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THE METHOD OF TEMPERATURE GREEN'S FUNCTIONS IN THE THEORY OF THE MÖSSBAUER EFFECT ON IMPURITY NUCLEI

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The method of temperature Green's functions is used to determine the probability f of the Mössbauer effect for an impurity nucleus in solid solution, and the temperature shift δE of the Mössbauer line. General equations are found which give f and δE in terms of parameters of the ideal solvent lattice and the mass ratio of the impurity and crystal-solvent atoms, as well as quantities characterizing the interaction of the impurity atom and the atoms of the solvent. Specific computations are made for a monatomic cubic crystal-solvent in the Debye approximation. The computed values of f and δE are compared with the available experimental data.

INTRODUCTION

THE study of the Mössbauer effect[1] for impurity nuclei in solid solution is of considerable interest since it offers some possibility of changing the intensity of the Mössbauer line from a single radioactive nucleus by a suitable choice of the crystal-solvent.

A complete computation of the intensity of the Mössbauer line and its temperature shift for the general case is possible if the solution of the vibration problem of the solvent lattice is known. Attempts at such a solution for certain models have been made previously (cf. [2-4]). Kagan and Iosilevskiĭ[5] tried to solve the dynamical problem of a substitutional solution in a monatomic cubic crystal; the solution was then used to determine the Mössbauer fraction. But there are many difficulties in doing this.

It has been shown earlier[6-7] that the method of temperature Green's functions[8-10] enables one to avoid solving the dynamical problem for a substitutional solution (except for the determination of the local frequencies, if any are present, and this only for the determination of the temperature dependence of the intensity of the Mössbauer line); all the quantities of interest are expressed in terms of the dynamical parameters of the ideal solvent lattice.

If we write the Hamiltonian for the vibrations of the nuclei of the lattice containing the impurity nucleus as

$$H = H_0 + V, \qquad (1)$$

where

$$H_0 = \sum_{\mathbf{n}} \frac{\mathbf{p}_{\mathbf{n}}^2}{2M} + \frac{1}{2} \sum_{\mathbf{n},\mathbf{n}'} u_{\mathbf{n}}^{\alpha} A_{\mathbf{n}\mathbf{n}'}^{\alpha\alpha'} u_{\mathbf{n}'}^{\alpha'},$$

$$V = \frac{\mathbf{p}_0^2}{2M}\mu + \varkappa \sum_{\mathbf{n}} u_0^{\alpha} A_{0\mathbf{n}}^{\alpha\alpha'} u_{\mathbf{n}}^{\alpha'} - \frac{\varkappa}{2} u_0^{\alpha} A_{00}^{\alpha\alpha'} u_0^{\alpha'};$$

$\mathbf{u}_{\mathbf{n}}$, $\mathbf{p}_{\mathbf{n}}$ are the displacement and momentum of the **n**-th nucleus, $A_{\mathbf{nn}'}^{\alpha\alpha'}$ are the force constants of the ideal lattice, κ is a factor which takes account of the change in the force constants when an atom of the ideal lattice with mass M is replaced by an impurity atom of mass m, $\mu = M/m - 1$, then the expression for the probability of a γ-transition in the impurity nucleus with emission of a γ quantum of energy E is expressed as

$$W(E) = \frac{2|L_{l_1 l_0}|^2}{\gamma} \operatorname{Re} \int_0^{\infty} dt \exp\left\{it(E_0 - E) - \frac{\gamma t}{2}\right\}$$
$$\times \exp\{k^{\alpha} k^{\alpha'} \langle u^{\alpha}(t) u^{\alpha'}(0)\rangle - k^{\alpha} k^{\alpha'} \langle u^{\alpha}(0) u^{\alpha'}(0)\rangle\}. \qquad (2)$$

Here

$$\langle u^{\alpha}(t) u^{\alpha'}(0)\rangle = Z^{-1} \operatorname{Sp}\{e^{-\beta H} u^{\alpha}(t) u^{\alpha'}(0)\},$$

$\beta = 1/k_B T$, k_B is the Boltzmann constant, Z is the partition function for phonons, E_0 is the difference in energy between the ground and excited states of the impurity nucleus, k is the wave vector of the radiated γ quantum.

1. INTENSITY OF THE MÖSSBAUER LINE FOR IMPURITY NUCLEI

The expression (2) determines the shape of the spectrum of emission of γ quanta by nuclei for an arbitrary temperature and an arbitrary form of the operator H in the harmonic approximation; its form is independent of the symmetry of the crystal and of the number of atoms per unit cell. In particular, if the crystal has translational symmetry, $k^{\alpha}k^{\alpha'}\langle u^{\alpha}(t)u^{\alpha'}(0)\rangle$ determines the phonon part of the emission spectrum, while $k^{\alpha}k^{\alpha'}\langle u^{\alpha}(0)u^{\alpha'}(0)\rangle$ gives the Mössbauer fraction.

If, however, the lattice contains an atom with a γ-emitting nucleus, then because of the appearance of local vibrations, the term $k^{\alpha}k^{\alpha'}\langle u^{\alpha}(t)u^{\alpha'}(0)\rangle$ in (2) will also contribute to the intensity of the Mössbauer line, and one can easily show that the Mössbauer fraction is then given by

$$f = f_1 I_0\left(2|a_{\lambda_0}|^2\sqrt{\bar{n}_{\lambda_0}(\bar{n}_{\lambda_0}+1)}\right), \tag{3}$$

where

$$f_1 = \exp\{-k^{\alpha}k^{\alpha'}\langle u^{\alpha}(0)\,u^{\alpha'}(0)\rangle\}, \qquad a_{\lambda_0} = k^{\alpha}w_0^{\alpha}(\lambda_0),$$

$w_0^{\alpha}(\lambda_0)$ are coefficients relating the operators u_n to the operators for creation and annihilation of elementary excitations of the nonideal crystal, $\bar{n}_{\lambda_0} = (e^{\beta\hbar\omega_{\lambda_0}} - 1)^{-1}$, ω_{λ_0} is the frequency of the local vibration, $I_0(z)$ is the Bessel function of zeroth order and imaginary argument. For $T = 0$ the second factor in (3) is equal to unity, so that knowledge of $\langle u^{\alpha}(0)u^{\alpha'}(0)\rangle$ is sufficient to determine the Mössbauer line.

To calculate $\langle u^{\alpha}(0)u^{\alpha'}(0)\rangle$ we note that this function is the boundary value of the Green's function:

$$G^{\alpha\alpha'}(\tau, \tau') = \langle Tu^{\alpha}(\tau)\,u^{\alpha'}(\tau')\,S(\beta)\rangle / \langle S(\beta)\rangle; \tag{4}$$

$$u^{\alpha}(\tau) = e^{\tau H_0}u^{\alpha}(0)\,e^{-\tau H_0}, \qquad V(z) = e^{zH_0}Ve^{-zH_0},$$
$$S(\beta) = T\exp\{-\int_0^{\beta} dz\,V(z)\}. \tag{5}$$

Using the temperature form of the generalized Wick theorem,[11] we get the following system of equations for the Fourier transform of $G^{\alpha\alpha'}(\tau,\tau')$:

$$\begin{aligned} G^{\alpha\alpha'}(\varepsilon_n) = {} & G_0^{\alpha\alpha'}(\varepsilon_n) - (\mu/M)\,D^{\alpha\gamma}(\varepsilon_n)\,D_0^{\alpha'\gamma}(-\varepsilon_n) \\ & - \varkappa X^{\alpha\gamma}(\varepsilon_n)\,G_0^{\alpha'\gamma}(-\varepsilon_n) \\ & - \varkappa G^{\alpha\gamma}(\varepsilon_n)[X_0^{\alpha'\gamma}(-\varepsilon_n) - A_{00}G_0^{\alpha'\gamma}(-\varepsilon_n)], \end{aligned} \tag{6a}$$

$$\begin{aligned} D^{\alpha\alpha'}(\varepsilon_n) = {} & D_0^{\alpha\alpha'}(\varepsilon_n) - \mu D^{\alpha\gamma}(\varepsilon_n)\,F_0(-\varepsilon_n) - \varkappa X^{\alpha\gamma}(\varepsilon_n)\,D_0^{\gamma\alpha'}(\varepsilon_n) \\ & - \varkappa G^{\alpha\gamma}(\varepsilon_n)\,[Y_0^{\gamma\alpha'}(\varepsilon_n) - A_{00}D_0^{\gamma\alpha'}(\varepsilon_n)], \end{aligned} \tag{6b}$$

$$\begin{aligned} X^{\alpha\alpha'}(\varepsilon_n) = {} & X_0^{\alpha\alpha'}(\varepsilon_n) \\ & - \frac{\mu}{M}D^{\alpha\gamma}(\varepsilon_n)\,Y_0^{\alpha'\gamma}(-\varepsilon_n) - \varkappa X^{\alpha\gamma}(\varepsilon_n)\,X_0^{\gamma\alpha'}(\varepsilon_n) \\ & - \varkappa G^{\alpha\gamma}(\varepsilon_n)\,[Z_0^{\gamma\alpha'}(-\varepsilon_n) - A_{00}X_0^{\gamma\alpha'}(\varepsilon_n)], \end{aligned}$$

where $\epsilon_n = 2\pi n/b$, $n = 0, \pm 1, \pm 2, \ldots$; $D^{\alpha\alpha'}(\epsilon_n)$, $D_0^{\alpha\alpha'}(\epsilon_n)$, $X^{\alpha\alpha'}(\epsilon_n)$, $G_0^{\alpha\alpha'}(\epsilon_n)$, etc are the Fourier transforms of the functions

$$G_0^{\alpha\alpha'}(\tau, \tau') = \overbracket{u^{\alpha}(\tau)\,u^{\alpha'}}(\tau'), \qquad D_0^{\alpha\alpha'}(\tau, \tau') = \overbracket{u^{\alpha}(\tau)\,p^{\alpha'}}(\tau'),$$
$$MF_0^{\alpha\alpha'}(\tau, \tau') = \overbracket{p^{\alpha}(\tau)\,p^{\alpha'}}(\tau'),$$
$$X_0^{\alpha\alpha'}(\tau, \tau') = \sum_{\mathbf{n}} A_{0\mathbf{n}}^{\alpha'\gamma}\,\overbracket{u^{\alpha}(\tau)\,u_n^{\gamma}}(\tau'),$$
$$D^{\alpha\alpha'}(\tau, \tau') = \frac{\langle Tu^{\alpha}(\tau)\,p^{\alpha'}(\tau')\,S(\beta)\rangle}{\langle S(\beta)\rangle},$$
$$X^{\alpha\alpha'}(\tau, \tau') = \sum_{\mathbf{n}} A_{0\mathbf{n}}^{\alpha'\gamma}\,\frac{\langle Tu^{\alpha}(\tau)\,u_{\mathbf{n}}^{\gamma}(\tau')\,S(\beta)\rangle}{\langle S(\beta)\rangle},$$
$$Y_0^{\alpha\alpha'}(\tau, \tau') = \sum_{\mathbf{n}} A_{0\mathbf{n}}^{\alpha\gamma}\,\overbracket{u_{\mathbf{n}}^{\gamma}(\tau)\,p^{\alpha'}}(\tau'),$$
$$Z_0^{\alpha\alpha'}(\tau, \tau') = \sum_{\mathbf{n}} A_{0\mathbf{n}}^{\alpha'\gamma}X_{\mathbf{n}0}^{\gamma\alpha}(\tau, \tau'),$$
$$X_{\mathbf{n}0}^{\gamma\alpha}(\tau, \tau') = \sum_{\mathbf{n}'} A_{0\mathbf{n}'}^{\alpha\gamma'}\,\overbracket{u_{\mathbf{n}}^{\gamma}(\tau)\,u_{\mathbf{n}'}^{\gamma'}}(\tau'),$$
$$\overline{AB} = \langle TAB\rangle, \qquad A_{00}^{\alpha\alpha'} = A_{00}\delta_{\alpha\alpha'}. \tag{7}$$

If the dynamical problem is solved for the ideal crystal-solvent, the system (6) completely determines the Mössbauer fraction as a function of μ and κ. But in the overwhelming majority of cases the solution of this problem is not known for the crystal-solvents in which the Mössbauer effect on impurities is studied. So for a qualitative estimate of the intensity of the Mössbauer line and its temperature shift we treat the Debye model of a crystal with degenerate branches, assuming that $\kappa = 0$.

The system (6) then has the form

$$\begin{aligned} G_0^{\alpha\alpha'}(\varepsilon_n) &= G_0^{\alpha\alpha'}(\varepsilon_n) - (\mu/M)\,D^{\alpha\gamma}(\varepsilon_n)\,D_0^{\alpha'\gamma}(-\varepsilon_n), \\ D^{\alpha\alpha'}(\varepsilon_n) &= D_0^{\alpha\alpha'}(\varepsilon_n) - \mu D^{\alpha\gamma}(\varepsilon_n)\,F_0^{\alpha'\gamma}(\varepsilon_n), \end{aligned} \tag{8}$$

where for the model under consideration

$$G_0^{\alpha\alpha'}(\varepsilon_n) = \frac{\hbar^2}{MN}\sum \frac{\delta_{\alpha\alpha'}}{\varepsilon_n^2 + \varepsilon_{\mathbf{f}}^2} \equiv \delta_{\alpha\alpha'}G_0(\varepsilon_n),$$
$$D_0^{\alpha\alpha'}(\varepsilon_n) = -\frac{\hbar}{N}\sum_{\mathbf{f}} \frac{\varepsilon_n\delta_{\alpha\alpha'}}{\varepsilon_n^2 + \varepsilon_{\mathbf{f}}^2} = \delta_{\alpha\alpha'}D_0(\varepsilon_n),$$
$$F_0^{\alpha\alpha'}(\varepsilon_n) = \frac{1}{N}\sum_{\mathbf{f}} \frac{\delta_{\alpha\alpha'}\,\varepsilon_{\mathbf{f}}^2}{\varepsilon_n^2 + \varepsilon_{\mathbf{f}}^2} \equiv \delta_{\alpha\alpha'}F_0(\varepsilon_n), \tag{9}$$

where $\epsilon_{\mathbf{f}} = \hbar\omega_{\mathbf{f}}$, and N is the number of atoms in the fundamental unit of the crystal.

From (8) we find

$$G(\varepsilon_n) = G_0(\varepsilon_n) - \frac{\mu}{M}\,\frac{D_0(\varepsilon_n)\,D_0(-\varepsilon_n)}{1 + \mu F_0(-\varepsilon_n)}; \tag{10a}$$

substituting the values of $D_0(\epsilon_n)$, $F_0(-\epsilon_n)$, and $G_0(\epsilon_n)$ from (9), we get

$$G(\varepsilon_n) = \frac{\hbar^2}{m}\,\frac{\psi(\varepsilon_n)}{1+\mu\,[1-\varepsilon_n^2\psi(\varepsilon_n)]}, \quad \psi(\varepsilon_n) = \frac{1}{N}\sum_{\mathbf{f}}(\varepsilon_n^2+\varepsilon_{\mathbf{f}}^2)^{-1}. \tag{10b}$$

The expression for the Mössbauer fraction is

$$f = \exp\left\{-\frac{3R}{\beta}\sum_{n=-\infty}^{\infty}\frac{\psi(\varepsilon_n)}{1+\mu-\mu\varepsilon_n^2\,\psi(\varepsilon_n)}\right\}. \tag{11}$$

By elementary transformations this can be brought to the form

$$f = \exp\{-3R\Lambda(\xi)/2\varepsilon_0\}, \qquad R = \hbar^2\mathrm{k}^2/2m,$$

$$\Lambda(\xi) = \frac{2\xi}{\pi}\sum_{n=-\infty}^{\infty}\frac{1-n\xi\,\mathrm{arc\,tg}\,(1/n\xi)}{1+\mu-3\mu\,(n\xi)^2\,[1-n\xi\,\mathrm{arc\,tg}\,(1/n\xi)]},$$

$$\xi = 2\pi\frac{T}{\Theta}. \tag{12)*}$$

The dependence of $\Lambda(\xi)$ on T/Θ is shown in Fig. 1.

The computation of the Mössbauer fraction using (12) for Fe^{57} nuclei in a Be lattice[12] gives the following results ($\Theta_{Be} = 1160°K$)

$$\frac{f\,(295^\circ\,\mathrm{K})}{f\,(80^\circ\,\mathrm{K})} = 0{,}895, \qquad \frac{f\,(425^\circ\,\mathrm{K})}{f\,(80^\circ\,\mathrm{K})} = 0.828.$$

We note that for $\mu < 0$ (no local frequencies present) in the limiting case of a heavy nucleus, when $\mu \to -1$, the main contribution to the sum over n in (11) comes from small ϵ_n. Using this one can bring the expression for f to the form

$$f \approx \exp\{(R/\mu\varepsilon')\,[2\,(e^{\beta\varepsilon'}-1)^{-1}+1]\},$$

where $\epsilon' = [-(1+\mu)/\mu\psi(0)]^{1/2}$. Thus for $T > (M/m)^{1/2}\Theta$ and $\mu < 0$ the intensity of the Mössbauer line drops exponentially with increasing temperature; this agrees with the conclusions of of Kagan and Iosilevskiĭ.[5]

To determine the Mössbauer fraction when $\mu > 0$, when a local frequency is present in the frequency spectrum of the nonideal crystal, one must find the quantity $|a_{\lambda_0}|^2$, which gives the contribution of the local frequency to the time correlation function $\langle u^{\alpha}(t)\,u^{\alpha'}(t')\rangle$. It is known that[13]

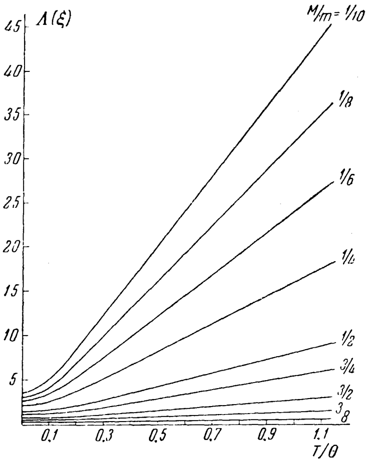

FIG. 1

$$\langle u^{\alpha}(t)\,u^{\alpha'}(t')\rangle = \int_{-\infty}^{\infty} d\varepsilon\, e^{-i\varepsilon(t-t')}\,J_{\alpha\alpha'}(\varepsilon), \tag{13}$$

where

$$J_{\alpha\alpha'}(\varepsilon) = -i\,(1-e^{-\beta\varepsilon})^{-1}\,[K_r^{\alpha\alpha'}(\varepsilon+i\delta) - K_a^{\alpha\alpha'}(\varepsilon-i\delta)],\ \delta\to 0, \tag{14}$$

while $K_{r,a}^{\alpha\alpha'}(\epsilon)$ is the analytic continuation of the Fourier transform of the function

$$K_r^{\alpha\alpha'}(t,t') = i\theta(t-t')\langle[u^{\alpha}(t),u^{\alpha'}(t')]\rangle,\ K_a^{\alpha\alpha'}(t,t') = -i\theta(t-t')\langle[u^{\alpha}(t),u^{\alpha'}(t')\rangle.$$

On the other hand one can show that the functions $K_{r,a}^{\alpha\alpha'}(\epsilon_n)$ are the analytic continuation of the Fourier transform of the temperature Green's function $G^{\alpha\alpha'}(\epsilon_n)$ into the upper and lower half-planes, respectively, i.e., the equations[10]

$$K_r^{\alpha\alpha'}(\varepsilon) = G^{\alpha\alpha'}(-i\varepsilon)/2\pi \text{ for } \mathrm{Im}\,\varepsilon > 0,$$
$$K_a^{\alpha\alpha'}(\varepsilon) = G^{\alpha\alpha'}(-i\varepsilon)/2\pi \text{ for } \mathrm{Im}\,\varepsilon < 0;$$

hold, so that, using (10b), we find

$$K_{r,a}^{\alpha\alpha'}(\varepsilon) = \delta_{\alpha\alpha'}\frac{\hbar^2}{2\pi m}\frac{\Phi(\varepsilon)}{1+\mu r(\varepsilon)} \quad \text{for } \mathrm{Im}\,\varepsilon \neq 0. \tag{15}$$

Here

$$\Phi(\varepsilon) = \frac{1}{N}\sum_{\mathbf{f}}(\varepsilon_{\mathbf{f}}^2-\varepsilon^2)^{-1}, \qquad r(\varepsilon) = \frac{1}{N}\sum_{\mathbf{f}}\varepsilon_{\mathbf{f}}^2(\varepsilon_{\mathbf{f}}^2-\varepsilon^2)^{-1}.$$

The functions $K_{r,\alpha}^{\alpha\alpha'}(\epsilon)$ form one function, analytic in the whole ϵ plane, except for a possible cut along the real axis;[13] the poles of this function on the real axis determine the spectrum of the elementary excitations of the system. In our case for determining the vibration frequencies of the lattice we get the equation

$$1 + \mu r(\varepsilon) = 0. \tag{16}$$

To determine the time correlation function, we substitute (15) and (14) in (13); then, computing the integral by the method of residues, we get

$$\langle u^{\alpha}(t)\,u^{\alpha'}(t')\rangle = \eta(\varepsilon_1)\,[\bar{n}_{\varepsilon_1}e^{i\varepsilon_1(t-t')} + (\bar{n}_{\varepsilon_1}+1)\,e^{-i\varepsilon_1(t-t')}] + K;$$
$$\eta(\varepsilon_1) = \frac{\hbar^2\Phi(\varepsilon_1)}{2m\varepsilon_1\mu\,(\partial r(\varepsilon)/\partial\varepsilon^2)_{\varepsilon=\varepsilon_1}}, \quad \bar{n}_{\varepsilon_1} = (e^{\beta\varepsilon_1}-1)^{-1}, \tag{17}$$

where ϵ_1 is the energy of the localized vibration, determined by (16); K gives the contribution to the time correlation function of all frequencies except the localized one.

Using (16) we also find that

$$\eta(\varepsilon_1) = \frac{\hbar^2(1+\mu)}{2m\varepsilon_1}\frac{\partial\ln\varepsilon_1^2}{\partial\mu}. \tag{18}$$

From (17) and (18) one can show that

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*arctg = $\tan^{-1}$.

$$|a_{\varepsilon_1}|^2 = \frac{R(1+\mu)}{\varepsilon_1}\frac{\partial \ln \varepsilon_1^2}{\partial \mu}. \tag{19}$$

Thus for $\mu > 0$ the Mössbauer fraction is given by the expression

$$f = \exp\left\{-\frac{2R}{\beta}\sum_n \frac{\psi(\varepsilon_n)}{1+\mu-\mu\varepsilon_n^2\psi(\varepsilon_n)}\right\}$$
$$\times\ I_0\left\{\frac{2R(1+\mu)}{\varepsilon_1}\sqrt{\bar{n}_{\varepsilon_1}(\bar{n}_{\varepsilon_1}+1)}\frac{\partial \ln \varepsilon_1^2}{\partial \mu}\right\}.$$

Finally we proceed to consider the general case when $\mu \neq 0$ and $\kappa \neq 0$. If we start from the model of a crystal with degenerate branches, Eqs. (6) can be solved easily. In this case we find for $G(\epsilon_n)$ the expression

$$G(\varepsilon_n) = \frac{\hbar^2(1+\mu)}{M(1+\varkappa)}\psi(\varepsilon_n)\Big\{(1+\mu)(1+\varkappa)$$
$$-\left[\varkappa(1+\mu)+\mu+\frac{\varkappa}{1+\varkappa}\right]\varepsilon_n^2\psi(\varepsilon_n)-\varkappa(1+\mu)a^2\psi(\varepsilon_n)\Big\}^{-1},$$
$$a^2 = \hbar^2 A_{00}/M.$$

If the spectrum of normal vibrations includes a localized frequency, its contribution to the time correlation function is given by the coefficient $|a_{\epsilon_1}|^2$, which in the case of $\kappa \neq 0$ is determined from the equation

$$(1+\mu)(1+\varkappa) + [\varkappa(1+\mu)+\mu+\varkappa/(1+\varkappa)\ \ \varepsilon_1^2\Phi(\varepsilon_1)$$
$$-\varkappa(1+\mu)a^2\Phi(\varepsilon_1) = 0. \tag{20}$$

Thus the intensity of the Mössbauer line is given in the general case by the expression

$$f = I_0\left\{\frac{2R(1+\mu)}{\varepsilon_1}\sqrt{\bar{n}_{\varepsilon_1}(\bar{n}_{\varepsilon_1}+1)}\frac{\partial \ln \varepsilon_1^2}{\partial \mu}\right\}$$
$$\times\ \exp\Big\{-\frac{2R}{\beta(1+\varkappa)}\sum_n \psi(\varepsilon_n)\ \Big[(1+\mu)(1+\varkappa)$$
$$-\left(\varkappa(1+\mu)+\mu+\frac{\varkappa}{1+\varkappa}\right)\varepsilon_n^2\psi(\varepsilon_n)$$
$$-\varkappa(1+\mu)a^2\psi(\varepsilon_n)\Big]^{-1}\Big\}, \tag{21}$$

The last expression can be used for numerical computations, for example on the Debye model.

In the case of T = 0, the first factor in (21) is unity, while the sum over n can be replaced by an integral. The position of the localized frequency can be computed numerically for arbitrary μ and κ, using (20). We also note that the method of temperature Green's functions also allows one to calculate f for more complicated lattices than those considered in this paper.

2. TEMPERATURE SHIFT OF THE MÖSSBAUER LINE

The temperature shift of the Mössbauer line from a γ-active nucleus in an ideal lattice was treated by Josephson.[14] Here we consider this problem for an impurity nucleus.

When a γ quantum of energy E is emitted, the mass of the impurity nucleus changes by an amount $\delta m = -E/c^2$. According to (1), the vibrational energy of the solvent changes by

$$\delta E = \langle \delta H \rangle = -\langle \mathbf{p}^2 \rangle E/2mc^2,$$
$$\langle \mathbf{p}^2 \rangle = Z^{-1}\,\mathrm{Sp}\,\{e^{-\beta H}\sum_\alpha p^\alpha(0)\,p^\alpha(0)\}, \tag{22}$$

where p is the momentum of the impurity nucleus. Just as in the preceding section, we find

$$\langle \mathbf{p}^2 \rangle = \sum_\alpha \frac{\langle S(\beta)\,p^\alpha(0)\,p^\alpha(0)\rangle}{\langle S(\beta)\rangle}, \tag{23}$$

where $S(\beta)$ is given by (5), while the statistical averaging is done with the Hamiltonian H_0.

To calculate (23), we consider the Green's function

$$F^{\alpha\alpha'}(\tau,\tau') = \langle T p^\alpha(\tau)\,p^{\alpha'}(\tau')\,S(\beta)\rangle/\langle S(\beta)\rangle,$$

which differs from (4) only by the replacement of $u^\alpha(t)$ by $p^\alpha(t)$; for $\tau = \tau'$ it goes over into (23). Obviously, for the Fourier transform of this function we can get a system of equations similar to (6). If the solutions of the dynamical problem for the ideal lattice are known, this system is easily solved and we can thus calculate $F^{\alpha\alpha'}(0,0)$. Thus the problem of the temperature shift of the Mössbauer line is solved completely rigorously.

Since, however, the solutions for the ideal lattice are not known, we restrict ourselves to considering monatomic crystals in the Debye approximation with degenerate branches. We then find for $F^{\alpha\alpha}(0,0)$ the expression

$$F^{\alpha\alpha}(0,0) = \frac{M}{\beta}\sum_{n=-\infty}^{\infty}\frac{F_0(-\varepsilon_n)}{1+\mu F_0(-\varepsilon_n)},$$

where $F_0(-\epsilon_n)$ is given by (9).

Thus in this case

$$\frac{\delta E}{E} = -\frac{3}{2mc^2\beta}(1+\mu)\sum_{n=-\infty}^{\infty}\frac{F_0(-\varepsilon_n)}{1+\mu F_0(-\varepsilon_n)}.$$

Setting $\xi = 2\pi T/\Theta$, we find $\delta E/E = -3k_B \times \Theta\chi(\xi)/2mc^2$;

$$\chi(\xi) = \frac{T}{\Theta}\Big\{1+2(1+\mu)$$
$$\times\sum_{n=1}^{\infty}\frac{1-3[n\xi]^2[1-n\xi\,\mathrm{arc\,tg}\,(1/n\xi)]}{1+\mu-3(n\xi)^2\mu\,[1-n\xi\,\mathrm{arc\,tg}\,(1/n\xi)]}\Big\}.$$

The dependence of $\chi(\xi)$ on the ratio T/Θ for different μ is shown in Fig. 2. From it we easily determine the temperature shift for Fe^{57} in a Be lattice. Taking $\Theta_{Be} = 1160°K$, for changes of tem-

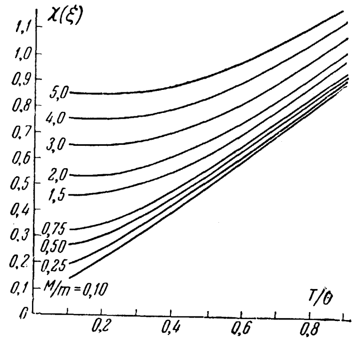

FIG. 2

perature from 80 to 295°K and from 295 to 425°K we get, respectively, temperature shifts of 0.118 and 0.093 mm/sec.

In conclusion we thank N. N. Bogolyubov for valuable comments and his interest in the work. We are also grateful to Dr. W. Marshall, who acquainted us with the experimental data of Heberle, Parks, and Schiffer.

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244