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A Galerkin Method for the Arbitrary Order Expansion in Momentum Space of the Boltzmann Equation using Spherical Harmonics

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Abstract

We have implemented a Galerkin method for the solution of the Boltzmann equation which allows arbitrary order spherical harmonic expansions in momentum space. The implementation of the method in one real space dimension shows the importance of including harmonics beyond first order to accurately calculate the distribution function in high field regions.

I Introduction

An approach to solving the Boltzmann equation using the basis function expansion for the distribution in momentum space was first proposed in [1]. As this was done for the homogeneous real space case, the problem was considerably simplified and only needed discretization in energy (momentum) space. More recent work in [2] has extended this idea to the inhomogeneous real space problem. In the method in [2], the distribution function is written as a sum of spherical harmonics at each point in real space, and this expansion is substituted into the Boltzmann equation. A set of coupled partial differential equations is then derived by matching coefficients of the spherical harmonics. Finally, this set of partial differential equations along with Poisson's equation is discretized to solve the problem. One difficulty with such an approach is that the order of the expansion is fixed *a priori*, and the set of partial differential equations is determined by the order. If a higher order solution is needed then a new expansion and discretization must be done and therefore it is difficult to extend the method to arbitrary order. To overcome this difficulty, we propose a Galerkin method in this paper which allows arbitrary order expansion.

II A Galerkin Method for Arbitrary Order Expansion

As in [2] we expand the distribution function in spherical harmonics:

$$f(\mathbf{r},\mathbf{k}) = \sum_{lm} f_{lm}(\mathbf{r},k)\, Y_{lm}(\theta,\phi) \tag{1}$$

Substituting the spherical harmonic expansion into the Boltzmann equation, multiplying by the conjugate spherical harmonic and integrating over a sphere in k-space yields:

$$\int Y^*_{l'm'}(\theta,\phi)\,\mathbf{v}(\mathbf{k})\cdot\frac{\partial}{\partial\mathbf{r}}\sum_{lm} f_{lm}(\mathbf{r},k)Y_{lm}(\theta,\phi)d\Omega - \int Y^*_{l'm'}(\theta,\phi)\frac{q\mathbf{F}(\mathbf{r})}{\hbar}\cdot\frac{\partial}{\partial\mathbf{k}}\sum_{lm} f_{lm}(\mathbf{r},k)Y_{lm}(\theta,\phi)d\Omega$$
$$= \int Y^*_{l'm'}(\theta,\phi)\;\mathcal{S}\left(\sum_{lm} f_{lm}(\mathbf{r},k)Y_{lm}(\theta,\phi)\right)d\Omega \quad (2)$$

where $\mathcal{S}$ denotes the scattering operator, $\mathbf{v}(\mathbf{k})$ is the electron velocity and $\mathbf{F}(\mathbf{r})$ is the electric field. For brevity, the expansion above will be written out only for the first term, assuming parabolic bands, and in one real space dimension, z. A two point approximation for the space derivative is:

$$\frac{\partial}{\partial z}f_{lm}(z,k) \approx \frac{f^{i+1,j}_{lm} - f^{i,j}_{lm}}{\Delta z} \quad (3)$$

where the i index denotes discretization in space and the j index denotes discretization in energy. The first term of the BTE can then be written as

$$v^j \sum_{lm} \frac{f^{i+1,j}_{lm} - f^{i,j}_{lm}}{\Delta z} G_{l'm';lm} \quad (4)$$

where v^j is the magnitude of the velocity vector and the the matrix elements $G_{l'm';lm}$ and $H_{l'm';lm}$ are given by

$$G_{l'm';lm} = \int_0^{2\pi}\int_0^{\pi} Y^*_{l'm'}(\theta,\phi)Y_{lm}(\theta,\phi)\cos\theta\,\sin\theta\,d\theta\,d\phi$$
$$H_{l'm';lm} = \int_0^{2\pi}\int_0^{\pi} Y^*_{l'm'}(\theta,\phi)\frac{\partial Y_{lm}(\theta,\phi)}{\partial\theta}\sin\theta\,\sin\theta\,d\theta\,d\phi\,. \quad (5)$$

This procedure is repeated for each term in the expansion, leading to the matrix equation, shown below, for the f_{lm}. First some notation is introduced to simplify the final form:

$$G^{i,j}_1 = (-c^{i,j} + a^{i,j})\,G + b^{i,j}\,H, \quad G^{i,j}_2 = c^{i,j}\,G, \quad G^{i,j}_3 = -a^{i,j}\,G$$
$$a^{i,j} = \frac{qF^i}{\Delta E}v^j, \quad b^{i,j} = \frac{qF^i}{2E^j}v^j, \quad c^{i,j} = \frac{v^j}{\Delta z}.$$

$$\begin{bmatrix} \ddots & \ddots & & \ddots & & & 0 \\ & G^{i,j}_1 & G^{i,j}_2 & & G^{i,j}_3 & & \\ & & G^{i+1,j}_1 & G^{i+1,j}_2 & & G^{i+1,j}_3 & \\ & & & \ddots & \ddots & & \ddots \\ & & & & & & \\ & & & & & & \\ 0 & & & & 0 & & \end{bmatrix} \begin{bmatrix} \vdots \\ \alpha^{i,j} \\ \alpha^{i+1,j} \\ \vdots \\ \alpha^{i,j+1} \\ \alpha^{i+1,j+1} \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ 0 \\ 0 \\ \vdots \\ \\ \\ \end{bmatrix}$$

The above equation (after including the scattering terms and boundary conditions) can be solved for $\alpha^{i,j}$, the coefficient vector of spherical harmonics at a given point (i, j) in the energy-space mesh. The order of the expansion enters only through the block matrices G and H and the size of the vector α, otherwise the formulation is the same. G and H can be computed up to any desired order. Although we have assumed a particular form for the discrete approximation to the derivatives in space and energy, the development described above holds equally well for a different discrete approximation, the only change being that the non-zero blocks would be at a different position in the matrix.

III Implementation and Results

Currently parabolic bands are assumed and scattering by acoustic phonons, optical phonons and ionized impurities (Brooks-Herring model) is included. In one dimension in real space, due to the symmetry of the distribution about the electric field direction, the spherical harmonic expansion reduces to a Legendre polynomial expansion and no ϕ dependence is needed. Fig. 1 shows the computed spherical harmonics coefficients for an n^+nn^+ diode as a function of position at different energy values (separated by 25 meV). In Fig. 2 the distribution functions obtained using different orders of spherical harmonics are compared. Although the electron temperature obtained in the two cases are close, the current differs by about 8%. The actual discretization stencil used for the coefficients in space and energy is shown in Fig. 3. At the boundaries, f_0 is assumed to be a Maxwellian and f_2 and higher even order coefficients are set to zero; all odd order coefficients are computed for all points in real space. This discretization is not unconditionally stable and if the mesh is coarse or the doping step large then instabilities of the type shown in Fig. 3 can result.

IV Conclusion and Future Work

We have solved the Boltzmann equation self-consistently with Poisson's equation using a Galerkin method. The advantage of the Galerkin method is that a higher order expansion only increases the size of the matrix generated from the algebraic equations, whereas in earlier methods the set of coupled partial difference equations would need to be augmented and discretized anew. Another benefit of a Galerkin method is that it seamlessly allows the use of different order expansions in different space regions. Finally we show that including higher order harmonics can significantly alter the calculated distributions in the high field regions. Further work will focus on developing a more stable method of discretization and on using higher order approximations to the derivatives.

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References

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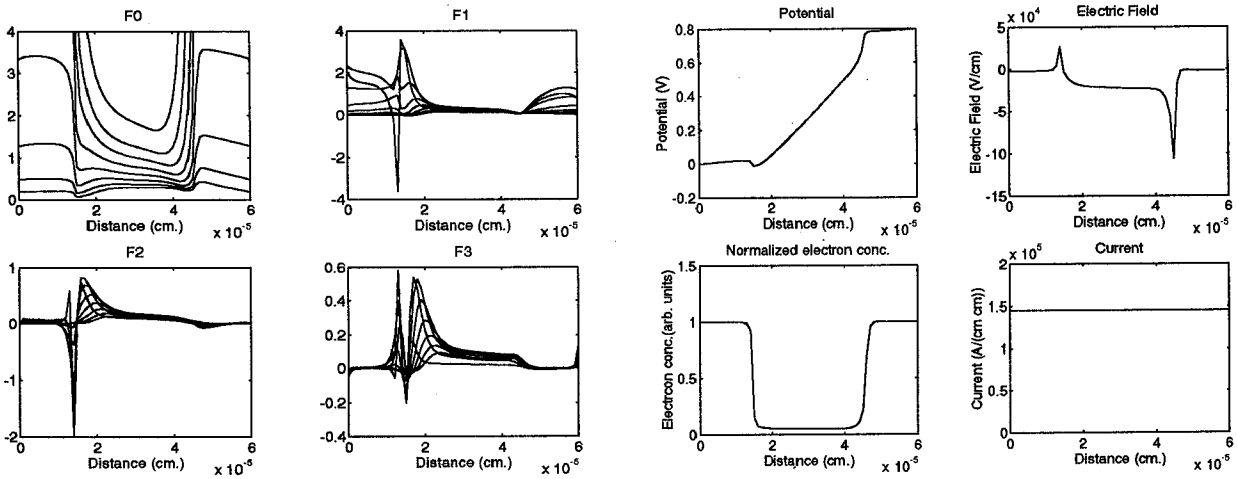

Figure 1: Spherical harmonic coefficients and Poisson equation solution for a 0.6 μm n^+nn^+ diode with a doping of $2 \times 10^{18} cm^{-3}$ and $1 \times 10^{17} cm^{-3}$ in the n^+ and n regions and a bias of $0.8V$.

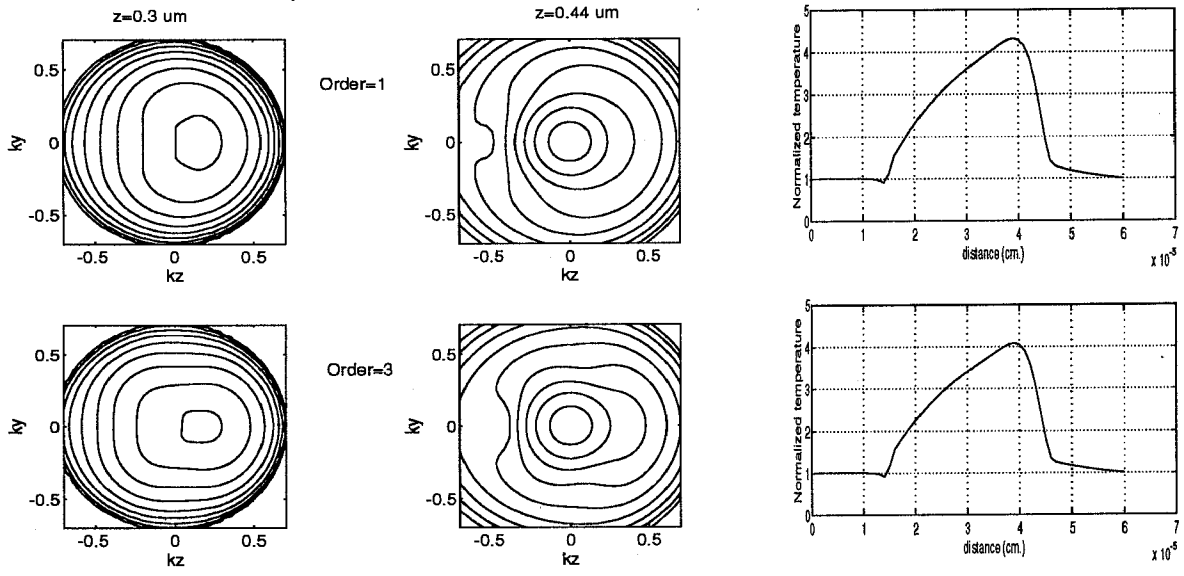

Figure 2: Contours of constant distribution function (separated by 3x) over a normalized k_z, k_y plane for the device of Fig. 1 up to the first and up to third order harmonic expansions at z=0.3 μm and z = 0.44 μm. On the right, the associated electron temperatures are shown.

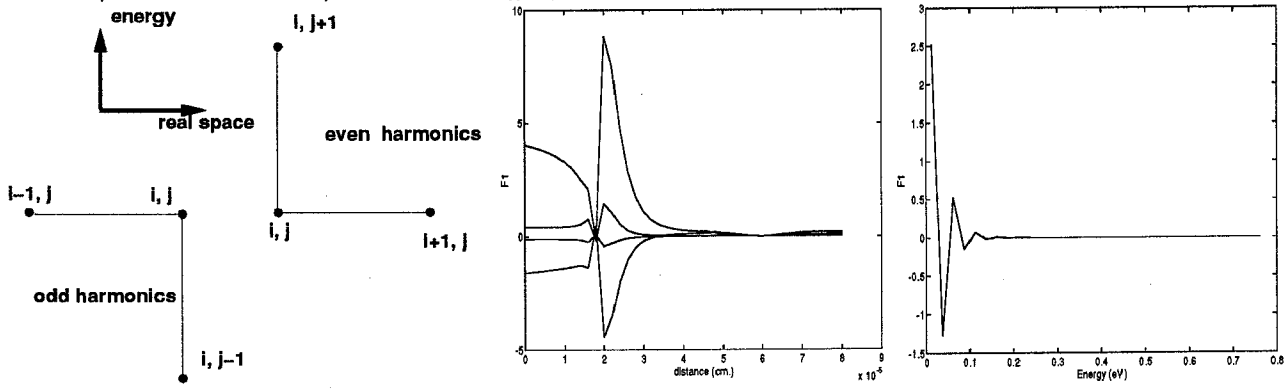

Figure 3: On the left is shown the discretization used for the coefficients and on the right the instability that can result if too coarse a mesh size is used in the spatial discretization.