partial \gamma_1}{\partial x} \right) \left( \sqrt{\frac{1}{3} w_1} \right) - \frac{q \hbar}{24 \epsilon} \frac{\partial \rho}{\partial x} \left[ \hat{K}_0 \left( \frac{3}{5} \sqrt{\frac{1}{3} w_1} \right) \right] = \left[ \frac{\partial w_0}{\partial t} \right]_{coll}
\]  
\text{(26)}

\[
v \left( \frac{\partial}{\partial x} \sqrt{\frac{1}{3} w_0} \right) - \frac{q \hbar}{24 \epsilon} \frac{\partial \rho}{\partial x} \left[ \hat{K}_1 \left( \frac{3}{5} \sqrt{\frac{1}{3} w_0} \right) \right] = -\frac{w_1}{\tau}
\]  
\text{(27)}

Where equations (24) and (27) are obtained by projecting the formulated Boltzmann/Wigner equation onto harmonics \( P_0 \) and \( P_1 \), respectively.

Next, we use substitution to algebraically eliminate the equation for \( w_1 \) to obtain the following single equation for the quantum energy distribution function \( w_0 \):

\[
v \left( \frac{\partial}{\partial x} \right) \left[ \gamma \tau \left( \frac{\partial w_0}{\partial x} + \frac{q \hbar^2}{24 \epsilon v} \frac{\partial \rho}{\partial x} \hat{K} w_0 \right) \right] = \left[ \frac{\partial w_0}{\partial t} \right]_{coll}
\]  
\text{(28)}

where \( \hat{K} = \hat{K}_0 + \hat{K}_1 \).

We now include the collision integral, which has been formulated previously using spherical harmonics[?, ?], and is provided in the Appendix. We then discretize the Boltzmann/Wigner equation using an analytical fitting method similar to the one used for the Boltzmann equation[?]. The equation is first discretized directly. Then the homogeneous
part of the discretized equations are solved analytically between mesh points. The nonhomogeneous part is then solved on the mesh points. This gives a discretized equation for $w_0$. The hole-current continuity equation is then discretized with a Scharfetter-Gummel approach, and the Poisson equation is discretized with standard central differences[?]. The resulting nonlinear algebraic system is then solved iteratively in a decoupled manner, using the solution of the Boltzmann equation as the initial guess.

**2-Dimensional Spherical Harmonic Boltzmann/Wigner Equation**

The derivation for 2-D applications is analogous to the 1-D approach. Of course we must use the complete spherical harmonic $Y_{lm}(\theta_k, \phi_k)$ to account for three dimensional angular dependence of momentum space. Thus, for 2-D, the Wigner function is expressed as:

$$w(\vec{r}, \vec{k}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} w_{lm}(\vec{r}, k) Y_{lm}(\theta_k, \phi_k)$$

(29)

The derivation now follows the 1-D approach but is significantly more tedious. Thus we only provide the results, details can be found in reference [?]. The resulting equations for 2-D simulation are analogous to (24) and (27), and are given by:

$$l = 0, \ m = 0, \ \text{term } Y_0^0$$

$$v \left[ \frac{\partial}{\partial x} + \frac{\gamma_1}{\gamma_x} \left( \frac{1}{2} \sqrt{\frac{2}{3}} w_1^{-1} - \frac{1}{2} \sqrt{\frac{2}{3}} w_1^1 \right) \right] + \left( \frac{\partial}{\partial y} + \frac{\gamma_1}{\gamma_y} \right) \left( \sqrt{\frac{1}{3}} w_1^0 \right)$$

$$= \left[ \frac{\partial w_0^0}{\partial t} \right]_{\text{cold}} - q \hbar^2 \frac{\partial \rho}{24e \partial x} \left[ \tilde{K}_0 \frac{3}{10} \sqrt{\frac{2}{3}} \left( w_1^{-1} - w_1^1 \right) \right] + \frac{\partial \rho}{\partial y} \left[ \tilde{K}_0 \left( \frac{3}{7} \sqrt{\frac{1}{3}} w_1^0 \right) \right]$$

(30)

$$l = 1, \ m = -1, \ \text{term } Y_1^{-1}$$

$$v \left( \frac{\partial}{\partial x} \frac{1}{2} \sqrt{\frac{2}{3}} w_0^0 \right) = \frac{-w_1^{-1}}{\tau} - q \hbar^2 \left\{ \frac{\partial \rho}{24e \partial x} \left[ \tilde{K}_1 \left( \frac{3}{10} \sqrt{\frac{2}{3}} w_0^0 \right) \right] \right\}$$

(31)

$$l = 1, \ m = 0, \ \text{term } Y_1^0$$
\begin{equation}
v \left( \frac{\partial}{\partial x} \sqrt{\frac{1}{3} w_0^0} \right) = \frac{-w_1^{-1}}{\tau} - \frac{q \hbar^2}{24 e} \left\{ \frac{\partial \rho}{\partial x} \left[ \hat{K}_1 \left( \frac{3}{5} \sqrt{\frac{1}{3} w_0^0} \right) \right] \right\}
\end{equation}

(32)

\begin{equation}
-v \left( \frac{1}{2} \frac{\partial}{\partial x} \sqrt{\frac{2}{3} w_0^0} \right) = \frac{-w_1^{-1}}{\tau} - \frac{q \hbar^2}{24 e} \left\{ \frac{\partial \rho}{\partial x} \left[ \hat{K}_1 \left( -\frac{3}{10} \sqrt{\frac{2}{3} w_0^0} \right) \right] \right\}
\end{equation}

(33)

Following methodology developed for the semiclassical Boltzmann equation\[^{[?]}\], we solve equations (31,32,33) for \(w_1^{-1}, w_0^0, w_1^1\), respectively, then back substitute into (30), to obtain the following equation for the 2-D quantum energy distribution function\[^{[?]}\]:

\begin{equation}
\frac{v}{3\gamma} \left\{ \frac{\partial}{\partial x} \left[ \gamma v \tau \left( \frac{\partial w_0^0}{\partial x} + \frac{q \hbar^2}{24 e \upsilon} \frac{\partial \rho}{\partial x} \hat{K} w_0^0 \right) \right] \right\} + \frac{\partial}{\partial y} \left[ \gamma v \tau \left( \frac{\partial w_0^0}{\partial y} + \frac{q \hbar^2}{24 e \upsilon} \frac{\partial \rho}{\partial y} \hat{K} w_0^0 \right) \right] = \left[ \frac{\partial w_0^0}{\partial t} \right]_{\text{coll}}
\end{equation}

(34)

Discretization and Self-Consistent Solution

Equation (34) is discretized using a Scharfetter-Gummel like strategy. The discretized Boltzmann/Wigner equation is then solved using a conjugate gradient method. The resulting Wigner function is then integrated to obtain the electron concentration throughout the device, which is then inserted into the RHS of the Poisson equation and the recombination term in the hole-current continuity equation. The Poisson and hole-current continuity equations are then discretized and solved using relatively standard methods\[^{[?], [?], [?]}. The entire coupled nonlinear system is then solved self-consistently using an iterative Gummel-like process for the Wigner function, the electrostatic potential and hole concentration throughout the device.

3 Results

We have applied our method of investigating quantum effects on semiclassical transport to a 2-D MOSFET and a 1-D NPN bipolar junction transistor (BJT).

1-D BJT Results
The doping structure of the BJT, which has a very narrow 50nm p-type base, is shown in Fig. 1. The emitter begins at \( x = 0 \mu m \), the base-emitter junction is at \( x = 0.05 \mu m \), and the base-collector junction is at \( x = 0.1 \mu m \). Fig. 2 shows the electrostatic potential inside the device with the applied biases of \( V_{BE} = 0.7 V \) and \( V_{CB} = 0.5, 1.0 \) and \( 2.0 V \), respectively. The potential was determined by self-consistent solution of the Poisson equation. It can be seen that the forward biased emitter-base barrier has its maximum magnitude at \( 0.07 \mu m \) into the device. It will be seen below that quantum mechanics influences the effects of this emitter-base barrier. Fig. 3 is the log of the Wigner (which we also call the quantum electron distribution) function calculated by solution to the Boltzmann/Wigner Equation along the device, at the bias \( V_{BE} = 0.7 \) and \( V_{BC} = 1.0 \). We see that in the emitter near the ideal classical ohmic contact, where the field is small, the quantum distribution function can be described by a Maxwellian, whereas in the high field region in the collector the quantum distribution function departs from equilibrium behavior with more electrons occupying the high energy region. This general behavior is predicted by both the Boltzmann/Wigner equation and the semiclassical BTE\[?\]. In Figs. 4 and 5 we compare values for electron densities determined from classical and quantum calculations for two different biases. The quantum electron concentration is obtained from the integration of the quantum distribution function over momentum, as calculated by the Boltzmann/Wigner equation. The classical values for electron concentration are obtained by integrating the semiclassical distribution function, as obtained by the BTE, over momentum. It is clear that the electron densities calculated by the two methods are very similar near the ideal classical ohmic contacts, while they show differences in the interior device active region. The electron density calculated by Boltzmann/Wigner equation is lower than that calculated by the BTE starting at \( x = 0.06 \mu m \). Then the percentage difference reaches its maximum at \( x = 0.07 \mu m \), where the emitter-base depletion region and the potential barrier peaks are located. This phenomenon suggests that the quantum effect should be included where the potential is rapidly varying, especially near the base-emitter barrier. We interpret the lower carrier concentration for the quantum calculation at the barrier peak to be due to the well-known quantum mechanical result that the electron wave function will reach its minimum value in the vicinity of a confining barrier peak, such as at the base-emitter junction. After the B-E junction, we also find that the semiclassical electron concentration predicted by the BTE is larger than that predicted by the Boltzmann/Wigner, especially for higher values of \( V_{CE} \). This follows since there are substantially fewer electrons to be thermionically emitted into the base due
to the reduced concentration at the BE junction. In terms of standard BJT parameters, quantum effects should therefore give rise to slightly reduced values of current gain $\beta$, a slightly greater tendency to modulate the base-collector junction and hence a lower Early voltage. Calculation of total collector current shows approximately 2% current less for the Boltzmann/Wigner case than that of the BTE for a fixed $V_{BE}$.

A detailed comparison of the quantum and semiclassical electron energy distribution function by position is also instrumental for understanding quantum effects. For comparison, we take the ratio of the semiclassical electron distribution function to the quantum distribution function (the semiclassical is in the numerator). The distribution function ratio is shown in Fig. 6. The ratio of the semiclassical to quantum distribution is very close to unity at the classical ohmic contacts. This is because the potential in these regions is relatively constant indicating little quantum confinement. As a result, semiclassical and quantum results coincide. The ratio starts to increase near $0.05\mu m$ and reach its peak near $0.07\mu m$, where the barrier region is located. Again, the calculations indicate that quantum effect suppresses the carrier concentration in the vicinity of a barrier. This is due to the added constraints that quantum mechanics places on the system. The quantum distribution function predicts less electrons at high energy than that predicted by the classical result. Once the electrons are injected into the base, semiclassical transport dominates. As can be seen from the figure, variations due to quantum constraints in the base-emitter junction, ultimately lead to subsequent variations in the distribution function in the unconfined base-collector region as well. This variation results from satisfying current continuity.

2-D MOSFET Results

We also solve the Boltzmann/Wigner equation for a 2-D MOSFET with the doping profile given by Fig. 7. This is achieved by solving equation (34) numerically as described above. The collision integral matrix elements are provided using Fermi’s golden rule.[7]

In Fig. 8, the ratio of electron concentration predicted by the BTE to that calculated by the Boltzmann/Wigner equation is shown for the whole device at the bias $V_{GS} = 3.0$, $V_{DS} = 3.0$. (The quantum results are in the denominator.) It is obvious to see that deep in the substrate, the carrier concentrations show no difference. However, near the source-channel junction, the channel region and the drain region, the carrier concentration predicted by the BTE is larger than that given by Boltzmann/Wigner equation. The ratio indicates that in regions near energy barriers (oxide interface, and source-channel junction) quantum effects
tend to decrease the carrier concentration. This relative decrease is then continued during semiclassical transport in the drain region due to dynamic effects and current continuity requirements. In Fig. 9, we show I-V characteristics for the MOSFET. The calculations give the expected results with quantum simulations predicting approximately 7% less drain current than the semiclassical model.

4 Conclusion

In this paper, a new approach is presented to investigate how semiclassical transport is influenced by quantum effects inside MOSFET and BJT devices. First, a quantum correction term is added to the Boltzmann equation to give rise to the Boltzmann/Wigner equation. This quantum correction term is expressed with spherical harmonics using a new third derivative operator. The effects of scattering are included explicitly by evaluating the semiclassical collision integral. The Boltzmann/Wigner equation is solved self-consistently with the Poisson and hole-current continuity equations for a 1-D BJT and a 2-D MOSFET. The results show that the carrier concentration predicted by the Boltzmann/Wigner equation near potential barriers is less than that predicted by the semiclassical Boltzmann model. The Boltzmann/Wigner also predicts reduced population of the quantum distribution function’s high energy tail. The lower concentrations in the quantum models give rise to reduced terminal currents in both the BJT and the MOSFET ranging from 2% to 7%.

In summary we have developed a new method for investigating quantum effects in largely semiclassical nanoscale devices. The solution of the Boltzmann/Wigner equation takes advantage of the Spherical Harmonics Expansion method. The results give the quantum corrected distribution function throughout the device. From the distribution function, most transport characteristics can be obtained.
5 Appendix

For optical phonons the contribution to the collision integral becomes:

\[
\left[ \frac{\partial w_0}{\partial t} \right]_{op} = \frac{D_i^2}{2\pi \rho \hbar^3 \omega_{op}} \sqrt{2m^{*3}} \left\{ \left[ w_o(\varepsilon_k + \hbar \omega_{op}) e^{\beta_{op}} - w(\bar{k}) \right] \gamma^{1/2}(\varepsilon_k + \hbar \omega_{op}) \gamma'(\varepsilon_k + \hbar \omega_{op}) + w_o(\varepsilon_k - \hbar \omega_{op}) - w(\bar{k}) e^{\beta_{op}} \right\} \gamma^{1/2}(\varepsilon_k - \hbar \omega_{op}) \gamma'(\varepsilon_k - \hbar \omega_{op}) \right\}
\]

where \(\beta_{op} = \frac{\hbar \omega_{op}}{k_B T}\), and \(\gamma^{1/2} \gamma'\) is proportional to the density of states.

The optical phonon scattering rate is:

\[
\frac{1}{\tau_{op}(\varepsilon_k)} = \frac{D_{op}^2}{2\pi \rho \hbar^3 \omega_{op}} \sqrt{2m^{*3}} \left\{ \gamma^{1/2}(\varepsilon_k + \hbar \omega_{op}) \gamma'(\varepsilon_k + \hbar \omega_{op}) + e^{\beta_{op}} \gamma^{1/2}(\varepsilon_k - \hbar \omega_{op}) \gamma'(\varepsilon_k - \hbar \omega_{op}) \right\}
\]

For elastic scattering the symmetrical part of the collision term vanishes. In the elastic approximation, the acoustic phonon scattering rate is:

\[
\frac{1}{\tau_{ac}(\varepsilon_k)} = \frac{k_B T D_{ac}^2}{\hbar^4 \rho u_0^2} \sqrt{2m^{*3}} \gamma^{1/2} \gamma'(\varepsilon_k) \left[ 1 + \frac{1}{3} \left( \frac{m u_0^2 \gamma(\varepsilon)}{(k_B T)^2} \right) \right]
\]

We also include elastic ionized impurity scattering \(\frac{1}{\tau_{ion}}\) using the expression given in \[?\].

The expression for the total scattering rate is given by

\[
\frac{1}{\tau} = \frac{1}{\tau_{op}} + \frac{1}{\tau_{ac}} + \frac{1}{\tau_{ion}}
\]

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Figure 1: The doping profile of the simulated NPN BJT.
Figure 2: The calculated electrostatic potential of the NPN BJT for the three different biases indicated. The barrier peak is located as $0.07\mu m$. 
Figure 3: The log of the quantum electron energy distribution function throughout the device as calculated by the Boltzmann/Wigner equation at the applied bias $V_{BE} = 0.7\text{V}$ and $V_{CB} = 1.0\text{V}$. The emitter contact is at $x = 0$. 
Figure 4: Comparison of the electron concentration as calculated by semiclassical Boltzmann equation and the Boltzmann/Wigner equation. The applied bias is $V_{BE} = 0.7V, V_{CB} = 0.5V$. The emitter contact is at $x = 0$. 
Figure 5: Comparison of the electron concentration as calculated by the semiclassical Boltzmann equation and the Boltzmann/Wigner equation. The applied bias is $V_{BE} = 0.7V$, $V_{CB} = 2.0V$. The emitter contact is at $x = 0$. 
Figure 6: The ratio of semiclassical distribution function to the quantum distribution function for $V_{BE} = 0.7\text{V}, V_{CB} = 0.5\text{V}$. The emitter contact is at $x = 0$. 
Figure 7: The doping profile of the simulated MOSFET.
Figure 8: Ratio of the electron concentration as calculated by the semiclassical Boltzmann equation to Boltzmann/Wigner equation. The applied bias is $V_{GS} = 3.0V$, $V_{DS} = 3.0V$. 
Figure 9: The MOSFET drain current comparison as calculated by Boltzmann/Wigner and BTE.