

# Application of Cumulant Expansion to the Modeling of Non-local Effects in Semiconductor Devices

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## Abstract

*The cumulant expansion method is proposed to solve the Boltzmann transport equation (BTE) in semiconductors. This method involves deriving a set of partial differential equations for the expansion coefficients from a Fourier transformation of the BTE. The collision terms for phonon emission and absorption scattering are obtained directly from quantum computed scattering transition rates, without invoking the relaxation time approximation. Unlike the moment expansion method used in hydrodynamic models, the cumulant expansion converges much faster when the distribution function is close to a drifted Maxwellian because, for this case, only the first three cumulants are non-zero. This method also provides a way to construct an arbitrary distribution function from the computed cumulants, without being limited to a shifted Maxwellian.*

## I. Introduction

Hydrodynamic models have the best mixture of physical sophistication for modeling of non-local effects in submicron devices and affordable computation efficiency in the TCAD environment. Major progress has been made in the last thirty years since hydrodynamic models were first proposed by Blotekjaer [1] and Stratton [2]. Hydrodynamic models have been used successfully in modeling carrier heating and velocity overshoot effects. However difficulties still exist, especially in modeling the collision terms. Most hydrodynamic models even use energy independent relaxation times. The relaxation time approximation (RTA) requires a long list of pre-conditions, including that the distribution function can only be a perturbation to a local equilibrium distribution and that scattering has to be either isotropic or elastic. These conditions clearly break down in deep submicron devices where the electric field can vary rapidly and thus the resulting distribution function is far from equilibrium. Furthermore, the relaxation times are usually extracted from bulk Monte Carlo simulation and applied in hydrodynamic models as a function of energy. This method is in gross error, because a distribution function in a

homogenous field can be very different from one in a device, despite sharing the same average energy after integration. As first pointed out by Lee and Tang[3] and more recently by Anile et al. [4], the collision terms are more correctly a function of current density and energy flux. Their empirical formulas are based on the first three terms of a moment expansion of the collision term proposed by Hansch et al. [5]. However, his approach, though more accurate, suffers slow convergence. Hydrodynamic models also limit themselves to only shifted-Maxwellian distributions, in spite of the fact that this implicitly assumes the heat flux is zero, which is generally not the case in a device. In this paper, we propose a complete hydrodynamic model based on the cumulant expansion method to address the above problems.

The cumulant expansion[6-7] has been used in many fields of statistics. It is especially efficient in treating random process whose distribution function is close to a shifted Gaussian. In this paper, we will show first that only three cumulants are needed to represent a shifted Gaussian instead of the infinite number of terms required by the moment expansion method upon which hydrodynamic models are based. Even when the distribution functions are distorted from a shifted Gaussian in high fields, the higher order cumulants should be small and converge fast.

Section II applies Fourier transformation to the BTE. A set of partial differential equations is obtained by comparing the coefficients of the conjugate variable of the random momentum. Next, the collision terms from phonon emission and absorption are examined, without employing the RTA, in section III. The last section summarizes our results. Possible future work is also discussed.

## II. Cumulant Expansion of the Boltzmann Transport Equation

One popular approach to solve the BTE is by expanding the distribution function into a series of known base functions. The coefficients of the expansion satisfy a set of hierarchical PDEs. The faster the series converges the less error is produced due to truncation. The benefit of the cumulant expansion is obvious because only the first

three terms in the expansion are needed to represent a shifted maxwellian. Moreover, as long as the distribution is close to a shifted maxwellian, the higher order cumulants will be small and reduce to zero very quickly. In contrast, the moments of a shifted maxwellian distribution function never go to zero until the number of moments tends to infinity.

Cumulants are defined as the coefficients of a Taylor expansion of the logarithm of the characteristic function. A characteristic function  $g$  is defined as the Fourier transform of its distribution function  $f(x,p,t)$ :

$$g(\bar{x}, \bar{\xi}, t) = \int f(\bar{x}, \bar{p}, t) \exp(i\bar{\xi} \cdot \bar{p}) d^3 p \quad (1)$$

$$\ln(g) = \sum_{n=0}^{\infty} \frac{i^n}{n!} C_{i_1 \dots i_n}^{(n)} \xi_1 \dots \xi_n \quad (2)$$

The index  $i$  runs through  $x, y, z$  in three dimensions. The  $n$ th cumulants  $C_{i_1 \dots i_n}^{(n)}$  usually depends on position and time and is a tensor with  $n$  symmetric indexes. Let's use the shifted maxwellian as an example to show the effectiveness of the expansion. Assuming the system has a temperature of  $T$ , effective mass of  $m^*$  and average momentum of  $\bar{p}^0$ , the characteristic function is then:

$$g(\bar{x}, \bar{\xi}, t) = \frac{n}{\sqrt{2\pi k_B T}} \int \exp\left(-\frac{(\bar{p} - \bar{p}^0)^2}{2m^* k_B T}\right) \exp(i\bar{\xi} \cdot \bar{p}) d^3 p$$

$$= \exp(\ln(n) + i\bar{p}^0 \cdot \bar{\xi} + \frac{i^2}{2} m^* k_B T \bar{\xi} \cdot \bar{\xi})$$

It is easy to see that the first three cumulants are  $\ln(n)$ , average momentum  $\bar{p}^0$  and  $m^*k_B T$ , where  $T$  is the scalar temperature. All other cumulants are zero. If the distribution function is expanded in moments, on the other hand, the series will need an infinite number of terms. Figure 1 compares the decay of the cumulants and the increase of moments as the order increases for a shifted gaussian distribution function with both shift and spreading of unity. The moments increase geometrically with the increase of the order, while the cumulants are all zero for the orders larger than 2.

The relationship between moments and cumulants can be obtained by taking the Taylor expansion of the characteristic function into moments and comparing the coefficients  $1, \bar{\xi}_i, \bar{\xi}_i \bar{\xi}_j, \dots$ :

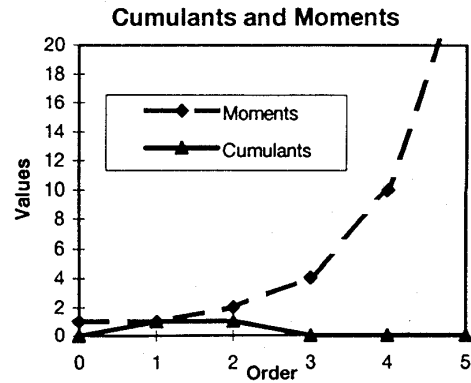


Figure 1. The comparison of cumulants and moments from a shifted gaussian distribution. The moments clearly diverge as the order increases while cumulants drop to zero for those with order larger than 2.

$$\sum_{n=0}^{\infty} \frac{i^n}{n!} m_{i_1 \dots i_n}^{(n)} \xi_1 \dots \xi_n = \exp\left(\sum_{n=1}^{\infty} \frac{i^n}{n!} C_{i_1 \dots i_n}^{(n)} \xi_1 \dots \xi_n\right)$$

Note that we have adapted Einstein's notation: repeated indices mean summation. It is useful to relate the first few cumulants with the moments of a distribution:

$$C^{(0)} = \ln(n)$$

$$C_i^{(1)} = \langle p_i \rangle = \bar{p}_i$$

$$C_{i,j}^{(2)} = \langle (p_i - \bar{p}_i)(p_j - \bar{p}_j) \rangle = \langle \Delta p_i \Delta p_j \rangle$$

$$C_{i,j,k}^{(3)} = \langle \Delta p_i \Delta p_j \Delta p_k \rangle$$

$$C_{i,j,k,l}^{(4)} = \langle \Delta p_i \Delta p_j \Delta p_k \Delta p_l \rangle - \langle \Delta p_i \Delta p_j \rangle \langle \Delta p_k \Delta p_l \rangle$$

$$- \langle \Delta p_i \Delta p_k \rangle \langle \Delta p_j \Delta p_l \rangle - \langle \Delta p_i \Delta p_l \rangle \langle \Delta p_j \Delta p_k \rangle$$

High order cumulants decrease fast because they contain only the higher order correlation of random variables left after subtracting the best possible correlation constructed with lower order cumulants.

In general, cumulants depend on the position and time, just as the distribution function they represent. Similar to hydrodynamic equations, the cumulants satisfy a set of partial differential equations imposed by the BTE. By multiplying the BTE by  $\exp(i\bar{\xi} \cdot \bar{p})$  and integrating over  $\bar{p}$ , a set of PDEs can be obtained by comparing the coefficients of  $1, \bar{\xi}_i, \bar{\xi}_i \bar{\xi}_j, \dots$  after factoring out a characteristic function from each term:

$$\begin{aligned}
\frac{\partial \mathcal{C}^{(0)}}{\partial t} + \frac{C_i^{(1)}}{m^*} \frac{\partial \mathcal{C}^{(0)}}{\partial x_i} + \frac{1}{m^*} \frac{\partial \mathcal{C}_i^{(1)}}{\partial x_i} &= f^{(0)} \\
\frac{\partial \mathcal{C}_i^{(1)}}{\partial t} + \frac{C_{i,j}^{(2)}}{m^*} \frac{\partial \mathcal{C}^{(0)}}{\partial x_j} + \frac{C_j^{(1)}}{m^*} \frac{\partial \mathcal{C}_i^{(1)}}{\partial x_j} + \frac{1}{m^*} \frac{\partial \mathcal{C}_{i,j}^{(2)}}{\partial x_j} - qF_i &= f_i^{(1)} \\
\frac{\partial \mathcal{C}_{i,j}^{(2)}}{\partial t} + \frac{C_{i,j,k}^{(3)}}{m^*} \frac{\partial \mathcal{C}^{(0)}}{\partial x_k} + \frac{1}{m^*} (C_{j,k}^{(2)} \frac{\partial \mathcal{C}_i^{(1)}}{\partial x_k} + C_{i,k}^{(2)} \frac{\partial \mathcal{C}_j^{(1)}}{\partial x_k}) \\
+ \frac{C_k^{(1)}}{m^*} \frac{\partial \mathcal{C}_{i,j}^{(2)}}{\partial x_k} + \frac{1}{m^*} \frac{\partial \mathcal{C}_{i,j,k}^{(3)}}{\partial x_k} &= f_{i,j}^{(2)}
\end{aligned}$$

where the  $f$ 's on the right hand side are collision dissipation terms related to the cumulants. Note that the electric field vector  $F_i$  only appears in the PDE for the second order cumulant. After the cumulants are solved from the PDEs, an arbitrary distribution function can be constructed via a reverse Fourier transform. If the 3<sup>rd</sup> or higher order cumulants are included, the resultant distribution function will be more general than a shifted Maxwellian. The first equation is the particle conservation equation. The second and third, however, are mixtures of particle conservation, momentum conservation and energy conservation equations.

### III. Modeling the Collision Terms Without Relaxation Time Approximation

Traditionally, collision terms are modeled by the RTA. As pointed out in [8], the distribution function is very different at the rising and falling edge of a changing field, even if the average energies are exactly the same. As a result, the collision term, which depends on the distribution function, is also very different. This indicates that the average energy is not sufficient to represent the distribution function or the collision terms. Thus, the traditional approach of extracting relaxation times from bulk Monte Carlo simulation is inaccurate: the distribution function in the bulk (constant fields) has little correlation with the distribution function in areas of a device where the fields change rapidly. In response to this limitation, Lee and Tang [3] proposed to characterize the collision terms by current density  $\mathbf{J}$  and energy flux  $\mathbf{S}$  instead of energy alone. They rely on Monte Carlo simulation of rising and falling fields (similar to the fields found in a MOSFET) to extract the dependence of the collision terms. Recently Anile et al. [4] also proposed a similar version of the collision term. However both models are empirical and the linear dependence on  $\mathbf{J}$  and  $\mathbf{S}$  is not well justified.

Here we apply our method to the collision terms using first principles. Similar to Section II, we apply a Fourier transform to the collision term and factor out a characteristic function:

$$\begin{aligned}
\left( \frac{\partial f}{\partial t} \right)_{col} &= \int f(\bar{x}, \bar{p}', t) S(\bar{p}', \bar{p}) d^3 p' \\
&- \int f(\bar{x}, \bar{p}, t) S(\bar{p}, \bar{p}') d^3 p \\
\int \left( \frac{\partial f}{\partial t} \right)_{col} \exp(i\bar{\xi} \cdot \bar{p}) d^3 p &= g(\bar{\xi}, \bar{x}) \{ f^{(0)} + \\
if_i^{(1)} \xi_i + \frac{i^2}{2!} f_{i,j}^{(2)} \xi_i \xi_j + \dots + \frac{i^n}{n!} f_{i_1 \dots i_n}^{(n)} \xi_{i_1} \dots \xi_{i_n} + \dots \}
\end{aligned}$$

where  $f_{i_1 \dots i_n}^{(n)}$  are collision terms for  $n$ -th cumulant,  $S(\mathbf{p}, \mathbf{p}')$  is the transition rate from  $\mathbf{p}$  to  $\mathbf{p}'$  due to scattering. The first three are expressed as:

$$\begin{aligned}
f^{(0)} &= 0 \\
f_i^{(1)} &= \exp(-C^{(0)}) \int d^3 p' d^3 p \{ f(\bar{x}, \bar{p}') S(\bar{p}', \bar{p}) (p'_i - p_i) \} \\
f_{i,j}^{(2)} &= \exp(-C^{(0)}) \int d^3 p' d^3 p \{ f(\bar{x}, \bar{p}') S(\bar{p}', \bar{p}) \\
(p'_i p'_j - p_i p_j) \} - C_i^{(1)} f_j^{(1)} - C_j^{(1)} f_i^{(1)} \\
f_{i,j,k}^{(3)} &= \exp(-C^{(0)}) \int d^3 p' d^3 p \{ f(\bar{x}, \bar{p}') S(\bar{p}', \bar{p}) \\
(p'_i p'_j p'_k - p_i p_j p_k) \} - C_{i,k}^{(2)} f_j^{(1)} - C_{j,k}^{(2)} f_i^{(1)} - C_{i,j}^{(2)} f_k^{(1)} \\
- C_k^{(1)} f_{i,j}^{(2)} - C_j^{(1)} f_{i,k}^{(2)} - C_i^{(1)} f_{j,k}^{(2)}
\end{aligned}$$

where  $S(\mathbf{p}, \mathbf{p}')$  is the transition rate due to scattering. The expressions for various scattering mechanisms can be derived from Fermi's golden rule based on quantum perturbation theory. Since the collision terms in the BTE linearly depend on the transition rate due to each scattering, the total collision contribution for each cumulant is the sum of the contributions from each scattering mechanism:

$$f_{total} = f_{phonon-em} + f_{phonon-abs} + f_{impurity} + \dots$$

The resultant collision terms therefore are explicit functions of the cumulants and other physical constants related to the scattering mechanisms. Thus, with this method no relaxation time approximation is needed.

Let's use optical phonon scattering as an example for the scattering dissipation calculation. The optical phonon transition rate  $S(\mathbf{p}, \mathbf{p}')$  is obtained by quantum perturbation:

$$\begin{aligned}
S(\bar{p}, \bar{p}') &= \frac{\pi (DtK)^2}{\rho V \omega_{op}} \left( \frac{N_{op}}{N_{op} + 1} \right) \times \\
\delta[\varepsilon(\bar{p}') - \varepsilon(\bar{p}) \mp \hbar \omega_{op}],
\end{aligned}$$

where  $DtK$  is the optical phonon coupling constant,  $N_{op}$  is the phonon occupation number,  $\omega_{op}$  is the angular

frequency of the optical phonon. The plus and minus signs correspond to the absorption and emission of the phonon. The collision term for the first cumulant can be obtained by plugging the scattering rate into the expression of the collision dissipation:

$$\begin{aligned} f_i^{(1),opt} &= \langle \int d^3 p S(\vec{p}', \vec{p})(p_i - p'_i) \rangle \\ &= -\frac{(DtK)^2 m^{*3/2}}{\sqrt{2\pi\hbar^3} \rho \omega_{op}} \left[ \frac{N_{op}}{N_{op} + 1} \right] \\ &\times \langle p_i \sqrt{\epsilon \pm \hbar\omega_{op}} \rangle \end{aligned}$$

The square root of final energy comes from the density of states in the above equation. Recall that the first order cumulant represents the average momentum, and the dissipation rate of average momentum is proportional to the initial momentum averaged over the density of states. Of course, the dissipation rate is also proportional to the phonon population for phonon absorption and proportional to phonon population plus 1 for phonon emission. The scattering dissipation rate for the second order cumulants can also be computed similarly:

$$\begin{aligned} f_{i,j}^{(2),opt} &= -\frac{(DtK)^2 m^{*3/2}}{\sqrt{2\pi\hbar^3} \rho \omega_{op}} \left[ \frac{N_{op}}{N_{op} + 1} \right] \times I_{i,j} \\ &- C_i^{(1)} f_j^{(1)} - C_j^{(1)} f_i^{(1)} \end{aligned}$$

where  $I_{i,j}$  is given by

$$I_{i,j} = \begin{cases} \langle p_i p_j \sqrt{\epsilon \pm \hbar\omega_{op}} \rangle & i \neq j \\ \langle [p_i^2 - \frac{2}{3} m^* (\epsilon \pm \hbar\omega_{op})] \sqrt{\epsilon \pm \hbar\omega_{op}} \rangle & i = j \end{cases}$$

The averages in the scattering dissipation terms can be expressed in cumulants that represent the distribution function. As a matter of fact, the average of any function  $S(\mathbf{p})$  can be expressed in cumulants through the following equation:

$$\begin{aligned} \langle S(\vec{p}) \rangle &= \frac{1}{(2\pi)^3} \int d^3 p \int d^3 \xi \cdot S(\vec{p}) \times \exp(-i\vec{p} \cdot \vec{\xi}) \\ &\times \exp(iC_i^{(1)} \xi_i + \frac{i^2}{2} C_{i,j}^{(2)} \xi_i \xi_j + \frac{i^3}{3!} C_{i,j,k}^{(3)} \xi_i \xi_j \xi_k + \dots) \end{aligned}$$

In this way the relaxation time approximation is removed completely. The expression of the collision dissipation terms are thus the functions of cumulants and the physical constants such as effective masses, Plank's constant, optical phonon energy and coupling constants.

We have constructed the framework for a simulation model for using cumulant expansion technique. This technique can treat collision terms without RTA. Thus no

empirical parameters are introduced and no calibration to Monte Carlo simulators are necessary. Without any assumption on the shape of the distribution function, this method extends the hydrodynamic model into an efficient BTE solver, and offers all capabilities which are available only from more complex methods such as spherical harmonic expansions. At the same time it is much simpler to solve than that of the spherical harmonic expansion.

So far we have only addressed the phonon scattering mechanisms. Several more scattering mechanisms, such as impurity scattering, surface roughness and carrier-carrier scattering will be published elsewhere together with the truncation scheme of the PDEs. More work is needed in verification of the model against Monte Carlo simulation in bulk, 1d and 2d simulations.

#### IV. Summary

We have proposed a new way of expanding the carrier distribution function in semiconductors. Without any assumption on the shape of the distribution function, a set of partial differential equations for cumulants is obtained by a Fourier transformation of the BTE. The collision terms are obtained without using the relaxation time approximation, thus lifting a major assumption which severely limits the accuracy of hydrodynamic methods in modeling submicron devices. In addition, only the three lowest cumulants are needed to represent a shifted maxwellian, which offers convergence advantages over moment-based methods such the traditional hydrodynamic model. Similar to the spherical harmonic expansion the cumulant expansion does not introduce empirical transport parameters and therefore no calibration is needed. More work is needed to make the cumulant expansion a viable model for device simulation for modern device technologies.

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