Interparticle collisions and hot-electron velocity fluctuations in GaAs at 80 K

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(Received 18 July 1996; revised manuscript received 26 February 1997)

The microwave spectral density of longitudinal current fluctuations in silicon-doped n-type GaAs at 80 K at moderate electric fields (<1 kV/cm) is calculated. Electron collisions with phonons, impurities, and among themselves are taken into account by a modified Monte Carlo procedure. The important role of interelectron collisions is disclosed, and velocity-velocity cross correlation under nonequilibrium conditions is calculated. The quantitative fitting to the available experimental data on the spectral density of current fluctuations is achieved, and the range of fields is defined for interparticle collisions to manifest themselves in the noise. [S0163-1829(97)04623-7]

I. INTRODUCTION

Investigation of fluctuations is indispensable while seeking a deeper understanding of relations between microscopic processes in a physical system and its macroscopic properties. Fluctuation phenomena in a nonequilibrium electron gas contain information difficult to obtain in other ways, and techniques based on hot-electron noise measurements have been demonstrated to be a powerful tool of diagnostics of solid state plasma.[1,2] Electron velocity fluctuations in doped semiconductors are predicted to be strongly influenced by interelectron collisions responsible, in particular, for additional correlation.[1,3,4]

We report an attempt to interpret results of microwave noise measurements in doped GaAs (Refs. 5 and 6) by comparing them with those of simulation performed, by means of a specially adopted Monte Carlo technique, within a framework of the model sufficient to evaluate effects of interelectron collisions. The theoretical investigation of effects of carrier-carrier scattering on high-electric-field properties of semiconductors goes back to Fröhlich and Paranjape[7] and Stratton.[8] Interelectron collisions, though conserving energy and momentum in the electron system, have an indirect effect on high-field transport[7–9] and—even more direct—on velocity fluctuations.[3,4] In the limiting cases when electron distribution in energy or even in energy and momentum is shaped by frequent interelectron collisions, the Boltzmann equation, though initially nonlinear in electron density, can be treated analytically in terms of ''electron temperature'' or ''drifted Maxwellian'' approximation. This allows an analytic treatment of hot-electron fluctuation problem with the important physical features of fluctuations in nonlinear-in-density nonequilibrium systems being preserved in these limiting cases.[1,4,10]

However, investigation of the analytically tractable models is not sufficient for understanding of field-dependent noise behavior over a wide range of electron densities. A semianalytical seminumerical method has been proposed in Ref. 11 to illuminate a role of interelectron collisions in fluctuation phenomena in the case of ''warm'' electrons. A wide interval of electron densities was covered, from those low enough for interelectron collisions to be neglected up to those high enough to ensure the validity of the electron temperature approximation. However, by definition, only the corrections quadratic in electric field strength were taken into account in Ref. 11. Regretfully, the experimental investigation of E^2 terms in noise characteristics is not an easy task, with most of the experimental results being obtained at intermediate and higher fields.[1,5,6]

So, a system of intercolliding hot electrons being known to have fluctuation properties differing from those in equilibrium, and adequate Monte Carlo techniques being proposed,[12,13] the results of practical interest are seldom found in the literature. Lugli and Reggiani[14] were the first to calculate separately electron velocity auto- and cross-correlation at different electron densities, but only a new generation of computers ensured safe resolving of equal-time cross correlation specific to a nonequilibrium system of intercolliding electrons.[15–17] Nevertheless, no effect of interelectron collisions on the total correlation function and the spectral density of velocity fluctuations was obtained for the considered model of n-type GaAs in investigated electric fields over 1 kV/cm at low lattice temperatures.

On the other hand, the experimental results[5,6] at moderate fields for doped n-type GaAs (impurity densities exceeding 10^{17} cm^{-3}) cannot be even qualitatively interpreted[18] within a framework of the model neglecting interelectron collisions. Thus, microscopic simulation at moderate fields outside the ''warm'' electron region and below 1 kV/cm with necessary scattering mechanisms taken into account is called for in order to resolve effects of interelectron collisions on observables and to interpret the available experimental data.

Definitions of correlation functions are given in Sec. II. The combined scattering rate technique is described in Sec. III. Section IV considers the dependence of calculated correlation functions and spectral densities of velocity fluctuations upon the electron number under simulation. In Sec. V, the calculation of current fluctuations for a realistic model of an electron gas in a doped semiconductor is performed and the results of computation are compared to the experimental data.

II. CORRELATION FUNCTIONS AND THEIR PROPERTIES

Let us introduce the time-dependent drift velocity of N free electrons weakly interacting among themselves and with

an unperturbed thermal bath, i.e., the velocity of the mass center of the electron system:

$$v_d(t)=\frac{1}{N}\sum_{i=1}^{N} v_i(t), \tag{1}$$

where $v_i(t)$ is the instantaneous velocity of the ith electron. Under a steady state (at equilibrium as well), the drift velocity of the electron system fluctuates around its average (over time, or over an ensemble of the systems) value

$$V_d=\overline{v_d(t)}. \tag{2}$$

The total electron energy and momentum of the electrons being conserved during an interelectron collision, the fluctuations of the drift velocity,

$$\delta v_d(t)=v_d(t)-V_d, \tag{3}$$

are caused only by electron interaction with the thermal bath (phonons and impurities in the case of semiconductor). On the other hand, the instantaneous velocity of the ith electron $v_i(t)$ in respect to its long-time average V_d,

$$\delta v_i(t)=v_i(t)-V_d, \tag{4}$$

is influenced by all scattering mechanisms in action. As far as electron velocity fluctuations are considered along a chosen direction (that in which a constant electric field will be applied), the vector indices are omitted.

The time-displaced drift-velocity to drift-velocity correlation function is

$$\Phi(t)=N\overline{\delta v_d(t_1+t)\,\delta v_d(t_1)}, \tag{5}$$

where the average is taken over t_1 with the time interval between two observations, t, being kept fixed. The function $\Phi(t)$ can be presented as

$$\Phi(t)=\Phi_{\text{auto}}(t)+\Phi_{\text{cross}}(t), \tag{6}$$

where

$$\Phi_{\text{auto}}(t)=\frac{1}{N}\overline{\sum_i \delta v_i(t_1+t)\,\delta v_i(t_1)} \tag{7}$$

and

$$\Phi_{\text{cross}}(t)=\frac{1}{N}\overline{\sum_{i\neq j} \delta v_i(t_1+t)\,\delta v_j(t_1)} \tag{8}$$

will be referred to as autocorrelation and cross-correlation functions.

The main features of time-displaced correlation of the electron velocities in the presence of interelectron collisions can be illustrated[19] by the case when the interaction of electrons with the thermal bath is weak as compared to that between themselves, i.e., when the interelectron relaxation time τ_{ee} is shorter than that of the electron momentum relaxation time τ_p caused by an interaction with the thermal bath: $\tau_{ee}\ll\tau_p$. In this case the autocorrelation function, starting from its equal-time ($t=0$) value,

$$\Phi_{\text{auto}}(0)=\overline{v_i^2}, \tag{9}$$

decreases with t due to interelectron collisions mainly: any collision causes a loss of one-electron velocity autocorrelation, and the shortest time constant, τ_{ee}, dominates the rate of decay of the autocorrelation function $\Phi_{\text{auto}}(t)$ in a short time scale.

In equilibrium there is no equal-time cross correlation: $\Phi_{\text{cross}}(0)=0$. On the other hand, any interelectron collision, conserving energy, and momentum, cause the correlation of velocities of the two electrons involved, and, for small t, the cross-correlation function $\Phi_{\text{cross}}(t)$ grows proportionally to t. The opposite tendencies in the evolution of $\Phi_{\text{auto}}(t)$ and $\Phi_{\text{cross}}(t)$ counterbalance each other, and the resultant total (drift-velocity to drift-velocity) correlation function $\Phi(t)$ changes slowly, its decay being caused only by the interaction of the electrons with the thermal bath. So, frequent interelectron collisions tend to redistribute the correlation between the diagonal and off-diagonal terms in favor of the cross correlation, the total correlation function for $t\ll\tau_p$ being kept approximately constant.

At $t\gg\tau_{ee}$ the autocorrelation function becomes small enough, and the cross-correlation function $\Phi_{\text{cross}}(t)$ follows closely the total correlation function $\Phi(t)$, both decaying with the time constant determined mainly by τ_p. So, the cross-correlation function passes over the maximum, its maximum value being under kT/m at equilibrium.[19]

III. MODIFIED MONTE CARLO TECHNIQUE

Let us simulate motion in a uniform electric field of N electrons undergoing different types of scattering events. All electrons move without scattering for the time between two successive ''events in the electron system.'' By the event we mean either a scattering of an electron by the thermal bath or a mutual collision between two electrons. The time between two successive events in the electron system will be referred to as the ''time of free flight of the system.''

For independent scattering events the time of free flight of the system is defined by the combined scattering rate:[16]

$$\lambda_{\text{comb}}(\mathbf{v}_1,\mathbf{v}_2,\ldots,\mathbf{v}_N)=\sum_{i=1}^{N}\lambda_i(\mathbf{v}_i)+\frac{1}{N-1}\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\lambda_{ij}^{ee}(\mathbf{v_i},\mathbf{v_j}), \tag{10}$$

where λ_i and λ_{ij}^{ee} are the integral rates of scattering of the ith electron by the thermal bath and by the jth electron, respectively. The factor $(N-1)^{-1}$ normalizes the e-e scattering rate, so that each electron under simulation is weighted by n/N where n is the electron density. Equation (10) reduces to that written down in Ref. 20 for $N=2$.

The combined scattering rate λ_{comb} depends on the electron velocity distribution. Our Monte Carlo procedure deals with the instantaneous velocity distribution rather than its time-average function. Thus the fluctuations of electron distribution are not ignored. In order to cope with the time-dependent combined scattering rate the Rees self-scattering procedure[9] is applied: a fictious ''scattering rate'' is added to

the instantaneous combined scattering rate to make the resultant total scattering rate independent of time.

Now, the simulation of synchronous motion of N electrons is straightforward. The procedure starts from a chosen electron velocity distribution. A random number is generated to simulate a realization of the ''time of free flight of the system'' determined by the total scattering rate. Since all electrons move without any scattering during the time of free flight, the velocities of all electrons before the scattering event are available, and this is sufficient to calculate the integral scattering rates of each possible scattering event, to make up the combined scattering rate, and to determine the self-scattering rate. Now, another random number is generated to select a type of the scattering event in proportion to its integral scattering rate. Provided the choice falls on the self-scattering, nothing happens in the system, and another free flight is simulated. Provided the choice falls on the ith electron to be scattered by one of the lattice-related mechanisms (phonon, impurity) the consequences of the collision are simulated in the standard way.[9] If the pair collision of the ith electron with the jth electron is selected, then a random number is generated to choose the scattering angle in the $(\mathbf{v}_i, \mathbf{v}_j)$ plane according to the differential interelectron scattering rate, and the final velocities of the two electrons involved are determined respecting the energy and momentum conservation.

The final velocity of the electron, or those of the electrons of the pair are used to renew the set of initial velocities for the next free flight. So, the velocities of all electrons are known at any time, and the simulation continues as long as required.

The simulated realization of the events in the electron system contains information on fluctuations around the steady state. The velocity correlation functions $\Phi(t)$, $\Phi_{\text{auto}}(t)$, and $\Phi_{\text{cross}}(t)$ [Eqs. (6)–(8)] are obtained as averages over the simulation time t_1 for any fixed time difference t.

The proposed ''combined scattering rate'' technique avoids the short-time-step procedure inherent to conventional ensemble Monte Carlo methods.[9,12,13,21] Since in the ensemble Monte Carlo technique the time step should be chosen essentially shorter than the mean time of free flight of the system, while each step is accompanied by a selection of a type of scattering event (the latter procedure is the same in both techniques), the combined scattering rate technique seems to be beneficial.

Evidently, Eq. (10) can be modified to consider interparticle collisions of different quasiparticles: electrons and holes, light and heavy holes, Γ and X electrons, etc.

IV. DEPENDENCE ON NUMBER OF ELECTRONS UNDER SIMULATION

In this section we consider the possibility of reducing the number of electrons under simulation without a loss of information on fluctuation properties of the system. In order to demonstrate the effect of interelectron collisions on fluctuations, we show in Fig. 1 the calculated velocity correlation functions in a heating electric field for a model corresponding to n-type GaAs at 80 K with the impurity scattering neglected. The curves in Fig. 1 have similar features to those

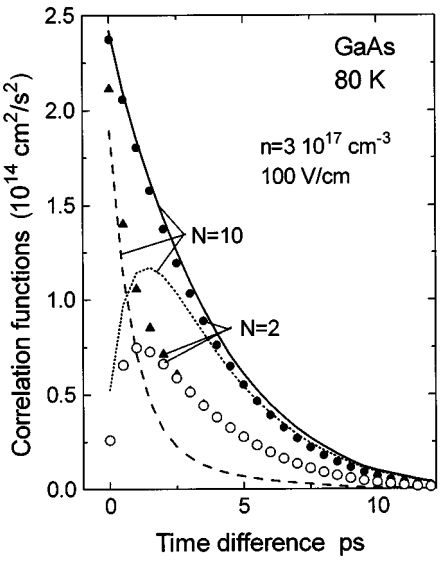

FIG. 1. Time-displaced hot-electron velocity correlation functions for a different number of electrons under simulation: $N=10$ (lines) and $N=2$ (symbols). Drift-velocity correlation functions: total (solid line and closed circles), autocorrelation (dashed line and triangles), cross correlation (dotted line and open circles). Phonon and interelectron scattering mechanisms are taken into account, impurity scattering is neglected.

described in Sec. II, except for the nonzero equal-time cross correlation appearing in the nonequilibrium steady state due to interelectron collisions.[15–17,19]

The correlation functions Φ, Φ_{auto}, and Φ_{cross} presented in Fig. 1 are obtained for electron systems with different numbers of simulated electrons, $N=2$ and $N=10$. It is noteworthy that the results on the total correlation function $\Phi(t)$ almost coincide for these two-electron numbers (Fig. 1, closed circles and solid line).

Knowledge of the correlation functions Φ, Φ_{auto}, and Φ_{cross} makes the calculation straightforward of the spectral densities of electron velocity fluctuations. Figure 2 illustrates the results on the corresponding spectral densities, S_v, S_{auto}, and S_{cross} in their dependence on the electron number N. In consistence with the results of Fig. 1, the results for the total spectral density demonstrate a weak if any dependence on N (Fig. 2, closed circles). In a similar way (and it has been checked during the simulation), the results on macroscopic variables such as electron drift velocity and average energy do not depend on the number of simulated electrons.

On the other hand, the partial spectral densities, S_{auto} and S_{cross}, are found to be linear functions of $1/N$ as expected from the analytic treatment of the electron system in thermal equilibrium.[19] The limits of S_{auto} and S_{cross} for N tending to infinity can be obtained by extrapolating the simulation data obtained for low N.

Simulation of 3×10^6 real interelectron collisions within the above model leads to the value of S_v with 4% rms deviation when the number of simulated electrons is $N=10$. The rms deviation of the total S_v comes mainly from the cross correlation. The CPU time on 100 MHz Pentium, being 150 min for 3×10^6 real interelectron collisions at $N=10$, increases almost proportionally to the product of N and the number of real events. These estimations suggest simulation

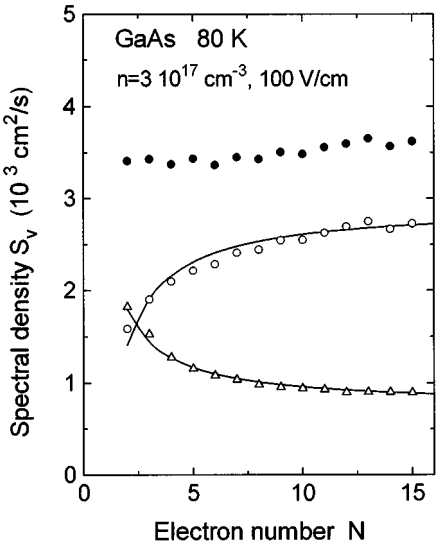

FIG. 2. Spectral density of hot-electron drift-velocity fluctuations (closed circles) versus the number of electrons under simulation, N. Triangles and open circles are contributions of autocorrelation and cross correlation; solid lines are fitted linear functions of $1/N$. Phonon and interelectron scattering mechanisms are taken into account, impurity scattering is neglected.

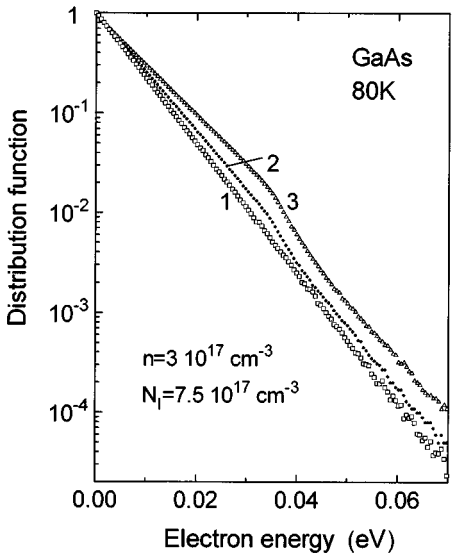

FIG. 3. Electron energy distribution function in n-type GaAs at 80 K ($n=3\times10^{17}$ cm^{-3}, $N_I=7.5\times10^{17}$ cm^{-3}) at different applied electric field: 1–50 V/cm, 2–250 V/cm, 3–500 V/cm.

of $N\sim10$ electrons in order to obtain the correct results on all three correlation functions with a reasonable consumption of CPU time. As a result, the proposed procedure seems efficient in comparison to those ensemble Monte Carlo techniques where a large number of electrons are to be simulated.

V. COMPARISON TO EXPERIMENTAL DATA

It remains to perform calculations for a realistic model of an electron gas in a doped semiconductor in the case where experimental data on microwave noise are available,[5,6] namely, for silicon-doped n-type GaAs, $n=3\times10^{17}$ cm^{-3}, at an 80 K lattice temperature. Since interelectron collisions are expected to be important at not too high electric fields (as is well known, the Coulomb scattering mechanisms gradually switches off with an increase of electron energies), calculations are performed within a framework of a parabolic one-valley (Γ-valley) model, thus ignoring intervalley transitions. Nonelastic acoustic and optical scattering by phonons (acoustic deformation potential, polar optical) is considered, with the phonons remaining in thermal equilibrium. The ionized impurity scattering and interelectron pair collisions are taken into account in the screened Coulomb approach. The effect of electron heating on the screening is neglected.

The experimental data on noise are available[5,6] for silicon-doped n-type GaAs demonstrating mobility of electrons, $\mu = 4000$ cm^2/V s at 80 K, essentially lower than predicted for acceptor-free n-type GaAs (see Ref. 22). It is evident that acceptors are present, and the compensation of donors is important (silicon is an amphoteric impurity in GaAs, and Si atoms in Ga sites act as donors while those occupying As sites act as acceptors). The technique to evaluate the degree of compensation in GaAs and other compound semiconductors is based on the low-field mobility measurements (see Refs. 23 and 24). For example, in the range of electron densities over 10^{17} cm^{-3} the typical degree of compensation in Sn-doped n-type GaAs was found[22] to be $N_I/n\gtrsim2$.

We estimated the degree of partial compensation of donors by acceptors in the silicon-doped n-type GaAs samples in the following way.[25] The dependence of electron drift velocity on the electric field was calculated for electron density 3×10^{17}cm^{-3} at different densities of the ionized impurities. The low-field mobility and the deviations from the Ohm law were found to be sensitive to the degree of compensation. A reasonable fit to the experimental data of Refs. 5 and 25 was obtained for the ionized impurity density $N_I\approx 7.5\times10^{17}$ cm^{-3}.

Figure 3 presents the hot-electron energy distribution obtained in the framework of the above model. Interelectron collisions set a rather good one-temperature distribution at 50 V/cm (Fig. 3, curve 1). At higher fields a kink develops at the optical phonon energy (0.036 eV, curves 2 and 3).

The results on the spectral density of drift-velocity fluctuations are presented in Fig. 4. The spectral density of current fluctuations was measured at 10 GHz frequency.[5] The frequency was high enough to avoid $1/f$ and generation-recombination noise, but it was low in comparison to the inverse time constants of the kinetic processes related to electron scattering in the conduction band. The experimental data on the spectral density of drift-velocity fluctuations (Fig. 4, squares) are obtained from the current fluctuation data through normalization at zero field by using mobility data and the Nyquist formula in the way described elsewhere.[1,6] The results are available in the field range embracing the intermediate fields where the interelectron scattering is expected to be most efficient. The closed circles in Fig. 4 give the electric field dependence of the spectral density resulting from the calculated total correlation function. For comparison, the results of the simulation neglecting interelectron collisions are shown (Fig. 4, diamonds).

One can see that the interelectron collisions have little

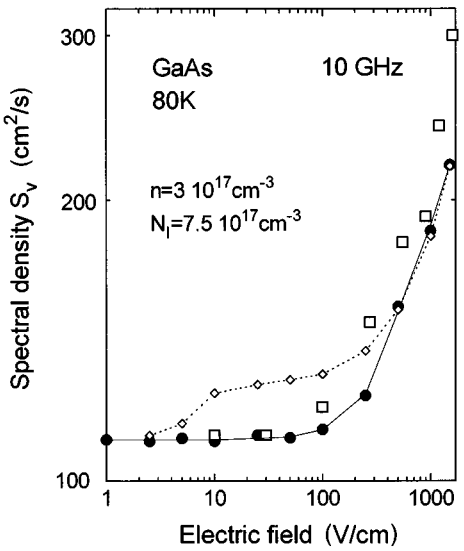

FIG. 4. Dependence of the spectral density of electron drift-velocity fluctuations at 10 GHz for silicon-doped n-type GaAs at 80 K ($n=3\times10^{17}$ cm^{-3}, $N_I=7.5\times10^{17}$ cm^{-3}). Monte Carlo simulation: with phonon, impurity, and interelectron scattering taken into account (closed circles), without interelectron scattering (diamonds). Experimental data—open squares (Ref. 5). Solid and dotted lines are guides to the eye.

influence on the fluctuation spectra at very low- and at high-electric fields (cf. diamonds and closed circles in Fig. 4). The most pronounced effect is obtained at intermediate fields ranging from 5 V/cm to 500 V/cm. The interelectron collisions cause an essential increase in the field strength required for the excess hot-electron fluctuations to manifest themselves.

The calculated dependence with the interelectron collisions taken into account (Fig. 4, closed circles) fits the experimental one (Fig. 4, squares). These results indicate an important role of the Coulomb scattering mechanisms (interelectron and ionized impurity scattering) in the formation of the spectral density of current fluctuations at the intermediate electric fields.

The spectral density of velocity fluctuations remains nearly constant at fields up to 200 V/cm (Fig. 4, closed circles and squares). This behavior can be explained by enhanced energy loss by electrons on optical phonons in the presence of interelectron scattering:[26] the interelectron-collision-dependent energy losses include spontaneous optical phonon emission by the electrons having acquired enough energy in the result of collisions with other electrons. The role of interelectron scattering diminishes at higher fields: an increase of electron energy causes the interelectron scattering rate to decrease and the spontaneous optical phonon emission to become the dominant scattering mechanism.

VI. CONCLUSIONS

The proposed Monte Carlo procedure was demonstrated to be an efficient tool for studying hot-electron noise in the presence of carrier-carrier scattering. The fluctuation properties of nonequilibrium electron gas in a semiconductor are shown to be sensitive to the presence of interelectron collisions. Taking them into account is crucial for an explanation of experimental data on microwave noise in doped GaAs at 80 K at moderate electric fields (5 ... 500 V/cm).

ACKNOWLEDGMENTS

This work was supported by the European Commision through the projects East ELEN 940020 and COPERNICUS 941180, and the Lithuanian State Science and Studies Foundation (Grant No. P5/94).

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