Relaxation of nonequilibrium carrier-density matrix in semiconductors with degenerate bands

M. I. D'yakonov and A. V. Khaetskiĭ

A. F. Ioffe Physicotechnical Institute, USSR Academy of Sciences
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A general method is developed for the description of kinetic phenomena in cubic-symmetry semiconductors with degenerate bands (such as p-Ge or HgTe). It is shown that the investigation of the relaxation of the carrier-density matrix in quasi-elastic collisions is substantially simplified if it is expanded in finite-rotation matrices. It is found that equations in closed form exist for the momentum distribution functions only in the Born approximation. Outside the limits of this approximation there arise specific effects due to the strong spin-orbit coupling. An expression is obtained in the quasiclassical limit for the field terms in the equation for the density matrix. The relaxation times of certain physical quantities are found.

1. INTRODUCTION

We propose here a general approach to the description of kinetic phenomena in cubic-symmetry semiconductors with complicated valence band (such as p-Ge), as well as in zero-gap semiconductors (such as HgTe). The energy spectrum of the carriers in such materials consists of two bands with different effective masses. At the center of the Brillouin zone there is fourfold degeneracy (Γ_8 representation). The state of the carriers is characterized by a rigid coupling of their angular momentum and the momentum due to the strong spin-orbit interaction.

Galvanomagnetic effects in type p-Ge semiconductors were first investigated theoretically by Pikus, Bir, and Normantas.[1,2] They derived and solved kinetic equations for the momentum distribution functions of light and heavy holes with allowance for the possibility of the conversion of some particles into others on scattering. Within the framework of such an approach the presence of spin-orbit coupling affects only the numerical values of the relaxation times and of the interband-transition probabilities. The premises developed in Refs. 1 and 2 have by now become universally accepted.

A nonequilibrium state of the carriers in a complicated band, however, cannot be described solely by the momentum distribution function. Moreover, in the general case there are no closed equations for the distribution functions of the particles, since the scattering is accompanied by mutual conversions of the particle fluxes and their spin fluxes. In the presence of a magnetic field, its interaction with the spin leads, owing to spin-orbit coupling, to additional action on the orbital motion (and vice versa). The spin and transport phenomena can generally speaking not be separated. This circumstance, not taken into account in Refs. 1 and 2, may turn out to be significant in galvanomagnetic phenomena.

A complete description of the nonequilibrium state calls for the use of a density matrix that describes, besides the distribution in momenta, also the spin state of the carriers. The present paper is devoted mainly to the relaxation of the density matrix in elastic (or quasi-elastic) collisions. It is known that for electrons in a simple band with isotropic dispersion law one can introduce, after expanding the distribution function in spherical functions, the relaxation times of its different moments. In the considered case of a complicated band this approach is inapplicable in view of the strong coupling between the angular momentum of the carrier and its momentum. We shall show that the problem is greatly simplified if the density matrix is expanded in finite-rotation matrices. The initial integro-differential equation breaks up then into a system of unrelated pairs of differential equations with constant coefficients. This makes it easy to determine the character of the relaxation of any physical quantity.

It will be shown that equations in closed form can be obtained for the momentum distribution functions only in the Born approximation. Therefore if this approximation holds (which is the case as a rule in semiconductors of the p-Ge type), the approach used in Refs. 1 and 2 is perfectly applicable. If, however, the Born approximation is not valid, as, e.g., in the case of resonant scattering of electrons by impurities in zero-gap semiconductors, the aforementioned relation between the flux of the particles and their spin flux becomes substantial. It alters, for example, the expression for the effective relaxation time that determines the electric conductivity.

In Sec. 2 we introduce the carrier-density matrix, which is next expanded in finite-rotation matrices. The connection is established between the corresponding moments of the density matrix with the mean values of the physical quantities.

In Sec. 3 are obtained simple equations for the relaxation of the density-matrix moments in quasi-elastic collisions.

In Sec. 4 we discuss the character of the relaxation of various physical quantities. We consider for simplicity the case of a zero-gap semiconductor, when there are no interband transitions in elastic scattering. An expression is obtained for the electric conductivity of the electrons in an alternating field, with allowance for effects that occur outside the limits of the Born approximation. The hole spin-relaxation time is obtained.

The final Sec. 5 is devoted to the derivation of the field terms in the kinetic equation for the density matrix in the quasiclassical limit. Owing to the presence of the spin-orbit coupling the field terms differ in form from the usual ones.

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An equation of motion is obtained for the average spin of heavy holes in a magnetic field.

We confine ourselves in this paper to the spherical approximation, neglecting the corrugation of the equal-energy surfaces. This is precisely the approximation in which is valid the method developed here, which explains fully the character of the relaxation of an arbitrary physical quantity. In the band of light holes (electrons in a zero-gap semiconductor) the corrugation is negligible. In the heavy-band hole, however, it is generally speaking not small. One can hope, however, that the main qualitative features of the phenomena due to spin-orbit coupling are correctly described even in the spherical approximation.

2. DENSITY MATRIX

The energy spectrum near the band degeneracy point in semiconductors such as Ge or in zero-gap semiconductors such as HgTe is described by the Luttinger Hamiltonian.[3] In the spherical approximation it is given by

$$\mathcal{H}(\mathbf{p})=\frac{1}{2m_0}\left[\left(\gamma_1+\frac{5}{2}\gamma\right)\mathbf{p}^2-2\gamma(\mathbf{pJ})^2\right], \tag{1}$$

where m_0 is the mass of the free electron, $\gamma=(2\gamma_2+3\gamma_3)/5$; $\gamma_1,\gamma_2,\gamma_3$ are the Luttinger parameters, $\mathbf{p}$ is the quasimomentum operator; J_x, J_y, J_z are 4×4 matrices corresponding to an angular momentum 3/2.

It is known that the Schrödinger equation with Hamiltonian (1) yields two energy-spectrum branches corresponding to the free motion of particles with effective masses

$$m_1=m_0/(\gamma_1+2\gamma), \quad m_2=m_0/(\gamma_1-2\gamma).$$

Depending on the values of the Luttinger parameters, these branches correspond either to the bands of the light and heavy holes in semiconductors such as Ge (at $\gamma_1+2\gamma>0$, $\gamma_1-2\gamma>0$), or to the electron and hole bands in a zero-gap semiconductor such as HgTe (at $\gamma_1+2\gamma>0$, $\gamma_1-2\gamma<0$).

The states are characterized by the projection of the angular momentum M on the quasimomentum direction (by the helicity), with $M=\pm1/2$ corresponding to the band with effective mass m_1, and the values $M=\pm3/2$ to the band with effective mass m_2. Each of the bands is doubly degenerate. The wave functions of these states can be written in the form[4]

$$\Psi_{M\mathbf{p}}=\exp(i\mathbf{pr}/\hbar)\chi_{M\mathbf{p}}, \quad \chi_{M\mathbf{p}}=\sum_{\mu}D^{(3/2)}_{\mu M}(\omega_{\mathbf{p}})u_{\mu}, \tag{2}$$

where u_μ are the eigenfunctions of the matrix J_z ($\mu=\pm1/2, \pm3/2$), $D^{(3/2)}_{\mu M}$ is the finite-rotation matrix,[1)] and $\omega_{\mathbf{p}}$ is the rotation that aligns the z axis of the laboratory frame with the direction of the momentum $\mathbf{p}$. The rotation is defined by the Euler angles φ,θ,ψ, with φ and θ obviously coinciding with the polar angles of the vector $\mathbf{p}$ in the lab, while the angle ψ is arbitrary and determines the phase factor of the wave function: $\exp(-iM\psi)$.

We introduce the single-particle density matrix $f_{MM'}(\omega_{\mathbf{p}})$ that characterizes the state of the ensemble of the particles described by the Hamiltonian (1). Its dependence on the Euler angle ψ is determined by the factor $\exp(i(M-M')\psi)$. Since the angle ψ is arbitrary, we could set it equal to zero (in the given coordinate frame). We shall find it more convenient, however, not to fix this angle and regard the density matrix as a function of the rotation $\omega_{\mathbf{p}}$. The density matrix depends as usual also on the energy ε, on the coordinates, and on the time.[2)] For the sake of brevity we shall not write out these arguments.

The elements of the density matrix with $|M|=|M'|=1/2$ describe particles in the band with mass m_1 (light holes in Ge or electrons in HgTe), while the elements with $|M|=|M'|=3/2$ describe particles in the band with mass m_2 (heavy holes).

The off-diagonal elements with $|M|\neq|M'|$ describe the coherence of the states belonging to different bands. It can be shown that in the absence of alternating fields that induce interband transitions such elements are small in the parameter $\hbar\tau^{-1}|\varepsilon_1(p)-\varepsilon_2(p)|^{-1}$, where τ is the characteristic relaxation time, and $\varepsilon_1(p)$ and $\varepsilon_2(p)$ are the energies in bands 1 and 2 at the characteristic momentum p. If the masses m_1 and m_2 differ noticeably, this parameter is small under the conditions of applicability of the kinetic equations. Off-diagonal elements with $|M|\neq|M'|$ can be not small in the presence of an alternating field that causes transitions between bands 1 and 2. Such transitions are not considered in the present paper, and we shall therefore neglect hereafter density-matrix elements with $|M|\neq|M'|$. There exist then two density matrices, containing four elements each and describing the particles in bands 1 and 2.

For further investigation of the isotropic relaxation it is convenient to resolve the density matrix into parts that transform in accord with irreducible representations of the rotation group. This can be done by expanding $f_{MM'}(\omega_{\mathbf{p}})$ in terms of finite-rotation matrices $D^{(\varkappa)}_{qq'}(\omega_{\mathbf{p}})$ with integer values of $\varkappa$. Since the density matrix depends on the angle ψ like $\exp(i(M-M')\psi)$, we must have $q'=M'-M$. Thus, the sought expansion is

$$f_{MM'}(\omega_p)=\sum_{\varkappa=0}^{\infty}\sum_{q=-\varkappa}^{\varkappa}(2\varkappa+1)f^{\varkappa q}_{MM'}D^{(\varkappa)}_{q,M'-M}(\omega_{\mathbf{p}}). \tag{3}$$

The moments $f^{\varkappa q}_{MM'}$ are expressed as follows in terms of the density matrix $f_{MM'}$:

$$f^{\varkappa q}_{MM'}=\int\frac{d\omega_{\mathbf{p}}}{8\pi^2}f_{MM'}(\omega_{\mathbf{p}})D^{(\varkappa)}_{q,M'-M}(\omega_{\mathbf{p}}), \tag{4}$$

where $d\omega_{\mathbf{p}}=\sin\theta d\theta d\varphi d\psi$.

An expansion similar to (3) was first used in Ref. 6. It is a generalization of the usual expansion of a distribution function in spherical functions $Y_{\varkappa q}$, and the diagonal elements of both coincide, since $D^{(\varkappa)}_{q0}(\omega_{\mathbf{p}})\propto Y^{*}_{\varkappa q}(\theta,\varphi)$.

Let us discuss certain properties and the physical meaning of the momenta $f^{\varkappa q}_{MM'}$. From the fact that the density matrix is Hermitian and from (4) we obtain

$$(f^{\varkappa q}_{MM'})^{*}=(-1)^{q+M-M'}f^{\varkappa-q}_{M'M}. \tag{5}$$

It follows next from the definition that the momenta differ from zero at $|M-M'|\leqslant\varkappa$. Therefore the elements that are not diagonal in M exist in band 1, where $|M|=1/2$, only at $\varkappa\geqslant1$, and in band 2, where $|M|=3/2$, only at $\varkappa\geqslant3$.

The mean value calculated with the aid of the density matrix $f_{MM'}$ for any operator $\hat{A}^{\varkappa q}q(\nu)$ that depends on the unit vector along the $\mathbf{p}$ direction and constitutes a tensor of rank is expressed only in terms of angular momenta having the same $\varkappa$. We write the mean value of such an operator in one of the bands in the form

$$\langle A^{\varkappa q}\rangle = \int_0^\infty d\varepsilon \rho(\varepsilon)\bar{A}^{\varkappa q}, \tag{6}$$

where $\rho(\varepsilon)$ is the density of states in one of the subbands of the corresponding band,

$$\bar{A}^{\varkappa q} = \int \frac{d\omega_{\mathbf{p}}}{8\pi^2} \mathrm{Sp}(\hat{f}\hat{A}^{\varkappa q}). \tag{7}$$

When calculating the trace in (7) account should be taken of only states pertaining to the band in question.

The matrix elements in (7) of the operator $\hat{A}^{\varkappa q}$ on the functions $\chi_{M\mathbf{p}}$ defined by Eq. (2) can be expressed in terms of matrix elements of the same operator in a coordinate frame in which the z axis coincides with the direction of $\mathbf{p}$ ($\chi_{M\mathbf{p}} = u_M$ in this system):

$$(\chi_{M\mathbf{p}}|A^{\varkappa q}(\nu)|\chi_{M'\mathbf{p}}) = D^{(\varkappa)*}_{q,M-M'}(\omega_{\mathbf{p}})(u_M|A^{\varkappa,M-M'}(\nu)|u_{M'}). \tag{8}$$

In the calculation of the matrix elements in the right-hand side of (8) the unit vector ν must be assumed directed along the z axis. With the aid of (3), (7), and (8) we get

$$\bar{A}^{\varkappa q} = \sum_{MM'} f^{\varkappa q}_{MM'}(u_{M'}|A^{\varkappa,M'-M}(\nu)|u_M). \tag{9}$$

Calculations with Eq. (9) yield, particularly for the band 1, where $|M| = 1/2$:

$$\overline{(\mathbf{J}\nu)} = {}^1/_2(f^{00}_{1/2\,1/2} - f^{00}_{-1/2\,-1/2}), \tag{10}$$

$$\bar{\nu}_q = f^{1q}_{1/2\,1/2} + f^{1q}_{-1/2\,-1/2}, \qquad \overline{\nu_q(\mathbf{J}\nu)} = {}^1/_2(f^{1q}_{1/2\,1/2} - f^{1q}_{-1/2\,-1/2}), \tag{11}$$

$$\bar{J}_q = {}^1/_2(f^{1q}_{1/2\,1/2} - f^{1q}_{-1/2\,-1/2}) + 2^{1/2}(f^{1q}_{1/2\,-1/2} - f^{1q}_{-1/2\,1/2}), \tag{12}$$

$$\overline{[\mathbf{J}\times\nu]}_q = 2^{1/2}i(f^{1q}_{1/2\,-1/2} + f^{1q}_{-1/2\,1/2}), \tag{13}$$

where the circular components of the vector are determined from the rule $\nu_0 = \nu_z$, $\nu_1 = -(\nu_x + i\nu_y)/2^{1/2}$, $\nu_{-1} = (\nu_x - i\nu_y)/2^{1/2}$. For band 2, where $|M| = 3/2$, we have

$$\overline{(\mathbf{J}\nu)} = {}^3/_2(f^{00}_{3/2\,3/2} - f^{00}_{-3/2\,-3/2}), \tag{14}$$

$$\bar{\nu}_q = f^{1q}_{3/2\,3/2} + f^{1q}_{-3/2\,-3/2}, \qquad \overline{\nu_q(\mathbf{J}\nu)} = {}^3/_2(f^{1q}_{3/2\,3/2} - f^{1q}_{-3/2\,-3/2}), \tag{15}$$

$$\bar{J}_q = {}^3/_2(f^{1q}_{3/2\,3/2} - f^{1q}_{-3/2\,-3/2}), \qquad \overline{[\mathbf{J}\times\nu]} = 0. \tag{16}$$

The combinations $f^{00}_{1/2\,1/2} + f^{00}_{-1/2\,-1/2}$ determine the number of the particles (with specified energy) in bands 1 and 2, respectively.

We note that for the velocity operator

$$\hat{\mathbf{V}} = m_0^{-1}[(\gamma_1 + {}^5/_2\gamma)\mathbf{p} - \gamma(\mathbf{J}(\mathbf{pJ}) + (\mathbf{pJ})\mathbf{J})] \tag{17}$$

the relation $\bar{\mathbf{V}} = (p/m)\bar{\nu}$ holds in each band (m is the effective mass in the considered band).

3. COLLISION INTEGRAL

The relaxation of the nonequilibrium density matrix $f_{MM'}(\omega_{\mathbf{p}})$ in elastic collisions is described by the following equation (see, e.g., Ref. 6):

$$\frac{\partial f_{MM'}(\omega_{\mathbf{p}})}{\partial t} = \int \frac{d\omega_{\mathbf{p}1}}{8\pi^2}\Big\{\sum_{M_1M_1'} K^{MM'}_{M_1M_1'} f_{M_1M_1'}(\omega_{\mathbf{p}1}) - \frac{1}{2}\sum_{M_1M_2}[K^{MM_1}_{M_2M_2} f_{M_1M'}(\omega_{\mathbf{p}}) + f_{MM_1}(\omega_{\mathbf{p}})K^{M_1M'}_{M_1M_2}]\Big\}. \tag{18}$$

This equation is a generalization of the usual kinetic equation for the distribution function to include the case when the system is characterized by a nondiagonal density matrix. The kernel K, just as the density matrix, depends on the energy ε as a parameter. The integration with respect to $d\omega_{\mathbf{p}1}$ includes integration with respect to the Euler angles $\varphi_1, \theta_1, \psi_1$ that determine the rotation that aligns the z axis in the lab with the direction of the momentum p_1. The dependence of the matrix $K^{MM'}_{M_1M_1'}$ on the angles ψ and ψ_1 can be readily shown to be determined by the factor $\exp[i(M - M')\psi - i(M_1 - M_1')\psi_1]$. The integrand is in fact independent of the angle ψ_1, and the integration with respect to this angle was added for convenience.

As already noted in the preceding section, the density-matrix elements that are not diagonal in the bands 1 and 2 can be neglected as small. Accordingly, account should be taken in both sides of (18) of only $f_{MM'}$ elements with $|M| = |M'|$. The quantities $K^{MM'}_{M_1M_1'}$ should therefore be regarded as different from zero only at $|M| = |M'|$, $|M_1| = |M_1'|$.

The intraband transitions are determined by the elements of the matrix $K^{MM'}_{M_1M_1'}$ that have $|M| = |M'| = |M_1| = |M_1'|$, and the interband transitions by the elements with $|M| = |M'| \neq |M_1| = |M_1'|$. In scattering by impurities, the values of K are expressed in terms of the scattering amplitude $F^{M\mathbf{p}}_{M_1\mathbf{p}_1}$ for the transition from the initial state $M_1\mathbf{p}_1$ to the final state $M\mathbf{p}$ as follows:

$$K^{MM'}_{M_1M_1'} = 4\pi N \frac{(2\varepsilon m_f)^{1/2}}{m_i} F^{M\mathbf{p}}_{M_1\mathbf{p}_1}(F^{M'\mathbf{p}}_{M_1'\mathbf{p}_1})^*, \tag{19}$$

where N is the impurity density and m_i and m_f are respectively the masses in the initial and final states:

$$m_i = \begin{cases} m_1 & \text{for} \quad |M_1| = |M_1'| = {}^1/_2 \\ m_2 & \text{for} \quad |M_1| = |M_1'| = {}^3/_2 \end{cases}$$
$$m_f = \begin{cases} m_1 & \text{for} \quad |M| = |M'| = {}^1/_2 \\ m_2 & \text{for} \quad |M| = |M'| = {}^3/_2 \end{cases}. \tag{20}$$

The elements of K with $M = M'$ and $M_1 = M'_1$ are the probabilities of the transitions from the state $(M_1\mathbf{p}_1)$ to $(M\mathbf{p})$.

The isotropy of the relaxation process means that the kernel K is a function of the parameters that determine the rotation $\omega_{\mathbf{p}\,\mathbf{p}\,1} = \omega_{\mathbf{p}}^{-1}\omega_{\mathbf{p}\,1}$ which transforms the coordinate system connected with $\mathbf{p}_1$ into the system connected with $\mathbf{p}$. This circumstance allows us to represent the kernel K in the form of an expansion in finite-rotation matrices:

$$K^{MM'}_{M_1M_1'} = \sum_{\varkappa=0}^{\infty}(2\varkappa+1)W^{MM'}_{M_1M_1'}(\varkappa)D^{(\varkappa)*}_{M'-M,M_1'-M_1}(\omega_{pp_1}), \tag{21}$$

where the expansion coefficients are determined by the inverse transformation

$$W^{MM'}_{M_1M_1'}(\varkappa)=\int\frac{d\omega_{\mathbf{pp}_1}}{8\pi^2}K^{MM'}_{M_1M_1'}D^{(\varkappa)}_{M'-M,M_1'-M_1}(\omega_{\mathbf{pp}_1}). \quad (22)$$

Substituting the expansion (21) in Eq. (18), using Eqs. (3) and (4) as well as the addition theorem for finite-rotation matrices,[5] we obtain a system of equations for the angular momenta $f^{\varkappa q}_{MM'}$:

$$\frac{\partial f^{\varkappa q}_{MM'}}{\partial t}=\sum_{M_1M_1'}W^{MM'}_{M_1M_1'}(\varkappa)f^{\varkappa q}_{M_1M_1'}$$
$$-\frac{1}{2}f^{\varkappa q}_{MM'}\sum_{M_1}(W^{MM}_{M_1M_1}(0)+W^{M'M'}_{M_1M_1}(0)). \quad (23)$$

Equation (23) describes the relaxation of any physical quantity that is a tensor of rank $\varkappa$ via intraband as well as interband transitions. It is important that momenta with different $\varkappa$ and q relax independently.

Additional simplifications occur when the symmetry properties of the coefficients W are used. To determine these properties we consider first the properties of the kernel K. From the definition of this quantity [see (19)] it follows that

$$(K^{MM'}_{M_1M_1'}(\omega_{\mathbf{pp}_1}))^*=K^{M'M}_{M_1'M_1}(\omega_{\mathbf{pp}_1}). \quad (24a)$$

Invariance to time reversal (the reciprocity theorem[7]) leads to the condition

$$m_a^{1/2}K^{MM'}_{M_1M_1'}(\omega_{\mathbf{pp}_1})=m_b^{1/2}(-1)^{M-M_1+M'-M_1'}K^{M_1M_1'}_{MM'}(\omega_{-\mathbf{p}_1-\mathbf{p}}), \quad (24b)$$

where m_a is the mass in the state $M_{\mathbf{p}}$ and m_b the mass in the state $M_1\mathbf{p}_1$. In addition, if the crystal has an inversion center we have[3)]

$$K^{MM'}_{M_1M_1'}(\omega_{\mathbf{pp}_1})=K^{-M-M'}_{-M_1-M_1'}(\omega_{-\mathbf{p}-\mathbf{p}_1}). \quad (24c)$$

An additional symmetry property appears in the Born approximation. Inasmuch as in this approximation[7]

$$F^{M\mathbf{p}}_{M_1\mathbf{p}_1}=(F^{M_1\mathbf{p}_1}_{M\mathbf{p}})^*,$$

it follows that

$$m_a^{1/2}K^{MM'}_{M_1M_1'}(\omega_{\mathbf{pp}_1})=m_b^{1/2}(K^{M_1M_1'}_{MM'}(\omega_{\mathbf{p}_1\mathbf{p}}))^*. \quad (24d)$$

Using Eq. (21) and the properties of D-matrices, we obtain from Eqs. (24) the following relations for the coefficients W:

$$W^{MM'}_{M_1M_1'}=(-1)^{M-M'+M_1-M_1'}(W^{M'M}_{M_1'M_1})^*, \quad (25a)$$
$$m_a^{1/2}W^{MM'}_{M_1M_1'}=m_b^{1/2}W^{M_1M_1'}_{MM'}, \quad (25b)$$
$$W^{MM'}_{M_1M_1'}=W^{-M-M'}_{-M_1-M_1'}, \quad (25c)$$
$$m_a^{1/2}W^{MM'}_{M_1M_1'}=m_b^{1/2}(W^{M_1M_1'}_{MM'})^*. \quad (25d)$$

We emphasize that Eq. (25d), just as (24d), is valid only in the Born approximation.

4. DENSITY-MATRIX RELAXATION

In this section we consider for simplicity the case of a zero-gap semiconductor, when there are no interband transitions. The relaxation in each band is then described at arbitrary $\varkappa$ by a system of four equations.

Using the properties (25a)–(25c), we can represent this system in the form

$$\frac{\partial}{\partial t}(f_{++}^{\varkappa q}+f_{--}^{\varkappa q})=-\frac{1}{\tau_1(\varkappa)}(f_{++}^{\varkappa q}+f_{--}^{\varkappa q})$$
$$+i\alpha(\varkappa)(f_{+-}^{\varkappa q}+f_{-+}^{\varkappa q}), \quad (26)$$
$$\frac{\partial}{\partial t}(f_{+-}^{\varkappa q}+f_{-+}^{\varkappa q})=i\alpha(\varkappa)(f_{++}^{\varkappa q}+f_{--}^{\varkappa q})-\frac{1}{\tau_2(\varkappa)}(f_{+-}^{\varkappa q}+f_{-+}^{\varkappa q}),$$
$$\frac{\partial}{\partial t}(f_{++}^{\varkappa q}-f_{--}^{\varkappa q})=-\frac{1}{\tau_3(\varkappa)}(f_{++}^{\varkappa q}-f_{--}^{\varkappa q})$$
$$+\beta(\varkappa)(f_{+-}^{\varkappa q}-f_{-+}^{\varkappa q}), \quad (27)$$
$$\frac{\partial}{\partial t}(f_{+-}^{\varkappa q}-f_{-+}^{\varkappa q})=\beta(\varkappa)(f_{++}^{\varkappa q}-f_{--}^{\varkappa q})-\frac{1}{\tau_4(\varkappa)}(f_{+-}^{\varkappa q}-f_{-+}^{\varkappa q}),$$

where

$$\tau_1^{-1}(\varkappa)=W_{++}^{++}(0)+W_{--}^{++}(0)-W_{++}^{++}(\varkappa)-W_{--}^{++}(\varkappa),$$
$$\tau_2^{-1}(\varkappa)=W_{++}^{++}(0)+W_{--}^{++}(0)-W_{-+}^{+-}(\varkappa)-W_{+-}^{+-}(\varkappa),$$
$$\tau_3^{-1}(\varkappa)=W_{++}^{++}(0)+W_{--}^{++}(0)-W_{++}^{++}(\varkappa)+W_{--}^{++}(\varkappa),$$
$$\tau_4^{-1}(\varkappa)=W_{++}^{++}(0)+W_{--}^{++}(0)+W_{-+}^{+-}(\varkappa)-W_{+-}^{+-}(\varkappa), \quad (28)$$
$$i\alpha(\varkappa)=W_{+-}^{++}(\varkappa)+W_{-+}^{++}(\varkappa),$$
$$\beta(\varkappa)=W_{+-}^{++}(\varkappa)-W_{-+}^{++}(\varkappa). \quad (29)$$

The symbols $(+)$ and $(-)$ denote here $(+|M|)$ and $(-|M|)$, respectively, where $|M|=1/2$ for band 1 and $|M|=3/2$ for band 2. Thus, $f^{\varkappa q}_{+-}$ and $W^{++}_{--}(\varkappa)$ should be understood as $f^{\varkappa q}_{1/2\,-1/2}$ and $W^{1/2\,1/2}_{-1/2\,-1/2}(\varkappa)$ (for band 1) or as $f^{\varkappa q}_{3/2\,-3/2}$ and $W^{3/2\,3/2}_{-3/2\,-3/2}(\varkappa)$ (for band 2). We note that the quantities τ, α, and β defined by (28) and (29) are real.

The system (23) was thus broken up into two independent systems (26) and (27) of two equations each. These equations make it easy to determine the character of the relaxation of an arbitrary physical quantity.

At $\varkappa=0$ we have $f^{00}_{+-}=f^{00}_{-+}=0$, $\alpha(0)=\beta(0)=0$, and in addition $1/\tau_1(0)=0$. The first equation of (26) describes the particle-number conservation. The first equation of (27) describes at $\varkappa=0$ the relaxation of the helicity [see Eqs. (10) and (14)]. The quantity $\tau_3(0)$ is thus the helicity relaxation time

$$\tau_3^{-1}(0)=2W_{--}^{++}(0). \quad (30)$$

For band 2 ($|M|=3/2$) the off-diagonal components of the momenta are equal to zero, $\alpha(\varkappa)=\beta(\varkappa)=0$, not only at $\varkappa=0$ but also at $\varkappa=1$ and 2. At $\varkappa\leqslant 2$ Eqs. (26) and (27) reduce therefore for this band to two independent equations that describe the relaxation of the quantities $f^{\varkappa q}_{++}+f^{\varkappa q}_{--}$ and $f^{\varkappa q}_{++}-f^{\varkappa q}_{--}$. The relaxation of these quantities is characterized respectively by the times $\tau_1(\varkappa)$ and $\tau_3(\varkappa)$. According to (15) and (16) the quantities $\tau_1(1)$ and $\tau_3(1)$ are respectively the momentum and spin relaxation times in band 2.

In the Born approximation, as follows from (25a), (25b), and (25d), we have $\alpha(\varkappa)=0$ at all $\varkappa$. The system (26) breaks up then into two independent equations that describe the

relaxation of the quantities $f^{\varkappa q}_{++}+f^{\varkappa q}_{--}$ and $f^{\varkappa q}_{+-}+f^{\varkappa q}_{-+}$, with relaxation times $\tau_1(\varkappa)$ and $\tau_2(\varkappa)$, respectively. The time $\tau_2(1)$ characterizes, according to (13), the relaxation of the vector $\overline{\mathbf{J}\times\mathbf{v}}$ (in band 1).

In the Born approximation, the kernel K takes the form

$$K^{MM'}_{M_1M_1'}=D^{(3/2)}_{MM_1}(\omega_{pp_1})D^{(3/2)*}_{M'M_1'}(\omega_{pp_1})w(\theta), \tag{31}$$

where $w(\theta)$ is a function of the scattering angle and is given, e.g., in the case of scattering by impurities, by

$$w(\theta)=\frac{2\pi}{\hbar}|U(p-p_1)|^2\rho_f(\varepsilon)N, \tag{32}$$

where $U(p-p_1)$ is the Fourier component of the impurity potential and $\rho_f(\varepsilon)$ is the density of the final states.

Using (22) and (31) we then obtain the following expressions for the coefficients W in the Born approximation:

$$W^{MM'}_{M_1M_1'}(\varkappa)=(-1)^{M-M_1}\sum_{lj}(2l+1)(2j+1)\times\begin{pmatrix} l & j & \varkappa \\ 0 & M-M' & M'-M\end{pmatrix}\times\begin{pmatrix} l & j & \varkappa \\ 0 & M_1-M_1' & M_1'-M_1\end{pmatrix}\begin{pmatrix} 3/2 & 3/2 & j \\ M & -M' & M'-M\end{pmatrix}\times\begin{pmatrix} 3/2 & 3/2 & j \\ M_1 & -M_1' & M_1'-M_1\end{pmatrix}w_l, \tag{33}$$

where

$$w_l=\frac{1}{2}\int_0^\pi w(\theta)P_l(\cos\theta)\sin\theta\,d\theta, \tag{34}$$

and P_l is a Legendre polynomial.

We present expressions for certain relaxation times in terms of the coefficients w_l in the Born approximation. The momentum-relaxation time (in bands 1 and 2):

$$1/\tau_1(1)=(w_0+w_2)/2-{}^7/_{10}w_1-{}^3/_{10}w_3. \tag{35}$$

The relaxation time of the vector $\overline{\mathbf{J}\times\mathbf{v}}$ (in band 1):

$$1/\tau_2(1)=(w_0+w_2)/2-{}^2/_5w_1-{}^3/_5w_3. \tag{36}$$

The helicity relaxation time:

$$\begin{aligned}1/\tau_3(0)&=(w_0+w_2)/2-{}^1/_{10}w_1-{}^9/_{10}w_3\ \text{(band 1)},\\ 1/\tau_3(0)&=(w_0+w_2)/2-{}^9/_{10}w_1-{}^1/_{10}w_3\ \text{(band 2)}.\end{aligned} \tag{37}$$

The spin relaxation time (in band 2):

$$1/\tau_3(1)={}^1/_5w_0-{}^1/_7w_2-{}^2/_{35}w_4. \tag{38}$$

We note that the coefficients w_l are different for bands 1 and 2 (owing to the difference of the effective masses). Calculation of the momentum relaxation times using Eq. (35), in scattering by charged impurities and acoustic phonons, leads to the results obtained by Bir, Normantas, and Pikus.[2] It is interesting that in scattering by charged impurities the spin relaxation time in band 2 is equal to the momentum-relaxation time: $\tau_3(1)=\tau_1(1)$.

Thus, in the Born approximation the quantities $f^{\varkappa q}_{++}+f^{\varkappa q}_{--}$ relax independently with relaxation times $\tau_1(\varkappa)$. This means that in this approximation there exists a closed equation for the particle-momentum distribution function in a given band (with both helicities). The quantities $f^{\varkappa q}_{++}+f^{\varkappa q}_{--}$ are the moments of the distribution function, viz., the coefficients of its expansion in spherical functions. Therefore under conditions when the Born approximation is valid all the kinetic phenomena that are not connected with spin proceed as if there exist two particle species with masses m_1 and m_2. It will be shown in Sec. 5 that this statement remains valid also in the presence of a magnetic field. (The spinor character of the wave functions of the particles influences only the numerical values of the relaxation time $\tau_1(\varkappa)$ and of the interband-transition probabilities.) Thus, the analysis of the kinetic phenomena in Refs. 1 and 2, in which no account was taken of the density-matrix elements that are not diagonal in the helicity, is perfectly valid under conditions when the Born approximation is applicable.

Generally speaking (not in the Born approximation), there is no closed equation for the momentum-distribution function. The relaxation of this function is described by the system (26). Let us explain the physical meaning of the effects that occur outside the range of the Born approximation. Consider the system (26) at $\varkappa=1$ for band 1. Using (11) and (13), we represent this system in the form

$$\begin{aligned}\frac{d\mathbf{p}}{dt}&=-\frac{\mathbf{p}}{\tau_1}+\frac{\alpha}{2^{1/2}}\overline{[\mathbf{J}\times\mathbf{p}]},\\ \frac{d}{dt}\overline{[\mathbf{J}\times\mathbf{p}]}&=-2^{1/2}\alpha\bar{\mathbf{p}}-\frac{1}{\tau_2}\overline{[\mathbf{J}\times\mathbf{p}]}.\end{aligned} \tag{39}$$

The coefficient α establishes the connection between the flux of the particles (of given energy) and their spin flux. Indeed, the spin flux of particles with a given energy is proportional to

$$q_{jk}={}^1/_2\overline{(J_i\hat{V}_k+\hat{V}_kJ_i)},$$

where $\hat{\mathbf{V}}$ is the velocity operator (17). It is easy to show the existence of the relation $\varepsilon_{ijk}\,g_{jk}=m_1^{-1}\,[\,\overline{\mathbf{J}\times\mathbf{p}}\,]_i$ where ε_{ijk} is a unit antisymmetric tensor. Equations (39) describe thus the mutual transformations of the particle flux and their spin flux, and the relaxation of these quantities in scattering. The terms containing the coefficient α lead to the anomalous Hall effect (see, e.g., Ref. 8) and to the onset of a spin flux when electric current flows.[9] It is known that these effects are due to spin-orbit interaction and occur only in the approximation higher than the Born approximation. In the case of electrons in a simple band, the corresponding coefficient has an additional smallness connected with the weakness of the spin-orbit coupling.[10] In the situation considered here the coupling between the spin of the particles and their momentum is strong. We note that in band 2 there is no mutual transformation of the fluxes since, as indicated above, $\overline{\mathbf{J}\times\mathbf{p}}=0$.

The Born approximation is certainly valid for the analysis of kinetic phenomena in a zero-gap semiconductor under conditions when a substantial role is played by resonant scattering of the electrons by charged acceptors that lead to quasidiscrete energy levels in the conduction band.[11] Bearing this in mind, we present the results of a calculation of the conductivity of electrons in a zero-gap semiconductor in an alternating electric field.

In the approximation linear in the electric field, it is necessary, at $\varkappa = 1$, to add to the left-hand side of the first equation of (26) the term $2/3eE_q \partial f_0/\partial p$, where f_0 is the Fermi function. Obtaining from (26) the value of $f^{1q}_{1/2\,1/2} + f^{1q}_{-1/2\,-1/2}$ and calculating the current density with the aid of (6), (7), (11), and (17), we obtain the following expression for the electric conductivity:

$$\sigma(\omega) = \frac{ne^2}{m_1} \frac{\tau_1(1+i\omega\tau_2)}{(1+i\omega\tau_1)(1+i\omega\tau_2)+\alpha^2\tau_1\tau_2}, \tag{40}$$

where n is the electron density, and the quantities τ_1, τ_2, and α must be calculated at an energy equal to the Fermi energy. In the static limit the effective relaxation time is $\tau_1/(1+\alpha^2\tau_1\tau_2)$. In the most interesting case of resonant scattering the problem of calculating the scattering amplitudes has not been solved to this day. We cannot therefore obtain explicit expressions for τ_1, τ_2, and α. In the Born approximation, when $\alpha = 0$, Eq. (40) reduces to the Drude equation.

We do not consider in this section interband transitions, which play a substantial role in semiconductors with a complicated valence band, such as p-Ge. When account is taken of the interband transitions, Eq. (23) together with the symmetry properties (25a)–(25c) yields in lieu of Eqs. (26) and (27) two systems of four equations each. In this case the density matrices of the light and heavy holes are interrelated. The corresponding equations are similar to (26) and (27), but are more cumbersome and will not be given here. In the Born approximation, calculation of the hole conductivity with allowance for the interband transitions leads to the results of Ref. 2.

5. FIELD TERMS IN THE KINETIC EQUATION

Let us establish the form of the field term in the kinetic equation for the density matrix $f_{MM'}$. We shall assume in this case that the quasiclassical conditions are satisfied, viz., the magnetic field is assumed nonquantizing and the characteristic scales of the spatial inhomogeneities are assumed large compared with the de Broglie wavelength. The collision terms of the kinetic equations are not considered in this section.

We start from the equation for the density operator ρ:

$$i\hbar \frac{\partial \rho}{\partial t} = [\tilde{\mathscr{H}}, \rho], \tag{41}$$

where

$$\tilde{\mathscr{H}} = \hat{\mathscr{H}}\left(-i\hbar\nabla - \frac{e}{2c}[\mathbf{H}\times\mathbf{r}]\right) - e\mathbf{E}\mathbf{r}, \tag{42}$$

$\mathbf{E}$ and $\mathbf{H}$ are the respective electric and magnetic field strengths, and $\hat{\mathscr{H}}$ is the Luttinger Hamiltonian[4] in the presence of a magnetic field. It differs from the Hamiltonian (1) by the substitution $\mathbf{p} \to \mathbf{p} - (e/2c)\mathbf{H}\times\mathbf{r}$, by the symmetrization of the term $(\mathbf{p}\cdot\mathbf{J})^2$, and by the addition of a term $(e\hbar/m_0c)k\,\mathbf{J}\cdot\mathbf{H}$ (k is the Luttinger constant). The matrix elements of the operator ρ in the momentum representation will be denoted by $\rho_{\mathbf{qq}'}$. These quantities are 4×4 matrices in the spin indices.

As usual, in the quasiclassical limit it is convenient to introduce the Wigner density matrix $\hat{f}(\mathbf{p},\mathbf{r})$, which is connected with the quantities $\rho_{\mathbf{qq}'}$ as follows:

$$f(\mathbf{p},\mathbf{r}) = \int \frac{d^3\varkappa}{(2\pi\hbar)^3} \exp(i\varkappa\mathbf{r}/\hbar)\,\rho_{\mathbf{p}+\varkappa/2,\mathbf{p}-\varkappa/2}, \tag{43}$$

where $\mathbf{P} = \mathbf{p} + (e/2c)\mathbf{H}\times\mathbf{r}$. The quantities $\mathbf{P}$ and $\mathbf{p}$ are respectively the generalized and kinematic momenta.

From (41) we get the following equation for the matrix $\hat{f}$:

$$i\hbar\frac{\partial \hat{f}}{\partial t} = \hat{\mathscr{H}}(\mathbf{p}+\mathbf{Q}/2)\hat{f} - (\hat{\mathscr{H}}(\mathbf{p}-\mathbf{Q}/2)\hat{f})^{+} - i\hbar e\mathbf{E}\frac{\partial \hat{f}}{\partial \mathbf{p}}, \tag{44}$$

where $\mathbf{Q} = -i\hbar(\nabla + (e/c)\mathbf{H}\times\partial/\partial\mathbf{p})$ is a differential operator acting on the matrix $\hat{f}(\mathbf{p},\mathbf{r})$.

Equation (44) is exact. When the quasiclassics conditions are satisfied we can expand the right-hand side of this equation in powers of the operator $\mathbf{Q}$ and confine ourselves to the linear terms. We have $\hat{\mathscr{H}}(\mathbf{p}+\mathbf{Q}/2) = \hat{\mathscr{H}}(\mathbf{p}) + (\hat{\mathbf{V}}\mathbf{Q} + \mathbf{Q}\hat{\mathbf{V}})/4$, where $\hat{\mathbf{V}} = \partial\hat{\mathscr{H}}(\mathbf{p})/\partial\mathbf{p}$ is the velocity operator whose explicit form is given by Eq. (17). With the aid of this formula we can readily verify that $\hat{\mathbf{V}}\mathbf{Q} = \mathbf{Q}\hat{\mathbf{V}}$. Taking this into account, we obtain an equation for the density matrix f:

$$\frac{\partial \hat{f}}{\partial t} + \{\hat{\mathbf{V}}, \nabla f\} + \left\{ e\mathbf{E} + \frac{e}{c}[\hat{\mathbf{V}}\times\mathbf{H}], \frac{\partial \hat{f}}{\partial \mathbf{p}} \right\} + \frac{i}{\hbar}[\hat{\mathscr{H}}(\mathbf{p}), \hat{f}] = 0. \tag{45}$$

Here $\{A,B\} = (AB + BA)/2$.

Equation (45) is a direct generalization of the usual classical kinetic equation for the distribution function to include the case when the Hamiltonian and the distribution function itself are matrices in the spin variables. It differs from the usual kinetic equation by the presence of a term with the commutator $[\hat{\mathscr{H}}, \hat{f}]$ and also in that the field and gradient terms are symmetrized, since the velocity vector is a matrix.

We proceed now to the equation for the density matrix $f_{MM'}$ considered in the preceding sections. To this end we must rewrite Eq. (45) in the basis of the functions (2), in which the Hamiltonian (1) is diagonal. It must be borne in mind here that the function (2) depends on the direction of the vector $\mathbf{p}$, therefore the matrix elements of the derivative $\partial\hat{f}/\partial\mathbf{p}$ in the new basis do not coincide with the quantities $\partial f_{MM'}/\partial\mathbf{p}$:

$$\left(\frac{\partial \hat{f}}{\partial \mathbf{p}}\right)_{MM'} = \frac{\partial f_{MM'}}{\partial \mathbf{p}} - \frac{i}{\hbar}[\hat{\mathbf{a}}, \hat{f}]_{MM'}. \tag{46}$$

The matrix elements of the operator $\hat{\mathbf{a}}$ are determined here by the formula $\mathbf{a}_{MM'} = i\hbar\chi^{*}_{M\mathbf{p}}(\partial\chi_{M'\mathbf{p}}/\partial\mathbf{p})$.

On going to the basis $\chi_{M\mathbf{p}}$, the equations for the density matrix elements that are not diagonal in the bands 1 and 2 (at $|M| \neq |M'|$) acquire terms of the form $(\varepsilon_1(p) - \varepsilon_2(p))f_{MM'}$, which stem from the commutator $[\hat{\mathscr{H}}, \hat{f}]$ in Eq. (45). In the absence of an alternating field that causes interband transitions, these terms make the elements that are not diagonal in the bands small (see the discussion of this question in Sec. 2). Therefore the off-diagonal elements can be discarded and we can write down uncoupled equations (disregarding the interband transitions due to collisions) for the density matrices in each band. Using the relation (46) as well as the property $\varepsilon_{ikl}\partial\hat{V}_k/\partial p_l = 0$, we can rewrite Eq. (45) in the basis of the functions (2) as follows:

$$\frac{\partial f_{MM'}}{\partial t}+\mathbf{v}\nabla f_{MM'}+\left(e\mathbf{E}+\frac{e}{c}[\mathbf{v}\times\mathbf{H}]\right)\frac{\partial f_{MM'}}{\partial \mathbf{p}}$$

$$+\frac{i}{\hbar}[\hat{h},\hat{f}]_{MM'}=0, \tag{47}$$

where the subscripts M and M' pertain to one band ($|M|=|M'|$), $\mathbf{v}=\mathbf{p}/m$, with m the effective mass in the corresponding band.

The matrix $\hat{h}$ can be represented in the form

$$\hat{h}=-\mathbf{E}\hat{\mathbf{D}}-\mathbf{H}\mathbf{M}, \quad \hat{\mathbf{D}}=e\mathbf{a}=ie\hbar\frac{\partial}{\partial\mathbf{p}},$$

$$\mathbf{M}=-\frac{ie\hbar}{c}\left[\frac{\hat{\mathbf{V}}+\mathbf{v}}{2}\frac{\partial}{\partial\mathbf{p}}\right]-\frac{e\hbar}{m_0c}k\mathbf{J}. \tag{48}$$

The matrix $\hat{h}$ is the effective "spin" Hamiltonian that determines the change of the helicities of the particles in each band under the action of external field. Expressions (48) coincide with the results obtained by Gorbovitskiĭ and Perel'[12] in an investigation of quasiclassical quantization for matrix Hamiltonians.[4)] In the presence of a magnetic field, the Hamiltonian h determines the energy distance between the degenerate (in the absence of a field) subbands of a given band, and by the same token the value of the effective g-factor in the quasiclassical limit.[12]

Equation (47) differs from the usual equation for the distribution function only in the presence of a term with a commutator $[\hat{h}\hat{f}]$. We note that this term drops out when an equation is set up for the summary distribution function $f_{++}+f_{--}$. As shown in Sec. 4, in the Born approximation this quantity relaxes independently. Therefore when using the Born approximation, in all the phenomena that are not connected with the spin, the difference between the field terms in (47) and the usual ones does not manifest itself. Outside the framework of the Born approximation, the spin fluxes and the particle fluxes are coupled, therefore the term with the commutator $[\hat{h}\hat{f}]$ can play a substantial role for phenomena such as electric conductivity in a magnetic field.

The complete equation for the density matrix is obtained by adding to the right-hand side of (47) the collision integral (18). As shown in Sec. 3, the collision integral becomes much simpler when the density matrix element is expanded in terms of the angular momenta in accord with Eq. (3), since momenta with different $\varkappa$ and q relax independently. The field terms in (47) lead to a connection between the momenta and the values of $\varkappa$ that differ by unity. The complete equations for the $f^{\varkappa q}_{MM'}$ are too long to be presented here. We confine ourselves to some of the results.

1) In the approximation linear in E and ∇f, the corresponding terms in (47) acquire, after expansion in the momenta, the form $\frac{1}{3}eE_q\delta_{\varkappa 1}\delta_{MM'}\partial f_0/\partial p$ and $\frac{1}{3}\delta_{\varkappa 1}\delta_{MM'}(p/m)\nabla_q f_0$. The quantity $E\hat{D}$ in (48) should be neglected here.

2) For band 2 at $\varkappa\leqslant 2$ the off-diagonal elements of the momenta are zero. The equations for the corresponding momenta do not contain the term $[\hat{h},\hat{f}]$ and the action of the magnetic field reduces only to the Lorentz force. The term containing the Lorentz force takes the form

$$i\frac{e}{m_2c}\{H_{-1}[(\varkappa-q)(\varkappa+q+1)/2]^{1/2}f^{\varkappa q+1}_{MM}+qH_0f_{MM}{}^{\varkappa q}$$

$$-H_1[(\varkappa+q)(\varkappa-q+1)/2]^{1/2}f^{\varkappa q-1}_{MM}\}. \tag{49}$$

3) With the aid of expression (49) at $\varkappa=1$ and Eq. (16) we can find the equation of motion for the average spin vector in band 2 (given the energy ε)

$$\frac{d\bar{\mathbf{J}}}{dt}=\frac{e}{m_2c}[\bar{\mathbf{J}}\times\mathbf{H}]-\frac{\mathbf{J}}{\tau_3(1)}, \tag{50}$$

where $\tau_3(1)$ is the spin relaxation time determined by Eq. (38). It is interesting that no direct interaction of the spin with the magnetic field $(e\hbar/m_0c)k\,\mathbf{J}\cdot\mathbf{H}$ manifests itself. The only cause of the spin precession in band 2 is the Lorentz force. The particle rotation caused by it leads to spin precession because of the rigid coupling between the particle spin and its momentum.

Equation (47), supplemented by the collision integral (18), makes it possible, by expanding the density matrix in terms of the momenta, to investigate arbitrary (not quantum) kinetic phenomena due to carriers in a complicated band.

[1)] We follow Edmonds[5] in the definition of these matrices.

[2)] The translational motion of the particles is assumed classical. The quantity $f_{MM'}$ considered by us is in fact the Wigner density matrix (see Sec. 5).

[3)] In semiconductors such as GaAs and HgTe there is no inversion center. The resultant additional terms in the Hamiltonian are, however, small and we neglect them.

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