Analysis of the stationary and transient autocorrelation function in semiconductors

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A theoretical analysis of velocity fluctuations in semiconductors is presented both in steady-state and in transient-regime conditions. Results obtained from a Monte Carlo procedure are shown for Si and GaAs. It has been found in particular that (i) off-diagonal contributions to the autocorrelation function must be taken into account; (ii) the convective contribution is positive; (iii) a long tail in the autocorrelation function, due to intervalley fluctuations, may be present; (iv) the negative part in the longitudinal autocorrelation function is due to the thermal contribution and is related to the increasing efficiency of the scattering mechanisms at increasing energies. Furthermore, the transport transient and the correlation transient are analyzed separately but simultaneously through the two-time autocorrelation function, and their effects on the results are discussed for real cases.

I. INTRODUCTION

This paper presents a general analysis of velocity fluctuations of carriers in semiconductors both in transient and in steady-state conditions. In recent times the analysis of velocity fluctuations of charge carriers in semiconductors in the presence of high external electric fields has received renewed attention.[1–12] Modern microelectronics technology, in fact, has reached the submicrometer scale of miniaturization, to which deeper insight into the physics of transport phenomena is required,[13] and fluctuations come to play an increasing role in the design and characterization of a device. Furthermore, a theoretical analysis of fluctuations at sufficiently high frequencies can yield significant information on the physical properties of the scattering sources present in the material under consideration and, more generally, on the microscopic interpretation of its transport properties.

Several papers have appeared on this subject in recent years. However, no rigorous account has yet been given of the different sources for such fluctuations,[14] and very few results have been reported on transient fluctuations.[15]

We present here a unified analysis of diffusion and noise problems obtained by means of the velocity autocorrelation function. This method can be used to describe both steady-state (Sec. II) and transient (Sec. III) phenomena, and also to analyze the different contributions to the diffusivity due to the different physical sources of fluctuations which arise in the presence of an applied electric field.

Results obtained with a Monte Carlo procedure will be shown for covalent (silicon) and polar (gallium arsenide) materials.

II. AUTOCORRELATION FUNCTION DIFFUSION, AND NOISE IN STATIONARY CONDITIONS

A. Theoretical analysis

Let us consider a homogeneous ensemble of carriers subject to a uniform static electric field $\vec{E}$ in steady-state conditions. The diffusion phenomenon is strictly related to noise. This is so because both of them are essentially due to the stochastic velocity fluctuations $\delta\vec{v}(t)$ of each particle over the drift value v_d. The mathematical quantity which describes the common origin of diffusion and noise is the autocorrelation function of velocity fluctuations, which, in one dimension, is defined as

$$C(t)=\langle \delta v(t')\delta v(t'+t)\rangle \ , \tag{1}$$

where the angular brackets indicate ensemble average, and the mean value, in steady-state conditions, is independent of t'. This quantity carries the information on how large these fluctuations are and how they decay in time.

$C(t)$ is related to the diffusion coefficient D through the equation[16]

$$D=\int_0^{+\infty} C(t)dt \ . \tag{2}$$

Thus D can be determined by Eq. (2) from the evaluation of $C(t)$. It is worth noting that the calculation of $C(t)$ is of interest in itself, because its analysis, as we shall see, yields a lot of physical information on the time evolution of the dynamic system under investigation.

Another important relation exists between the diffusion coefficient and the noise spectrum of velocity fluctuations, defined as

$$S_v(\omega)=\lim_{t\to+\infty}\frac{1}{T}\left\langle \left| \int_0^T \delta v(t)e^{i\omega t}dt \right|^2 \right\rangle . \tag{3}$$

With the use of the Wiener-Kintchine theorem[17] the well-known relation

$$D=\tfrac{1}{2}S_v(0) \tag{4}$$

is found. In what follows we shall describe the different origins of the various terms which can contribute to the diffusion process of carriers in semiconductors. In doing so, we shall consider a many-valley semiconductor with two types of valleys (this is the case, for example, of n-Si with the external field along a [100] direction).

Let us consider an electron that, at time t, is in a valley

of type $V(t)$ [$V(t)=1$ or 2] with energy between ϵ and $\epsilon+d\epsilon$. We may then define v_d as the drift velocity, i.e., mean velocity of all electrons; $v_V(t)$ as the valley drift velocity, i.e., mean velocity of all electrons in valley $V(t)$; $v_{\epsilon V}(t)$ as the mean velocity of electrons in valley V with energy between ϵ and $\epsilon+d\epsilon$.

The instantaneous velocity of each electron $v(t)$ can then be written as the drift velocity plus a number of fluctuating terms:[12]

$$\begin{aligned} v(t)&=v_d+[v_V(t)-v_d]+[v_{\epsilon V}(t)-v_V(t)] \\ &\quad+[v(t)-v_{\epsilon V}(t)] \\ &=v_d+\delta v_V(t)+\delta v_\epsilon(t)+\delta v_\kappa(t)\ , \end{aligned} \tag{5}$$

where $\delta v_V(t)$ is the fluctuation associated with the drift velocity of the valley in which the electron is at time t, $\delta v_\epsilon(t)$ is the fluctuation associated with the electron energy, and $\delta v_\kappa(t)$ is the fluctuation associated with the electron momentum.

By using the expression in Eq. (1) the steady-state autocorrelation function becomes

$$C(t)=\sum_{i,j}\langle \delta v_i(t')\delta v_j(t'+t)\rangle=\sum_{i,j}C_{ij}(t)\ , \tag{6}$$

where

$$C_{ij}(t)=\langle \delta v_i(t')\delta v_j(t'+t)\rangle\ , \tag{7}$$

and $i,j=V,\ \epsilon,\ k$. It has sometimes been implicitly assumed in the literature that the total noise due to velocity fluctuations is given by the sum of the three "diagonal" contributions $C_{ii}(t)$ in Eq. (6), at the origin of intervalley (C_{VV}) (Refs. 18 and 19) convective ($C_{\epsilon\epsilon}$) (Ref. 20), and thermal ($C_{\kappa\kappa}$) (Ref. 20) noise, respectively. This restrictive assumption is correct only when the relaxation times of the various fluctuating terms have well-differentiated values,[20] so that in calculating the "off-diagonal" terms one of the two fluctuations can be assumed as constant, while the other fluctuation averages to zero. In general, however, off-diagonal terms C_{ij} also contribute to the autocorrelation function and therefore to diffusion and noise. As an example, $C_{\kappa\epsilon}(t)$ is the contribution to the autocorrelation of velocity fluctuations associated with correlations of momentum and energy fluctuations.

Owing to the linearity of Eqs. (2) and (4) we can also associate specific terms in the autocorrelation function with corresponding terms in the diffusion constant and in noise, thus making explicit their physical origins.

B. Monte Carlo procedure

The Monte Carlo procedure used for the theoretical calculations is of the standard type, and only a few features of interest will be summarized here. The evaluation of the autocorrelation function of δv in steady-state conditions can easily be performed from a Monte Carlo simulation as follows. Let T be the time interval in which the autocorrelation function is to be sampled, which is usually taken as larger than the autocorrelation time [i.e., such that $C(t)\approx 0$ for $t\geq T$]. Then T is divided into a number M of intervals of duration $\Delta T=T/M$ in order to determine $C(t)$ at the times

$$0,\ \Delta t,\ 2\Delta t,\ \ldots,M\,\Delta T=T\ .$$

During the simulation, the velocity of the sampled particle is recorded at the time values $i\,\Delta T, i=0,1,2,\ldots$. When i becomes greater than M, the products

$$v(i\,\Delta T)v[(i-j)\Delta T],\quad j=0,1,\ldots,M \tag{8}$$

are evaluated for each i and j. Products corresponding to the same value of j are averaged over the simulation, thus obtaining

$$\langle v(t)v(t+j\,\Delta T)\rangle_t=C(i\,\Delta T)+v_d^2 \tag{9}$$

(angular brackets with subscript t indicate time average), since in steady-state conditions the time average is equivalent to the ensemble average.

The noise spectrum can be obtained from a Monte Carlo procedure as a Fourier transform of $C(t)$.[2] In order to determine the diffusion coefficient by means of a Monte Carlo simulation, the second central moment

$$M(t)=\langle[z(t)-\langle z(t)\rangle]^2\rangle \tag{10}$$

can be evaluated as a function of the simulation time t,

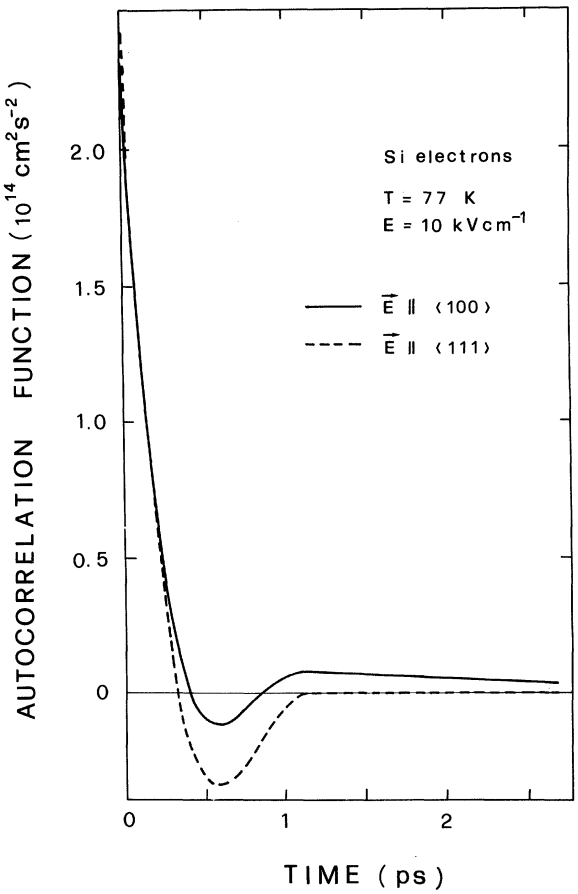

FIG. 1. Velocity autocorrelation function for electrons in Si, as obtained from a Monte Carlo simulation, at 77 K for $E=10$ kV/cm applied along a ⟨100⟩ (continuous line) and ⟨111⟩ (dashed line) directions, respectively.

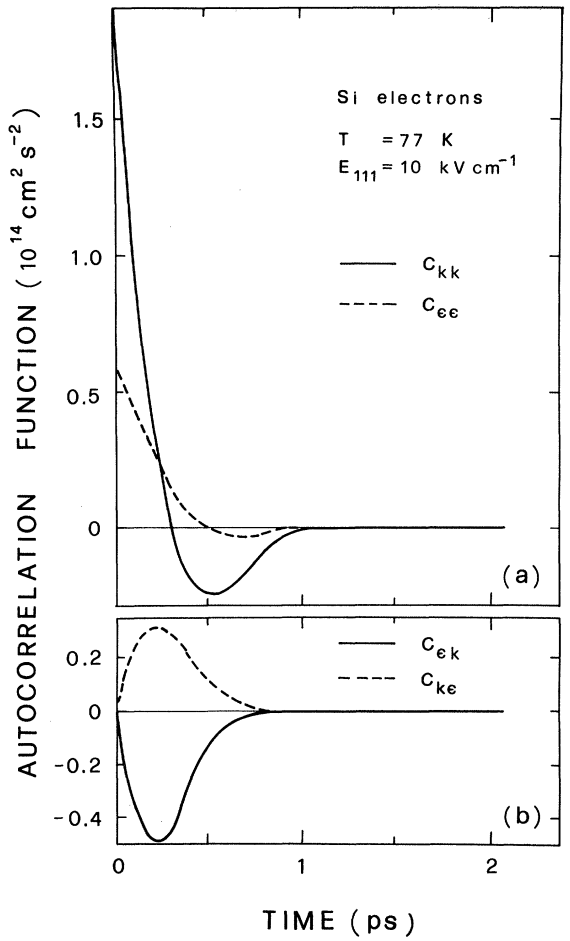

FIG. 2. (a) Autocorrelation function of thermal and convective fluctuations for electrons in Si at 77 K and $E=10$ kV/cm (see Sec. II); (b) Off-diagonal terms $C_{K\epsilon}(t)$ and $C_{\epsilon K}(t)$ which contribute significantly to the total velocity autocorrelation function for the case shown in (a).

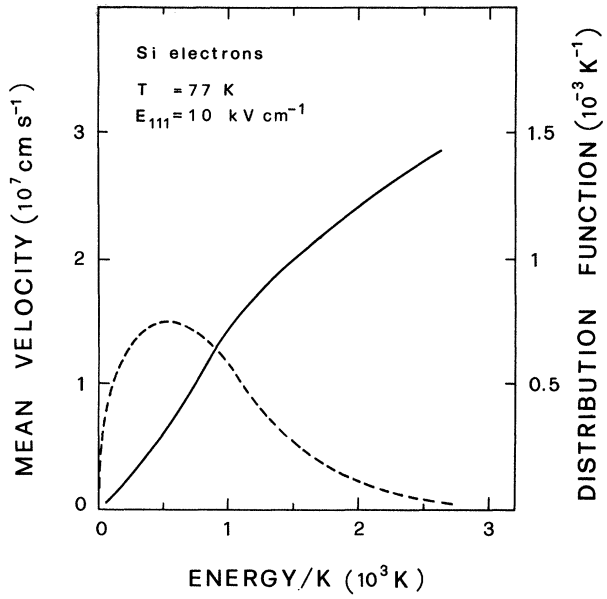

FIG. 3. Mean velocity (continuous line and left scale) and distribution function (dashed line and right scale) as functions of energy for electrons in Si at the indicated temperature and field.

where the average is performed over many different particles. For times larger than the initial transient, the time dependence of $M(t)$ becomes linear and yields the diffusion coefficient as

$$D=\frac{1}{2}\frac{d}{dt}M(t)\,. \tag{11}$$

D can also be obtained from a numerical evaluation of the integral in Eq. (2) once $C(t)$ has been obtained. The physical models used in the calculations for Si and GaAs used in this paper are those reported by Brunetti *et al.*[21] and Ruch,[22] respectively.

C. Results for silicon

Results for electrons in Si have been obtained with an applied electric field $E=10$ kV/cm and a crystal temperature of 77 K. The simplest physical situation to discuss is that with the valleys symmetrically oriented with respect to the direction of the external field ($\vec{E}||[111]$).

Figures 1 and 2 report the autocorrelation function of velocity fluctuations and the different contributions, respectively, as analyzed in Sec. II A, for the case $\vec{E}||[111]$. Within this analysis it is seen that a negative part in the total autocorrelation function is present, which is mostly due to the thermal contribution. Furthermore, the off-diagonal term $C_{\epsilon K}(t)$ of the autocorrelation function, as defined in Eq. (6), also gives an appreciable contribution to the negative part, largely compensated by a positive contribution of $C_{K\epsilon}(t)$. The particular form of these contributions is related to the energy dependence of the scattering mechanisms. In fact, if at a given time t a positive fluctuation of electron momentum occurs, at a later time, due to the larger absorbed power, a positive fluctuation of energy is likely to occur; this, in turn, leads to an increase in the scattering efficiency, so there is a greater probability that a scattering will occur. Since each scattering is momentum randomizing, at larger times negative fluctuations of momentum will follow.

In order to connect this sequence of events to the shapes of the different terms $C_{ij}(t)$, we need to relate energy fluctuations to velocity fluctuations $\delta v_\epsilon(t)$. Figure 3 shows $v_{\epsilon V}$ as a function of energy in Si for the same temperature and field considered above. It can be seen here that $v_{\epsilon V}$ is an increasing function of ϵ, so that a positive $\delta\epsilon$ will correspond to a positive $\delta v_\epsilon(t)$.

By collecting the above considerations, it can be understood why $C_{K\epsilon}$ is positive, $C_{\epsilon K}$ is negative, and C_{KK} is positive at smaller t and negative at larger t, with a minimum which is reached at times greater than the extrema of $C_{K\epsilon}$ and $C_{\epsilon K}$ (see Fig. 2).

In this case, therefore, the fact that the scattering probability is an increasing function of energy yields a negative contribution to longitudinal diffusivity through a negative part of C_{KK} and not through a negative convective contribution $C_{\epsilon\epsilon}$, which exhibits a regular behavior with a small

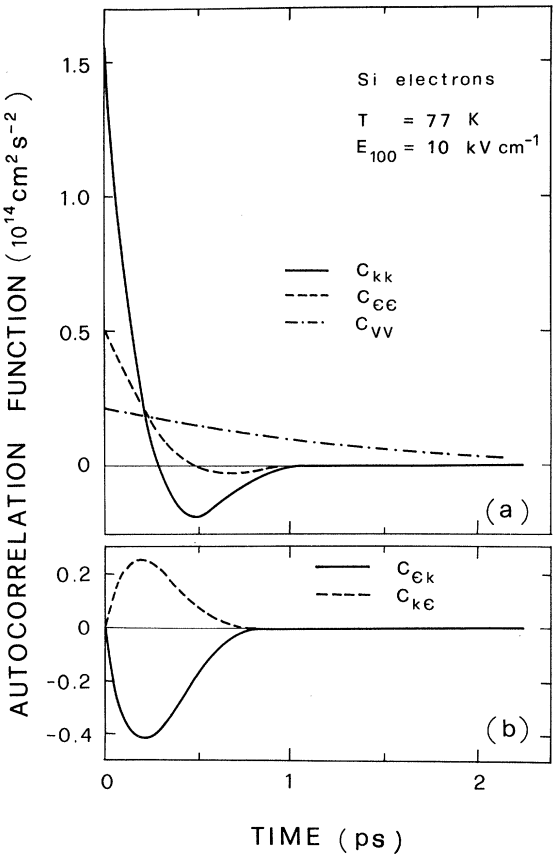

FIG. 4. (a) Autocorrelation function of thermal, convective, and intervalley fluctuations for electrons in Si at 77 K and $E=10$ kV/cm (See Sec. II); (b) off-diagonal terms $C_{k\epsilon}(t)$ and $C_{\epsilon k}(t)$ which contribute to the total autocorrelation function for the case shown in (a).

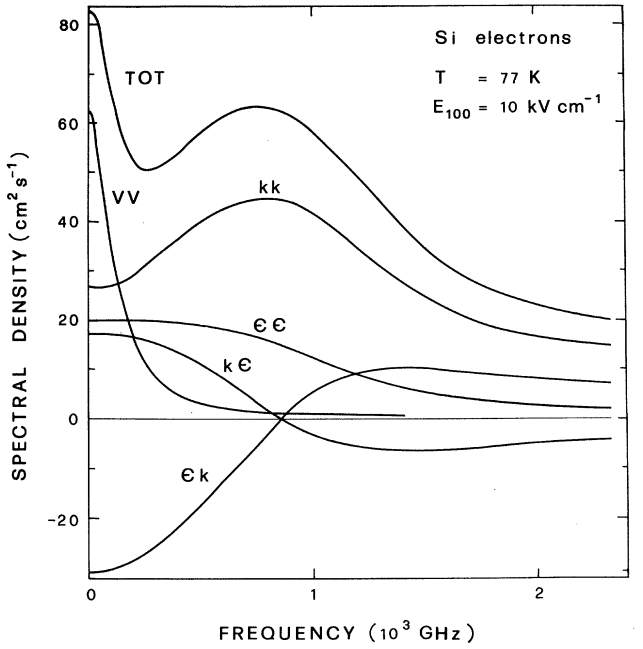

FIG. 5. Spectral density of velocity fluctuations and its components for electrons in Si at the indicated temperature and field obtained as Fourier transforms of the autocorrelation function shown in Figs. 1 and 4. The lettering of the curves is defined in the text.

negative part. Other off-diagonal terms are, in this case, much smaller.

Figures 1 and 4 report the autocorrelation function of velocity fluctuations and its different contributions, respectively, as analyzed in Sec. II A for $\vec{E}||[100]$. In this case the different valleys have nonequivalent orientations with respect to the field direction, and therefore different components of the drift velocity along the direction of $\vec{E}$, so that the phenomenon of longitudinal intervalley diffusion occurs.[21] The intervalley contribution to $C(t)$ is responsible for the long tail of the total autocorrelation function, absent for the case $\vec{E}||[111]$ (see Fig. 1), since the intervalley transition time is the largest of the characteristic times of the process under investigation in these conditions of field and temperature. If we evaluate the integral of the intervalley contribution C_{VV} we find for the intervalley diffusion coefficient the value $D_{VV}=24$ cm^2/s, which is very close to the difference $D^l_{100}-D^l_{111}=21$ cm^2/s (Ref. 21).

The conclusion that such a difference is due to intervalley fluctuations is confirmed by the observation that the thermal and convective contributions to the total autocorrelation function are very similar for the two field orientations (see Figs. 2 and 4).

In a transverse direction, for $\vec{E}||[100]$ velocity fluctuations are due only to thermal fluctuations ($v_V=v_{\epsilon V}=v_d=0$); their autocorrelation is always positive, since no energy transfer is associated with velocity fluctuations. For this reason D_t is always larger than D_l, when the scattering efficiency is an increasing function of ϵ.

Figure 5 shows the noise spectral density $S_v(\omega)$ for the case of $\vec{E}||[100]$ discussed above. Again, the peculiar shape of the total $S_v(\omega)$ can be understood from the analysis of the partial contributions, also shown in Fig. 5. The white-noise value of the total spectrum, corresponding to a diffusion coefficient of 41 cm^2/s, is strongly influenced by the large intervalley contribution ($D_{VV}=31$ cm^2/s). This term shows the most rapid decrease at increasing frequencies due to the largest relaxation time of the intervalley velocity fluctuations. The thermal term gives a relatively small contribution ($D_{kk}=14$ cm^2/s) to the white-noise level as an effect of the cancellation of the negative and positive parts of C_{kk}, and has a bump, due to the strong oscillation of C_{kk}. The convective contribution, with a white-noise level corresponding to $D_{\epsilon\epsilon}=10$ cm^2/s, is present with a monotonically decreasing behavior, and is always positive. The off-diagonal terms $S_{k\epsilon}$ and $S_{\epsilon k}$ have similar shapes of opposite signs; their cumulative contribution, which is relatively small, is negative at low frequencies, corresponding to a negative contribution to diffusivity, and becomes positive at high frequencies.

The total noise spectrum corresponding to the sum of the different terms seen above shows a non-Lorentzian behavior with a fast initial decrease due to the decrease in the intervalley term followed by a bump due to the

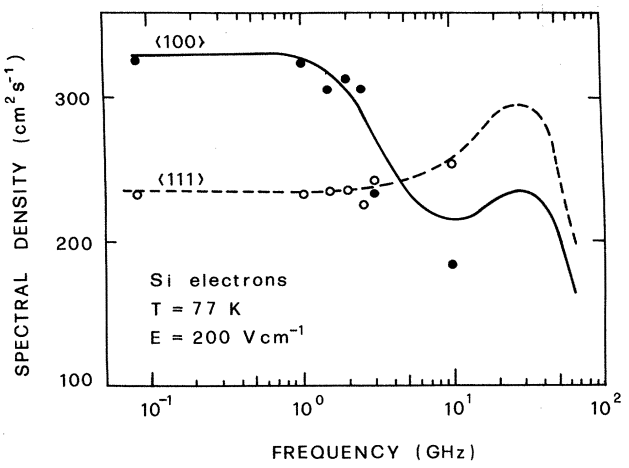

FIG. 6. Spectral density of velocity fluctuations for electrons in Si at 77 K and $E=200$ V/cm along a ⟨100⟩ and a ⟨111⟩ directions. Points refer to experimental data of Bareikis (Ref. 23) and lines refer to Monte Carlo calculations.

thermal contribution and by the final ω^{-2} dependence. Owing to the high frequencies involved, it may be difficult to detect experimentally the maximum of $S_v(\omega)$ at 800 GHz. In experiments, however, it must be taken into account that an initial decrease in $S_v(\omega)$ after a white-noise level does not indicate the cutoff of velocity fluctuations, but rather yields information on the intervalley relaxation time.

Results consistent with the above interpretation have been obtained with calculations performed at other temperatures and fields. In particular, for $T=77$ K and $E=200$ V/cm along ⟨100⟩ and ⟨111⟩ directions, agreement has been found with experimental data of Bareikis,[23] as shown in Fig. 6.

D. Results for gallium arsenide

Results for electrons in GaAs have been obtained with an applied electric field $E=10$ kV/cm and a crystal temperature of 300 K. Figure 7(a) reports the autocorrelation function of velocity fluctuations together with its three diagonal terms. The thermal fluctuations at the chosen field strength are much higher than for the case of Si, owing to the higher electron energy.

Figure 7(b) reports the off-diagonal terms. They are all of the same order of magnitude, but much smaller than the thermal contribution, so that in this part of the figure a different vertical scale has been used.

The interpretation of the diagonal terms, as well as of the off-diagonal terms $C_{\epsilon\kappa}$ and $C_{\kappa\epsilon}$, is similar to that given for the case of Si. Figure 8 shows, in fact, that v_ϵ is a monotonous function of energy also for the case of GaAs. This figure also shows two interesting features. By increasing the field above threshold for negative differential mobility, the whole v_ϵ curve (not only its high-energy part) is reduced, due to the randomizing effect of intervalley scattering. The effect is related to the intervalley collisions with the final $\vec{k}$ in the central valley with direction opposite to the electric force.[24] Furthermore, at

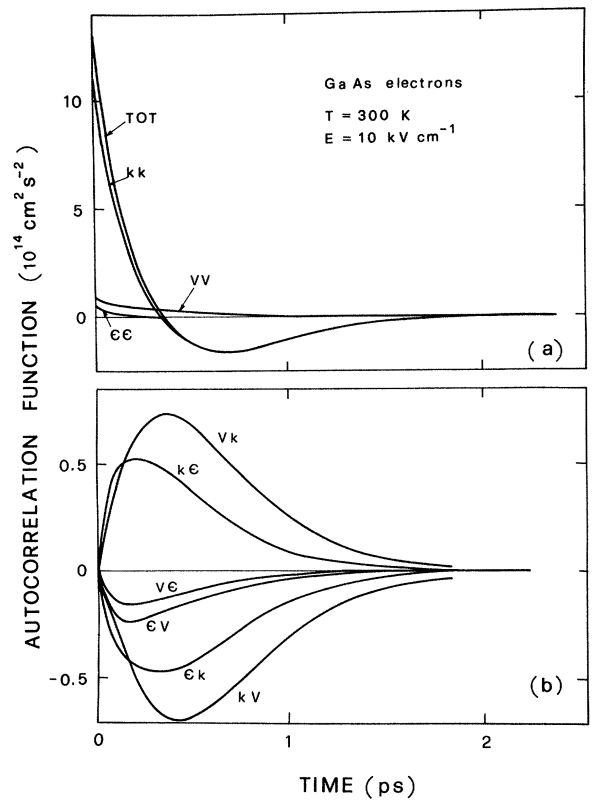

FIG. 7. (a) Autocorrelation function of velocity fluctuations and its diagonal terms and (b) off-diagonal terms for the case of electrons in GaAs at the indicated temperature and field. In (b) a different vertical scale has been used.

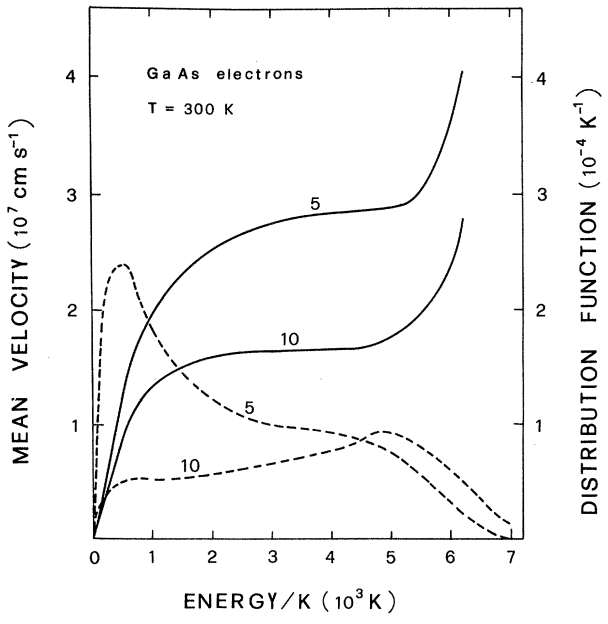

FIG. 8. Mean velocity (solid lines and left scale) and distribution function (dashed lines and right scale) as functions of energy for electrons in the central valley in GaAs at $T=300$ K. The numbers on the curves indicate the field strength in kV/cm.

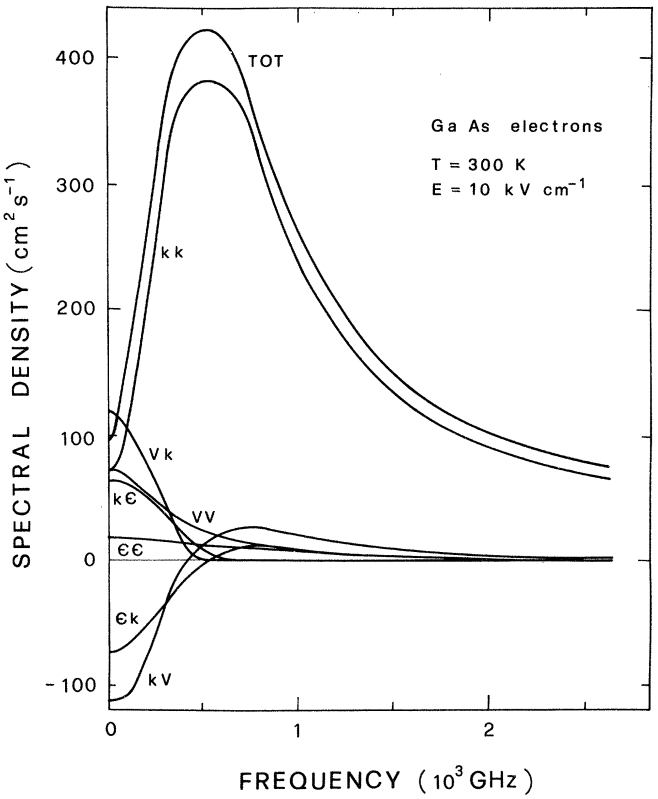

FIG. 9. Spectral density of velocity fluctuations and its components for electrons in GaAs at the indicated temperature and field obtained as Fourier transforms of the autocorrelation functions shown in Fig. 7. The lettering on the curves is defined in the text.

energies above threshold for intervalley scattering, the curve v_ϵ increases more sharply, because electrons enter this region of energy mainly because of acceleration due to the field.

In order to discuss the results for the other off-diagonal terms, we shall refer to the succession of electron states described in Ref. 24. Electrons in the upper valley will eventually be scattered in the negative half $\vec{k}$ space of the lower valley into a state with high energy; as an effect of the field, their energy will first decrease, and then increase until the electron will again be scattered into the upper valley, in this way beginning a new cycle. Therefore, when an electron is in the "slow" upper valley ($\delta v_V < 0$), a positive fluctuation of energy will most probably follow, corresponding to a positive δv_ϵ, with a negative $\vec{k}$ in the central valley. This is the main reason for having $C_{V\epsilon}$ negative and $C_{V\kappa}$ positive. When $\delta\vec{k}$ (and consequently δv_κ) is positive, a large energy will follow ($\delta v_\epsilon > 0$) and the electron will lie predominantly in the slow valley ($\delta v_V < 0$) until its energy has been decreased by successive intervalley scatterings; when, instead, $\delta\vec{k}$ is negative ($\delta v_\kappa < 0$), then the energy will be decreased by the field action ($\delta v_\epsilon < 0$) and the electron will lie in the "fast" valley ($\delta v_V > 0$) until it again reaches an energy comparable with that necessary to emit an intervalley phonon. This explains why $C_{\kappa V}$ and $C_{\epsilon V}$ are negative.

Figure 9 shows the spectral densities calculated from the autocorrelation functions shown in Fig. 7. $S_{V\epsilon}$ and $S_{\epsilon V}$ are smaller than the other contributions and have not been reported for the sake of clarity.

With regard to the noise spectrum, at high frequencies the thermal contribution $S_{\kappa\kappa}$ is dominant, while for the white noise, owing to the large cancellation of the positive and negative part of $C_{\kappa\kappa}$, $S_{\kappa\kappa}$ becomes comparable with other terms.

III. TRANSIENT AUTOCORRELATION FUNCTION AND DIFFUSION

A. Transient correlations

The diffusion process of a carrier ensemble comes from the particle space-velocity correlations which arise during the evolution in time of the system. Starting from an initial condition in which the particle positions and velocities are totally uncorrelated, the process which occurs during the time necessary for setting up the correlations will be defined as the correlation transient. Furthermore, when a high electric field is applied at a certain time to the electron ensemble, the transport process itself must pass through a transient regime which is necessary for attaining the stationary distribution $f(\vec{k})$ in $\vec{k}$ space. This process will be called transport transient.

In what follows we shall discuss how these two different transients can be analyzed separately, but simultaneously, and how their effects influence the transient of the diffusivity of the electron ensemble. The definition of the transient diffusion coefficient has been given by a generalization of Eq. (11) to arbitrary small times:[25–27]

$$D(t)=\frac{1}{2}\frac{d}{dt}\langle[z(t)-\langle z(t)\rangle]^2\rangle\ , \tag{12}$$

where $z(t)$ is the space position of a carrier at time t along the z direction parallel to $\vec{v}_d$.

This generalization can be put in an equivalent form in terms of the autocorrelation function, which is easily interpretable from a physical point of view. By using

$$z(t)=z(0)+\int_0^t v(t)dt \tag{13}$$

in Eq. (12) we have

$$D(t)=\frac{1}{2}\frac{d}{dt}\left[\langle\delta z^2(0)\rangle+2\left\langle\delta z(0)\int_0^t\delta v(t')dt'\right\rangle+\int_0^t dt'\int_0^t dt''\langle\delta v(t')\delta v(t'')\rangle\right]$$

$$=\langle\delta z(0)\delta v(t)\rangle+\int_0^t dt'\langle\delta v(t)\delta v(t')\rangle\ . \tag{14}$$

If there is no correlation between the initial positions and velocities of the particles, Eq. (14) becomes

$$D(t)=\int_0^t d\tau C_t(\tau)\,, \tag{15}$$

with

$$C_t(\tau)=\langle \delta v(t)\delta v(t-\tau)\rangle,\quad 0\le\tau\le t \tag{16}$$

where we have set in Eq. (15) $\tau=t'-t$. Equation (15) reduces to Eq. (2) in steady-state conditions ($t\to\infty$).

By comparing these two expressions, we see that in the present case (i) the integration interval does not extend to $+\infty$ but toward the past, back only as far as the initial conditions; this finite integration brings about the effect of correlation transient, and (ii) the autocorrelation function to be integrated in the transient analysis [Eq. (16)] is not time independent; it is given by the specific ensemble average at a particular time, and its shape provides information about the transport transient.

The transient autocorrelation function $C_t(\tau)$, also called two-time autocorrelation function[15] can be calculated with a Monte Carlo procedure through the simulation of the dynamics of an ensemble of electrons. At fixed times 0, Δt, $2\Delta t$, ..., the direct calculation of the velocity fluctuations is performed with respect to the mean value, calculated at the same time over the carrier ensemble. The products $v(i\Delta t)v(j\Delta t)$, $j=0,1,\ldots,i$ are then averaged over the ensemble and they give $i+1$ values of the transient autocorrelation function at the time $t=i\Delta t$.

The analysis of the various contributions to the autocorrelation function [see Eq. (6)], according to the separation in Eq. (5), can also be obtained for the transient case in a similar way. The present analysis holds also if the field is switched on at a time t_S larger than the time $t=0$ of the initial conditions.[28] In this case the effect of the transport transient is separated in time from the initial correlation transient of the zero-field diffusion (see the next section).

B. Results for silicon

As an application of the general theory outlined in the preceding section, we now discuss a few special examples which contain the significant features of most of the interesting cases. All the results have been obtained with the Monte Carlo technique for electrons in Si with the silicon model referenced in Sec. II B.

Figure 10 presents results for the second central moment, the transient longitudinal diffusion coefficient, obtained with Eq. (12), and the mean velocity, as functions of time for electrons in Si with $E_{111}=10$ kV/cm. The following initial conditions have been taken: electrons are randomly situated in one of the six valleys with equal probability; the velocities are chosen according to an equilibrium Maxwellian distribution, and the electrons are all positioned at $r=0$.

Figure 10 shows that the second central moment first increases quadratically with time, as predicted by ballistic behavior. At intermediate times (0.2—1 ps) an irregular behavior is exhibited by the diffusivity: a tendency to level off, followed by an overshoot ($t\simeq 0.8$ ps). Then, at sufficiently long times, the second central moment shows the linear dependence on time with the slope corresponding to the steady-state diffusion.

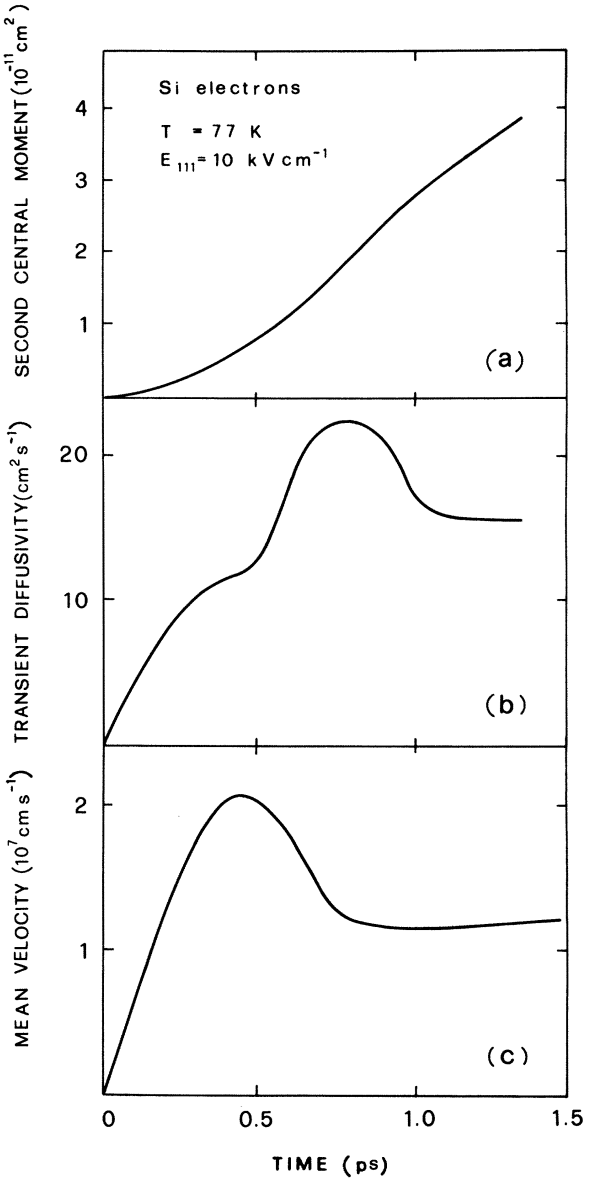

FIG. 10. Second central moment (a), longitudinal diffusion coefficient (b), and mean velocity (c) as functions of time for electrons in Si at 77 K and $E=10$ kV/cm along a ⟨111⟩ direction.

This behavior is due essentially to the combined action of the acceleration impressed by the external field and of the dissipation of energy and momentum associated with intervalley scattering. At the very beginning the field accelerates the electron gas, and all the particles move toward the region of energy where intervalley emission becomes possible. In this interval of time (0—0.2 ps) we have the ballistic regime, in which both mean velocity and diffusivity increase linearly with time [see Figs. 10(b) and 10(c)]. The fastest electrons will then undergo intervalley scattering, becoming in this way very slow; as a consequence mean velocity and diffusivity tend to level off ($t\simeq 0.5$ ps). Later, as an effect of the scattering, we have a

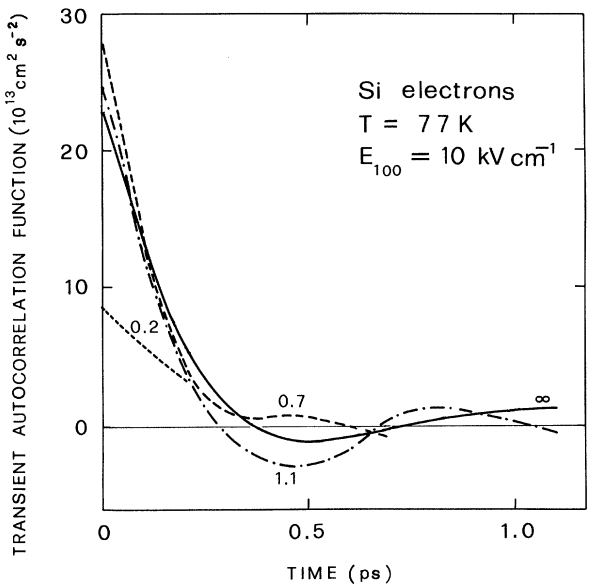

FIG. 11. Transient velocity autocorrelation function vs correlation time τ at fixed times t (reported in ps over each curve in the figure) for electrons in Si at 77 K and $E=10$ kV/cm along a $\langle 100 \rangle$ direction. Each curve is interrupted at $\tau=t$ when the correlation with the initial conditions is reached. The stationary autocorrelation function (continuous line) is shown for comparison.

separation between fast electrons (those which have not yet undergone scattering) and slow electrons (which did undergo scattering), which causes a fast increase in the diffusivity [see Fig. 10(b)] and a decrease in the mean velocity [see Fig. 10(c)] after its maximum value ($t \simeq 0.8$ ps). Finally, due to the randomness of the scattering, the randomized steady distribution of velocities will be set up, and both $\langle v \rangle$ and D reach the steady-state value; the steady diffusivity is lower than the overshoot value because each particle becomes, in steady-state conditions, alternatively slow and fast, with a reduction in the spreading rate at long times, as indicated by the negative part in the stationary autocorrelation function.

As previously noted, the results on transient diffusion can be analyzed and understood in terms of the transient autocorrelation function $C_t(\tau)$. The examples presented below (Figs. 11 and 12) refer to the silicon case with $E=10$ kV/cm.

However, here the field has been chosen along a $\langle 100 \rangle$ direction in order to add to the discussion the effect of the intervalley contribution to the diffusivity. Figure 11 shows the transient autocorrelation function, as a function of τ at various times t; the same initial conditions used in Fig. 10 have been taken. Each of these curves is interrupted at $\tau=t$ when the correlation with the initial conditions is reached. The area under each curve gives the corresponding value at time t of the transient diffusion coefficient. At very short times this area is very small both because $C_t(\tau)$ starts from low values, and because it is interrupted at short τ. The first effect is a consequence of the transport transient, the electrons being still "cold," while the second effect is present because at small times the correlations are not yet established (correlation transient). As t increases, the area reaches larger values, and it is maximum when the positive part of the $C_t(\tau)$ is totally present and a negative part is not yet present. This leads to the overshoot of the transient diffusivity. When negative correlations are established, $D(t)$ decreases toward the steady-state value, which is attained when the shape of $C_t(\tau)$ reproduces the steady-state function and the integral of the autocorrelation function is extended to all significant values of τ.

It is particularly interesting to reproduce the same analysis for the intervalley contribution alone. Figure 12 shows the transient autocorrelation function $C_{VV_t}(\tau)$ for

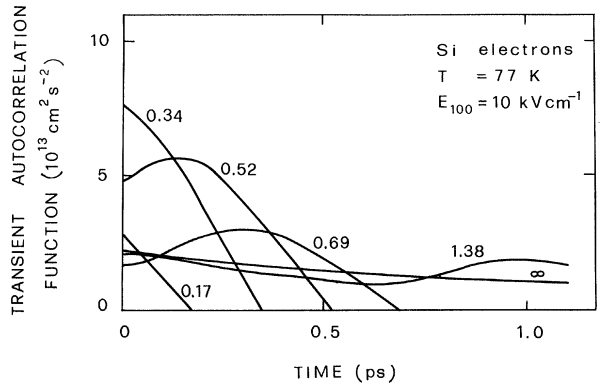

FIG. 12. Transient intervalley autocorrelation function vs correlation time τ at fixed times t (reported in ps over each curve in the figure) for electrons in Si at 77 K and $E=10$ kV/cm along a $\langle 100 \rangle$ direction. Each curve is interrupted at $\tau=t$, when the correlation with the initial conditions is reached. The stationary intervalley autocorrelation function ($t \to \infty$) is shown for comparison.

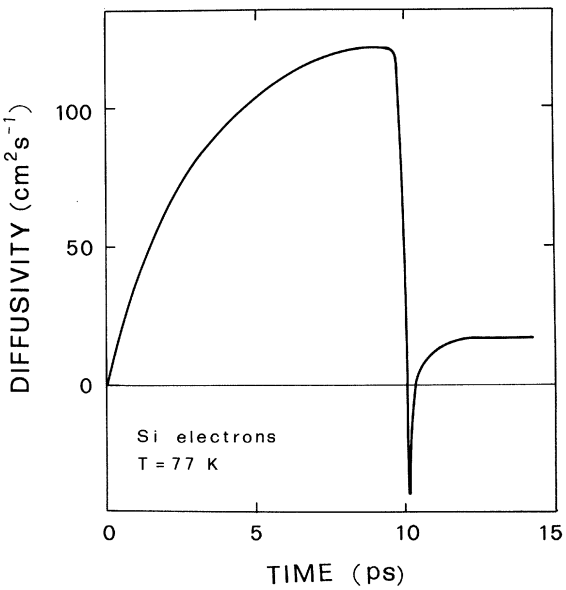

FIG. 13. Transient diffusivity as a function of time for electrons in Si at 77 K, in a physical situation in which a field $E_{111}=10$ kV/cm is switched on at time $t_s=9.57$ ps after the initial conditions ($t=0$) of uncorrelated particles.

the intervalley velocity fluctuations $\delta v_V(t)$, defined in Sec. III A, as a function of τ for various times t. The most striking aspect of this set of curves is the presence of a bump which is shifted toward a greater value of τ as t increases. This phenomenon is clearly due to the velocity overshoot in the two types of valleys which increases the value of $\delta v_V(t)$ with respect to the steady state. As t increases, this overshoot recedes more and more in the past, so that it is seen at larger correlation times until it vanishes, when any memory of the overshoot effect is lost.

The overshoot of the GaAs diffusivity[29] can be analyzed in a similar way, and a negative part of the transient autocorrelation function prevails over the positive part at the times when D is found negative.[29] This strong negative correlation is a consequence of the electron transfer back and forth from central to upper valleys, as discussed above.

As a final result, we report in Fig. 13 an analysis of the transient diffusivity in a case in which the electric field is applied after the onset of the zero-field correlations. Before application of the field, the diffusivity slowly reaches the steady-state value in about 10 ps. When the electric field is applied, a transport transient occurs, with heating of the carriers, on a shorter time scale (in about 2 ps); during this time new correlations are established and the diffusivity reaches the new lower steady value, passing through a minimum with a region of negative values. This negative region is in great contrast with the overshoot of D seen for the case in Fig. 10. This can be explained by considering that the first electrons which undergo intervalley scattering after the field application are the fastest electrons in the direction of the field; during the first part of the process (zero-field correlation transient) the distributions of carriers have fully developed the space-velocity correlations at the basis of the diffusion process, so that a slowing down of the fastest particles due to intervalley scattering produces a shrinking of the space distribution, corresponding to the negative D. It may be useful to compare the behavior of D after the onset of the field in Fig. 13 with Fig. 10(b) in order to appreciate the influence of initial conditions in the transient diffusion.

IV. CONCLUSIONS

This paper reports a theoretical analysis of the velocity fluctuations in semiconductors both in steady-state and in transient conditions. Two points of novelty have been introduced into the discussion. The first concerns the separation of the different contributions to the diffusivity due to the different physical sources of velocity fluctuations in the material. This analysis is important in that it enables a deeper insight into the microscopic evaluation of the carrier ensemble subject to an external field.

The second contribution concerns theoretical analysis of the transient diffusivity. Starting from a generalization to transient regimes of the steady-state relation which connects the diffusion coefficient and the velocity autocorrelation function, a separate analysis of the correlation transient and of the transport transient has been presented. These results are important particularly in connection with the realization of very small (submicrometer) semiconductor devices, for which the transit time is comparable with the time necessary to attain the steady-state conditions. Through the use of the Monte Carlo simulative technique, results have been obtained for Si and GaAs.

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