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The study of the emission and absorption of γ-quanta by nuclei located in a crystal lattice is of interest both for nuclear physics and for solid-state physics ([1–7]). The interpretation of the experimental data carried out in ([1]) was based on Lamb' s work ([8]). Bearing in mind that it is experimentally possible to detect very small changes (10^{-7} eV) in the positions of the maxima of the emission (or absorption) cross section of γ-quanta, and also to study the shape of the reabsorption curve, it is of considerable interest to take into account the change in the equilibrium positions and normal frequencies of lattice vibrations depending on the state of the nucleus. The question of the criteria determining the shape of the intensity curve of emission (or absorption) and the presence of an unshifted Mössbauer line in the spectrum is very important. The present paper considers this circle of questions.

Let us consider a solid containing, as an impurity, γ-radioactive nuclei; we shall assume that the impurity concentration is small and, on this basis, neglect the interaction between impurity atoms. The coupling of the impurity atom with the host may change as a result of the fact that the magnetic moment of the impurity nucleus is different depending on the state of the nucleus. For example, in the case of a ferromagnetic host, the dipole coupling of the nuclear magnetic moment with the spins of the electronic d shell of the nearest atoms is significant.

Using the adiabatic method, one can show that the equilibrium positions of the host nuclei and the normal frequencies of vibrations of its lattice will be different depending on the state of the impurity nucleus. In calculating the emission and absorption of γ-quanta by nuclei located in a solid, we shall take these possibilities into account. Then, in the adiabatic approximation, the wave function of the system nucleus + host + electromagnetic field will have the form

$$\Phi_{ln_sN_\sigma} = \psi_l|N_\sigma\rangle S_l|n_s\rangle, \qquad (1)$$

where ψ_l is the wave function of the nucleus and electrons in the state l; $|n_s\rangle$ and $|N_\sigma\rangle$ are, respectively, the wave functions of the lattice vibrations and of the radiation field. The operator S_l, indicating that the equilibrium positions of the host nuclei are different for different states of the impurity-atom nucleus, has the form

$$S_l = \exp\left\{\sum_s \xi_{sl}\left(b_s^+ - b_s\right)\right\}, \tag{2}$$

where b_s^+, b_s are the phonon creation and annihilation operators; ξ_{sl} are the displacements of the nuclei in normal coordinates; the index s numbers the values of the wave vector and the branches of the normal vibrations of the host.

Having the functions (1), let us consider the emission of γ-quanta by an impurity nucleus in the transition $l_1 \to l_0$. Using the Weisskopf-Wigner method ([9]) for

for the probability of the transition $l\{n_s\}, \{0\} \to l_0, \{n'_s\}, \{1_\sigma\}$, we obtain the expression

$$\left|a_{l_0,\{n'_s\},\{1_\sigma\}}(\infty)\right|^2 = \left|\langle l_0\{n'_s\}\{1_\sigma\}|V|l_1\{n_s\}\{0\}\rangle\right|^2 \times \frac{\Gamma/2}{\left[E - E_0 + \sum_s\left(\hbar\omega_{sl_0}n'_s - \hbar\omega_{sl_1}n_s\right)\right]^2 + \Gamma^2/4}, \tag{3}$$

where

$$\langle l_0\{n'_s\}\{1_\sigma\}|V|l_1\{n_s\}\{0\}\rangle = L\prod_s\left\langle n'_s\middle|\exp\left\{-i\sum_s\left(q_s b_s + q_s^* b_s^+\right)S_{l_1}\right\}\middle|n_s\right\rangle;$$

$$q_{sl_1} = \frac{(\mathbf{p}\cdot\mathbf{e}_s)}{\sqrt{2M\hbar\omega_{sl_1}N}};$$

$\mathbf{p}$ is the momentum of the emitted γ-quantum; $\mathbf{e}_s$ are orthonormal solutions of the equations of lattice-nucleus vibrations; L is the nuclear matrix element on the functions ψ_{l_1} and ψ_{l_0}. For simplicity we have put $S_{l_0} = 1$. The level width Γ appearing in (3), as the calculation shows, is practically independent of the state of the lattice $\{n_s\}$ and, consequently, of the temperature, and is equal to the natural width of the excited nuclear level.

Summing (3) over all final states and averaging over all initial ones, we obtain, analogously to ([2,8]), the total cross section for emission of γ-quanta of energy E

$$\sigma_e(E) = \frac{\Gamma^2}{4}\sigma_0 W_e(E). \tag{4}$$

Here

$$W_e(E) = \frac{2}{\Gamma}\,\mathrm{Re}\int_0^{\infty} \exp\left\{ i\mu(E - E_0') - \mu\frac{\Gamma}{2} + g_e(\mu) \right\} d\mu;$$

$$E_0' = E_0 + \sum_s \overline{n}_{sl_0}\left(\hbar\omega_{sl_1} - \hbar\omega_{sl_0}\right);$$

$$g_e(\mu) = \sum_s \left|\xi_{sl_1} + iq_{sl_1}\right|^2 \left\{ (\overline{n}_{sl_0} + 1)e^{i\mu\hbar\omega_{sl_0}} + \overline{n}_{sl_0} e^{-i\mu\hbar\omega_{sl_0}} - 2\overline{n}_{sl_0} - 1 \right\};$$

σ_0 is the total absorption cross section of γ-quanta by a free nucleus at resonance; E_0 is the energy difference between the excited and ground states of the impurity nucleus, taking into account its interaction with the electrons and the solvent.

To establish the form of the function $W_e(E)$, we divide the integration interval $[0, \infty]$ into two intervals $[0, \mu_0]$ and $[\mu_0, \infty]$. Under the condition $\mu_0\omega_{\max} < 1$, in the integral $\int_0^{\mu_0} \ldots\, d\mu$ the function $g_e(\mu)$ can be expanded in a power series. Introducing the notation

$$R_e = \sum_s \left|\xi_{sl_1} + iq_{sl_1}\right|^2 \hbar\omega_{sl_0}, \qquad B_e^2 = \frac{1}{2}\sum_s \left|\xi_{sl_1} + iq_{sl_1}\right|^2 (2\overline{n}_{sl_0} + 1)(\hbar\omega_{sl_0})^2,$$

$$C_e = \frac{1}{3!}\sum_s \left|\xi_{sl_1} + iq_{sl_1}\right|^2 (\hbar\omega_{sl_0})^3, \qquad D_e = \frac{1}{4!}\sum_s \left|\xi_{sl_1} + iq_{sl_1}\right|^2 (2\overline{n}_{sl_0} + 1)(\hbar\omega_{sl_0})^4,$$

we obtain that, under the condition

$$\frac{1}{2}\sum_s \left|\xi_{sl_1} + iq_{sl_1}\right|^2 (2\overline{n}_{sl_0} + 1)\left(\frac{\omega_{sl_0}}{\omega_{sl_0}^{\max}}\right)^2 > 1, \tag{5}$$

$$W_1^e(E) = \frac{2}{\Gamma}\,\mathrm{Re}\int_0^{\mu_0} \exp\left\{ i\mu(E - E_0') - \mu\frac{\Gamma}{2} + g_e(\mu) \right\} d\mu =$$

$$= \frac{4}{\Gamma^2}\left\{ 1 - \frac{C_e}{8B_e^6}(E - E_0' + R_e)^3 + \frac{D_e}{16B_e^8}(E - E_0' + R_e)^4 + \ldots \right\}\psi(x, \eta), \tag{6}$$

where

$$\psi(x, \eta) = \int_0^{\infty} \cos xy\, e^{-y - y^2\eta^2/4}\, dy, \qquad x = \frac{2(E - E_0' + R_e)}{\Gamma}, \quad \eta = \frac{4B_e}{\Gamma}.$$

The integral

$$W_{11}^{e}(E) = \frac{2}{\Gamma}\,\mathrm{Re}\int_{\mu_0}^{\infty} \exp\left\{ i\mu(E - E_0') - \mu\frac{\Gamma}{2} + g_e(\mu) \right\} d\mu = e^{-G}\frac{1}{(E - E_0')^2 + \Gamma^2/4} \tag{7}$$

under the condition

$$\frac{1}{2}\sum_s \left|\xi_{sl_1} + iq_{sl_1}\right|^2 (2\bar{n}_{sl_0} + 1)\frac{\Gamma}{\hbar\omega_{sl_0}^{\max}} < 1, \tag{8}$$

where

$$G = \sum_s \left|\xi_{sl_1} + iq_{sl_1}\right|^2 (2\bar{n}_{sl_1} + 1).$$

Thus, under conditions (5) and (8), the cross section for emission of γ-quanta in the neighborhood of the point $E = E_0' - R_e$ is represented as a curve that decreases rapidly on both sides of this point and is not symmetric with respect to it; at the point $E = E_0'$ there is a peak of the unshifted line, whose intensity is proportional to $\exp\{-G\}$. As the temperature is raised, $W_e(E)$ takes the form of a Gaussian curve with half-width $2B_e(\ln 2)^{1/2}$ and with a maximum at the point $E = E_0' - R_e$; the intensity of the Mössbauer line drops sharply.

At low temperatures, when condition (5) is not fulfilled, $W_e(E)$ is represented as a sum of superposed Lorentzian curves and has the form

$$W_e(E) = e^{-G}\prod_s \sum_{n_s', n_s} \frac{{\alpha_s}^{n_s}\beta_s^{n_s'}}{n_s!\,n_s'!}\,\frac{1}{[E - E_0' - \hbar\omega_{sl_0}(n_s' - n_s)]^2 + \Gamma^2/4}, \tag{9}$$

where

$$\alpha_s = \left|\xi_{sl_1} + iq_{sl_1}\right|^2 (\bar{n}_{sl_0} + 1), \qquad \beta_s = \left|\xi_{sl_1} + iq_{sl_1}\right|^2 \bar{n}_{sl_0}.$$

The contribution to the Mössbauer component is given by that part of the sum in which $n_s' = n_s$.

An analogous consideration of the problem of absorption of γ-quanta in the transition $l_0 \to l_1$ gives the following result for the absorption cross section:

$$\sigma_a(E) = \frac{\Gamma^2}{4}\sigma_0 W_a(E), \tag{10}$$

$$W_a(E) = \frac{2}{\Gamma} \operatorname{Re} \int_0^\infty \exp\left\{ i\mu(E_0' - E) - \mu\frac{\Gamma}{2} + g_a(\mu) \right\} d\mu,$$

$$g_a(\mu) = \sum_s \left| \xi_{sl_1} + i q_{sl_0} \right|^2 \left\{ (\bar{n}_{sl_1} + 1) e^{i\mu\hbar\omega_{sl_1}} + \bar{n}_{sl_1} e^{-i\mu\hbar\omega_{sl_1}} - 2\bar{n}_{sl_1} - 1 \right\}.$$

The analysis of the function $W_a(E)$ is carried out in the same way as in the case of emission. At the point $E = E_0'$ there is an unshifted line of natural width; at the point $E = E_0' + R_a$ lies the maximum of that part of the spectrum which is associated with the processes of creation and annihilation of phonons. Criteria (5) and (8) remain the same; in them one need only make the replacements $q_{sl_1} \to q_{sl_0}$, $\omega_{sl_0} \to \omega_{sl_1}$, and $\bar{n}_{sl_0} \to \bar{n}_{sl_1}$.

Examination of expressions (6) and (7) shows that, when the change in the equilibrium positions of the nuclei and the change in the normal frequencies of vibrations are taken into account,

lattice: a) the Mössbauer line shifts with temperature by the amount $\Delta E = \sum_s \bar{n}_{sl_0}(\hbar\omega_{sl_1} - \hbar\omega_{sl_0})$; b) the maxima at the points $E = E_0' \mp R_{e(a)}$, respectively for emission and absorption, are separated from the Mössbauer line by the distance $R_{e(a)} > \frac{\mathbf{p}^2}{2M}$, the recoil energy of the nucleus; c) the intensity of the Mössbauer line is additionally reduced as a result of the presence of the displacement ξ_{sl_1} in the expression for G.

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