

# Solution of the Boltzmann Transport Equation in Two Real-Space Dimensions using a Spherical Harmonic Expansion in Momentum Space

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## Abstract

In this paper we present results obtained by solving the Boltzmann equation in two real space dimensions using a spherical harmonic expansion in momentum space. We show that if the coordinate system in momentum space is rotated to be aligned with the electric field then the magnitude of most of the harmonics can be assured to be small and thus they can be neglected without a significant loss of accuracy, which considerably reduces the complexity of the problem. Numerical results are presented for two dimensional structures in which flow occurs through both drift and diffusion.

## Introduction

To accurately model hot carrier phenomena such as gate and substrate currents in advanced semiconductor devices, it is necessary to solve the Boltzmann transport equation to obtain the carrier distribution functions. The most common approach to solve the Boltzmann equation is the Monte Carlo method [1] [2] [3]. Although such a method can be accurate, it is computationally expensive and, because of its stochastic nature, rare events are hard to model well. Recently, another approach using a basis function expansion of the distribution has been suggested [4] [5]. The simulation results presented in earlier work were mostly for the homogeneous or the one-dimensional examples and low order, which considerably reduced their complexity. In this work we present results from the solution of the Boltzmann transport equation in two real space dimensions using a spherical harmonic expansion in momentum space which is rotated to be aligned with the field direction at all points. As described in [6], we use a Galerkin method to generate a set of coefficients (to arbitrary order in principle) for the spherical harmonics at each point in two-dimensional real space.

When expanding the distribution in spherical harmonics in momentum space one obvious method is to

use a fixed coordinate system for all space. But this choice implies that when the electric field changes direction, the polar direction,  $k_z$ , will not be aligned with the electric field and therefore any symmetry in the distribution function about the electric field would not be exploited. Consequently, many of the 'off-diagonal' harmonics (eg.  $f_{1,-1}$ ,  $f_{2,2}$ ) would be non-zero. An alternate approach is to rotate the  $k$ -axes in such a way that the polar direction is always aligned with the electric field and thus minimize the 'off-diagonal' harmonics. This effect is demonstrated in Fig. 1. With a rotated coordinate system we therefore expect to be able to neglect off-diagonal terms, without a significant loss in accuracy. The real impact of this would be for higher orders where retaining all the coefficients will become prohibitively expensive and therefore a method which allows those coefficients to be neglected without a high penalty in accuracy would be greatly advantageous.

## Formulation Using A Rotated Coordinate System

Consider the case where the electric field direction is at an angle  $\mu$  from a fixed  $k_z$  direction, and we wish to expand the distribution function in terms of local spherical harmonics using the electric field direction as the polar direction. Then the relationship between the local variables, in the  $z, y$  frame which is rotated by an angle  $\mu$  from a global  $\hat{z}, \hat{y}$  frame (see Fig.2), and the variables in the global frame is given by

$$\begin{bmatrix} \sin \hat{\theta} \cos \hat{\phi} \\ \sin \hat{\theta} \sin \hat{\phi} \\ \cos \hat{\theta} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos \mu & \sin \mu \\ 0 & -\sin \mu & \cos \mu \end{bmatrix} \begin{bmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{bmatrix} \quad (1)$$

Thus the harmonic expansion can be written in terms of either the local or the global coordinate system:

$$f = \sum_{lm} f_{lm}(\mathbf{r}, k) Y_{lm}(\theta, \phi) = Y^T f = \hat{Y}^T R f \quad (2)$$

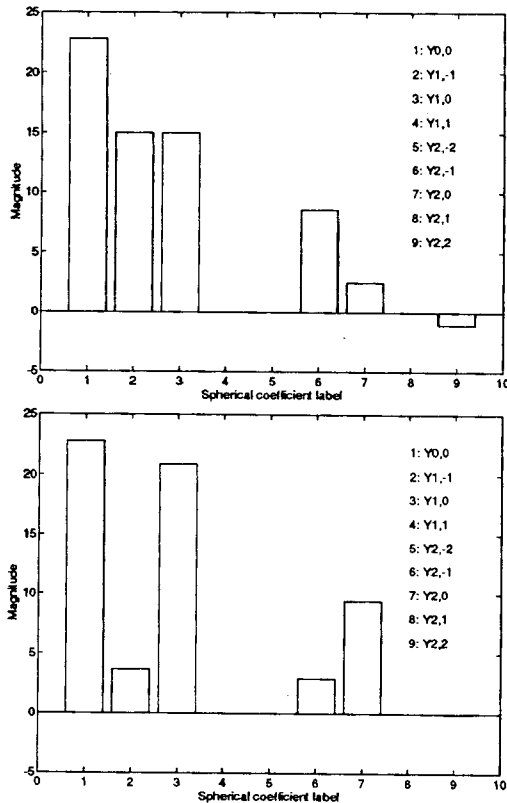


Figure 1: Coefficients of the spherical harmonics for a Maxwellian distribution displaced from the  $k_z$  direction along directions  $45^\circ$  (top) and  $10^\circ$  (bottom) from the  $k_z$  axis.

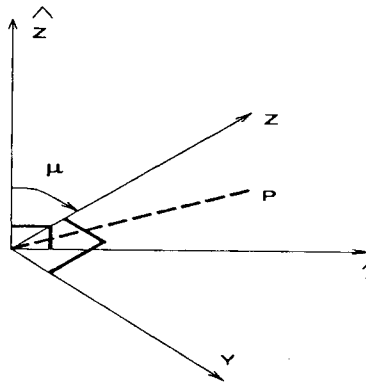


Figure 2: Rotated coordinate system

where  $Y, \hat{Y}$  are the vectors of the local and global spherical harmonics functions respectively and  $f$  is the vector of coefficients. The rotation matrix,  $R$ , up to first order, was given in (1). Note that the rotation matrix reduces to an identity matrix when  $\mu = 0$ . A rotation matrix can also be constructed for higher orders.

The approach we will follow for the solution of the

two-dimensional ( $y, z$ ) problem is summarized below:

1. Expand the distribution function in local coordinates.
2. Insert the expansion in the drift, diffusion and scattering terms of the BTE in local coordinates.
3. Convert to global harmonics by multiplying by the rotation matrix.
4. Discretize in space and energy.
5. Multiply by conjugate harmonics and integrate over a unit sphere in  $k$ -space to form the coefficient matrix.
6. Solve the matrix problem to obtain the coefficients at all points in real space.

This approach only differs in Step 3 from that followed in the one-dimensional problem [6]. In the following section, for brevity, we only illustrate the above steps for the diffusion term and acoustic phonon scattering.

### The Diffusion Term

The diffusion term of the BTE is

$$\mathbf{v}(\mathbf{k}) \cdot \nabla_r f(\mathbf{r}, \mathbf{k})$$

which after substituting the spherical harmonic expansion can be written as

$$\mathbf{v}(\mathbf{k}) \cdot \nabla_r Y^T f = \mathbf{v}(\mathbf{k}) \cdot \nabla_r (\hat{Y}^T R f).$$

If we assume spherical bands then  $\mathbf{v}(\mathbf{k})$  is in the radial  $k$  direction and its projection onto the  $z$ -axis is  $v(k) \cos \theta$  and onto the  $y$ -axis is  $v(k) \sin \theta \sin \phi$ . Then the diffusion term is

$$v(k) \left( Y^T \frac{\partial(Rf)}{\partial z} \cos \theta + Y^T \frac{\partial(Rf)}{\partial y} \sin \theta \sin \phi \right).$$

Finally the derivatives in space and energy must be discretized to generate a matrix problem for the coefficients in space and energy for any desired order. The discretized version of the diffusion term is:

$$v(E) [G_z (R^{i+1} f^{i+1} - R^i f^i) + G_y (R^{j+1} f^{j+1} - R^j f^j)]$$

where

$$G_z = \frac{1}{\Delta z} \int d\Omega Y^* Y^T \cos \theta \quad (3)$$

$$G_y = \frac{1}{\Delta y} \int d\Omega Y^* Y^T \sin \theta \sin \phi \quad (4)$$

form the non-zero blocks in the sparse coefficient matrix and  $i$  and  $j$  are the indices for the discretized variables in the  $z$  and  $y$  directions, respectively.

### The Scattering Term

We include acoustic and optical phonon and ionized impurity scattering; and for all three cases assume a single spherical band for simplicity. The scattering term

is handled in the same way as in the one-dimensional case with the important difference that we convert local harmonics to global ones, as done for the other terms, by multiplying by the rotation matrix. For example the expression for acoustic scattering is given as

$$c_{ac}g(E)Y^T S_{ac} f$$

where  $S_{ac}$  is understood to be the operator (matrix) for acoustic phonons scattering,  $c_{ac}$  is the scattering rate and  $g(E)$  is the density of states. With rotation this is modified as follows:

$$c_{ac}g(E)Y^T S_{ac} R f.$$

The last step is to generate the coefficient matrix entry by multiplying the conjugate harmonics and integrating over the unit sphere in k-space:

$$\int d\Omega Y^* Y^T c_{ac}g(E)S_{ac} R f.$$

### Equations to First Order

Although in our approach we do not need to explicitly write down the set of PDE's that arise in the problem, we give below the PDE's up to first order, for the rotated formulation:

$$\begin{aligned} & \frac{\partial(-\sin \mu f_{1,-1})}{\partial z} + \frac{\partial(\cos \mu f_{1,0})}{\partial z} \\ & + \frac{\partial(\cos \mu f_{1,-1})}{\partial y} + \frac{\partial(\sin \mu f_{1,0})}{\partial y} \\ & - \mathcal{E} \left[ \frac{\partial(f_{1,0})}{\partial E} + \frac{f_{1,0}}{E} \right] = \frac{1}{v'(E)} \left( \frac{\partial f_{0,0}}{\partial t} \right) \\ v' \left[ \frac{\partial(f_{0,0})}{\partial y} - \mathcal{E}_y \frac{\partial(f_{0,0})}{\partial E} \right] & = \cos \mu \frac{-f_{1,-1}}{\tau(E)} + \sin \mu \frac{-f_{1,0}}{\tau(E)} \\ v' \left[ \frac{\partial(f_{0,0})}{\partial z} - \mathcal{E}_z \frac{\partial(f_{0,0})}{\partial E} \right] & = -\sin \mu \frac{-f_{1,-1}}{\tau(E)} + \cos \mu \frac{-f_{1,0}}{\tau(E)} \end{aligned} \quad (5)$$

where  $\mathcal{E}$  is the magnitude of the electric field and  $v'(E) = \frac{v(E)}{\sqrt{3}}$ .

### Numerics

#### Boundary Conditions

To solve the discretized problem we need to impose physically consistent boundary conditions. For ohmic contacts we assume that the isotropic part of the distribution,  $f_{0,0}$ , is Maxwellian; otherwise we assume a boundary condition which ensures that the current normal to the boundary is zero, but the distribution itself at the boundary is not explicitly constrained.

#### Self-Consistent Solution

We obtain a self-consistent solution by using a decoupled Gummel type iteration between Poisson's equation and the Boltzmann equation. Specifically, the electron

concentration obtained from the Boltzmann equation solution is used to solve the non-linear Poisson equation, and the electric field obtained from this is in turn used in the Boltzmann equation. We have usually achieved convergence in approximately ten iterations.

#### Matrix Solution

In two real space dimensions, the matrix problem is equivalent to solving a three dimensional problem. When the problem size is less than 10,000 or so unknowns, direct sparse matrix solution is feasible but for much larger problems we use an iterative solver. Both preconditioned GMRES and CGS yield acceptable results, converging in about 150 iterations. For the preconditioner we use the matrix formed when only the energy coupling is considered. Thus only a block diagonal matrix needs to be factored to form the preconditioner, which can be done quite efficiently.

### Simulation Results

A simple test to check if the coordinate rotation approach works as expected is to use this method to simulate flow in a resistive structure as shown in Fig. 3. Here the potential and the electron concentration at the two contacts is fixed, and a boundary condition enforcing no normal current flow is imposed elsewhere. Fig. 4 shows the results obtained from a structure which mimics the channel region of a MOSFET with a factor of 10 change in the doping concentration.

### Conclusions

The work reported in this paper has demonstrated:

1. Self-consistent simulations of the Boltzmann and Poisson equations using a Gummel type iteration scheme.
2. Successful implementation of ohmic contacts and no normal current boundaries.
3. The effectiveness of a rotated momentum space coordinate system in reducing the off-diagonal coefficients.
4. Simulation of two-dimensional structures.
5. Use of an iterative sparse matrix solver with a preconditioner.

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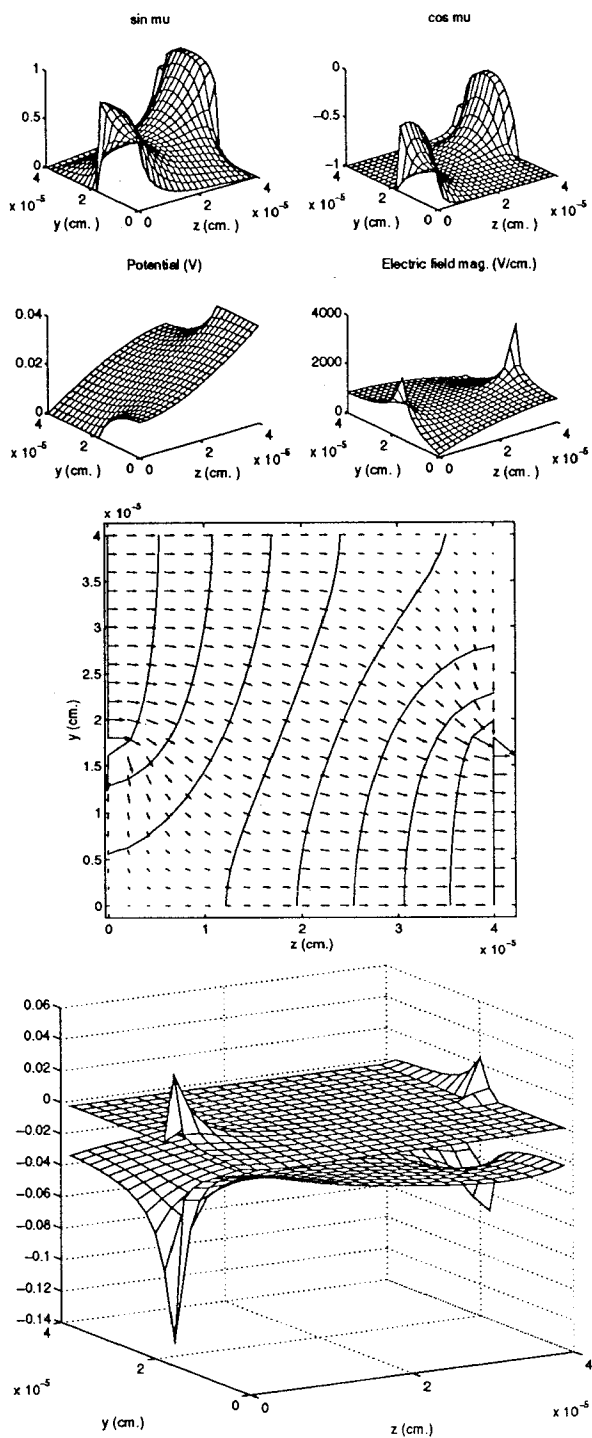


Figure 3: In the top figure the sine and the cosine of the rotation angle, the electric potential and the electric field are shown for a resistive structure. In the center the current flow lines and the equipotentials are shown for the same structure. The bottom plot shows the harmonic coefficients  $f_{1,0}$  and  $f_{1,-1}$  at an energy of 50meV. Note that  $f_{1,-1}$  is zero almost everywhere except at the contact corners, even though the current has significant components in both directions.

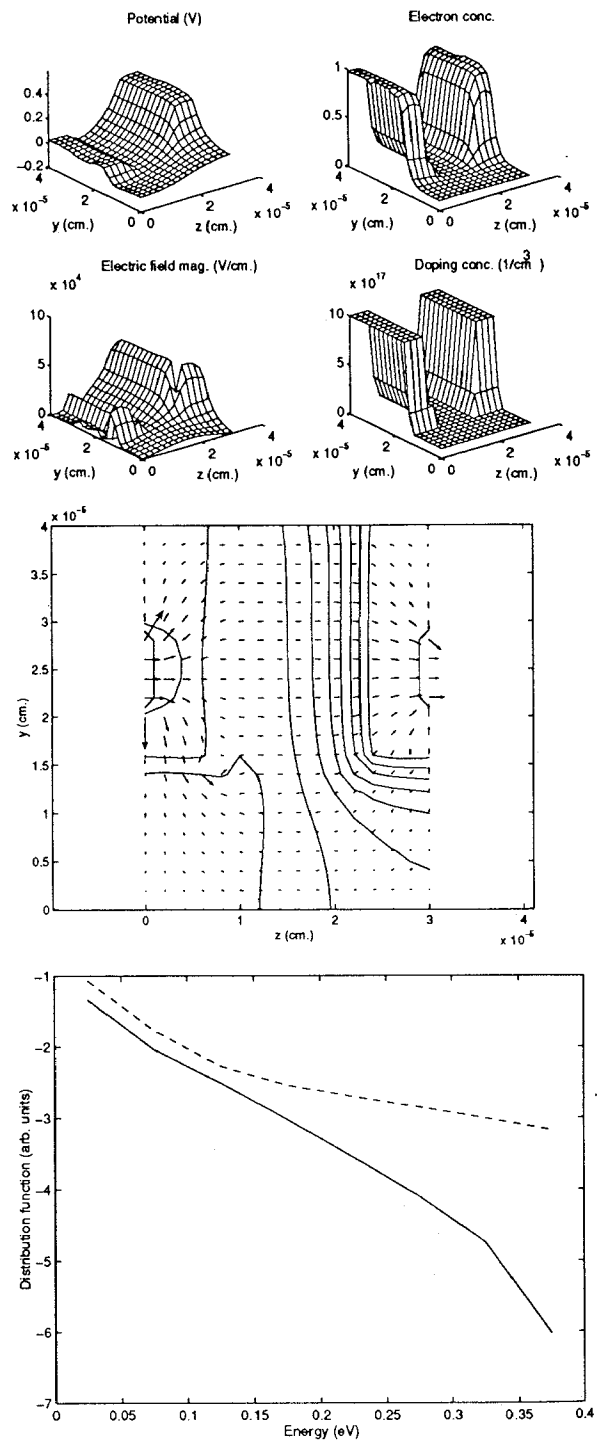


Figure 4: In the top figure the the electric potential, the electron concentration (normalized by  $1.0 \times 10^{18}$ ), the electric field and the doping profile are shown for a two dimensional structure which mimics the flow near the surface of a MOSFET. In the middle figure the current flow lines and the equipotentials are shown for the same structure. The bottom plot shows the  $f_{0,0}$  spherical harmonic coefficient as a function of energy at  $(z=0.12 \mu\text{m}, y=0.22 \mu\text{m})$  solid, and  $(z=0.22 \mu\text{m}, y=0.22 \mu\text{m})$ , dash.

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