Long-Time Tail of the Autocorrelation Function for Electron Drift in High Electric Fields in Silicon

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The velocity autocorrelation $\varphi(t)$ function is calculated for electrons moving along a high electric field in n-type silicon. For short times t, it varies as $\exp(-t/\tau_0)$, but for times greater than approximately $1.5\tau_0$, the short-time exponential decay appears to go over to a $t^{-3/2}$ decay. This representation covers the initial relaxation, but a second exponential also appears as relaxation to the nonequilibrium steady state occurs.

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The Brownian motion of a relatively large impurity in a classical liquid has been taken as descriptive of a typical fluctuating system. Since Alder and Wainwright[1] first discovered long-time tails on the velocity autocorrelation function by molecular dynamic calculations for these systems, considerable theoretical interest has centered on this problem.[2,3] Experimental verification has been limited and confined to such classical liquids or gases.[4] That such phenomena, and particularly the $t^{-3/2}$ tail of the velocity autocorrelation function, might be more generally applicable is suggested by much of the theoretical work, but particularly by that of Zwanzig and Bixon,[3] who showed that such behavior followed from the frequency dependence of the frictional damping constant. The behavior found by these latter workers was more complicated, in that $\varphi'(t) = \langle [v(t+t_0) - \langle v\rangle][v(t_0) - \langle v\rangle]\rangle$ became negative and decayed to zero, at long times, with a $t^{-3/2}$ behavior, after passing through a local minimum.

The general case for high-field transport in semiconductors differs in that relaxation of the fluctuation is to a nonequilibrium steady state,[5] and the process is nonlinear.[6,7] However, the response is similar to that found by Zwanzig and Bixon[3] in that $\varphi'(t)$ becomes negative, passes a local minimum, and relaxes finally to $\langle v\rangle^2$,[7] a behavior suggested by the fact that the velocity fluctuation is composed of two portions: $v' = v(t) - \langle v\rangle = v'' + u'$, where u' is the velocity fluctuation arising from a fluctuation of carrier energy, $u' = u(\epsilon + \Delta\epsilon) - u(\epsilon)$, and v'' arises from momentum fluctuations about u'.[7] This general behavior has recently been observed in Monte Carlo calculations.[8] The principal difficulty in calculating transport parameters in these latter systems lies in the complicated energy dependence of the many scattering processes.[9] In the past few years, however, ensemble Monte Carlo techniques have been developed which can be used to calculate these transport parameters with high resolution.[10] In this Letter, we report results for the autocorrelation function of the longitudinal velocity of electrons in a high electric field in Si. These results suggest that a long-time tail exists on the initial, momentum decay of the autocorrelation function and that this tail decays with the characteristic $t^{-3/2}$ behavior discussed above.

As developed by Lebwohl and Price,[10] and subsequently used by Ferry and Barker,[11] the ensemble Monte Carlo technique is a hybrid method in which an ensemble of electrons is adopted. This ensemble is composed of N electrons, with variables R_i, $i = 1, 2, \ldots, N$, where the set $R_i = \{k_i, x_i, \ldots\}$ includes all necessary descriptors of each electron's state. At each time step, all R_i are calculated by a Monte Carlo process, and the set $\{R_i\}$ is treated as an ensemble evolving in time. The ensemble Monte Carlo method is characterized by an ensemble distribution function that evolves with $\{R_i\}$. Variables such as velocity or position are calculated from an ensemble average over $\{R_i\}$ at each time step and the variance is controlled by a sufficiently large value for N. One should be aware, however, of the vagaries of stochastic simulations on a computer, and we have used a variety of fields, number of electrons, and seeds for the random-number generators without affecting these results. In the calculations reported here, a value of $N = 2500$ was used. This value is sufficiently large to give good results for the transient dynamic response of the electrons to a high electric field,[11] for example. Thus the method is capable of yielding good results for the transport characteristics.

In the calculations reported here, the ensemble Monte Carlo method was used to calculate the correlation function for the total velocity, $\varphi(t) = \langle v(t+t_0)v(t_0)\rangle = \varphi'(t) + \langle v\rangle^2$ [all calculations shown in the figures have $\varphi(t)$ normalized to $\langle v^2\rangle$].[12] The ensemble of electrons was initialized as a Max-

wellian at the lattice temperature, 300 K, and was assumed to reside at $x=0$ at $t=0$. A homogeneous electric field of 25 kV/cm was applied at $t=0$, and the ensemble allowed to evolve in time. After approximately 0.4 psec, the ensemble was in a pseudoequilibrium with the field and had a drift velocity near 9×10^6 cm/sec.[13] After this pseudoequilibrium was achieved, the longitudinal velocity autocorrelation function $\varphi(t) = \langle v(t_0+t)v(t_0)\rangle$ was calculated for several initial times t_0. The stationarity of the system was therefore verified as well, and the averaging process was carried out over the ensemble as well as over various initial times. In Fig. 1 is shown the variation of $\varphi(t)$ as a function of time t. The initial fall of $\varphi(t)$ is primarily due to momentum relaxation, with the local minimum and subsequent rise due to energy relaxation as suggested by Price.[7] The error bars indicate the spread of data points from the calculations and averaging procedures.

The initial exponential decay portion is significant. The time constant of this portion of the decay of $\varphi(t)$ is closely related to, and slightly larger than, the momentum relaxation time τ_m associated with the chordal mobility $\mu = v_d/E$, rather than the differential mobility dv_d/dE (here we define the effective or average $\tau_m = m^*\mu/e$). The latter quantity has been suggested as the appropriate quantity for longitudinal diffusion.[14] At 25 kV/cm, the velocity is becoming very nearly saturated, so that the differential mobility is more than an order of magnitude smaller than the chordal mobility. This difference is readily distinguished from the data in Fig. 1. The decay of $\varphi(t) \sim \exp(-t/\tau_0)$ is best fitted with a τ_0 of 7×10^{-14} sec, while $\tau_m \sim 5.4\times10^{-14}$ sec. The result of the decay constant of the exponential portion of $\varphi(t)$ being slightly larger than τ_m appears to be a general result, as it was checked at several other values of electric field. Van Kampen[6] has suggested such a difference would occur. If $v(t)$ decays as $\exp(-t/\tau_m)$, he suggests that a fully nonlinear treatment of noise would have the correlation function decay with a characteristic time $\tau_0 = \tau_m/(1-\epsilon)$, where $\epsilon \sim 1.5\langle v\rangle^2/\langle v^2\rangle$. This gives $\tau_0 \sim 6.8\times10^{-14}$ sec, for the τ_m given above, and this is within the accuracy of the present calculations.

It is clear from Fig. 1, that the initial decay, the momentum relaxation portion, deviates substantially from an exponential for times greater than about 0.1 psec. This initial portion of $\varphi(t)$, for $0 \le t \le 0.3$ psec, is shown in Fig. 2. Here, it is evident that although $\varphi(t)$ decays initially as an exponential, it deviates noticably from this be-

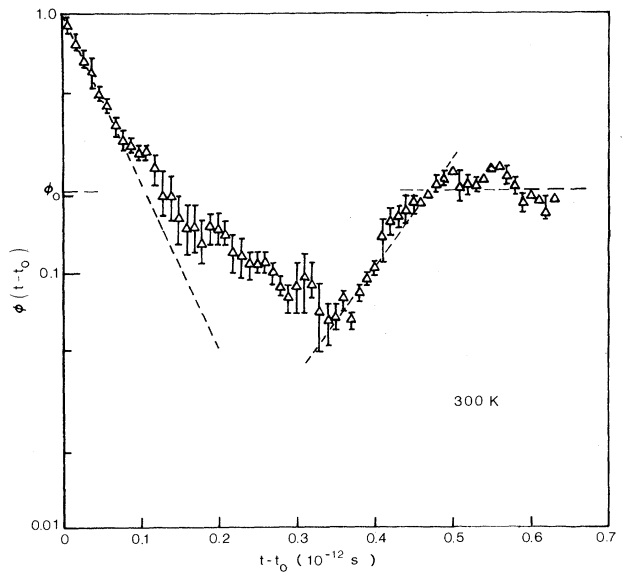

FIG. 1. The correlation function for the total velocity, $\varphi(t) = \langle v(t+t_0)v(t_0)\rangle/\langle v^2\rangle$, for electron motion along a 25-kV/cm electric field in silicon. The horizontal dashed curve is the value of $\langle v^2\rangle$, while the initial decay (dashed curve) shows exponential behavior, at first, with a characteristic time $\tau_0 \sim 7\times10^{-14}$ sec.

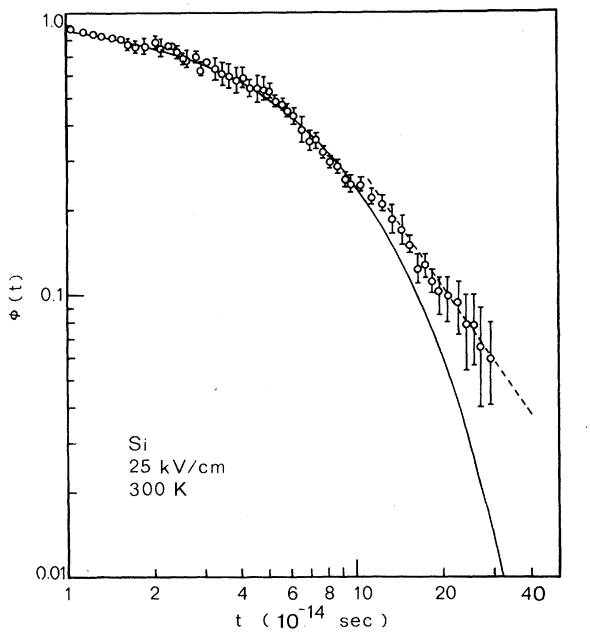

FIG. 2. The initial decay of $\varphi(t)$ from Fig. 1. Here, only the portion for $t \le 0.3$ psec is illustrated to highlight the $t^{-3/2}$ behavior for $t \ge 0.1$ psec. The solid curve is an exponential decay with $\tau_0 \sim 7\times10^{-14}$ sec. The dashed curve is a $t^{-3/2}$ decay.

havior at long times, and begins to decay as $t^{-3/2}$. This behavior differs from that reported by Fauquemberque *et al.*,[8] but appears to be intrinsic to the momentum relaxation process. Gurevich[15] examined the behavior of velocity fluctuations in semiconductors in high electric fields. He pointed out that the correlation function satisfies a differential equation which is described by the same Green's function as solutions of the Boltzmann equation, complete with collision operator.[16] We have carried out preliminary calculations with a Shockley model including elastic collisions.[17] Although a simple model, it is one in which the Green's function can be found and gives results in good agreement with experiment.[18,19] These results indicate that a $t^{-3/2}$ behavior does occur in the high-field case. While the long-time tail on the momentum relaxation portion of $\varphi(t)$ appears to be correct mathematically, its detailed physical origin is not yet clear. However, it does appear to arise from the elastic scattering processes and possibly may be related to streaming (in energy space) allowed by such scattering.[20]

The longitudinal diffusion coefficient can be found by integrating $\varphi'(t)$.[21] This gives a value of $D_l \cong 12$ cm^2/V·sec, where the uncertainty comes from the noise on $\varphi(t)$ and on $v_d(t)$. This yields, as it should, the value found from $\langle(\Delta x)^2\rangle/2t_f$, where $\Delta x = x - v_d t$ and t_f is the final time of calculation (in the limit $t_f \to \infty$), which is also computed simultaneously in these calculations. This value agrees well with the calculations and measurements of Canali *et al.*[22]

In summary, we have found that the longitudinal diffusivity, along a high-electric field in silicon, is characterized by a velocity autocorrelation function which appears to show a $t^{-3/2}$ tail, on its momentum relaxation portion, for long times.

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[12]The use of $\varphi(t)$, rather than the more normal $\varphi'(t)$, follows from the long-time tails investigated. The use of $\varphi(t)$ allows log-log or semilog plots to be used without zero-crossing complications. The two are of course identical for equilibrium cases, but the second equality follows if the process is at least wide-sense stationary. This latter is not a foregone conclusion in nonlinear processes (Ref. 5), and must be checked in each case. As discussed in the text, this was done and calculations with either $\varphi'(t)$ or $\varphi(t)$ were found to agree.

[13]It is generally found that at 25 kV/cm, the transient and overshoot velocity effects decay in less than 0.3 psec (Ref. 11).

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