Generalization of Nyquist-Einstein Relationship to Conditions Far from Equilibrium in Nondegenerate Semiconductors

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We present for the first time an exact decomposition procedure for the current spectral density in the presence of generation-recombination mechanisms. The correct microscopic analysis shows that the cross correlation between velocity and number fluctuations plays an essential role in the noise properties of semiconductors. This, in turn, yields a generalization of the Nyquist-Einstein relationship in the presence of an applied electric field when statistical generation and recombination mechanisms are active.

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At equilibrium the Nyquist-Einstein relationship relates the current spectral density at low frequency S_I with the diffusion coefficient D of a classical ensemble of charge carriers interacting with a thermal bath. For a homogeneous semiconductor device of length L, where the charge carriers responsible for the current are supplied by a single type of impurity levels (donor or acceptor), by definition it is

$$S_I(\omega\to 0)=4\int_0^\infty \langle \delta I(0)\delta I(t)\rangle dt=\frac{4e^2}{L^2}N_0uD, \quad (1)$$

where $I(t)=I(t)-\langle I\rangle$ is the current fluctuation around the steady-state value $\langle I\rangle$, the angular brackets denote a time average (the explicit time dependence will herewith indicate instantaneous quantities), e is the electron charge, N_0 is the number of impurities, and u is the fraction which is ionized. Equation (1) is a consequence of the fluctuation-dissipation theorem[1,2] and thus strictly valid only at equilibrium. The remarkable property of Eq. (1) is that the "many-particle" quantity S_I, which describes current correlations, is related to the "single-particle" quantity D describing one-particle velocity correlations. This occurs only at equilibrium because here the choice of a Maxwell-Boltzmann velocity distribution implies a vanishing contribution of the two-particle interaction, as first pointed out by Gantsevich, Gurevich, and Katilius.[3]

In this Letter we will prove that, provided two-particle interaction can be neglected, Eq. (1) can be generalized to conditions far from equilibrium when, because of an electric field which is externally applied, the device supports a stationary current. When $1/f$ contributions are negligible, an increase of S_I with current towards a quadratic dependence has been observed.[4-6] Such a behavior is usually attributed to the generation-recombination (GR) mechanism which occurs statistically between the conducting band and the impurity levels when these are not fully ionized.[7,8] Microscopically, this interpretation implies a decomposition of the noise sources in terms of two independent contributions,[9] one which is associated with fluctuations in the velocity of carriers while they move in the conducting band (Johnson noise), and the other associated with fluctuations in their number (GR noise). However, these two sources of noise are, in general, coupled. As we shall show, an exact decomposition procedure reveals that an important role can be played by this coupling term.[10] As a starting point, we recall that, from the Ramo-Shockley theorem and its generalization,[11] the total current $I(t)$, as measured in the outside circuit, can be expressed in the following equivalent forms:

$$I(t)=(e/L)N_0v_d^r(t)=(e/L)N(t)v_d(t), \quad (2)$$

where

$$v_d^r(t)=\frac{1}{N_0}\sum_{i=1}^{N_0}v_i(t)$$

is the reduced carrier drift velocity (which accounts for the time spent by the carriers on the impurities, the so-called trapping time), $N(t)$ is the number of carriers in the conducting band (free carriers), and

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

is the free-carrier drift velocity (which neglects the trapping time). The excitation of carriers from bound to conducting states can be viewed as an extreme case of a two-valley transition process, studied by Price,[12] Shockley, Copeland, and James,[13] and Brunetti, Jacoboni, and

Reggiani,[14] when zero velocities are assigned to carriers in one valley. The last expression on the right-hand side of Eq. (2) lends itself to an exact decomposition of S_I in terms of different noise sources. Indeed, from Eq. (2) S_I can be given the two following equivalent expressions:

$$S_I=(4e^2/L^2)N_0^2\int_0^\infty \langle \delta v_d^r(0)\delta v_d^r(t)\rangle dt, \tag{3a}$$

$$S_I=(4e^2/L^2)\int_0^\infty dt\{\langle N\rangle^2\langle \delta v_d(0)\delta v_d(t)\rangle+\langle v_d\rangle^2\langle \delta N(0)\delta N(t)\rangle+\langle N\rangle\langle v_d\rangle[\langle \delta N(0)\delta v_d(t)\rangle+\langle \delta v_d(0)\delta N(t)\rangle]\}. \tag{3b}$$

If two-particle interaction can be neglected, then we have

$$\begin{aligned}\langle \delta v_d^r(0)\delta v_d^r(t)\rangle &=(1/N_0)\langle \delta v^r(0)\delta v^r(t)\rangle;\\ \langle \delta v_d(0)\delta v_d(t)\rangle &=(1/\langle N\rangle)\langle \delta v(0)\delta v(t)\rangle,\end{aligned} \tag{4}$$

where $\delta v^r(t)=v^r(t)-v_d^r$ and $\delta v(t)=v(t)-v_d$.

In terms of the fluctuations of $v_d^r(t)$, from Eqs. (3a) and (4) there follows

$$S_I=(4e^2/L^2)N_0\int_0^\infty \langle \delta v^r(0)\delta v^r(t)\rangle dt. \tag{5}$$

In terms of the fluctuations of $N(t)$ and $v_d(t)$, from Eqs. (3b), (4), and (5) we have

$$S_I=\frac{4e^2}{L^2}N_0D_{\text{tot}}=\frac{4e^2}{L^2}N_0(uD_{vf}+D_{\text{GR}}+D_{\text{cross}}), \tag{6}$$

$$D_{\text{tot}}=\int_0^\infty \langle \delta v^r(0)\delta v^r(t)\rangle dt, \tag{7}$$

$$D_{vf}=\int_0^\infty \langle \delta v(0)\delta v(t)\rangle dt, \tag{8}$$

$$D_{\text{GR}}=(\langle v_d\rangle^2/N_0)\int_0^\infty \langle \delta N(0)\delta N(t)\rangle dt, \tag{9}$$

$$D_{\text{cross}}=u\langle v_d\rangle\int_0^\infty [\langle \delta N(0)\delta v_d(t)\rangle+\langle \delta v_d(0)\delta N(t)\rangle]dt. \tag{10}$$

Equations (6)-(10) represent, in the absence of two-particle interaction, a generalized Nyquist-Einstein relationship which relates noise and diffusion under conditions far from equilibrium. In particular, Eq. (6) generalizes Price's relationship[15] when the velocity of the carriers accounts for trapping and detrapping processes. We notice that under nonlinear response in the applied electric field, also D_{vf} and u become field dependent. By addition of a factor $\exp(i\omega t)$ to the integrands inside Eqs. (7)-(10), the frequency dependence of S_I and D_{tot} can be easily recovered. The total diffusion coefficient D_{tot}, as seen from Eq. (7), can be decomposed into the sum of three terms which are related respectively to fluctuations in free-carrier velocity (D_{vf}), number (D_{GR}), and correlation between number and velocity (D_{cross}). For the isotropic case here considered, D_{tot} and D_{vf} have a longitudinal and a transverse component with respect to the electric field. From their definition in terms of correlation functions [see Eqs. (9) and (10)], it appears that D_{GR} and D_{cross} are proportional to $\langle v_d\rangle^2$ and $\langle v_d\rangle$, respectively. Therefore, they describe excess noise and, as expected, vanish at equilibrium and/or when the noise is measured in a direction perpendicular to the applied field. Clearly, D_{GR} and D_{cross} are identically zero when the traps are fully ionized (i.e., $u=1$), since that implies $\delta N(0)=\delta N(t)=0$.

To give a quantitative example of the above results, a Monte Carlo simulation has been performed for the case of p-type silicon (boron doped) at 77 K where recent experiments performed by Vaissiere and co-workers[6,16] are available. From a standard simulation[17] in the presence of GR mechanism we obtain D_{tot}. Although possible in principle, a direct evaluation of the single terms in Eqs. (8)-(10) is, at present, beyond our computational capabilities, because of the large difference in the characteristic times governing trapping versus scattering processes. To provide an estimate of the cross correlation term, the following procedure has been followed. Without losing in accuracy, but saving computing time, D_{vf} is calculated from the transverse rather than the longitudinal diffusion coefficient. Then D_{GR} is calculated from the standard expression,[7] $D_{\text{GR}}=[\langle v_d\rangle^2u^2(1-u)]/[\gamma(2-u)^2]$, where u and the generation rate γ are consistently estimated from the simulation. Within these approximations, D_{cross} is evaluated by difference following Eq. (6). The details of the numerical calculations are given elsewhere[18] and the results are reported in Figs. 1-3. Figure 1 shows the different contributions to the total diffusion coefficient as a function of the applied electric field. The only experi-

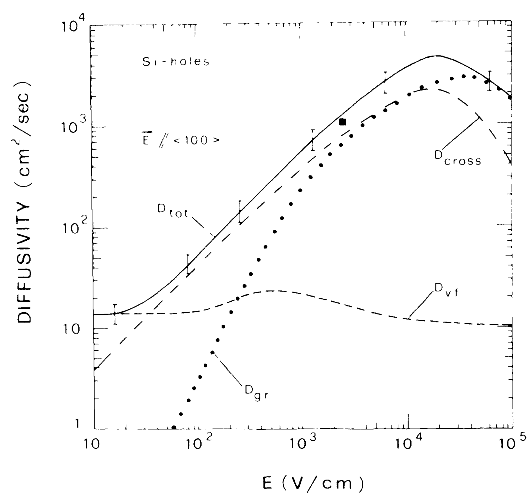

FIG. 1. Total (continuous curve) and individual (broken curves) diffusion coefficients as functions of the electric field for the case of p-type silicon (boron doped) at 77 K with $N_0=3\times10^{15}$ cm^3. Curves report Monte Carlo calculations with bars indicating uncertainties. The point presents the only experimental result available at present (see Refs. 6 and 16).

mental result available at present[6,16] is reported for comparison with theory. At the lowest electric fields only the velocity-fluctuation contribution is present, in agreement with the equilibrium Nyquist-Einstein relationship (1). At increasing fields the three components of the diffusion coefficient exhibit quite different field dependences. While D_{vf} varies very slowly, $D_{\rm GR}$ and $D_{\rm cross}$ have respectively a quadratic and a linear field dependence, as anticipated above, up to about 10^3 V/cm. $D_{\rm GR}$ becomes predominant at 10^4 V/cm. Then, on further increase of the field, both $D_{\rm GR}$ and $D_{\rm cross}$ are found to reach a maximum and then decrease. This behavior should be attributed to the onset of hot-electron conditions, here starting above 100 V/cm. As known,[19] under these conditions the energy distribution function deviates from its equilibrium Maxwell-Boltzmann shape, and the average carrier energy increases with the electric field. As a consequence, $\langle v_d \rangle$ tends to saturate and, because of the lower efficiency of the recombination processes, u tends to unity. This, in turn, yields the high-field dependence of $D_{\rm GR}$ shown in Fig. 1. In other words, at high fields $D_{\rm GR}$ is much more sensitive to the carrier mean energy than to the detailed shape of the carrier distribution function. In the field region where $D_{\rm cross}$ dominates over $D_{\rm GR}$, we ascribe its larger value to the strong coupling between velocity and number fluctuations of carriers. From a microscopic point of view, this coupling occurs in the low-energy region (below about 1 meV in this case) of the carrier distribution function where the scattering rate for recombination processes is comparable with or larger than those for interaction with the lattice. This can be seen in Fig. 2, where we show the energy dependence of the scattering rates due to the different mechanisms which have been used in the Monte Carlo simulations. Physically, the importance of $D_{\rm cross}$ is connected with the fact that the carriers, when first thermally ionized, do not have the same energy distribution as the steady one in the conducting band (and correspondingly for capture). They differ over what Price called the "aging time" in his pioneer paper on intervalley noise.[12] However, carrier heating, by decreasing the population in the low to the advantage of the high region of the energy distribution function, weakens this velocity-number correlation, in fact, decoupling the velocity and number noise sources. As a result $D_{\rm cross}$ is found to reach a maximum value (which corresponds to $u \simeq 0.7$) and then to decrease at the highest fields. Similar results for $D_{\rm cross}$ are found for different acceptor concentrations, as reported in Fig. 3. Here we observe that, with increasing impurity concentration, the value of $D_{\rm cross}$ decreases at low fields and its maximum shifts to higher fields. The former behavior is determined by the smaller value assumed by the factor $\langle v_d \rangle u$ at larger impurity concentrations. The latter is associated with the fact that higher fields are also necessary in order to have u close to unity (and consequently a vanishing value of $D_{\rm cross}$).

In conclusion, we have proven that, when two-particle interactions are neglected, the Nyquist-Einstein relationship can be generalized to conditions far from equilibrium to include statistical carrier generation and recombination through traps. This implies a reinterpretation of the diffusion coefficient which, in addition to velocity fluctuations, includes contributions from the fluctuations in carrier number and their cross correlation. This last contribution represents a new term which is responsible for an extra source of noise in the presence of a stationary current (excess noise). A numerical calculation has

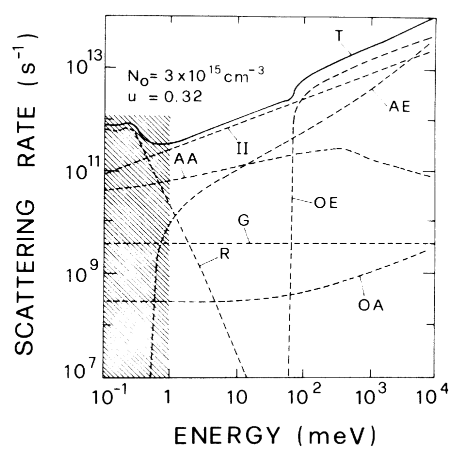

FIG. 2. Scattering rate as a function of energy for holes in Si at 77 K. AA, acoustic absorption; AE, acoustic emission; OA, optical absorption; OE, optical emission; II, ionized impurities; G, generation; R, recombination; T, total. The shaded region emphasizes the range of energy where the recombination rate prevails over other scattering rates. Notice that the generation rate is independent of the carrier energy, which represents now the energy level of the trap.

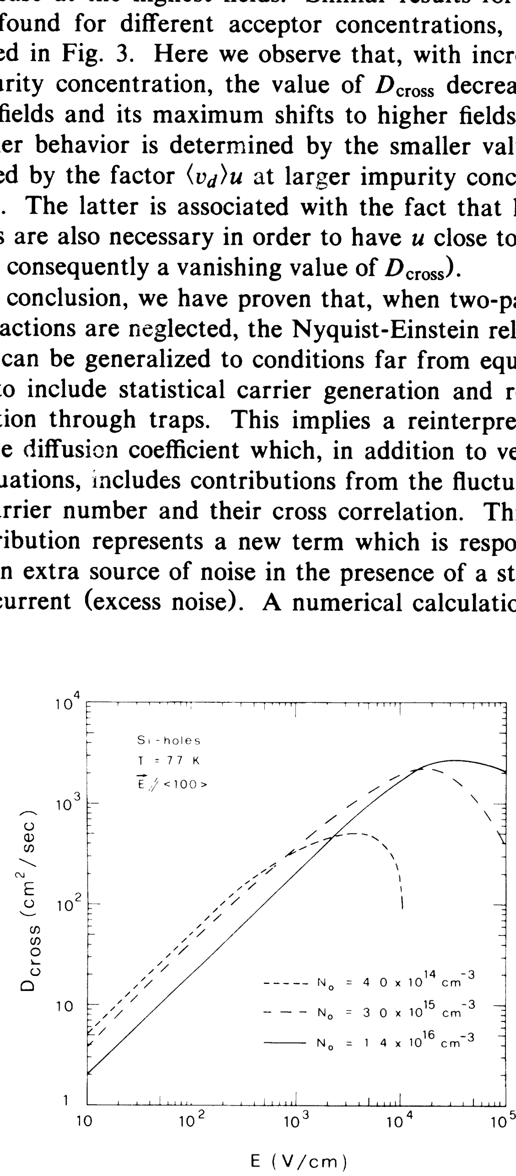

FIG. 3. Diffusion coefficient associated with cross correlations in carrier number and velocity fluctuations as a function of the electric field for different impurity concentrations.

been performed for the case of p-type silicon. In agreement with available experiments, the relevance of this extra term is clearly evidenced when an exact decomposition procedure is used to interpret noise-diffusion quantities as a function of the electric field.

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