ANALYSIS OF CARRIER TRANSPORT IN SEMICONDUCTORS WITH INFINITE SERIES EXPANSION OF THE MOMENTUM DISTRIBUTION FUNCTION

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ABSTRACT

The main objective of this study is to generalize recent work on the Legendre polynomial expansion method of solving Boltzmann's Transport Equation (BTE) in semiconductors [1,2,3,4,5,6]. With this generalization, we extend the typical first or second order approaches to solving the BTE to include an arbitrary number of Legendre polynomials. The generalization is accomplished by using recurrance relations to automatically generate a quasi-infinite system of equations from the original BTE. The system is them solved for the quasi-infinite unknown Legendre coefficients to obtain the distribution function to arbitrary Legendre order. The Legendre polynomial (LP) expansion method for solving the BTE has the advantage that much of the work can be performed analytically, thus requiring much less computation type than the Monte Carlo method. In this paper, we introduce the methodology of the LP expansion, and discuss the results for applied homogeneous static and time dependent fields.

I. Introduction

To solve the Boltzmann equation to arbitrary Legendre order, we begin by writing the BTE in 1 space dimension:

$$\frac{\partial f}{\partial t} + v_{\parallel}\frac{\partial f}{\partial x_{\parallel}} + qE\frac{\partial f}{\partial p_{\parallel}} = \left[\frac{\partial f}{\partial t}\right]_c \tag{1}$$

where $f = f(t, x_{\parallel}, \vec{p})$ is the distribution function, and $a_{\parallel}$ designates the component of $\vec{a}$ parallel to the applied field (where $a = x, v, p$). (In writing this equation, we have assumed that the applied field always points in the same direction, and the variation of the field is in only one dimension.) With this equation, it can be shown that the distribution function can be written in terms of the following infinite LP expansion:

$$f(t, x_{\parallel}, \vec{p}) = \sum_{n=0}^{\infty} f_n(t, x_{\parallel}, p)P_n(\chi) \tag{2}$$

In the above expression, $P_n(\chi)$ are the known basis functions of the LP expansion; and $\chi \equiv cos\theta$, where θ is chosen to represent the direction of the carrier momentum with respect to the applied electric field; f_n represent the unknown coefficients of the basis functions, which depend on $t, x_{\parallel}$, and on the magnitude of the carrier momentum only. The dependence of the distribution function on the momentum's direction is given by the LP basis functions.

The objective is to solve the BTE by determining the coefficients f_n of the LP expansion. Once the coefficients are ascertained, they can be substituted into Eqn. (2) to determine the distribution function. Since an infinite number of unknown coefficients f_n have been introduced, the orthogonality property of Legendre polynomials is utilized to generate an infinite number of equations to determine the unknown coefficients. The equation corresponding to the nth coefficient, for example, is the following:

$$\int_{-1}^{1} d(cos\theta)P_n(cos\theta)\left\{\frac{\partial f}{\partial t} + v_{\parallel}\frac{\partial f}{\partial x_{\parallel}} + qE\frac{\partial f}{\partial p_{\parallel}} - \left[\frac{\partial f}{\partial t}\right]_c\right\} = 0 \tag{3}$$

In order to generate this equation explicitly, one has to express the operators in Boltzmann's equation in terms of Legendre polynomials. The next section shows how this is done.

II. Operators in terms of Legendre Polynomial Basis

Time Operator: To begin with, the time operator, $\frac{\partial}{\partial t}$ acts only on the coefficients f_n, hence no further reduction into the LP basis elements is necessary. The time derivative of the distribution function can therefore be expressed directly as

$$\frac{\partial f(t,\vec{x},\vec{p})}{\partial t} = \sum_{n=0}^{\infty} P_n(\chi)\frac{\partial f_n(t,\vec{x},p)}{\partial t} \tag{4}$$

Momentum Operator: In contrast to the time operator, expressing the momentum operator is more complicated. This is because the effect of the derivative operator $\frac{\partial}{\partial p_{\parallel}}$ on the LP elements will interfere with their linear independence. Thus, we must represent the momentum operator such that it preserves the integrity of the individual Legendre polynomials.

It can be shown that the momentum operator takes the following form:

$$\frac{\partial f}{\partial p_{\parallel}} = \sum_{n=0}^{\infty} \frac{\partial f_n}{\partial p}\chi P_n(\chi) + \frac{f_n}{p}(1-\chi^2)\frac{\partial P_n}{\partial \chi} \tag{5}$$

Then, to re-express this operator in terms of the original basis elements, we enlist the help of the following well known recurrance relations for Legendre polynomials [7]:

$$\begin{aligned} \chi P_n(\chi) &= \alpha_n P_{n+1}(\chi) + \frac{n}{n+1}\alpha_n P_{n-1}(\chi) \\ (1-\chi^2)\frac{dP_n(\chi)}{d\chi} &= -n\chi P_n(\chi) + nP_{n-1}(\chi) \end{aligned} \tag{6}$$

where we have introduced the notation $\alpha_n = \frac{n+1}{2n+1}$.

Upon substitution of the above recurrance relations into Eqn. (5), and some re-arrangement of terms under the summation, we arrive at the following expression for the momentum operator:

$$qE\frac{\partial f}{\partial p_{\parallel}} = qE\sum_{n=0}^{\infty}\left[\left(\frac{\partial}{\partial p} - \frac{n-1}{p}\right)\alpha_{n-1}f_{n-1} + \left(\frac{n+1}{n+2}\frac{\partial}{\partial p} + \frac{n+1}{p}\right)\alpha_{n+1}f_{n+1}\right]P_n(\chi) \tag{7}$$

Velocity-Displacement Operator: Formulation of this operator is straightforward once the following form is recognized:

$$v_{\parallel}\frac{\partial f}{\partial x_{\parallel}} = v(p)\sum_{n=0}^{\infty}\frac{\partial f_n}{\partial x_{\parallel}}\chi P_n(\chi) \tag{8}$$

Upon using the recurrence relation in (6), the following expression for the velocity-displacement operator can be obtained:

$$v_{\parallel}\frac{\partial f}{\partial x_{\parallel}} = v(p)\sum_{n=0}^{\infty}\left[\alpha_{n-1}\frac{\partial f_{n-1}}{\partial x_{\parallel}} + \frac{n+1}{n+2}\alpha_{n+1}\frac{\partial f_{n+1}}{\partial x_{\parallel}}\right]P_n \tag{9}$$

Collision Operators: Generally, the collision operator representation in the LP basis is obtained by performing the following integration:

$$\left[\frac{\partial f_n}{\partial t}\right]_c = \frac{2n+1}{2}\int_{-1}^{1} d(cos\theta)\left[\frac{\partial f}{\partial t}\right]_c P_n(cos\theta) \tag{10}$$

Here, we have explicitly utilized the orthogonality of the Legendre polynomials to generate the terms for the individual coefficients. This integration can be performed either numerically, or analytically, depending on the complexity of the collision expression involved.

III. Total Boltzmann Equation in LP Basis

Putting the various operators together, and using the orthogonality of the Legendre polynomials, an infinite set of equations is obtained. The interesting result is that all the equations have identical form, and can thus be generated automatically. The equation for the n'th coefficient, f_n, is given by

$$\frac{\partial f_n}{\partial t} + \left[v(p)\frac{\partial}{\partial x_{\|}} + qE\left(\frac{\partial}{\partial p} - \frac{(n-1)}{p}\right)\right]\alpha_{n-1}f_{n-1} + \left[\frac{n+1}{n+2}v(p)\frac{\partial}{\partial x_{\|}} + qE\left(\frac{n+1}{n+2}\frac{\partial}{\partial p} + \frac{(n+1)}{p}\right)\right]\alpha_{n+1}f_{n+1} = \left[\frac{\partial f_n}{\partial t}\right]_c \quad (n>0) \quad (11)$$

IV. Relationship of LP Coefficients to Hydrodynamic Model

In addition to providing the complete distribution function, the LP approach can be useful for evaluating the the hydrodynamic approach to device modeling. In the hydrodynamic method, the focus is not on determining the distribution function, but rather, on determining statistical averages which have physical significance. The LP approach can be used to calculate statistical averages for comparison with hydrodynamic models. From the orthogonality property of Legendre polynomials, it is easily demonstrated that the carrier concentration and average energy depend only on f_0, where as the drift velocity depends only on f_1. Other hydrodynamic quantities are not as simple such as electron temperature and heat flow which depend on f_0 and f_2, and f_1 and f_3, respectively.

Thus, the moments which are usually sought in hydrodynamic calculations depend only on the lowest order coefficients. Hence, it can be said that most quantities of physical interest to hydrodynamic formulations depend on specific symmetry properties of the momentum distribution function. Furthermore, the relative importance of various hydrodynamic quantities can be investigated by examining the magnitude of specific Legendre coefficients.

V. Results

The BTE was solved using the infinite series method for the homogeneous and time-dependent cases. All calculations were for silicon and included the effect of a multivalley, nonparabolic band structure, intervalley phonons and acoustic phonons. The transport model used is identical to the one employed in standard MC calculations[8]. Fig. 1 shows values for the isotropic part of the distribution function calculated using the presented technique are in excellent agreement with MC calculations. Fig. 2 shows the distribution function for a homogeneous 100kV/cm electric field, obtained with a 40th order solution to the BTE. It is interesting to note that at low electron energy the distribution function is strongly peaked in the direction of the field, but at high energy the distribution is essentially isotropic. Fig. 3 shows the f_0, f_2, f_5, f_{10}, f_{15} and f_{20} coefficients of the LP expansion. In Fig. 4 time-dependent values for average electron energy and velocity are calculated with a 20th order solution to the time-dependent BTE are shown.

VI. Conclusion

We have developed a new method for analyzing carrier transport by solving the Boltzmann transport equation. With this method, we represent the distribution function in terms of a LP expansion to arbitrarily high order. An infinite system of equations can be automatically generated from the original BTE using LP recurrence relations. The set of equations can easily be solved using numerical sparse matrix algebra for the coefficients of the infinite LP expansion. Once the coefficients are obtained, the distribution function is calculated. We found that there is excellent agreement between the Monte Carlo method and the infinite LP expansion technique, while requiring approximately 1/100 the CPU time to evaluate. Values for the distribution function using as many forty Legendre polynomials are readily determined, requiring only 5 minutes on a Sun 3/60 workstation to calculate. Finally, it is worth noting that, while we have only shown application of the method for the homogeneous, steady-state case, the new method lends itself well to space and time-dependent situations.

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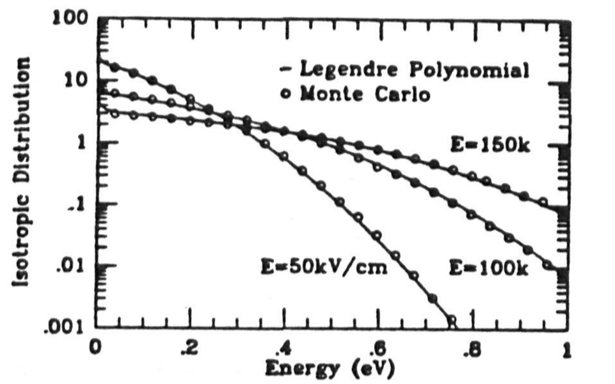

Fig. 1: Comparison of the isotropic distributions f_o obtained from the Monte Carlo and P_n method for 3 fields.

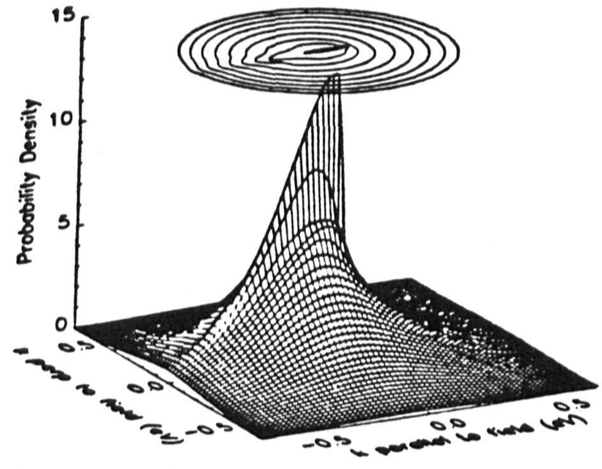

Fig. 2: The total $k - space$ distribution for the $100\frac{kV}{cm}$ case.

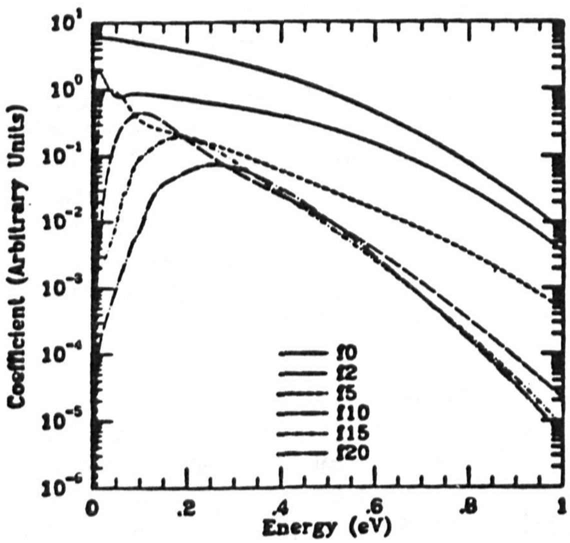

Fig. 3: Selected P_n coefficients determined by Legendre Polynomial method to 40th order for the $E = 100\frac{kV}{cm}$ case.

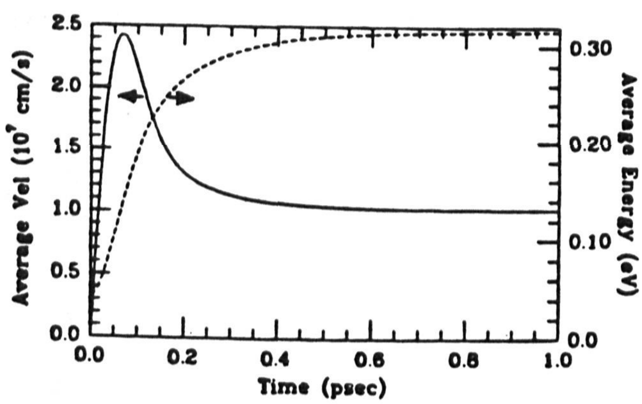

Fig. 4: Average Energy and velocity versus time for $100\frac{kV}{cm}$ step function