2-Dimensional Solution to the Boltzmann Transport Equation to Arbitrarily High-Order Accuracy

Ken Hennacy, Neil Goldsman and I.D. Mayergoyz

Department of Electrical Engineering,
University of Maryland,
College Park, MD 20742

Abstract

In this work, we present a general 2-dimensional spherical harmonic formulation of Boltzmann's transport equation. Until recently, numerical implementation of this approach has been discussed for either 1-dimensional geometries, or only a few of the spherical harmonics [1, 2]. In this paper, a formulation is presented that includes an arbitrary number of spherical harmonics.

I. Introduction

Device modeling by direct solution to the Boltzmann transport equation is usually not performed because of dimensionality problems and difficulties in evaluating the collision integral. To directly account for 2-dimensional device operation with the Boltzmann equation, we would normally have to perform calculations in 5 dimensions (2 dimensions in real-space and 3 dimensions in momentum-space). To overcome this 'curse of dimensionality' a new approach to solve the BTE in device models is being developed which uses a spherical harmonic (SH) or a Legendre polynomial expansion.

II. Indefinite Spherical Harmonics Expansion

One of the reasons why we are interested in this method is that it gives us the ability to produce differential-difference operators for the evaluation of the collision integral to all orders in the expansion. Finding expressions for the rest of the BTE operators, however, involves some work. To solve the 2-D BTE to high-order accuracy, the distribution function is expressed in terms of an infinite spherical harmonic expansion with unknown coefficients that depend on energy and position:

$$f(\mathbf{r},\mathbf{k}) = \sum_{lm} f_l^m(\mathbf{r},\varepsilon) Y_l^m(\theta,\phi) \tag{1}$$

$Y_l^m(\theta,\phi)$ are the spherical harmonics[3]; $f_l^m(\mathbf{r},\varepsilon)$ are the coefficients which are to be determined; $l = 0, 1, 2, ...$; and for each l, the superscript $m = -l, -l+1, ..., 0, ...l-1, l$.

The spherical harmonics give the angular dependence of the distribution function in momentum space, and the coefficients provide its magnitude. The SH-numerical formulation allows us to account for the angular dependence of the distribution function in momentum space (θ,ϕ) analytically, thereby reducing the dimensionality of our calculations from 5 to 3.

III. SH Formulation to Arbitrarily High Order Accuracy

The objective is now to determine the unknown coefficients $f_l^m(\mathbf{r},\varepsilon)$, which can be used to construct the distribution function. Furthermore, to minimize the possibility of truncation errors in the SH approach, we have developed a technique to determine the coefficients to arbitrarily high order. The basic idea behind the approach is to automatically generate a system of equations for all the unknown SH coefficients $f_l^m(\mathbf{r},\varepsilon)$, and then solve the system and construct the distribution function using the above summation.

To generate this set of equations, we first substitute the above summation into the BTE. Next, we project the BTE onto each of the SH basis functions. The projection onto the $l,m'th$ SH basis function, which yields an equation for the $l,m'th$ coefficient, is illustrated by the following operation,

$$\int d\Omega Y_l^{m*}(\theta,\phi)\left\{\left(\frac{1}{\hbar}\nabla_k\varepsilon\cdot\nabla_r-\frac{e}{\hbar}E(\mathbf{r})\cdot\nabla_k-\left[\frac{\partial}{\partial t}\right]_c\right)f_l^m(\mathbf{r},\varepsilon)Y_l^m(\theta,\phi)\right\}=0\ .$$

By performing a similar projection onto each of the SH basis functions, the angular dependence of the distribution function is integrated out, and an infinite system of coupled equations is generated for the unknown coefficients.

In principle, this set of projections could be performed as is, leaving a system of differential-difference-integral equations for the unknown coefficients $f_l^m(\mathbf{r},\varepsilon)$. However, the initial substitution of the SH expansion into the various terms of the BTE gives rise to many nonlinear products of SH basis functions. Projecting these nonlinear products by performing the indicated integrations would become unwieldy. Furthermore, since an infinite SH expansion is present, each equation would contain an infinite number of terms, and each equation would therefore be directly coupled to all the other generated equations.

To simplify the system, we take advantage of the SH recurrence relations[3]. These relations allow us to re-express all nonlinear products of SH basis functions in terms of linear combinations. Once each term in the BTE is expressed as a linear combination, we can take advantage of the orthogonality of spherical harmonics and easily perform the projections indicated by Eqn. (2).

IV. Generalized System of SH Equations

After using recursion and performing the indicated integrations, we obtain the remarkable result that almost all of the infinite terms in each equation vanish identically due to orthogonality. Furthermore, we find that the coupling between equations is only through neighbors. Another extremely useful result is that each equation has an identical form. The system can therefore be automatically generated to arbitrarily high order and then be solved numerically. The equation for the l,m SH coefficient is given below. The equation for any of the other SH coefficients is obtained by appropriately changing the value of the indices l,m to other allowed integers:

$$\left\{\sum_{i=1}^{2} v(\varepsilon)\left[\frac{\partial}{\partial x_i} - eE_i\left(\frac{\partial}{\partial \varepsilon} - \frac{l-1}{2}\frac{\gamma'}{\gamma}\right)\right]\hat{a}_i^+ + v(\varepsilon)\left[\frac{\partial}{\partial x_i} - eE_i\left(\frac{\partial}{\partial \varepsilon} + \frac{l+2}{2}\frac{\gamma'}{\gamma}\right)\right]\hat{a}_i^-\right\} f_l^m$$

$$= \left[\frac{\partial f_l^m}{\partial t}\right]_c \tag{2}$$

where $v(\varepsilon) = \frac{\sqrt{2m\gamma}}{m\gamma'}$, $\gamma' = d\gamma/d\varepsilon$, and γ represents the dispersion relation; the sum is over the 2 directions in the $x - z$ plane; and the operators $\hat{a}$ have been defined as,

$$\hat{a}_1^- f_l^m \equiv \frac{1}{2}\left\{-\alpha_{l-1}^m \alpha_l^m f_{l-1}^{m-1} + \alpha_{l-1}^{-m} \alpha_l^{-m} f_{l-1}^{m+1}\right\} \tag{3}$$

$$\hat{a}_1^+ f_l^m \equiv \frac{1}{2}\left\{\alpha_{l+1}^{-m+1} \alpha_l^{-m+1} f_{l+1}^{m-1} - \alpha_{l+1}^{m+1} \alpha_l^{m+1} f_{l+1}^{m+1}\right\} \tag{4}$$

$$\hat{a}_3^- f_l^m \equiv \alpha_{l-1}^{-m+1} \alpha_l^m f_{l-1}^m \tag{5}$$

$$\hat{a}_3^+ f_l^m \equiv \alpha_{l+1}^m \alpha_l^{-m+1} f_{l+1}^m \tag{6}$$

where $\alpha_l^m \equiv \sqrt{\frac{l+m}{2l+1}}$. Due to the need to consider self-consistent boundary conditions in multi-dimensional problems, it is necessary to produce a set of 2nd order equations from this set of 1st order equations. Before doing this, however, it is possible to eliminate mixed partial derivative operators such as $\frac{\partial^2}{\partial\varepsilon\partial x_i}$ that would occur from such a substitution procedure by introducing the guage transformation,

$$\varepsilon \rightarrow \varepsilon' - e\phi(\vec{x}) \equiv H \tag{7}$$

as discussed in Ref. [2]. Here, the effect of the transformation is to produce the same set of equations as Eqn. (2) except that now, the energy derivatives are no longer present. This is because the derivatives with respect to position now have a new meaning, i.e. they are evaluated for fixed values of H.

V. Results

We have solved this generalized system for the 2-D space-independent case. This system is truncated, discretized and solved numerically. Solving the space independent BTE to 10 orders requires less than a minute of CPU time on a Sun4 work-station. Fig. 1 shows the SH coefficients coresponding to $l = 0, 2, 4$ for a $100\frac{kV}{cm}$ electric field 45 degrees from the p_3 axis in the 111 direction. Fig. 2 shows a comparison of this result with the case of the electric field in the direction of the p_3 axis. The purpose is to demonstrate how different SH coefficients become important to resolve the 2-dimensional angular dependence of the distribution function. Calculation of the isotropic coefficient remains the same, while the magnitude of higher order coefficients change in response to the changing values of the spherical harmonics. It is believed that some numerical error is present at low energy for the higher order coefficients as it was expected that the shapes of the coefficients of the same order in l should be the same.

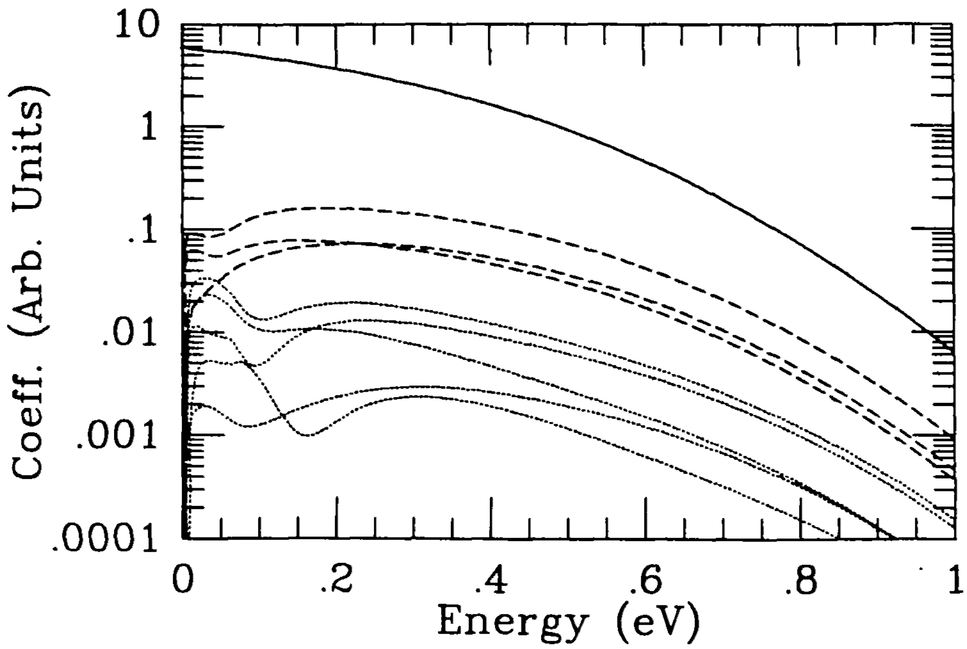

Fig. 1. SH Coefficients corresponding to l=0,2,4 for a 100 kV/cm electric field in the 111 direction.

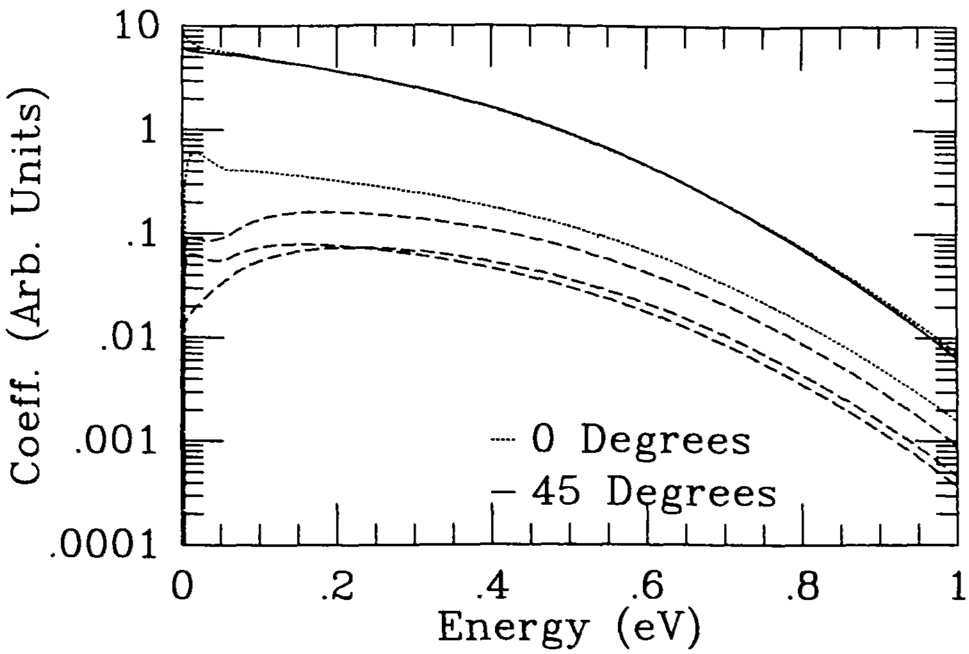

Fig. 2. A comparison of SH coefficients calculated for two different field orientations.

VI. Summary

We have developed a new method for solving the BTE for 2-dimensional geometries. The method reduces the dimensionality of the problem from 5 to 3. Theoretically, the orientation of the coordinate system should not affect the calculation of the distribution function, however in practice with the direct method, a small numerical difference is noticed.

References

[1] K. A. Hennacy and N. Goldsman, "A Generalized Legendre Polynomial/Sparse Matrix Approach for Determining the Distribution Function in Non-Polar Semiconductors." 1993.

[2] D. Ventura, A. Gnudi, G. Baccarani, and F. Odeh, "Multidimensional Spherical Harmonics Expansion Of Boltzmann Equation For Transport In Semiconductors," *Appl. Math. Lett.*, vol. 5, 1992.

[3] G. B. Arfken, *Mathematical Methods for Physicists.* New York: Academic Press, 1966.

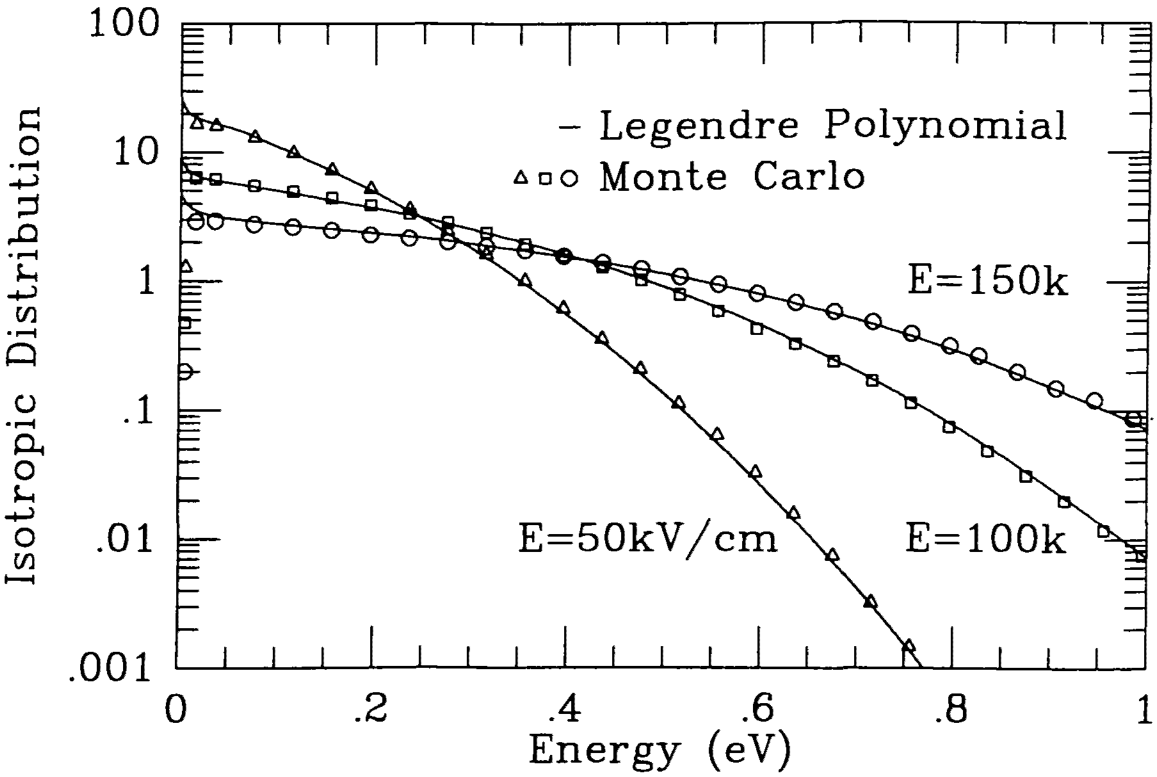

Fig. 3. Isotropic coefficient f_0 for different homogeneous applied electric fields. Comparison of the LP calculation with the Monte Carlo method was excellent up to energies higher than 2eV.