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Quantum transport in the coupled electron–acoustic-phonon system: Application to energy transport in Si and Ge

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The ambipolar carrier and energy transport in highly excited semiconductors is studied within a hydrodynamic model in the relaxation-time approximation, which is rederived quantum mechanically. The electronic sybsystem is considered to be scattered by acoustic-phonon deformation potential. In particular, the ambipolar transport coefficients of diffusion and thermal conductivity, as well as those describing cross effects (Dufour and Soret coefficients), are theoretically derived.

I. INTRODUCTION

The problem of irreversible processes in solids and especially the evaluation of nonequilibrium quantities like transport coefficients has mainly been treated within two methods: the Boltzmann equation approach[1–3] and the linear-response method.[4–7]

In the linear-response method and its variants (Kubo method,[4] Mori projection-operator formalism,[5] and various Green's function techniques[6,7]) one assumes that the response of the electronic system is proportional to the applied fields and that the constant of proportionality can be found by means of correlation functions evaluated in equilibrium. These methods have been extensively used in calculations of transport coefficients like electronic conductivity when the system is acted upon by external fields. Apart from the difficulties one has with divergences in perturbation expansions of the thermal averages in these methods, there are some open questions concerning their validity itself, namely the expansion of the response in a power series of the driving force and consideration of the first-order term only,[8] and the problem of dissipation of energy, since the linear-response formalism treats the system adiabatically.[9] Efforts to overcome these drawbacks have led towards a refinement of the Kubo method, the so-called resolvent approach,[5,10–12] and also to a formulation of nonlinear-response theory.[13,14]

In a somewhat parallel way, Mori,[15] Jackson and Mazur,[16] and later Zubarev[17] have tried to treat thermal transport coefficients like heat conductivity, diffusion coefficient, and viscosity, which cannot be described by terms in the Hamiltonian but are due to spatial inhomogeneities. The common thread in these theories is the local-equilibrium concept, which is also extended to the many-particle distribution function.

Within the framework of transport theory one assumes that field gradients cause only slight deviations of electron or hole distribution functions from equilibrium. In the Boltzmann-equation method, which is the one adopted here, one constructs a transport equation, i.e., a self-consistent equation for the perturbed distribution function, by suitably decoupling correlations in particle motions which are contained in the collision integral.

In the present work an effort is made to deduce the ambipolar transport coefficients of diffusion, thermal conductivity, thermodiffusion, and Dufour coefficient for Si and Ge by means of a Boltzmann equation linearized around a homogeneous nonequilibrium state. We work in the hydrodynamic approximation (mean free time of carriers is very much less than relaxation time), and the scattering mechanism is assumed to be the isotropic deformation potential due to acoustic phonons.

II. THE HAMILTONIAN

We start from the familiar idea of considering the semiconductor as a "gas" of excitations with respect to the vacuum state, $|0\rangle$. If we restrict ourselves to two electronic bands, this vacuum state means zero number of electrons (e) in the conduction band and of holes (h) in the valence band ($N_e = N_h = 0$). This also defines the zero-point momentum $\mathbf{p}_0 = 0$ and energy $E_0 = 0$.

Nonpolar-optical-phonon scattering depends on the symmetry of the band structure being very weak for carriers at the Γ point or for $\langle 100 \rangle$ minima (case of GaAs, etc.). It is, however, strong for minima along $\langle 111 \rangle$ directions. Polar-optical-phonon scattering for intermediate and higher temperatures remains the most important scattering mechanism in compound semiconductors in general. Other less important scattering mechanisms like ionized- or neutral-impurity scattering (the former being of long-range Coulomb type and the latter of much shorter range and weaker), are neglected in the present work, since we deal with perfect materials. Carrier-carrier interactions in semiconductors usually affect transport properties very little,[18] since they simply redistribute momentum and energy among carriers and no dissipation takes place. Numerical efforts concerning this interaction have been made by various authors.[19,20] Carrier–acoustic-phonon interactions are due to deformations of the local crystal parameters, as a result of the acoustic-phonon-induced strain, causing in turn a variation of the local band-structure characteristics of the material. The corresponding perturbation potential has the form

$$\hat{U}^{\lambda\text{-ph}}(\mathbf{r}) = C^{\lambda}\nabla\cdot\hat{\mathbf{u}}(\mathbf{r}) \; . \tag{2.1}$$

Here C^λ ($\lambda=e,h$) is the deformation potential parameter and $\hat{\mathbf{u}}$ the elastic displacement field. This type of carrier-phonon interaction is usually most important for covalent semiconductors (for a review see Ref. 21). Thus in the present work subsystems to be considered in detail are the electron field, the hole field, and the longitudinal displacement field with given dispersion relations (modes) $E^\lambda(\mathbf{p}^\lambda)$ and $\hbar\omega(k)$, respectively. The Hamiltonian operator for the coupled electron (hole)-phonon system, reads

$$\hat H=\hat H^{\lambda}+\hat H^{\mathrm{ph}}+\hat H^{\lambda\text{-ph}},\quad \lambda=e,h\ . \tag{2.2}$$

The Wigner operator $\hat N^\lambda$ for the subsystem λ can be written in terms of the field operators $\hat\Psi^\dagger_\lambda,\hat\Psi_\lambda$ as follows:[22-24]

$$\hat N^{\lambda}(x,t)=\hbar^3\int d\gamma\, e^{-i\gamma\cdot\mathbf{p}}\hat\Psi^\dagger_\lambda(\mathbf{r}-\tfrac{1}{2}\hbar\boldsymbol{\gamma},t)\hat\Psi_\lambda(\mathbf{r}+\tfrac{1}{2}\hbar\boldsymbol{\gamma},t)\ , \tag{2.3}$$

where $x=(\mathbf{r},\mathbf{p})$ with the inverse relation

$$\int \hat N^{\lambda}(\mathbf{r},\mathbf{p},t)d\mathbf{p}=(2\pi\hbar)^3\hat\Psi^\dagger_\lambda(\mathbf{r},t)\hat\Psi_\lambda(\mathbf{r},t)\ . \tag{2.4}$$

In the Wigner representation $\hat H^\lambda$ has the following form:

$$\hat H^{\lambda}=\int_V\int_{\mathrm{BZ}}\frac{d^6x}{(2\pi\hbar)^3}E_0^\lambda(|\mathbf{p}|)\hat N^{\lambda}(\mathbf{r},\mathbf{p},t)\ . \tag{2.5}$$

Here V is the volume of the system, $d^6x=d^3r\,d^3p$, and the momentum integral is taken over the first Brillouin zone. $E_0^\lambda(|\mathbf{p}|)$ represents the energy-dispersion relations of the noninteracting quasiparticles λ. The second term on the right-hand side of (2.2) describes the phonon subsystem, while the third term describes the electron- or hole-phonon interaction. In terms of $\hat N^\lambda$ it has the form

$$\hat H^{\lambda\text{-ph}}=C^\lambda\int\frac{d^6x}{(2\pi\hbar)^3}\nabla\cdot\hat{\mathbf{u}}(\mathbf{r},t)\hat N^{\lambda}(\mathbf{r},\mathbf{p},t)\ . \tag{2.6}$$

The elastic field displacement $\hat{\mathbf{u}}$ is given through the following relation:

$$\hat{\mathbf{u}}(\mathbf{r},t)=\frac{1}{(2\pi)^3}\left[\frac{\hbar V}{2\rho}\right]^{1/2}\times\int d\mathbf{k}\frac{e^{-i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{\omega(\mathbf{k})}}\mathbf{e}(\mathbf{k})[\hat b^\dagger(-\mathbf{k})-\hat b(\mathbf{k})]\ , \tag{2.7}$$

where $\hat b^\dagger,\hat b$ represent phonon creation and annihilation operators in the Heisenberg representation. It is to be noted that the Wigner operator $\hat N^\lambda$ is bilinear with respect to $\hat\Psi^\dagger_\lambda$ and $\hat\Psi_\lambda$, whereas $\hat{\mathbf{u}}$ depends linearly on $\hat b^\dagger$ and $\hat b$. It is therefore impossible to express the interaction term $\hat H^{\lambda\text{-ph}}$ via a Wigner operator for the phonon field. In the Appendix the collision integral appropriate for the electron (hole)–acoustic-phonon interaction is rederived quantum mechanically and the corresponding relaxation time $\tau^{\lambda\text{-ph}}$ is used in Sec. IV for the linearization of the Boltzmann equation.

III. THE HOMOGENEOUS STATE: PARAMETRIZATION

In order to describe relaxation of the homogeneous systems to equilibrium within the Boltzmann picture, two different time scales are introduced: mean collision time $\tau_c^{\lambda\lambda'}$ and relaxation time $\tau_r^{\lambda\lambda'}$ ($\tau_c^{\lambda\lambda'}\ll\tau_r^{\lambda\lambda'}$). The second occurs in turn in two different time scales: while fast processes (*e*-*e*, *h*-*h*, and *e*-*h* scattering) are assumed to establish a temperature in each subsystem, the slow ones (*e*-ph and *h*-ph scattering, *e*-*h* recombination) control deviations of the subsystems from equilibrium. The equilibrium state is characterized by (a) the electronic distributions ($\lambda=e,h$)

$$f_0^\lambda(\mathbf{p}^\lambda)=\frac{1}{N}\langle\hat N^{\lambda}\rangle_0=\left[1+\exp\left[\frac{E^\lambda(\mathbf{p})-\mu^\lambda}{k_BT^\lambda}\right]\right]^{-1}, \tag{3.1}$$

where μ^λ is the respective chemical potential, (b) vanishing collision integrals $I^{\lambda\lambda'}=0$ for every pair of subsystems λ,λ', and (c) the elastic field displacement $\hat{\mathbf{u}}$ satisfying the equations

$$\mathbf{u}_0=\langle\hat{\mathbf{u}}\rangle_0=0\ , \tag{3.2}$$

$$\langle\hat{\mathbf{u}}^2\rangle_0=\frac{\hbar}{\rho V}\sum_{\mathbf{k}}\frac{1}{\omega(\mathbf{k})}[\tfrac{1}{2}+f_0^{\mathrm{ph}}(\mathbf{k})]\neq0\ , \tag{3.3}$$

where $f_0^{\mathrm{ph}}(\mathbf{k})=\langle\hat b^\dagger(\mathbf{k})\hat b(\mathbf{k})\rangle_0$. With respect to the above parameters the following is assumed.[25]

(i) Electronic subsystems are in quasiequilibrium. The chemical potentials are in general unequal, $\mu^e(n,T)\neq\mu^h(n,T)$, while equality holds in the case of equilibrium. The carrier densities $n^e=n^h=n$ are therefore independent of T. The corresponding relaxation time towards equilibrium ($\mu^e=\mu^h$) is long compared with the lifetime τ of *e*-*h* pairs and can be considered as infinite.

(ii) There is nonequilibrium between subsystems:

$$T^e=T^h=T,\quad \Delta T=T-T^{\mathrm{ph}}\neq0\ . \tag{3.4}$$

The relaxation to the state $\Delta T=0$ due to inelastic scattering is also taken to be slow.

(iii) The phonon system remains in thermal equilibrium. The present state is thus characterized by the parameter set $\{T,n,T^{\mathrm{ph}}\}$. An additional drift can be included, as has been discussed in Ref. 25.

IV. THE INHOMOGENEOUS STATE: LINEARIZATION

The evolution of an inhomogeneous electronic system proceeds as a superposition of the following processes: (a) collisions, classified as a fast process and the only source of irreversibility, (b) free flow, characterized by position-dependent drift velocities $\mathbf{w}^\lambda(\mathbf{r})$, and (c) average field, i.e., Vlassov-like terms in the case of an inhomogeneous plasma. The last two processes, classified as slow ones, are nondissipative and reversible.

General functions f^λ satisfying $I^{\lambda\lambda'}=0$ have the form (3.1), where all intensive parameters depend on $\mathbf{r}^\lambda$. The first-order correction for elastic collisions is obtained by linearizing the kinetic equation for the distribution function f^{λ}:

$$\left[\frac{\partial}{\partial t}+\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{r}}\right]f^{\lambda}(x,t)=I^{\lambda\text{-ph}}(x,t) \tag{4.1}$$

by means of the relaxation time $\tau_r^{\lambda\text{-ph}}$. The collision integral assumes the following form:

$$I^{\lambda\text{-ph}}=-\frac{f^{\lambda}-f_0^{\lambda}}{\tau_r^{\lambda\text{-ph}}},\quad \lambda=e,h \tag{4.2}$$

where f_0^{λ} is the quasiequilibrium distribution function (3.1). Using the equipartition approximation for the equilibrium phonon system one finds[18,26]

$$\tau^{\lambda\text{-ph}}(|\mathbf{p}^{\lambda}|)=A_{-1}^{\lambda\text{-ph}}|\mathbf{p}^{\lambda}|^{-1}, \tag{4.3}$$

where

$$A_{-1}^{\lambda\text{-ph}}=\frac{\pi\rho\hbar^4 s^2}{m^{\lambda}(C^{\lambda})^2 k_B T^{\text{ph}}} . \tag{4.4}$$

$A_{-1}^{\lambda\text{-ph}}$ contains the material parameters C^{λ}, m^{λ}, the mass density ρ, and sound velocity s. Substituting (4.2) in (4.1) leads to

$$f^{\lambda}(x,t)=f_0^{\lambda}(x,t)-\frac{\partial f_0^{\lambda}}{\partial \mathbf{p}^{\lambda}}\tau_r^{\lambda\text{-ph}}(\mathbf{p}^{\lambda})T^{\lambda}[E^{\lambda}(x)X_u^{\lambda}+X_n^{\lambda}] ,\qquad \lambda=e,h \tag{4.5}$$

where

$$\mathbf{X}_n^{\lambda}=\nabla\left[-\frac{\mu^{\lambda}}{T^{\lambda}}\right]+\frac{\mathbf{F}^{\lambda}}{T^{\lambda}} , \tag{4.6}$$

$$\mathbf{X}_u^{\lambda}=\nabla\left[\frac{1}{T^{\lambda}}\right] \tag{4.7}$$

are the thermodynamic forces. $\mathbf{F}^{\lambda}$ is the local electrostatic force exerted on the particle λ.

V. THE HYDRODYNAMIC QUANTITIES

In the hydrodynamic picture for electrons and holes a characteristic length l_H^{λ} associated with the inhomogeneities of the system can be introduced:

$$(l_H^{\lambda})^{-1}=\max\frac{\nabla|f^{\lambda}(x,t)|}{f^{\lambda}(x,t)} , \tag{5.1}$$

and a characteristic time $\tau_H^{\lambda\text{-ph}}=l_H^{\lambda}/v_{\tau}^{\lambda}$ for which $\tau_c^{\lambda\text{-ph}}\ll\tau_r^{\lambda\text{-ph}}\ll\tau_H^{\lambda\text{-ph}}$ is assumed to be valid. In this case an adequate description can be given in terms of local macroscopic fields: mass, velocity, and energy density. If $\xi^{\lambda}(x)$ represents a microscopic one-particle property, the corresponding current density is obtained from the following averages with respect to $f^{\lambda}(\mathbf{r},\mathbf{p},t)$:

$$\mathbf{j}_{\xi}^{\lambda}(\mathbf{r},t)=n^{\lambda}\left\langle\xi^{\lambda}\frac{\partial E^{\lambda}}{\partial \mathbf{p}_{\lambda}}\right\rangle , \tag{5.2}$$

from which for $\xi^{\lambda}=1$ one obtains the particle current density

$$\mathbf{j}_n^{\lambda}=n^{\lambda}\left\langle\frac{\partial E^{\lambda}}{\partial \mathbf{p}_{\lambda}}\right\rangle , \tag{5.3}$$

and for $\xi^{\lambda}=E^{\lambda}$ the local energy current density

$$\mathbf{j}_u^{\lambda}=n^{\lambda}\left\langle E^{\lambda}\frac{\partial E^{\lambda}}{\partial \mathbf{p}_{\lambda}}\right\rangle . \tag{5.4}$$

By carrying out the averages in (5.3) and (5.4) by means of the distribution function (4.5) we are led to the following results for the current densities:

$$\mathbf{j}_n^{\lambda}=\overleftrightarrow{\mathbf{L}}_{nn}^{\lambda}\mathbf{X}_n^{\lambda}+\overleftrightarrow{\mathbf{L}}_{nu}^{\lambda}\mathbf{X}_u^{\lambda} , \tag{5.5}$$

$$\mathbf{j}_u^{\lambda}=\overleftrightarrow{\mathbf{L}}_{un}^{\lambda}\mathbf{X}_n^{\lambda}+\overleftrightarrow{\mathbf{L}}_{uu}^{\lambda}\mathbf{X}_u^{\lambda},\quad \lambda=e,h \tag{5.6}$$

where $\overleftrightarrow{\mathbf{L}}_{jk}=\overleftrightarrow{\mathbf{L}}_{kj}$ are the transport tensors, local properties which can be expressed as momentum averages with respect to f_0^{λ}:

$$\overleftrightarrow{\mathbf{L}}_{nn}^{\lambda}=T^{\lambda}n^{\lambda}\left\langle\frac{\partial}{\partial \mathbf{p}_{\lambda}}\otimes\left[\tau^{\lambda\text{-ph}}(\mathbf{p}_{\lambda})\frac{\partial E^{\lambda}}{\partial \mathbf{p}_{\lambda}}\right]\right\rangle_0 , \tag{5.7}$$

$$\overleftrightarrow{\mathbf{L}}_{nu}^{\lambda}=T^{\lambda}n^{\lambda}\left\langle\frac{\partial}{\partial \mathbf{p}_{\lambda}}\otimes\left[\tau^{\lambda\text{-ph}}(\mathbf{p}_{\lambda})\frac{\partial E^{\lambda}}{\partial \mathbf{p}_{\lambda}}E^{\lambda}\right]\right\rangle_0 , \tag{5.8}$$

$$\overleftrightarrow{\mathbf{L}}_{uu}^{\lambda}=T^{\lambda}n^{\lambda}\left\langle\frac{\partial}{\partial \mathbf{p}_{\lambda}}\otimes\left[\tau^{\lambda\text{-ph}}(\mathbf{p}_{\lambda})\frac{\partial E^{\lambda}}{\partial \mathbf{p}_{\lambda}}(E^{\lambda})^2\right]\right\rangle_0 , \tag{5.9}$$

where $\otimes$ means dyadic product. The explicit dependence on the relaxation time can be seen. With $\tau^{\lambda\text{-ph}}$ in the deformation potential model (4.3) and (4.4) (isotropic case), $\partial E^{\lambda}/\partial \mathbf{p}_{\lambda}$ just cancels the $\mathbf{p}$ dependence of $\tau^{\lambda\text{-ph}}(\mathbf{p}_{\lambda})$. Furthermore, only the diagonal matrix elements $(\overleftrightarrow{\mathbf{L}}_{jk}^{\lambda})_{xx}=(\overleftrightarrow{\mathbf{L}}_{jk}^{\lambda})_{yy}=(\overleftrightarrow{\mathbf{L}}_{jk}^{\lambda})_{zz}$ are nonzero:

$$L_{nn}^{\lambda}=\frac{1}{3\pi^2\hbar^3}g^{\lambda}k_B T^2 A_{-1}^{\lambda\text{-ph}}F_0^{\lambda} , \tag{5.10}$$

$$L_{nu}^{\lambda}=\frac{2}{3\pi^2\hbar^3}g^{\lambda}k_B^2 T^3 A_{-1}^{\lambda\text{-ph}}F_1^{\lambda} , \tag{5.11}$$

$$L_{uu}^{\lambda}=\frac{1}{\pi^2\hbar^3}g^{\lambda}k_B^3 T^4 A_{-1}^{\lambda\text{-ph}}F_2^{\lambda} . \tag{5.12}$$

Here, g^{λ} is the degeneracy factor for particle λ and the parameters F_{ν}^{λ} stand for the Fermi integrals of the νth order:

$$F_{\nu}^{\lambda}(\eta^{\lambda})=\int_0^{\infty}\frac{x^{\nu}}{e^{x-\eta^{\lambda}}+1}dx,\quad \nu \text{ real} , \tag{5.13}$$

and

$$\eta^{\lambda}=\frac{\mu^{\lambda}}{k_B T^{\lambda}}$$

is the reduced chemical potential.

VI. THE AMBIPOLAR TRANSPORT

Despite the fact that interactions within the electronic system are neglected, the e and h subsystems are macroscopically correlated by means of the electric field, which results because of the local charge imbalance due to the fact that electrons and holes tend to diffuse at different speeds. This field is given by the Poisson equation

$$\nabla\cdot\mathbf{E}=\frac{|e|}{\epsilon_0}(n^h-n^e)\ . \tag{6.1}$$

Due to this field the electron and hole currents are correlated. In the ambipolar approximation we set $n^h \simeq n^e$ but require that

$$\mathbf{j}_n^e=\mathbf{j}_n^h=\mathbf{j}_n\ , \tag{6.2}$$

$$\mathbf{j}_u^e+\mathbf{j}_u^h=\mathbf{j}_u\ . \tag{6.3}$$

We are thus left with only one particle and one energy current controlled by the following thermodynamic forces:

$$\mathbf{X}_n=\mathbf{X}_n^e+\mathbf{X}_n^h\ , \tag{6.4}$$

$$\mathbf{X}_u=\mathbf{X}_u^e=\mathbf{X}_u^h\ . \tag{6.5}$$

By expressing the currents (5.5) and (5.6) in terms of these forces and taking into account the continuity equation for electrons and holes, one gets the following ambipolar expressions for the transport coefficients:

$$L_{nn}=\frac{L_{nn}^eL_{nn}^h}{L_{nn}^e+L_{nn}^h}\ , \tag{6.6}$$

$$L_{nu}=\frac{L_{nu}^eL_{nn}^h+L_{nu}^hL_{nn}^e}{L_{nn}^e+L_{nn}^h}\ , \tag{6.7}$$

$$L_{uu}=L_{uu}^e+L_{uu}^h-\frac{(L_{nu}^e-L_{nu}^h)^2}{L_{nn}^e+L_{nn}^h}\ . \tag{6.8}$$

VII. THE AMBIPOLAR TRANSPORT COEFFICIENTS

By introducing instead of $\mathbf{X}_n,\mathbf{X}_u$ a new set of forces, namely gradients of temperature ∇T and particle number density ∇n, we obtain the following expressions for the currents (5.5) and (5.6):

$$\mathbf{j}_n=-D_T\frac{\nabla T}{T}-D\nabla n\ , \tag{7.1}$$

$$\mathbf{j}_u=-K\nabla T-B_T\nabla n\ , \tag{7.2}$$

where the coefficients are explained below.

(a) D is the ambipolar diffusion coefficient at constant temperature for (e,h) pairs:

$$D=\frac{L_{nn}}{T}\left[\frac{\partial\mu}{\partial n}\right]_T\ . \tag{7.3}$$

The isothermal derivative of the chemical potential is given by

$$\left[\frac{\partial\mu}{\partial n}\right]_T=\frac{2k_BT}{n}\left[\frac{F_{1/2}^e}{F_{-1/2}^e}+\frac{F_{1/2}^h}{F_{-1/2}^h}\right]\ . \tag{7.4}$$

The coefficient D is plotted as a function of the carrier density for Si and Ge in Fig. 1 for $T=20$, 60, and 100 K. The various parameters used for the calculations are taken from Table I. The results show that in the classical domain, i.e., for $n<10^{18}$ cm^{-3}, D remains practically constant, its classical value being for Si $\simeq 40$, 50, and 85 cm^{2}sec^{-1} at temperatures $T=20$, 60, and 100 K and for Ge $\simeq 100$, 130, and 220 cm^{2}sec^{-1} at the same temperatures. The onset of the quantum regime (carrier degeneracy) is marked by an abrupt increase of the diffusion parameter.

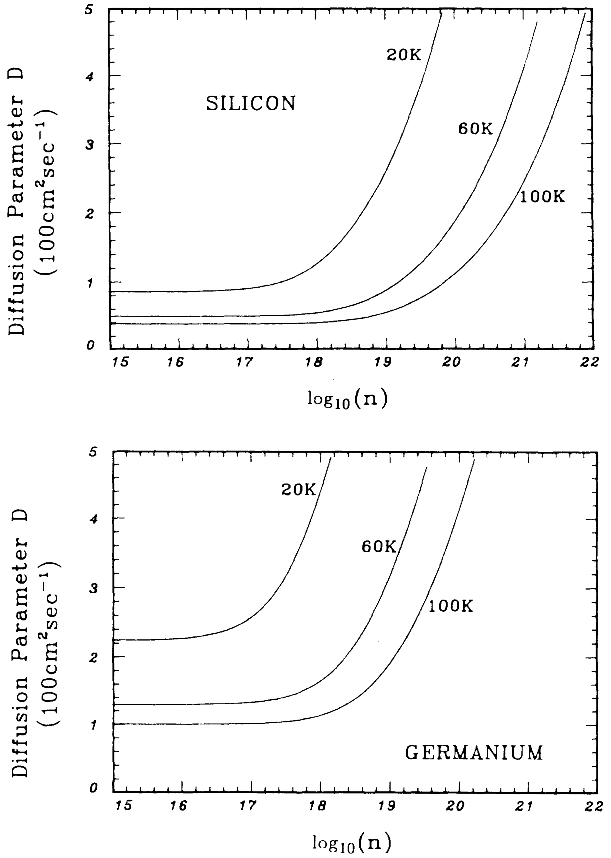

FIG. 1. Isothermal ambipolar diffusion coefficient for Si and Ge as a function of carrier density: it is almost constant in the classical limit while in the quantum limit it grows fast.

(b) D_T is the thermodiffusion coefficient:

TABLE I. Material parameters used for the calculation of transport coefficients. m^e, m^h are density-of-states effective masses. m_0^e is the bare electron mass. E_g stands for the energy gap.

	Si	Ge
ρ (g/cm^3)	2.33	5.32
s (10^5 cm/sec)	9.01	5.33
m^e/m_0^e	0.322	0.216
m^h/m_0^e	0.56	0.37
C^e (eV)	-7.0^a	-11.3^b
C^h (eV)	-10.2^a	-8.2^a
E_g (eV)	1.12	0.72
g^e	12	8
g^h	2	2

[a] Reference 39.

[b] Reference 40.

$$D_T=\frac{1}{T}\left[L_{nu}-L_{nn}\left[\frac{\partial u}{\partial n}\right]_T\right], \tag{7.5}$$

where

$$\left[\frac{\partial u}{\partial n}\right]_T=3k_BT\left[\frac{F^e_{1/2}}{F^e_{-1/2}}+\frac{F^h_{1/2}}{F^h_{-1/2}}\right]. \tag{7.6}$$

The coefficient D_T describes the transport of (e,h) pairs induced by temperature gradients (Soret effect). As shown in Fig. 2 for Si and Ge, D_T vanishes in the classical limit whereas in the degenerate case it increases at a fast rate.

(c) K is the thermal conduction coefficient:

$$K=\frac{1}{T^2}\left[L_{uu}-L_{nu}\left[\frac{\partial u}{\partial n}\right]_T\right], \tag{7.7}$$

which, when plotted versus carrier density (Fig. 3) shows a similar behavior to that of D_T.

(d) B_T is the Dufour coefficient:

$$B_T=\frac{1}{T}L_{nu}\left[\frac{\partial \mu}{\partial n}\right]_T . \tag{7.8}$$

It describes the energy transport due to concentration gradients (Dufour effect). In Fig. 4 the ratio B_T/T versus carrier density for Si and Ge is plotted. Its overall behavior resembles that of the D coefficient.

The drift mobility μ_d^λ of electrons and holes can be obtained by means of the Einstein relation:

$$\mu_d^\lambda=\frac{D^\lambda\,|\,e\,|}{2k_BT}\frac{F^\lambda_{-1/2}}{F^\lambda_{1/2}},\quad \lambda=e,h . \tag{7.9}$$

The mobility μ_d^λ has been plotted versus carrier density in Fig. 5 for Si and Ge for various temperatures. The onset of the degenerate regime is accompanied by a fast decrease of μ_d^λ, approaching zero values at very high densities. For increasing temperatures μ_d^λ assumes systematically lower values, as expected. Figure 6 displays μ_d^λ as a function of temperature in the nondegenerate case for Si and Ge. In this approximation $(\mu^e \rightarrow -\infty)$ the Fermi integrals can be approximated as follows:

$$\lim_{\eta\rightarrow-\infty} F_\nu(\eta)=\Gamma(\nu+1)e^{\eta} , \tag{7.10}$$

where $\Gamma(z)$ is the gamma function.

The mobility obtained in this approximation behaves according to a $T^{-3/2}$ law. The results of the present

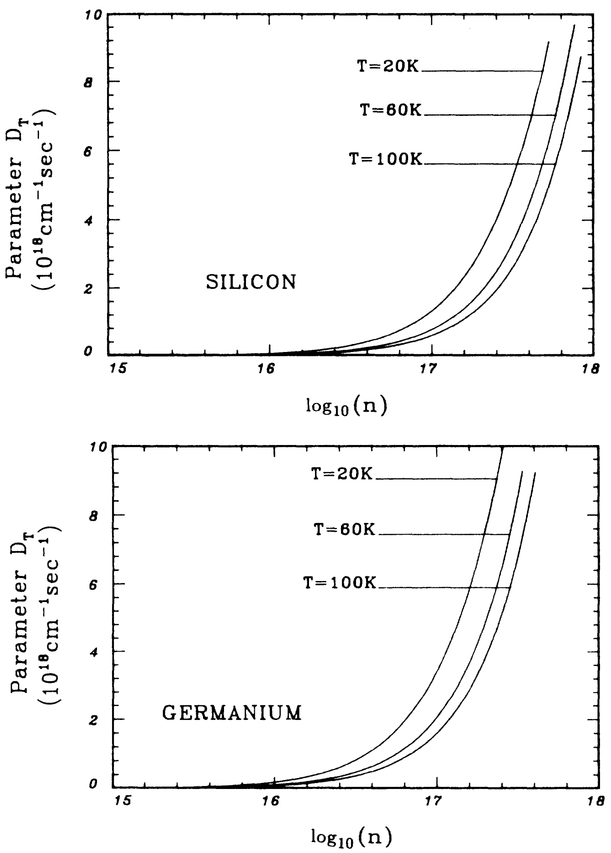

FIG. 2. Ambipolar thermodiffusion coefficient as a function of carrier density n for Si and Ge. In the nondegenerate case it declines to zero.

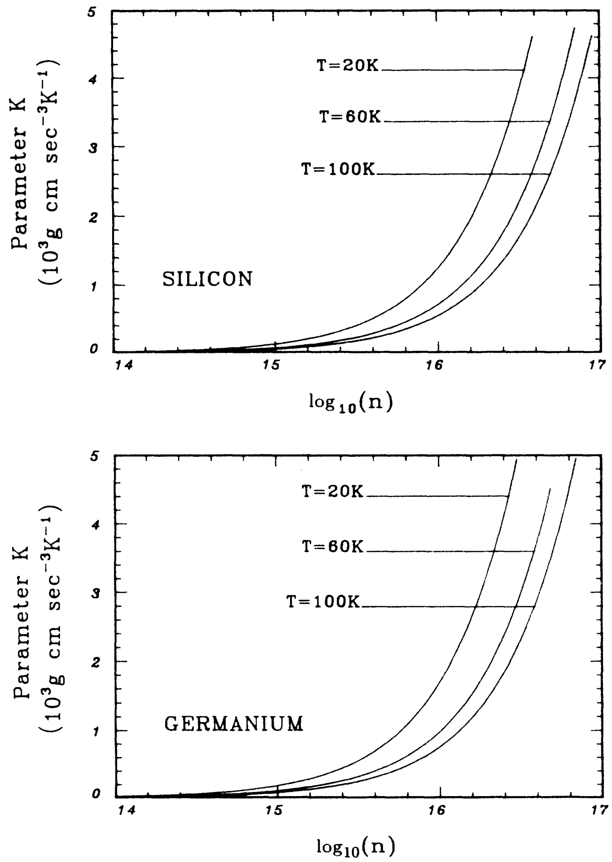

FIG. 3. Ambipolar thermal conduction coefficient as a function of the carrier density n for Si and Ge. A qualitatively similar behavior to the case of the thermodiffusion coefficient is to be noted.

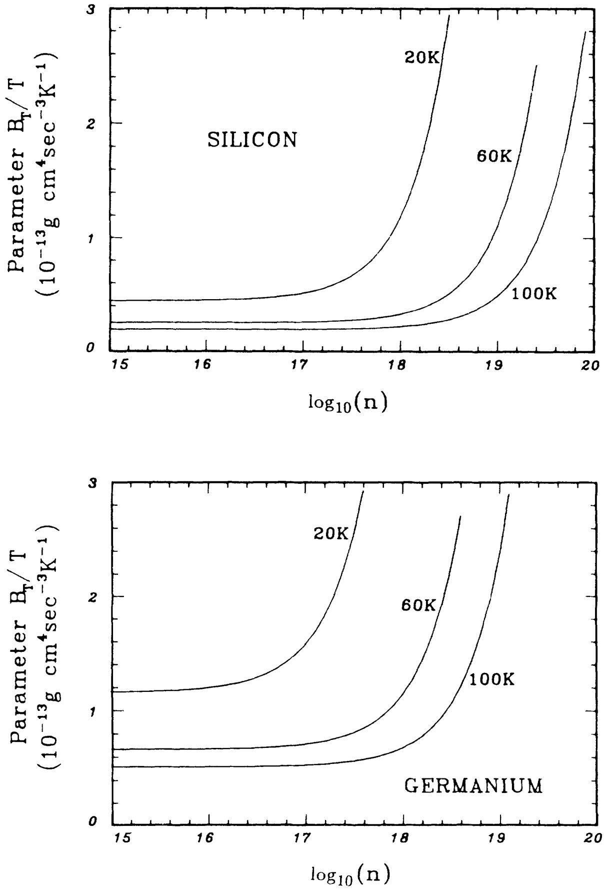

FIG. 4. Ambipolar Dufour coefficient as a function of the carrier density n for Si and Ge. It displays a qualitatively similar behavior to that of the diffusion coefficient.

work are represented in the figures by the straight line, together with experimental results. In the nondegenerate case one recovers the Wiedemann-Franz-Lorenz law:

$$\frac{K^e}{\sigma^e T^e}=3\frac{k_B^2}{e^2} , \qquad (7.11)$$

where $\sigma^e=n^e e \mu_d^e$ is the electronic conductivity. At very high carrier densities many-body effects (exchange and correlation) are expected to play an important role in the carrier transport,[27] especially in three ways: higher scattering rates within the carrier subsystem, energy-gap narrowing, and renormalization of the effective mass via self-energy corrections. The last effect can be taken into account by introducing self-consistent potentials $U^{\lambda\lambda'}$, $\lambda,\lambda'=e,h$ (see also Ref. 22), just as is done for the electron-phonon interaction in the Appendix. Meyer and Glicksman[28] have reported that at high densities carrier-carrier scattering has a considerable effect on the drift mobility while, as concluded theoretically,[29] ambipolar diffusivity does not seem to undergo changes, at least in first order. Effective-mass renormalization does not seem to play a significant role[30] for densities less than 10^{21} cm^{-3}. Band-gap narrowing and band-gap gradients can be induced at high densities either by self-energy shifts of the quasiparticles and density gradients, or by heating of the lattice as a result of increased carrier-phonon interactions. Their effect will be a decrease of the ambipolar diffusivity.[27,31]

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APPENDIX: QUANTUM-MECHANICAL DERIVATION OF THE COLLISION INTEGRAL

The equations of motion for the fields $\hat{\mathbf{u}}$ and $\hat{N}$ can be found by means of the Heisenberg equations:

$$\frac{\partial^2\hat{\mathbf{u}}}{\partial t^2}-s^2\nabla^2\hat{\mathbf{u}}=\frac{C^\lambda}{\rho(2\pi\hbar)^3}\boldsymbol{\nabla}\int \hat{N}^\lambda(\mathbf{r},\mathbf{p},t)d\mathbf{p} , \qquad (\mathrm{A1})$$

where ρ is the mass density of the material, T_σ the tension coefficient, and $s^2=T_\sigma/\rho$ is the sound velocity. The corresponding equation of motion for $\hat{N}$ is

$$\left[\frac{\partial}{\partial t}+\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{r}}\right]\hat{N}^\lambda(\mathbf{r},\mathbf{p},t)=\frac{i}{\hbar(2\pi)^3}\int d\boldsymbol{\gamma}\, d\boldsymbol{\eta}\, e^{i\boldsymbol{\gamma}\cdot(\boldsymbol{\eta}-\mathbf{p})}[\hat{U}^{\lambda\text{-ph}}(\mathbf{r}-\tfrac{1}{2}\hbar\boldsymbol{\gamma})-\hat{U}^{\lambda\text{-ph}}(\mathbf{r}+\tfrac{1}{2}\hbar\boldsymbol{\gamma})]\hat{N}^\lambda(\mathbf{r},\boldsymbol{\eta},t) , \qquad (\mathrm{A2})$$

where

$$\hat{U}^{\lambda\text{-ph}}(\mathbf{r})=C^\lambda\boldsymbol{\nabla}\cdot\hat{\mathbf{u}}(\mathbf{r}) . \qquad (\mathrm{A3})$$

$\hat{U}^{\lambda\text{-ph}}$ can be viewed as the potential operator for the quasiparticle-phonon coupling. From the operator equations we go over to equations for the moments of $\hat{N}^\lambda$. By statistically averaging the Wigner operator one gets[23]

$$\langle \hat{N}^\lambda(x,t)\rangle=N^\lambda f^\lambda(x,t) , \qquad (\mathrm{A4})$$

where f^λ stands for the one-particle distribution function and N^λ is the total particle number. The kinetic equations for the distribution function f (we suppress the index λ in the following) can be obtained by averaging (A2). One can easily verify that the resulting equation has the form

$$\hat{L}_a f=I(\mathbf{r},\mathbf{p},t) , \qquad (\mathrm{A5})$$

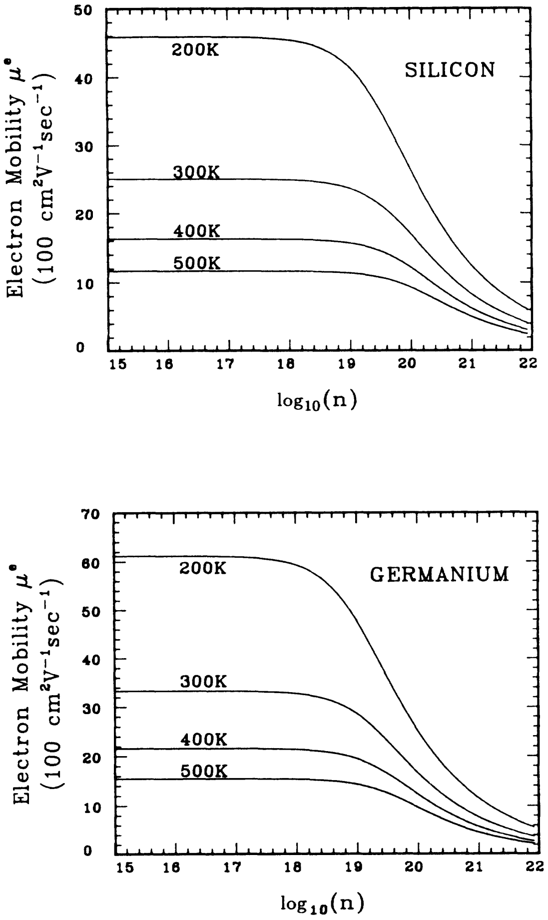

FIG. 5. Electronic drift mobility as a function of the carrier density in Si and Ge. In the classical case it remains practically constant, whereas in the degenerate case it vanishes.

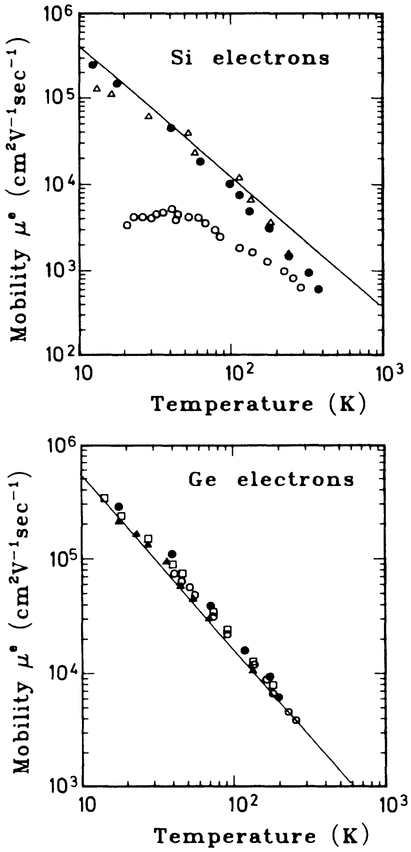

FIG. 6. Electron mobility in Si and Ge as a function of the temperature, in the nondegenerate regime. The straight line refers to the results of the present work. The experimental data are, for Si, (a) open circles, Ref. 32, (b) solid circles, Ref. 33, and (c) open triangles, Ref. 34; and for Ge, (a) open circles, Ref. 35, (b) solid circles, Ref. 36, (c) solid triangles, Ref. 37, and (d) open squares, Ref. 38.

where $\hat{L}_a$ is defined as follows:[23]

$$\hat{L}_a A(\mathbf{r},\mathbf{p},t)=\left[\frac{\partial}{\partial t}+\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{r}}\right]A(\mathbf{r},\mathbf{p},t)-\frac{iN}{\hbar(2\pi)^3}\int d\gamma\, d\eta\, e^{i\gamma\cdot(\eta-\mathbf{p})}\langle[\hat{U}(\mathbf{r}-\tfrac{1}{2}\hbar\gamma)-\hat{U}(\mathbf{r}+\tfrac{1}{2}\hbar\gamma)]\rangle A(\mathbf{r},\eta,t)\ . \tag{A6}$$

The term involving $\hat{U}$ describes a mean-field-type self-energy renormalization due to the carrier-phonon coupling. Expanding this term, the operator $\hat{L}_a$ in (A5) takes the conventional form for quasiparticles (compare Ref. 22):

$$\hat{L}_a=\frac{\partial}{\partial t}+\frac{\partial E}{\partial \mathbf{p}}\cdot\frac{\partial}{\partial \mathbf{r}}+\frac{\partial E}{\partial \mathbf{r}}\cdot\frac{\partial}{\partial \mathbf{p}} \tag{A7}$$

with

$$E(\mathbf{r},\mathbf{p})=E_0(p)+\langle\hat{U}^{\lambda\text{-ph}}\rangle\ . \tag{A8}$$

Since the phonon subsystem is treated in the harmonic approximation, one finds that $\langle\hat{U}\rangle=C\nabla\cdot\langle\hat{\mathbf{u}}\rangle=0$ (in equilibrium). Thus the operator $\hat{L}_a$ in (A7) can further be simplified:

$$\hat{L}_a=\frac{\partial}{\partial t}+\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{r}}\ . \tag{A9}$$

On the other hand, the collision integral $I(\mathbf{r},\mathbf{p},t)$ on the right-hand side of (A5) has the form

$$I(\mathbf{r},\mathbf{p},t)=\frac{1}{N\hbar(2\pi)^3}\int d\gamma\, d\eta\, e^{i\gamma\cdot(\eta-\mathbf{p})}(\langle\delta\hat{U}\delta\hat{N}\rangle_{\mathbf{r}-(1/2)\hbar\gamma,\mathbf{r},\eta,t}-\langle\delta\hat{U}\delta\hat{N}\rangle_{\mathbf{r}+(1/2)\hbar\gamma,\mathbf{r},\eta,t})\ . \tag{A10}$$

This form for the collision integral has been used by Klimontovich[23] for his treatment of the electron-ion plasma. We work further in terms of the spectral densities $(\delta\hat{U}\delta\hat{N})_{\omega,\mathbf{k},\mathbf{p}}$ which are involved in the collision integral (A10). If spatial homogeneity and stationary conditions are assumed for $\delta\hat{U}$ and $\delta\hat{N}$, correlations of the type $\langle\delta\hat{U}\delta\hat{N}\rangle$ depend on the differences $t-t'$ and $\mathbf{r}-\mathbf{r}'$. In the time-asymptotic limit one obtains

$$(\delta U\delta N)_{\omega,\mathbf{k},\mathbf{p}}=\frac{N\pi C^2k^2}{\rho A}\delta(\omega-\mathbf{k}\cdot\mathbf{v})[f(\mathbf{p}+\tfrac{1}{2}\hbar\mathbf{k})+f(\mathbf{p}-\tfrac{1}{2}\hbar\mathbf{k})]-\frac{N}{\hbar}C^2k^2(\delta\hat{\mathrm{u}}\delta\hat{\mathrm{u}})_{\omega,\mathbf{k}}\frac{f(\mathbf{p}+\frac{1}{2}\hbar\mathbf{k})-f(\mathbf{p}-\frac{1}{2}\hbar\mathbf{k})}{\omega-\mathbf{k}\cdot\mathbf{v}-i\Delta}\ . \tag{A11}$$

Substitution of the above expressions for the spectral densities in the formula for the collision integral leads to the normal Bloch form without exchange:

$$I(\mathbf{p})=\frac{\pi C^2}{\rho s^2(2\pi)^3}\int\omega_k[\delta(\hbar\omega_k-E_{p,p-\hbar k})+\delta(\hbar\omega_k+E_{p,p-\hbar k})][N_k(f_{p-\hbar k}-f_p)-f_p]d\mathbf{k}\ , \tag{A12}$$

where N_k is the Bose factor:

$$N_k=[\exp(\hbar\omega_k/k_BT)-1]^{-1},\quad \omega_k=sk\ . \tag{A13}$$

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