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Kinetic properties of a superconductor with a structural transformation

Yu. V. Kopaev, V. V. Manyailenko, and S. N. Molotkov

P. N. Lebedev Physics Institute, USSR Academy of Sciences
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The kinetic properties (absorption of high frequency ultrasound, relaxation of nuclear spin) of superconductors with partial dielectrization of the conduction electrons with a charge density wave are considered. It is shown that in the case of simultaneous Cooper and electron-hole pairing the ultrasound absorption coefficient has a maximum at the superconducting-transition temperature T_c . The rate of relaxation of the nuclear spin can have a maximum both at T_c and at a lower temperature. It is shown that if T_c is much lower than the structural-transition temperature, the kinetic properties differ insignificantly from the properties obtained in the BCS theory. Intraband Cooper pairing in a semimetal is investigated. It is shown that when account is taken of Hamiltonian terms with transition of a pair of particles from one band to another, the relative phase difference of the order parameters is fixed at either 0 or π . The order-parameter phase shifts due to the phase transitions can lead to observable physical phenomena. The results (in the case $T_p \gtrsim T_c$) agree qualitatively with the experimentally observed singularities of the kinetic properties of semiconductors with β -W structure.

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1. INTRODUCTION

It is well known that the compounds having the highest superconducting transition temperature undergo a structural transformation near this temperature.¹ The influence of the structural distortions on the critical superconducting transition temperature was investigated in a number of studies, using the model of a semimetal with almost identical electron and hole Fermi surfaces,² the model of a single-band metal with flat sections of the Fermi surface,^{3,4} as well as the model of a quasi-one-dimensional metal.⁵ In all the foregoing cases the system turned out to be unstable to electron-hole pairing. In addition, the singularities of the single-particle electron spectrum lead also to instability of the photon subsystem,⁶ i. e., to structural distortions. As a result of the electron-hole pairing,

the state density at the edges of the dielectric gap can increase significantly. If, following the dielectric pairing, the Fermi level of the system is at least partially outside the dielectric gap (this occurs if the Fermi surfaces of the electrons and holes are not completely congruent), superconducting pairing becomes possible. The latter takes place against a background of increased state density, on account of which a substantial rise of T_c is possible. It has also been shown,^{2,3} that there exist optimal conditions at which T_c can substantially exceed the superconducting-transition temperature in the absence of dielectric pairing (and hence in the absence of the structural transformation).

We consider in this paper the kinetic properties (the absorption of high-frequency ultrasound, the rate of

nuclear spin-lattice relaxation) of such superconducting systems. It is known from experiments that the ultrasound absorption coefficient of superconducting compounds with β -W structure has a maximum at the superconducting-transition temperature,^{7,8} a fact that cannot be explained within the framework of the BCS model.⁹

The kinetic properties of a system with only electron-hole pairing were considered by Iddis and one of us.¹⁰ It was also shown there that the ultrasound absorption coefficient has a maximum somewhat below the transition point (we recall that in ordinary superconductors the absorption coefficient is a monotonically increasing function of the temperature). The different behavior of the absorption coefficient in a superconductor and in an excitonic dielectric is due to the different renormalization of the matrix elements of the electron-phonon interaction in the restructured phase. The simultaneous coexistence of electron-hole and Cooper pairings leads, within the framework of this model, to a sharp increase of the absorption at the superconducting transition temperature. The rate of nuclear spin-lattice relaxation, depending on the ratio of the system parameters, can have a maximum either at T_c or at a somewhat lower temperature.

So far we have dealt with the kinetic properties of a superconductor whose structural transition temperature T_p exceeds insignificantly the superconducting transition temperature ($T_p \geq T_c$). In addition, it was assumed that the cutoff energy for the Cooper pairing ω_D satisfies the condition $\epsilon_F \gg \omega_D \gg \Sigma$ (Σ is the dielectric gap). In Sec. 4 we consider another limiting situation, namely when $T_p \gg T_c$. Following the dielectric pairing, the excess carriers (which are present because of the doping) remain above the gap, and the superconducting pairing (at $\omega_D \ll \bar{\mu}$ and $\omega_D \ll \Sigma$, where $\bar{\mu}$ is the Fermi-level shift in the dielectric phase) causes a restructuring of the spectrum only near the chemical-potential level $\bar{\mu}$. It turns out that in this situation the kinetic properties of the system differ only insignificantly from the properties of a superconductor in the BCS model.

In the Appendix we consider the kinetic properties of a semimetal, in which only intraband Cooper pairing is realized (the electron-hole pairing is assumed to be suppressed because of the strong non-congruence of the Fermi surfaces of the electrons and holes). It turns out that when account is taken in the Hamiltonian of the interaction terms connected with the transition of the particle pair upon scattering from one band to another (of the type $\lambda_2 a_1^\dagger a_1^\dagger a_2 a_2$) leads to the appearance of two poles in the vertex part that corresponds to the intraband Cooper channel. It will be shown that one solution corresponds to fixing the phase difference between the order parameters in the first and second bands at a value zero, and the other at a value π . Depending on the intraband transitions, the relative phase shift of the order parameter leads to observable physical phenomena.

2. ULTRASOUND ABSORPTION

We consider the absorption of ultrasound in a superconductor with partial dielectrization of the electrons.

We start with the model of a doped semimetal, where dielectric and Cooper pairings are simultaneously possible. The influence of the electron-hole pairing on the superconducting pairing was investigated in detail within the framework of this model by Rusinov *et al.*²

We confine ourselves here to high-frequency ultrasound ($\omega\tau \gg 1$, where ω and τ are the sound frequency and the momentum relaxation time of the quasiparticles). In this limit we can neglect the relaxation processes and regard sound absorption as a process wherein acoustic quanta are absorbed by free quasiparticle excitations.

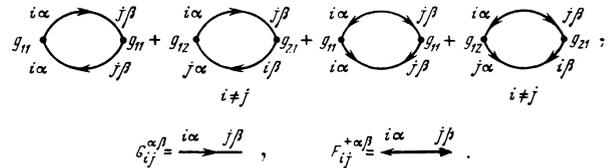
We assume that the Hamiltonian of the electron-phonon interaction is of the form

$$H_{e1-ph} = \sum_{\mathbf{k}, \mathbf{k}', \alpha} g_{ij} a_{i\alpha}^+(\mathbf{k}') a_{j\alpha}(\mathbf{k}) (b_{\mathbf{q}} + b_{-\mathbf{q}}^+), \quad (1)$$

where $a_{i\alpha}^+(\mathbf{k})$ is the operator of creation of an electron in band i with momentum \mathbf{k} and with spin α , g_{ij} are the matrix elements of the electron-phonon interaction, and $b_{\mathbf{q}}^+$ is the operator for the production of a phonon with momentum \mathbf{q} . We assume that the momentum conservation law $\mathbf{k}' = \mathbf{k} + \mathbf{q}$ is satisfied in expression (1) for H_{e1-ph} . The phonon damping is determined from the usual equation

$$D_0^{-1}(\mathbf{q}, \omega) - \Pi(\mathbf{q}, \omega) = 0, \quad (2)$$

where $D_0(\mathbf{q}, \omega)$ is the phonon Green's function. The sound absorption coefficient is given by the imaginary part of the polarization operator $\Pi(\mathbf{q}, \omega)$, which is determined by the sum of the following diagrams:



We assume here that singlet electron-hole pairing (responsible for the structural transition) and singlet Cooper pairing take place. With this taken into account, the spin structure of the Green's functions becomes

$$G_{ij}^{\alpha\beta} = G_{ij} \delta_{\alpha\beta}, \quad F_{ij}^{\alpha\beta} = i\sigma_{\alpha\beta} \nu F_{ij}. \quad (3)$$

In analytic form, the expressions for the polarization operator $\Pi(\mathbf{q}, \omega)$ can be represented as

$$\Pi(\mathbf{q}, \omega) = \sum_{i=1}^4 \Pi_i(\mathbf{q}, \omega),$$

where

$$\Pi_1(\mathbf{q}, \omega_n) = -\frac{T}{(2\pi)^3} \sum_{\substack{\epsilon_n, i, j \\ \alpha, \beta}} \int g_{ij}^2 G_{ii}^{\alpha\beta}(\mathbf{p}, \epsilon_n) G_{jj}^{\beta\alpha}(\mathbf{p}-\mathbf{q}, \epsilon_n - \omega_n) d\mathbf{p}, \quad (4)$$

$$\begin{aligned} \Pi_2(\mathbf{q}, \omega_n) = & -\frac{T}{(2\pi)^3} \sum_{\substack{\epsilon_n, i, j \\ \alpha, \beta}} \int [g_{ij}^2 G_{ij}^{\alpha\beta}(\mathbf{p}, \epsilon_n) G_{ji}^{\beta\alpha}(\mathbf{p}-\mathbf{q}, \epsilon_n - \omega_n) \\ & + g_{i2}^2 G_{ij}^{\alpha\beta}(\mathbf{p}, \epsilon_n) G_{ij}^{\beta\alpha}(\mathbf{p}-\mathbf{q}, \epsilon_n - \omega_n)] d\mathbf{p}, \quad (5) \end{aligned}$$

$$\Pi_3(\mathbf{q}, \omega_n) = -\frac{T}{(2\pi)^3} \sum_{\substack{\epsilon_n, i, j \\ \alpha, \beta}} \int g_{ij}^2 F_{ii}^{+\alpha\beta}(\mathbf{p}, \epsilon_n) F_{jj}^{\beta\alpha}(\mathbf{p}-\mathbf{q}, \epsilon_n - \omega_n) d\mathbf{p}, \quad (6)$$

$$\begin{aligned} \Pi_4(\mathbf{q}, \omega_n) = & -\frac{T}{(2\pi)^3} \sum_{\substack{\epsilon_n, i, j \\ \alpha, \beta}} \int [g_{ii}^2 F_{ij}^{+\alpha\beta}(\mathbf{p}, \epsilon_n) F_{ji}^{\beta\alpha}(\mathbf{p}-\mathbf{q}, \epsilon_n - \omega_n) \\ & + g_{i2}^2 F_{ij}^{+\alpha\beta}(\mathbf{p}, \epsilon_n) F_{ij}^{\beta\alpha}(\mathbf{p}-\mathbf{q}, \epsilon_n - \omega_n)] d\mathbf{p}. \quad (7) \end{aligned}$$

We assume here that $g_{11} = g_{22}$ and $g_{12} = g_{21}$. The Green's functions in (4)–(7) are of the form²

$$G_{11}(\mathbf{p}, \omega_n) = \{ (i\omega_n - \varepsilon_2(\mathbf{p})) [(i\omega_n + \varepsilon_1(\mathbf{p})) (i\omega_n + \varepsilon_2(\mathbf{p})) - |\Sigma|^2] - \Delta_{21} [\Delta_{21}^* (i\omega_n + \varepsilon_2(\mathbf{p})) - \Delta_{22} \Sigma] + \Delta_{22} [\Delta_{21}^* \Sigma^* - \Delta_{22} (i\omega_n + \varepsilon_1(\mathbf{p}))] \} \text{Det}^{-1}, \quad (8)$$

$$G_{21}(\mathbf{p}, \omega_n) = \{ -\Sigma [(i\omega_n + \varepsilon_1(\mathbf{p})) (i\omega_n + \varepsilon_2(\mathbf{p})) - |\Sigma|^2] - \Delta_{21} [\Delta_{11}^* (i\omega_n + \varepsilon_2(\mathbf{p})) - \Delta_{12}^* \Sigma] + \Delta_{22} [\Delta_{11}^* \Sigma^* - \Delta_{12}^* (i\omega_n + \varepsilon_1(\mathbf{p}))] \} \text{Det}^{-1}, \quad (9)$$

$$F_{11}^+(\mathbf{p}, \omega_n) = \{ -\Sigma [\Delta_{12} (i\omega_n + \varepsilon_1(\mathbf{p})) - \Delta_{22}^* \Sigma] - (i\omega_n - \varepsilon_2(\mathbf{p})) [\Delta_{11}^* (i\omega_n + \varepsilon_2(\mathbf{p})) - \Delta_{12}^* \Sigma] + \Delta_{22} [\Delta_{11}^* \Delta_{22}^* - \Delta_{12}^* \Delta_{21}^*] \} \text{Det}^{-1}, \quad (10)$$

$$F_{21}^+(\mathbf{p}, \omega_n) = \{ -\Sigma [\Delta_{21} \Sigma^* - \Delta_{22}^* (i\omega_n + \varepsilon_1(\mathbf{p}))] - (i\omega_n - \varepsilon_2(\mathbf{p})) [\Delta_{11}^* \Sigma^* - \Delta_{12}^* (i\omega_n + \varepsilon_1(\mathbf{p}))] + \Delta_{21} [\Delta_{11}^* \Delta_{22}^* - \Delta_{12}^* \Delta_{21}^*] \} \text{Det}^{-1}, \quad (11)$$

where $\text{Det} = (\omega_n^2 + \omega_1^2(\mathbf{p}))(\omega_n^2 + \omega_2^2(\mathbf{p}))$, $\Delta_{11,22}$ is the superconducting gap in the first and second bands, while Δ_{12} and Σ are the interband superconducting and dielectric gaps. We consider hereafter only the symmetrical case (in the terminology of Ref. 2, i. e., $\Delta_{11} = \Delta_{22}$). In principle an antisymmetrical solution $\Delta_{11} = -\Delta_{22}$ is also possible. However, as shown in Ref. 2, in the presence of a structural transition the symmetrical solution is energywise favored over the antisymmetrical one.

The spectrum of the elementary excitations in the system is given by

$$\omega_{\pm}(\mathbf{p}) = [(E(\mathbf{p}) \pm \mu)^2 + \bar{\Delta}^2]^{1/2},$$

where

$$E(\mathbf{p}) = (\varepsilon^2(\mathbf{p}) + \bar{\Sigma}^2)^{1/2}, \quad \bar{\Sigma} = (\mu \Sigma + \Delta \Delta_{21}) / \mu, \\ \bar{\Delta} = (\Delta \mu - \Delta_{21} \Sigma) / \mu, \quad \Delta_{11,22} = \Delta, \quad \mu^2 = \mu^2 + \Delta_{21}^2.$$

The spectrum of the electrons in the initial phase is assumed isotropic

$$\varepsilon_{1,2}(\mathbf{p}) = \mu \pm \varepsilon(\mathbf{p}), \quad \varepsilon(\mathbf{p}) = p^2 / 2m - \varepsilon_F,$$

where μ is the shift of the Fermi level as a result of doping.

In the calculation of the integrals (4)–(7) it is convenient to change from integration with respect to momentum to integration with respect to energy, in accordance with the rule

$$\int (\dots) \frac{d\mathbf{p}}{(2\pi)^3} \rightarrow \frac{m p_F}{(2\pi)^2} \int_{-\infty}^{+\infty} (\dots) d\varepsilon_p dx \rightarrow \frac{m^2}{(2\pi)^2 |q|} \int_{-\infty}^{+\infty} d\varepsilon_p \int_{\varepsilon_{p-q}}^{\varepsilon_{p+q}} (\dots) d\varepsilon_{p-q}, \quad (12)$$

where $\varepsilon_{p\pm q} = \varepsilon_p \pm v_F |q| x$, $x = \cos \theta$ (θ is the angle between the vectors \mathbf{p} and \mathbf{q}). Further simplification of the formulas is possible only under the assumption that $v_F |q| / \Delta, \Sigma \gg 1$ (which is usually made for ordinary superconductors⁹). We can then make the change $\varepsilon_{p\pm q} \rightarrow \pm \infty$ in the limits of integration in (12), the integration with respect to ε_p and ε_{p-q} being carried out independently.

After substituting (8)–(11) in (4)–(7), we sum the obtained expressions over the frequencies, and then, after analytic continuation to the real frequency axis ($i\omega_n \rightarrow \omega + i\delta$ sign ω) and taking (12) into account we obtain for the imaginary parts of $\Pi_{1,4}(\mathbf{q}, \omega)$ the expressions

$$\text{Im} \Pi_1(\mathbf{q}, \omega) = \frac{4}{\pi} \bar{g}^2 \frac{m^2}{|q|} \sum_{i,j} \int_{\Delta_{ij}}^{\infty} \frac{1}{2} [u_i^2(\varepsilon + \omega) u_j^2(\varepsilon) + v_i^2(\varepsilon + \omega) v_j^2(\varepsilon)] \times N_i(\varepsilon + \omega) N_j(\varepsilon) (f(\varepsilon) - f(\varepsilon + \omega)) d\varepsilon, \quad (13)$$

$$\text{Im} \Pi_2(\mathbf{q}, \omega) = \frac{4}{\pi} \bar{g}^2 \frac{m^2}{|q|} \sum_{i,j} \int_{\Delta_{ij}}^{\infty} 2(-1)^{i+j} [p_i^2(\varepsilon + \omega) p_j^2(\varepsilon) + l_i^2(\varepsilon + \omega) l_j^2(\varepsilon)] N_i(\varepsilon + \omega) N_j(\varepsilon) (f(\varepsilon) - f(\varepsilon + \omega)) d\varepsilon, \quad (14)$$

$$\text{Im} \Pi_3(\mathbf{q}, \omega) = -\frac{4}{\pi} \bar{g}^2 \frac{m^2}{|q|} \sum_{i,j} \int_{\Delta_{ij}}^{\infty} \frac{\Delta^2 N_i(\varepsilon + \omega) N_j(\varepsilon)}{4\varepsilon(\varepsilon + \omega)} (f(\varepsilon) - f(\varepsilon + \omega)) d\varepsilon, \quad (15)$$

$$\text{Im} \Pi_4(\mathbf{q}, \omega) = -\frac{4}{\pi} \bar{g}^2 \frac{m^2}{|q|} \sum_{i,j} \int_{\Delta_{ij}}^{\infty} \frac{\Delta_{2i}(\varepsilon + \omega) \Delta_{2j}(\varepsilon)}{\varepsilon(\varepsilon + \omega)} N_i(\varepsilon + \omega) \times N_j(\varepsilon) (f(\varepsilon) - f(\varepsilon + \omega)) d\varepsilon. \quad (16)$$

The functions in the integrals of (13)–(16) are defined in the following manner:

$$u_i^2(\varepsilon) = 1/2(1 - \xi_i(\varepsilon)/\varepsilon), \quad v_i^2(\varepsilon) = 1/2(1 + \xi_i(\varepsilon)/\varepsilon), \\ \xi_i(\varepsilon) = \mu - (-1)^i E_i(\varepsilon), \quad E_i(\varepsilon) = (\varepsilon^2 - \Delta^2)^{1/2} + (-1)^i \mu, \\ p_i^2(\varepsilon) = 1/2(1 - \xi_i(\varepsilon)/\varepsilon) \Sigma / 2E_i(\varepsilon), \quad l_i^2(\varepsilon) = 1/2(1 + \xi_i(\varepsilon)/\varepsilon) \Sigma / 2E_i(\varepsilon), \\ \Delta_{2i}(\varepsilon) = (-1)^i \Sigma \Delta / 2E_i(\varepsilon), \\ N_i(\varepsilon) = [(\varepsilon^2 - \Delta^2)^{1/2} + (-1)^i \mu] / \{ [(\varepsilon^2 - \Delta^2)^{1/2} + (-1)^i \mu \}^2 - \Sigma^2 \}^{1/2} (\varepsilon^2 - \Delta^2)^{1/2}, \quad \Delta_{\pm} = [(\Sigma \pm \mu)^2 + \Delta^2]^{1/2}, \\ f(\varepsilon) = (\exp(\varepsilon/T) + 1)^{-1}, \quad \bar{g}^2 = g_{11}^2 + g_{12}^2, \\ \Delta_{ij} = \begin{cases} \Delta_+, & i=j=1 \\ \Delta_+ - \omega, & i=1, j=2 \\ \Delta_+, & i=2, j=1 \\ \Delta_-, & i=j=2 \end{cases}$$

We have retained in (13)–(16) only the terms of the scattering channel (i. e., those containing the distribution functions in the combination $f - f'$). The recombination terms (which contain f and f' in the form $1 - f - f'$) have been left out, since we assume that $\omega/\Delta \ll 1$ and $\Sigma \ll 1$, so that no production of new particles takes place. It was shown² that the interband superconducting parameter Δ_{21} is always small ($\Delta_{21} \ll \Delta_{11,22}, \Sigma$), and it was therefore left out of (13)–(16).

The sound absorption coefficient is given by

$$\alpha_{us} = \text{Im} \Pi(\mathbf{q}, \omega) = \text{Im}(\Pi_1(\mathbf{q}, \omega) + \Pi_2(\mathbf{q}, \omega) + \Pi_3(\mathbf{q}, \omega) + \Pi_4(\mathbf{q}, \omega)). \quad (17)$$

To calculate the integrals (13)–(16) we must know the temperature dependence of the order parameters Δ and Σ and of the chemical potential μ . The equations for the order parameters at finite temperatures were obtained in Refs. 2 and 3. To determine the qualitative $\alpha_{us}(T)$ dependence, however, it suffices to use the BCS approximation for the behavior of $\Delta(T)$ and $\Sigma(T)$. The $\mu(T)$ dependence is determined from the electroneutrality equation where the given $\Delta(T), \Sigma(T), \delta n(\delta n = N/4N(0))$ (is the concentration of the excess carriers

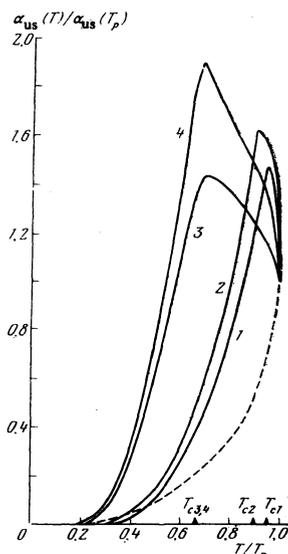


FIG. 1. Absorption of ultrasound, case $T_p \geq T_c$.

due to doping, in energy units). The results of the numerical calculations are shown in Fig. 1. The values of the parameters T_c/T_p , ω/T_p , and $\delta n/T_p$ respectively for curves 1-4 are the following: 1-0.95, $0.5 \cdot 10^{-3}$, 3.06; 2-0.9, $0.5 \cdot 10^{-3}$, 3.01; 3-0.665, $0.4 \cdot 10^{-3}$, 2.92; 4-0.665, $0.4 \cdot 10^{-3}$, 2.0. The dashed line shows the behavior of $\alpha_{us}(T)$ in accord with the BCS theory⁹ (for the case $T_c = T_p$). A distinguishing feature of these curves is the presence of a maximum at the superconducting transition temperature. From a comparison of curves 1 and 2 or 3 and 4 it is seen that the intensity of the absorption at the maximum increases with decreasing doping. The latter, as is well known,² leads to an increase of the state density on the Fermi level at temperatures below the structural-transition temperature. Similar relations were experimentally observed for the ultrasound absorption coefficient in V_3Si and in Nb_3Sn .^{7,8}

The anomalies of sound absorption in superconductors with β -W lattice can apparently be treated as the consequence of dielectric correlation of the conduction electrons, which can lead to a structural transformation from the cubic into the tetragonal phase. Within the framework of this simple model we can expect only qualitative agreement with experiment. We note that the qualitative character of the curves does not change substantially even though dielectric correlations may not lead to a structural transition (for example because of insufficient perfection of the sample). An attempt to explain the anomalies in the absorption of ultrasound on the high-temperature side ($T > T_p$) in V_3Si was made by Schuster and Dieterich.¹¹

3. NUCLEAR-SPIN RELAXATION

We proceed now to consider the rate of nuclear-spin relaxation. The Hamiltonian of the hyperfine interaction of the electrons with a given nuclear spin takes, according to Ref. 12, the form

$$H_{is} = \frac{8\pi}{3} \gamma_e \gamma_n \sum_{\mathbf{k}, \mathbf{k}'} u_{i\mathbf{k}_F}(0) u_{j\mathbf{k}'_F}(0) \left[I_z (a_{i+}(k') a_{j+}(k) - a_{i+}(k) a_{j+}(k')) + \frac{1}{2} (I_+ a_{i+}(k') a_{j+}(k) + I_- a_{i+}(k) a_{j+}(k')) \right], \quad (18)$$

where $u_{i,j\mathbf{k}_F}(0)$ are the Bloch amplitudes of bands i and j (at $|\mathbf{k}| = k_F$) at the nucleus, γ_e and γ_n are the gyromagnetic ratios for the spins of the electrons and of the nucleus, I_z is the z -component of the nuclear angular-momentum operator, and as usual $\hat{I}_\pm = \hat{I}_x \pm i\hat{I}_y$ are the nuclear angular momentum creation and annihilation operators.

The procedure for calculating the time of the nuclear spin-lattice relaxation was described in detail,^{12,13} and we present therefore the final expressions. We have

$$\frac{1}{T_1} = \text{Im}(\Pi_1(\omega) + \Pi_2(\omega) - \Pi_3(\omega) - \Pi_4(\omega)), \quad (19)$$

where ω is an energy of the order of the hyperfine interaction, and

$$\text{Im} \Pi_1(\omega) = 2\pi \bar{A}^2 N(0)^2 \sum_{i,j} \int_{\Delta_{ij}}^{+\infty} \frac{1}{2} [u_i^2(\epsilon + \omega) u_j^2(\epsilon) + v_i^2(\epsilon + \omega) v_j^2(\epsilon)] N_i(\epsilon + \omega) N_j(\epsilon) (-T \partial f(\epsilon) / \partial \epsilon) d\epsilon,$$

$$\text{Im} \Pi_2(\omega) = 2\pi \bar{A}^2 N(0)^2 \sum_{i,j} \int_{\Delta_{ij}}^{+\infty} 2(-1)^{i+j} [p_i^2(\epsilon + \omega) p_j^2(\epsilon) + l_i^2(\epsilon + \omega) l_j^2(\epsilon)] N_i(\epsilon + \omega) N_j(\epsilon) (-T \partial f(\epsilon) / \partial \epsilon) d\epsilon,$$

$$\text{Im} \Pi_3(\omega) = -2\pi \bar{A}^2 N(0)^2 \sum_{i,j} \int_{\Delta_{ij}}^{+\infty} (\Delta_{z_1}^2 N_i(\epsilon + \omega) N_j(\epsilon) / 4\epsilon(\epsilon + \omega)) \times (-T \partial f(\epsilon) / \partial \epsilon) d\epsilon,$$

$$\text{Im} \Pi_4(\omega) = -2\pi \bar{A}^2 N(0)^2 \sum_{i,j} \int_{\Delta_{ij}}^{+\infty} (\Delta_{z_2}(\epsilon + \omega) \Delta_{z_2}(\epsilon) / \epsilon(\epsilon + \omega)) \times N_i(\epsilon + \omega) N_j(\epsilon) (-T \partial f(\epsilon) / \partial \epsilon) d\epsilon,$$

where $\bar{A}^2 = A_{11}^2 + A_{12}^2$, $A_{ij}^2 = 64/9 \pi^2 \gamma_e^2 \gamma_n^2 |u_{i\mathbf{k}_F}(0)|^2 |u_{j\mathbf{k}_F}(0)|^2$, and $N(0)$ is the state density on the Fermi level.

It is seen from (19) that $\pi_{3,4}(\omega)$ enter with different signs than in (17). This is a reflection of the antisymmetry of the superconducting anomalous mean values over the spin index (3).

The results of the numerical calculations are shown in Fig. 2, where the parameters T_c/T_p , ω/T_p , $\delta n/T_p$ for curves 1-4 are respectively 1-0.95, $0.5 \cdot 10^{-3}$, 3.06; 2-0.9, $0.5 \cdot 10^{-3}$, 3.01; 3-0.665, $0.4 \cdot 10^{-3}$, 2.92; 4-0.665, $0.4 \cdot 10^{-3}$, 2.0. It is seen from Fig. 2 that, depending on the system parameters, the maximum of the nuclear-spin relaxation rate can occur either at T_c or at somewhat lower temperatures (according to the BCS theory the maximum lies always below T_c , Ref. 9). All the curves are characterized by a kink at $T_c < T < T_p$. Similar relations were observed in experiment for a number of V_3X compounds,¹⁴ where the maximum was reached always at the superconducting-transition temperature.

4. ULTRASOUND ABSORPTION, SPIN-LATTICE RELAXATION RATE AT $T_p \gg T_c$

In the preceding sections we considered the case when the temperatures of the structural and superconducting transitions were close. It was assumed in addition that the cutoff energy ω_D for the Cooper pairing satisfies the conditions $\epsilon_F \gg \omega_D \gg \epsilon$. Physically this means that the electrons of the completely filled valence band also take part in the superconducting pairing, because of the narrow dielectric gap. In the opposite limiting case $\bar{\mu} \gg \omega_D$ and $\epsilon \gg \omega_D$, however ($\bar{\mu}$ is the shift of the Fermi level in the dielectric phase as a result of doping), which corresponds to the situation $T_p \gg T_c$ (in this case the temperature of the structural transition

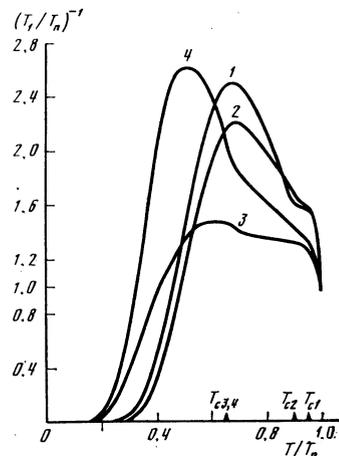


FIG. 2. Rate of nuclear-spin relaxation, case $T_p \geq T_c$.

T_p may turn out to be higher than the melting temperature, i. e., it may be unobservable, and T_p becomes simply a parameter of the problem), the problem must be solved differently: it is necessary to consider first the transition from the semimetallic state to the dielectric phase, and then take into account the Cooper pairing. The latter causes, at $\bar{\mu} \gg \omega_D$ and $\epsilon \gg \omega_D$, a restructuring of the spectrum only near the chemical-potential level $\bar{\mu}$. In essence, this was how the problem of the joint electron-hole and Cooper-pairing was solved by Mattis and Langer.⁴

In this approach it is more convenient to investigate the kinetic properties in the language of the Bogolyubov canonical transformation.¹⁵ In singlet dielectric pairing, the Bloch states $\psi_{1k}^\alpha(\mathbf{r})$ and $\psi_{2k}^\alpha(\mathbf{r})$ from different bands become intermixed. This fact is taken into account by the canonical transformation¹⁶

$$\begin{aligned} a_{1\alpha}(\mathbf{k}) &= A_k \alpha_{1\alpha}(\mathbf{k}) + B_k \alpha_{2\alpha}(\mathbf{k}), \\ a_{2\alpha}(\mathbf{k}) &= A_k \alpha_{2\alpha}(\mathbf{k}) - B_k \alpha_{1\alpha}(\mathbf{k}), \end{aligned} \quad (20)$$

where $\alpha_{1,2\alpha}(\mathbf{k})$ and $\alpha_{1,2\alpha}(\mathbf{k})$ are the unrenormalized and the new quasiparticle operators, and

$$\begin{aligned} A_k^2, B_k^2 &= 1/2(1 \pm \epsilon(\mathbf{p})/E(\mathbf{p})), \\ E(\mathbf{p}) &= (\epsilon^2(\mathbf{p}) + \Sigma^2)^{1/2}. \end{aligned}$$

In superconducting pairing it is necessary to intermix the electronic states (\mathbf{k}, α) and $(-\mathbf{k}, -\alpha)$ in the dielectric phase only in the upper band in the case of an n -type semiconductor (and in the lower band in the case of a p -type semiconductor), since the electrons of the completely filled valence band, in contrast to the preceding case, do not take part in the Cooper pairing. According to Ref. 14, we have

$$\begin{aligned} \alpha_{1\alpha}(\mathbf{k}) &= u_k c_{\alpha}(\mathbf{k}) + v_k c_{-\alpha}(-\mathbf{k}), \\ \alpha_{1-\alpha}(-\mathbf{k}) &= u_k c_{-\alpha}(-\mathbf{k}) - v_k c_{\alpha}(\mathbf{k}), \end{aligned} \quad (21)$$

where $c_{\pm\alpha}(\mathbf{k})$ are the new quasiparticle operators, and

$$\begin{aligned} u_k^2, v_k^2 &= 1/2(1 \pm \xi(\mathbf{k})/E(\mathbf{k})), \quad \xi(\mathbf{k}) = E(\mathbf{k}) - \bar{\mu}, \\ E(\mathbf{k}) &= (\xi^2(\mathbf{k}) + \Delta^2)^{1/2}, \quad \bar{\mu}^2 = \mu^2 + \Sigma^2. \end{aligned}$$

After applying the canonical transformation (20) to the Hamiltonian (1), and after transforming in the resultant expression the operators of only the first band by means of (21), we obtain the expression for the ultrasound absorption coefficient:

$$\begin{aligned} \alpha_{us} &= 4\pi \int \frac{d\mathbf{p}}{(2\pi)^3} \{g_{11} n^2(\mathbf{p}, \mathbf{p}') - 2g_{12} g_{11} m(\mathbf{p}, \mathbf{p}') n(\mathbf{p}, \mathbf{p}') \\ &+ g_{12}^2 m^2(\mathbf{p}, \mathbf{p}')\} l^2(\mathbf{p}, \mathbf{p}') \delta(\mathbf{p}' - \mathbf{p} - \mathbf{q}) \delta(E' - E - \omega) (f(E) - f(E')), \end{aligned} \quad (22)$$

where the coherence factors are

$$\begin{aligned} n^2(\mathbf{p}, \mathbf{p}') &= (A_p A_{p'} + B_p B_{p'})^2 = 1/2(1 + (\epsilon(\mathbf{p})\epsilon(\mathbf{p}') + \Sigma^2)/E(\mathbf{p})E(\mathbf{p}')), \\ m^2(\mathbf{p}, \mathbf{p}') &= (A_p B_{p'} + B_p A_{p'})^2 = 1/2(1 - (\epsilon(\mathbf{p})\epsilon(\mathbf{p}') - \Sigma^2)/E(\mathbf{p})E(\mathbf{p}')), \\ l^2(\mathbf{p}, \mathbf{p}') &= (u_p u_{p'} - v_p v_{p'})^2 = 1/2(1 + (\xi(\mathbf{p})\xi(\mathbf{p}') - \Delta^2)/E(\mathbf{p})E(\mathbf{p}')). \end{aligned}$$

Changing from integration with respect to momentum to integration with respect to energy between limits symmetrical about $\bar{\mu}$, we get

$$\begin{aligned} \alpha_{us} &= (2m^2 \bar{\mu} / \pi |q| \mu) \int_{\Delta}^{\bar{\mu}} \{g_{11}^2 n^2(\xi, \omega) \\ &- 2g_{12} g_{11} n(\xi, \omega) m(\xi, \omega) \\ &+ g_{12}^2 m^2(\xi, \omega)\} ((\xi + \omega) \\ &- \Delta^2) / (\xi^2 - \Delta^2)^{1/2} [(\xi + \omega)^2 - \Delta^2]^{1/2} (f(\xi) - f(\xi + \omega)) d\xi, \end{aligned} \quad (23)$$

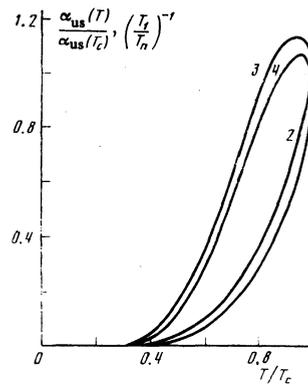


FIG. 3. Absorption of ultrasound (curves 1 and 2) and rate of nuclear spin-lattice relaxation (curves 3, 4) in the case $T_p \gg T_c$.

where

$$\begin{aligned} n^2(\xi, \omega) &= 1/2(1 + (\epsilon(\xi)\epsilon(\xi + \omega) \\ &+ \Sigma^2)/E(\xi)E(\xi + \omega)), \\ m^2(\xi, \omega) &= 1/2(1 - (\epsilon(\xi)\epsilon(\xi + \omega) \\ &- \Sigma^2)/E(\xi)E(\xi + \omega)), \\ \epsilon(\xi) &= (E^2(\xi) - \Sigma^2)^{1/2}, \\ E(\xi) &= (\xi^2 - \Delta^2)^{1/2} + \bar{\mu}. \end{aligned}$$

The results of the numerical calculation are shown in Fig. 3 (curves 1 and 2). It was assumed in the calculations that the $\Delta(T)$ dependence is given by the BCS equation, in which the state density $N(0)$ on the Fermi level in the semimetal, is replaced by the state density at the chemical-potential level in the dielectric phase, $N(\bar{\mu}) = N(0)\bar{\mu}/\mu$. The values of the parameters Σ/T_c , g_{12}/g_{11} , μ/T_c , ω/T_c for curves 1 and 2 are then 1—10.0, 0.1, 5.0, 0.1; 2—10², 1.0, 10.0, 0.1. In addition, since $T_p \gg T_c$, we replaced $\Sigma(T)$ by its value of $T = 0$.

The calculation of the nuclear-spin relaxation rate is completely analogous to the preceding case, except that $l(\mathbf{p}, \mathbf{p}')$ is replaced by another coherence factor $P(\mathbf{p}, \mathbf{p}')$, which is responsible for electron scattering with spin flips. As a result we obtain

$$\begin{aligned} \frac{1}{T_1} &= 4\pi(N(0)\bar{\mu}/\mu)^2 \int_{\Delta}^{\bar{\mu}} \{A_{11}^2 n^2(\xi, \omega) - 2A_{11} A_{12} n(\xi, \omega) m(\xi, \omega) + A_{12}^2 m^2(\xi, \omega)\} \\ &\times ((\xi + \omega) + \Delta^2) / (\xi^2 - \Delta^2)^{1/2} [(\xi + \omega)^2 - \Delta^2]^{1/2} (-T \partial f(\xi) / \partial \xi) d\xi. \end{aligned} \quad (24)$$

The coherence factor responsible for processes with spin slip is the following:

$$P^2(\mathbf{p}, \mathbf{p}') = (u_p u_{p'} + v_p v_{p'})^2 = 1/2(1 + (\xi(\mathbf{p})\xi(\mathbf{p}') + \Delta^2)/E(\mathbf{p})E(\mathbf{p}')).$$

The matrix elements A_{ij} in (24) are defined as follows:

$$A_{ij}^2 = \frac{1}{\pi} \int_{\Delta}^{\bar{\mu}} \gamma_i^2 \gamma_j^2 |u_{i\mathbf{p}}(0)|^2 |u_{j\mathbf{p}'}(0)|^2.$$

The temperature dependences of the rate of the nuclear spin-lattice relaxation are given in Fig. 3 (curves 3 and 4, the parameters Σ/T_c , A_{12}/A_{11} , μ/T_c , ω/T_c being 3—10², 1.0, 10.0, 5 · 10⁻³; 4—10², 1.0, 10.0, 0.1. It is seen thus from Fig. 3 that in the limit $T_p \gg T_c$ the renormalization of the matrix elements on account of the dielectric pairing does not change the temperature dependence of the kinetic coefficients, and therefore the results differ little from the results of the BCS theory.⁹

The results are valid for the description of the kinetic properties of strongly doped superconducting semiconductors, in which the forbidden band width satisfies the condition $\Sigma \gg \omega_D$. In the opposite limiting case $\omega_D \gg \Sigma$ we must use the results of the preceding sections.

We consider the kinetic properties of a two-band superconductor with substantially noncongruent electron and hole Fermi surfaces. The dielectric correlations turn out to be inessential in this case and there is no structural transition. We consider for the sake of argument a semimetal, although the results of this Appendix are fully applicable to a two-band metal (for example, with overlapping *s* and *d* bands). We show first that the inclusion, in the Hamiltonian, of interaction terms connected with the transition of a particle pair from one band to another via scattering, fixes the relative phase difference of the order parameters in the different bands.

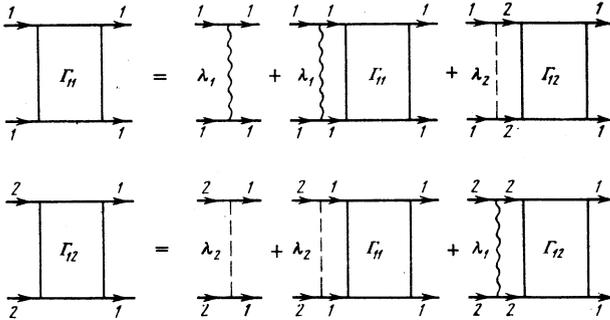
We consider a semimetal with Hamiltonian

$$H = \sum_{i=1}^2 \left\{ \sum_{\mathbf{k}} \varepsilon_i(\mathbf{k}) a_i^+(\mathbf{k}) a_i(\mathbf{k}) + \frac{\lambda_i}{2} \sum_{\mathbf{k}, \mathbf{k}'} a_i^+(\mathbf{k}) a_i^+(-\mathbf{k}) a_i(\mathbf{k}') a_i(-\mathbf{k}') \right\} + \left[\frac{\lambda_2}{2} \sum_{\mathbf{k}} a_1^+(\mathbf{k}) a_1^+(-\mathbf{k}) a_2(\mathbf{k}') a_2(-\mathbf{k}') + \text{H.c.} \right], \quad (\text{A.1})$$

where $\varepsilon_{1,2}(\mathbf{k})$ is the dispersion law of the electrons in the first and second bands,

$$\varepsilon_{1,2}(\mathbf{k}) = \pm (k^2/2m_{1,2} - \varepsilon_F).$$

The investigation of the stability of the system relative to Cooper pairing within the limits of each band reduces to a system of equations for the vertex functions Γ_{11} and Γ_{12} at a small total momentum $q = \{i\omega_n^0, \mathbf{q}\}$:



The solution of this system at $q = 0$ is

$$\Gamma_{11} = \frac{\lambda_1 + (\lambda_2^2 - \lambda_1^2) N_2 L}{\text{Det}}, \quad \Gamma_{12} = \frac{\lambda_2}{\text{Det}},$$

where

$$\text{Det} = (1 - \lambda_1 N_1 L)(1 - \lambda_2 N_2 L) - \lambda_2^2 N_1 N_2 L^2, \quad L = -\ln(2\gamma\omega_D/\pi T),$$

$N_{1,2}$ are the state densities at the Fermi level in the first and second bands. The vertex parts have two poles:

$$L(T_c) = \frac{\lambda_1(N_1 + N_2) \pm [\lambda_1^2(N_1 + N_2)^2 - 4N_1 N_2(\lambda_1^2 - \lambda_2^2)]^{1/2}}{2N_1 N_2(\lambda_1^2 - \lambda_2^2)}. \quad (\text{A.2})$$

Let us ascertain what corresponds to the different poles in the vertex parts. Writing down the system of equations for the orders parameters in the first and second bands at $T = T_c$, we get

$$\begin{aligned} \Delta_{11} &= \lambda_1 N_1 L(T_c) \Delta_{11} + \lambda_2 N_2 L(T_c) \Delta_{22}, \\ \Delta_{22} &= \lambda_1 N_2 L(T_c) \Delta_{22} + \lambda_2 N_1 L(T_c) \Delta_{11}. \end{aligned} \quad (\text{A.3})$$

The system is compatible if $L(T_c)$ satisfies the condi-

tion (A.2), where the minus sign in (A.2) corresponds to a solution of the form

$$\Delta_{11} = |\Delta_{11}| e^{i\varphi}, \quad \Delta_{22} = |\Delta_{22}| e^{i(\varphi + 2n\pi)},$$

with n an integer. The plus sign corresponds to a solution of the type

$$\Delta_{11} = |\Delta_{11}| e^{i\varphi}, \quad \Delta_{22} = |\Delta_{22}| e^{i(\varphi + (2n+1)\pi)}.$$

In the limit $N_1 = N_2 = N$ we get

$$L(T_c) = 1/(\lambda_1 \pm \lambda_2) N, \quad \Delta_{11} = \pm \Delta_{22}.$$

Two-band superconductors were investigated in a number of studies.^{17,18} No attention was paid there, however, to the possible existence of the second solution. Depending on the sign of the constant λ_2 , the minimum of the free energy corresponds to the first solution at $\lambda_2 < 0$ and to the second solution at $\lambda_2 > 0$ (we assume $\lambda_1 < 0$). In Secs. 2 and 3 we confine ourselves to the first (symmetrical) type of solution, since it corresponds to an energy minimum in the presence of a structural transition.

The relative phase shift of Δ_{11} and Δ_{22} can lead to observable physical phenomena as a result of interband transitions. Consider, for example, sound absorption and relaxation of nuclear spin. Calculations in the two-band model and in the BCS model⁹ are analogous, and we present therefore the final formulas. For the sound absorption coefficient we have

$$\begin{aligned} \alpha_{\text{us}} &= \frac{2g_{11}^2}{\pi |q|} \sum_{i=1,2} \int_{|\Delta_i|}^{\infty} \frac{[e(\varepsilon \pm \omega) - |\Delta_i|^2] m_i^2}{(\varepsilon^2 - |\Delta_i|^2)^{1/2} [(e + \omega)^2 - |\Delta_i|^2]^{1/2}} (f(e) - f(e + \omega)) d\varepsilon \\ &+ \frac{g_{12}^2}{\pi |q|} \sum_{i,j=1,2} \int_{\tilde{\Delta}}^{\infty} \frac{[e(\varepsilon + \omega) - \cos \varphi_{12} |\Delta_i| |\Delta_j|] m_i^2 v_{iF} v_{jF}}{(\varepsilon^2 - |\Delta_j|^2)^{1/2} [(e + \omega)^2 - |\Delta_i|^2]^{1/2}} (f(e) - f(e + \omega)) d\varepsilon, \end{aligned} \quad (\text{A.4})$$

where $\tilde{\Delta} = \max\{|\Delta_i| - \omega, |\Delta_j|\}$ and φ_{12} is equal either to 0 or to π , and $\Delta_{i,j} = \Delta_{11,22}$.

Similarly for the nuclear-spin relaxation we have

$$\begin{aligned} \frac{1}{T_1} &= 4\pi A_{11}^2 \sum_{i=1,2} \int_{|\Delta_i|}^{\infty} \frac{[e(\varepsilon + \omega) + |\Delta_i|^2] N_i^2}{(\varepsilon^2 - |\Delta_i|^2)^{1/2} [(e + \omega)^2 - |\Delta_i|^2]^{1/2}} \left(-T \frac{\partial f(e)}{\partial e}\right) d\varepsilon \\ &+ 2\pi A_{12}^2 \sum_{i,j=1,2} \int_{\tilde{\Delta}}^{\infty} \frac{[e(\varepsilon + \omega) + \cos \varphi_{12} |\Delta_i| |\Delta_j|] N_i N_j}{(\varepsilon^2 - |\Delta_j|^2)^{1/2} [(e + \omega)^2 - |\Delta_i|^2]^{1/2}} \left(-T \frac{\partial f(e)}{\partial e}\right) d\varepsilon. \end{aligned} \quad (\text{A.5})$$

The coherence of the paired electrons in states with opposite momenta and spins in the superconducting phase makes the transitions of the electrons bound into a Cooper pair interdependent. Depending on the scattering mechanism, a distinction is made between processes of two types, for which the transition probabilities differ greatly because of the coherence effects. The first type includes electron scattering without spin flip (for example, interaction with phonons, which leads to absorption of ultrasound waves). The second type includes processes with spin flip (hyperfine interaction of conduction electrons with nuclear spin, which determines the rate of nuclear relaxation). It is seen from the first terms in expressions (A.4) and (A.5) that the coherence factors of the two types of processes differ in structure ($|\Delta_i|^2$ enters in the coherence factor with minus sign (A.4) for the process of interaction with phonons, and with plus sign (A.5) for the process with

spin flip). It is precisely this difference in the sign of $|\Delta_i|^2$ in the coherence factors which is responsible for the different temperature dependences of the kinetic coefficients (a monotonic increase of the ultrasound absorption with increasing temperature, as against a plot with a maximum below the transition point in the case of nuclear-spin relaxation). From the terms responsible to the interband scattering in (A.4) and (A.5) it is seen that the signs of $|\Delta_i|$ and $|\Delta_j|$ are different for the solution with $\varphi_{12} = \pi$ than for the intraband processes, and therefore at $g_{12} \sim g_{11}$ the temperature dependence of the sound absorption has a maximum, just as in the case of the spin-lattice relaxation rate.

We note that in the case of the second solution the system is more stable to impurity scattering, since the intraband scatterings are partially compensated by the interband scatterings (because the diagrams for the interband scattering enter with opposite signs).

Thus, the relative phase difference of the order parameters Δ_{11} and Δ_{22} , as a result of interband transitions, should lead to observable physical phenomena.

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Possible types of magnetic ordering of S ions in the garnet structure

D. A. Yablonskiĭ

Donetsk Physicotechnical Institute, Ukrainian Academy of Sciences

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A model approach is proposed to determine and classify, within the framework of the exchange approximation, the types of magnetic ordering that are produced when a crystal goes over into a magnetically ordered state. Within the framework of this approach, the possible types of ordering in the garnet structure are determined for the case when the magnetic and crystal-chemical cells coincide. It is shown that some magnetic structures cause tetragonal or trigonal lattice distortions due to exchange striction. All the obtained exchange structures are in correspondence with the exchange classes introduced by Andreev and Marchenko.

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The magnetic properties of antiferromagnetic garnets are the subject of a rather larger number of studies (see the review of Belov and Sokolov¹). A theoretical analysis of some types of magnetic ordering in such structures was carried out by the Bertaut method² in a number of studies³⁻⁶. This method is based on an analysis of a model quadratic spin Hamiltonian. It will be shown in this paper, however, that inclusion of only the interactions that are quadratic in the spin is insufficient for a complete determination of all the possible magnetic configurations.

A preferable method that determines all the possible types of magnetic ordering in crystals with different symmetries is the expansion of the spin-density vector in irreducible representations of the symmetry group of the paramagnetic state of the crystal.^{7,8} It is precisely by this method that von Prandl⁹ obtained and classified by symmetry type all the possible types of magnetic configurations of the spins in the garnet structure. He took into account to an equal degree both the exchange and the relativistic interactions. At the same time, for crystals with magnetic S ions, a much sim-