Correlation functions of hot electrons in semiconductors

Paolo Lugli
Dipartimento di Ingegneria Meccanica, II Università di Roma, via O. Raimondo, I-00173 Roma, Italy

Lino Reggiani
Dipartimento di Fisica dell'Università degli Studi di Modena Centro Interuniversitario di Struttura della Materia del Ministero della Pubblica Istruzione, via Campi 213/A, I-41100 Modena, Italy

Jean Jacques Niez
Laboratoire d'Electronique et de Technique de l'Informatique, Institut de Recherche Technique et de Développement Industriel (LETI-IRTDI) du Commisariat à L'Energie Atomique, Boîte Postale 85X, 38041 Grenoble CEDEX, France
(Received 27 February 1989)

We present a general theory of the correlation functions for a steady state which is valid for arbitrary strengths of an applied electric field, as obtained in high-field transport in semiconductors. When limiting to the first two moments of the distribution function, we find a closed set of equations coupling energy and velocity which are amenable to an analytical solution. Thus, the theory provides an interpolation formula which gives smooth, analytical expressions for the correlation functions. These expressions can be made to fit the computer simulation by using these simulations to estimate the various parameters. The theory is found to be in excellent agreement with numerical calculations for a simple model semiconductor performed with an ensemble Monte Carlo technique.

I. INTRODUCTION

Since the work initiated by Green and Kubo,[1] the use of the velocity autocorrelation function has been proven to be a fundamental tool for the description of the thermodynamic state of a physical system. For example, near equilibrium the velocity autocorrelation function unifies the physical interpretation of both mobility and diffusivity (the Callen-Welton-Kubo fluctuation-dissipation theorem[2,3]). Furthermore, the analysis of the decay in time of the velocity and energy autocorrelation functions provides valuable information on the momentum and energy relaxation rate of the system. It is interesting to remark that under linear response in an applied electric field the two rates, and hence the two correlation functions, are independent of each other.

The aim of this paper is to generalize the above formalism to the case of far-from-equilibrium conditions, when a high electric field originates hot-electron conditions.[4] Starting from a first-principles approach, we formulate the problem within the quantum-mechanical Heisenberg picture. Then a generalized Langevin equation for the macroscopic variables of interest is obtained. This, in turn, enables us to write the equation of motion for the relevant correlation functions. At this stage we make a relaxation-time assumption which, by separating the fast from the slow part of the dynamics (coarse graining in time), allows us to write the classical counterpart of the quantum correlation functions. Thus, we succeed in obtaining a closed set of coupled first-order differential equations for the velocity and energy correlation functions which is solved analytically. Because of the high field, these equations are coupled and the time behavior of the correlations deviates from a simple exponential decay. Analytical results will be proven to agree quite well with the numerical simulations performed through an ensemble Monte Carlo (EMC) technique. Since the theory correctly recovers the Kubo formalism under linear response in the applied field,[3] this methodology can be viewed as a generalization of Kubo formalism under far-from-equilibrium conditions.[5]

The paper is organized as follows. In Sec. II we define the physical system and introduce the correlation functions of interest. In Sec. III the generalized Langevin equation for the relevant macroscopic variables is derived from first principles. In Sec. IV the theory is applied to the simple case of a semiconductor with a single spherical and parabolic band. For this model we succeed in obtaining a closed set of equations for the correlation functions relating velocity and energy. The analytical results so obtained are compared with an appropriate EMC simulation in Sec. V. Section VI draws the main conclusions of this work.

II. THE PHYSICAL MODEL

We consider a homogeneous ensemble of electrons in a semiconductor subject to a uniform static field E_0 of arbitrary strength. The Hamiltonian H_0 of the whole system may be written as

$$H_0 = H_e + H_{e\text{-}F} + H_{e\text{-}L} + H_L \ , \tag{1}$$

where H_e is the electronic Hamiltonian, $H_{e\text{-}F}$ is the time-

independent electric field term (assumed to be switched on adiabatically), $H_{e\text{-}L}$ is the electron-lattice interaction, and H_L is the Hamiltonian of the lattice variables (usually limited to those terms representing the phonon field).

We now introduce the set of thermodynamical macroscopic variables, P_m, of the problem. For example, in our case the usually chosen P_m's are $\mathbf{P}_e$, H_e, and H_L ($\mathbf{P}_e$ being the total momentum of the electronic system). Their time variation is governed by two components: a slow one, which has essentially a thermodynamical character, and a fast one, which reflects the fluctuations. The completeness of the chosen set remains a matter of physical intuition (see Refs. 6–8). As a matter of fact, the physical plausibility for a proper choice of the macroscopic variables is that their correlation functions have the slowest decay time. However, if the set is not complete, although the following mathematical development keeps its formal aspect, the introduction of a relaxation-time approximation will be not valid.

In the steady state, one can always write the density matrix ρ of the problem as[9]

$$\rho=\exp(-\Sigma) , \tag{2}$$

where Σ is an appropriate operator which can be obtained through the far-from-equilibrium Zubarev method.[9] Following Refs. 10 and 11, it can be proven that Σ is the sum of two terms: Σ_I and Σ_R. The first term, having a memory of the past dynamics, carries ultimately the irreversibility of motion while the second gives the dissipationless part.

Let us introduce the following set of correlation functions designed for the steady state:[12,13]

$$(P_m;P_n)_z=(P_n;P_m)_z$$

$$=\int_0^1 d\alpha \,\mathrm{Tr}\{P_m e^{-\alpha\Sigma}(P_n-\langle P_n\rangle)e^{(\alpha-1)\Sigma}\} , \tag{3}$$

where Tr is the quantal trace operator and $\langle\ \rangle$ stands for ensemble average. Equation (3) differs from the ones which were previously used[10–12] by the appearance of Σ in place of Σ_R. Let us stress that Eq. (3) corresponds to the evaluation of correlation functions of macroscopic variables for the steady nonequilibrium state. Their form comes from the fact that, first, we want the involved density matrix to be that of the steady state, and second, we want their expression to be obtained through analytical continuation from the equilibrium state. We notice that the first requirement is absolutely essential if we want to compare the theory with any experimental and/or numerical result. In Refs. 10 and 12, looking at the evaluation of the macroscopic variables (or their mean values) in a transient regime, the initial condition of which being the equilibrium, use has been made of the correlation functions associated with Σ_R to be able to separate the dissipative from the nondissipative part of the motion. However, these correlation functions appear in the results only through the kernels of the integrals of the theory; one does not use them for any direct fitting with numerical data. In Ref. 11 use has been made of the correlation functions associated with Σ_R because they are an essential step of the expansion of any mean value calculated through Eq. (2). Then, one uses mathematical techniques coming from the equilibrium-state problem to evaluate these correlation functions. In short, the correlation functions defined by Eq. (3) are the quantal counterparts of the classical ones for a steady nonequilibrium state one can obtain by EMC techniques. It is natural to extend the aforementioned works[11,12] by introducing the operator Π_z defined such that (for any quantal operator X)

$$\Pi_z X=\mathrm{Tr}\{\rho X\}+\sum_{i,j}(X;P_i)_z\{(P;P)_z^{-1}\}_{ij}(P_j-\langle P_j\rangle) . \tag{4}$$

Here, and in the following, we shall take P to be the column matrix whose elements are the individual P_m's. Thus, all the equations involving P without an index have to be interpreted as having matrix products and sums. Notice that Π_z, for the steady state considered here, is time independent. It is an easy task to check that Π_z is a projection operator such that

$$\Pi_z P_m=P_m , \tag{5a}$$

$$(X;\Pi_z Y)=(\Pi_z X;Y) , \tag{5b}$$

$$\mathrm{Tr}\{\rho(1-\Pi_z)X\}=0 . \tag{5c}$$

III. THE LANGEVIN EQUATION FOR THE MACROSCOPIC VARIABLES

We now want to derive a Langevin equation for our set of macroscopic variables, the P_m's, starting from the Heisenberg equation. This can be written as ($\hbar=1$)

$$\frac{dP_m(t)}{dt}=iU_0^\dagger(t-s)[H_0,P_m(s)]U_0(t-s) \tag{6}$$

(because P_m's do not depend on time explicitly), where $[H_0, X]$ has the meaning of a quantal commutator and $U_0(t-s)=\exp[-i(t-s)H_0]$, with $0\le s\le t$, is the usual time-evolution operator associated with the Hamiltonian H_0 of Eq. (1). By using superoperator technique,[7] Eq. (6) becomes

$$\frac{dP_m(t)}{dt}=iS(t-s)L_0P_m(s) , \tag{7}$$

where $S(t-s)$ and L_0 are defined by

$$L_0X=[H_0,X] \tag{8a}$$

$$S(t-s)X=U_0^\dagger(t-s)XU_0(t-s) . \tag{8b}$$

From Eqs. (8) it is easily found that the operator $S(t-s)$ obeys the following equations:

$$\frac{\partial S(t-s)}{\partial t}=iS(t-s)L_0 , \tag{9a}$$

$$S(0)=1 . \tag{9b}$$

Equation (7) can be given the following convenient form:

$$\frac{dP_m(t)}{dt}=iS(t)\Pi_z L_0P_m(0)+iS(t)(1-\Pi_z)L_0P_m(0) \tag{10}$$

in which the first term is the projected motion on the

$P_m(t)$'s, see Eq. (4). The aim of the following is to show that the second term bears all the memory part of the dynamics as well as all its fluctuating component.

Following a previous work,[12] we introduce the operator $G_0(t-s)$ as a single-time Green's function given by

$$G_0(t-s)=\exp[i(t-s)L_0(1-\Pi_z)] \tag{11a}$$

and satisfying

$$\frac{\partial G_0(t-s)}{\partial t}=iG_0(t-s)L_0(1-\Pi_z)\ , \tag{11b}$$

$$G_0(0)=1\ . \tag{11c}$$

It is easily stated that $G_0(t-s)$ obeys the following property:

$$(1-\Pi_z)G_0(t-s)(1-\Pi_z)=(1-\Pi_z)G_0(t-s)\ . \tag{12}$$

From Eqs. (11) it is possible to derive a relation linking $S(t-s)$ and $G_0(t-s)$ (see the Appendix):

$$S(t-s)=G_0(t-s)+i\int_s^t ds'\,S(s'-s)L_0\Pi_z G_0(t-s')\ . \tag{13}$$

By integrating Eq. (13) by part and using Eqs. (9) and (11), we obtain

$$S(t)(1-\Pi_z)=(1-\Pi_z)G_0(t)+i\int_0^t ds'\,S(s')\Pi_z L_0(1-\Pi_z)G_0(t-s')\ , \tag{14}$$

which, when substituted in Eq. (10), gives

$$\frac{dP_m(t)}{dt}=iS(t)\Pi_z L_0 P_m(0)+i\int_0^t ds'\,S(s')\Pi_z L_0(1-\Pi_z)G_0(t-s')\dot{P}_m(0)+(1-\Pi_z)G_0(t)\dot{P}_m(0)\ , \tag{15}$$

where $\dot{P}_m$ stands for iL_0P_m.

Equation (15) is the "generalized Langevin equation" appropriate to our system. The first term is the projected motion on the $P_m(t)$'s, the second term bears the memory of the past, and the last term describes the fluctuations in a "Langevin way," since both its mean value and its correlation with the P_m's at time $t=0$ are zero [see Eqs. (5)].

Usually the P_m's are such that the dissipationless motion ($H_{e\text{-}L}=0$) is described by equations of the following type:

$$\dot{P}_m(t)=\sum_n a_{mn}P_n(t)\ . \tag{16}$$

As an example, for the chosen P_m's and in an isotropic effective-mass situation, the dissipationless motion is given by

$$\dot{\mathbf{P}}_e=eN_e\mathbf{F}\ , \tag{17a}$$

$$\dot{H}_e=\frac{e}{m}\mathbf{F}\cdot\mathbf{P}_e\ , \tag{17b}$$

$$\dot{H}_L=0\ , \tag{17c}$$

where e is the electron charge, N_e is the total number of electrons, and m is the carrier effective mass.

Being in the framework of Eq. (16), with the aid of Eq. (5), we can write

$$(1-\Pi_z)\dot{P}_m(0)=(1-\Pi_z)\dot{P}_{m,L}(0)\ , \tag{18}$$

where $\dot{P}_{m,L}=i[H_{e\text{-}L},P_m]$ is the part of $\dot{P}_m$ restricted to H_{e-L} only. Using the definition of Π_z and Eqs. (12) and (18), Eq. (15) becomes

$$\frac{dP_m(t)}{dt}=\sum_{i,j}(\dot{P}_m;P_i)_z\{(P;P)_z\}_{ij}^{-1}(P_j(t)-\langle P_j\rangle)-\int_0^t ds'\sum_{i,j}[G_0(t-s')\dot{P}_{m,L};(1-\Pi_z)\dot{P}_{i,L}]_z\{(P;P)_z^{-1}\}_{ij}(P_j(s')-\langle Pj\rangle)+(1-\Pi_z)G_0(t)\dot{P}_{m,L}(0)\ , \tag{19}$$

where we have used the property $(L_0X;Y)_z=-(X;L_0Y)_z$.

Coming from first principles, Eq. (19) can be seen as a starting point for a set of coherent approximations. The easier way of doing it is to go into a relaxation-time paradigm. To do that, one has to suppose that the kernels of the integral in Eq. (19) are rapidly varying functions whose ultimate effect is to select the value of the macroscopic variable at time $s'=t$.[14,15] This can be supported by the fact that, the P_m's being supposedly a complete set of macroscopic variables, all the slow parts of the dynamics are taken away from $G_0(t-s')$. Thus the possible failure of the relaxation-time approach could come from an incomplete choice of the P_m's or, in other words, from the impossibility of decomposing the time scale into a slow and fast component.

Within the relaxation-time approach, Eq. (19) reads

$$\frac{dP_m(t)}{dt}=\sum_j\alpha_{m,j}(P_j(t)-\langle Pj\rangle)+(1-\Pi_z)G_0(t)\dot{P}_{m,L}(0)\ , \tag{20}$$

where

$$\alpha_{m,j}=\sum_i \left[(\dot{P}_m;P_i)_z\{(P;P)_z\}^{-1}_{ij}-\int_0^\infty ds'[G_0(t-s')\dot{P}_{m,L};(1-\Pi_z)\dot{P}_{i,L}]_z\{(P;P)_z^{-1}\}_{ij}\right] . \tag{21}$$

By recalling the stochastic nature of the last term in the right-hand side of Eq. (21), Eq. (20) recovers the usual Langevin equation when $m=j=1$ and $P_1=P_e$. It is the one we want to use for describing the evolution of our relevant correlation functions. For example, using Eqs. (5) one gets

$$\frac{d}{dt}(P_m(t);P_l)_z=\sum_j \alpha_{mj}(P_j(t);P_l)_z . \tag{22}$$

IV. EQUATIONS OF MOTION FOR A CLOSED SET OF CORRELATION FUNCTIONS

Taking for simplicity a single spherical and parabolic band model semiconductor, then four correlation functions, which couple velocity and energy fluctuations, can be taken as a complete set. These can be written in matrix notation as

$$\begin{bmatrix}\phi_{vv}(t) & \phi_{v\varepsilon}(t)\\ \phi_{\varepsilon v}(t) & \phi_{\varepsilon\varepsilon}(t)\end{bmatrix}=\begin{bmatrix}\langle \delta v\,\delta v(t)\rangle & \langle \delta v\,\delta\varepsilon(t)\rangle\\ \langle \delta\varepsilon\,\delta v(t)\rangle & \langle \delta\varepsilon\,\delta\varepsilon(t)\rangle\end{bmatrix} . \tag{23}$$

According to Eq. (22) , the set in Eq. (23) is found to satisfy the following closed system of coupled first-order differential equations:

$$\frac{d}{dt}\phi_{vv}=-\alpha_{11}\phi_{vv}-\alpha_{12}\phi_{v\varepsilon} , \tag{24a}$$

$$\frac{d}{dt}\phi_{v\varepsilon}=-\alpha_{21}\phi_{vv}-\alpha_{22}\phi_{v\varepsilon} , \tag{24b}$$

$$\frac{d}{dt}\phi_{\varepsilon v}=-\alpha_{11}\phi_{\varepsilon v}-\alpha_{12}\phi_{\varepsilon\varepsilon} , \tag{24c}$$

$$\frac{d}{dt}\phi_{\varepsilon\varepsilon}=-\alpha_{21}\phi_{\varepsilon v}-\alpha_{22}\phi_{\varepsilon\varepsilon} , \tag{24d}$$

where the coefficients α_{ij} (which depend on the external field but not on time) describe the microscopic properties of the physical system.

At equilibrium ($F=0$) the diagonal terms α_{11} and α_{22} coincide with the momentum and energy relaxation rate, respectively. [This is the reason for keeping explicitly the negative signs in Eq. (24).] The off-diagonal terms α_{12} and α_{21} are zero at equilibrium when, as known, the relaxation of momentum and energy are independent. Under hot-electron conditions these rates are no longer independent and the off-diagonal terms describe the coupling between them. Indeed, as we shall see in the next section, under high fields the sign of the α_{ij} coefficients will depend on the thermodynamic state at hand and the general nonexponential decay in time of the correlation functions does not allow for a proper definition of a velocity and energy relaxation rate. A microscopic determination of the α_{ij} coefficients remains a formidable problem which has not yet been considered.

The analytical solution of Eqs. (24) in normalized form is given by

$$\begin{aligned}
\phi_{vv}(t)&=\frac{e^{-\lambda t}}{\bar{\alpha}_{21}\omega_0}\{\bar{\alpha}_{21}[\omega_0\cosh(\omega_0 t)+(\lambda-\alpha_{11})\sinh(\omega_0 t)]+[(\lambda-\alpha_{11})^2-\omega_0^2]\sinh(\omega_0 t)\} ,\\
\phi_{v\varepsilon}(t)&=\frac{e^{-\lambda t}}{\omega_0}\{\omega_0\cosh(\omega_0 t)-[(\lambda-\alpha_{11})+\bar{\alpha}_{21}]\sinh(\omega_0 t)]\} ,\\
\phi_{\varepsilon v}(t)&=\frac{e^{-\lambda t}}{\bar{\alpha}_{21}\omega_0}\{\bar{\alpha}_{21}[\omega_0\cosh(\omega_0 t)+(\lambda-\alpha_{11})\sinh(\omega_0 t)]+[(\lambda-\alpha_{11})^2-\omega_0^2]\sinh(\omega_0 t)\} ,\\
\phi_{\varepsilon\varepsilon}(t)&=\frac{e^{-\lambda t}}{\omega_0}\{\omega_0\cosh(\omega_0 t)-[(\lambda-\alpha_{11})+\bar{\alpha}_{21}]\sinh(\omega_0 t)]\} ,
\end{aligned} \tag{25}$$

where $\lambda=\frac{1}{2}(\alpha_{11}+\alpha_{22})$, $\omega_0^2=\frac{1}{4}(\alpha_{11}-\alpha_{22})^2+\alpha_{12}\alpha_{21}$, $\beta=\langle \delta v\,\delta\varepsilon\rangle/\langle \delta v^2\rangle$; $\lambda=\langle \delta v\,\delta\varepsilon\rangle/\langle \delta\varepsilon^2\rangle$; $\bar{\alpha}_{21}=\alpha_{21}/\beta$; $\tilde{\alpha}_{21}=\alpha_{21}\gamma$. We notice that λ and ω_0 are two frequencies which characterize the main features of the time evolution of the correlation functions. As a matter of fact, λ, which is always real, is responsible for a damping, while ω_0, when imaginary, determines an oscillatory behavior.

V. COMPARISON WITH AN ENSEMBLE MONTE CARLO SIMULATION

The analytical results in Eq. (25) can be made to fit computer simulations by using these simulations to estimate the various parameters. Accordingly, we have performed an EMC calculation for a simple Si-like model semiconductor with $\mathbf{F}\|\langle 111\rangle$.[16] To this end, the α_{ij} coefficients as well as the values of β and γ have been taken from the values of the correlation functions and their derivatives at $t=0$ as obtained through the EMC simulation and then inserted in Eq. (25).

We have considered here scattering with acoustic and nonpolar optical (or intervalley) phonons. In the calculation we have taken 10^4 and 4×10^4 particles finding a good coincidence of the numerical results within a maximum uncertainty of about 5%.

To check the reliability of the functional form given by

Eq. (25), we have prepared the EMC simulation for the two following cases of interest.

A. Quasielastic regime

This condition, which corresponds to a carrier momentum distribution function with the even part dominating over the odd part, is well reproduced at the temperature of 300 K. Figures 1 and 2 show the time behavior of the normalized correlation functions as obtained from the EMC simulation and calculated from Eq. (25) for a typical low and high value of the electric field. The agreement found is excellent and covers the entire range of fields here examined, $1 \leq F \leq 200$ kV/cm. We have noticed that at the lowest fields the agreement slightly degrades because the resolution of the EMC data becomes poorer, especially for the case of the cross-correlation functions. At all fields we have found that $\lambda > |\omega_0|$ and the autocorrelation function of velocity exhibits a faster decay than that of energy, a well-known behavior associated to the property of the scattering mechanisms here considered which relaxes the velocity faster than the energy. At increasing fields the velocity and energy correlation functions do not follow a simple relaxation-time behavior. In particular, starting from fields of 20 kV/cm, the velocity autocorrelation function exhibits a minimum, thus going to negative values. This behavior can be associated to the distinct contribution given to the velocity autocorrelation function by fluctuations in momentum and energy. Firstly, proposed on the basis of intuition years ago by Price,[17] this behavior is established here on firm mathematical grounds on the basis of the Heisenberg equations of motion.

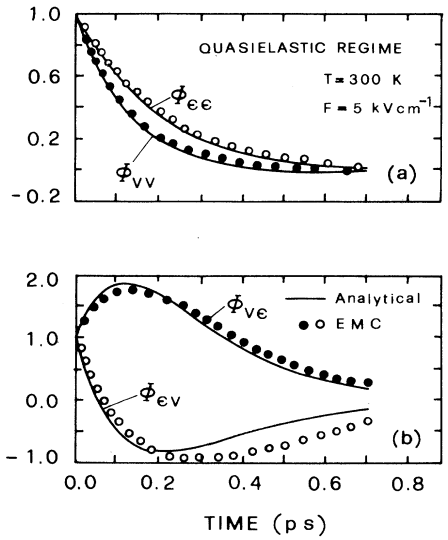

FIG. 1. Normalized correlation functions as a function of time for the case of "quasielastic regime" at $F=5$ kV/cm. Solid curves and points refer to present theory and EMC calculations, respectively. (a) and (b) refer to autocorrelation and cross-correlation terms, respectively.

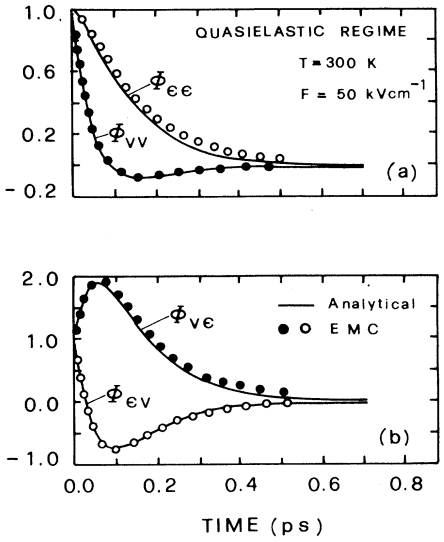

FIG. 2. Normalized correlation functions as a function of time for the case of quasielastic regime at $F=50$ kV/cm. Solid curves and points refer to present theory and EMC calculations, respectively. (a) and (b) refer to auto correlation and cross-correlation terms, respectively.

The peculiar form of the cross-correlation functions is analogous to that given in Ref. 18 for the case of Si at 77 K. Its interpretation is related to the energy dependence of the scattering mechanisms, which in our case always leads to an increase of the scattering rate with increasing energy. Therefore, when considering the velocity-energy correlation function, we argue the following. If initially a positive fluctuation of velocity occurs, at a later time, due to the large absorbed power, a positive fluctuation of energy is likely to occur; for the same reason an initial negative fluctuation of velocity will lead to a negative fluctuation of energy. Thus, the initial slope of $\langle \delta v\, \delta\varepsilon(t) \rangle$ will always be positive. On the other hand, when considering the energy-velocity correlation function, we find that if initially a positive fluctuation of energy occurs, at a later time, due to the increased efficiency of the scattering, a negative fluctuation of velocity is likely to occur; for the same reason an initial negative fluctuation of energy will lead to a positive fluctuation of velocity. Thus the initial slope of $\langle \delta\varepsilon\, \delta v(t) \rangle$ will always be negative. At later times, the zero-property tendency of the correlation functions will imply a maximum for $\langle \delta v\, \delta\varepsilon(t) \rangle$ and a minimum for $\langle \delta\varepsilon\, \delta v(t) \rangle$.

For a better understanding of the correlation decay rates, Figs. 3 and 4 present the spectral functions $g_{ij}(\omega) = \int_0^\infty \phi_{ij}(t) \exp(i\omega t) dt$ at a typical field value of 50 kV/cm. Figure 3 reports the diagonal components g_{vv} and $g_{\varepsilon\varepsilon}$. The real part of g_{vv} shows a maximum associated with the negative region of ϕ_{vv} and then goes to zero with a typical Lorentzian shape. As discussed above, this maximum can be related to the correlation between energy and momentum fluctuations which originates because

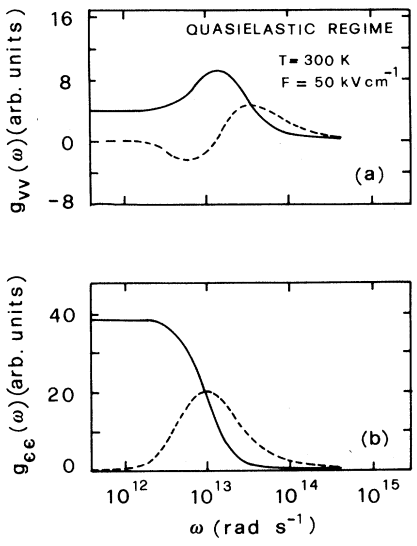

FIG. 3. Spectral density of (a) velocity and (b) energy fluctuations as a function of angular frequency for the case of quasielastic regime at $F=50$ kV/cm. Solid and dashed lines refer to the real and imaginary part, respectively.

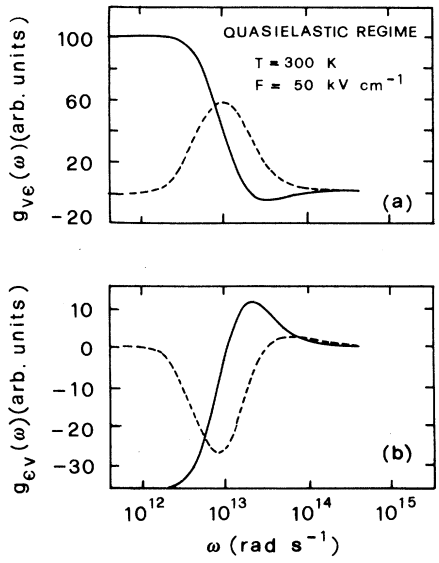

FIG. 4. Spectral density of (a) velocity-energy and (b) energy-velocity fluctuations as a function of angular frequency for the case of quasielastic regime at $F=50$ kV/cm. Solid and dashed lines refer to the real and imaginary part, respectively.

of the far-from-equilibrium conditions (hot electrons). At low frequencies both kinds of fluctuations concur in determining g_{vv}. However, at frequencies $\omega > 1/\tau_\varepsilon$, τ_ε being the energy relaxation time, the contribution of energy fluctuations tends to disappear. Since this contribution (usually called convective[4,6]) is, in our case, negative, g_{vv} exhibits a maximum. At higher frequencies the region $\omega > 1/\tau_m$, τ_m being the momentum relaxation time, is reached and g_{vv} will tend eventually to zero. The real part of $g_{\varepsilon\varepsilon}$ shows a decay to zero faster than g_{vv} because of a larger value of the energy with respect to the momentum relaxation time. The imaginary parts of g_{vv} and $g_{\varepsilon\varepsilon}$ are reported in the same figure for completeness.

Figure 4 reports the off-diagonal components $g_{v\varepsilon}$ and $g_{\varepsilon v}$. We notice that the real part of $g_{v\varepsilon}$ decays to zero similar to $g_{\varepsilon\varepsilon}$ while the real part of $g_{\varepsilon v}$ achieves a maximum and then decays to zero similar to g_{vv}. These similarities are found to be present in the whole region of electric fields examined. Again, the imaginary parts of $g_{v\varepsilon}$ and $g_{\varepsilon v}$ are reported in the same figure for completeness.

Figure 5 shows the dependence on electric field of the α_{ij} coefficients. The diagonal terms are both positive and satisfactorily agree (see solid and dashed lines in the figure) with the expected momentum and energy relaxation rates which, within the balance equation approach, are given, respectively, by

$$\alpha_{11}=\frac{1}{\tau_m}=\frac{e}{\mu m}\ , \tag{26a}$$

$$\alpha_{22}=\frac{1}{\tau_\varepsilon}=\frac{e\mu F^2}{\langle\varepsilon\rangle-\langle\varepsilon_0\rangle}\ , \tag{26b}$$

where μ and $\langle\varepsilon\rangle$ are, respectively, the chord mobility and the average carrier energy at the given field obtained

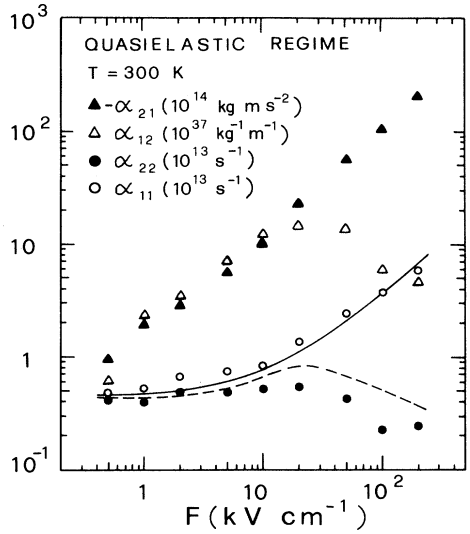

FIG. 5. Set of α_{ij} coefficients as a function of the electric field for the case of quasielastic regime. Different points refer to EMC calculations; the solid and dashed lines refer, respectively, to the momentum and energy relaxation rates evaluated within an electron temperature model [see Eqs. (26a) and (26b) of text].

from the EMC calculations and $\langle \varepsilon_0 \rangle = \frac{3}{2} k_B T$, k_B being the Boltzmann constant and T the equilibrium bath temperature.

The off-diagonal terms α_{12} and α_{21} have to be odd in the field since changing the field direction implies the change in the sign of velocity and its time derivative but not of energy and its time derivative. In particular, the term α_{21} is found to be negative and to exhibit a substantial linear dependence with the electric field. On the contrary, the term α_{12} is found to be positive and to exhibit a linear dependence up to fields of 10 kV/cm; then, in concomitance with the flattening of α_{22}, it reaches a maximum and eventually decreases.

Figure 6 reports the initial values ($t=0$) of the correlation functions as a function of the electric field. Here, EMC results are compared with analytical calculations obtained within an electron temperature model which should approximate well the quasielastic regime. Accordingly, by assuming $\langle \varepsilon \rangle = \frac{3}{2} k_B T_e$, T_e being the electron temperature, it is found that

$$\langle (\delta v)^2 \rangle = \frac{k_B T_e}{m} , \tag{27a}$$

$$\langle (\delta \varepsilon)^2 \rangle = \tfrac{1}{2} (k_B T_e)^2 , \tag{27b}$$

$$\langle \delta v \, \delta \varepsilon \rangle = \tfrac{1}{4} v_d k_B T_e , \tag{27c}$$

where v_d is the drift velocity and the factor $\frac{1}{4}$ in the last expression comes from the assumption that the momentum relaxation time is inversely proportional to the square root of the energy.

The excellent agreement between the data of the simulation and the analytical results further confirms that the physical system is really well described in terms of the quasielastic regime at any field.

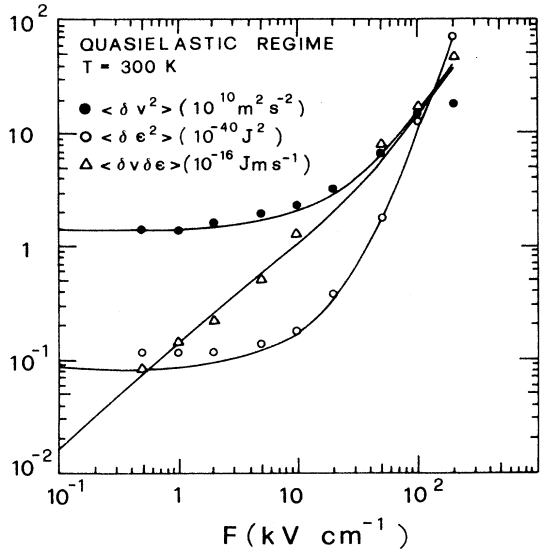

FIG. 6. Initial values ($t=0$) of the correlation functions for the quasielastic regime as a function of the electric field. Points refer to EMC calculations, curves to analytical expressions evaluated within an electron temperature model [see Eqs. (27a), (27b), and (27c) of text].

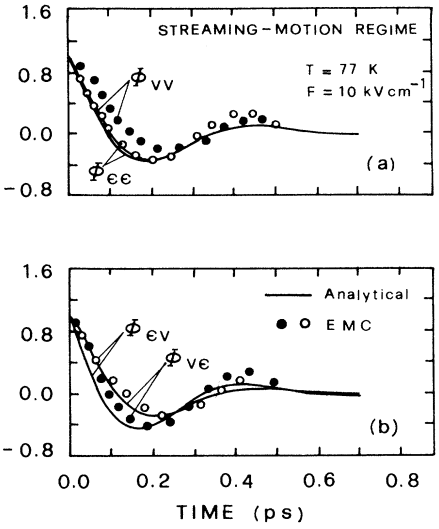

FIG. 7. Normalized correlation functions as a function of time for the case of "streaming-motion regime" at $F=10$ kV/cm. Solid curves and points refer to present theory and EMC calculations, respectively. (a) and (b) refer to autocorrelation and cross-correlation terms, respectively.

B. Streaming-motion regime

Under this condition the odd part of the distribution strongly prevails over the even part, and the shape of the

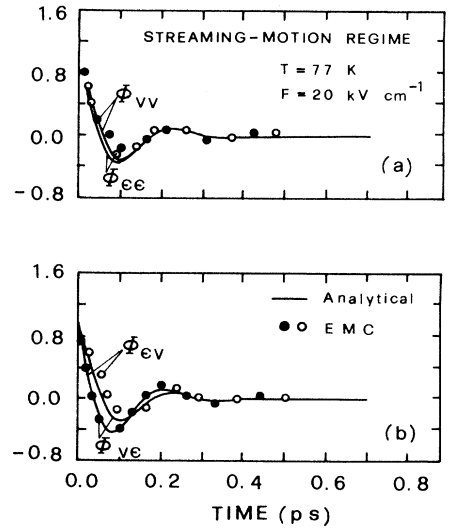

FIG. 8. Normalized correlation functions as a function of time for the case of streaming-motion regime at $F=20$ kV/cm. Solid curves and points refer to present theory and EMC calculations, respectively. (a) and (b) refer to autocorrelation and cross-correlation terms, respectively.

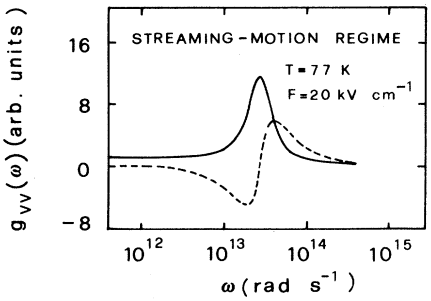

FIG. 9. Spectral density of velocity fluctuations as a function of angular frequency for the case of streaming-motion regime at $F=20$ kV/cm. Solid and dashed lines refer to the real and imaginary part, respectively.

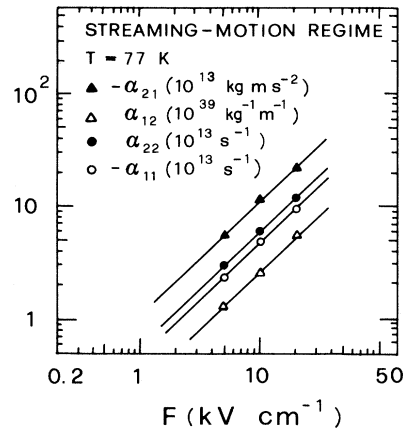

FIG. 10. Set of α_{ij} coefficients as a function of the electric field for the case of the streaming-motion regime. Different points refer to EMC calculations; the lines evidence the linear dependence with the electric field.

distribution function becomes needlelike.[4] To this purpose, the optical phonon coupling has been arbitrarily increased (by a factor 5) with respect to the previous case and the lattice temperature lowered at 77 K.

Figures 7 and 8 show the time behavior of the correlation functions as obtained from the EMC simulations and calculated from Eqs. (25). The agreement between the simulated and calculated values should be considered satisfactory. (We remark that in this case the calculated values are quite sensitive to small variations of β, γ, and of the α_{ij} coefficients.) The wavy behavior of the correlation functions is associated to the streaming character of the distribution function which now describes a quite ordered motion of the carriers. Indeed, the carriers at rest move up to the optical phonon energy and then repeat again this path after emission of an optical phonon. In this case we find that $\lambda<|\omega_0|$ at all fields and, in agreement with the expectations,[4] the relationship $\omega_0=2\pi F(2e^2m\hbar\omega_{\rm op})^{-1/2}$, $\hbar\omega_{\rm op}$ being the optical phonon energy, is verified by the simulation with an accuracy of 15%.

The periodicity in time of the correlation functions is better evidenced by their spectral functions which, apart from irrelevant details, all exhibit the characteristic features as reported in Fig. 9 for the case of $g_{vv}(\omega)$. Here the characteristic frequency ω_0 is clearly identified by the peak in the real part of $g_{vv}(\omega)$.

Figure 10 shows the dependence with electric field of the α_{ij} coefficients. They all exhibit a linear dependence with the electric field and, both α_{21} and α_{11} have been found to be negative. The fact is that now α_{11} can no longer be interpreted as a momentum relaxation rate since, in its ideal form, the streaming-motion regime does not have a truly thermodynamic behavior. This regime falls into the category of what is called "deterministic chaos."[19] Indeed, for $F\neq0$ the fixed point of the distribution function has the needlelike shape previously discussed whatever the strength of the electric field is. This fixed point, however, never has a Boltzmann shape (the velocity distribution no longer having any Gaussian character), which implies that the motion does not correspond to ordinary thermodynamics. In fact, the field drives "deterministically" the electron gas into a state which looks thermodynamical being characterized by a given shape of the distribution function.

The initial values ($t=0$) of the correlation functions are now expected to be independent of the electric field. Their values are reported in Table I together with the theoretical values obtained from Eqs. (27) with $k_BT_e=\frac{2}{9}\hbar\omega_{\rm op}$ and $v_d=(\hbar\omega_{\rm op}/2m)^{1/2}$ according to the streaming-motion model.[4] The agreement is good for $\langle(\delta v)^2\rangle$, while for the other correlation functions a more detailed calculation, accounting for the actual shape of the distribution function, is needed for a better fit. In any case, such a comparison confirms that the physical system is really well described in terms of the streaming-motion regime.

TABLE I. Initial values of the correlation functions under streaming-motion regime.

	$\langle(\delta v)^2\rangle$ [10^{10} (m/s)^2]	$\langle(\delta\varepsilon)^2\rangle$ (10^{-41} J^2)	$\langle\delta\varepsilon\,\delta v\rangle$ (10^{-17} J m/s)	
At any field	0.63	0.17	5.5	Theory
$F=5$ kV/cm	0.68	0.31	12	EMC
$F=10$ kV/cm	0.55	0.33	13	EMC
$F=20$ kV/cm	0.75	0.35	15	EMC

VI. CONCLUSIONS

Within the framework of a quantum Langevin approach we have presented a general theory of the correlation functions for the steady state in far-from-equilibrium conditions driven by an external electric field. By making a coarse graining in time, the slow part of the dynamics is separated from the fast part, thus going into a relaxation-time paradigm. By taking velocity and energy as the relevant macroscopic variables we have succeeded in giving an analytical solution to the closed set of correlation functions coupling velocity and energy fluctuations. The result is found to generalize the linear-response theory to the far-from-equilibrium case (hot electrons).

A numerical simulation based on an ensemble Monte Carlo calculation performed for a simple Si-like model semiconductor has provided a significative test of the analytical theory. Thus we have confirmed the importance of cross-correlation terms in determining the time dependence of the correlation functions. In particular, deviations from simple exponential behavior of the velocity and energy correlation functions are proven here on the grounds of a first-principles calculation based on the Heisenberg equation of motion.

ACKNOWLEDGEMENTS

The authors wish to thank Dr. R. Brunetti and Professor C. Jacoboni for very valuable discussions on the subject. The financial support of Ministero Pubblica Istruzione (MPI) and the Centro Interdipartimentale di Caliolo Automatico e Informatica Applicata (CICAIA) of Modena University is gratefully acknowledged.

APPENDIX

We want here to derive Eq. (13) of the main text linking $S(t-s)$ and $G_0(t-s)$. For this purpose, we introduce the operator $S_R(t-s)$ defined by

$$\frac{\partial S_R(t-s)}{\partial t} = -iL_0 S_R(t-s) , \tag{A1a}$$

$$\frac{\partial S_R(t-s)}{\partial s} = iS_R(t-s)L_0 , \tag{A1b}$$

$$S_R(0)=1 . \tag{A1c}$$

Since here L_0 is time independent, it is clear that $S_R(t-s)=S(s-t)$. More generally, from Eqs. (9) and (A1) one can easily prove that

$$S(t-s)S_R(t-s)=1 . \tag{A2}$$

Now, if we introduce the operator $K(t-s)$ by

$$K(t-s)=S_R(t-s)G_0(t-s) , \tag{A3}$$

it is easy to show from Eqs. (11) and (A1) that

$$\frac{\partial K(t-s)}{\partial s} = iS_R(t-s)L_0\Pi_z G_0(t-s) . \tag{A4}$$

By integrating Eq. (A4) on s, one gets

$$K(t-s)-1=i\int_t^s ds' S_R(t-s')L_0\Pi_z G_0(t-s') , \tag{A5}$$

which reads

$$1-S_R(t-s)G_0(t-s) = i\int_s^t ds' S_R(t-s')L_0\Pi_z G_0(t-s') . \tag{A6}$$

By multiplying Eq. (A6) by $S(t-s)$ and using Eq. (A2), one gets

$$S(t-s)-G_0(t-s) = i\int_s^t ds' S(t-s)S_R(t-s')L_0\Pi_z G_0(t-s') . \tag{A7}$$

Now, it is easily stated that $S(t-s)S_R(t-s')=S(s'-s)$, and from that and Eq. (A7) one gets Eq. (13) of the main text.

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