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Drift velocity correlations in semiconductors in the presence of interparticle collisions

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Abstract

Drift velocity correlation functions are investigated analytically in a phenomenological approach and numerically through Monte Carlo simulation. The simulation takes into account electron–phonon and electron–electron scattering. The thermodynamic equilibrium state is investigated. Analytical results are in good agreement with those obtained by the Monte Carlo method.

1. Introduction

Fluctuation phenomena in semiconductors have been intensively investigated over the last three decades [1–3]. They are particularly important in electron transport in semiconductors. Fluctuation effects have been conventionally investigated without taking into account Coulomb electron–electron (e–e) scattering. However at sufficiently high electron densities, it is necessary to take into account the e–e scattering contribution to the total distribution function and related correlators.

The correlators of various kinetic quantities in the presence of e–e collisions have been studied recently by the numerical Monte Carlo (MC) method [4–8]. The cross-correlation has been found to be essential for the noise properties of semiconductors (see also [9, 10]). However, it is interesting to describe the behaviour of the correlators analytically.

The present paper is aimed at the analytical and MC description of electron drift velocity-to-drift velocity correlation functions in the presence of e–e collisions.

Problem specification and definitions of velocity correlation functions are given in section 2. Phenomenological theory is described in section 3. The results of the analytical approach are compared with the numerical data in section 4. Conclusions are made in section 5.

2. Problem specification

The electron drift velocity-to-drift velocity correlation function is defined as an average of the product of two separated in time electron drift velocities $V_d(t)$. It splits naturally into two

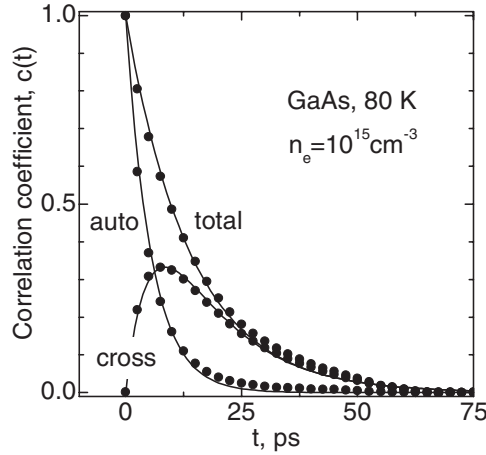


Figure 1. Relaxation of electron velocity-to-velocity correlation function coefficients in GaAs. Thermodynamic equilibrium state. Phonons and e–e scattering mechanisms are included. Points—MC, curves—analytical approximation by equations (11).

parts, namely the auto- and cross-correlator:

$$\overline{\delta V_d(t_1)\delta V_d(t_1+t)} = \frac{1}{N} \left\{ \frac{1}{N} \sum_i \overline{\delta V_i(t_1)\delta V_i(t_1+t)} + \frac{1}{N} \sum_{i \neq j} \overline{\delta V_i(t_1)\delta V_j(t_1+t)} \right\}. \quad (1)$$

Here $V_d(t) = \sum_{i=1}^N \frac{V_i(t)}{N}$ is the instantaneous drift velocity at time moment t , $V_i(t)$ is the velocity of the i th electron, and N is the number of electrons in the ensemble. The bars denote averaging over time t_1 , or over the ensemble at different t_1 and $t_1 + t$.

Equation (1) allows for defining the average electron velocity-to-velocity correlator as

$$\Phi_{\text{total}}(t) \equiv N \overline{\delta V_d(t_1)\delta V_d(t_1+t)} = \Phi_{\text{auto}}(t) + \Phi_{\text{cross}}(t). \quad (2)$$

If the e–e scattering is neglected, the cross-correlation function $\Phi_{\text{cross}}(t)$ is zero, because the motion of individual electrons is independent. In the case of high electron density, the contribution of the cross-correlation function $\Phi_{\text{cross}}(t)$ to the total correlation $\Phi_{\text{total}}(t)$ appears to be significant.

The values of correlators at thermodynamic equilibrium have been calculated for the parabolic model of the Γ valley in GaAs. The material parameters correspond to those listed in [11]. Electron scattering on nonelastic acoustic and optical modes of lattice vibrations, as well as e–e scattering (at the electron density of $n_e = 10^{15} \text{ cm}^{-3}$) is taken into account. Inter-electron collisions are treated in the Brooks–Herring approximation. Standard expressions [12] for electron scattering rates are used. The calculations are performed by the modified combined scattering rate (CSR) method proposed in [6–8]. The main features of this method consist of synchronous N electron ensemble motion. The ‘time of free flight of the system’ is defined from the sum of the each electron scattering rate on the thermal bath and on the all remaining electrons. The CSR technique avoids the short-time step procedure and a large electron number inherent to conventional ensemble MC simulation.

The typical result of MC calculations of the velocity-to-velocity correlator obtained in the case of GaAs is shown in figure 1. The plotted correlation coefficient $c(t)$ is determined as the ratio of the respective correlation function to initial total correlation function $\Phi_{\text{total}}(0)$. In thermodynamic equilibrium, when $\Phi_{\text{cross}}(0) = 0$, the latter is equal to $\Phi_{\text{total}}(0) = \Phi_{\text{auto}}(0) =$

$\overline{V^2} = kT/m$. In our case the lattice temperature is $T = 80$ K and the mean square of electron velocity is $\overline{V^2} \approx 1.81 \times 10^{10} \text{ m}^2 \text{ s}^{-2}$.

As is seen from figure 1, strong velocity-to-velocity cross-correlation arises in the presence of e–e collisions, with a maximum at the time moment when the auto-correlation function decay is the fastest.

We shall describe further the features of electron velocity-to-velocity correlation functions analytically in a phenomenological way and compare with numerical MC calculations. It is well known that the e–e scattering intensity rapidly decreases with electric field strength. The role of the e–e scattering contribution in the correlation manifests significantly at the thermodynamic equilibrium, which will be considered hereafter for the sake of simplicity.

3. Phenomenological theory

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

$$\frac{d\delta F_p(t)}{dt} = -\frac{\delta F_p(t)}{\tau_p} - \frac{\delta F_p(t) - \delta F_p^M(t)}{\tau_{ee}} + y_p(t). \quad (3)$$

Here $F_p(t)$ is the instantaneous electron momentum distribution function, $F_p^M(t)$ is the drifted Maxwellian distribution corresponding to the $F_p(t)$ distribution at time t and $y_p(t)$ describes the Langevin random force (for example, see [1]). 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 (3) 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 [13, 14]. 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. Liboff in his textbook gives considerable attention to this approach [14] (see also [15]). 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 the impurity scattering.

The term $\delta F_p^M(t)$ describes the relaxation of a drifted Maxwellian distribution. Electron–electron scattering does not tend to bring either $F_p^M(t)$ or $F_p(t)$ to the thermodynamic equilibrium form, because the average energy and momentum do not change during mutual 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 equation (3) by the initial distribution function fluctuation $\delta F_{p1}(t_1)$, and average the product over time or over the ensemble. 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 can write the correlator dynamic equation as:

$$\frac{d\overline{\delta F_{p1}(0)\delta F_p(t)}}{dt} = -\frac{\overline{\delta F_{p1}(0)\delta F_p(t)}}{\tau_p} - \frac{\overline{\delta F_{p1}(0)\delta F_p(t)} - \overline{\delta F_{p1}(0)\delta F_p^M(0)} \exp(-t/\tau_p)}{\tau_{ee}}. \quad (4)$$

The last term in equation (3) representing a random force vanishes because this force is δ -correlated in time. We have here the term $\overline{\delta F_{p1}(0)\delta F_p^M(0)}$, which describes the correlation between the initial fluctuations of an actual distribution and the drifted Maxwellian distribution.

The drifted Maxwellian distribution corresponds to the actual electron distribution function at any instant. These two fluctuations are related in the following way:

$$\delta F_p^M(0) = \delta F_p(0) + \Delta F_p(0), \quad (5)$$

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

$$\overline{\delta F_{p1}(0)\delta F_p^M(0)} = \overline{\delta F_{p1}(0)\delta F_p(0)}. \quad (6)$$

We are interested in the velocity-to-velocity correlators; therefore we multiply the equation (4) 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 $c_{\text{total}}(t) = c_{\text{auto}}(t) + c_{\text{cross}}(t)$ in the thermodynamic equilibrium

$$\frac{dc_{\text{total}}(t)}{dt} = -\frac{c_{\text{total}}(t)}{\tau_p} - \frac{c_{\text{total}}(t) - c_{\text{total}}(0) \exp(-t/\tau_p)}{\tau_{ee}}. \quad (7)$$

Now the separate parts of the correlation function will be described. The equation of auto-correlation follows directly from a simple reasoning that a single electron feels both the lattice and neighbouring electrons as a scattering background and lose its instant velocity due to these scattering mechanisms (see below equation (8)). The remaining terms in equation (7) describe the relaxation of the cross-correlation function. The first-order linear differential equations for the velocity-to-velocity correlator coefficients can be then written as

$$\frac{dc_{\text{auto}}(t)}{dt} = -\frac{c_{\text{auto}}(t)}{\tau_p} - \frac{c_{\text{auto}}(t)}{\tau_{ee}} \quad (8)$$

and

$$\frac{dc_{\text{cross}}(t)}{dt} = -\frac{c_{\text{cross}}(t)}{\tau_p} - \frac{c_{\text{cross}}(t)}{\tau_{ee}} + \frac{\exp(-t/\tau_p)}{\tau_{ee}}. \quad (9)$$

Equation (9) is nonhomogeneous: the last positive term reflects the tendency of electrons to conserve the lattice noise between themselves.

Taking into account the known initial conditions [1] under equilibrium:

$$c_{\text{auto}}(0) = 1, \quad \text{and} \quad c_{\text{cross}}(0) = 0, \quad (10)$$

the auto- and cross-correlation coefficients are given in the form of

$$\begin{aligned} c_{\text{auto}}(t) &= e^{-t/\tau_c}, \\ c_{\text{cross}}(t) &= e^{-t/\tau_p} (1 - e^{-t/\tau_{ee}}). \end{aligned} \quad (11)$$

As 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

$$c_{\text{total}}(t) = c_{\text{auto}}(t) + c_{\text{cross}}(t) = \exp(-t/\tau_p), \quad (12)$$

which shows that it does not depend on e-e scattering. In accordance with Price and Einstein relations the diffusion coefficient and the zero-field mobility also do not depend on e-e scattering. In our model (lattice and electron relaxation time approximation) this conclusion is obvious because, as is accepted, the electrons do not create any noise but tend to redistribute lattice noise between them.

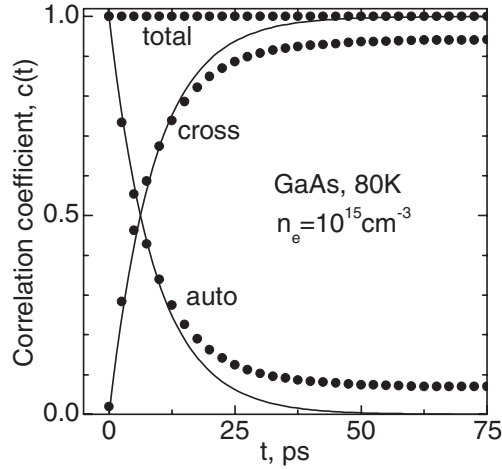


Figure 2. Electron velocity-to-velocity correlation coefficients of $\delta(\omega)$ type noise. Thermodynamic equilibrium state. Points—MC, curves—approximation by τ_{ee} relaxation time.

4. Monte Carlo modelling data

Having the results from a simple analytical model and comparing it with the MC calculations one can easily estimate various kinetic parameters. We have found the electron scattering time by lattice of $\tau_p \sim 14$ ps from the MC data on total correlation decay (figure 1). Then, one finds that the e–e scattering time is $\tau_{ee} \sim 9$ ps from the auto-correlation function decay. Using these times, the analytical dependencies calculated with equation (11) coincide reasonably well with those from the MC data (figure 1).

The characteristic time at which the cross-correlation function reaches its maximum value in the case of rare lattice scattering is

$$t_{\max} \approx \tau_{ee} \ln \left(1 + \frac{\tau_p}{\tau_{ee}} \right). \quad (13)$$

In our case $t_{\max} \sim 8.4$ ps and $c_{\text{cross}}(t_{\max}) \sim 0.33$, in agreement with the numerical results (figure 1).

With the aim of explaining more thoroughly the role of e–e scattering in the velocity-to-velocity fluctuation phenomena the following two problems were also investigated.

- (1) Let the $\delta(\omega)$ -type noise having spectrum $S = A\delta(\omega)$, (ω is the frequency), i.e. with zero frequency, be generated, for example, only at the initial moment $t = 0$, and in accordance with equilibrium electron distribution. This situation is opposite to the $\delta(t)$ -type noise situation (white noise). Then all the lattice scattering mechanisms are switched off and the electron ensemble is allowed to evolve only under the influence of e–e collisions. Here we used averaging over the ensemble. The total correlation coefficient then is $c_{\text{total}} = \frac{1}{A} \int S d\omega = 1$, i.e. the total correlation function remains constant. In this situation electrons tend to conserve the lattice noise and redistribute it among themselves in a such way that the auto-correlation function decrease is accompanied by the appearance of increasing cross-correlation at the same time (figure 2). The latter increases symmetrically from zero, tending to approach the initial auto-correlation value. It also follows from equations (11) that in the case of the limit $\tau_p \rightarrow \infty$ the auto-correlation coefficient decreases within time τ_{ee} , and the cross-correlation coefficient increases within the same

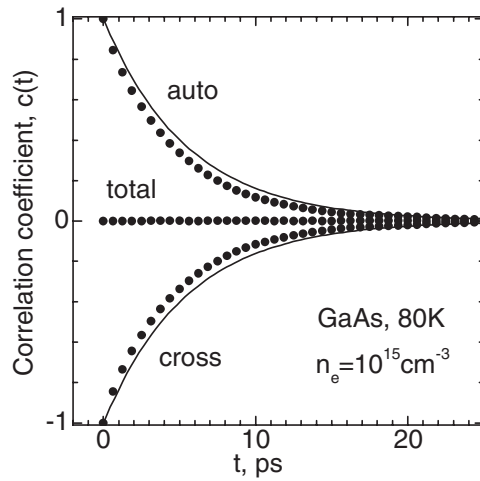


Figure 3. Electron velocity-to-velocity correlation coefficients of the chaotic part of electron velocity. Phonon and e–e scattering are included. Thermodynamic equilibrium state. Points—MC, curves—analytical approximation by τ_c relaxation time.

time τ_{ee} , while their sum remains equal 1. This analytical scenario is in accordance with the MC results presented in figure 2 and with considerations presented in [7, 8]. Note that the obtained difference in figure 2 between saturated Monte Carlo values and analytical ones is about 0.067. It is related to the peculiarities of CSR method used, which is intended to adjust the saturated coefficients to the values

$$c_{\text{auto}} \approx \frac{1}{N} \quad \text{and} \quad c_{\text{max}} \approx \frac{N-1}{N} \quad (14)$$

reported elsewhere [7, 8]. It can be seen that the saturated simulation values depend on the number N of simulated electrons in the MC ensemble. In our case this number is equal to $N = 15$. When the thermostat scattering mechanisms are included together with the e–e scattering, then, it should be noted, the number of particles in the simulated ensemble for the convergence of simulation must be taken to be dependent on how much the relaxation time τ_p differs from τ_{ee} . In our case (figure 1) 1–3% accuracy was achieved when the particle number was equal to $N \sim 10$ –20 (see also [7, 8]).

The calculation results in figure 2 clearly demonstrate the nature of cross-correlation and confirm the validity of our phenomenological approach.

- (2) One should pay attention to an interesting situation observed for the chaotic part of the electron velocity $\delta v_i^*(t) = v_i(t) - v_d(t)$, i.e. the difference at any instant t between the drift velocity and the instantaneous electron velocity. The chaotic part of the drift velocity in the drifting coordinate system does not fluctuate, and the corresponding total correlation function is equal to zero. In addition, electrons interact among themselves and with the lattice vibrations. Then it follows from equations (1) and (2) that at any instant one has

$$\Phi_{\text{auto}}(t) = -\Phi_{\text{cross}}(t). \quad (15)$$

The results of calculations (figure 3) show indeed that the total correlation function is equal to zero and consists of the exponentially decreasing positive auto-correlation and the symmetrically increasing negative cross-correlation functions. This calculation, as well as the simulation presented in figure 2, can also serve for MC testing data.

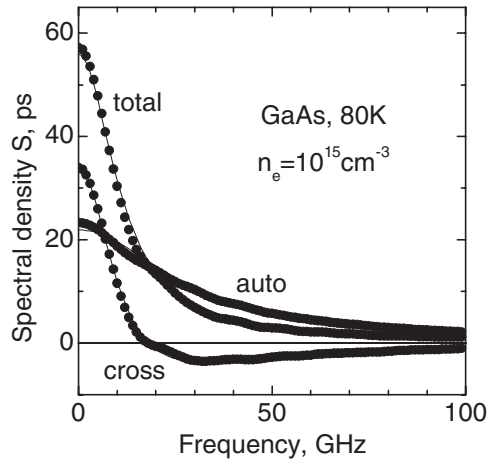


Figure 4. Electron noise spectral density versus frequency. Thermodynamic equilibrium state. Points—MC, curves—approximation by equations (16).

In experiments, the spectral density of noise is usually measured. It can be evaluated from the spectral density of correlation functions in the framework of the presented phenomenological treatment. The known formulas (for example, see [16]) can be used for exponentially relaxing total and auto-correlation coefficients. The expression of the cross-correlation spectrum density can be obtained as the difference between the total and auto-correlation spectral densities. They are

$$\begin{aligned} c_{\text{total}}^{\omega} &= \frac{4\tau_p}{(\omega\tau_p)^2 + 1}, \\ c_{\text{auto}}^{\omega} &= \frac{4\tau_c}{(\omega\tau_c)^2 + 1} \end{aligned} \quad (16)$$

and

$$c_{\text{cross}}^{\omega} = c_{\text{total}}^{\omega} - c_{\text{auto}}^{\omega}.$$

One can see from figure 4 that the results of our simple analytical consideration and the results of MC calculations are also in a good agreement.

5. Conclusions

The phenomenological approach shows that, in equilibrium, the auto-correlation function decreases exponentially during the combined scattering time τ_c when the lattice and e–e scattering mechanisms are included. The cross-correlation function tends to increase during the time of the order of τ_{ce} , but then goes over to zero per lattice scattering time. The total correlation function decreases during the lattice scattering time τ_p . The total correlation function, as well as diffusion coefficient and low-field mobility, do not depend on e–e scattering. The results of analytical approach are in good agreement with the Monte Carlo simulation, which confirms the usefulness of our simple analytical model. In fact the obtained results have a more general meaning. For example, they can be applied to describe the Brownian particle motion, which includes the interparticle collisions. Up until now only the single particle auto-correlation behaviour has been describe analytically in the textbooks of fluctuation phenomena (for example, see [17]).

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