TEMPERATURE VARIATION OF THE WIDTH AND SHIFT OF THE RESONANCE LEVEL WHEN PARTICLES MOVE IN A CRYSTAL

A. M. AFANAS'EV and Yu. KAGAN

Submitted to JETP editor July 5, 1966

J. Exptl. Theoret. Phys. (U.S.S.R) 52, 191–207 (January, 1966)

We investigate the influence of the regularity of the crystal lattice on the change in the parameters of the nuclear resonance level in the presence of lattice vibrations, and also with due allowance for the spin and isotopic incoherent scattering. A consistent derivation is presented of a system of dynamic equations for the motion of particles in regular crystals, for both particles satisfying the Schrödinger equation and for γ quanta and x rays. In the case of resonant interaction, we analyze the question of the influence of the change in the resonance parameters of the level on the coefficients of this system. We also consider the temperature dependence of the coefficients of the dynamic systems under potential scattering (neutrons and x rays) with a consistent account taken of the processes of coherent scattering of particles with excitation (absorption) of phonons.

1. INTRODUCTION

THE authors have shown in an earlier paper [1] that when particles resonantly interacting with nuclei move in regular crystals, the true resonance width is not the total width Γ of the resonance level of the nucleus, but also the inelastic part Γ_2 of the width. This result was obtained under the assumption that the spin of the ground state of the nucleus is zero, and that the nuclei themselves do not vibrate. Physically, such a strong change in the width is connected with the fact that the presence of translational symmetry gives rise to the absence of elastic scattering even in the case of pure resonance interaction.

The situation is different in a vibrating lattice. Indeed, in this case it becomes possible for particles to be scattered with simultaneous emission or absorption of phonons. This should give rise to an increase in the width as compared with Γ_2. The resonance width should then depend on the temperature. Another cause of the increase in width for a regular crystal, compared with Γ_2, is the dependence of the resonant interaction on the spin of the nucleus in the ground state (spin incoherence), and also the isotopic incoherence in the case when the concentration of the resonant nuclei differs from unity.

The question of the change of the resonant nuclear width in regular crystals is important in the general case also for the dynamic theory. Such a theory, for particles moving in crystal and experiencing resonant nuclear interaction, was developed in connection with the effect of suppression of inelastic channels in papers by the authors.[2,3] The derivation of a general dynamic system of equations, which takes into account both the presence of inelastic nuclear channels and the vibrations of the nuclei, the spin, and the isotopic coherence, was based on the assumption that the amplitude of the scattering by the nucleus in the crystal has the same value as in the case of an isolated nucleus. In connection with the possibility of changing the elastic part of the resonance width in the crystal, such an assumption, as already noted, corresponds to the assumption that the inelastic part of the nuclear width is large compared with the elastic one. A consistent allowance for a change in the width makes it possible to develop the dynamic theory to include the general case.

The method developed in this paper allows us to consider not only the case of resonant interaction, but also pure potential interaction, which is characteristic, in particular, of x rays and neutrons. This raises the analogous problem of determining the coefficients of the system of dynamic equations, a problem connected with a consistent allowance for the processes of the coherent particle scattering and excitation (absorption) of phonons.

All the questions noted above are considered in the present paper.

2. DERIVATION OF GENERAL SYSTEM OF EQUATIONS

Let us consider a regular crystal made up of nuclei with low-lying resonant energy level E_0.

The state of the crystal will be described by an aggregate of occupation numbers n of the phonons and an aggregate of spin projections j of all the nuclei. For simplicity, where possible, we shall use a unified index ν, characterizing the state of the system as a whole. The state of the particle will be described by a wave vector $\mathbf{k}$ with spin projection σ (in the case of γ quanta, σ will define the polarization).

We shall analyze the problem of particle motion in such a crystal by a method similar to that used in the analysis of resonance fluorescence within the framework of the usual nonstationary perturbation theory [4]. We introduce the following state amplitudes: $C_{k\sigma\nu}$—all the nuclei of the crystal in the ground state, the particle has parameters $k\sigma$; $C_{s\nu}$—the s-th nucleus in the crystal is excited (in this case the aggregate index ν contains the projection of the spin of the s-th nucleus in the excited state); $C_{sp\nu}$—state arising after the decay along the inelastic channel, with s characterizing the new nucleus in the s-th lattice point (in the case of conversion—new state of the atom); p—momentum of the emitted secondary particle. (We do not distinguish explicitly the spin indices of the outgoing particles and of the nucleus in the new state.)

For these amplitudes, in the energy representation, we get the following system of equations:

$$\begin{aligned}
&(E-E_{\mathbf{k}}-\Delta E_{\nu})C_{\mathbf{k}\sigma\nu}=\sum_{s} H^{\mathbf{k}\sigma\nu}_{s\nu'}C_{s\nu'},\\
&(E-E_0-\Delta E_{\nu})C_{s\nu}=H^{s\nu}_{\mathbf{k}'\sigma'\nu'}C_{\mathbf{k}'\sigma'\nu'}+H^{s\nu}_{sp\nu'}C_{sp\nu'},\\
&(E-E_{\mathbf{p}}-\tilde{E}_0-\Delta E_{\nu})C_{sp\nu}=H^{sp\nu}_{s\nu'}C_{s\nu'}.
\end{aligned}\tag{2.1}$$

Here E_0 is the energy of the nucleus produced as a result of the reaction ΔE_ν includes both the phonon energy (the crystal vibrations are considered in the harmonic approximation), and the energy of the hyperfine interaction of the nuclei in the ground and excited states, reckoned from the energy E_{ν_0} of the ground state of the crystal as a whole. The particle energy E_k is assumed independent of the spin. Summation is implied over repeated indices in the right side of (2.1) (the summation with respect to the index s is marked explicitly).

Eliminating the amplitudes $C_{sp\nu}$ in the second equation, we get

$$(E-E_0-\Delta E_{\nu})C_{s\nu}=H^{s\nu}_{\mathbf{k}'\sigma'\nu'}C_{\mathbf{k}'\sigma'\nu'}+R^{s}_{\nu\nu'}C_{s\nu'},\tag{2.2}$$

$$R^{s}_{\nu\nu'}=\sum_{\mathbf{p}\nu''}\frac{H^{s\nu}_{sp\nu''}H^{sp\nu''}_{s\nu'}}{E-\tilde{E}_0-E_{\mathbf{p}}-\Delta E_{\nu''}+i\delta}.\tag{2.3}$$

As usual, in equations of type (2.1) E contains a small positive imaginary addition, which we have separated in explicit form in (2.3).

For the matrix elements of the operator H, which are contained in (2.3), the following formulas apply in the most general case:

$$H^{s\nu}_{sp\nu'}=(H^{sp\nu'}_{s\nu})^{*}=L(\mathbf{p}i_s)e^{i\mathbf{p}\mathbf{R}_s}(e^{i\mathbf{p}\mathbf{u}_s})_{nn'}.\tag{2.4}$$

We have separated here the index i_S, which characterizes the spin projections of the excited state of the s-th nucleus (this matrix element is of course diagonal in the spin variables of the remaining nuclei); $\mathbf{R}_S$ is the equilibrium position of the s-th nucleus and u_S is the displacement relative to the equilibrium position, connected with the crystal vibrations.

Usually the energy of the secondary particle E_p is much larger than either the characteristic energy of the photons ω_0, or the energies of the hyperfine interaction. Therefore in summing over p in the right side of (2.3) we can omit $\Delta E_\nu''$ from the denominator. Using this circumstance, and also formula (2.4), we get

$$R^{s}_{\nu\nu'}=\Big[\sum_{\mathbf{p}}\frac{L(\mathbf{p}i_s)L^{*}(\mathbf{p}i_s')}{E-\tilde{E}_0-E_{\mathbf{p}}+i\delta}\Big]\delta_{nn'}.\tag{2.5}$$

The expression in the square brackets of (2.5) is diagonal in the indices i_S and i_S'. Indeed, this expression can be regarded as matrix elements of a certain operator $\hat{R}$, acting on the spin variables of the nucleus in the excited state. But the only scalar operator from which $\hat{R}$ can be constructed is $\hat{I}^2$ ($\hat{I}$ is the operator of the total momentum of the nucleus). As a result we obtain

$$R^{s}_{\nu\nu'}=R_2\delta_{\nu\nu'},\quad R_2=\sum_{\mathbf{p}}\frac{|L(\mathbf{p}i)|^2}{E-\tilde{E}_0-E_{\mathbf{p}}+i\delta}=\Delta E_2-\frac{i\Gamma_2}{2},\tag{2.6}$$

$$\Delta E_2=\operatorname{Re}R_2,$$

$$\Gamma_2=-2\operatorname{Im}R_2=2\pi\sum_{\mathbf{p}}|L(\mathbf{p}i)|^2\delta(E-E_{\mathbf{p}}-\tilde{E}_0).\tag{2.7}$$

We shall be interested in the values of $E\sim E_{k_0}\sim E_0$. Taking this circumstance into account, Γ_2 is simply the probability, per unit time, of the decay of the excited state of the nucleus with emission of a secondary particle, i.e., the inelastic part of the nuclear level; ΔE_2 is the renormalization of the nuclear-level energy, connected with the presence of inelastic channels. Substituting now (2.3), with allowance for (2.5)—(2.7), in (2.2), we arrive at the equation

$$(E-E_0-\Delta E_2-\Delta E_{\nu}+i\Gamma_2/2)C_{s\nu}=H^{s\nu}_{\mathbf{k}\sigma\nu}C_{\mathbf{k}\sigma\nu'}.\tag{2.8}$$

We now express the amplitudes $C_{S\nu}$ from this equation and substitute them in the first equation

of (2.1). As a result we obtain an equation relating only the amplitudes $C_{\mathbf{k}\sigma\nu}$:

$$(E-E_{\mathbf{k}}-\Delta E_{\nu})C_{\mathbf{k}\sigma\nu}=\sum_{s\nu''}\frac{H_{s\nu''}^{\mathbf{k}\sigma\nu}H_{\mathbf{k}'\sigma'\nu'}^{s\nu''}}{E-E_0'-\Delta E_{\nu''}+i\Gamma_2/2}C_{\mathbf{k}'\sigma'\nu'}; \tag{2.9}$$

$$E_0'=E_0+\Delta E_2. \tag{2.10}$$

Let us determine the character of the motion of a particle with definite wave vector $\mathbf{k}_0$ and spin projection σ_0. To this end we shall consider formally the right side of (2.9) as a perturbation, and express, as usual, all other amplitudes in terms of $C_{\mathbf{k}_0\sigma_0\nu_0}$, and then substitute them in the equation of the system (2.9) with $\mathbf{k}\sigma\nu=\mathbf{k}_0\sigma_0\nu_0$. However, in the case when the particle is incident on the crystal at a Bragg angle, it is necessary to separate the system of equations for $C_{\mathbf{k}_0\sigma_0\nu_0}$ and $C_{\mathbf{k}_i\sigma'\nu_0}$, where $\mathbf{k}_i$ are the wave vectors of the particles scattered at Bragg angles, since these amplitudes are of the same order as $C_{\mathbf{k}_0\sigma_0\nu_0}$. We confine ourselves for simplicity to the case where not more than one diffracted wave is produced (with wave vector $\mathbf{k}_1=\mathbf{k}_0+\mathbf{K}_1$, where $\mathbf{K}_1$ is the reciprocal-lattice vector multiplied by 2π), and write the system of equations for $C_{\mathbf{k}_0\sigma\nu_0}$ and $C_{\mathbf{k}_1\sigma'\nu_0}$, which we shall henceforth denote simply by $C_{\mathbf{k}_0\sigma}$ and $C_{\mathbf{k}_1\sigma'}$. Eliminating successively all the remaining amplitudes from the system (2.9), we get

$$\begin{aligned}(E-E_{\mathbf{k}_0})C_{\mathbf{k}_0\sigma}&=V_{00}^{\sigma\sigma'}C_{\mathbf{k}_0\sigma'}+V_{01}^{\sigma\sigma'}C_{\mathbf{k}_1\sigma'},\\ (E-E_{\mathbf{k}_1})C_{\mathbf{k}_1\sigma}&=V_{10}^{\sigma\sigma'}C_{\mathbf{k}_0\sigma'}+V_{11}^{\sigma\sigma'}C_{\mathbf{k}_1\sigma'}.\end{aligned} \tag{2.11}$$

The coefficients $V_{\alpha\beta}^{\sigma\sigma'}$ ($\alpha,\beta=0,1$) are determined by the following series:

$$\begin{aligned}\hat{V}_{\alpha\beta}=&\sum_s\hat{v}_{p_\alpha p_\beta}^s+\sum_{ss'}{\sum_p}'\hat{v}_{p_\alpha p}^s\hat{G}_p(E)\,\hat{v}_{pp_\beta}^{s'}\\ &+\sum_{ss's''}{\sum_{pp'}}'\hat{v}_{p_\alpha p}^s\hat{G}_p(E)\,\hat{v}_{pp'}^{s'}\hat{G}_{p'}(E)\,\hat{v}_{p'p_\beta}^{s''}+\ldots\end{aligned} \tag{2.12}$$

We have written out this expansion in operator form with respect to the spin variables. With this

$$(v^s)_{pp}^{\sigma\sigma'}=\sum_{\nu''}\frac{H_{s\nu''}^{\mathbf{k}\sigma\nu}H_{\mathbf{k}'\sigma'\nu'}^{s\nu''}}{E-E_0'-\Delta E_{\nu''}+i\Gamma_2/2}, \tag{2.13}$$

$$G_p^{\sigma\sigma'}=\delta^{\sigma\sigma'}(E-E_{\mathbf{k}}-\Delta E_\nu+i\delta)^{-1}. \tag{2.14}$$

Here p is the aggregate of the quantum numbers $\mathbf{k}\nu$, $p_\alpha=\mathbf{k}_\alpha\nu_0$, and $p_\beta=\mathbf{k}_\beta\nu_0$. The matrix elements of the operator H which enter in (2.13) can be represented in the most general case in the form

$$H_{s\nu'}^{\mathbf{k}\sigma\nu}=(H_{\mathbf{k}\sigma\nu}^{s\nu'})^*=\mathcal{M}_{i_s}^{\mathbf{k}\sigma j_s}e^{i\mathbf{k}\mathbf{R}_s}(e^{i\mathbf{k}\mathbf{u}_s})_{nn'} \tag{2.15}$$

(as in the case (2.4), this matrix element is diagonal in the spin variables of the remaining nuclei).

We confine ourselves to cases in which the particle energy $E_{\mathbf{k}}$ is much larger than either the characteristic phonon energy ω_0 or the energy of the hyperfine interaction. In this case we can neglect in (2.14) ΔE_ν compared with $E_{\mathbf{k}}$. As a result we obtain

$$G_p^{\sigma\sigma'}=\delta^{\sigma\sigma'}(E-E_{\mathbf{k}}+i\delta)^{-1}. \tag{2.16}$$

The primed summation signs in (2.12) denote that $p=p_0, p_1$.

In the analysis of the motion of the particles described by the Schrödinger equation, we confine ourselves to a consideration of s-scattering only. Then the operators $V_{\alpha\beta}^{\sigma\sigma'}$ are diagonal in the spin indices:

$$V_{\alpha\beta}^{\sigma\sigma'}=V_{\alpha\beta}\delta^{\sigma\sigma'}, \tag{2.17}$$

and the system (2.11) breaks up into (2S + 1) pairs of identical equations (S is the particle spin). This pair of equations is written in the following form:

$$\begin{aligned}(k_0^2/\varkappa^2-1)C_{\mathbf{k}_0}&=g_{00}C_{\mathbf{k}_0}+g_{01}C_{\mathbf{k}_1},\\ (k_1^2/\varkappa^2-1)C_{\mathbf{k}_1}&=g_{10}C_{\mathbf{k}_0}+g_{11}C_{\mathbf{k}_1}.\end{aligned} \tag{2.18}$$

we have introduced here the notation $\varkappa^2=2mE$, where m is the particle mass

$$g_{\alpha\beta}=-V_{\alpha\beta}/E. \tag{2.19}$$

In the problem involving the motion of photons (γ quanta and x rays), $\hat{V}_{\alpha\beta}$ remains an operator in the variable σ, which in this case describes the polarization values. By virtue of the transversality of the electromagnetic waves, σ acquires two values for a given $\mathbf{k}$. It is convenient to introduce formally a third longitudinal polarization. Then the matrix elements $V_{\alpha\beta}^{il}$ and $(v^s)_{pp}^{il}$, (the indices i and l run already through three values) can be regarded as components of ordinary second-rank tensors, and the amplitudes C_{kl} can be regarded as components of a certain vector $\mathbf{C}_{\mathbf{k}}$.

In order that formula (2.12) remain in force, it is sufficient to use in place of the function $\hat{G}_p(E)$, defined by means of formula (2.16), the following formula:

$$G_p^{il}(E)=(\delta^{il}-k^ik^l/k^2)(E-E_{\mathbf{k}}+i\delta)^{-1}. \tag{2.20}$$

The vector amplitude $\mathbf{C}_{\mathbf{k}}$ has the meaning of the Fourier component with respect to time of the photon wave function in the momentum representation (cf.[5]; in the notation of[5] $\mathbf{C}_{\mathbf{k}}$ is the temporal Fourier component of $\mathbf{f}_{\mathbf{k}}$) and is connected with the corresponding Fourier components of the

electric field intensity $\mathscr{E}_{\mathbf{k}}^{l}$ by the relation

$$(E + ck)\,\mathscr{E}_{\mathbf{k}}{}^{l} = 2kN(k)C_{kl},$$

where N(k) is a certain normalization factor and c is the speed of light.

For $\mathscr{E}_{\mathbf{k}_\alpha}^{l}$ it is now easy to obtain the following system of equations:

$$\begin{aligned}(k_0^2/\varkappa^2 - 1)\,\mathscr{E}_{\mathbf{k}_0}{}^{i} &= g_{00}{}^{il}\mathscr{E}_{\mathbf{k}_0}{}^{l} + g_{01}{}^{il}\mathscr{E}_{\mathbf{k}_1}{}^{l},\\ (k_1^2/\varkappa^2 - 1)\,\mathscr{E}_{\mathbf{k}_1}{}^{i} &= g_{10}{}^{il}\mathscr{E}_{\mathbf{k}_0}{}^{l} + g_{11}{}^{il}\mathscr{E}_{\mathbf{k}_1}{}^{l},\end{aligned} \qquad (2.21)$$

$$k_{\alpha'}{}^{l}\mathscr{E}_{\mathbf{k}_{\alpha'}} = 0,$$

where $\kappa = E/c$, and

$$g_{\alpha\beta}{}^{il} = -2V_{\alpha\beta}{}^{il}/E. \qquad (2.22)$$

In writing out (2.22) we have used also the fact that E and ck_0 are close in magnitude, and we have put $E + ck_0 \approx 2E$.

The systems (2.18) and (2.21) correspond exactly to the systems of dynamic equations obtained earlier by the authors [2,3] in connection with the problems of neutron motion (cf. (2.14) in [3]) and γ quanta (cf. (3.1) in [2]). The expressions contained in these papers for the coefficients $g_{\alpha\beta}$ and $g_{\alpha\beta}^{il}$ actually corresponded to the assumption that the inelastic width of the resonance level Γ_2 is much larger than the elastic width Γ_1. The formulas obtained above for these coefficients solve the problem in the general case, for an arbitrary ratio of Γ_2 to Γ_1. In comparing the results of the present paper with the results of [2] it should be remembered that the term $(k_\alpha^i k_\beta^l/\kappa^2)\,\delta_{\alpha\beta}$, which enters in the expression for $g_{\alpha\beta}^{il}$ in [2] but is missing in the present paper, is insignificant by virtue of the transversality of the waves.

Far from the Bragg condition we have $C_{k_1} = 0$, and the motion of the particle in the crystal is described by the equation

$$(k_0^2/\varkappa^2 - 1 - g_{00})C_{k_0} = 0,$$

in other words, by a dispersion equation of the form

$$k_0^2/\varkappa^2 - 1 - g_{00} = 0. \qquad (2.23)$$

Equation (2.23), together with the formulas that determine g_{00}, is a generalization of the problem considered earlier by the authors, concerning the change in the resonance nuclear parameters [1], which occurs when the particles move in a regular crystal, to include the case of a vibrating lattice, a nonzero spin of the ground state of the nucleus, and an arbitrary concentration of the resonant nuclei. With this, the intensity of the beam moving over the crystal is defined as $\exp(-\mu x)$, where

$$\mu = 2\,\mathrm{Im}\,k_0 \approx \varkappa\,\mathrm{Im}\,g_{00}. \qquad (2.24)$$

Before we proceed to calculate the coefficients $g_{0\beta}$ and $g_{\alpha\beta}^{il}$, let us write out for $\hat{V}_{\alpha\beta}$ the following formula, which follows directly from (2.12):

$$\begin{aligned}\hat{V}_{\alpha\beta} = &\sum_s \hat{\tilde{v}}^s_{p_\alpha p_\beta} + \sum_{s\neq s'}{\sum_{p}}' \hat{\tilde{v}}^s_{p_\alpha p}\,\hat{G}_p(E)\,\hat{\tilde{v}}^{s'}_{pp_\beta} \\ &+ \sum_{\substack{s\neq s'\\ s'\neq s''}}{\sum_{pp'}}' \hat{\tilde{v}}^s_{p_\alpha p}\hat{G}_p(E)\,\hat{\tilde{v}}^{s'}_{pp'}\hat{G}_{p'}(E)\,\hat{\tilde{v}}^{s''}_{p'p_\beta} + \ldots,\end{aligned} \qquad (2.25)$$

where

$$\hat{\tilde{v}}^s_{pp'} = \hat{v}^s_{pp'} + \sum_{p''}\hat{v}^s_{pp''}\hat{G}_{p''}(E)\,\hat{\tilde{v}}^s_{p''p'}. \qquad (2.26)$$

A solution of this equation, as can be readily verified by direct substitution, is determined by the expression

$$\hat{\tilde{v}}^s_{pp'} = \sum_{\substack{\mathbf{k}\sigma\nu\\ s''\nu''}} \frac{H^{\mathbf{k}\sigma\nu}_{s\nu''}H^{s\nu''}_{\mathbf{k}'\sigma'\nu'}}{E - E_0 - \Delta E_{\nu''} + i\Gamma/2}. \qquad (2.27)$$

Here $\Gamma = \Gamma_1 + \Gamma_2$ is the total width of the resonance level of the individual nucleus. The elastic part of the width Γ_1 is determined in this case by the expression

$$\Gamma_1 = 2\pi \sum_{\mathbf{k}\sigma j} |\mathscr{M}^{i}_{\mathbf{k}\sigma j}|^2\,\delta(E_0 - E_{\mathbf{k}}); \qquad (2.28)$$

E_0 is the true value of the resonance level, corresponding to an isolated nucleus:

$$E_0 = E_0' + \Delta E_1, \qquad \Delta E_1 = \mathrm{P}\sum_{\mathbf{k}j}\frac{|\mathscr{M}^{i}_{\mathbf{k}\sigma j}|^2}{E_0 - E_{\mathbf{k}}} \qquad (2.29)$$

(the symbol P signifies that the sum is taken in the sense of the principal value). In the derivation of (2.27)—(2.29) it is necessary to use formula (2.15). The diagonality in the spin indices i_s follows from the same reasons as in the case of (2.5).

We shall stop to analyze only the limiting cases: that of a narrow line, when

$$\Gamma \ll \omega_0, \qquad (2.30)$$

and a wide line, when

$$\Gamma \gg \omega_0. \qquad (2.31)$$

Here ω_0 is the characteristic frequency of the phonon spectrum. In both cases, the expressions for $\hat{\tilde{v}}^s_{pp'}$ are greatly simplified. In addition, in this paper we confine ourselves to cases when there is no hyperfine splitting (it is clear that this limitation is important only for narrow lines). Then $\Delta E_\nu \equiv \Delta E_n$.

In the case of a narrow line, when the inequality (2.30) occurs, we should confine ourselves in

summing with respect to ν'' in (2.27), as usual, to terms for which $n'' = n_0$. Using this circumstance, as well as (2.15), we readily obtain

$$\hat{\tilde{v}}^s_{pp'} = \frac{\hat{a}(\mathbf{k}j_s, \mathbf{k}'j_s')}{E - E_0 + i\Gamma/2} e^{i(\mathbf{k}-\mathbf{k}')\mathbf{R}_s} (e^{i\mathbf{k}\mathbf{u}_s})_{nn_0} (e^{-i\mathbf{k}'\mathbf{u}_s})_{n_0n'}, \quad (2.32)$$

where

$$a^{\sigma\sigma'}(\mathbf{k}j_s, \mathbf{k}'j_s') = \sum_{i_s} \mathscr{M}^{\mathbf{k}\sigma j_s}_{i_s} \mathscr{M}^{i_s}_{\mathbf{k}'\sigma' j_s'}. \quad (2.33)$$

In the opposite limiting case, when the inequality (2.31) holds, we can neglect $\Delta E_{\nu''}$ compared with $\Gamma/2$ in the denominators of (2.27). As a result we obtain

$$\hat{\tilde{v}}^s_{pp'} = \frac{\hat{a}(\mathbf{k}j_s, \mathbf{k}'j_s')}{E - E_0 + i\Gamma/2} e^{i(\mathbf{k}-\mathbf{k}')\mathbf{R}_s} (e^{i(\mathbf{k}-\mathbf{k}')\mathbf{u}_s})_{nn'}. \quad (2.34)$$

For a particle with spin $S = 1/2$ and for s-scattering (this is precisely the case of interest to us) the general expression for the operator $\hat{a}$ is

$$\hat{a}(j_s, j_s') = a_0\delta_{j_s j_s'} + a_1 (\mathbf{I}_0\mathbf{S})_{j_s j_s'}. \quad (2.35)$$

With the aid of (2.33) and (2.28) we easily get

$$a_0 = \frac{\pi}{m\varkappa}\zeta\Gamma_1, \quad \zeta = \frac{2I+1}{2(2I_0+1)}. \quad (2.36)$$

Here I_0 and I are the spins of the nuclei in the ground and in the excited states. The constants a_0 and a_1 are interrelated in the same manner as the ordinary coherent and incoherent amplitudes in the case of pure resonance scattering:

$$a_1 = \pm 4a_0/(2I+1). \quad (2.37)$$

The plus sign corresponds to the case $I = I_0 + 1/2$, and the minus sign to $I = I_0 - 1/2$.

In the case of phonons, using in H, owing to the resonance character of the interaction, only the term which is linear in the vector potential, we can easily obtain for (2.33) the formula

$$a^{il}(\mathbf{k}j_s, \mathbf{k}'j_s') = \frac{2\pi}{E} \sum_{i_s} (\hat{j}_1^i(\mathbf{k}))_{j_s i_s} (\hat{j}_1^l(\mathbf{k}'))_{i_s j_s'}. \quad (2.38)$$

We have used here the notation of the earlier paper [2].

It will be convenient in what follows to represent $a^{il}(\mathbf{k}j_s, \mathbf{k}'j_s')$ in a form similar to (2.35):

$$a^{il}(\mathbf{k}j_s, \mathbf{k}'j_s') \equiv a_0^{il}(\mathbf{k}\mathbf{k}')\delta_{j_s j_s'} + a_1^{il}(\mathbf{k}j_s, \mathbf{k}'j_s'), \quad (2.39)$$

$$a_0^{il}(\mathbf{k}\mathbf{k}') = \frac{1}{2I_0+1} \sum_{j_s} a^{il}(\mathbf{k}j_s, \mathbf{k}'j_s). \quad (2.40)$$

From the definitions of (2.40) and (2.39) it follows that

$$\sum_{j_s} a_1^{il}(\mathbf{k}j_s, \mathbf{k}'j_s) = 0. \quad (2.41)$$

This tensor is proportional to the tensor I^{il} introduced in [2]. Using the results of that paper, we find directly that in the case of M1 and E2 transitions we have respectively

$$a_0^{il}(\mathbf{k}\mathbf{k}_1) = b'[(\mathbf{k}\mathbf{k}_1)\delta^{il} - k_1^i k^l],$$
$$a_0^{il}(\mathbf{k}\mathbf{k}_1) = b'[(\mathbf{k}\mathbf{k}_1)\delta^{il} + k_1^i k^l - {}^2/_3 k^i k_1^l], \quad (2.42)$$

where

$$b' = \frac{\pi c}{2\varkappa} \frac{2I+1}{2I_0+1} \Gamma_1. \quad (2.43)$$

Following the reasoning used in [2] to determine I^{il}, we can easily obtain an expression for $a_0^{il}(\mathbf{k}\cdot\mathbf{k}_1)$ for the case of the E1 transition, too;

$$a_0^{il}(\mathbf{k}\mathbf{k}_1) = b'\varkappa^2\delta^{il}. \quad (2.44)$$

We shall henceforth consider only E1, M1, and E2 transitions.

3. CHANGE IN WIDTH AND SHIFT OF RESONANCE NUCLEAR LEVEL IN CRYSTAL

1. In this section we consider the change in the resonance parameters in the case when the particles satisfy the Schrödinger equation. We begin the analysis with the case of a narrow resonance line (see (2.30)) and assume at first that the spin I_0 of the lower state of the nuclei is equal to zero and the concentration η of the resonant isotopes is equal to unity.

Let us find the explicit form of $g_{\alpha\beta}$ (2.19) by using the representation (2.25). To this end we substitute in (2.25) the expression (2.32) with allowance for (2.35) and (2.36). After simple transformations we obtain

$$g_{\alpha\beta} = -f_\alpha f_\beta \Big\{ N_0 \frac{\pi\Gamma_1/m\varkappa}{E - E_0 + i\Gamma/2} + \frac{(\pi\Gamma_1/m\varkappa)^2}{(E - E_0 + i\Gamma/2)^2} \sum_{s' \neq s} \mathscr{F}(s, s') + \Big(\frac{\pi\Gamma_1/m\varkappa}{E - E_0 + i\Gamma/2}\Big)^3 \sum_{s''\neq s',\, s'\neq s} \mathscr{F}(s, s')\mathscr{F}(s', s'') + \ldots, \quad (3.1)$$

$$\mathscr{F}(s, s') = \sum_{\mathbf{k}}{}' \frac{\exp\{i(\mathbf{k}_0 - \mathbf{k})(\mathbf{R}_s - \mathbf{R}_{s'})\}}{E - E_{\mathbf{k}} + i\delta} \times (\exp\{i\mathbf{k}(\mathbf{u}_{s'} - \mathbf{u}_s)\})_{n_0 n_0}, \quad (3.2)$$

where N_0 is the number of atoms per unit volume.

The quantity f_α in (3.1) has the following meaning

$$f_\alpha = (\exp\{i\mathbf{k}_\alpha \mathbf{u}_s\})_{n_0 n_0} = \exp\{-{}^1/_2 Z(\mathbf{k}_\alpha)\},$$
$$Z(\mathbf{k}_\alpha) = \frac{1}{2MN_0} \sum_{\mathbf{q}\mu} \frac{|\mathbf{k}_\alpha \mathbf{e}(\mathbf{q}, \mu)|^2}{\omega(\mathbf{q}, \mu)} [2\bar{n}(\mathbf{q}, \mu) + 1]. \quad (3.3)$$

Here $\mathbf{q}$ and μ are the wave vector and the number of the branch of the phonon, $\omega(\mathbf{q}, \mu)$ is the pho-

non frequency, $\mathbf{e}(\mathbf{q}, \mu)$ the polarization vector, $\bar{n}(\mathbf{q}, \mu)$ the average phonon occupation numbers, and M the mass of the atom in the lattice (for simplicity we consider a monatomic crystal lattice).

We note that taking the diagonal matrix element with respect to the stationary state of the microscopic system n_0 is equivalent to averaging over the thermodynamic equilibrium. We have used this circumstance in writing out (3.3), and we shall use it throughout in what follows.

In a regular crystal $\mathcal{F}(s, s')$ depends only on the difference $\mathbf{R}_s - \mathbf{R}_{s'}$. It follows directly therefore that the sum $\Sigma\mathcal{F}(s, s')$ over $s' \neq s$ does not depend on s. The series (3.1) is then a geometric progression and contracts to the expression

$$g_{\alpha\beta} = -f_\alpha f_\beta \frac{2\pi}{\Omega_0 \varkappa^3} \frac{\Gamma_1}{E - E_0 + i\Gamma/2 + R(E)}, \tag{3.4}$$

$$R(E) = -\frac{\pi\Gamma_1}{m\varkappa} \times \sum_{s\neq 0} \sum_{\mathbf{k}}{}' \frac{\exp\{i(\mathbf{k}_0 - \mathbf{k})\mathbf{R}_s\} (\exp\{i\mathbf{k}(\mathbf{u}_s - \mathbf{u}_0)\})_{n_0 n_0}}{E - E_{\mathbf{k}} + i\delta}, \tag{3.5}$$

where $\Omega_0 = 1/N_0$ is the volume of the unit cell. Thus, the width and the position of the resonance level change significantly by amounts

$$\Delta\Gamma = 2 \operatorname{Im} R(E_0), \quad \Delta E = -\operatorname{Re} R(E_0). \tag{3.6}$$

Let us determine in explicit form the matrix element contained in (3.5). Direct calculations yield

$$(\exp\{i\mathbf{k}(\mathbf{u}_s - \mathbf{u}_0)\})_{n_0 n_0} = \exp\{-Z(\mathbf{k}) + Y_s(\mathbf{k})\},$$

$$Y_s(\mathbf{k}) = \frac{1}{2MN_0} \sum_{\mathbf{q}, \mu} \frac{|\mathbf{k}\mathbf{e}(\mathbf{q}, \mu)|^2}{\omega(\mathbf{q}, \mu)} [2\bar{n}(\mathbf{q}, \mu) + 1] \cos \mathbf{q}\mathbf{R}_s. \tag{3.7}$$

At temperatures that are large compared with ω_0, this expression decreases exponentially with increasing T. By virtue of this, R vanishes in this limiting case and the resonance dependence of the quantities $g_{\alpha\beta}$ remains practically the same as for the individual nucleus.

In the opposite case, at low temperatures and in a sufficiently rigid lattice, (3.7) can be replaced by unity. Taking into account the fact that we have eliminated from the sum over $\mathbf{k}$ the values $\mathbf{k} = \mathbf{k}_0$ and $\mathbf{k} = \mathbf{k}_1$, we obtain directly for the change in the width

$$\Delta\Gamma = -\frac{2\pi^2\Gamma_1}{m\varkappa} \int \frac{d\mathbf{k}}{(2\pi)^3} \delta(E_0 - E_{\mathbf{k}}) = -\Gamma_1 \tag{3.8}$$

and for the shift

$$\Delta E = -\frac{2\pi\Gamma_1}{\varkappa\Omega_0} \left[\sum_{\mathbf{K}}{}' \frac{1}{(\mathbf{k}_0 + \mathbf{K})^2 - k_0^2} - \frac{\Omega_0}{(2\pi)^3} \int\!\!\!\!\!\!\diagup \frac{d\mathbf{q}}{q^2 - k_0^2} \right]. \tag{3.9}$$

The prime in the summation over $\mathbf{K}$ denotes exclusion of the term with $\mathbf{K} = 0$, as well as $\mathbf{K} = \mathbf{K}_1$ if the Bragg condition is satisfied.

The expressions obtained for the width and for the shift coincide exactly with the results obtained in [1] by another method.

The greatest interest attaches in our case to the intermediate region, where the change in the width and the shift of the nuclear resonance level begin to depend on the temperature. To analyze this case we expand the exponential (3.7), which enters in (3.5), in powers of $Y_s(\mathbf{k})$. In this expansion, a significant term besides the first, is the second one, inasmuch as $Y_s(\mathbf{k})$ itself decreases slowly with increasing $\mathbf{R}_s$, which leads to a logarithmic divergence in the summation over s. The remaining terms decrease with increasing $\mathbf{R}_s$ sufficiently rapidly, and will be disregarded in the analysis that follows. Then

$$R(E) \approx -\frac{\pi\Gamma_1}{m\varkappa} \sum_{s\neq 0} \sum_{\mathbf{k}}{}' \frac{\exp\{i(\mathbf{k}_0 - \mathbf{k})\mathbf{R}_s\}}{E - E_{\mathbf{k}} + i\delta} e^{-Z(\mathbf{k})} (1 + Y_s(\mathbf{k})). \tag{3.10}$$

As shown by direct calculations, the contribution made to Re R(E) by the second term in the brackets in (3.10) is small. We then get for the line shift

$$\Delta E \approx -\frac{2\pi\Gamma_1}{\varkappa\Omega_0} \left[\sum_{\mathbf{K}}{}' \frac{\exp\{-Z(\mathbf{k}_0 + \mathbf{K})\}}{(\mathbf{k}_0 + \mathbf{K})^2 - k_0^2} - \frac{\Omega_0}{(2\pi)^3} \int\!\!\!\!\!\!\diagup \frac{e^{-Z(\mathbf{q})}}{q^2 - k_0^2} d\mathbf{q} \right]. \tag{3.11}$$

For the change in width we get after simple calculations, assuming cubic symmetry of the crystal

$$\Delta\Gamma = -\Gamma_1 e^{-Z(\mathbf{k}_0)} + \Delta\Gamma'. \tag{3.12}$$

The quantity $\Delta\Gamma'$, which is the result of the second term in the brackets in (3.10), is given by

$$\Delta\Gamma' = \frac{2\pi^2\Gamma_1}{m\varkappa} \left\{ \sum_{\mathbf{K}} \rho(\mathbf{k}_0 + \mathbf{K}) - \frac{\Omega_0}{(2\pi)^3} \int \frac{d\mathbf{k}}{(2\pi)^3} \rho(\mathbf{k}_0 + \mathbf{k}) \right\}, \tag{3.13}$$

where

$$\rho(\mathbf{k}) = \frac{1}{2M} \sum_{\mu} \int \frac{d\mathbf{q}}{(2\pi)^3} e^{-Z(\mathbf{k}+\mathbf{q})} \frac{|(\mathbf{k} + \mathbf{q})\mathbf{e}(\mathbf{q}, \mu)|^2}{\omega(\mathbf{q}, \mu)} \times [2\bar{n}(\mathbf{q}, \mu) + 1] \delta(E - E_{\mathbf{k}+\mathbf{q}}). \tag{3.14}$$

A special role in the sum over $\mathbf{K}$ is played by

the term with $\mathbf{K} = 0$, and if the Bragg condition is satisfied also by the term with $\mathbf{K} = \mathbf{K}_1$. Indeed, as can be readily verified directly, in these cases the integral (3.14) diverges logarithmically at small values of q:

$$\rho(\mathbf{k}_i) \approx \frac{m\varkappa}{(2\pi)^2}\frac{3T}{M\overline{c_{зв}^2}}e^{-Z(\mathbf{k}_i)}\ln\left(\frac{q_0}{q_{min}}\right), \quad (3.15)$$

$$\frac{1}{\overline{c_{зв}^2}} = 3\lim_{q\to 0}\sum_{\mu}\int\frac{d\Omega_{\mathbf{q}}}{2\pi}\frac{|\mathbf{n}_i\mathbf{e}(\mathbf{q},\mu)|^2}{\overline{c_\mu^2(\mathbf{q})}}\delta\left(\frac{\mathbf{q}\mathbf{n}_i}{q}\right), \quad \mathbf{n}_i = \frac{\mathbf{k}_i}{k_i}. \quad (3.15')$$

Here q_0 is a quantity on the order of the limiting wave vector of the phonons; as regards q_{min}, it can be shown that its limiting value is determined by the larger of the two quantities $1/L$ or Γ (L is the linear dimension of the crystal); $c_\mu(q) = \omega(q, \mu)/q$.

The result (3.15) is connected with the logarithmic divergence of the cross section for single-phonon scattering, which is known for the case of Bragg scattering of x rays. It is exceedingly interesting that in the case of a narrow line this section diverges also for small-angle scattering (the term with $\mathbf{K} = 0$). We note that the remaining part in (3.13) is as a rule much smaller than (3.15).

For limited values of the temperature, $T \ll \Theta_D$ (Θ_D is the Debye temperature), and for low-lying resonance levels, when $Z(k_0) \ll 1$, we get $\Delta\Gamma \approx -\Gamma_1$, and the vanishing of the elastic width occurs in full measure. With increasing temperature, a noticeable decrease takes place in $|\Delta\Gamma|$. For large values of k_0, the decisive role will then be played by the drop in the probability $\exp[-Z(\mathbf{k}_0)]$ of the Mossbauer effect, and for small k_0 the role of the term (3.15) in $\Delta\Gamma'$ becomes very important.

We note that the change in width in the presence of Bragg scattering is different than in its absence.

As to the temperature dependence of ΔE, we note only a general tendency for the shift to decrease with temperature. The presence of factors that depend on the vibrations of the nuclei leads here to a rapid convergence of the terms of the series in K and of the integral in (3.11).

2. Unlike the case of a narrow resonance line, the case of a broad line is much more complicated. The situation becomes even more complicated if we consider simultaneously nuclei with $I_0 \neq 0$ and $\eta \neq 1$. By virtue of this, in the analysis of all these factors we confine ourselves to an examination of the most interesting case, when the change in the width and the shift of the level are small compared with Γ. Then the series (2.25) converges rapidly and we can confine ourselves to allowance for only the first two terms. Substituting in (2.25) the expressions (2.32) or (2.34) we get, with account of (2.35)

$$V_{\alpha\beta} = f_{\alpha\beta}\tilde{\sum_s}\frac{(a_0 + a_1\mathbf{I}_s\mathbf{S})_{j_0 j_0}}{E - E_0 + i\Gamma/2} + \tilde{\sum_{s'\neq s}}\frac{(a_0 + a_1\mathbf{I}_s\mathbf{S})_{j_0 j}(a_0 + a_1\mathbf{I}_{s'}\mathbf{S})_{jj_0}}{(E - E_0 + i\Gamma/2)^2}\Phi_{\alpha\beta}(s, s'), \quad (3.16)$$

where in the case of a narrow line (see (3.2), (2.32))

$$f_{\alpha\beta} = f_\alpha f_\beta, \quad \Phi_{\alpha\beta}(s, s') = f_\alpha f_\beta \mathcal{F}(s, s'), \quad (3.17)$$

and in the case of a broad line

$$f_{\alpha\beta} = (\exp\{i(\mathbf{k}_\alpha - \mathbf{k}_\beta)\mathbf{u}_s\})_{n_0 n_0} = \exp\{-1/2 Z(\mathbf{k}_\alpha - \mathbf{k}_\beta)\},$$

$$\Phi_{\alpha\beta}(s, s') = \sum_{\mathbf{k}}{}' \frac{(\exp\{i(\mathbf{k}_\alpha - \mathbf{k})\mathbf{u}_s + i(\mathbf{k} - \mathbf{k}_\beta)\mathbf{u}_{s'}\})_{n_0 n_0}}{E - E_{\mathbf{k}} + i\delta} \times \exp\{i(\mathbf{k}_0 - \mathbf{k})(\mathbf{R}_s - \mathbf{R}_{s'})\}. \quad (3.18)$$

The tilde over the summation sign in (3.16) means that the summation over s and s′ is taken only over the lattice points where the resonance nuclei are situated. It is natural to assume here that these nuclei are randomly distributed over the crystal-lattice points.

In the case of unpolarized nuclei, the terms that depend on the nuclear spins vanish upon summation over the lattice points in (3.16), since all the projections of the nuclear spins are equally probable. Going over to summation over all the lattice sites, we get

$$V_{\alpha\beta} = \eta f_{\alpha\beta}\sum_s\frac{a_0}{E - E_0 + i\Gamma/2} + \eta^2\sum_{\substack{s,\,s'\\ s'\neq s}}\frac{a_0^2}{(E - E_0 + i\Gamma/2)^2}\Phi_{\alpha\beta}(s, s'). \quad (3.19)$$

Using the fact that $\Phi_{\alpha\beta}(s, s')$ depends only on the difference $\mathbf{R}_s - \mathbf{R}_{s'}$, and also formula (2.36), and going over to the expression for $g_{\alpha\beta}$ (2.19), we get

$$g_{\alpha\beta} = -\frac{2\pi\eta\zeta f_{\alpha\beta}}{\Omega_0\varkappa^3}\frac{\Gamma_1}{E - E_0 + i\Gamma/2}\left(1 - \frac{R_{\alpha\beta}}{E - E_0 + i\Gamma/2}\right).$$

Alternately, with the same accuracy with which (3.16) is determined, we have

$$g_{\alpha\beta} = -\frac{2\pi\eta\zeta f_{\alpha\beta}}{\Omega_0\varkappa^3}\frac{\Gamma_1}{E - E_0 + i\Gamma/2 + R_{\alpha\beta}}. \quad (3.20)$$

Here

$$R_{\alpha\beta} = -\frac{\pi\Gamma_1\eta\zeta}{m\varkappa} f_{\alpha\beta}^{-1} \sum_{s\neq 0} \Phi_{\alpha\beta}(s,0). \qquad (3.21)$$

In the case of a narrow line $R_{\alpha\beta}$ does not depend on the indices α and β:

$$R_{\alpha\beta} = \eta\zeta R, \qquad (3.22)$$

where R coincides with the value in (3.5).

Thus, the change of the width and the shift of the resonance line (3.6) turn out to be directly proportional to the concentration and to the spin factor (2.36), which determines the coherent part of the scattering amplitude. The presence of these factors in the general case leads to a decrease in $|\Delta\Gamma|$ and $|\Delta E|$, which is connected with the appearance of an isotopic and spin incoherent-scattering channel. For a sufficiently low concentration, $R_{\alpha\beta}$ turns out to be small, and the resonance parameters, naturally, tend to their values for the isolated nucleus.

In the case of a broad line, calculating (3.18) in explicit form, we get

$$R_{\alpha\beta} = -\eta\zeta \frac{\pi\Gamma_1 f_{\alpha\beta}^{-1}}{m\varkappa} \times \sum_{s\neq 0} \sum_{\mathbf{k}}{}' \frac{\exp\{i(\mathbf{k}_0-\mathbf{k})\mathbf{R}_s - Z_{\alpha\beta}(\mathbf{k}) + X_s^{\alpha\beta}(\mathbf{k})\}}{E - E_{\mathbf{k}} + i\delta}; \qquad (3.23)$$

$$Z_{\alpha\beta}(\mathbf{k}) = {}^1/_2(Z(\mathbf{k}_\alpha-\mathbf{k}) + Z(\mathbf{k}_\beta-\mathbf{k})),$$

$$X_s^{\alpha\beta}(\mathbf{k}) = \frac{1}{2N_0M} \sum_{\mathbf{q},\mu} \frac{[(\mathbf{k}_\alpha-\mathbf{k})\mathbf{e}(\mathbf{q},\mu)][(\mathbf{k}_\beta-\mathbf{k})\mathbf{e}(\mathbf{q},\mu)]}{\omega(\mathbf{q},\mu)} \times (2\bar{n}(\mathbf{q},\mu)+1)\cos\mathbf{q}\mathbf{R}_s. \qquad (3.24)$$

As in the case of the narrow line, we expand the exponential in (3.23) in powers of $X_s^{\alpha\beta}$, confining ourselves to the first two terms of the series. Here again the real part of $R_{\alpha\beta}$ is determined essentially by the first term of the expansion, and the ratio $\Delta E_{\alpha\beta} f_{\alpha\beta}/\eta\zeta$ (the shift and the change in the width enter differently in the different coefficients $g_{\alpha\beta}$) will be described by formula (3.11), in which the exponential $\exp[-Z(\mathbf{k})]$, which enters in the sum over K and in the integral, must be replaced by $\exp[-Z_{\alpha\beta}(\mathbf{k})]$. For $\Delta\Gamma_{\alpha\beta}$ we have in the case of cubic crystal symmetry

$$\Delta\Gamma_{\alpha\beta} = -\eta\zeta\Gamma_1 f_{\alpha\beta}^{-1} \frac{k_0 \exp\{-2Z(\mathbf{k}_0)\}}{2|\mathbf{k}_\alpha+\mathbf{k}_\beta|Z(\mathbf{k}_0)} \left[\exp\left\{\frac{|\mathbf{k}_\alpha+\mathbf{k}_\beta|}{k_0} Z(\mathbf{k}_0)\right\} - \exp\left\{-\frac{|\mathbf{k}_\alpha+\mathbf{k}_\beta|}{k_0} Z(\mathbf{k}_0)\right\}\right] + f_{\alpha\beta}^{-1}\eta\zeta\Delta\Gamma'_{\alpha\beta}, \qquad (3.25)$$

where $\Delta\Gamma'_{\alpha\beta}$ is determined by formula (3.12) with

$$\rho_{\alpha\beta}(\mathbf{k}) = \frac{1}{2M}\sum_{\mu} \int \frac{d\mathbf{q}}{(2\pi)^3} \exp\{-Z_{\alpha\beta}(\mathbf{k}+\mathbf{q})\} \times \frac{[(\mathbf{k}_\alpha-\mathbf{k}-\mathbf{q})\mathbf{e}(\mathbf{q},\mu)][(\mathbf{k}_\beta-\mathbf{k}-\mathbf{q})\mathbf{e}(\mathbf{q},\mu)]}{\omega(\mathbf{q},\mu)} \times [2\bar{n}(\mathbf{q},\mu)+1]\delta(E-E_{\mathbf{k}+\mathbf{q}}). \qquad (3.26)$$

It is interesting that, unlike the case of a narrow line, the diverging term in (3.13) in the sum over K appears only in the presence of Bragg scattering. Therefore, in the penetration problem, when there is no Bragg scattering, $\Delta\Gamma'$ is small and the expression for the change in the width is defined by

$$\Delta\Gamma \approx -\eta\zeta\Gamma_1 \frac{1-\exp\{-4Z(\mathbf{k}_0)\}}{4Z(\mathbf{k}_0)}. \qquad (3.27)$$

We note that in the case of a broad line the temperature dependence of $\Delta\Gamma$, has an entirely different character than in the case (3.12)—(3.15) of a narrow one. In particular, at high temperatures, when $Z(\mathbf{k}_0) \sim T$, $\Delta\Gamma$ tends to zero exponentially in the case of a narrow line, and only like $1/T$ in the case of a broad one.

On the other hand, in the case of Bragg scattering there appear in $\Delta\Gamma'_{\alpha\beta}$ with $\alpha = \beta$ diverging terms corresponding to $\rho_{00}(K_1)$ and $\rho_{11}(0)$ and playing a decisive role in $\Delta\Gamma'_{\alpha\alpha}$. It is interesting that when $\alpha \neq \beta$ there is no divergence and $\Delta\Gamma_{\alpha\beta}$ in this case again is determined essentially only by the first term of (3.25). Then

$$\rho_{00}(\mathbf{K}_1) = \rho_{11}(0) \approx \frac{m\varkappa}{(2\pi)^2} \frac{3T}{M\overline{c_{s\,\mathrm{sound}}^2}} \frac{K_1^2}{\varkappa^2} e^{-Z(\mathbf{K}_1)} \ln\frac{q_0}{q_{min}}, \qquad (3.28)$$

where $\overline{c_{s\,\mathrm{sound}}^2}$ is determined by (3.15′) with $n_i = K_1/K_1$. Unlike the case of a narrow line, here q_{min} is determined by the larger of the quantities $1/L$ or $g_{00}\varkappa$.

4. CHANGE IN WIDTH AND SHIFT OF RESONANCE NUCLEAR LEVEL IN CRYSTAL. CASE OF γ QUANTA

1. In this section we confine ourselves to only the most important case, that of a narrow resonance line (see (2.30)).

We separate again the case when the spin of the ground state of the nucleus I_0 is equal to zero, and $\eta = 1$. We determine the values of $g_{\alpha\beta}^{il}$ (2.22), using the expansion (2.25). We substitute formulas (2.32) and (2.39) in (2.25) and take account of the fact that when $I_0 = 0$ we have $a_1^{il} = 0$. Then in the case of an E1 transition, using expression (2.44),

and making the same transformations as in the derivation of (3.1), we get

$$g_{\alpha\beta}^{il} = -f_\alpha f_\beta \frac{2b'\varkappa}{c\Omega_0}\left\{\frac{\delta^{il}}{E-E_0+i\Gamma/2} - \frac{R^{il}}{(E-E_0+i\Gamma/2)^2} + \frac{R^{ip}R^{pl}}{(E-E_0+i\Gamma/2)^3} - \ldots\right\}, \quad (4.1)$$

$$R^{il} = -b'\varkappa^2 \sum_{s\neq 0}\sum_{\mathbf{k}}{}' \frac{\exp\{i(\mathbf{k}_0-\mathbf{k})\mathbf{R}_s\}\exp\{-Z(\mathbf{k})+Y_s(\mathbf{k})\}}{E-E_{\mathbf{k}}+i\delta} \times\left(\delta^{il}-\frac{k^ik^l}{k^2}\right). \quad (4.2)$$

In the coordinate system in which the tensor R^{il} reduces to its diagonal form, all the tensors $g_{\alpha\beta}^{il}$ are diagonal, and the series (4.1) turns into geometric series. As a result we obtain

$$g_{\alpha\beta}^{11} = -f_\alpha f_\beta \frac{2b'\varkappa}{c\Omega_0}\frac{1}{E-E_0+i\Gamma/2+R^{11}} \quad (4.3)$$

and analogous expressions for the other two principal values of the tensor.

We note that in the general case $R^{11} \neq R^{22} \neq R^{33}$, and thus, coefficients with different values of the resonance parameters enter in the dynamic problem. (It must be emphasized that the reduction of the tensors $g_{\alpha\beta}^{il}$ to diagonal form does not mean that the corresponding equations (2.21) will separate in this coordinate frame into three independent equations, or into the transversality condition $k_\alpha^l \mathscr{E}_{k_\alpha}^l = 0$.) In the particular problem involving the penetration of a γ quantum through a crystal in the absence of Bragg scattering, it is obviously sufficient to know the properties of the tensor $g_{00}^{\lambda\rho}$, where λ and ρ are the coordinates in the plane perpendicular to the direction of the vector $\mathbf{k}_0$. From the first equation of (2.21), we obtain in this case, putting $\mathscr{E}_{k_1}^l = 0$, the following dispersion equation:

$$|(k_0^2/\varkappa^2-1)\delta^{\lambda\rho} - g_{00}^{\lambda\rho}| = 0. \quad (4.4)$$

This equation gives a value of k_0 in the crystal corresponding to two values of polarization.

If we assume for simplicity that $\mathbf{k}_0$ is directed along the symmetry axis, then

$$g_{00}^{\lambda\rho} = g_{00}\delta^{\lambda\rho}, \quad (4.5)$$

and we obtain two identical roots for k_0

$$k_0 \approx \varkappa(1+{}^1/_2 g_{00}). \quad (4.6)$$

With this, g_{00} takes the form (4.3) with

$$R = -\pi c\varkappa\Gamma_1 \times \sum_{s\neq 0}\sum_{\mathbf{k}}{}' \frac{\exp\{i(\mathbf{k}_0-\mathbf{k})\mathbf{R}_s\}\exp\{-Z(\mathbf{k})+Y_s(\mathbf{k})\}}{E-E_{\mathbf{k}}+i\delta}\varphi(\mathbf{k}), \quad (4.7)$$

$$\varphi(\mathbf{k}) = {}^3/_2[1-(k^\lambda)^2/k^2]. \quad (4.8)$$

In writing out (4.7) we used the explicit form of (2.43), and also the fact that in the case of E1 transitions and when $I_0 = 0$ we always have $I = 1$.

If we make in (4.7) the same transformations as in the transition from (3.5) to (3.10)—(3.14), then we readily get

$$\Delta E = -\frac{\pi\Gamma_1}{\Omega_0\varkappa^2}\left\{\sum_{\mathbf{K}}\frac{\varphi(\mathbf{k}_0+\mathbf{K})e^{-Z(\mathbf{k}_0+\mathbf{K})}}{|\mathbf{k}_0+\mathbf{K}|-k_0} - \frac{\Omega_0}{(2\pi)^3}\int\!\!\!\!\!\!\diagup\frac{\varphi(\mathbf{q})e^{-Z(\mathbf{q})}}{q-k_0}d\mathbf{q}\right\}, \quad (4.9)$$

and for $\Delta\Gamma$ we again obtain (3.12) with

$$\Delta\Gamma' = \pi c\varkappa\Gamma_1\left\{\sum_{\mathbf{K}}\varphi(\mathbf{k}_0+\mathbf{K})\rho(\mathbf{k}_0+\mathbf{K}) - \frac{\Omega_0}{(2\pi)^3}\int d\mathbf{k}\,\varphi(\mathbf{k}_0+\mathbf{k})\rho(\mathbf{k}_0+\mathbf{k})\right\}, \quad (4.10)$$

where $\rho(\mathbf{k})$ is determined by formula (3.14). Thus, the shift and change in width have qualitatively the same character of the temperature dependence as in the case of particles experiencing s scattering (see the preceding section).

A similar analysis can be made for M1 transitions. The problem reduces completely to that of the preceding case of E1 transition, if we go over from $\mathscr{E}_{\mathbf{k}}^l$ to the Fourier components of the magnetic-field vector.

2. We now proceed to the general case, when $I_0 \neq 0$ and $\eta \neq 1$. As in the preceding section, we confine ourselves to the case when $|\Delta\Gamma|$ and $|\Delta E|$ are small compared with Γ. Then, if we retain only the first two terms in the expansion (2.25), the reasoning remains exactly the same as in Heading 2 of the preceding section. In summing over the spin variables it is necessary to use here Eq. (2.41), which leads to the vanishing of terms containing a_1^{il}. All the results of the preceding part of this section remain in force, with the substitution

$$R^{il} \to \eta\zeta R^{il}, \qquad \zeta = (2I+1)/(2l+1)(2I_0+1) \quad (4.11)$$

(l is the multipolarity of the transition).

The character of the influence of the spin and isotopic incoherence on the change in the width and on the shift of the nuclear level turn out to be the same as in the case of particles experiencing s scattering.

5. DYNAMIC SYSTEM OF EQUATIONS IN A CRYSTAL

The results obtained in the preceding sections show that the vibrations of the nuclei as well as

spin and isotopic incoherence can lead to a change in the resonance parameters of the nuclei, and at the same time lead to a rather nontrivial change in the coefficients $g_{\alpha\beta}$ in the system of the dynamic equations (2.18) and (2.21), compared with those values obtained in earlier papers [2,3], with account taken of the vibrations of the crystal lattice and also of the spin and isotopic scattering. In most cases $\Gamma_2 \gg \Gamma_1$, and thus the change in the resonance parameters is really small. However, we can indicate a whole number of cases when Γ_1 is comparable with Γ_2 and, consequently it becomes necessary to use the general expressions for $g_{\alpha\beta}$ obtained in the present paper.

The method developed here can, of course, be used for an analysis of the dynamic problem also in the case of potential scattering of particles, such as ordinary scattering of x rays, neutrons, and electrons. Taking into account all the inelastic processes connected with the interaction with an individual atom we arrive at the system of equations (2.11) and (2.12) with

$$(v^s)_{pp'}^{\sigma\sigma'} = v_{\mathbf{kk}'}^{\sigma\sigma'} e^{i(\mathbf{k}-\mathbf{k}')\mathbf{R}_s} (e^{i(\mathbf{k}-\mathbf{k})\mathbf{u}_s})_{nn'}, \tag{5.1}$$

$$v_{\mathbf{kk}'}^{\sigma\sigma'} = v_0^{\sigma\sigma'}(\mathbf{k},\mathbf{k}') - iv_2^{\sigma\sigma'}(\mathbf{k},\mathbf{k}'). \tag{5.2}$$

Here $v_0^{\sigma\sigma'}(\mathbf{k},\mathbf{k}')$ corresponds to the amplitude of the Born scattering and $v_2^{\sigma\sigma'}(\mathbf{k},\mathbf{k}')$ characterizes the imaginary part of the scattering amplitude, due to the inelastic processes.

As usual, we shall assume that the interaction with the individual atom is weak, and that $|v_2| \ll |v_0|$. We therefore confine ourselves in (2.12) to the first two terms of the expansion

$$V_{\alpha\beta}^{\sigma\sigma'} = \frac{\exp\{-{}^1/_2 Z(\mathbf{k}_\alpha - \mathbf{k}_\beta)\}}{\Omega_0} \times \Big[v_{\mathbf{kk}'}^{\sigma\sigma'} + \sum_s \sum_{\mathbf{k}\sigma''}{}' \frac{v_0^{\sigma\sigma''}(\mathbf{k}_\alpha,\mathbf{k}) v_0^{\sigma''\sigma'}(\mathbf{k},\mathbf{k}_\beta)}{E - E_{\mathbf{k}} + i\delta} \times \exp\{i(\mathbf{k}_0 - \mathbf{k})\mathbf{R}_s - Z_{\alpha\beta}(\mathbf{k}) + X_s^{\alpha\beta}(\mathbf{k})\}\Big]. \tag{5.3}$$

We have used here the notation given in (3.3) and (3.24).[1)] The second term in (5.3) is actually a small correction to the first. However, strictly speaking, this statement is valid only for the real part, since the imaginary correction, by virtue of the condition $|v_2| \ll |v_0|$, may turn out to be significant. We confine ourselves below only to the analysis of Im $V_{\alpha\beta}^{\sigma\sigma'}$.

In the case of sufficiently high temperatures, all the terms of the sum over s in (5.3) vanish, with the exception of s = 0. Then

$$\operatorname{Im} V_{\alpha\beta}^{\sigma\sigma'} = \frac{\exp\{-{}^1/_2 Z(\mathbf{k}_\alpha - \mathbf{k}_\beta)\}}{\Omega_0} [v_2^{\sigma\sigma'}(\mathbf{k}_\alpha,\mathbf{k}_\beta) + v_1^{\sigma\sigma'}(\mathbf{k}_\alpha,\mathbf{k}_\beta)], \tag{5.4}$$

$$v_1^{\sigma\sigma'}(\mathbf{k}_\alpha,\mathbf{k}_\beta) = \pi \sum_{\mathbf{k}\sigma''} v_0^{\sigma\sigma''}(\mathbf{k}_\alpha,\mathbf{k}) v_0^{\sigma''\sigma'}(\mathbf{k},\mathbf{k}_\beta)\delta(E - E_{\mathbf{k}}); \tag{5.5}$$

v_1 actually determines that part of the total cross section of the interaction connected with pure elastic coherent scattering by an individual atom.

At low temperatures, when we can neglect the lattice vibrations, the second term in (5.3) turns out to be pure real because we have excluded from the sum over **K** the terms with K = 0 and K = K_1. Then Im $V_{\alpha\beta}^{\sigma\sigma'}$ is determined only by the first term in (5.4), i.e., only by inelastic processes.

The approximate value for arbitrary temperatures can be obtained by the same method as in the derivation of (3.12)—(3.14), if we separate first in explicit form the term with s = 0. As a result we add to (5.4) the expression

$$\frac{\pi}{\Omega_0} \sum_{\mathbf{k}\sigma''} v_0^{\sigma\sigma'}(\mathbf{k}_\alpha,\mathbf{k}) v_0^{\sigma''\sigma'}(\mathbf{k},\mathbf{k}_\beta) e^{-Z_{\alpha\beta}(\mathbf{k})}\delta(E - E_{\mathbf{k}}) + \frac{\pi}{\Omega_0}\Big\{ \sum_{\mathbf{K}} \rho_{\alpha\beta}^{\sigma\sigma'}(\mathbf{k}_0 + \mathbf{K}) - \frac{\Omega_0}{(2\pi)^3}\int d\mathbf{k}\, \rho_{\alpha\beta}^{\sigma\sigma'}(\mathbf{k}_0 + \mathbf{k})\Big\}; \tag{5.6}$$

$$\rho_{\alpha\beta}^{\sigma\sigma'} = \frac{1}{2M}\sum_{\mu}\int \frac{d\mathbf{q}}{(2\pi)^3}\Big(\sum_{\sigma''} v_0^{\sigma\sigma''}(\mathbf{k}_\alpha,\mathbf{k}+\mathbf{q}) v_0^{\sigma''\sigma'}(\mathbf{k}+\mathbf{q},\mathbf{k}_\beta) \cdot \exp\{-Z_{\alpha\beta}(\mathbf{k}+\mathbf{q})\} \times \frac{[(\mathbf{k}_\alpha - \mathbf{k} - \mathbf{q})\mathbf{e}(\mathbf{q},\mu)][(\mathbf{k}_\beta - \mathbf{k} - \mathbf{q})\mathbf{e}(\mathbf{q},\mu)]}{\omega(\mathbf{q},\mu)} \times (2\bar{n}(\mathbf{q},\mu) + 1)\delta(E - E_{\mathbf{k}+\mathbf{q}}). \tag{5.7}$$

From this expression it follows that the imaginary part of the coefficients of the dynamic system of equations contains a temperature dependence which is more complicated than that determined by the Debye-Waller factor. This result is significant when the scattering cross section is comparable with the absorption cross section. In the opposite case, we can neglect the term (5.6) and we arrive at the values obtained in [2,3] for the coefficients of the dynamic system in the case of a broad line. (In the case of a broad nuclear line ($\Gamma \gg \omega_0$) potential scattering and resonance scattering are physically equivalent.)

In the case of x rays we have

$$v_0^{il}(\mathbf{q}) = -\frac{2\pi e^2}{m_e \varkappa c} F(\mathbf{q})\delta^{il}, \tag{5.8}$$

where F(q) is the atomic form factor and m_e is

[1)] In the derivation of (5.3) we have also assumed that the energy of the incident particle E_{k_0} is much larger than ω_0.

the electron mass. In this case in the coefficients $\Delta g_{\alpha\beta}^{il}$ (2.22) of the system (2.21), connected with scattering by the phonons (second term in the brackets in (5.4) and the term (5.6)), is given by

$$\Delta g_{\alpha\beta}{}^{il} \approx i\frac{4\pi}{\Omega_0\varkappa}\left(\frac{e^2}{m_e c^2}\right)^2 \left\{ \int F(\mathbf{k}_\alpha - \mathbf{k}) F(\mathbf{k} - \mathbf{k}_\beta) \left(\delta^{il} - \frac{k^i k^l}{k^2}\right) \right.$$
$$\times [\exp\{-{}^1/_2 Z(\mathbf{k}_\alpha - \mathbf{k}_\beta)\} - \exp\{-Z_{\alpha\beta}(\mathbf{k})\}] \frac{d\Omega_{\mathbf{k}}}{4\pi}\Big|_{k=k_0}$$
$$+ \delta_{\alpha\beta}\left(\delta^{il} - \frac{k_\gamma{}^i k_\gamma{}^l}{k_\gamma{}^2}\right) |F(\mathbf{K}_1)|^2$$
$$\left. \times \exp\{-Z(\mathbf{K}_1)\} \frac{K_1{}^2}{\varkappa^2} \frac{3T}{2Mc_{\text{зв}}{}^2} \ln\frac{q_0}{q_{min}} \right\}. \quad \gamma \neq \alpha,$$
$$q_{min} = \max\{1/L, g_{00}\varkappa\}. \qquad (5.9)$$

Here the tensor $\delta^{il} - k^i k^l/k^2$ picks out, upon integration over the directions of the vector k, only the transverse polarizations (see the derivation of the systems (2.10) and (2.11)).

We have retained in the last term of (5.6) only the diverging logarithmic part. It is interesting that it appears only for the diagonal coefficients of the dynamic system. This is very important for anomalous penetration.

[1] Yu. Kagan and A. M. Afanas'ev, JETP 50, 271 (1966), Soviet Phys. JETP **23**, 178 (1966).

[2] A. M. Afanas'ev and Yu. Kagan, JETP 48, 327 (1965), Soviet Phys. JETP 21, 215 (1965).

[3] Yu. Kagan and A. M. Afanas'ev, JETP 49, 1504 (1965), Soviet Phys. JETP 22, 1032 (1966).

[4] W. Heitler, The Quantum Theory of Radiation, Oxford, 1954.

[5] A. I. Akhiezer and V. B. Berestetskiĭ, Kvantovaya élektrodinamika (Quantum Electrodynamics), Fizmatgiz, 1959.

Translated by J. G. Adashko
26