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EFFECT OF CRYSTALLINE FIELDS ON THE SHAPE OF THE SPECTRUM OF RESONANCE ABSORPTION OF GAMMA RAYS

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By treating simultaneously the quadrupole interaction of the nucleus with the crystalline field and the interaction with the radiation field, a discussion is given of the effect of crystalline fields on the shape of the spectrum for resonance absorption of γ rays. Problems relating to the dynamics of the particles constituting the crystal are treated under highly simplified assumptions; nevertheless the method used can easily be revised for any other model for the dynamic properties of the crystal.

1. INTRODUCTION

The splitting of nuclear levels by crystalline fields, which previously was observed by radiofrequency spectroscopic methods, has recently been seen in experiments on resonance absorption of γ quanta. In this connection one naturally asks to what extent the interaction of the nucleus with the crystalline fields affects the shape of the resonance absorption spectrum for γ rays and the results of measurements of physical quantities. The formulation of problems of this kind for resonance absorption of γ rays differ essentially from the case for rf spectroscopy since the radiation widths of nuclear levels are comparable to typical values of the splittings. Thus to include the dynamical aspect of the crystalline field one must treat simultaneously the interactions of the nucleus with the perturbing fields and the radiation field.

The need for including dynamic components of the crystalline field is seen from new experimental data (cf. [1]) which cannot be understood on the basis of purely static splittings of the nuclear levels. In this connection we note that the effect on the parameters of the observed spectrum of small splittings of the nuclear levels by static fields can be calculated completely by the method described in [2], so that experimental study of static splittings does not involve any difficulties of principle.

Taking account of the dynamical component of the crystalline fields may also be significant for the interpretation of the temperature dependence of the probability f′ for recoilless absorption. Usually f′ is determined from the dependence of the maximum absorption $\epsilon(0)$ on absorber thickness, but as explained in [2], $\epsilon(0)$ is extremely sensitive to line shape, which in turn is more or less determined by the dynamic component of the crystalline field.

Using as an example electric quadrupole interaction, the present paper treats the simultaneous effect of static and dynamic crystalline fields on the shape of the resonance absorption of γ quanta (obviously the results are equally applicable to the emission spectrum). To be specific, we choose a nucleus with ground-state spin $^1/_2$ and spin $^3/_2$ in the excited state.

2. FORMULATION OF THE PROBLEM

The Hamiltonian for the quadrupole interaction of the nucleus with an electric field has the form

$$\hat{H} = \sum_{i,j} \hat{Q}_{ij} V_{ij}, \tag{1}$$

where $\hat{Q}_{ij}$ is the quadrupole moment operator, a symmetric tensor of rank two with zero trace. The operator $\hat{Q}_{ij}$ is related to the spin operator $\hat{J}_i$ as follows:

$$\hat{Q}_{ij} = \frac{eQ}{6J(2J-1)}\left[{}^3/_2\{\hat{J}_i\hat{J}_j\} - \delta_{ij}J(J+1)\right], \tag{2}$$

where Q is the nuclear quadrupole moment; the curly brackets denote the anticommutator, $V_{ij} = \partial^2 V/\partial x_i \partial x_j$, where V is the potential produced by the nucleus.

We assume the electric field in the crystal to consist of two parts: a static field $V^{(0)}$ and a variable field V(t). The static field is determined by the equilibrium configuration of the unit cells and, on the assumption of strictly harmonic thermal vibrations, is independent of temperature; on the other hand, the dynamical component of the field is induced by the thermal motion of the particles making up the crystal, and consequently depends on the temperature. So we shall set

$$V = V^{(0)} + V(t). \tag{3}$$

The eigenvalues of the operator for the static quadrupole interaction are determined by the anisotropy coefficient $g^{(0)}$ of the tensor $V_{ik}^{(0)}$:

$$g^{(0)2} = \tfrac{1}{2}\left[(V_{xx}^{(0)} - V_{yy}^{(0)})^2 + (V_{yy}^{(0)} - V_{zz}^{(0)})^2 + (V_{zz}^{(0)} - V_{xx}^{(0)})^2 + 6\,(V_{xy}^{(0)2} + V_{yz}^{(0)2} + V_{zx}^{(0)2})\right]. \tag{4}$$

In particular, for a system with spin $^3/_2$ the static splitting $\Delta^{(0)}$ is given by the relation

$$\Delta^{(0)} = eQg^{(0)}/3. \tag{5}$$

In the system of the principal axes of the tensor $V_{ik}^{(0)}$, the expression for $g^{(0)}$ is considerably simplified:

$$g^{(0)} = \sqrt{^3/_2}\,[V_{xx}^{(0)2} + V_{yy}^{(0)2} + V_{zz}^{(0)2}]^{1/2} = {}^3/_2 V_{zz}^{(0)} \sqrt{1 + \eta^2/3}, \tag{6}$$

where $\eta = (V_{xx}^{(0)} - V_{yy}^{(0)})/V_{zz}^{(0)}$ is the asymmetry coefficient of the field.

The eigenfunctions of the quadrupole operator for spin $^3/_2$ are

$$\Psi_{\rm I}^{(1)} = \begin{pmatrix} \lambda \\ 0 \\ A\lambda \\ 0 \end{pmatrix}, \quad \Psi_{\rm I}^{(2)} = \begin{pmatrix} 0 \\ A\lambda \\ 0 \\ \lambda \end{pmatrix}; \quad \Psi_{\rm II}^{(1)} = \begin{pmatrix} 0 \\ \lambda \\ 0 \\ -A\lambda \end{pmatrix}, \quad \Psi_{\rm II}^{(2)} = \begin{pmatrix} -A\lambda \\ 0 \\ \lambda \\ 0 \end{pmatrix},$$

$$E_{\rm I} = +eQg^{(0)}/6, \quad E_{\rm II} = -eQg^{(0)}/6, \tag{7}$$

where $A = \eta/(\sqrt{3} + \sqrt{3 + \eta^2})$; $\lambda^2 = 1/(1 + A^2)$ is a normalization factor.

For the tensor of the dynamical field it is natural to assume

$$V_{ik}(t) = \sum_{\omega_s} \tilde{V}_{ik}(\omega_s) \cos[\omega_s t + \varphi_{ik}(\omega_s)], \tag{8}$$

where ω_s are the frequencies of the phonon spectrum of the crystal; $V_{ik}(\omega_s)$ and $\varphi_{ik}(\omega_s)$ are the corresponding amplitudes and phases. Because of the negligibly small width of the ground state of the nucleus, the effect of the perturbing field (8) on the shape of the γ ray resonance absorption spectrum can be treated, in the one-quantum approximation, in two successive stages:

1) a solution of the problem is found for an individual component of the expansion (8);

2) the distortions of the absorption spectrum caused by the harmonic perturbations of frequency ω_s are summed in accordance with (8).

The Hamiltonian for quadrupole interaction of the nucleus with a harmonic field has the form

$$\hat{H}_s(t) = \hat{H}_s \exp[i\omega_s t] + \hat{H}_s^+ \exp[-i\omega_s t], \tag{9}$$

$$\hat{H}_s = \frac{eQ}{4\sqrt{3}} \begin{pmatrix} \tilde{V}_0 & \tilde{V}_{-1} & \tilde{V}_{-2} & 0 \\ \tilde{V}_{+1} & -\tilde{V}_0 & 0 & \tilde{V}_{-2} \\ \tilde{V}_{+2} & 0 & -\tilde{V}_0 & -\tilde{V}_{-1} \\ 0 & \tilde{V}_{+2} & -\tilde{V}_{+1} & \tilde{V}_0 \end{pmatrix}. \tag{9'}$$

We have introduced the notation

$$\tilde{V}_0 = \frac{\sqrt{3}}{2}\tilde{V}_{zz}, \qquad \tilde{V}_{\pm 1} = \tilde{V}_{xz} \exp[i\varphi_{xz}] \pm i\tilde{V}_{yz} \exp[i\varphi_{yz}],$$

$$\tilde{V}_{\pm 2} = \tfrac{1}{2}\,\widetilde{(V_{xx} - V_{yy})} \exp[i\varphi_{(xx-yy)}] \pm i\tilde{V}_{xy} \exp[i\varphi_{xy}]. \tag{9''}$$

3. DERIVATION OF GENERAL FORMULAS

Let us consider the effect of interaction of the nucleus with a harmonic perturbing field on the spectral characteristics of the resonance transition. The behavior of the system is given by the Schrödinger equation, which for such problems is conveniently treated in E-space. Without giving the initial equations, we enumerate the unperturbed states which must be taken into account in formulating such equations:

1) $A^{\pm}0$—the nucleus is in its ground state; the radiation field is characterized by the energy distribution function of the quanta, $W_e(E_\gamma)$, which describes the perturbing flux. The superscripts ± give the sign of the projection of the nuclear spin:

2) $B_{\rm I\gamma}^{(1,2)}$—the nucleus is in the excited state $B_{\rm I}^{(1,2)}$ (the energy of the state is $E_{B_{\rm I}} = E_B + \Delta^{(0)}/2$, where E_B is the excitation energy of the nucleus in the absence of the splitting); a quantum of energy E_γ is absorbed from the distribution $W_e(E_\gamma)$; the superscripts (1, 2) denote the form of the spin function for the excited state of the nucleus;

3) $B_{\rm II\gamma}^{(1,2)}$—the nucleus is in the excited state $B_{\rm II}^{(1,2)}$ (the energy of the state is $E_{B_{\rm II}} = E_B - \Delta^{(0)}/2$; a quantum of energy E_γ is absorbed;

4) $A^{\pm}kp$—the nucleus is in the ground state; a quantum of wave vector k and polarization p is radiated; the quantum of energy E_γ remains absorbed.

The purely radiative effects described by the initial system of equations can be included consistently using the results of the general damping theory (cf. [3]), which, in particular leads to the appearance in the equations of Γ and Γ_A, the radiation widths of the excited and ground states of the nucleus. Making use of the familiar properties of stimulated processes of interaction with the radiation field, we eliminate the amplitudes $A^{\pm}0$ and $A^{\pm}kp$, and arrive at the following equations for the Fourier amplitudes for the excited states of the nucleus:

$$
\begin{aligned}
f_{\mathrm{I}}(E)\,C_{B^{(1)}_{\mathrm{I}}\gamma}(E) &= Hf_A(E)\left[D^1_{-1-p_\gamma}+\frac{A}{\sqrt{3}}D^1_{1-p_\gamma}\right]\\
&+\frac{eQ}{4\sqrt{3}}[KC_{B^{(1)}_{\mathrm{I}}\gamma}(E^+)+K^*C_{B^{(1)}_{\mathrm{I}}\gamma}(E^-)+L^*_-C_{B^{(1)}_{\mathrm{II}}\gamma}(E^+)\\
&+L^*_+C_{B^{(1)}_{\mathrm{II}}\gamma}(E^-)+M^*_-C_{B^{(2)}_{\mathrm{II}}\gamma}(E^+)+M^*_+C_{B^{(2)}_{\mathrm{II}}\gamma}(E^-)],\\
f_{\mathrm{I}}(E)\,C_{B^{(2)}_{\mathrm{I}}\gamma}(E) &= Hf_A(E)\left[\sqrt{\frac{2}{3}}AD^1_{0-p_\gamma}\right]\\
&+\frac{eQ}{4\sqrt{3}}[KC_{B^{(2)}_{\mathrm{I}}\gamma}(E^+)+K^*C_{B^{(2)}_{\mathrm{I}}\gamma}(E^-)+M_+C_{B^{(1)}_{\mathrm{II}}\gamma}(E^+)\\
&+M_-C_{B^{(1)}_{\mathrm{II}}\gamma}(E^-)-L_+C_{B^{(2)}_{\mathrm{II}}\gamma}(E^+)-L_-C_{B^{(2)}_{\mathrm{II}}\gamma}(E^-)],\\
f_{\mathrm{II}}(E)\,C_{B^{(1)}_{\mathrm{II}}\gamma}(E) &= Hf_A(E)\left[\sqrt{\frac{2}{3}}D^1_{0-p_\gamma}\right]\\
&+\frac{eQ}{4\sqrt{3}}[L_+C_{B^{(1)}_{\mathrm{I}}\gamma}(E^+)+L_-C_{B^{(1)}_{\mathrm{I}}\gamma}(E^-)+M^*_-C_{B^{(2)}_{\mathrm{I}}\gamma}(E^+)\\
&+M^*_+C_{B^{(2)}_{\mathrm{I}}\gamma}(E^-)-KC_{B^{(1)}_{\mathrm{II}}\gamma}(E^+)-K^*C_{B^{(1)}_{\mathrm{II}}\gamma}(E^-)],\\
f_{\mathrm{II}}(E)\,C_{B^{(2)}_{\mathrm{II}}\gamma}(E) &= Hf_A(E)\left[\sqrt{\frac{1}{3}}D^1_{1-p_\gamma}-AD^1_{-1-p_\gamma}\right]\\
&+\frac{eQ}{4\sqrt{3}}[M_+C_{B^{(1)}_{\mathrm{I}}\gamma}(E^+)+M_-C_{B^{(1)}_{\mathrm{I}}\gamma}(E^-)-L^*_-C_{B^{(2)}_{\mathrm{I}}\gamma}(E^+)\\
&-L^*_+C_{B^{(2)}_{\mathrm{I}}\gamma}(E^-)-KC_{B^{(2)}_{\mathrm{II}}\gamma}(E^+)-K^*C_{B^{(2)}_{\mathrm{II}}\gamma}(E^-)], \qquad (10)
\end{aligned}
$$

where C(E) are the Fourier amplitudes for the corresponding states; $H = \lambda H_{B\gamma|A0}$ where $H_{B\gamma|A0}$ is the reduced matrix element for the radiative transition; $D^1_{mp_\gamma}$ are the matrices for finite rotations for L = 1; p_γ is the index for circular polarization of the initial quantum; the argument of the D-function should be taken in the form $(\varphi_0, \theta_0, 0)$, where φ_0, θ_0 are the azimuthal and polar angles of the initial quantum; A and λ are defined in (7); in addition

$$
f_A(E) = 1/(E - E_{A0} + i\Gamma_A/2), \qquad f_{\mathrm{I}} = 1/(E - E_{B_{\mathrm{I}}\gamma} + i\Gamma/2),
$$

$$
f_{\mathrm{II}} = 1/(E - E_{B_{\mathrm{II}}\gamma} + i\Gamma/2);
$$

$$
K = \lambda^2\left\{\frac{\sqrt{3}}{2}\widetilde{V}_{zz}(1-A^2) + A\,(\widetilde{V_{xx}-V_{yy}})\exp\left(i\varphi_{(xx-yy)}\right)\right\},
$$

$$
L_{\pm} = \{\widetilde{V}_{xz}\exp(\pm i\varphi_{xz}) + i\widetilde{V}_{yz}\exp(\pm i\varphi_{yz})\},
$$

$$
\begin{aligned}
M_{\pm} = \lambda^2\{&(1-A^2)\tfrac{1}{2}(\widetilde{V_{xx}-V_{yy}})\exp[\pm i\varphi_{(xx-yy)}]\\
&+ i(1+A^2)\widetilde{V}_{xy}\exp(\pm i\varphi_{xy}) - \sqrt{3}A\widetilde{V}_{zz}\}.
\end{aligned}
$$

The symbol $E^{\pm}$ denotes $(E \pm \hbar\omega_s)$; the system (10) is written for the case where initially the nucleus is in the state A^+0.

For the kind of problem considered here the solution of (10) can be constructed by iteration, and we thus obtain an expression for the spectrum in the form of an expansion in the perturbation parameter $(eQ)^2$. If we limit ourselves to terms in this expansion linear in $(eQ)^2$, it is sufficient to consider only the first and second iterations of (10), taking as the zeroth approximation for C(E) the following expressions:

$$
\begin{aligned}
C^{(0)}_{B^{(1)}_{\mathrm{I}}\gamma}(E) &= H\left[D^1_{-1-p_\gamma}+\frac{A}{\sqrt{3}}D^1_{1-p_\gamma}\right]f_A(E)f_{\mathrm{I}}(E),\\
C^{(0)}_{B^{(2)}_{\mathrm{I}}\gamma}(E) &= H\left[\sqrt{\frac{2}{3}}AD^1_{0-p_\gamma}\right]f_A(E)f_{\mathrm{I}}(E),\\
C^{(0)}_{B^{(2)}_{\mathrm{II}}\gamma}(E) &= H\left[\sqrt{\frac{2}{3}}D^1_{0-p_\gamma}\right]f_A(E)f_{\mathrm{II}}(E),\\
C^{(0)}_{B^{(2)}_{\mathrm{II}}\gamma}(E) &= H\left[\sqrt{\frac{1}{3}}D^1_{1-p_\gamma}-AD^1_{-1-p_\gamma}\right]f_A(E)f_{\mathrm{II}}(E). \qquad (11)
\end{aligned}
$$

From the standard relation between spectral functions and the Fourier amplitudes for the states of the system, we get an expression for the absorption spectrum in this approximation:

$$
\begin{aligned}
W_A(x) = {}& [2N(d,p)]^{-1}\{D(x-d/2)\\
&\times[1+\alpha^2F(x-d/2;\ x-d/2;\ p)\\
&+\beta^2F(x+d/2;\ x-d/2;\ p)] + D(x+d/2)\,[1+\alpha^2F(x\\
&+d/2;\ x+d/2;\ p)+\beta^2F(x-d/2;\ x+d/2;\ p)]\}. \qquad (12)
\end{aligned}
$$

We have used the notation

$$
\frac{E_\gamma - E_B}{\Gamma/2} = x; \qquad \frac{\Delta^{(0)}}{\Gamma/2} = d; \qquad \frac{\hbar\omega_s}{\Gamma/2} = p;
$$

the functions D(x) and F(x,y,z) are defined as:

$$
D(x) = 1/(1+x^2),
$$

$$
\begin{aligned}
F(x,y,z) = {}& D(x-z) + D(x+z) + 2D(x)\\
&\times\{[x(y+z)-1]D(y+z)\\
&+[x(y-z)-1]D(y-z)\};
\end{aligned}
$$

α^2 and β^2, the diagonal and off-diagonal parameters of the dynamical quadrupole interaction, are given by the relations

$$
\begin{aligned}
\alpha^2 &= \delta^2\left[\tfrac{3}{4}\mu^2\widetilde{V}^2_{zz} + 4A^2\widetilde{V}^2_{(xx-yy)} + 2\sqrt{3}A\mu\widetilde{V}_{zz}\widetilde{V}_{(xx-yy)}\cos\varphi\right],\\
\beta^2 &= \delta^2[3A^2\widetilde{V}^2_{zz} + \mu^2\widetilde{V}^2_{(xx-yy)} + \lambda^{-4}(\widetilde{V}^2_{xy} + \widetilde{V}^2_{yz} + \widetilde{V}^2_{zx})\\
&\quad - 2\sqrt{3}A\mu\widetilde{V}_{zz}\widetilde{V}_{(xx-yy)}\cos\varphi], \qquad (13)
\end{aligned}
$$

where

$$
\mu = (1-A^2), \quad \delta^2 = \frac{1}{48}\left(\frac{eQ}{\Gamma/2}\right)^2\lambda^4, \quad \varphi = \varphi_{(xx-yy)},
$$

$$
\widetilde{V}_{(xx-yy)} = \tfrac{1}{2}(\widetilde{V_x - V_{yy}});
$$

N(d, p) is a normalization factor given by the expression

$$N(d,p) = \pi\{1 + 8\alpha^2 E(p) + 4\beta^2 [E(d+p) + E(d-p)]\},$$
$$E(x) = x^2/(x^2+4)^2.$$

From (13) it follows that

$$\alpha^2 + \beta^2 = \left(\frac{eQ}{\Gamma/2}\right)^2 \left(\frac{\tilde{g}}{12}\right)^2 = \left(\frac{\tilde{d}}{4}\right)^2. \qquad (14)$$

Here $\tilde{g}$ is the anisotropy coefficient of the "amplitude tensor" $\tilde{V}_{ik}$; $\tilde{d} = \tilde{\Delta}/(\Gamma/2)$, where $\tilde{\Delta}$ is the splitting in the static field described by the tensor $\tilde{V}_{ik}$. Relation (14) shows in particular that $\alpha^2 + \beta^2$ is independent of the structure of the static electric field; the latter is significant only for the separation of the dynamical interaction into a diagonal and an off-diagonal part.

For an axially symmetric static field, expressions (13) simplify, and the physical meaning of α^2 and β^2 becomes clear:

$$\alpha^2 = \left(\frac{eQ}{2\Gamma}\right)^2 \tilde{V}^2_{zz},$$

$$\beta^2 = \left(\frac{eQ}{2\Gamma}\right)^2 [\tilde{V}^2_{(xx-yy)} + \tilde{V}^2_{xy} + \tilde{V}^2_{yz} + \tilde{V}^2_{zx}]/3. \qquad (15)$$

By comparing $W_A(x)$ from (12) for $p \rightarrow 0$ with the exact spectrum, one can obtain a sufficient condition for the validity of (12), in the form

$$\tilde{\Delta} \leqslant \Gamma. \qquad (16)$$

4. EFFECT OF A HARMONIC PERTURBATION ON THE ABSORPTION SPECTRUM

As we see from (12), the dynamic field causes a significant change in the shape of the spectrum as a whole (and not just in its width), so that one should compare $W_A(x)$ with the natural spectrum on the basis of several different parameters. We shall consider two such parameters.

1. The integral width of the spectrum

$$\varkappa_{\text{int}} = \int_{-\infty}^{\infty} W_A(x)\,dx/\pi W_A(0). \qquad (17)$$

The physical meaning of this quantity is that κ_{int} is a direct measure of the degree of nonmonochromaticity of the radiation (in the sense of the lifetime of the radiator), as can easily be seen by a Fourier transformation.

2. The half-width of the distribution at half height, $\kappa_{1/2}$. This quantity is, strictly speaking, only a purely "geometrical" characteristic of the spectrum, but $\kappa_{1/2}$ is a very convenient parameter from the point of view of experiment.

For a dispersion distribution $\kappa_{\text{int}} = \kappa_{1/2}$, so that the difference $\kappa_{\text{int}} - \kappa_{1/2}$ can be taken as a measure of the deviation from a normal distribution.

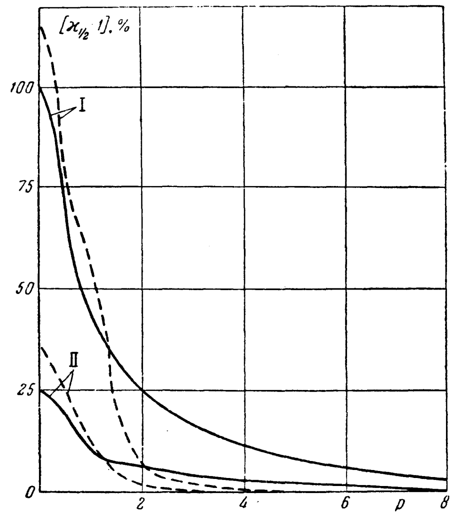

FIG. 1. Dependence of $\varkappa_{1/2} - 1$ and $\varkappa_{\text{int}} - 1$ on the "perturbing" frequency for the unsplit line (d = 0). The dashed curves are for the halfwidth, the solid curves for the full width; I and II correspond to $\tilde{d} = 2$ and $\tilde{d} = 1$.

Using the example of the unsplit line (d = 0), we see the following (cf. Fig. 1):

a) The finite lifetime of the excited state of the system leads to a strong dependence of the distortions produced in the absorption spectrum by the dynamic interaction of the nucleus on the "perturbing" frequency ω_s. The nature of this dependence is such that "high frequency" fields ($\omega_s\tau \gg 1$, where τ is the lifetime of the nucleus) produce a much smaller distortion of the spectrum than do the "low frequency" fields ($\omega_s\tau \ll 1$).

b) The sign of the difference $\kappa_{\text{int}} - \kappa_{1/2}$ depends on whether ω_s lies to one or the other side of a limiting value which is near to $\Gamma/\hbar$. Thus in principle one can imagine a case where the result of summation of the distortions due to the individual "perturbing" frequencies gives a line for the resonance transition which is broadened, but almost the same shape as a normal distribution.

The "nondiagonal" part of the dynamic interaction leads to further peculiarities, which include the following (cf. Fig. 2):

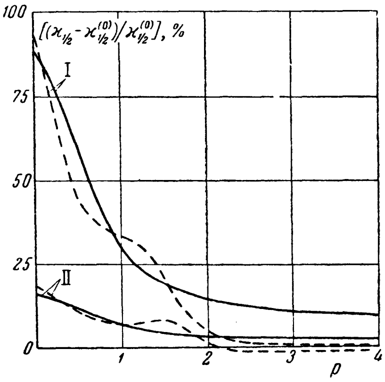

FIG. 2. Dependence of $(\varkappa_{1/2} - \varkappa^{(0)}_{1/2})/\varkappa^{(0)}_{1/2}$ and $(\varkappa_{\text{int}} - \varkappa^{(0)}_{\text{int}})/\varkappa^{(0)}_{\text{int}}$ on the "perturbing" frequency for the split line (d = 1). The dashed curves are for the half-width, the solid curves are for the integral width; I and II correspond to $\tilde{d} = 2$ and $\tilde{d} = 1$.

a) For "perturbing" frequencies $\omega_s > \omega_s^{\lim}(\tilde{d}) \sim \Gamma/\hbar$, the geometrical width of the spectrum $\kappa_{1/2}$ is less than the unperturbed value. However one should remember that such a narrowing of the spectrum cannot be interpreted as an increase in the selectivity of the absorber (or the monochromaticity of the radiator), since the integral width of the spectral distribution κ_{int} always exceeds the corresponding unperturbed value.

b) There is a small band of "perturbing" frequencies near $\Delta^{(0)}/\hbar$ which is singled out by its effect on the parameter $\kappa_{1/2}$.

c) As we see from (12), the action of the "nondiagonal" perturbation on the spectrum depends essentially on the degree of "overlap" of the unperturbed components, so that for $\Delta^{(0)} \gg \Gamma$ the "nondiagonal" perturbations have practically no effect.

5. EFFECT OF TEMPERATURE ON THE SHAPE OF THE RESONANCE SPECTRUM OF A GAMMA TRANSITION

Looking at experiments whose purpose is not the study of the dynamics of thermal motion of particles in a crystal, we consider the problem of the temperature dependence of the shape of the spectrum for a resonance transition under the following extremely simplified assumptions (cf. [4]):

1) the phonon spectrum of the crystal is given by a Debye function

$$f(\omega) = 3V\omega^2/2\pi^2 v^3, \tag{18}$$

where v is the velocity of thermal waves in the crystal and V is the crystal volume;

2) the relation between the relative displacement of neighboring particles, r, and the amplitude of the corresponding normal vibration, ζ, is taken in the form

$$r = 2\pi R\zeta/\lambda, \tag{19}$$

where R is the interatomic spacing and λ is the wavelength of the corresponding vibration;

3) we take for the average energy of the oscillator the classical expression

$$M\omega_s^2\zeta^2 = kT, \tag{20}$$

where M is the mass of the crystal;

4) the relation of the dynamic field to r is taken in the form

$$\tilde{V}_{ik}(\omega_s) = e\gamma_{ik}R^{-4}r(\omega_s), \tag{21}$$

where the γ_{ik} are geometrical coefficients determined by the structure of the unit cell of the crystal.

Using formulas (12), (18)-(21), we get the expression for the spectrum of the resonant γ transition:

$$\begin{aligned} W_A(x) = \frac{1}{2N(d)} \Big\{ & D(x - d/2)\Big[1 + C\gamma_{\mathrm{D}}^2\Big(\frac{T}{\Theta}\Big)H(x - d/2) \\ & + C\gamma_{\mathrm{ND}}^2\Big(\frac{T}{\Theta}\Big)H(x + d/2)\Big] + D(x + d/2) \\ & \Big[1 + C\gamma_{\mathrm{D}}^2\Big(\frac{T}{\Theta}\Big)H(x + d/2) + C\gamma_{\mathrm{ND}}^2\Big(\frac{T}{\Theta}\Big)H(x - d/2)\Big]\Big\}, \end{aligned} \tag{22}$$

where H(x) = 1 − 2D(x); T is the absolute temperature and Θ is the Debye temperature. The parameters γ^2 are given by the relations

$$\begin{aligned} \gamma_{\mathrm{D}}^2 &= \lambda^4\left[\frac{\mu^2}{4}\gamma_{zz}^2 + \frac{4A^2}{3}\gamma_{(xx-yy)}^2 + \frac{2A\mu}{\sqrt{3}}\gamma_{zz}\gamma_{(xx-yy)}\cos\varphi\right], \\ \gamma_{\mathrm{ND}}^2 &= \lambda^4\Big[A^2\gamma_{zz}^2 + \frac{\mu^2}{3}\gamma_{(xx-yy)}^2 + \frac{\lambda^{-4}}{3}(\gamma_{xy}^2 + \gamma_{zy}^2 + \gamma_{zx}^2) \\ &\quad - \frac{2A\mu}{\sqrt{3}}\gamma_{zz}\gamma_{(xx-yy)}\cos\varphi\Big]; \end{aligned} \tag{23}$$

N(d) is a normalization factor:

$$N(d) = \pi\left\{1 + C\gamma_{\mathrm{ND}}^2\left(\frac{T}{\Theta}\right)\left(\frac{d^2}{4 + d^2}\right)\right\},$$

$$C = \frac{9}{16\pi^2}\left(\frac{k^2e^4Q^2}{\hbar^3}\right)\frac{\Theta^2}{\rho v^5 R^6}; \tag{24}$$

ρ is the density of the crystal; the subscripts "N" and "ND" denote diagonal and nondiagonal parameters γ^2.

We also note that since the assumptions about the dynamics of the thermal motion made above are extremely simplified, the calculation of C using formula (24) is hardly justified, and it is

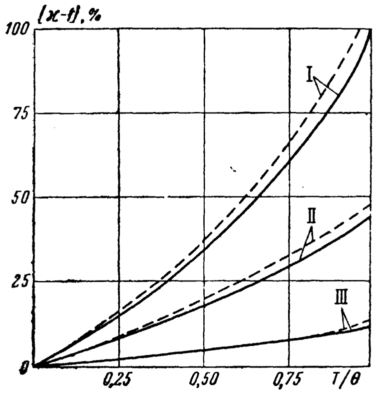

FIG. 3. Temperature dependence of $\kappa - 1$ for the unsplit line (d = 0). The dashed lines are the halfwidth, the solid lines, the integral width, I, II and III correspond to $C\gamma^2$ = 0.5, 0.3 and 0.1.

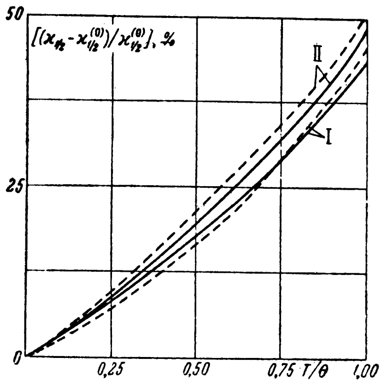

FIG. 4. Temperature dependence of $(\varkappa_{1/2} - \varkappa_{1/2}^{(0)})/\varkappa_{1/2}^{(0)}$ and $(\varkappa_{\text{int}} - \varkappa_{\text{int}}^{(0)})/\varkappa_{\text{int}}^{(0)}$ for the split line (d = 1). The dashed lines are the half-width, the solid lines, the integral width; I – $C\gamma_D^2 = 0.5$, $C\gamma_{ND}^2 = 0$; II – $C\gamma_D^2 = 0$, $C\gamma_{ND}^2 = 0.5$.

more reasonable to determine C from experimental data.

The dependence of $\kappa_{1/2}$ and κ_{int} on temperature is shown in Figs. 3 and 4. One can judge the effect of the perturbations on the measured quantity f′ from the dependence of the maximum absorption $\epsilon(0)$ for infinitely thin source and absorber. In this case, for the unsplit line one has the relation

$$\varepsilon(0)/\varepsilon^{(0)}(0) = [1 - {}^1\!/_2 C\gamma^2 T/\Theta], \qquad (25)$$

where $\epsilon^{(0)}(0)$ is the maximum absorption in the absence of perturbing fields.

We also note the characteristic narrowing of the spectrum (decrease of $\kappa_{1/2}^{\text{obs}}$, $\kappa_{\text{int}}^{\text{obs}}$) with temperature, which can occur for the split line (for $\Delta^{(0)} > 2\Gamma$) for certain values of the parameters $C\gamma_D^2$ and $C\gamma_{ND}^2$.

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