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Electron-electron Collisions and Drift Velocity Fluctuations in n-GaAs at T=80 K

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Abstract: Modified combined scattering rate Monte Carlo technique is proposed. Electron collisions with phonons, impurities and among themselves are taken into account. The proposed technique avoids the short-time-step procedure inherent to conventional ensemble Monte Carlo method. All *N* modelled electrons move using the total probability for the scattering of each electron by the thermal bath and mutual scattering between electrons pairs ("events in the electron system"). The quantitative fitting to the available experimental data on the spectral density is achieved and the range of moderate fields is defined for interparticle collisions to manifest themselves in the noise. In the second part of the presented report a drift velocity correlator is investigated numerically by Monte Carlo simulation and for the fist time analytically by a phenomenological approach taking into account electron-phonon and electron-electron scattering between free carriers. The thermodynamic approach is investigated. The results of the velocity-to-velocity correlation functions and electron noise spectrum obtained analytically are in quite good agreement with those given by the Monte Carlo method.
Keywords: Monte Carlo, Electron-electron collisions, Drift velocity fluctuations, Spectral density.

1. Introduction

Fluctuations phenomena in semiconductors have been intensively investigated during the last three decades [1-3]. Fluctuation effects have been conventionally investigated without an account on the Coulomb electron-electron (e-e) scattering. However at sufficiently high electron densities, it is necessary to take into account e-e scattering to the total distribution function and related correlators.

Interparticle collisions though conserving energy and momentum of the electron system have an indirect effect on transport and – even more direct – on velocity correlations. In the presented report the 'combined scattering method' (CSR) Monte Carlo method [4] is used to interpret the results of microwave noise.

The important role of e-e collisions is demonstrated, and drift-velocity to drift-velocity cross-correlation under non-e1uilibrium conditions is calculated. In the second part drift velocity correlation functions are investigated analytically in a

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phenomenological approach and numerically through Monte Carlo simulation. Thermodynamic equilibrium state is investigated. Analytical results are in good agreement with those obtained by Monte Carlo method in the GaAs crystal.

2. Electron-electron collisions. Drift velocity fluctuations

It can be shown [4] that the "time of free flight" for independent scattering events of the N electron system with $\mathbf{k}_i$ wave-vectors is defined by the combined scattering rate:

$$\lambda_{comb}(\mathbf{k}_1, \mathbf{k}_2, ..., \mathbf{k}_N) = \sum_{i=1}^{N} \lambda_i(\mathbf{k}_i) + \frac{1}{N-1} \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \lambda_{ij}^{ee}(\mathbf{k}_i, \mathbf{k}_j), \quad (1)$$

where $\lambda_i(\mathbf{k}_i)$ and $\lambda_{ij}^{ee}(\mathbf{k}_i, \mathbf{k}_j)$ are conventional integral rates of scattering of the ith electron by the thermal bath and by the jth electron respectively [5]. Equation (1) reduces to that written down in [6] for N=2. All N electrons move without scattering for the "time of free flight of the system" between two successive events of an electron scattering by the thermal bath or mutual collision between two electrons occurs. The "time of free flight" is defined from the sum of the each electon scattering rate on the thermal bath and on the all remaining electrons. CSR technique avoids the short-time step procedure and a large electron number inherent to conventional ensemble MC simulation.
The time-displaced drift-velocity correlation function is

$$\Phi_{total} = N\overline{\delta v_d(t_1 + t)\delta v_d(t_1)} = \Phi_{auto} + \Phi_{cross}, \quad (2)$$

where the auto- and cross-correlation functions are defined as:

$$\Phi_{auto} = \overline{\frac{1}{N}\sum_i \delta v_i(t_1 + t)\delta v_i(t_1)}, \quad \Phi_{cross} = \overline{\frac{1}{N}\sum_{i \neq j} \delta v_i(t_1 + t)\delta v_j(t_1)}, \quad (3)$$

In order to demonstrate the effect of e-e collisions on fluctuations, the calculated velocity correlation functions in a heating electric field are shown in Figure 1 for the model corresponding to n-type GaAs with the impurity scattering neglected. In our case $\tau_{ee} \leq \tau_p$ strong cross-correlation appears. The equal-time cross-correlation also appears in non-equilibrium system as it was predicted in [1]. The auto-correlation decreases mainly in time τ_{ee}. The decay of Φ_{total} is caused by the electron interaction with thermostat. In thermodynamic equilibrium, when $\Phi_{cross}(0) = 0$, the latter is equal to $\Phi_{total}(0) = \Phi_{auto}(0) = \overline{V^2} = kT/m$.

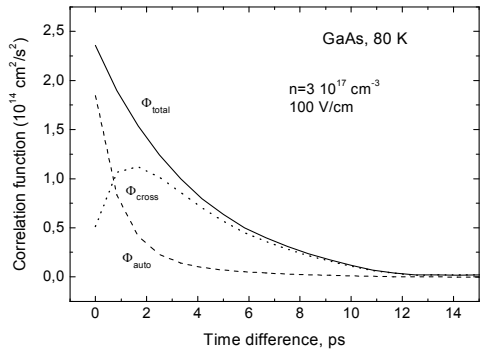

Fig. 1. Drift-velocity correlation functions: total (solid line), auto-correlation (dashed line) and cross-correlation (dotted line). Phonon and interelectron scattering is taken into account, impurity scattering is neglected

The results of the spectral density of drift velocity fluctuations are presented in Figure 2. The experimental data are obtained from the current fluctuations data through normalization at zero field by using mobility data and Nyquist formula [7]. One can see that the most pronounced effect is obtained at intermediate fields ranging from 5 V/cm to 500 V/cm

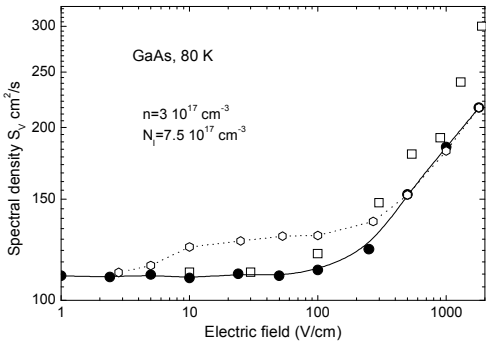

Fig. 2. Dependence of the spectral density of electron drift velocity fluctuations for compensated n-GaAs. MC with phonon, impurity and e-e scattering: (closed circles), without e-e scattering (diamonds). Experimental data–open squares [7].

The nearly constant behavior at fields up to 100 V/cm can be explained by enhanced energy loss by electrons on optical phonons in the presence of e-e collisions. The role of e-e collisions diminishes at higher field.

3. Drift velocity correlations in semiconductors in the thermodynamic equilibrium state.

The values of correlators at the thermodynamic equilibrium have been calculated for the parabolic model of Γ valley in GaAs. The material parameters correspond to these listed in [8]. Electron scattering on non-elastic acoustic and optical modes of lattice vibrations, as well as e-e scattering ($n_e = 10^{15}$ cm^{-3}) is taken into account. Inter-electron collisions are treated in the Brooks-Herring approximation. Standard expressions for electron scattering rates are used [5]. The calculations are performed by the CSR MC method.

Let us start with the simplified Boltzmann-Langevin equation for the fluctuation distribution function. In the state of thermodynamic equilibrium it can be written as

$$\frac{d\delta F_p(t)}{dt} = -\frac{\delta F_p(t)}{\tau_p} - \frac{\delta F_p(t) - \delta F_p^M(t)}{\tau_{ee}} + y_p(t) \qquad (4)$$

Here $F_p(t)$ is the instantaneous electron momentum distribution function, $F_p^M(t)$ is the drifted Maxwellian distribution corresponding to the $F_p(t)$ at time t, $y_p(t)$ describes the Langevin random force. In our case the rate of fluctuation relaxation is governed by the lattice and e-e scattering mechanisms.

The first term on the right-hand side of equation (4) ensures the relaxation of instantaneous distribution $F_p(t)$ to the equilibrium distribution during lattice relaxation time τ_p. The second term is written in accordance with the Gross-Bhatnager-Krook approach [9]. Its form is based on the property of the instantaneous electron distribution function to acquire symmetric form (the drifted Maxwellian distribution) in the e-e scattering time τ_{ee} under the influence of e-e scattering. R. Liboff in his textbook [10] gives considerable attention to this approach (see also [11]). Electron momentum can be intensively scattered by impurity centres too, but the energy of electrons is conserved in this scattering process. Even in this simple approach we cannot predict the final distribution that will result under the influence of impurity scattering. Therefore, we will omit further the impurity scattering.

The therm $\delta F_p^M(t)$ describes the deviation of a drifted Maxwellian distribution.

E-e scattering does not tend to bring either $F_p^M(t)$ or $F_p(t)$ to the thermodynamic equilibrium, because the average energy and momentum do not change during e-e collisions. So, the drifted Maxwellian distribution is supposed to relax only under the influence of lattice scattering during the corresponding scattering time τ_p. Therefore, we have used $\delta F_p^M(t) = \delta F_p^M(0)\exp(-t/\tau_p)$.

Then, we multiply the equation (4) by the initial distribution function fluctuation $\delta F_{p1}(t_1)$, and average the product. Let us denote the correlator $\overline{\delta F_{p1}(t_1)\delta F_p(t_1+t)}$ as $\overline{\delta F_{p1}(0)\delta F_p(t)}$). Now we write the dynamic equation:

$$\frac{d\overline{\delta F_{p1}(0)\delta F_p(t)}}{dt} = -\frac{\overline{\delta F_{p1}(0)\delta F_p(t)}}{\tau_p} - \frac{\overline{\delta F_{p1}(0)\delta F_p(t)} - \overline{\delta F_{p1}(0)\delta F_p^M(0)}\exp(-t/\tau_p)}{\tau_{ee}} \tag{5}$$

The last term in Eq. (4) representing a random force, vanishes because this force is δ-correlated in time. Initial fluctuations of an actual distribution and the drifted Maxwellian distribution are related in the following way:

$$\delta F_p^M(0) = \delta F_p(0) + \Delta F_p(0) \tag{6}$$

where $\Delta F_p(0)$ is deviation between them. Because of the chaotic behaviour of $\Delta F_p(0)$ we assume that

$$\overline{\delta F_{p1}(0)\delta F_p^M(0)} = \overline{\delta F_{p1}(0)\delta F_p(0)} \tag{7}$$

We are interested in the velocity-to-velocity correlators; therefore we multiply the equation (5) by $V_{i1}(0)V_j(t)$ and sum it up by p_1 and p. Finally, we obtain the phenomenological equation describing the relaxation of the total velocity-to-velocity correlator coefficient $c_{total}(t) = c_{auto}(t) + c_{cross}(t)$ in the thermodynamic equilibrium:

$$\frac{dc_{total}(t)}{dt} = -\frac{c_{total}(t)}{\tau_p} - \frac{c_{total}(t) - c_{total}(0)\exp(-t/\tau_p)}{\tau_{ee}} \tag{8}$$

The first-order linear differential equations for the velocity-to-velocity correlator coefficients can be then written as

$$\begin{aligned} \frac{dc_{auto}(t)}{dt} &= -\frac{c_{auto}(t)}{\tau_p} - \frac{c_{auto}(t)}{\tau_{ee}} \\ \frac{dc_{cross}(t)}{dt} &= -\frac{c_{cross}(t)}{\tau_p} - \frac{c_{cross}(t)}{\tau_{ee}} + \frac{\exp(-t/\tau_p)}{\tau_{ee}} \end{aligned} \tag{9}$$

Taking into account the known initial conditions [1] under equilibrium: $c_{auto}(0) = 1$, and $c_{cross}(0) = 0$, the correlation coefficients are given as

$$c_{auto}(t) = e^{-t/\tau_c},$$
$$c_{cross}(t) = e^{-t/\tau_p}(1 - e^{-t/\tau_{ee}}). \tag{10}$$

As it is seen the auto-correlation coefficient in equilibrium decreases exponentially with a combined relaxation time $\tau_c = \tau_p \tau_{ee}/(\tau_p + \tau_{ee})$. This result describes conventionally the relaxation of the probe particle velocity correlator. We obtain from the second equation that the cross-correlation coefficient tends to increase during the time τ_{ee}, but then decreases to zero per lattice scattering time.
One can see an important result of the total correlation coefficient:

$$c_{total}(t) = c_{auto}(t) + c_{cross}(t) = \exp(-t/\tau_p). \tag{11}$$

This shows that it does not depend on e-e scattering.
The analytical dependencies calculated with equation (11) reasonably well coincide with those from the MC data (Fig. 3).

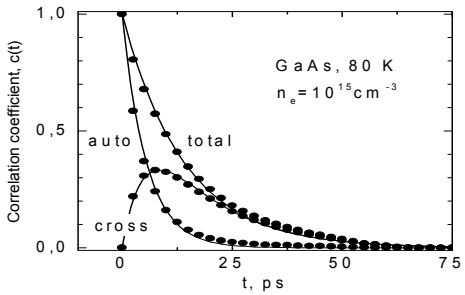

Fig. 3. Relaxation of velocity correlation coefficients in n-GaAs. Points - MC, curves - by equations (10).

The characteristic time at which the cross-correlation function reached its maximum in the case of $\tau_{ee} \le \tau_p$ is $t_{\max} \approx \tau_{ee} \ln(1 + \tau_p/\tau_{ee})$. The more details of the corelation functions bechavior (spectral density, etc.) can be found in [12].

4. Conclusions

The presented MC procedure was demonstrated to be an efficient tool for studying electron noise in the presence of e-e scattering. Taking them in accordance is crucial for explanation of experimental data on microwave noise in doped GaAs.
The results of analytical approach are in good agreement with the Monte Carlo simulation, what confirms the usefulness of our simple analytical model. Till

now only the single particle autocorrelation behaviour has been describe analytically in the textbooks of fluctuation phenomena (for example, see [13]).

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