

Inclusion of Electron-Electron Scattering in the Spherical Harmonics Expansion Treatment of the Boltzmann Transport Equation

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Abstract

A new methodology is proposed to include the short range electron-electron interaction in the Spherical Harmonics Expansion approach to the Boltzmann Transport Equation, in the frame of spherical and non-parabolic bands. The electron energy distribution is computed in the uniform field case, and large corrections in the high-energy tail are observed.

1. Introduction

Short-range electron-electron (e-e) scattering is currently thought to have a major influence on the high-energy part of the electron population in semiconductor devices. Its implementation is therefore almost mandatory in every model of carrier transport aimed at the investigation of typical hot-electron effects such as current multiplication factors due to impact ionization and gate oxide injection. It is well known that this mechanism has been found difficult to treat even in Monte Carlo (MC) simulators, due to the non-linearity of the effect and to the cumbersome integrals required to find the scattering rates.

The Spherical Harmonics Expansion (SHE) scheme [1, 2, 3] has been developed recently as an alternative to both moment-based solutions of the Boltzmann Transport Equation (BTE) and Monte Carlo simulators since it allows a deterministic approximate solution of the BTE by reducing the dimension of the argument of the unknown carrier density $f(\mathbf{r}, \mathbf{k})$.

The purpose of this work is that of incorporating the e-e scattering in the program described in [1], which deals with the homogeneous case and spherical symmetric bands, without introducing any simplifying assumptions on the scattering integral calculations other than those intrinsically involved in the SHE method.

2. The mathematical procedure

Consider the expression of the e-e scattering operator

$$-f(\mathbf{k}) \int S(\mathbf{k}, \mathbf{k}_0, \mathbf{k}', \mathbf{k}'_0) f(\mathbf{k}_0) d\mathbf{k}_0 d\mathbf{k}' d\mathbf{k}'_0 + \int S(\mathbf{k}', \mathbf{k}'_0, \mathbf{k}, \mathbf{k}_0) f(\mathbf{k}') f(\mathbf{k}'_0) d\mathbf{k}_0 d\mathbf{k}' d\mathbf{k}'_0 \quad (1)$$

with the scattering matrix (Born approximation)

$$S(\mathbf{k}, \mathbf{k}_o, \mathbf{k}', \mathbf{k}'_o) = c_{ee} \delta(\mathbf{k} + \mathbf{k}_o - \mathbf{k}' - \mathbf{k}'_o) \delta(E + E_o - E' - E'_o) \frac{1}{(\beta^2 + q^2)^2} \quad (2)$$

where \mathbf{k} and \mathbf{k}_o are the initial states of the two scattering electrons, the corresponding primed vectors are the final states, \mathbf{q} is defined as $\mathbf{q} = \mathbf{k} - \mathbf{k}'$, and β is the inverse screening length. The following procedure is adopted:

- 1) as requested by the SHE scheme $f(\mathbf{a})$ is expanded as $f_o(a) + f_1(a) \cos(\theta)$, where θ is the angle between \mathbf{a} and the reference axis, and the expansion is truncated at the second term;
- 2) the integration over $d\mathbf{k}'_o$ in the first integral and over $d\mathbf{k}_o$ in the second integral is performed by eliminating the momentum δ function;
- 3) the $d\mathbf{k}_o$ integral in the first term of (1) and the $d\mathbf{k}'_o$ integral in the second term are computed analytically in their angular parts using the energy δ function;
- 4) in both terms in (1) the angular part of the integral in $d\mathbf{k}'$ is performed analytically;
- 5) the remaining double integrals in $dk_o dk'$ for the first term, and $dk'_o dk'$ for the second term, are numerically computed.

The most peculiar part of this scheme is point 3) above. Actually, the energy δ function has usually been eliminated by an integration over the modulus of one of the \mathbf{k} vectors involved in (1). This choice brings about overwhelming mathematical complications when applied to a band shape other than parabolic, thus forcing a choice between using an oversimplified band shape which fails at high energies, and a fully numeric integration scheme. We have taken a different stance by integrating the energy δ function on the cosine of one of the angles involved in (1). For instance, in the first integral in (1) we can write

$$\begin{aligned} & \delta(E + E_o - E' - E'_o) = \\ & = \frac{\gamma'(E + E_o - E')}{2\sqrt{q^2\gamma(E_o)}} \delta\left(\cos(\widehat{\mathbf{k}_o\mathbf{q}}) - \frac{\gamma(E + E_o - E') - \gamma(E_o) - q^2}{2\sqrt{q^2\gamma(E_o)}}\right) \end{aligned} \quad (3)$$

where

$$\gamma(E(\mathbf{k})) \equiv k^2 \quad (4)$$

and γ' stands for the derivative of γ with respect to the energy. We proceed in an analogous way with the second integral in (1).

The non-linearities of quadratic type in the unknown density function are treated via an iterative method, where the density functions inside the integrals are frozen from the previous iteration step.

We stress the fact that no assumption on the band-shape other than spherical symmetry is required. In fact a set of non-parabolic bands is used in our simulations.

The procedure described above can partially be applied in the frame of the MC method. Since MC does not extract the angular dependence of f , we are left with double integrals in $dk_o dk'$ to be performed numerically in the computation of the total scattering rate.

3. Results

Figs. 1 and 2 show the results of the homogeneous SHE simulations for two different electric fields and various electron densities; β is set equal to the inverse Debye length. Even for low densities the significant effect of e-e scattering on the high-energy tail of the electron distribution is clearly seen. The effect is much less pronounced at electric fields higher than 300 kV/cm and lower than 30 kV/cm, since in this case the distribution is closer to a maxwellian shape.

Consider the expression (1) divided by $f(\mathbf{k})$. The zero order term of the SHE of such term describes the electron balance due to e-e scattering at a given energy, and represents an e-e effective scattering rate (ESR). Notice that such ESR is positive if the electron in-rate is larger than the electron out-rate. In Fig. 3 the positive part of the ESR is plotted for the same electric field and electron densities as for Fig. 1. The ESR for energies lower than 0.3 eV, not represented in the figure, is negative, reflecting the fact that cold electrons tend to be scattered to more energetic states. At larger energies one can note a very rapid growth of the ESR, which in the tail becomes comparable with the optical phonon scattering rate. This accounts for the major changes exhibited by the tail of the electron distribution in Figs. 1 and 2. It should be noticed that the increase of the ESR is related to the deviation of the distribution function from the maxwellian shape: a maxwellian distribution would result in a zero ESR.

The accuracy of the SHE method strictly depends on the fact that the coefficients of the expansion of the unknown distribution become negligible after a few terms. A comparison with MC data, where the e-e scattering was neglected, showed good agreement when two terms of the expansion were considered, and an excellent agreement with three terms [1]. Fig. 4 shows the ratio of the first two terms f_0 and f_1 for a 200 kV/cm field. It is apparent that f_1 loses much of its weight in the high-energy region, thus suggesting that the e-e scattering leads to a more spherical distribution. This makes us confident about the appropriateness of the truncation at the second term of the SHE.

4. Acknowledgments

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References

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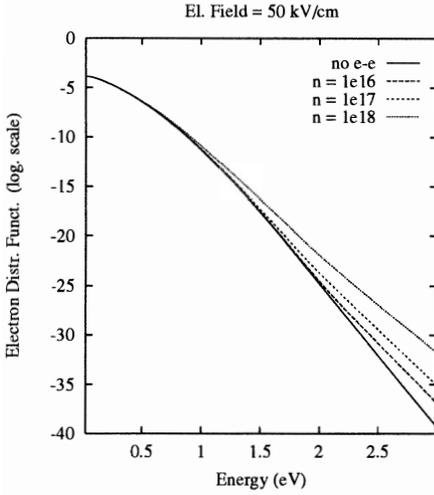


Figure 1: Electron distribution function for a 50 kV/cm electric field and various electron concentrations.

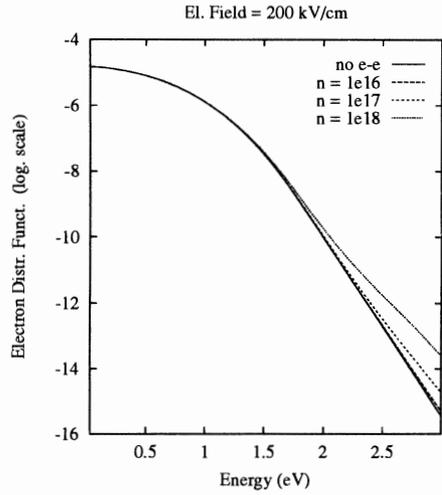


Figure 2: Electron distribution function for a 200 kV/cm electric field and various electron concentrations.

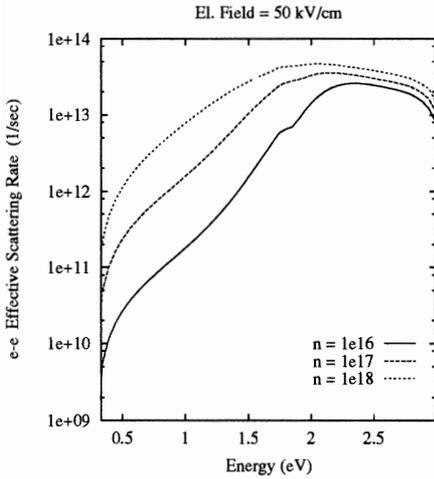


Figure 3: Short-range e-e effective scattering rate for various electron concentrations and a 50 kV/cm electric field.

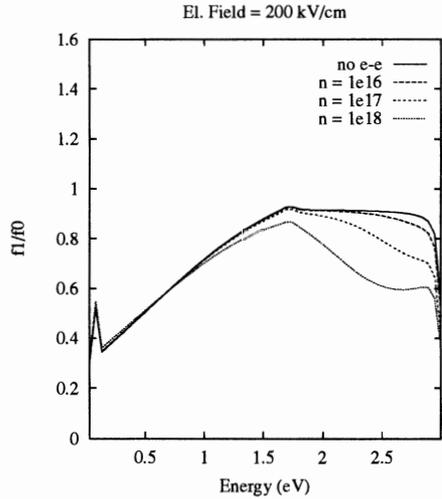


Figure 4: The ratio between the first two SHE components for various electron concentrations and for a 200 kV/cm electric field compared with the ratio obtained without e-e scattering.