NUCLEAR POLARIZATION IN SEMICONDUCTORS AND SEMIMETALS BY A DIRECT CURRENT

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The influence of an electric current in a semiconductor or semimetal on the magnetization of the electron and nuclear spin subsystems is investigated. Two mechanisms for the interaction of the conduction electron spins with the lattice are considered: interaction with acoustic and with optical phonons. The spin relaxation time of the conduction electrons, associated with their interaction with optical phonons, is calculated for equilibrium and for "hot" electrons. It is shown that the interaction with optical phonons may be the principal mechanism in the establishment of nuclear and electron polarization.

$\mathbf{I}$T is well known that in a semiconductor or semimetal in the presence of a temperature difference of the electrons—spin temperature T_S and kinetic temperature T_e—the magnetization of the nuclear subsystem differs from the equilibrium magnetization corresponding to the temperature of the lattice. For example, in the Overhauser effect the difference between T_S and T_e is achieved by saturation of the electron spin resonance. Feher [1] and Feher and Clark [2] proposed and experimentally verified another scheme for nuclear polarization. Here the difference $T_e - T_S$ is achieved by heating the conduction electrons by a direct current. In this connection, as a consequence of the spin-lattice relaxation the spin temperature may differ from the kinetic temperature. In the present article we consider several mechanisms for establishing a difference between spin and electron temperatures, and also the resulting nuclear magnetization of the system in the presence of drift and heating of the electron gas.

1. Let us consider a system of nuclear spins interacting with the conduction electrons. For simplicity, let us assume the nuclear spin is equal to $\frac{1}{2}$. The Hamiltonian for the magnetic interaction of nuclear spins with conduction electrons has the form [3]

$$\mathcal{H}_1 = A \mathbf{IS} \delta (\mathbf{r}_S - \mathbf{r}_I), \tag{1}$$

where $\mathbf{S}$ is the electron spin, $\mathbf{I}$ is the nuclear spin, $\mathbf{r}_S$ is the electron coordinate, and $\mathbf{r}_I$ is the coordinate of the nucleus. Here the nonsecular part of the interaction is omitted, it is usually negligibly small for conduction electrons having s-type wave functions.

The equations for the rates of change of the nuclear subsystem level populations have the form

$$dN_- / dt = -N_- W_{(+-)\to(-+)} + N_+ W_{(-+)\to(+-)}, \quad N_- + N_+ = 1,$$

$$W_{(+-)\to(-+)} = \frac{2\pi}{\hbar} \sum_{\mathbf{pp'}} |\langle +-|\mathcal{H}_1|-+\rangle|^2 f_+ (\mathbf{p}_+)$$

$$\times [1 - f_- (\mathbf{p}_-')] \, \delta (\varepsilon_{\mathbf{p}_+} - \varepsilon_{\mathbf{p}_-'} - 2\Delta_N), \tag{2}$$

where $N_{\mp}$ are the relative populations of the nuclear subsystem levels with $I_z = \mp \frac{1}{2}$, $|-+\rangle$ is the state corresponding to $S_z = -\frac{1}{2}$, $I_z = \frac{1}{2}$, $f_{\pm} (\mathbf{p})$ are the distribution functions of the electrons with spin $S_z = \pm \frac{1}{2}$, $W_{(+-)\to(-+)}$ and $W_{(-+)\to(+-)}$ are the probabilities of simultaneous reversal of the electron and nuclear spins (it is easy to see that only such transitions are allowed for an interaction of the type (1)); β is the Bohr magneton, H_0 is the external magnetic field.

We note here that the simple description of the kinetics of nuclear spins given by Eqs. (2) is valid under the condition that the Zeeman energy of the nucleus is greater than the energy of the magnetic interactions of the nucleus giving rise to the width of the nuclear resonance line, which is usually satisfied in experiments on nuclear polarization.

Let us determine the stationary value of the nuclear magnetization associated with the presence of an electric current in the system of conduction electrons. In order to determine the functions $f_{\pm} (\mathbf{p})$ it is necessary to solve the kinetic equations for the conduction electrons, with heating of the electron gas taken into account. Such a problem, without taking the spin and spin-orbit interaction of the electrons into consideration, has been investigated by a number

of authors in the theory of nonlinear galvanomagnetic phenomena.

One of the methods frequently applied here is the method of "effective parameters." The nonequilibrium distribution function is approximated by the equilibrium distribution in a system of coordinates moving with the average velocity of the electrons, and by an effective electron temperature T_e which is different from the lattice temperature. This approximation is admissible for sufficiently large electron-gas density. It is possible to take account of the spin and spin-orbit interaction in this scheme, using then the fact that the frequency of collisions of electrons with scatterers without spin flip is usually several orders of magnitude larger than the collision frequency with spin flip. Therefore, one can assume that both subsystems in the drifting coordinate system have identical temperatures, but different chemical potentials. We note that essentially the same approximation is used for consideration of electron spin resonance and the Overhauser effect.

Thus, the electron distribution functions have the form

$$f_\pm(\mathbf{p}) = \left\{ 1 + \exp\frac{\varepsilon(\mathbf{p} - m\mathbf{v}) \pm \Delta_e - \zeta^\pm}{T_e} \right\}^{-1}, \qquad (3)$$

where $\Delta_e = g\beta H/2$, g is the gyromagnetic ratio of the electron; $\mathbf{v}_e$, T_e, and $\zeta^\pm$ are functions of the electric current in the system. It is easy to see that

$$I_{\text{stat}}^z \equiv \frac{N_- - N_+}{2} = \frac{1}{2}\left(\sum_{\mathbf{pp'}}\{f_-(\mathbf{p'})[1-f_+(\mathbf{p})]-f_+(\mathbf{p})[1-f_-(\mathbf{p'})]\} \right.$$
$$\times \delta\left(\varepsilon_{\mathbf{p}_+} - \varepsilon_{\mathbf{p}_-'} - 2\Delta_N\right) \left)\left(\sum_{\mathbf{pp'}}\{f_-(\mathbf{p'})[1-f_+(\mathbf{p})]+f_+(\mathbf{p}) \right.$$
$$\times [1-f_-(\mathbf{p'})]\}\,\delta\left(\varepsilon_{\mathbf{p}_+} - \varepsilon_{\mathbf{p}_-'} - 2\Delta_N\right)\right)^{-1}. \qquad (4)$$

Let us assume that $\zeta_\pm = \zeta_0 \pm \delta$. Expanding (4) in powers of δ/T_e, Δ_N/T_e, and $mv^2/2T_e$, and also using the condition $\Delta_e/T_e \ll 1$, we obtain with the aid of standard calculations, to the lowest order approximation in the parameters mentioned above,

$$\frac{I^z(j)}{I^z(0)} = \frac{T_N}{T_e}\left(1 - s'\frac{\gamma_e}{\gamma_N}\right), \qquad I^z(0) = \frac{\Delta_N}{2T_N},$$
$$s' = s - \frac{mv^2}{3\bar\varepsilon}, \qquad \bar\varepsilon = \begin{cases} T, & \zeta_0/T \ll -1, \\ \zeta_0, & \zeta_0/T \gg 1, \end{cases} \qquad (5)$$

where γ_e and γ_N are the gyromagnetic ratios of electrons and nuclei, T_N is the lattice temperature, $s = \delta/\Delta_e$ is the electron paramagnetic resonance saturation parameter. The latter is related to the spin temperature of the electrons

and to the average electron magnetization by the relations

$$s = (S^z(0) - S'^z(j))/S^z(0), \qquad T_s = -T_e/(1 - s),$$

where $S^z(0)$ and $S^z(j)$ are the equilibrium (for $T_s = T_e$) and, respectively, nonequilibrium values of the average electron spin, T_s is the temperature of the spin subsystem, T_e is the temperature of the electrons.

In semiconductors it is often necessary to consider, besides the contact interaction of the nuclei with the conduction electrons, also other relaxation mechanisms, for example, the interaction with paramagnetic impurities. In this case it is necessary to take the "leakage" of nuclear magnetization, caused by these additional interactions, into account. Let there be an additional relaxation mechanism with relaxation time τ_1', tending to establish a magnetization equal to the equilibrium value I_0^z; then the stationary value of the nuclear polarization is determined by the relation

$$\frac{I^z(j)}{I^z(0)} = \frac{T_N}{T_e}\left(1 - \frac{\gamma_e}{\gamma_N}s'\right)f + 1 - f,$$
$$f = \tau_1'/(\tau_1' + \tau_1). \qquad (6)$$

This relation is easily obtained from the equation for the nuclear level populations in the presence of two relaxation mechanisms.[2] We note that in our approximations the electron drift does not directly influence the nuclear polarization.

2. Since $\nu_s \ll \nu_e$ (ν_s and ν_e are the frequencies for collisions of electrons with scatterers with and without spin flip), then one can determine $T_e(j)$ and $\mathbf{v}(j)$, as this is usually done in the theory of nonlinear galvanomagnetic phenomena, by neglecting the spin. T_e and $\mathbf{v}$ strongly depend on the mechanisms for the scattering of momentum and energy of the electrons, on the magnitudes of the magnetic and electric fields, on the angle between the magnetic and electric fields, and on the boundary conditions. One can, for example, find an examination of these questions in the article by Bass.[5]

Let us consider the establishment of s for given T_e and $\mathbf{v}$. It is well known that the basic mechanism for relaxation of the conduction-electron spin is scattering by acoustic phonons, with the spin-orbit interaction taken into account; in this connection relaxation of momentum and energy may be accomplished by other mechanisms as well (for example, the momentum may relax through the impurities). The parameter δ (or s) in the distribution functions (3) is determined from the steady state condition for $M_z(t)$

(z ∥ H), where M_z is the density of the spin angular momentum of the electron gas.

It is possible to obtain an equation for M_z from simple considerations of the conservation of spin density during collisions:

$$\dot{M}_z = \frac{g\beta}{2} \sum_{\sigma\sigma'} \sum_{kq} (\sigma - \sigma') W_{k\sigma}{}^{k+q\sigma'} \{(N_q + 1)$$

$$\times f_{\sigma'}(k+q)[1 - f_\sigma(k)] - N_q f_\sigma(k)[1 - f_{\sigma'}(k+q)]\}$$

$$\times \delta(\varepsilon_{k+q,\sigma'} - \varepsilon_{k\sigma} - \hbar\omega_q), \qquad (7)$$

where N_q is the distribution function of the phonons with quasimomentum q, $W_{k\sigma}^{k'\sigma'}$ is the probability for the transition of an electron from the state $|k\sigma\rangle$ to the state $|k'\sigma'\rangle$. It is also possible to obtain this equation from the Boltzmann equations for $f_{\pm}(p)$, multiplying them by $\sigma g\beta/2$ and summing over σ.[6]

In order to calculate s, it is sufficient to know the dependence of $W_{k\sigma}^{k+q,\sigma'}$ on k and q. In contrast to the probability for a transition without spin flip, the probability for a transition with spin flip strongly depends on the energy spectrum of the crystal, on the symmetry of the crystal under space reflection, on the position of the bottom of the conduction band in the Brillouin zone, and so forth. For the simple case when the bottom of the conduction band and the top of the valence band are located at the center of the Brillouin zone (InSb, in which Feher and Clark [2] observed nuclear polarization, has just such an energy spectrum), Yafet [7] showed that the transition probability is given by

$$W_{k\sigma}{}^{k+q,\sigma'} \sim \begin{cases} |q|, & \sigma = \sigma', \\ |k+k'|^2 |q|^3, & \sigma \neq \sigma'. \end{cases} \qquad (8)$$

We note that in a number of articles [6,8] a value of the transition probability equal to $|k + k'|^2 |q|^{-1}$ was used to calculate of electron and nuclear polarization. This result, obtained by Elliott [9] is incorrect, [7] since Elliott takes the spin-orbit interaction into account only in the wave functions, but he does not consider it in the electron-phonon interaction energy.

Now let us deduce the solution of the transcendental equation (7) for a nondegenerate electron gas. We shall seek the solution δ in the form of a series in powers of the small parameter $\gamma = (mc_0^2/T_e)^{1/2}$; for example, for InSb the value of $mc_0^2 \sim 10^{-2}$ °K. In this connection, Δ_e/T_e and mv^2/T_e are assumed to be small. Expanding (7) in a series in powers of γ and collecting terms of like order, we obtain with the aid of standard but tedious calculations the following result for

an electron gas subject to Maxwell-Boltzmann statistics

$$s \cong \frac{mc_0^2}{T_e} \left\{ \frac{1}{3} \left(\frac{v}{c_0} \right)^2 \right.$$

$$\left. - \sqrt{\frac{mc_0^2}{T_e}} \, 3\sqrt{\pi} \left(\frac{T_e}{T_p} - 1 \right) \left(1 - \frac{1}{4} \left(\frac{v}{c_0} \right)^2 \right) \right\}; \qquad (9)$$

c_0 is the velocity of sound in the crystal, T_p is the temperature of the phonons. We note that in articles [6,8] strongly overestimated results corresponding to $s \sim \gamma$ are obtained.

For a degenerate electron gas the saturation parameter s, correct to coefficients of the order of unity, has the same form as in Eq. (9), only in this case the small parameter γ is replaced by $(mc_0^2/\zeta_0)^{1/2}$ (ζ_0 is the Fermi energy). We see that both in the degenerate case as well as in the non-degenerate case, s is much smaller than unity. Taking account of the nonequilibrium of the phonons (phonon drag and heating) still further decreases this quantity.[6] We note that the same order of magnitude result is obtained for an examination of piezo-acoustic scattering, which may be essential for the scattering of hot electrons in InSb at 4.2 °K.[10]

3. From formula (9) it is evident that the saturation parameter s is proportional to the square (or to the cube, if $v/c_0 \cong 0$) of the ratio of the energy transferred by the electron to the phonon during a collision to the average electron energy. If the inelasticity of the scattering is neglected, then s vanishes. During the collision of an electron with an optical phonon, the electron emits or absorbs an energy quantum $\hbar\omega_0$ appreciably larger than for a collision with an acoustic phonon. This suggests that the interaction with optical phonons may lead to a large nuclear polarization.

The Hamiltonian for the interaction of conduction electrons with optical phonons has the form

$$\mathcal{H}_{ep} = -e\Phi - \frac{e\hbar}{4m^2c^2} (\sigma[\nabla\Phi, p]), \qquad (10)*$$

where in standard notation $e\Phi$ has the form [11]

$$-e\Phi = i \frac{2\pi ze^2}{a^3\sqrt{N}} \frac{M_1 + M_2}{\sqrt{M_1 M_2}} \sum_{qj} \frac{(n_{qj}q)}{q^2} (a_{qj}e^{iqr} - a_{qj}^* e^{-iqr}). \qquad (11)$$

The second term in Eq. (10) describes the change in the spin-orbit energy of an electron due to the lattice vibrations.

The matrix element determining the transition probability is given by

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* $[\nabla\Phi, p] \equiv \nabla\Phi \times p$.

$$\langle N_{\mathbf{q}}'\mathbf{k}'\sigma' \,|\, \mathcal{H}_{ep} \,|\, N_{\mathbf{q}}\mathbf{k}\sigma\rangle = \sum_{\mathbf{q}} C_{\mathbf{q}} \langle N_{\mathbf{q}}' \,|\, a_{\mathbf{q}} - a_{-\mathbf{q}}^* \,|\, N_{\mathbf{q}}\rangle$$

$$\times \left\langle \mathbf{k}'\sigma' \,\Big|\, e^{i\mathbf{q}\mathbf{r}} \left(1 + \frac{ie\hbar}{4m^2c^2}(\sigma\,[\mathbf{q}\mathbf{p}])\right) \Big|\, \mathbf{k}\sigma \right\rangle; \tag{12}$$

$$C_{\mathbf{q}} = i\,\frac{2\pi z e^2}{a^3\sqrt{N}}\,\frac{M_1 + M_2}{\sqrt{M_1 M_2}}\,\frac{1}{q}, \tag{13}$$

$$M_{\mathbf{k}'\sigma'}^{\mathbf{k}\sigma} \equiv \left\langle \mathbf{k}'\sigma' \,\Big|\, e^{i\mathbf{q}\mathbf{r}} \left(1 + \frac{ie\hbar}{4m^2c^2}(\sigma\,[\mathbf{q}\mathbf{p}])\right) \Big|\, \mathbf{k}\sigma \right\rangle$$

$$= \frac{1}{N} \int_V e^{-i\mathbf{k}'\mathbf{r}} u_{n\mathbf{k}'\sigma'}^* e^{i\mathbf{q}\mathbf{r}} \left(1 + \frac{ie\hbar}{4m^2c^2}(\sigma\,[\mathbf{q}\mathbf{p}])\right) e^{i\mathbf{k}\mathbf{r}} u_{n\mathbf{k}\sigma}\,d\mathbf{r}$$

$$\cong \delta_{\mathbf{k}'-\mathbf{k}-\mathbf{q},0} \int_\Omega u_{n\mathbf{k}'\sigma'}^*(\mathbf{r}) \left(1 + \frac{ie\hbar}{4m^2c^2}(\sigma\,[\mathbf{q}\mathbf{p}])\right) u_{n\mathbf{k}\sigma}(\mathbf{r})\,d\mathbf{r}. \tag{14}$$

In Eq. (13) the integral is to be evaluated over the volume of the crystal, in Eq. (14) it is over an elementary cell. $u_{n\mathbf{k}\sigma}(\mathbf{r})$ is the Bloch amplitude of the wave function with the spin-orbit interaction taken into account. In going from Eq. (13) to Eq. (14) we have neglected Umklapp processes.

The integral in Eq. (14) is a function of $\mathbf{k}$ and $\mathbf{k}'$. This function determines the spin relaxation in the crystal. In the same way as in the acoustic scattering case, it depends essentially on the energy spectrum of the crystal. Let us consider the behavior of the integral (14) for the simple case when the crystal has a center of inversion and the bottom of the conduction band and the top of the valence band are located at the center of the Brillouin zone. The maximum electron energy is appreciably smaller than the width of the forbidden gap. Such a situation occurs, for example, in InSb.[1]

We expand the integral (14) in a series in powers of $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ and $\mathbf{K} = (\mathbf{k}' + \mathbf{k})/2$. For calculations we can confine ourselves to the first nonvanishing term of the series, since this series converges rapidly. In fact, in the expansion of the integral (14) with respect to the quasimomentum, $\mathbf{k}\cdot\mathbf{p}$ perturbation theory gives for each power of $\mathbf{K}$ or $\mathbf{q}$ a factor of the order of $\hbar P/m\epsilon_g$ (or smaller), where P is the interband matrix element of the momentum and ϵ_g is the width of the forbidden gap. Usually $\hbar Pk/m\epsilon_g$ is a small quantity.[12] We have

$$R(\mathbf{K}\mathbf{q}) \equiv \left(u_{\mathbf{K}+\mathbf{q}/2,\sigma}^* \,\Big|\, 1 + \frac{ie\hbar}{4m^2c^2}(\sigma\,[\mathbf{q}\mathbf{p}]) \,\Big|\, u_{\mathbf{K}-\mathbf{q}/2,-\sigma}\right)$$

$$= a_0(\mathbf{K},0) + \sum_i q_i b_i + \sum_{ij} q_i K_j d_{ij} + \ldots \tag{15}$$

In what follows we shall omit the band index on the functions $u_{n\mathbf{k}\sigma}(\mathbf{r})$.

The first two terms in the expansion (15) are equal to zero. It is possible to prove this in general form by using the properties of the Bloch amplitudes under the operations of time reversal and space reflection. We introduce J—the operator for reflection of the coordinates, and $\mathbf{K} \equiv -i\sigma_y K_0$—the time reversal operator.[12] Then

$$a_0(\mathbf{K},0) = (u_{\mathbf{K}\sigma} u_{\mathbf{K}-\sigma}) = \int_\Omega u_{\mathbf{K}\sigma}^*(r)\,u_{\mathbf{K}-\sigma}(r)\,dr. \tag{16}$$

Taking account of the identity

$$JKu_{\mathbf{k}\sigma} \equiv Cu_{\mathbf{k}\sigma} = u_{\mathbf{k},-\sigma} \tag{17}$$

(correct to within a phase factor) and

$$(\varphi,\psi) = (C\psi, C\varphi), \qquad K^2 = -1, \quad C^2 = -1, \tag{18}$$

we obtain

$$(u_{\mathbf{K}\sigma}, u_{\mathbf{K},-\sigma}) = (u_{\mathbf{K}\sigma}, Cu_{\mathbf{K}\sigma}) = (C^2 u_{\mathbf{K}\sigma}, Cu_{\mathbf{K}\sigma})$$

$$= -(u_{\mathbf{K}\sigma}, u_{\mathbf{K};-\sigma}) = 0, \tag{19}$$

$$\sum_i q_i b_i = \sum_i q_i \left\{ \left(\left(\frac{\partial u_\sigma}{\partial K_i}\right)_{K=0}, u_{0,-\sigma}\right) - \left(u_{0\sigma}, \left(\frac{\partial u_{-\sigma}}{\partial K_i}\right)_{K=0}\right)\right.$$

$$\left. + \frac{ie\hbar}{4m^2c^2}\,[(u_{0,\sigma}\,|\,\mathbf{p}\,|\,u_{0,-\sigma}),\,\sigma]_i \right\}. \tag{20}$$

Considering that $Cp_j C^{-1} = p_j = (\tilde{p}_j)^*$, we obtain

$$(u_{0\sigma}p_j u_{0,-\sigma}) = (u_{0\sigma}p_j Cu_{0\sigma}) = (Cp_j Cu_{0\sigma}, Cu_{0\sigma})$$

$$= (Cp_j C^{-1}C^2 u_{0\sigma}, Cu_{0\sigma}) = (C^2 u_{0\sigma}, p_j u_{0,-\sigma})$$

$$= -(u_{0\sigma}p_j u_{0,-\sigma}) = 0. \tag{21}$$

We expand $u_{\mathbf{K},\sigma}$ in powers of $\mathbf{K}$:

$$u_{\mathbf{K}\sigma} = u_{0\sigma} + \sum_i K_i u_\sigma^{(1)}(r) + \ldots \tag{22}$$

Considering that

$$Ju_{\mathbf{K}\sigma} = u_{-\mathbf{K},\sigma}(r), \tag{23}$$

apart from a phase factor which is not important here, we obtain

$$u_{\mathbf{K}\sigma}(-r) = u_{0\sigma}(r) - \sum_i K_i u_{i\sigma}^{(1)}(r) + \ldots = u_{0\sigma}(-r)$$

$$+ \sum_i K_i u_{i\sigma}^{(1)}(-r) + \ldots \tag{24}$$

From here we see that $u_{i\sigma}^{(1)}(r)$ and $u_{0\sigma}(r)$ have opposite parities under space reflection. Then

$$(u_{i\sigma}^{(1)}(r), u_{0,-\sigma}(r)) = (u_{i\sigma}^{(1)}(-r),$$

$$u_{0\sigma}(-r)) = (u_{i\sigma}^{(1)}(-r), u_{0\sigma}^*(r)) = 0. \tag{25}$$

Similarly

$$\left(u_{0\sigma}(r), \left(\frac{\partial u_{-\sigma}}{\partial K_i}\right)_{K=0}\right) = 0.$$

And so, from Eqs. (19)–(21) we have

$$R(\mathbf{K},\mathbf{q}) = \sum_{ij} d_{ij} K_i q_j.$$

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[1]Although the InSb crystal is not invariant under reflection of the coordinates; however, in this case the noninvariance plays a small role in spin relaxation (see [7]).

One can calculate the constants d_{ij} by using $\mathbf{k} \cdot \mathbf{p}$ perturbation theory. However, for our purposes we can neglect the angular dependence of the function $R(\mathbf{K}, \mathbf{q})$ which is unimportant for calculation of the electron polarization and may give a factor of order unity in connection with the calculation of the electron spin relaxation time. Therefore we set

$$R(K, q) \cong dKq, \tag{26}$$

where in order of magnitude d is equal to $\delta g \hbar^2 / m_0 \epsilon_g$ (here $\delta g = |g - 2|$ may be appreciably greater than unity),[6] m_0 is the free electron mass.

Taking into consideration that [11]

$$\langle N_\mathbf{q}' | a_\mathbf{q} | N_\mathbf{q} \rangle = \left[\frac{\hbar N_\mathbf{q}}{2(M_1 + M_2) w_\mathbf{q}} \right]^{1/2} \delta_{N_\mathbf{q}', N_\mathbf{q}-1},$$

$$\langle N_\mathbf{q}' | a_\mathbf{q}^* | N_\mathbf{q} \rangle = \left[\frac{\hbar N_\mathbf{q}}{2(M_1 + M_2) w_\mathbf{q}} \right]^{1/2} \delta_{N_\mathbf{q}', N_\mathbf{q}+1}, \tag{27}$$

we obtain the following expressions for the probabilities of absorption and emission of a phonon per unit time:

$$W_{k\sigma}^{+k'\sigma'} = w(q) N_\mathbf{q} \delta(\epsilon_{k+q, \sigma'} - \epsilon_{k\sigma} + \hbar\omega_q), \tag{28a}$$

$$W_{k\sigma}^{-k'\sigma'} = w(q)(N_\mathbf{q} + 1) \delta(\epsilon_{k-q, \sigma'} - \epsilon_{k\sigma} + \hbar\omega_q), \tag{28b}$$

$$w(q) \cong \frac{(2\pi)^3 z^2 e^4}{N \mu a^6 \omega_0} (\delta g)^2 \frac{\hbar^4 K^2}{m_0^2 \epsilon_g^2} = w^0(q) \frac{\hbar^4 K^2 q^2}{m_0^2 \epsilon_g^2} (\delta g)^2. \tag{29}$$

Here μ is the reduced mass of the ions, $w^0(q)$ is the function determining the probability of the transition (28) without spin flip.

4. Now let us evaluate the electron polarization parameter s. We return to Eq. (7). The electron distribution function has the form (3). In Eq. (7) we change over to new integration variables $\mathbf{p} - m\mathbf{v} \to \mathbf{p}$, $\mathbf{p}' - m\mathbf{v} \to \mathbf{p}'$. Then

$$\dot{M}_z = g\beta \sum_{\sigma\sigma'} \sum_{kq} (\sigma - \sigma') \overline{w}_{k\sigma}^{k+q, \sigma'} \{(N_\mathbf{q} + 1) f_{\sigma'}(\mathbf{k})[1 - f_\sigma(\mathbf{k})]$$

$$- N_\mathbf{q} f_\sigma(\mathbf{k})[1 - f_{\sigma'}(\mathbf{k} + \mathbf{q})]\} \delta(\epsilon_{k+q, \sigma'} - \epsilon_{k\sigma} - \hbar\omega_q^*); \tag{30}$$

here

$$\hbar\omega_\mathbf{q}^* = \hbar\omega_0 + \hbar qv = \hbar\omega_0(1 + qv/\omega_0),$$

$$\overline{w}(\mathbf{K}, \mathbf{q}) = w(\mathbf{K}, \mathbf{q})|1 + mvk/\hbar K^2|^2.$$

We shall not take the dispersion of optical phonons into consideration.

It is easy to see that in the case of optical phonons one can, to a first approximation, neglect the drift of the carriers for $v \lesssim c_0$ over a wide temperature interval. In fact,

$$\frac{\hbar qv}{\hbar\omega_0} \cong \frac{v}{c} \left(\frac{T_{cr}\bar{\epsilon}}{T_{Debye}^2} \right)^{1/2} \ll 1,$$

since

$$T_{cr} \sim mc^2 \sim (10^{-2} - 1)^\circ K, \quad T_{Debye} = \hbar\omega_0 \sim 10^2 \,^\circ K,$$

$$\bar{\epsilon} \sim (10 - 10^2) \,^\circ K.$$

Similarly

$$\frac{mvk}{\hbar k^2} \cong \frac{v}{c} \left(\frac{T_{cr}}{\bar{\epsilon}} \right)^{1/2} \ll 1.$$

In order to solve the transcendental equation $\dot{M}_z = 0$, we assume that $\delta / T_e \ll 1$. This is a natural assumption since Eq. (7) is valid under the condition $\Delta_e / T_e \ll 1$. Expanding (30) in powers of δ / T_e and confining our attention to the lowest-order approximation, we obtain

$$s = -\Delta \left\{ \sum_{\sigma\sigma'} \sum_{kq} (\sigma - \sigma') w(\mathbf{k}, \mathbf{q})(N_p - N_e)[f_0(\epsilon_{k\sigma} + \hbar\omega_0) \right.$$

$$- f_0(\epsilon_{k\sigma})] \delta(\epsilon_{k'\sigma'} - \epsilon_{k\sigma} - \hbar\omega_0) \bigg\} \left\{ \sum_{\sigma\sigma'} \sum_{kq} (\sigma - \sigma') w(\mathbf{k}, \mathbf{q}) \right.$$

$$\times \left[\sigma' \frac{\partial f_0}{\partial \epsilon_{k'\sigma'}}(N_\mathbf{q} + 1 - f_0(\epsilon_{k\sigma})) - \sigma \frac{\partial f_0}{\partial \epsilon_{k\sigma}}(N_\mathbf{q} + f(\epsilon_{k'\sigma'})) \right]$$

$$\times \delta(\epsilon_{k'\sigma'} - \epsilon_{k\sigma} - \hbar\omega_0) \bigg\}^{-1},$$

$$f_0(\epsilon_{k\sigma}) = f_0 \left(\frac{\epsilon_{k\sigma} - \zeta_0}{T_e} \right), \quad N_{p,e} = N_0 \left(\frac{\hbar\omega_0}{T_{p,e}} \right), \tag{31}$$

where T_{lat} is the temperature of the lattice.

We note that s does not depend on the numerical factor in the matrix element (26). The calculation yields

$$s = -\frac{1}{2} \frac{\hbar\omega_0}{T_e} \left[N_0 \left(\frac{\hbar\omega_0}{T_{lat}} \right) - N_0 \left(\frac{\hbar\omega_0}{T_e} \right) \right] \psi_1 \left(\frac{\hbar\omega_0}{T_e}, z \right)$$

$$\times \psi_2^{-1} \left(\frac{\hbar\omega_0}{T_e}, z, \frac{\hbar\omega_0}{T_{lat}} \right),$$

$$\psi_1 \left(\frac{\hbar\omega_0}{T_e}, z \right) = \int_0^\infty dx \left[f_0(x - z) - f_0 \left(x + \frac{\hbar\omega_0}{T_e} - z \right) \right]$$

$$\times \left(1 + \frac{\hbar\omega_0}{T_e x} \right)^{-1/2} \left(1 + \frac{\hbar\omega_0}{2T_e x} \right), \tag{33}$$

$$\psi_2 \left(\frac{\hbar\omega_0}{T_e}, z, \frac{\hbar\omega_0}{T_{lat}} \right) = \int_0^\infty dx \left[\frac{\partial f_0(x + \hbar\omega_0/T_e - z)}{\partial x} \right.$$

$$\times \left(N_0 \left(\frac{\hbar\omega_0}{T_{lat}} \right) + 1 - f_0(x - z) \right)$$

$$+ \frac{\partial f_0(x - z)}{\partial x} \left[N_0 \left(\frac{\hbar\omega_0}{T_{lat}} \right) + f_0 \left(x + \frac{\hbar\omega_0}{T_e} - z \right) \right]$$

$$\times \left(x^2 + \frac{\hbar\omega_0}{T_e} x \right)^{1/2} \left(x + \frac{\hbar\omega_0}{2T_e} \right). \tag{34}$$

Let us consider certain special cases.

A. Nondegenerate electron gas. a) For $\hbar\omega_0/T_e \gg 1$ and $\hbar\omega_0/T_{lat} \gg 1$ we have

$$s = -\frac{1 - \exp[\hbar\omega_0(1/T_e - 1/T_{lat})]}{1 + \exp[\hbar\omega_0(1/T_e - 1/T_{lat})]}, \tag{35}$$

for $(\hbar\omega_0/T_e)[(T_e/T_{lat}) - 1] \ll 1$ we have

$$s = -\frac{\hbar\omega_0}{2T_e}\left(\frac{T_e}{T_{lat}} - 1\right), \tag{36}$$

and for $\hbar\omega_0/T_{lat} \gg \hbar\omega_0/T_e$ we find

$$s = -1. \tag{37}$$

Since $\hbar\omega_0/T_{lat}$ and $\hbar\omega_0/T_e$ are appreciably greater than unity, this case may be realized for a comparatively small difference between T_e and T_{lat}, namely

$$T_e/T_{lat} - 1 \gg T_e/\hbar\omega_0 \ll 1. \tag{38}$$

b) In the case $\hbar\omega_0/T_e \ll 1$ and $\hbar\omega_0/T_{lat} \ll 1$, we obtain

$$s = -\frac{1}{4}\left(\frac{\hbar\omega_0}{T_e}\right)^2\left(\frac{T_e}{T_{lat}} - 1\right). \tag{39}$$

c) For $\hbar\omega_0/T_e \ll 1$ and $\hbar\omega_0/T_{lat} \gg 1$, we have

$$s = -\frac{1}{4}\hbar\omega_0/T_e. \tag{40}$$

B. <u>Degenerate electron gas ($z \gg 1$).</u>
a) For $\hbar\omega_0/T_e \gg 1$, $\hbar\omega_0/T_{lat} \gg 1$, and $z \gg \hbar\omega_0/T_e$ we have

$$s = \begin{cases} -\dfrac{1}{4}\left(\dfrac{\hbar\omega_0}{\zeta_0}\right)^2, & \dfrac{\hbar\omega_0}{T_{lat}} \gg \dfrac{\hbar\omega_0}{T_e}, \\[2mm] -\dfrac{1}{8}\left(\dfrac{\hbar\omega_0}{\zeta_0}\right)^2\dfrac{\hbar\omega_0}{T_e}\left(\dfrac{T_e}{T_{lat}} - 1\right), & \hbar\omega_0\left(\dfrac{1}{T_{lat}} - \dfrac{1}{T_e}\right) \ll 1. \end{cases} \tag{41}$$

b) For $\hbar\omega_0/T_e \gg 1$, $\hbar\omega_0/T_{lat} \gg 1$, and $z \ll \hbar\omega_0/T_e$, we have

$$s = \begin{cases} -1, & \dfrac{\hbar\omega_0}{T_{lat}} \gg 1, \\[2mm] -\dfrac{\hbar\omega_0}{2}\left(\dfrac{1}{T_{lat}} - \dfrac{1}{T_e}\right), & \hbar\omega_0\left(\dfrac{1}{T_{lat}} - \dfrac{1}{T_e}\right) \ll 1. \end{cases} \tag{42}$$

These results show that in all limiting cases optical phonons give a considerably larger electron (and nuclear) polarization than acoustic phonons. This result has a simple physical interpretation. Let us consider, for example, the case $\hbar\omega_0 \gg T_{lat}, T_e$. In this case $N_q \ll 1$; therefore, processes involving the spontaneous radiation of optical phonons by "hot" electrons are dominant in the interaction of electrons with optical phonons. Here the following two processes accompanied by spin flip are possible: $(\epsilon_{k'} +| \rightarrow (\epsilon_k -|$ and $(\epsilon_{k'} -| \rightarrow (\epsilon_k +|$ (see Fig. 1), for which the energy conservation law has the form

$$\epsilon_{k'} - \epsilon_k = \hbar\omega_0 - 2\Delta_e, \tag{43a}$$

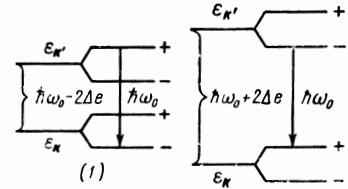$$\epsilon_{k'} - \epsilon_k = \hbar\omega_0 + 2\Delta_e. \tag{43b}$$

FIG. 1

Electrons with energies $\epsilon \geq \hbar\omega_0 - 2\Delta_e$ and $\epsilon \geq \hbar\omega_0 + 2\Delta_e$, respectively, may participate in processes of the type (43a) and (43b). Since the number of electrons with energies $\epsilon \geq \hbar\omega_0 - 2\Delta_e$ is greater than the number with energies $\epsilon \geq \hbar\omega_0 + 2\Delta_e$, then processes of type (43a) occur more often than processes of type (43b) (see Fig. 2). Processes of type (43a) increase the electron polarization. This effect must increase with increasing Δ_e/T_e and $\hbar\omega_q/T_e$.

We note here than in contrast to the Overhauser effect where the saturating radio frequency field increases the spin temperature of the electrons in comparison with the kinetic temperature and decreases the magnetization, in the effect on the "hot" electrons the spin temperature is lower than the temperature of the electrons and, correspondingly, the electron magnetization is increased (although it is less than for $T_e = T_{lat}$). A directed drift of the electrons, in contrast to their heating, increases the spin temperature of the electrons.

5. In order that the interaction with optical phonons may actually lead to a large electron (and nuclear) polarization, it is necessary that the spin relaxation time of the conduction electrons by optical phonons should be comparable with the spin relaxation time caused by other mechanisms, or smaller than it. The investigations of Overhauser, Elliott, Yafet, and others have shown that in semiconductors, over a broad range of temperatures and impurity concentrations, the dominant mechanism for conduction electron spin relaxation is relaxation by acoustic phonons (relaxation by optical phonons was not considered). The conditions under which relaxation by optical phonons may be essential will be shown below.

It is easy to obtain a formula for the relaxation time from Eq. (7) by substituting in it, as
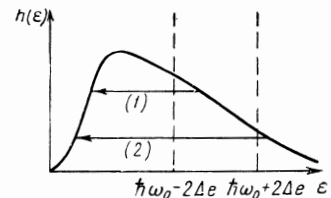

FIG. 2

usual, the distribution function $f(p, \sigma)$ in the form $f[(\epsilon_{k\sigma} - \zeta_\sigma)/T_e]$. Expanding Eq. (7) in a series in powers of $(\zeta_\sigma - \zeta_0)/T_e = -\sigma\delta/T_e$ and Δ_e/T_e, it is easy to reduce it to the form

$$\dot{M}_z = -\frac{M_z - M_0}{\tau_1},$$

where τ_1, according to definition, is the longitudinal relaxation time of the conduction electron spin. Having carried out this procedure, we obtain

$$\frac{1}{\tau_1} = \sum_{\sigma\sigma'}\sum_{kq}\left\{(\sigma - \sigma')|w_{k\sigma}^{k+q,\sigma'}|\left[\sigma\frac{\partial f}{\partial\epsilon_{k\sigma}}(N_q + f(\epsilon_{k'\sigma'}))\right.\right.$$
$$\left.\left. - \sigma'\frac{\partial f}{\partial\epsilon_{k'\sigma'}}(N_q + 1 - f(\epsilon_{k\sigma}))\right]\delta(\epsilon_{k'\sigma'} - \epsilon_{k\sigma} - \hbar\omega_q)\right\}$$
$$\times\left\{\sum_{\sigma\sigma'}\sum_{kq}\left(\frac{\sigma - \sigma'}{2}\right)\sigma\frac{\partial f_0}{\partial\epsilon_k}\right\}^{-1},$$

$$f_0(\epsilon_k) = f_0\left(\frac{\epsilon_k - \zeta_0}{T_e}\right), \tag{44}$$

where $\hbar\omega_q = \hbar\omega_0$, and we neglect the dispersion of the optical phonons.

It is convenient to study not the spin relaxation time proper, but the ratio of the relaxation time τ_0 without spin flip to the relaxation time with spin flip, since the relaxation without spin slip has been rather well studied. We shall define the relaxation time without spin flip in the following manner:

$$\frac{1}{\tau_0} = \sum_k\frac{1}{\tau_0(\epsilon)}\frac{\partial f_0}{\partial\epsilon_k}\bigg/\sum_k\frac{\partial f_0}{\partial\epsilon_k}. \tag{45}$$

Here $\tau_0(\epsilon)$ is a relaxation time approximating the collision integral in the Boltzmann equation. We note that, for optical phonons, such a definition is possible only in two limiting cases:

$$\hbar\omega_0 \gg T_e, \qquad T_e \gg \hbar\omega_0. \tag{46}$$

Using formulas (34) and (28c), carrying out the integration with respect to angles and with respect to the modulus of q in Eq. (44), we obtain

$$\frac{1}{\tau_1} = \frac{4\pi z^2 e^4 (m^*)^{1/2} T_e^{3/2}}{\sqrt{2}\,\mu a^3\hbar\omega_0 m_0^2\,\epsilon_g^2}(\delta g)^2$$

$$\times\psi_2\left(\frac{\hbar\omega_0}{T_e}, z, \frac{\hbar\omega_0}{T_{lat}}\right)\bigg/\int_0^\infty dx\cdot x^{1/2}\frac{\partial}{\partial x}f_0(x - z). \tag{47}$$

Let us consider certain limiting cases.

High temperatures ($T_e \gg \hbar\omega_0$, $T_{lat} \gg \hbar\omega_0$). The relaxation time of the conduction electrons, associated with scattering by optical phonons without spin flip, is given by the expression [11]

$$\tau_0(\epsilon) \cong \frac{\sqrt{2}}{4\pi}\frac{\mu a^3(\hbar\omega_0)^2\epsilon^{1/2}}{z^2 e^4 (m^*)^{1/2}T_{lat}}. \tag{48}$$

For the equilibrium system ($T_e = T_{lat}$) the ratio τ_0/τ_1, as one can easily see, is given by

$$\frac{\tau_0}{\tau_1} \cong \begin{cases} 8\left(\dfrac{m^*}{m_0}\right)^2(\delta g)^2\left(\dfrac{T_e}{\epsilon_g}\right)^2, & z \ll -1, \quad (49a) \\[2mm] 2\left(\dfrac{m^*}{m_0}\right)^2(\delta g)^2\left(\dfrac{\zeta_0}{\epsilon_g}\right)^2, & z \gg 1 \qquad (49b) \end{cases}$$

(Eq. (49a) is for Maxwell-Boltzmann statistics, Eq. (49b) is for Fermi-Dirac statistics).

Low temperatures ($\hbar\omega_0 \gg T_e$, $T_e = T_{lat}$). We have

$$\frac{\tau_0}{\tau_1} \cong \begin{cases} 2\left(\dfrac{m^*}{m_0}\right)^2(\delta g)^2\left(\dfrac{\hbar\omega_0}{\epsilon_g}\right)^2, & z \ll -1, \\[2mm] 1\left(\dfrac{m^*}{m_0}\right)^2(\delta g)^2\left(\dfrac{\hbar\omega_0}{\epsilon_g}\right)^2, & 1 \ll z < \dfrac{\hbar\omega_0}{T_e}, \quad (50) \\[2mm] 4\left(\dfrac{m^*}{m_0}\delta g\right)^2\left(\dfrac{\hbar\omega_0\zeta_0^3}{\epsilon_g^2}\right)^{1/2}, & z \gg \dfrac{\hbar\omega_0}{T_e}. \end{cases}$$

Let us compare the obtained results with the electron spin relaxation time associated with scattering by acoustic vibrations. Yafet [7] showed that

$$\frac{\tau_0^{ac}}{\tau_1^{ac}} \cong \left(\frac{m^*}{m_0}\right)^2(\delta g)^2\left(\frac{\epsilon}{\epsilon_g}\right)^2, \quad \epsilon = \begin{cases} T_e, & z \ll -1, \\ \zeta_0, & z \gg 1. \end{cases} \tag{51}$$

Using (48) and (49), we form the ratio of the spin relaxation times for scattering by acoustic phonons and by optical phonons:

$$\frac{\tau_1^{ac}}{\tau_1^{op}} \sim \frac{\tau_0^{ac}}{\tau_0^{op}}, \qquad T \gg \hbar\omega_0;$$

$$\frac{\tau_1^{ac}}{\tau_1^{op}} \sim \begin{cases} \dfrac{\tau_0^{ac}}{\tau_0^{op}}\left(\dfrac{\hbar\omega_0}{T_e}\right)^2, & z \ll -1 \text{ and } 1 \ll z < \dfrac{\hbar\omega_0}{T_e}, \\[2mm] \dfrac{\tau_0^{ac}}{\tau_0^{op}}\left(\dfrac{\hbar\omega_0}{\zeta_0}\right)^{1/2}, & z \gg \dfrac{\hbar\omega_0}{T_e}. \end{cases} \tag{53}$$

Relations (53) indicate that at low temperatures the relative role of optical phonons in spin scattering increases.

Formulas (49)—(53) are obtained under the assumption that the electrons are in equilibrium with the phonons. One can take the effect on the electron spin relaxation time of heating the electrons relative to the lattice into account by using formula (47). In fact, the ratio of the spin lattice relaxation time in the equilibrium system ($T_e = T_{lat}$) to the relaxation time in the non-equilibrium system ($T_e \neq T_{lat}$), taken at one temperature equal to T_e, is given by

$$\frac{\tau_1^{op}(T_e, T_{lat} = T_e)}{\tau_1^{op}(T_e, T_{lat} \neq T_e)} = \frac{\psi_2(\hbar\omega_0/T_e, z, \hbar\omega_0/T_{lat})}{\psi_2(\hbar\omega_0/T_e, z, \hbar\omega_0/T_e)} \equiv y. \tag{54}$$

In the case of low temperatures, $T_e \ll \hbar\omega_0$, this ratio is given by

$$y = \frac{1}{2}\left\{1 + \exp\left[-\hbar\omega_0\left(\frac{1}{T_{lat}} - \frac{1}{T_e}\right)\right]\right\}. \tag{55}$$

It is easy to see that even for relatively small heating, $(T_e/T_{lat}) - 1 \gg T_e/\hbar\omega_0 \ll 1$, the parameter y attains its own minimal value $y = \frac{1}{2}$.

For high temperatures $(\hbar\omega_0 < T_e, \hbar\omega_0 < T_{lat})$

$$y = T_{lat}/T_e. \tag{56}$$

From formula (44) it follows that for acoustic phonons when $T \gg T_{cr} = mc_0^2$, N_q will be approximately equal to $T_{lat}/\hbar c_0 q \gg 1$, and therefore

$$1/\tau_1 = T_{lat}\varphi(T_e).$$

Then it is easy to form the ratio of the spin relaxation times for acoustic phonons, analogous to relation (54):

$$\frac{\tau_1^{ac}(T_e, T_{lat} = T_e)}{\tau_1^{ac}(T_e, T_{lat} \neq T_e)} = \frac{T_{lat}}{T_e}. \tag{57}$$

We see that for appreciable heating $(T_e \gg T_{lat})$ the spin relaxation time by optical phonons is double the equilibrium relaxation time, whereas for acoustic phonons it may be considerably larger than the equilibrium value. Thus, relations (54), (56), and (57) indicate an increase of the relative role of the optical phonons in spin scattering (at low temperatures) in nonequilibrium systems too.

6. In order to estimate the dependence of the nuclear and electron polarizations on the electric field, sometimes it is necessary to consider several mechanisms for the spin-lattice relaxation of the conduction electrons. For example, in the presence of both acoustic and optical phonons, the saturation parameter s is given by

$$s = s_{ac}(1 - \xi) + s_{op}\xi, \tag{58}$$
$$\xi = \tau_1^{ac}/(\tau_1^{op} + \tau_1^{ac}). \tag{59}$$

Since s_{ac} is usually very small, for comparable values of τ_1^{ac} and τ_1^{op} the parameter s is determined by the second term in (58). The dependence of $I^z(j)/I^z(0)$ and s on the electric field has a complicated form and is determined by formulas (6) and (32) and by the dependence of the effective temperature on the electric field. It is possible to approximately determine the dependence of the parameter ξ on the effective temperature T_e from relations (54), (56), and (57) (for $z < \hbar\omega_0/T_e$):

$$\xi = \left[A\left(\frac{\hbar\omega_0}{T_e}\right)^{-3/2} \exp\left(\frac{\hbar\omega_0}{T_e}\right) + 1\right]^{-1},$$

where A is a constant approximately equal to

$$\frac{2T_{lat}}{\hbar\omega_0} \frac{\tau_0^{op}(T_{Debye})}{\tau_0^{ac}(T_{Debye})} \tag{60}$$

In the region $T_{lat} \ll \hbar\omega_0$, the electron polarization reaches its maximal value for $T_e \sim (\frac{2}{3})\hbar\omega_0$. The nuclear polarization also has a maximum in this region of temperatures and in order of magnitude amounts to

$$\frac{I^z(j)}{I^z(0)} \sim \frac{T_{lat}}{T_e}f(T_e)\frac{\gamma_e}{\gamma_N} \quad \left(T_e \sim \frac{2}{3}\hbar\omega_0\right). \tag{61}$$

At present there is still too little experimental data known for one to be able to make a detailed comparison of the calculated results with experiment. In the experiments of Clark and Feher on InSb, an increase of the nuclear polarization of In^{115}, Sb^{121}, and Sb^{123} by approximately 10 to 100 times was observed in fields up to 1 V/cm.[2,13] The electron temperature reached 20 to 50°K.[4] Under these conditions, the acoustic phonons lead to a polarization of the In^{115} nuclei on the order of 1.2 to 1.5 ($\zeta_0 \cong 60°K$). Consideration of the optical phonons apparently may explain the observed value of the nuclear polarization. However, it is impossible to make a quantitative comparison with this data, since the experiment was carried out in a magnetic field of 12,000 Oe, which corresponds to $\Delta_e \gtrsim T_e$.

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