Generalization of Thermal Conductivity and Lorenz Number to Hot-Carrier Conditions in Nondegenerate Semiconductors

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We present a generalization to high-field transport of the carrier thermal conductivity and Lorenz number in nondegenerate semiconductors. The theory is based on the correlation-function formalism. In its range of validity, it provides exact values and predicts an anisotropic behavior of the above parameters with respect to the direction of the applied field. Calculations for the case of *n*-Si at 300 K evidence a dramatic decrease, more than 2 orders of magnitude, of the longitudinal values at the highest fields of 100 kV/cm. [S0031-9007(96)00785-5]

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Small-signal kinetic coefficients are of fundamental and applied importance for the study and characterization of electronic transport in semiconductor materials and devices. Under linear response in the applied field, Onsager phenomenological relations and Kubo formalism provide a rigorous theoretical framework [1]. However, at increasing fields above the onset of hot-carrier conditions, no general relations are available and we rely on more or less attainable solutions of the kinetic equation [2]. To this extent, differential conductivity and diffusivity have been already thoroughly investigated and rigorous generalizations to hot-carrier conditions have been developed theoretically and verified experimentally [3,4]. On the contrary, for the case of thermoelectric coefficients only approximate approaches, mostly based on heated Maxwellian energy distributions [5,6], are available. To fill such a lack of knowledge, and point out the physical weakness of existing approaches, this Letter presents a generalization of the thermal conductivity associated with charge transport to conditions far from linear response. This generalization should be of basic interest in the field of physical kinetics, as well as of practical interest in the modeling of submicron semiconductor devices. Indeed, in ultrashort structures even small values of the applied voltage are responsible for local electric fields well above the limit of validity for a linear response analysis over thermal-equilibrium conditions. To this purpose a generalization of the Wiedemann-Franz law and the Lorenz number under high electric fields is of fundamental importance if not a crucial step for any microscopic modeling [7–10].

The present approach applies an extension of Kubo formalism [11–13] to far from equilibrium conditions. Accordingly, with respect to the standard definition of thermal conductivity near thermodynamic equilibrium, the correlation functions of microscopic fluxes are calculated with respect to stationary values at the given bias point and the thermodynamic temperature T_0 is replaced by the noise-temperature spectrum associated with velocity fluctuations at the given field E and angular frequency ω, $T_n(E,\omega)$, making use of the exact Price relationship [14]. The thermal conductivity along the direction of the field, $\kappa(E,\omega)$, and the corresponding Lorenz number, $L(E,\omega)$, generalized to hot-carrier conditions are thus given by

$$\kappa(E,\omega) = \frac{n}{KT_n^2(E,\omega)} \times \frac{I_{11}(E,\omega)I_{22}(E,\omega) - I_{12}(E,\omega)I_{21}(E,\omega)}{I_{11}(E,\omega)}, \quad (1)$$

$$T_n(E,\omega) = \frac{e^2 n}{K\sigma_d(E,\omega)} I_{11}(E,\omega), \quad (2)$$

$$I_{\nu\mu}(E,\omega) = \int_0^{+\infty} C_{\nu\mu}(t)\exp(-i\omega t)\,dt, \qquad \nu,\mu \equiv 1,2, \quad (3a)$$

$$C_{\nu\mu}(t) = \overline{\delta j_\nu(0)\delta j_\mu(t)}, \quad (3b)$$

$$L(E,\omega) = \frac{\kappa(E,\omega)}{\sigma_d(E,\omega)T_n(E,\omega)}. \quad (4)$$

Here n is the carrier concentration, K the Boltzmann constant, e the electron charge, $j_1 = v(\mathbf{k})$, $j_2 = v(\mathbf{k})\epsilon(\mathbf{k})$

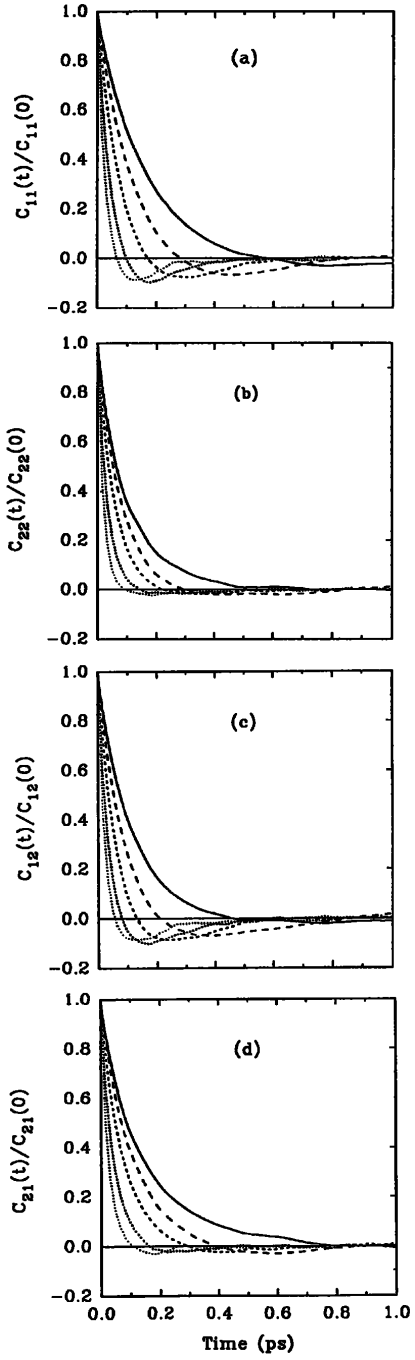

FIG. 1. Longitudinal correlation functions normalized to their initial value for extrinsic n-Si with doping concentration $n = 10^{17}$ cm^{-3} at 300 K and increasing electric-field strengths respectively of 5, 10, 20, 50, and 100 kV/cm in passing from the longest (continuous curve) to the shortest (finest dotted curve) time decay. Values refer to the direction of the electric field along the $\langle 111 \rangle$ crystallographic axes.

[$v(\mathbf{k})$ and $v(\mathbf{k})\epsilon(\mathbf{k})$ being the carrier velocity and energy flux as functions of wave vector $\mathbf{k}$ along the field direction], $\sigma_d(E, \omega)$ the differential electrical conductivity, and $\delta j_\mu(t)$ the fluctuation of $j_\mu(t)$ around its average value. In (3b) we assume ergodicity so that the overbar denotes time average. Properties of the above scheme are as follows: (i) Under thermal-equilibrium conditions (i.e., $E = 0$) $T_n(\omega) = T_0$, thus Onsager relations are fulfilled, and standard linear-response formalism is recovered [1]. (ii) The frequency dispersion of thermal conductivity contains in general several time scales, e.g., those related to momentum and energy relaxation. (iii) Under nonlinear response in the applied field, the constraint $\sigma_d > 0$, which implies electrical stability of the system, must be satisfied and thermal conductivity and Lorenz number become anisotropic with respect to the field direction. Values along the transverse direction of the field can be obtained from Eqs. (1)–(4) by calculating the correspondent correlation functions [15], and replacing the differential with the chord conductivity.

The correlation functions and conductivities entering the definition of κ and L are calculated using a Monte Carlo simulator [16]. We have considered the case of extrinsic n-Si, doping concentration 10^{17} cm^{-3}, at $T_0 = 300$ K with the field applied along the $\langle 111 \rangle$ crystallographic direction, being this a physical system of relevant interest for applied purposes. Figures 1(a)–1(d) report the four longitudinal correlation functions $C_{\nu\mu}(t)$ at increasing values of the electric field. Curves are normalized to their initial value to make better use of the time scales. In general, at increasing fields curves exhibit a faster decay and the presence of a negative part, a behavior associated with the shortening and coupling of both momentum and energy relaxation times due to hot-carrier effects. Even at vanishing fields, and thus for continuity at thermal equilibrium, $C_{22}(t)$ decays faster than other functions because its decay rate is practically the sum of momentum and energy rates. An analogous but less pronounced behavior is exhibited by the two cross-correlation functions. An important result is that, even at thermal

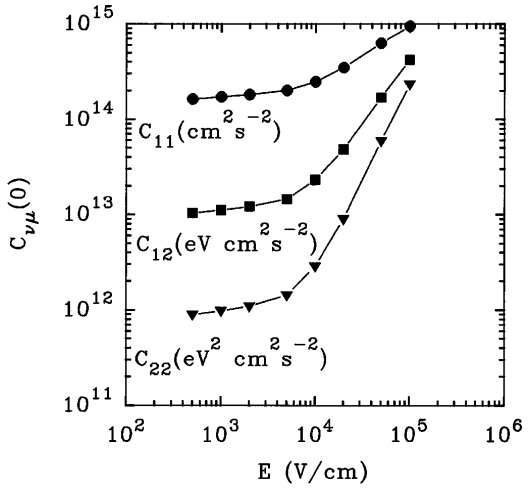

FIG. 2. Variance of the correlation functions of Fig. 1 as a function of electric-field strength.

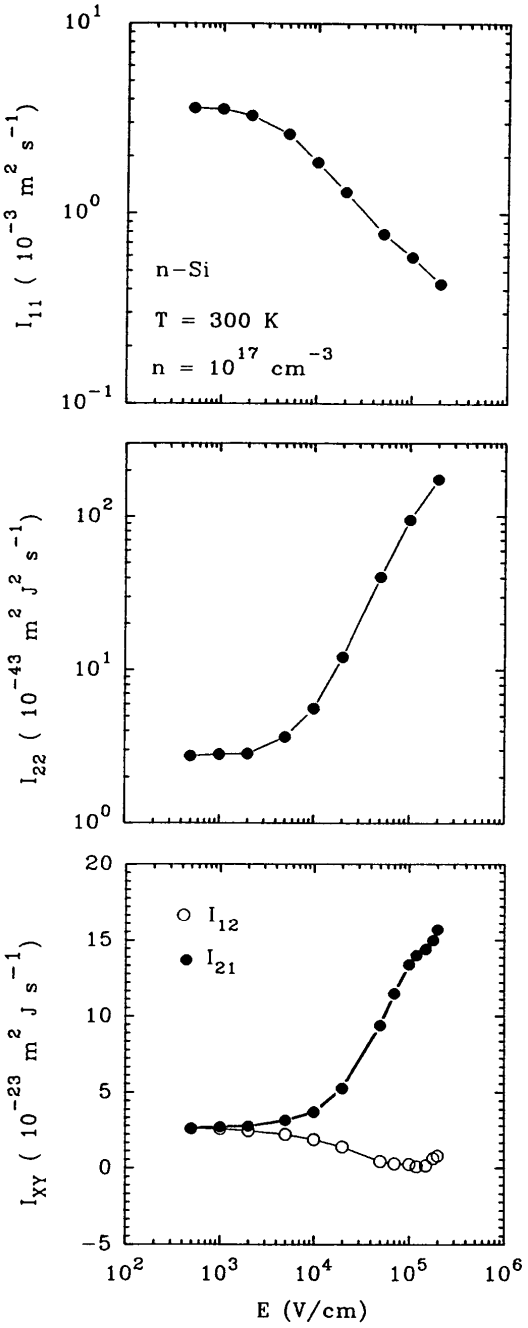

FIG. 3. Spectral densities of the correlation functions of Figs. 1 and 2 at $\omega = 0$ as a function of electric-field strength.

equilibrium, the simple relaxation time approach based on a single time scale is not valid. We remark that the couples of correlation functions $C_{11}(t)$, $C_{12}(t)$ and $C_{22}(t)$, $C_{21}(t)$ have similar features, being characterized by the initial fluctuation of the same variable: velocity for the former, energy for the latter. For the sake of completeness, the variances $C_{11}(0)$, $C_{22}(0)$, and $C_{12}(0) = C_{21}(0)$ are reported in Fig. 2 as a function of the electric field. Here hot-carrier effects are responsible for a systematic

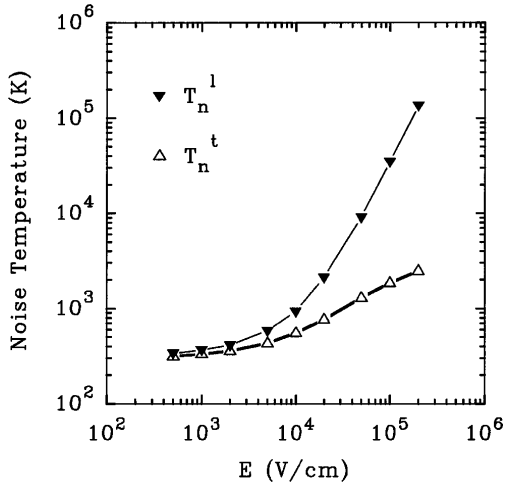

FIG. 4. Equivalent noise-temperature data in *n*-Si at 300 K as a function of electric-field strength. Full triangles refer to the longitudinal and open triangles to the transverse direction with respect to the electric field.

increase of all variances which exhibit asymptotic behaviors steeper for higher moments. Similar behaviors, apart from the absence of the negative part, are found for the transverse correlation functions. Figure 3 reports the low frequency ($\omega = 0$) spectral densities $I_{\nu\mu}(E, 0)$ of the respective correlation functions as a function of the electric field. The different behaviors exhibited by different spectral densities are the result of the competitive effect between shortening time scales and increasing variances of the corresponding correlation functions at increasing fields. Accordingly, $I_{11}(E, 0)$, which corresponds to the longitudinal diffusivity, decreases due to the prevailance of shortening time scale, while $I_{22}(E, 0)$ increases

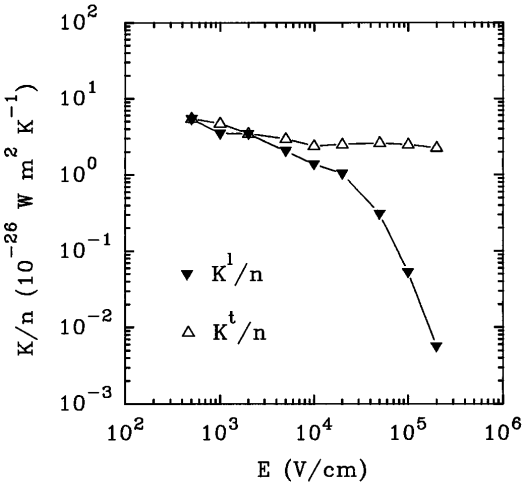

FIG. 5. Thermal conductivity per unit concentration in *n*-Si at 300 K as a function of electric-field strength. Full triangles refer to the longitudinal and open triangles to the transverse direction with respect to the electric field.

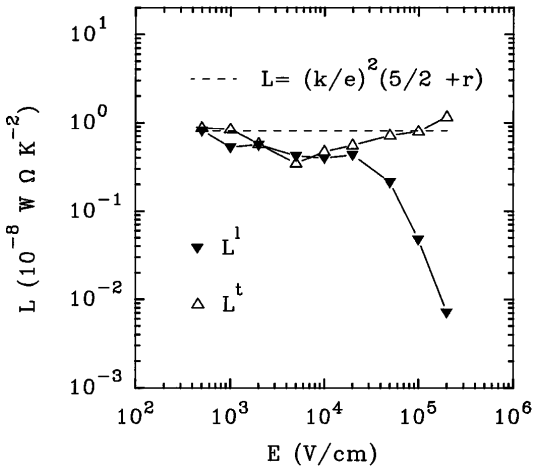

FIG. 6. Lorenz number in *n*-Si at 300 K as a function of electric-field strength. Full triangles refer to the longitudinal and open triangles to the transverse direction with respect to the electric field. Dashed line refers to the linear-response value obtained using an energy-dependent relaxation-time approach with the energy exponent $r = -1.4$ best fitted by the present calculations.

because of the prevailance of increasing variance. The cross-correlation spectral densities exhibit an interesting opposite feature. At the lowest field they are equal, thus fulfilling Onsager relations. At increasing fields, I_{21} parallels the I_{22} behavior, while I_{12} exhibits a nonmonotonic behavior with a minimum at 100 kV/cm. These significant differences between I_{21} and I_{12} due to the presence of a negative part in the correlation function C_{12} (with a maximum effect at 100 kV/cm) which is absent in C_{21}. The longitudinal and transverse noise-temperature data are reported in Fig. 4 as a function of electric fields. The faster increases of the longitudinal with respect to the transverse value reflects the difference between the differential and the chord conductivity. The carrier thermal conductivity at low frequency calculated from Eq. (1) is shown in Fig. 5. Here longitudinal and transverse values are reported for the sake of comparison. We remark that the large difference between the two values reflects the higher value of the longitudinal with respect to the transverse noise-temperature value. In particular, for semiconductors exhibiting negative differential conductivity (NDC) a thermal conductivity cannot be defined for fields above the threshold value for NDC. The generalized Lorenz number obtained for both cases is reported in Fig. 6. The dashed curve in the same figure represents the classical value $L = (K/e)^2(5/2 + r)$ [17] obtained within an energy-dependent relaxation-time approximation with $r = -1.4$ as best fit value. Again, the presence of hot carriers strongly modifies the linear-response value and, for the longitudinal case, a dramatic decrease for more than 2 orders of magnitude is predicted at the highest fields considered.

In conclusion, the carrier thermal conductivity and Lorenz number in semiconductors has been generalized to the case of high-field transport. Calculations applied to *n*-Si at 300 K show a strong anisotropic behavior, with the longitudinal value exhibiting a dramatic decrease for more than 2 orders of magnitude with respect to its linear-response value at the highest fields considered.

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