$$\Gamma_n = \sum_m V_{nm} N_m \frac{\pi}{\beta} \sum_\Omega \frac{1}{\sqrt{\bar{u}_m^2(\Omega)+1}}, \qquad (7)$$

where

$$\Omega = (2r+1)\frac{\pi}{\beta} \quad (r=0, \pm 1, \ldots), \quad \bar{u}_n(\Omega) = -iu_n \quad (s=i\Omega).$$

On the basis of (6) and (7), expressions were obtained in[4,6,8-12] for the energy gap ω_g and the state densities $n_n(\omega)$ of a two-band superconductor with a nonmagnetic impurity ($\beta_{nm} \neq 0$). It was possible in the extreme cases of large and small parameters α_n to obtain explicit expressions for ω_g and the function $n_n(\omega)$ over the entire frequency range[8-12]. N. I. Botoshan and M. I. Vladimir carried out computer calculations for intermediate values of the parameters of the theory. It was shown that for a system with a nonmagnetic impurity, ω_g is always larger than the smaller and smaller than the larger of the two system ordering parameters Γ_n. As the concentration of this impurity increases with $\Gamma_1 < \Gamma_2$, the value of ω_g/Γ_1 increases with it. At high impurity concentrations, when the inequality $\alpha_n \gg \hbar\omega_g/\Gamma_n$ is satisfied, we obtain for ω_g on the assumption of weak coupling

$$\omega_g \approx \frac{\Gamma_1\Gamma_2(\alpha_1+\alpha_2)}{\Gamma_1\alpha_1+\Gamma_2\alpha_2} \approx 2\omega_D e^{-1/\tau}. \qquad (8)$$

The relation of the single-band theory of Bardeen, Cooper, and Schrieffer[13] and Bogolyubov[14] holds between ω_g and T_c in this extreme case, thus demonstrating the single-band nature of the superconductive properties of the two-band model with a high nonmagnetic-impurity concentration.

Investigation of the electromagnetic properties of the two-band model with impurity[15] also confirms this conclusion.

Values of $n_n(\omega)$ were calculated on the basis of a method of analysis developed in[8,11] and based on separation of the nonanalytic dependence of these functions on the impurity parameters in Eq. (6) in the frequency ranges near the energy gap and near the larger of the two ordering parameters. At frequencies far from these values, the computation method was based on expansion of the functions $n_n(\omega)$ in powers of the small parameters of the theory. It was shown that at small concentrations of the nonmagnetic impurity, the state densities have sharp maxima near the respective ordering parameters. The heights of the maxima increase with decreasing impurity concentration, their half-widths decrease, and the frequencies of the maxima approach the values for the energy gaps of the pure substance.

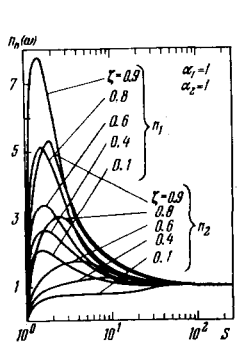

FIG. 1

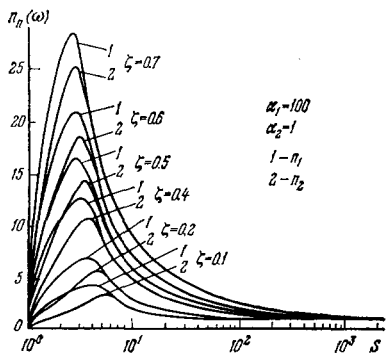

FIG. 2

Figures 1 and 2 present computer-generated curves[12] of $n_n(\omega)$ as functions of

$$\frac{\omega}{\Gamma_1} = \frac{\omega_g}{\Gamma_1} + \frac{Q}{3}(s-1),$$

where

$$Q = \frac{(\alpha_1\alpha_2)^{2/3}\omega_0^{1/3}(1-\zeta)^{1/3}(\omega_0-1)(1+\zeta\omega_0)}{\zeta\alpha_1^2+(\omega_0-1)(1+\zeta\omega_0)^2} \qquad \left(\omega_0 = \frac{\omega_g}{\Gamma_1}\right)$$

at various values of the parameters α_n and $\zeta = \Gamma_1/\Gamma_2$.

The entropy and thermal conductivity of a two-band superconductor with impurity[16] and its absorption of light and ultrasound[17] were computed on the basis of the method developed for investigation of the functions n_n and functions related to them.

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Yu. E. Perlin and B. S. Tsukerblat. Dichroism Effects in Systems with Dynamic Jahn-Teller Coupling. Insurmountable mathematical difficulties are encountered in attempts to calculate the shape of the optical bands that arise on transitions between Jahn-Teller electron vibrational states of a crystal impurity

center. Results obtained for molecular systems[1,2] with the aid of computers cannot be extended to local states of crystals because of the dispersion of the crystal vibrations that results from the strong dependence of the optical-spectrum parameters on the phonon-density distribution. By calculating the moments of the spectrum and their variations in dichroism effects, we can obtain information on the electron states and the electron-phonon interaction without resorting to a detailed calculation of the band contour.

Let us consider a transition from an orbital singlet initial state A to a multiplet Γ that is split by a perturbation **W** operating in the electronic subsystem. For the n-th central moment of the optical distribution we obtain the matrix expression

$$\sigma_n = (-1)^n \frac{d^n}{dt^n} \langle e^{-iWt} U(t) \rangle_{ph} \Big|_{t=0}, \quad (1)$$

where $\langle \ldots \rangle_{ph}$ represents statistical averaging over the vibrational subsystem,

$$U(t) = T \exp \left\{ \frac{i}{\hbar} \int_0^t [H_{eL}(t_1) + W(t_1)]\, dt_1 \right\} \quad (2)$$

is the evolution operator, and

$$H_{eL} = \sum_{\kappa} v_{\kappa} q_{\kappa} \quad (3)$$

is the operator of the electron-phonon interaction in the approximation linear in the normal coordinates q_K of the crystal vibrations. The matrix operators in formulas (1)—(3) are defined in the basis that diagonalizes the perturbation **W**. The moments (1) are reckoned from the center of gravity of the distribution

$$\bar{\Omega} = \omega_{\Gamma A} \mathbf{1} + \hbar^{-1} W, \quad (4)$$

where $\omega_{\Gamma A}$ is the Franck-Condon frequency in the absence of the perturbation. We obtain for the second and third moments

$$\sigma_2 = \frac{1}{2\hbar^2} \sum_{\kappa} v_{\kappa}^+ v_{\kappa} \operatorname{cth} \frac{\beta_{\kappa}}{2}, \quad (5)$$

$$\sigma_3 = \frac{1}{2\hbar^2} \sum_{\kappa} \left[\omega_{\kappa} v_{\kappa}^+ v_{\kappa} + \sum_{\kappa} v_{\kappa}^+ [W, v_{\kappa}] \operatorname{cth} \frac{\beta_{\kappa}}{2} \right] = \sigma_3' + \sigma_3'' \quad \left(\beta_{\kappa} = \frac{\hbar\omega_{\kappa}}{kT} \right). \quad (6)$$

It follows from (5) and (6) that σ_2 and σ_3' are invariants of the point group of the local center, so that the splitting of the band that is observed in dichroism effects is not accompanied by a change in the second moments of its components. The latter are therefore equal to the second moment of the unsplit band. At the same time, the third moment contains a correction σ_3'' proportional to the matrix **W**. The only contribution to the proportionality coefficient comes from vibrations that are active in the dynamic Jahn-Teller effect (JTE) and have $[\mathbf{W} \times \mathbf{v}] \neq 0$. Under the conditions of the JTE, therefore, an external field not only shifts the band, but also deforms it, so that the hypothesis of the so-called "rigid shift" becomes inapplicable.

The change in the third moment in external fields can be used to extract information on the parmaeters of the Jahn-Teller interaction. Let us demonstrate this for the case of a transition of the A → T type to an orbital triplet in a cubic center when the modes $\overline{\Gamma} = E$, T_2 are active in the JTE. In this case, the matrix $\sigma_3''(\text{trig})$, which corresponds to uniaxial compression along the axis C_3, takes the form

$$\sigma_{3\,(\text{trig})}'' = W_{\text{trig}} \left[-\frac{1}{2} \sigma_2(T_2) - \frac{3}{2} \sigma_2(E) \right], \quad (7)$$

where $\sigma_2(\overline{\Gamma})$ are the contributions of the respective modes to σ_2. For compression along the C_4 axis we obtain

$$\sigma_{3\,(\text{tetr})}'' = W_{\text{tetr}} \left[-\frac{3}{2} \sigma_2(T_2) \right]. \quad (8)$$

The matrices $\mathbf{W}_{\text{trig(tetr)}}$ can be determined from (4) for an observed change $\bar{\Omega}$ on transition from σ- to π-polarized light. Then Eqs. (7) and (8) are used to determine $\sigma_2(E)$ and $\sigma_2(T_2)$ from the measured values of σ_3'', i.e., to find the contributions of the Jahn-Teller vibrations to the second moment:

$$\sigma_2 = \sigma_2(A_1) + \sigma_2(E) + \sigma_2(T_2). \quad (9)$$

Measuring the total second moment σ_2, we also determine $\sigma_2(A_1)$. These results apply for arbitrary Jahn-Teller coupling and are equally valid for both local and crystal vibrations. Reference[3] gives a specific calculation of $\sigma_2(\overline{\Gamma})$ for the U band of ruby ($^4A_{2g} \rightarrow {}^4T_{2g}$ transition in the Cr^{3+} ion).

If the dynamic JTE is relatively small, the band retains its near-Gaussian bell shape on strong electron-phonon interaction. Using the well-known Edgeworth expansion for the band maximum, we obtain the formula

$$\Omega_{\max} = \bar{\Omega} - \frac{\sigma_3}{2\sigma_2}. \quad (10)$$

Accordingly, we have for trigonal dichroism

$$\Omega_{\max}(\pi) - \Omega_{\max}(\sigma) = W_{\text{trig}} \left[1 + \frac{3\sigma_2(E) + \sigma_2(T_2)}{4\sigma_2} \right]. \quad (11)$$

The second term of (11) is a small correction to the frequency of the band maximum, but in calculation of the shift of the maximum it yields a quantity of the same order as the change in the first moment. Relation (11) must be taken into account in determining the parameters of crystal fields of low symmetry from the dichroism of the band maxima. The multiplier in the square brackets is different for different A → T bands (for example, the U and Y bands in ruby), together with the multiplier $\mathbf{W}_{\text{trig}}$ (which is also, generally speaking, different for different bands). It is therefore more reliable to determine $\mathbf{W}_{\text{trig}}$ from the shift of the first moment instead of from the shift of the maximum. Estimates for ruby indicate that the multiplier in the square brackets of (11) equals 1.27 and 1.5 for the U and Y bands, respectively[3].

A detailed exposition will be submitted in the author's monograph "Effekty élektronno-kolebatel'nogo vzaimodeĭstviya v opticheskikh spektrakh primesnykh paramagnitnykh ionov" (Electron-Vibrational Interaction Effects in the Optical Spectra of Impurity Paramagnetic Ions), which will be publsihed in 1974 by "Shtiintsa" (Kishinev).

*$[W, v_{\mathcal{H}}] = W \times v_{\mathcal{H}}$.

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V. A. Kovarskiĭ. Features of the Absorption, Emission, and Scattering of Light by Atoms and Impurity Centers of Crystals with Degenerate Energy Spectra in a Strong Electromagnetic Field. The development of