

The interaction between phonons and degenerate centers (spin, pseudospin)

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The problem is considered as to how dynamic susceptibility arises in an isolated degenerate system as a result of interaction with phonons. This susceptibility consists of a narrow Lorentz peak and a smooth background. In the lowest approximation with respect to degenerate-center concentration, the centers clad with phonons lead to an anomalously strong (in a broad temperature range) and temperature-independent decay of phonons of the viscosity type. One consequence of such a decay is that the heat conductivity below the Debye temperature is proportional to the temperature. It is also found that the interaction between the phonons and the centers becomes strong at sufficiently low temperatures. The results are practically independent of the nature of the degenerate center and are of quantum origin.

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1. INTRODUCTION

Two questions are considered in this work. First is the dynamics of an individual center, which possesses an internal degenerate degree of freedom by virtue of the fact that the acoustic phonons produce transitions between the degenerate levels. The second is the reaction of such phonon-clad centers on the field of the acoustic phonons. Here the specific nature of the degenerate center is almost of no consequence to us. This can be either the spin S or the total angular momentum of the ion $J(S, J > \frac{1}{2})$ in the absence of a degeneracy-removing constant field, or the same thing in a field which only partially removes the degeneracy. Further, this can be different cases of degenerate or almost degenerate orbital motion, combined below in the term "pseudospin." For example, a dynamic Jahn-Teller system or else a tunnel state in the case when the level splitting can be neglected.

In all cases, only one thing is of importance to us, namely that the phonons produce transitions between levels in the first order in the interaction, and not merely modulate the levels. In other the interaction with the phonons must not be written down in the form of a single term that is the product of some function of J_x (or σ_x) with the phonon operator, but rather the presence is necessary of several terms which depend on different components of the vector J (or σ) and which do not commute with one another. Thus, the considered phenomena have a purely quantum nature and disappear in the classical limit $J \rightarrow \infty$.

This is the essential difference of the results obtained below from the usually considered effects connected with phonon broadening of local levels (see, for example, the work of Krivoglaz *et al.*^{1,2} and the work of Duke and Mahan³). Along with this, a very similar formulation of the problem is contained in the paper of Ivanov and Fishman,⁴ where the absorption of sound by a dynamic Jahn-Teller system is considered.

We now discuss qualitatively the picture that arises in the case in which an isolated center is clad by a field of phonons. First of all, we note that the results are practically identical for centers of different nature. The entire difference reduces to the form of the coef-

ficients that enter into the answer, and depend on the nature of the center and the specific form of its interaction with the phonons. For the sake of convenience, we shall frequently speak of spins in what follows.

As is well known, a free spin has in a zero external field only a static susceptibility $\chi \sim T^{-1}$, while the dynamic susceptibility $\chi(\omega)$ is identically equal to zero. Interaction with phonons leads to the result that each spin state survives a finite time and therefore should feel an external field of the corresponding frequency. Here the decisive role is played by the frequency dependence of the phonon field acting on the spin.

As is well known, in the low-frequency limit the spin interacts with the field of the strain tensor (for example, see the book of Al'tshuler and Kozyrev⁵). As a result, it turns out that the spectral density of the phonon field acting on the spin is proportional to ω^3 . This leads to the result that a Lorentzian line of finite width is not formed in lowest order perturbation theory, and the dynamic susceptibility $\chi(\omega)$ has the form of a smooth background that is temperature-independent. The width of this background is of the order of the Debye frequency Θ , with $\text{Im}\chi \sim \omega$ at $\omega \ll \Theta$. A Lorentzian peak of finite width Γ arises only upon taking into account the effects of the next higher perturbation theory, and it turns out that in the static limit $\omega \rightarrow 0$ the susceptibility is somewhat less than the static susceptibility of the free spin, although, as before, its smooth part is proportional to T^{-1} . The difference between the adiabatic and isothermal susceptibilities introduced by Kubo is, however, completely absent here.

It should be emphasized that such a coincidence of the two static susceptibilities does not always occur (see, for example, the work of Lazuta⁷). The general form of the function $\text{Im}\chi(\omega)\omega^{-1}$ is shown in Fig. 1. It should be remarked that the described picture of the frequency dependence of the susceptibility is a consequence of the weakness of the spin-phonon interaction as $\omega \rightarrow 0$. Such a weak coupling takes place only in three-dimensional systems. In the case of a lower dimensionality, the coupling is much greater; however, the discussion of the spin susceptibility in such sys-

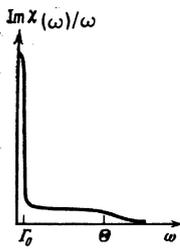


FIG. 1.

tems goes beyond the bounds of this work. It should also be noted that Krivoglaz and Los⁸ also studied the dynamics of an isolated spin in the presence of degeneracy. However, in their case (the field of critical fluctuations) the spectral density of the field acting on the spin was proportional to ω . As a result, a Lorentzian line of finite width appeared even in first order perturbation theory.

Up to now, in speaking about the susceptibility, we have not specified the type of interaction the response to which the susceptibility describes. In particular, it can be describing the reaction to a local strain. But in this case, in the case of a finite density of centers, the latter react on the phonon field. This leads, even in the case of a weak interaction, to anomalously strong viscous-type phonon damping proportional to ω^2 (we recall that damping from static defects is proportional to ω^4). Such a damping can be called (somewhat arbitrarily) "spin viscosity." In the range of frequencies away from the Lorentzian peak the damping is due to the background and does not depend on the temperature. In the case of a Jahn-Teller system, the damping has been discussed by Ivanov and Fishman⁴ from a somewhat different point of view. This damping leads to very important physical consequences. First, there arises an anomalous temperature dependence of the thermal conductivity: if we neglect other mechanisms, then at $T \ll \Theta$ the thermal conductivity turns out to be proportional to T , while at $T \gg \Theta$ it does not depend on the temperature. Second, a term proportional to ω appears in the spectral density of the phonon field that acts on the spin, thanks to which the spin-phonon interaction becomes strong at sufficiently low temperatures and the need arises of solving the self-consistent problem of the dynamics of the spin-phonon system. We propose to discuss the solution of this problem in the following.

2. CHOICE OF MODELS; DIAGRAM TECHNIQUE

As was already noted in the Introduction, the nature of the degenerate center is almost of no significance to us. However, it is nevertheless convenient in what follows to carry out the entire analysis while keeping in mind some specific models, to the description of which we now turn.

1. The spin (total angular momentum) in the field of elastic oscillations is in the isotropic case,

$$H_1 = g [\{ J_i, J_j \}^{-2/3} J(J+1) \delta_{ij}] \varepsilon_{ij}(\mathbf{R}_0), \quad (1)$$

where $\{ J_i, J_j \} = J_i J_j + J_j J_i$, \mathbf{R}_0 are the coordinates of the spin, and ε_{ij} is the strain tensor.

2. As is known, the crystalline field partially removes the degeneracy, and then, in place of the $(2J+1)$ -fold degeneracy of the levels, there arise several series of levels of lower multiplicity.⁹ If we are interested in the frequency of the phonons and in temperatures that are greater than corresponding splitting, then this splitting is unimportant and, as before, we can use the Hamiltonian (1). In the inverse limiting case, we are interested only in the lowest multiplet. It is only necessary that there be transitions between its components in the first order in the interaction. We shall not discuss the possible situations. We only note that there is no splitting in a field of cubic symmetry and in place of (1) we have

$$H_2 = 2g_1 [J_x^2 \varepsilon_{xx} + J_y^2 \varepsilon_{yy} + J_z^2 \varepsilon_{zz} - 1/3 J(J+1) \varepsilon_{ii}] + g_2 [\{ J_x, J_y \} \varepsilon_{xy} + \{ J_y, J_z \} \varepsilon_{yz} + \{ J_z, J_x \} \varepsilon_{zx}]. \quad (2)$$

3. In the case of the dynamic Jahn-Teller effect or of the tunnel state (when we can neglect in it splitting of the levels), in the case of twofold degeneracy, the Hamiltonian takes the form

$$H_3 = g (\sigma_x Z_{ij} \varepsilon_{ij} + \sigma_x X_{ij} \varepsilon_{ij}), \quad (3)$$

where Z and X are numerical matrices.

In what follows, it is necessary that the phonons not only modulate the degenerate levels, but also produce transitions among them. For this, there should not be a direction \mathbf{n} in the xz plane such that $(\sigma \cdot \mathbf{n})$ commutes with H_3 . It is not difficult to establish the fact that the corresponding commutator differs from zero in the case in which X is not proportional to Z , i.e., if $X_{ij} \neq CZ_{ij}$. In the Jahn-Teller case, the matrices Z and X are of the same order; there is a more detailed discussion of this, for example, in Ref. 4. In the case of the tunnel state, the matrix X is small in comparison with Z , since it should be proportional to the penetrability of the barrier.

For what follows, it is convenient to write down the interaction (1)–(3) in unified fashion:

$$H_1 = g \sum_{\mu} Q^{\mu} \varepsilon^{\mu}(\mathbf{R}_0) = g \sum_{\mu} Q^{\mu} c_{ij}^{\mu} \varepsilon_{ij}(\mathbf{R}_0), \quad (4)$$

where Q^{μ} are operators acting in the space of the functions of the degenerate state [the combinations J_i in (1) and (2) or σ_x and σ_z in (3)], while ε^{μ} are the combinations of components of the tensor ε_{ij} .

For calculation of the dynamic susceptibility below, we shall use the technique of Abrikosov, proposed by him for the study of the Kondo effect.¹⁰ We shall now formulate this technique briefly in a form that is convenient for us (see also the work of Walker¹¹). In place of the Hamiltonian (4) we introduce a new Hamiltonian, which describes an ensemble of infinitely heavy particles situated in the immediate vicinity of the point \mathbf{R}_0 and interacting with the phonons:

$$H = \lambda \sum_M a_M^{\dagger} a_M + g \sum_{M, M', \mu} a_M^{\dagger} Q_{M', M}^{\mu} a_M \varepsilon^{\mu}(\mathbf{R}_0) = H_0 + H_1. \quad (5)$$

Here a_M^{\dagger} and a_M are the creation and annihilation operators of the particles (for definiteness, fermions) at the point \mathbf{R}_0 , and M is a quantum number that distinguishes the states inside the multiplet (for example,

the projection of the angular momentum). If the mass of the particle approaches infinity, then its orbital motion becomes classical and classical statistics are applicable for its description. Here $-\lambda$ in (5) is the chemical potential, which tends to minus infinity, and the averages of the occupation numbers $\langle a_M^+ a_M \rangle = \langle n_M \rangle$ are proportional to $\exp(-\lambda/T)$, i.e., they tend to zero.

The ordinary temperature diagram technique is applicable to the Hamiltonian (5) (see, for example, the book of Abrikosov, Gor'kov and Dzyaloshinskii¹²). Since $\lambda \rightarrow \infty$, each closed fermion loop is proportional here to $\exp(-\lambda/T)$, i.e., it is exponentially small. Therefore, in the calculation of the susceptibility, it is necessary to consider only a single closed loop, and it is not necessary to take into account diagrams that have a large number of such loops and correspond to the interaction of two or more particles located at the point R_0 . In addition, since a single particle is located at the point R_0 , the susceptibility should be orthonormalized in a suitable way. As a result, we obtain the following for the susceptibility that describes the reaction to the action conjugate to the operator P :

$$\begin{aligned} \chi_P &= N^{-1} \text{Sp} \{ e^{-H_0/T} P(\tau), P(0) \}, \\ N &= \sum_M \text{Sp} e^{-H_0/T} a_M^+ a_M = \sum_M \langle n_M \rangle, \\ P &= \sum_{M, M'} a_M^+ P_{M, M'} a_M. \end{aligned} \quad (6)$$

In the case of magnetic susceptibility, P is the spin or total angular momentum, while in the case of reaction to a strain it is one of the operators Q^μ determined by the equations (1)–(4). We emphasize once again that in the calculation of χ it is necessary to keep only the part that is finite in the limit as $\lambda \rightarrow \infty$. Obviously, if there is more than one center, the normalizing factor in (6) should be the product of the numbers of particles N for all the centers.

The first few perturbation-theory diagrams for χ are shown in Fig. 2, where the lines with arrows correspond to the Green's functions of the particles

$$g_{M, M'}^{(0)} = \delta_{M, M'} (i\omega_n - \lambda)^{-1},$$

and the wavy lines are the Green's functions of the strain tensor $\Delta_{\mu, \nu}$. For calculation of the susceptibility at real frequencies, it is necessary to continue the temperature diagrams analytically. This is done in two stages. First, it is necessary to formulate a diagram technique for the complete Green's function g and the complete vertex part Γ , both continued to the real axis; the diagrams for these are shown in Fig. 3. We then must express the susceptibility in the form of an integral of these quantities.

The first part of this program in our case is very simple. We choose the frequencies of the wave lines

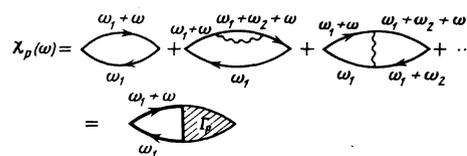


FIG. 2.

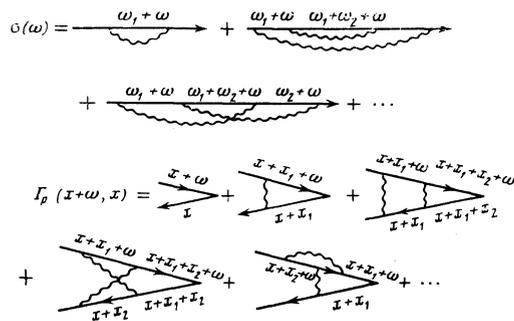


FIG. 3.

to be the independent frequencies over which the summation is carried out. This can be done so that they enter into the arguments of the g -functions with a positive sign (see Fig. 3). After this, it is necessary to replace the sums over the frequencies by contour integrals, introducing the Planck function $N(\omega)$ as a weighting factor. In the calculation of these integrals, it is not necessary to take the poles of the Green's function g_0 into account, since the residues at these poles are proportional to $N(\lambda) \approx \exp(-\lambda/T)$. Thanks to this circumstance, the integration contours can be deformed so that they encircle the real axis. But the function $\Delta(\omega)$ has on the real z axis a jump equal to $\text{Im}\Delta(\omega)$; as a result, the contour integrals are easily transformed into integrals along the real axis, and a simple diagram technique develops at real frequencies: to each wavy line there is juxtaposed a quantity $\pi^{-1}N(\omega)\text{Im}\Delta(\omega)$, and the frequencies of the wavy lines must be so chosen that they enter into the argument of g_0 with a positive sign; it is necessary to integrate from $-\infty$ to $+\infty$ over all the frequencies of the wavy lines.

It is seen from the specific analytic form of the expressions corresponding to the diagrams of Fig. 3 for $\Gamma(\omega_1 + \omega, \omega_1)$, that the vertex part is an analytic function of two independent variables: $\omega_1 + \omega$ and ω_1 , on each of which it has a cut along the real axis. The general proof of this assertion can be found in the work of the author.¹³ Since the analytic properties of the Green's functions are also known,¹² continuation of $\chi(\omega)$ to the real axis is easily carried out (see Ref. 13 and the work of Ginzburg¹⁴) and the following expression exists for the retarded susceptibility:

$$\begin{aligned} \chi_P(\omega) &= (2\pi i N)^{-1} e^{-\lambda/T} \int_{-\infty}^{\infty} dx e^{-x/T} \text{Sp} P \{ g(x+\omega) \Gamma_P^{++}(x+\omega, x) g(x) \\ &\quad - g^*(x) \Gamma_P^{--}(x, x-\omega) g^*(x-\omega) - g(x+\omega) \Gamma_P^{+-}(x+\omega, x) g^*(x) \\ &\quad + g(x) \Gamma_P^{-+}(x, x-\omega) g^*(x-\omega) \}. \end{aligned} \quad (7)$$

Here g is the retarded Green's function, the plus and minus signs on Γ_P indicate the signs of the imaginary parts of the corresponding arguments (for example,

$$\Gamma_P^{+-}(x, y) = \Gamma_P(x+i\delta, y-i\delta);$$

the trace is taken over the projections of M . In the derivation of this formula, a shift of all the energies by an amount λ was carried out. As a result, the factor $[\exp(x/T) + 1]^{-1}$ under the integral, which appears upon replacement of the sum over ω_1 by an integral,

was replaced by $\exp\{- (x + \lambda)/T\}$.

It remains to discuss the properties of the function $\text{Im}\Delta(\omega)$. For noninteracting phonons it has the form

$$\text{Im}\Delta_{q\nu q}(\omega) = -\frac{\pi v_0}{(2\pi)^3} \int d\mathbf{k} \sum_{\kappa} (e_{\kappa}^{\nu} k^{\nu} + e_{\kappa}^{\nu} k^{\nu}) (e_{\kappa}^{\nu} k^{\nu} + e_{\kappa}^{\nu} k^{\nu}) \times (8m\omega_{\kappa})^{-1} [\delta(\omega - \omega_{\kappa}) - \delta(\omega + \omega_{\kappa})], \quad (8)$$

where m is the mass of the elementary cell, v_0 is its volume, κ is the index of polarization. Obviously, $\text{Im}\Delta$ can be represented in the following fashion:

$$\text{Im}\Delta_{q\nu q}(\omega) = -(\omega/\Theta)^2 (ms^2)^{-1} \Lambda(\omega) d_{q\nu q}, \quad (9)$$

where Θ is the characteristic phonon frequency, which we shall call the Debye frequency, s is the mean sound speed, defined by the equation $3s^{-3} = 2s_t^{-3} + s_l^{-3}$; $\Lambda(\omega)$ is a cutoff factor, equal to unity at $\omega \ll \Theta$ and decreasing rapidly with increase in ω at $\omega \gg \Theta$, and d is a frequency-independent tensor, for which, in the Debye approximation, we have

$$d_{q\nu q} = d_0 \delta_{ij} \delta_{pq} + d_1 (\delta_{ip} \delta_{jq} + \delta_{iq} \delta_{jp}),$$

$$d_0 = \frac{1}{10} \left[\left(\frac{s}{s_t} \right)^2 - \left(\frac{s}{s_l} \right)^2 \right]; \quad d_1 = \frac{1}{20} \left[2 \left(\frac{s}{s_t} \right)^2 + 3 \left(\frac{s}{s_l} \right)^2 \right]. \quad (10)$$

3. SUSCEPTIBILITY

We shall use perturbation theory in the calculation of the susceptibility. This is valid if the dimensionless spin-phonon coupling constant $f^2 = g^2 (\Theta m s^2)^{-1}$ is small. Here, however, it is impossible to limit ourselves only to the first order perturbation theory, and it is necessary to take into account also that part of the contribution of second order (proportional to f^4) which leads to a finite width of the Lorentz line.

We need to know the Green's function g and the vertex part Γ_P for the calculation of the susceptibility. We shall first discuss the matrix structure of these quantities. We begin with the Green's function and consider, for example, the third diagram of Fig. 3 for σ . Since $g_0 \sim \delta_{M'M}$, this diagram is proportional to $Q^{\lambda} Q^{\mu} Q^{\lambda'} Q^{\mu'} d_{\lambda\lambda'} d_{\mu\mu'}$, where $d_{\lambda\lambda'}$ is the corresponding combination of components of the tensor d . In the case of interactions that are invariant to a transformation of any symmetry group [for example, (1) and (2)], this quantity is a scalar and is proportional to $\delta_{M'M}$. In the case of the interaction (3) $\varepsilon_x = X\varepsilon$ and $\varepsilon_z = Z\varepsilon$ can be regarded formally as components of some magnetic field with zero mean value. Naturally, this analogy is valid only if $\langle \varepsilon_x \varepsilon_z \rangle = 0$, which we shall assume in what follows for simplicity. After this, it is clear that in this case the diagram is proportional to $\delta_{M'M}$, since there is no constant magnetic field in the system. A similar consideration is obviously possible also for all other diagrams, and therefore $g \sim \delta_{M'M}$.

We now proceed to $\Gamma_P^{M'M}$ and show that if P is transformed according to the irreducible representation of the symmetry group, then $(\Gamma_P)_{M'M} \sim P_{M'M}$. For this we consider as an example the fourth diagram of Fig. 3; it is proportional to

$$(Q^{\nu} Q^{\mu} P Q^{\nu'} Q^{\mu'})_{M'M} d_{\nu\nu'} d_{\mu\mu'}.$$

It is quite obvious that this quantity should transform like P in symmetry transformations and, consequently,

that it is proportional to $P_{M'M}$. It is clear that this same reasoning is true also for all the remaining diagrams determining Γ_P . It is no longer necessary to consider the interaction (3) separately, since we have in fact reduced it above to the interaction of the spin with a plane fluctuating magnetic field. All these considerations of general character are confirmed by direct calculations, using a specific form of interaction.

We now proceed to the calculation of $g(\omega)$. We first consider the first diagram of Fig. 3 for σ ; to it corresponds the following analytic expression:

$$\sigma^{(1)}(\omega) = \frac{f^2 \alpha}{\pi \Theta^2} \int_{-\infty}^{\infty} dx g(x+\omega) x^2 N(x) \Lambda(x), \quad (11)$$

$$f^2 = g^2 (\Theta m s^2)^{-1}; \quad \alpha = Q^{\nu} Q^{\mu} d_{\nu\mu}.$$

In what follows it is convenient to make an energy shift, replacing $\omega - \lambda$ by ω . After this, obviously, $\sigma^{(1)}(0)$ describes the renormalization of the energy zero. Making use of the free Green's function $g_0 = \omega^{-1}$ for its calculation, we obtain

$$\sigma^{(1)}(0) = \frac{f^2 \alpha}{\pi \Theta^2} \int_{-\infty}^{\infty} dx x^2 N(x) \Lambda(x) = -\frac{f^2 \alpha}{\pi \Theta^2} \int_{-\infty}^{\infty} dx x^2 \Lambda(x), \quad (12)$$

where we have taken it into account that $\Lambda(x)$ is an even function. Since $\sigma_1(0)$ does not depend on the temperature, it can be included in λ . Then it is not difficult to write the Green's function of first order in the form

$$g^{(1)}(\omega) = \left[\omega Z^{-1} - \frac{\omega^2 f^2 \alpha}{\pi \Theta^2} \int_{-\infty}^{\infty} \frac{dx x N(x) \Lambda(x)}{x + \omega + i\delta} \right]^{-1} = \frac{Z}{\omega + i\delta} + g_2(\omega), \quad (13)$$

$$Z = 1 - \frac{\alpha f^2}{\pi \Theta^2} \int_{-\infty}^{\infty} dx x N(x) \Lambda(x), \quad g_2(\omega) = \frac{f^2 \alpha}{\pi \Theta^2} \int_{-\infty}^{\infty} \frac{dx x N(x) \Lambda(x)}{x + \omega + i\delta}. \quad (13a)$$

We see that in first order no finite damping arises in the Green's function, i.e., as before, there is a pole at $\omega = 0$; here, however, the residue at the pole becomes less than unity and a non-pole background increment $g_2(\omega)$ arises. It is also evident that the retention of terms of order f^2 in the denominator is an exaggeration of the accuracy.

Finite damping of g does arise only in the next order of perturbation theory, i.e., when account is taken of the second and third diagrams of Fig. 3. The contribution of the second diagram is easiest to obtain by substituting (12) in (10) and separating the terms proportional to f^4 , while the contribution of the third diagram must be calculated by using the functions g_0 . As a result, we obtain

$$\sigma^{(2)}(\omega) = -\left(\frac{f^2}{\pi \Theta^2} \right)^2 \int_{-\infty}^{\infty} \frac{dx_1 dx_2 x_1^2 x_2^2 N_1 N_2 \Lambda_1 \Lambda_2}{(x_1 + \omega)(x_2 + \omega)(x_1 + x_2 + \omega)} (\omega \alpha^2 + \beta x_2), \quad (14)$$

$$\beta = Q^{\nu} Q^{\mu} [Q^{\nu'}, Q^{\nu'}] d_{\nu\nu'} d_{\mu\mu'}.$$

In the function $\sigma^{(2)}(\omega)$ we can separate out the terms that vanish in the limit $\omega = 0$; they give a contribution of order f^4 to the renormalization of the residue Z and the background part of the Green's function and are of no interest in what follows. The part that is finite in the limit $\omega = 0$ leads first, to an additional shift in the energy zero and is also of no importance in what follows, and second, to a finite damping. As a result, the part of $\sigma^{(2)}$ that is of interest to us can be written

in the form

$$\sigma_1(\omega) = - \left(\frac{f}{\pi\Theta^2} \right)^2 \beta \int_{-\infty}^{\infty} dx_1 dx_2 (x_1 x_2)^2 N_1 N_2 \Lambda_1 \Lambda_2 \left(\frac{1}{x_1 + x_2 + \omega + i\delta} - \frac{1}{x_1 + x_2} \right), \quad (15)$$

where the integral in the first term is taken in the sense of the principal value.

As a result, we get for the Green's function

$$g(\omega) = g_1(\omega) + g_2(\omega), \quad g_1(\omega) = Z[\omega - \sigma_1(\omega)]^{-1}, \quad (16)$$

where Z and g_2 are determined by the expressions (13a). The function $g_1(\omega)$ has a pole with residue Z at the point $\omega = -i\Gamma_0$, where

$$\Gamma_0 = 2\pi\beta \left(\frac{f}{\pi\Theta^2} \right)^2 \int_0^{\infty} dx x^4 N(x) [N(x) + 1] \Lambda^2(x) = \begin{cases} \frac{2\beta f^4}{\pi} T \left(\frac{T}{\Theta} \right) c_0, & T \gg \Theta, \\ \frac{8\pi^3 \beta}{15} T \left(\frac{Tf}{\Theta} \right)^4, & T \ll \Theta, \end{cases} \quad (17)$$

$$c_0 = \Theta^{-3} \int_0^{\infty} dx x^2 \Lambda^2(x).$$

It is clear from the physical requirement $\Gamma_0 > 0$ that β is positive. This can be established with the help of actual calculations, using the interactions (1)–(3), and a general proof can also be given, based on the definition of β . However, we shall not concern ourselves with this. The functions σ_1 and g_2 possess an important property:

$$\text{Im } F(-\omega) = e^{-\omega/T} \text{Im } F(\omega). \quad (18)$$

In the order f^2 in which we are interested, the interaction does not change the normalization in (7), i.e., $N = G \exp(-\lambda/T)$, where G is the multiplicity of the degeneracy of the considered system. Actually, we represent the number of particles N in the form of an integral of the Green's function²:

$$N = - \sum_M \pi^{-1} \int_{-\infty}^{\infty} dx n(x) \text{Im } g_{MM}(x) = -e^{-\lambda/T} G \pi^{-1} \int_{-\infty}^{\infty} dx e^{-x/T} \text{Im } g(x), \quad (19)$$

where $n(x)$ is the Fermi function. By virtue of (18), the integrand on the right side of (19) does not increase exponentially. Substituting the expressions (16) and (13a) in (19), it is not difficult to verify that the terms of order f^2 actually cancel out.

We now proceed to the study of the vertex part $\Gamma_P(x + \omega, x)$. As is seen from (7), we need different branches of this analytic function of two variables. Here, obviously, Γ_P^{+-} and Γ_P^{-} can simply be calculated by perturbation theory since in this case the poles of all the functions g_1 lie on the same side of the contour of integration, and therefore the integrals over the intermediate frequencies are finite in the limit $\Gamma_0 \rightarrow 0$ and cannot compensate for the smallness of the interaction. As a result, we obtain

$$\Gamma_P^{++}(x + \omega, x) = 1 + \frac{f^2 a_P}{\pi\Theta^2} \int_{-\infty}^{\infty} dx_1 x_1^3 N_1 \Lambda_1 g_1(x_1 + x + \omega) g_1(x_1 + x), \quad (20)$$

$$a_P = \text{Sp} (Q^* P Q^* P) d_{vv'} (\text{Sp } P^2)^{-1} > 0, \quad \Gamma_P^{--} = (\Gamma_P^{++})^*.$$

The situation is more complicated in the case Γ_P^{+-} , since at $\omega = 0$ there is an intermediate state in which

$|g_1|^2$ is under the integral sign. Here the poles of the functions g_1 and g_1^* contract the contour of integration and the corresponding integrals diverge as $\Gamma_0 \rightarrow 0$. As a result, the integral equation for Γ_P^{+-} takes in our approximation the form

$$\Gamma_P^{+-}(x + \omega, x) = 1 + \frac{f^2 a_P}{\pi\Theta^2} \int_{-\infty}^{\infty} dx_1 x_1^3 N_1 \Lambda_1 g_1(x_1 + x + \omega) g_1^*(x_1 + x) \\ \times \Gamma_P^{+-}(x_1 + x + \omega, x_1 + x) + b_P \left(\frac{f}{\pi\Theta^2} \right)^2 \int_{-\infty}^{\infty} dx_1 dx_2 (x_1 x_2)^2 N_1 N_2 \Lambda_1 \Lambda_2 \\ \times g_1(x_1 + x + \omega) g_1^*(x_1 + x_2) g_1(x_1 + x_2 + x + \omega) g_1^*(x_1 + x_2 + x) \\ \times \Gamma_P^{+-}(x_1 + x_2 + x + \omega, x_1 + x_2 + x), \quad (21)$$

$$b_P = \text{Sp} (Q^* Q^* P Q^* Q^*) d_{vv'} d_{vv'} (\text{Sp } P^2)^{-1}.$$

We attempt to solve this equation by iteration. It is easy to show that a divergence develops in the second term at $\omega \sim \Gamma_0$ and $\Gamma_0 \rightarrow 0$ only in the second iteration, and it is of the same order as the divergence of the first iteration of the third term. This means that in the solution of Eq. (21), the first iteration of the second term must be taken into account by perturbation theory, while the second iteration is used for reconstruction of the kernel in the third term, so that this kernel takes into account not only the diagram with the cross (fourth diagram of Fig. 3) but also the two rungs of the ladder (third diagram). As a result, Eq. (21) must be rewritten in the form

$$\Gamma_P^{+-}(x + \omega, x) = 1 + \frac{f^2 a_P}{\pi\Theta^2} \int_{-\infty}^{\infty} dx_1 x_1^3 N_1 \Lambda_1 g_1(x_1 + x + \omega) g_1^*(x_1 + x) \\ + \left(\frac{f^2}{\pi\Theta^2} \right)^2 \int_{-\infty}^{\infty} dx_1 dx_2 (x_1 x_2)^2 N_1 N_2 \Lambda_1 \Lambda_2 g_1(x_1 + x + \omega) [b_P g_1^*(x_1 + x_2) + a_P^2 g_1^*(x_1 + x)] \\ \times g_1(x_1 + x_2 + x + \omega) g_1^*(x_1 + x_2 + x) \Gamma_P^{+-}(x_1 + x_2 + x + \omega, x_1 + x_2 + x). \quad (22)$$

This equation is easily solved if we note that at $\omega \ll T, \Theta$, the important region of integration over x_2 in the third term is close to the poles of the last two Green's functions. Since the remaining factors under the integral change little in the case of such x_2 , we can set $x_2 = -x - x_1$ in them and, moreover, neglect the dependence on ω . As a result, we obtain the following equation:

$$\Gamma_P^{+-}(x + \omega, x) = 1 + \frac{f^2 a_P}{\pi\Theta^2} \int_{-\infty}^{\infty} dx_1 x_1^3 N_1 \Lambda_1 g_1(x_1 + x + \omega) g_1^*(x_1 + x) \\ + K(x) \frac{2\pi i}{\omega + 2i\Gamma_0} \Gamma_P^{+-}(\omega, 0), \quad (23)$$

$$K(x) = \left(\frac{f}{\pi\Theta^2} \right)^2 \int_{-\infty}^{\infty} dx_1 [x_1^2 (x + x_1)^2 b_P - x_1^3 (x + x_1) a_P^2] N(x_1) \\ \times N(-x - x_1) \Lambda(x_1) \Lambda(x + x_1),$$

where the function g_1 has been substituted for g_0 in the calculation of $K(x)$.

The solution of this equation has the form

$$\Gamma_P^{+-}(x + \omega, x) = 1 + \frac{f^2 a_P}{\pi\Theta^2} \int_{-\infty}^{\infty} dx_1 x_1^3 N_1 \Lambda_1 g_1(x_1 + x + \omega) g_1^*(x_1 + x) \\ + [2\pi i K(x) Z_P / (\omega + 2i\Gamma_0)]; \\ \Gamma_P = 2\pi\gamma_P \left(\frac{f}{\pi\Theta^2} \right)^2 \int_{-\infty}^{\infty} dx x^4 N(x) [N(x) + 1] \Lambda^2(x), \quad (24)$$

$$\gamma_P = \beta + b_P - a_P^2 = \text{Sp} (Q^* Q^* P^* P) d_{vv'} d_{vv'} (\text{Sp } P^2)^{-1},$$

$$Z_P = 1 + \frac{f^2 a_P}{\pi\Theta^2} \int_{-\infty}^{\infty} dx x N \Lambda.$$

The temperature dependence of Γ_P is obviously the same as of Γ_0 . The same dependence is possessed by the paramagnetic-resonance linewidth due to the Raman scattering of the phonons (see the work of Al'tshuler and Kozyrev¹⁵). This is not accidental, since we have actually taken into account the very same process in the limit, when the resonance frequency is equal to zero. Everything said above about β can be said about γ_P . The substitution of (2), (13), (16) and (20) in (7) leads, after long calculations (see the Appendix), to the following rather complicated expression for the susceptibility:

$$\chi_P(\omega) = \overline{P^2} \left\{ \frac{2i\Gamma_P Z_P}{T(\omega + 2i\Gamma_P)} + \frac{f^2}{\pi\Theta^2} \frac{2i\Gamma_0}{T(\omega + 2i\Gamma_0)} \left[(a_P - 2\alpha) \int_{-\infty}^{\infty} dx x N \Lambda \right. \right. \\ \left. \left. - 2a_P \Theta T \right] + \frac{2f^2 \varphi_P}{\pi\Theta^2} \int_{-\infty}^{\infty} \frac{dx x \Lambda}{x + \omega + i\delta} \right\}; \quad (25)$$

$$\overline{P^2} = G^{-1} \text{Sp } P^2, \quad \varphi_P = \alpha - a_P = \text{Sp}(P[P, Q^\mu]Q^\mu) d_{mm} (\text{Sp } P^2)^{-1}.$$

In this expression, the first term is the usual Lorentz peak with width Γ_P , and with an amplitude somewhat changed by the interaction in comparison with the usual value $\overline{P^2} T^{-1}$ [for the magnetic susceptibility, $\overline{P^2} = S(S+1)/3$]. The second term is a Lorentz peak with width Γ_0 and with a small amplitude proportional to f^2 . Both these terms are calculated under the assumption that $\omega \ll T, \Theta$; at high frequencies allowance for them is an exaggeration in the accuracy, since they are proportional to f^4 . Finally, the last term is the background part of the susceptibility, which begins to fall off only at $\omega > \Theta$. The nature of the background is very simple. This is the amplitude of the elastic scattering of a quantum of the field conjugate to the operator P , accompanied by the emission of a virtual phonon. The ordinary energy dependence of this amplitude is due to the fact that, because of the degeneracy, the energy denominators corresponding to phonon-free intermediate states are equal to the energy of the quantum ω . In the next section, in the discussion of phonon damping, we shall return to this question.

The following expression is obtained from (25) for the static susceptibility:

$$\chi_P(0) = \frac{\overline{P^2}}{T} [1 - \delta(T)]; \\ \delta(T) = \frac{2f^2}{\pi\Theta} \left[\left(\int_{-\infty}^{\infty} dx x N \Lambda - 2T\Theta \right) \varphi_P + T\Theta a_P \right] = \begin{cases} 2Tf^2 a_P / \pi\Theta, & T \gg \Theta \\ 2f^2 \varphi_P c_1 / \pi, & T \ll \Theta \end{cases}, \quad (26) \\ c_1 = \Theta^{-2} \int_0^{\infty} dx x \Lambda.$$

We see that this susceptibility is somewhat smaller than for the free system, and the difference increases with increase in the temperature. This is not surprising, since the phonons always generate transitions between levels (spin flip) and the intensity of this process obviously increases with the temperature.

The expression (27) is identical with the ordinary isothermal susceptibility. This can be established if we check the fulfillment of the sum rule (see, for example, Ref. 7):

$$\overline{P^2} = \pi^{-1} \int_{-\infty}^{\infty} d\omega \text{Im } \chi_P(\omega) (1 - e^{-\omega/T})^{-1}. \quad (27)$$

The corresponding calculations are given in the Appendix. For what follows, it is necessary to neglect insignificant small increments in (25) and use the following simple expression for $\chi_P(\omega)$:

$$\chi_P(\omega) = \overline{P^2} \left\{ \frac{2i\Gamma_P}{T(\omega + 2i\Gamma_P)} + \frac{2f^2 \varphi_P}{\pi\Theta^2} \int_{-\infty}^{\infty} \frac{dx x \Lambda}{x + \omega + i\delta} \right\}, \quad (28) \\ \text{Im } \chi_P(\omega) = \overline{P^2} \left\{ \frac{2i\Gamma_P \omega}{T[\omega^2 + (2\Gamma_P)^2]} + \frac{2f^2 \varphi_P}{\Theta^2} \omega \Lambda(\omega) \right\}.$$

We see that the imaginary part of the background susceptibility does not depend on the temperature and is proportional to ω at $\omega \ll \Theta$. Comparing the imaginary parts of the background and peak, and taking (17) and (24) into account, it is not difficult to verify that the background gives the principal contribution to the susceptibility if the condition

$$\omega > \omega_0 = f\Theta \begin{cases} (T/\Theta)^{1/2}, & T \gg \Theta \\ (T/\Theta)^2, & T \ll \Theta \end{cases} \quad (29)$$

is satisfied. Since the sign of $\text{Im } \chi$ should be the same as the sign of ω , the constant φ_P is positive; we can say the same about it that was said above about β .

The widths Γ_0 and Γ_P , as well as the amplitude of the background φ_P , have a purely quantum nature, i.e., they vanish in the classical limit. It is easiest to understand this through the example of the interaction (1). Actually, the energy of the interaction is finite as $J \rightarrow \infty$ only if $g^2 \sim J^{-2}$. But here it follows immediately from (14), (24), and (25) that Γ_0 and φ_P are proportional to J^{-1} , and that $\Gamma_P \sim J^{-2}$.

4. THE EFFECT OF DEGENERATE CENTERS ON THE PHONONS

Thus, we have obtained the expression (28) for the susceptibility of a center clad with phonons. If the concentration of such centers is finite, they lead to a change in the phonon spectrum. We now consider this phenomenon and the physical effects connected with it in the case in which the quantity nf^4 is small, where n is the atomic concentration of the centers. Taking the expression (4) into account, we obtain

$$D_{ij}(\mathbf{k}, \omega) = D_{ij}^{(0)}(\mathbf{k}, \omega) - \frac{g^2 n}{m} D_{ip}^{(0)}(\mathbf{k}, \omega) k_q \chi_{pqim}(\omega) k_m D_{ij}(\mathbf{k}, \omega), \quad (30) \\ \chi_{pqim}(\omega) = \sum_{\mu} c_{p\mu} c_{i\mu} \chi_{\mu}(\omega)$$

for the phonon Green's function D in this approximation. In the derivation of this expression, we have taken into account the symmetry of χ in pq and lm .

We shall now assume that the phonons are described by the Debye model and limit ourselves to consideration of the isotropic case, in which

$$\chi_{pqim} = \chi_1 \delta_{pq} \delta_{im} + \chi_2 (\delta_{pi} \delta_{qm} + \delta_{pm} \delta_{qi}), \quad (31)$$

then we have for the transverse and longitudinal Green's functions

$$D_t(\mathbf{k}, \omega) = \{\omega^2 - (s_1 k)^2 + f^2 n (ks)^2 \Theta [\chi_1(\omega) + \chi_2(\omega)]\}^{-1}, \quad (32) \\ D_l(\mathbf{k}, \omega) = \{\omega^2 - (s_1 k)^2 + f^2 n (ks)^2 \Theta [\chi_1(\omega) + \chi_2(\omega)]\}^{-1}.$$

In the case of the interaction (1), the isotropy certainly exists, and $\chi_{ii pp} = 0$, and therefore, $\chi_1 = -\chi_0/15$,

$\chi_2 = \chi_0/10$, where $\chi_0 = \chi_{ijij}$. In the general case, there is no isotropy but this obviously has no influence on the basic physical results obtained below.

We first consider the region of high frequencies, where the condition (29) is satisfied and the susceptibility is determined by the background. In this case, the phonon damping of the κ -th branch ($\kappa = t, l$) and the renormalized sound speed s'_κ have at $\omega \ll \Theta$ the form

$$\gamma_\kappa = \frac{n^2 F_\kappa s^2 \omega^2}{2\Theta s_\kappa^3}, \quad s'_\kappa = s_\kappa \left(1 - \frac{n^2 F_\kappa s^2}{\pi s_\kappa^2} \right), \quad (33)$$

where F_κ is the combination of the products $(\overline{Q^\mu})^2 \varphi_\mu$, entering in the expression for D_κ .

Thus, in this region of frequencies, the damping does not depend on the temperature and is proportional to ω^2 , i.e., it is large in comparison with the damping by static defects, which is proportional to ω^4 . As was pointed out in the Introduction, such a damping for a Jahn-Teller system has been obtained in Ref. 4. One can connect the temperature-independent "spin viscosity" coefficients with the damping (33)

$$\eta_\kappa = F_\kappa n s^2 \rho \Theta^{-1}, \quad \zeta_\kappa = F_\kappa n s^2 \rho \Theta^{-1}, \quad (34)$$

where ρ is the density of the body.

It follows from (33) that the scattering cross section of a phonon by a center is proportional to ω^2 . The same frequency dependence exists also for resonance scattering of a phonon by a multi-level system if the frequency of the phonon is significantly greater than the energy of the resonances which is natural, since in our case these energies are equal to zero.¹⁾

We now consider the reverse limiting case, in which the background can be neglected. If $\omega \ll \Gamma$ the renormalized sound speed has the form

$$s'_\kappa = s_\kappa^2 (1 - \overline{Q^\mu}^2 n \Theta T^{-1}), \quad (35)$$

where $\overline{Q^\mu}^2$ is the corresponding combination of the constants $(\overline{Q^\mu})^2$. We see that upon a decrease in the temperature, one of the sound speeds vanishes and, consequently, the system loses stability. Below this temperature, a state ought to develop with nonzero mean values of the operators Q^μ . It should be emphasized that such a phase transition, due to interaction with phonons, could be realized only if the remaining forms of interaction (for example, exchange) were significantly weaker. Somewhat later we shall see that the simple theory developed above for the dynamics of an isolated center, which does not take into consideration the change in phonon damping by interaction with such centers, becomes inapplicable before the phase transition occurs. Therefore, the problem of the phase transition requires additional analysis beyond the framework of the present research.

The phonon damping at $\omega \ll \Gamma$ also has a viscous character, but it depends strongly on the temperature. The following expression holds for it:

$$\gamma_\kappa = f n \overline{Q^\mu}^2 \Theta s^2 \omega^2 / 4 s_\kappa^3 T \Gamma_\kappa. \quad (36)$$

We shall not write out the simple formulas for the range of frequencies $\Gamma_\kappa < \omega < \omega_0$.

Equation (9) is the basis of the theory developed above. According to this equation, the damping $\text{Im}\Delta \sim \omega^3$ at small ω . Such a frequency dependence was obtained for ideal harmonic phonons and can obviously change if allowance is made for their damping. However, the damping of the ordinary type, due to scattering by static inhomogeneities and anharmonism, depends on a high power of the phonon frequency (see, for example, the book by Krivoglaz¹⁶⁾ and therefore does not change this dependence.²⁾ Along with this, the contribution of the background part of the susceptibility to the damping turns out to be very important. In order to understand this, we must substitute $\text{Im}D$ in place of the combination of δ functions multiplied by $(2\omega_{kx})^{-1}$. As a result, as is not difficult to establish, the following increment appears at $T \rightarrow 0$ and $\omega > \omega_0$, in addition to the contribution to $\text{Im}\Delta$ in the form (9):

$$\text{Im}\Delta'(\omega) = -A f n F \omega (\Theta m s^2)^{-1}, \quad (37)$$

where the constant A depends on the form of the phonon spectrum at large k and on what combination of atomic displacements replaces the tensor ϵ_{ij} in (4) in the microscopic treatment (see, for example, Ref. 4).

It thus turns out that at

$$\omega < \omega_1 = \Theta f^2 (nF)^{1/2} \quad (38)$$

the dependence of $\text{Im}\Delta$ on the frequency is not cubic but linear. This means that the theory developed above is not applicable at such frequencies. In the calculation of the damping, a range of frequencies of the order of the temperature was important [see (17)]. Therefore, if $T > \omega_1$, but $\Gamma < \omega_1$, and the Lorentz peak is calculated correctly, only the expression for the background turns out to be incorrect at $\omega < \omega_1$. However, at $T < \omega_1$, all the obtained results are inapplicable and it is necessary to solve the entire problem of the self-consistent spin-phonon system. We propose to do this later in another work. We also note that if F is not too small, the frequency ω_1 is greater than that temperature at which, according to (35), the sound speed vanishes.

It remains for us to discuss the question as to how the interaction of the phonons with the degenerate centers affects the thermal properties. The corresponding calculations are rather cumbersome and we shall give them in the Appendix. It is shown there that the basic contribution to the heat capacity is made by the background and has the form

$$\Delta C = n f^2 \begin{cases} \Lambda_1 (T/\Theta)^2, & \omega_1 \ll T \ll \Theta \\ -\Lambda_2 T/\Theta, & T \gg \Theta \end{cases}, \quad (39)$$

where the constants Λ_1 and Λ_2 are given below by the formulas (A.15). We see that at all temperatures the degenerate centers lead to small corrections to the known temperature dependences for the lattice heat capacity.

The result for the heat capacity turns out to be the most interesting. As has already been mentioned above, the background part of the susceptibility leads to the result that the cross section for phonon scattering by the center is proportional to ω^2 . This means that the mean free path length of the phonon at $T \ll \Theta$

is proportional to T^{-2} and does not depend on the temperature at $T \gg \Theta$. This easily permits us to estimate the heat capacity if we use the well-known formula $\kappa = 1/3CIs$. As a result we get, with account of (33),

$$\kappa = \frac{\Theta^3}{f n_s} \begin{cases} K_1 T / \Theta, & \omega_1 < T < \Theta \\ K_2, & T > \Theta \end{cases} \quad (40)$$

where the constants K_1 and K_2 are of the order of unity. They can be calculated by the Kubo formula (see, for example, the book of Lifshitz and Pitaevskii¹⁷). This is done in the Appendix; their values are given there. Formula (40), of course, is applicable only in that range of values of the parameters in which the scattering by the degenerate centers determines the free path length of the phonons. We again emphasize that the expressions (39) and (40) are valid only if $T > \omega_1$.

5. DISCUSSION OF THE RESULTS. SOME GENERALIZATIONS

The obtained results are based on an assumption that f^2 is small; more exactly, the deviation of Z (13a) from unity should be small, which at high temperatures means smallness of the quantity $f^2 T \Theta^{-1}$. The question arises as to what values of f^2 are encountered in nature. Here, of course, too small an f^2 would be uninteresting, since the considered effects become unobservable.

We first discuss the case of rare earth ions. The spin-phonon interaction of such ions has been studied experimentally (see, for example, the works of Baker and Currell¹⁸ and Pela *et al.*¹⁹). It was found in these works that the value of g changes in order of magnitude from hundredths of an electron volt to several electron volts. If we use the definition (11) for f^2 and assume the atomic weight of the elementary cell to be of the order of one hundred then to this range of values of g there corresponds a change of f^2 from 10^{-4} to several units. In particular, this means that the characteristic energy ω_1 , defined by (38) and limiting the regions of applicability of the theory from below, can be found to be very large, lying in a range easily reached by experiment. Thus, if $f^2 \sim 0.1$ and $n \sim 0.1$, then $\omega_1 \sim 0.03\Theta$.

It should be noted that if $f^2 \ll 1$, then the effects considered above, which are associated with the influence of the centers on the phonon, take place even for concentrated systems ($n \sim 1$) if the characteristic energy Θf^4 of interaction of the centers through the phonon is greater than the exchange energy and the energy of the magnetic-dipole forces.

In the case of Jahn-Teller systems, the value of the coupling constant g is limited by the requirement that the effect be dynamic. Roughly speaking, this means that $g \lesssim \Theta$. But here f^2 turns out to be of the order of 10^{-2} – 10^{-3} and, consequently, the considered effects much less pronounced.

We now discuss the case of a tunnel state. Obviously, the developed theory is applicable only at frequencies that are greater than the separation of levels in the neighboring wells. In the interaction (3) the second term describes the transitions induced by phonons between the potential wells, and is proportional to the

amplitude of transmission through the barrier \mathcal{D} , which has the same exponential smallness as the tunnel splitting of the levels. In the case of interaction with phonons, according to (24) and (25), the observed quantities—the peak width and the background amplitude—are expressed in terms of the commutator and are therefore proportional to \mathcal{D}^2 and \mathcal{D} . Here, if the quantity ω_1 turns out to be much greater than the level splitting, the thermal properties described above should change strongly even before this splitting begins to appear.

The quantity g can be of the order of a single electron volt (see, for example, the work of Black and Halperin²⁰), to which corresponds $f^2 = 1$. Therefore, if the splitting is less than one degree, the effects connected with ω_1 should be taken into account at $n \sim 10^{-2}$ if $\mathcal{D} \geq 10^{-2}$. We have seen that there are cases in nature in which $f^2 \sim 1$. Strictly speaking, our theory is inapplicable there. However, we now advance arguments by virtue of which it can be thought that the results are valid at $T \ll \Theta$ and $\omega \ll \Theta$, with some changes, also at $f^2 \sim 1$. We begin with the width of the Lorentz peak. Account of diagrams with three phonon lines obviously leads to a contribution of the order of $\Theta f^6 (T/\Theta)^7$ and if $f^2 (T/\Theta)^2 \ll 1$, it can be neglected. Obviously one can also neglect the contribution from the more complicated diagrams. So far as the background and the amplitude of the Lorentz peak are concerned, account of the more complicated diagrams as $T \rightarrow 0$ should lead to a renormalization of the corresponding amplitudes, so that they will be functions of f^2 , and of the order of unity. The contribution linear in ω to the imaginary part of the background susceptibility must be regarded as the first term of the low-energy expansion of this quantity in ω/Θ .

All the results obtained above are the consequence of formula (9), according to which $\text{Im}\Delta \sim \omega^3$. Such a dependence of $\text{Im}\Delta$ on ω takes place only for three-dimensional systems. In the case of systems of lower dimensionality (two dimensional or quasi-one dimensional), this dependence is significantly weaker and, correspondingly, the spin-phonon interaction is much stronger at low frequencies.

The dependence of $\text{Im}\Delta$ on ω in low-temperature systems is easily determined by means of well-known formulas for the phonon frequencies of such systems (see the book by Landau and Lifshitz²¹). Thus, in two-dimensional systems or quasi-two-dimensional, if we neglect layer interaction, $\text{Im}\Delta_{\parallel} \sim \omega^2 \varepsilon(\omega)$ for the components of the tensor Δ parallel to the layer, where ε is the sign function, and $\text{Im}\Delta_{\perp} \sim \varepsilon(\omega)$ for mixed components. In quasi-one-dimensional systems, in the frequency range in which filament interaction is insignificant, $\text{Im}\Delta_{\parallel} \sim \omega$ for the longitudinal component and $\text{Im}\Delta_{\perp} \sim |\omega|^{-1/2} \varepsilon(\omega)$ for the mixed component. Obviously, each of the enumerated cases of behavior of $\text{Im}\Delta$ requires special analysis. As an illustration, we note that if $\text{Im}\Delta \sim \omega$, then the theory becomes logarithmic in order f^2 .

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APPENDIX

1. According to (20) and (24), the susceptibility can be separated into three terms; the first, χ_1 , is obtained if we replace the vertex in (7) by unity, the second, χ_2 , if we substitute in (7) terms from (20) and (24) that are linear in a_p , and, finally, the third, χ_3 , is obtained by substitution of the last term from (24) in (7).

The expression for χ_1 can be reduced to the form

$$\chi_1 = \bar{P}^2 (2\pi i)^{-1} \int_{-\infty}^{\infty} dx e^{-x/T} [g(x+\omega) + g^*(x-\omega)] \text{Im} g(x). \quad (\text{A.1})$$

Thanks to (18), there are no increasing exponents under the integral sign in the case of negative x . Taking (13a) and (16) into account, and also the fact that, in under our assumptions $\Gamma_0 \ll T$, we obtain after simple calculations

$$\chi_1 = \bar{P}^2 \left\{ \frac{2i\Gamma_0 Z^2}{T(\omega+2i\Gamma_0)} + \frac{2f^2 \alpha}{\pi\Theta^2} \int_{-\infty}^{\infty} \frac{dx x \Lambda}{x+\omega+i\delta} \right\}. \quad (\text{A.2})$$

The quantity χ_2 can easily be reduced to the form

$$\chi_2 = \bar{P}^2 a_p \frac{f^2}{\pi\Theta^2} [J(\omega) + J^*(-\omega)], \quad (\text{A.3})$$

$$J(\omega) = \frac{1}{\pi} \int_{-\infty}^{\infty} dx dx_1 \frac{(x_1-x)^3 \Lambda(x_1-x)}{\exp(x_1/T) - \exp(x/T)} g_1(x+\omega) g_1(x_1+\omega) \text{Im}[g_1(x) g_1(x_1)].$$

Here the integrand with respect to x and x_1 has in the upper half plane, besides the poles of the functions $g_1^*(x)$ and $g_1^*(x_1)$, only distant singularities, connected with Λ and $[\exp(x_1/T) - \exp(x/T)]^{-1}$, which lie above the real axis at distances of the order of Θ and T . We raise the contour of integration to these singularities. As a result, in addition to the contour integral, a term arises for J that is due to the poles of the functions g_1^* and is of the form

$$J_1(\omega) = -2Z g_1(\omega+i\Gamma_0) \int_{-\infty}^{\infty} \frac{dx (x-i\Gamma_0)^3 \Lambda(x)}{\exp(x/T) - \exp(i\Gamma_0/T)} g_1(x+\omega) g_1^*(x). \quad (\text{A.4})$$

The function g_1 can be replaced on the contour of integration by $g_0 + g_0^2 \sigma_1$, after which the integrand turns out to be proportional to σ_1 , and therefore account of the contour integral is an exaggeration of accuracy. We consider J_1 in more detail. Just as before, we raise the contour of integration, recognizing that now the residue at the pole of $g_1^*(x)$ is equal to zero. We then replace g_1 on the contour by $g_0 + g_0^2 \sigma_1$ and expand in Γ_0/T ; an expression is obtained in which there are no singularities up to the real axis, to which we and therefore one can return along it. As a result, we obtain

$$J_1(\omega) = -2g_1(\omega+i\Gamma_0) \int_{-\infty}^{\infty} \frac{dx}{x+\omega+i\delta} \left\{ x^2 N + \frac{i\Gamma_0}{T} x^2 N^2 - 3i\Gamma_0 x N + x^2 N \left[\frac{\sigma_1^*(x)}{x+i\delta} + \frac{\sigma_1(x+\omega)}{x+\omega+i\delta} \right] \right\}. \quad (\text{A.5})$$

Substituting this expression in (A.3) and taking into account that at $\omega \ll T$ and $\omega \ll \Theta$ we have

$$g_1(\omega+i\Gamma_0) = (\omega+2i\Gamma_0)^{-1},$$

we arrive at the expression

$$\chi_2(\omega) = \bar{P}^2 \frac{f^2 a_p}{\pi\Theta^2} \left\{ -2 \int_{-\infty}^{\infty} \frac{dx x \Lambda}{x+\omega+i\delta} + \frac{1}{\omega+2i\Gamma_0} \left[2i\Gamma_0 \int_{-\infty}^{\infty} \frac{dx x \Lambda}{x+\omega+i\delta} - 1 + \frac{2x}{T} \left(N + \frac{1}{2} \right) \right] - 2 \int_{-\infty}^{\infty} dx x^2 N \left[\frac{\sigma_1^*(x)}{x+i\delta} + \frac{\sigma_1(x+\omega)}{x+\omega+i\delta} \right] \frac{1}{x+\omega+i\delta} - \left[\frac{\sigma_1(x)}{x-i\delta} + \frac{\sigma_1^*(x-\omega)}{x-\omega-i\delta} \right] \frac{1}{x-\omega-i\delta} \right\}. \quad (\text{A.6})$$

In all the integrals here, with the exception of the first, we can set $\omega=0$, since the entire calculation is true only at $\omega \ll T, \Theta$, and large x are important under the integral. After this, the terms containing σ_1 vanish, since $\text{Re}\sigma_1(0)=0$, and we finally get for χ_2

$$\chi_2(\omega) = \bar{P}^2 \frac{a_p f^2}{\pi\Theta^2} \left\{ -2 \int_{-\infty}^{\infty} \frac{dx x \Lambda}{x+\omega+i\delta} + \frac{4i\Gamma_0}{\omega+2i\Gamma_0} \left[-\Theta + \frac{1}{T} \int_{-\infty}^{\infty} dx x N \Lambda \right] \right\}, \quad (\text{A.7})$$

$$\Theta = 1/2 \int_{-\infty}^{\infty} dx x \Lambda.$$

There remains the calculation of χ_3 . If we replace g by g_1 in the corresponding expression, then we can neglect the dependence of $K(x)$ on x , and, as a result, we get, in the case $\omega \ll T, \Theta$,

$$\chi_3 = -\frac{\bar{P}^2 Z_p Z^2 \cdot 2i(\Gamma_0 - \Gamma_p) \omega}{T(\omega+2i\Gamma_0)(\omega+2i\Gamma_p)} = \frac{\bar{P}^2}{T} Z^2 Z_p \left(\frac{2i\Gamma_p}{\omega+2i\Gamma_p} - \frac{2i\Gamma_0}{\omega+2i\Gamma_0} \right). \quad (\text{A.8})$$

It is also not difficult to verify that the interference term, which contains g_1 and g_2 , is negligibly small. Adding together (A.2), (A.7), and (A.8), we get formula (25).

2. We now prove that the susceptibility that we have calculated satisfies the sum rule (27). It is not possible to use (25) for this, since its terms proportional to Γ_0 at large ω are calculated incorrectly. Therefore, it is necessary to carry out the proof in general form, using (7), (20), and (24). It follows from (7) that

$$\text{Im} \chi(\omega) = (1 - e^{-\omega/T}) \bar{P}^2 e^{-N/T} N^{-1} \text{Im} G(\omega),$$

$$G(\omega) = (2\pi i)^{-1} \int_{-\infty}^{\infty} dx e^{-x/T} [g(x+\omega) g(x) \Gamma^{++}(x+\omega, x) - g(x+\omega) g^*(x) \Gamma^{+-}(x+\omega, x)]. \quad (\text{A.9})$$

Here $G(\omega)$ is a function that is regular in the upper half plane. Obviously, (27) is rewritten in the form

$$\int_{-\infty}^{\infty} d\omega \text{Im} G(\omega) = \pi e^{N/T} N G^{-1}. \quad (\text{A.10})$$

If we replace the quantity $\Gamma^{\alpha\beta}$ in $G(\omega)$ by unity and substitute in (A.10), then we obtain an identity. This follows from the definition (19) for N and the known sum rule for g^{12}

$$\int_{-\infty}^{\infty} dx \text{Im} g(x) = -\pi. \quad (\text{A.11})$$

The remaining part of G^1 falls off like ω^{-2} as $\omega \rightarrow \infty$ and therefore the corresponding integral is equal to zero. It is easy to verify this by writing it down in the form

$$(2\pi i)^{-1} \int_{-\infty}^{\infty} d\omega [G^1(\omega) - G^{1*}(\omega)].$$

The zero is obtained here because of the fact that the

contour of integration in each of the components can be deformed into an infinitely distant semicircle.

3. For the calculation of the heat capacity we use the formula for the correction that must be introduced in the thermodynamic potential Ω when the interaction is turned on.¹² This formula, after replacement of the sum over the frequencies by an integral, and with account of the expressions (32), can be transformed to the form

$$\Delta\Omega = \int_0^{\theta} \frac{df_1}{f_1} f_1^{2n} \Theta \frac{v_0}{(2\pi)^2} \sum_{\mu} \int dk \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{dx N(x) \text{Im} \chi_{\mu}(x, f_1) (ks)^2}{x^2 - (s_{\mu}k)^2}. \quad (\text{A.12})$$

Since we are interested in effects of order n , we have replaced the total Green's function of the phonon in this expression by the free Green's function. Making use of the sum rule (27) and discarding the terms known to be temperature independent, it is not difficult to obtain the following form (A.12)

$$\Delta\Omega = \int_0^{\theta} df_1 f_1 n \Theta \frac{v_0}{(2\pi)^3} \int dk \sum_{\mu} \left(\frac{s}{s_{\mu}}\right)^2 \frac{1}{\pi} \int_0^{\theta} \frac{dx x^2 \text{Im} \chi_{\mu}(x, f_1) (2N+1)}{x^2 - (s_{\mu}k)^2}. \quad (\text{A.13})$$

If we substitute the expression for the Lorentz peak in place of $\text{Im} \chi$ in this expression, then, because of the factor x^2 in the numerator, we do not have to take into account the damping Γ_x in the denominator. As a result, it turns out that this part of $\Delta\Omega$ is proportional to f^6 and is negligibly small. The contribution from the background can be written in the form

$$\Delta\Omega_{\text{pr}} = n \frac{f^2 v_0}{2\Theta (2\pi)^2} \int dk \sum_{\mu} F_{\mu} \left(\frac{s}{s_{\mu}}\right)^2 \frac{1}{\pi} \int_0^{\theta} \frac{dx x^2 N \Lambda}{x^2 - (s_{\mu}k)^2}. \quad (\text{A.14})$$

Now, using the well-known formula for the heat capacity

$$\Delta C = -T \frac{\partial^2}{\partial T^2} \Delta\Omega,$$

it is easy to obtain the expression (39) of the main text, where the constants Λ_1 and Λ_2 are determined by the expressions

$$\Lambda_1 = \frac{1}{20} \Theta^2 v_0 \int dk \sum_{\mu} \frac{s^2 F_{\mu}}{s_{\mu}^4 k^2}, \quad \Lambda_2 = \frac{\pi}{6} \sum_{\mu} F_{\mu} \left(\frac{s}{s_{\mu}}\right)^2. \quad (\text{A.15})$$

4. As is known, the operator of the thermal energy flux of the phonon gas has the form

$$q = \frac{1}{2N} \sum_{\mathbf{k}, \mu} \{a_{\mathbf{k}, \mu}^+, a_{\mathbf{k}, \mu}\} \frac{\partial \omega_{\mathbf{k}, \mu}}{\partial \mathbf{k}}. \quad (\text{A.16})$$

The Kubo formula¹⁷ for the thermal conductivity can be written in the following form:

$$\kappa(\omega) = (3T i \omega)^{-1} [\Phi_{\alpha\alpha}(\omega) - \Phi_{\alpha\alpha}(0)], \quad (\text{A.17})$$

where $\Phi_{\alpha\beta}$ is the retarded Green's function of the operators q_{α} . Since we neglect the dimensions of the centers, by virtue of the vector nature of the vertices in the diagram series in Φ we need retain only the first diagram, which is a simple loop, and, as a result, we have for κ :

$$\kappa(\omega) = (3(2\pi)^2 T i \omega)^{-1} \sum_{\mu} \int dk \omega_{\mathbf{k}, \mu}^2 \left(\frac{\partial \omega_{\mathbf{k}, \mu}}{\partial \mathbf{k}}\right)^2 [\Phi_{\mu}(\mathbf{k}, \omega) - \Phi_{\mu}(\mathbf{k}, 0)], \quad (\text{A.18})$$

$$\Phi_{\mu}(\mathbf{k}, \omega) = \frac{1}{\pi^2} \int_{-\infty}^{\infty} \frac{dx_1 dx_2 [N(x_1) - N(x_2)]}{x_2 - x_1 + i\delta} \text{Im} d_{\mu}(\mathbf{k}, x_1) \text{Im} d_{\mu}(\mathbf{k}, x_2),$$

where the expression for $\Phi_{\mu}(\mathbf{k}, \omega)$ is obtained after analytic continuation of the corresponding temperature diagram, and $d_{\mu}(\mathbf{k}, \omega)$ is the retarded Green's function of the operators $a_{\mathbf{k}, \mu}$ and $a_{\mathbf{k}, \mu}^+$. In the limit $\omega=0$, this expression is easily transformed to the form

$$\kappa = (3(2\pi)^2 T^2 \pi)^{-1} \sum_{\mu} \int dk (\omega_{\mathbf{k}, \mu})^2 \times \left(\frac{\partial \omega_{\mathbf{k}, \mu}}{\partial \mathbf{k}}\right)^2 \int_{-\infty}^{\infty} dx N(x) (N(x)+1) [\text{Im} d_{\mu}(\mathbf{k}, x)]^2. \quad (\text{A.19})$$

In this integral, the principal contribution at $T \ll \Theta$ is made by $x \sim T$ and at $T > \Theta$ we have $x \sim \Theta$. But, by virtue of (29), the Lorentz part of the susceptibility is small at such x and the entire damping is determined by the background. For free phonons κ is infinite. Therefore, we are interested in the contribution to κ which diverges in the limit as $f^4 n \rightarrow 0$. This contribution is obviously connected with the pole of the function d . But, from the definition of the function d or D and formula (33) for the damping, it is clear that near the pole,

$$d_{\mu}(\mathbf{k}, \omega) \approx (\omega - s_{\mu}k + i s_{\mu} \gamma_{\mu})^{-1}. \quad (\text{A.20})$$

After substitution of this expression in (A.14), we find

$$\kappa = \frac{\Theta}{6\pi^2 n f^4 T^2} \sum_{\mu} \frac{s_{\mu}}{F_{\mu} s^2} \int_0^{\theta} dx x^2 N(x) [N(x)+1]. \quad (\text{A.21})$$

In both limiting cases, this integral is easily evaluated and, as a result, we obtain

$$K_1 = 1/18 \sum_{\mu} s_{\mu} (F_{\mu} s)^{-1}, \quad K_2 = 3\pi^{-2} K_1. \quad (\text{A.22})$$

Note added in proof, (Oct. 3, 1980). In the paper of V.V. Kokshenev [J. Low Temp. Phys. 20, 373 (1979)], for the case of a mixture of orthohydrogen in solid para-hydrogen, a viscous-type damping of the photons was obtained, similar to (32), and the corresponding expression for the thermal conductivity is in satisfactory agreement with the experimental data.

Note added in proof (25 December 1980). In formula (A5), in the first term under the integral sign, a term $\Lambda'(x) x^0 x^2 N$ has been left out in the braces. Allowance for this term expression (A.6) somewhat, and an additional term

$$- \frac{P^2 f a_p}{\pi \theta^2} \frac{2i\Gamma_0}{\omega + 2i\Gamma_0} \int \frac{dx x^2 \Lambda'(x)}{x + \omega + i\delta}$$

appears in (25). At the same time, in expression (25) for δ no account need be taken of the term proportional to a_p , therefore in the high-temperature limit

$$\delta = \frac{\varphi P f^2 c_0}{3\pi} \left(\frac{\theta}{T}\right)^2$$

The phrase after (25) should be replaced by the following: "We see that this susceptibility is somewhat lower than for the free system, and in the high-temperature limit this difference vanishes; this is not surprising, since the investigated effect is of quantum origin."

¹⁷The author is grateful to V. L. Gurevich who called his attention to this circumstance.

²We are only considering dielectrics. In metals, the effect of electrons changes the entire picture.

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Translated by R. T. Beyer

ERRATUM

Erratum: Theory of pure short *S-c-S* and *S-c-N* microjunctions [Sov. Phys. JETP 51, 111 (1980)]

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In expression for I_{exc} in Eq. (42), the coefficient 16/3 should be replaced by 8/3. In Eqs. (45) (last two lines), (45'), and (45'') all the terms with the exception of V/R must be multiplied by $\frac{1}{2}$. The expression for $\sigma(V)$ at $T \ll \Delta$ should take the form

$$\sigma(V) = 2\sigma \left\{ \theta(\Delta - |V|) + \frac{V}{\Delta} \left[\frac{V}{\Delta} - \left(\left(\frac{V}{\Delta} \right)^2 - 1 \right)^{1/2} \right] \theta(|V| - \Delta) \right\}.$$

The value of $\sigma_0(T)$ is 2σ at $T \ll \Delta$ and $(1 + 4\Delta/3T)\sigma$ at $T \gg \Delta$.

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