Localized Mode Detection by Means of the Mössbauer Effect*

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The Mössbauer effect in a simple cubic crystal, disordered by light isotopes was studied for the possibility of observing the localized mode vibrational spectrum over the background of the continuum.

I. INTRODUCTION

A GREEN'S function solution for the motion of a three-dimensional crystal with defects and harmonic, nearest neighbor forces has been presented by Montroll.[1] The solution contains an integral which arises frequently in mathematical physics, and has consequently been tabulated in a short table for values of the argument in the neighborhood of the defect.[2] Its use in lattice defect problems is restricted, however, to solutions whose frequencies lie above the maximum frequency of the perfect crystal. With the tables, the contribution to the motion of a light isotopic defect from its localized mode has been obtained. It has been stated[3] that since the amplitude of this contribution is larger than that of any propagating mode in a large crystal, a considerable recoil in a Mössbauer type nucleus, of energy equal to the excitation energy for a phonon of this localized mode (LM), is probable. The presence of such modes would become observable by means of this recoil, as an additional peak in the cross section, shifted from the recoilless part by the LM excitation energy. A calculation of this alteration in the Mössbauer single phonon spectrum has already been performed, for the case of a single such impurity in a crystal. The calculation gives a value of 10^4 b for absorption with LM excitation.[4] This paper performs that calculation in a different manner, which directly demonstrates the effect of the LM coupling on the recoilless and nonrecoil-free spectrum.

The question of observability, however, is not settled on this basis. Additional considerations are first the fact that in a real crystal the phonons interact anharmonically, thereby attributing to each lattice vibration a natural width, considerably greater than that of the nuclear transition. Estimates of this width have been made from data on the thermal conductivity, leading to the conclusion that at absolute zero, the lifetime of a localized mode is only of the order of 100 periods,[5] a width of 10^{-3} or 10^{-4} eV, compared with 10^{-9} eV for the 14.4 keV level of Fe^{57}. Secondly, in a real crystal the situation to be treated is one of a certain concentration of defects. Considerable attention has been given to the treatment of disordered distributions of defects in linear chains, by means of perturbation theory, which demonstrates that the vibrational motion of such a system can be described by a superposition of phonon states, only for a brief interval, due to the scattering of phonons from the perturbing defects.[6] The spectrum of a disordered linear chain, of light impurities, has been given in orders of the concentration by means of a diagrammatic perturbation theory in which only proper diagrams need be considered.[7] This method is directly generalizable to the three-dimensional case, yielding a usable expression for the impurity band spectrum, which is simply related to that of the perfect crystal. Again reference is made to the tables mentioned above.

In Sec. II, the case of a single light Mössbauer isotope is developed for the absorption cross section at $T=0$. The amplitude of the LM motion, D_0, is calculated in Appendix I. In Sec. III, the spectrum for the LM band of a disordered cubic crystal is found for a concentration dilute enough to permit one to neglect superposing the localized mode of the nearest neighboring impurity. The cross section for absorption with such a concentration of Mössbauer isotopes is found in Sec. IV, by a procedure which underestimates, not too seriously, the cross section. The numerical evaluation of the cross section is discussed in Appendix III.

II. RESONANCE ABSORPTION BY A LIGHT ISOTOPE AT THE ORIGIN

The amplitude for a transition of the vibrational state of the crystal when a photon of momentum $\mathbf{p}$ is absorbed by the light isotopic impurity is

$$\langle\{\beta_s\}|\exp\left[\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{u}(0)\right]|\{\alpha_s\}\rangle, \tag{1}$$

where $\mathbf{u}(0)$ is the displacement of the center of mass of the Mössbauer impurity from its equilibrium position

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[1] E. W. Montroll and R. B. Potts, Phys. Rev. **100**, 525 (1955).

[2] A. A. Maradudin, E. W. Montroll, G. H. Weiss, Robert Herman, and H. W. Milnes, *Green's Functions for Monatomic Simple Cubic Lattices* (Mémoires, Classe des Sciences, Académie Royale de Belgique, Bruxelles, 1960).

[3] S. V. Maleev, Zh. Eksperim. i Teor. Fiz. **39**, 891 (1960) [translation: Soviet Phys.—JETP **12**, 671 (1961)]. Others who have made similar suggestions at about the same time are B. Mozer and G. H. Vineyard, Bull. Am. Phys. Soc. **6**, 135 (1961); and W. M. Visscher, *The Mössbauer Effect* (John Wiley & Sons, Inc., New York, 1962).

[4] W. M. Visscher, Phys. Rev. **129**, 28 (1963).

[5] P. G. Klemens, Phys. Rev. **122**, 443 (1961).

[6] A. A. Maradudin, G. H. Weiss, and D. W. Jepsen, J. Math. Phys. **2**, 349 (1961).

[7] J. S. Langer, J. Math. Phys. **2**, 584 (1961).

at the origin and where $|\{\alpha_s\}\rangle$ and $|\{\beta_s\}\rangle$ are the initial and final-phonon states of the crystal. The amplitude is expressed in normal modes of a crystal of N atoms,

$$\exp\left[\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{u}(0)\right]$$
$$=\exp\left[i\sum_{\mathbf{k}}\frac{D_{\mathbf{k}}}{\sqrt{N}}(a_{\mathbf{k}}+a_{\mathbf{k}}^{\dagger})+iD_0(a_0+a_0^{\dagger})\right], \quad (2)$$

where $D_{\mathbf{k}}/\sqrt{N}$ and D_0 are the contributions to the displacement from the propagating and LM's, respectively, and the a's are creation and annihilation operators. In finding the cross section, the analysis is similar to that in the original work by Lamb[8] on neutron resonance absorption in a perfect crystal: the propagating modes are still those of the perfect crystal as are the corresponding initial and final states. The use of these unperturbed modes as an approximation is based on the fact that the nonlocalized, perturbed normal modes have amplitudes which are of the same order $1/\sqrt{N}$, in determining the displacement, $\mathbf{u}(0)$. The analysis departs from Lamb's in summing over the initial and final states of the LM. These sums must be done separately, because the amplitude of this mode is not weakened, as are the amplitudes of the propagating modes, by the factor, $1/\sqrt{N}$. The independence of the modes allows the separation. The cross section is then

$$W_0(\mathcal{E},T)$$
$$=\frac{\sigma_0'\Gamma}{A}\int_{-\infty}^{\infty}\left(\exp\left[i\mu\mathcal{E}-|\mu|\frac{\Gamma}{2}+g(\mu,T)\right]\right)$$
$$\times\Big(\sum_{\alpha_0,\beta_0}e^{-i\mu\hbar\omega_0(\beta_0-\alpha_0)}d(\alpha_0)\,|\langle\beta_0|e^{iD_0(a_0+a_0^{\dagger})}|\alpha_0\rangle|^2\Big)d\mu,$$

$$g(\mu,T)=\sum_s\frac{(\mathbf{p}\cdot\mathbf{e}_s)^2}{2M\hbar\omega_sN}[(\bar{\alpha}_s+1)\exp(-i\hbar\omega_s\mu)$$
$$+\bar{\alpha}_s\exp(i\hbar\omega_s\mu)-2\bar{\alpha}_s-1], \quad \bar{\alpha}_s=(e^{(\hbar\omega_s/kT)}-1), \quad (3)$$

where σ_0' is the resonance absorption cross section for the first excited state, energy E_0, of the impurity nucleus; E, the energy of the incoming photon; Γ, the total width of the nuclear excited state; $\mathcal{E}=E-E_0$, $d(\alpha_0)=(1-e^{(-\hbar\omega_0/kT)})e^{-\alpha_0(\hbar\omega_0/kT)}$ and ω_0 is the LM frequency. For $T=0$, we may set $\alpha_0=0$ and

$$|\langle\beta_0|e^{iD_0(a_0+a_0^{\dagger})}|0\rangle|^2$$
$$=\langle 0|e^{-iD_0(a_0+a_0^{\dagger})}|\beta_0\rangle\langle\beta_0|e^{iD_0(a_0+a_0^{\dagger})}|0\rangle.$$

The sum over final states is performed by means of their completeness.

$$\sum_{\beta_0}e^{-i\mu\hbar\omega_0\beta_0}|\langle\beta_0|e^{iD_0(a_0+a_0^{\dagger})}|0\rangle|^2$$
$$=\langle 0|e^{-iD_0(a_0+a_0^{\dagger})}e^{-i\mu\hbar\omega_0a_0^{\dagger}a_0}e^{iD_0(a_0+a_0^{\dagger})}|0\rangle. \quad (4)$$

[8] W. E. Lamb, Jr., Phys. Rev. **55**, 190 (1939).

The evaluation of this expectation value (Appendix II) gives

$$\langle\ \rangle_{0,0}=e^{-D_0^2}\exp[D_0^2e^{-i\mu\hbar\omega_0}]. \quad (5)$$

The absorption cross section, at $T=0$, is

$$W_0(\mathcal{E},0)$$
$$=\frac{\sigma_0'\Gamma}{4}e^{-D_0^2}\int_{-\infty}^{\infty}\exp\left[i\mu\mathcal{E}-|\mu|\frac{\Gamma}{2}+g(\mu,0)+D_0^2e^{-i\mu\hbar\omega_0}\right]d\mu$$
$$=\sum_{n=0}^{\infty}e^{-D_0^2}\frac{{D_0}^{2n}}{n!}W(\mathcal{E}-n\hbar\omega_0,0), \quad (6)$$

where $W(\mathcal{E},0)$ is the cross section for a perfect crystal. In Appendix I, D_0^2 is found to be 7×10^{-3}, so that the first two terms in the sum predominate,

$$W_0(\mathcal{E},0)=e^{-D_0^2}W(\mathcal{E},0)$$
$$+D_0^2e^{-D_0^2}W(\mathcal{E}-\hbar\omega_0\,0),+O(D_0^4). \quad (7)$$

Thus, the LM resonance is about 1/100 of the recoilless absorption, or about 10^4 b.

III. THE LOCALIZED MODE SPECTRUM OF THE DISORDERED CRYSTAL

Langer has calculated the vibration spectrum of a disordered linear chain, $\bar{g}(\omega)$, from

$$\bar{g}(\omega)=\frac{2\omega}{\pi}\lim_{\epsilon\to0}\lim_{N\to\infty}\frac{1}{3N}\,\mathrm{Im}\,\mathrm{Tr}\bar{D}(\omega^2+i\epsilon), \quad (8)$$

where $\bar{D}(\omega^2)$ is the inverse of the secular matrix of the disordered chain, by a perturbation theory in orders of the concentration, q, of impurities of mass M', less than M, the mass of the host atoms. To first order in q, a diagonal element of $\bar{D}$ is, for the simple cubic crystal,

$$\bar{D}_{\mathbf{k}}=[{\omega_{\mathbf{k}}}^2-\omega^2+G_{\mathbf{k}}^{(1)}(\omega^a)]^{-1}, \quad (9)$$

where ${\omega_{\mathbf{k}}}^2$ is an eigenvalue of the unperturbed secular matrix of the simple cubic crystal, with nearest neighbor forces and force constants, γ_j,

$${\omega_{\mathbf{k}}}^2=\sum_{j=1}^{3}\frac{2\gamma_1}{M}\left(1-\cos\frac{2\pi K_j}{N^{1/3}}\right),$$
$$(K_j=-\tfrac{1}{2}N^{1/3},\ -\tfrac{1}{2}N^{1/3}+1,\ \cdots,\ \tfrac{1}{2}N^{1/3}), \quad (10)$$

$$G_{\mathbf{k}}^{(1)}(\omega^2)=\frac{q\kappa{\omega_{\mathbf{k}}}^2}{1+(\kappa\omega^2/3N)\sum_{\mathbf{k}'}({\omega_{\mathbf{k}'}}^2-\omega^2)^{-1}},$$
$$\kappa=1-\frac{M'}{M}>0. \quad (11)$$

Substituting (10) into the sum over the unperturbed

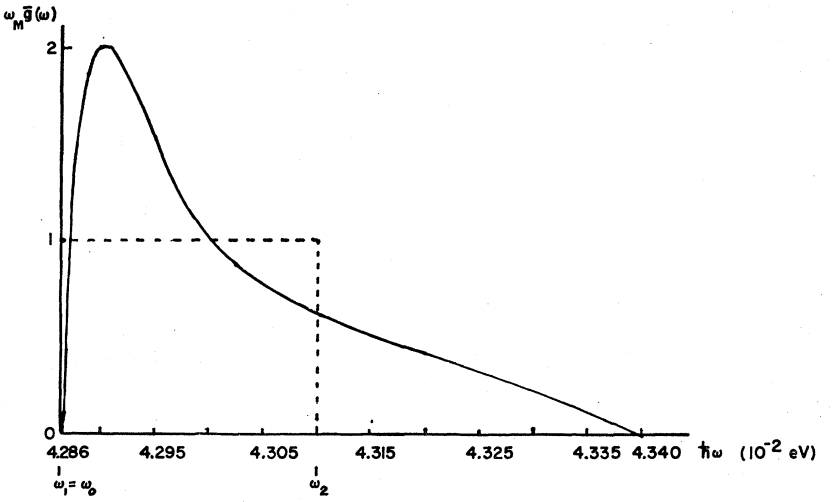

FIG. 1. LM spectrum for a disordered simple cubic crystal, with parameters $\kappa=0.4$, $q=0.01$, $\alpha=1$. For $\hbar\omega_M$, the Mössbauer effect fitted Debye energy for Fe^{57} of 4.22×10^{-2} eV is used. The dashed rectangle is the approximation employed in Sec. IV.

spectrum and passing to an integral as $N\to\infty$,

$$\frac{1}{3N}\sum_{\mathbf{k}'}(\omega_{\mathbf{k}'}{}^2-\omega^2)^{-1}\longrightarrow$$

$$-\frac{M}{2\gamma}\left\{\frac{1}{\pi^3}\int\int\int_0^\pi\frac{d^3k'}{(2+\alpha)\beta-\cos k_1'-\cos k_2'-\alpha\cos k_3'}\right\}. \tag{12}$$

For values of ω greater than the maximum frequency of the perfect simple cubic crystal, the expression in the brackets is tabulated as $I(0,0,0;\alpha;\beta)$, where $\gamma=\gamma_1=\gamma_2$, $\alpha=\gamma_3/\gamma$ the ratio of central to noncentral force constants, $\beta=2\omega^2/\omega_M{}^2-1$ and ω_M is the maximum unperturbed frequency. Thus,

$$G_{\mathbf{k}}{}^{(1)}=\frac{q\kappa\omega_{\mathbf{k}}{}^2}{1-(\kappa\omega^2M/2\gamma)I(0,0,0;\alpha;\beta)},\quad \omega>\omega_M \tag{13}$$

and

$$\bar{D}_{\mathbf{k}}(\omega^2+i\epsilon)=\frac{p}{f_{\mathbf{k}}{}^2-f^2p-i\epsilon},\quad f_{\mathbf{k}}{}^2=\frac{\omega_{\mathbf{k}}{}^2}{\omega_M{}^2},\quad f^2=\frac{\omega^2}{\omega_M{}^2}, \tag{14}$$

where

$$p=\frac{1-\kappa M\omega^2I/2\gamma}{1-\kappa M\omega^2I/2\gamma+q\kappa},\quad \omega>\omega_M. \tag{15}$$

To evaluate the trace of $\bar{D}$, the squared frequency function for the perfect cubic crystal, $G(\omega^2)$, is used to convert the sum to an integral.

$$\frac{1}{3N}\mathrm{Tr}\bar{D}(\omega^2+i\epsilon)=\int_0^1\frac{pG(\omega_M{}^2f_{\mathbf{k}}{}^2)}{f_{\mathbf{k}}{}^2-fp^2-i\epsilon}df_{\mathbf{k}}{}^2. \tag{16}$$

The imaginary part is just, $\pi pG(\omega^2p)$, and

$$\omega_M\bar{g}(\omega)=2fp\omega_M{}^2G(\omega_M{}^2fp^2),\quad \omega>\omega_M. \tag{17}$$

Referring to the table[2] for I and to a graphical representation[9] of $\omega_M{}^2G(\omega_M{}^2f^2p)$, $\alpha=1$, we find the spectrum shown in Fig. 1, for $q=0.01$, $\kappa=0.4$. The dashed figure was chosen to have almost the same area as the calculated spectrum, but is broadened to underestimate the cross section that will result from its use in the next section. The lower edge of the pulse coincides with the lowest frequency of the spectrum, which is the LM frequency found by Montroll for the case of the single light defect.

IV. ABSORPTION IN THE REGION OF THE LM SPECTRUM

The normalized spectrum found in the last part is taken to be a rectangular pulse of height $1/\omega_M$ over the interval (ω_1,ω_2). This is done to make the integration below simple. The probability that an absorbing nucleus has its LM in the interval $(\omega,\omega+d\omega)$ is

$$P(\omega)d\omega=\bar{g}d\omega\Big/\int_{\omega_1}^{\omega_2}\bar{g}d\omega=\frac{d\omega}{\Delta\omega},\quad \Delta\omega=\omega_2-\omega_1. \tag{18}$$

The cross section for absorption of a photon of energy $E_0+\mathcal{E}$ in the region of the LM spectrum is just the integral

$$\bar{W}(\mathcal{E},0)=\int_{\omega_1}^{\omega_2}W_0(\mathcal{E},0)P(\omega_0)d\omega_0. \tag{19}$$

$$\bar{W}(\mathcal{E},0)=e^{-D_0{}^2}W(\mathcal{E},0)+\frac{iD_0{}^2e^{-D_0{}^2}}{\hbar\Delta\omega}\frac{\sigma_0'\Gamma}{4}\int_{-\infty}^{\infty}\left(\exp\left[i\mu\mathcal{E}-|\mu|\frac{\Gamma}{2}+g\right]\right)\times\left(\frac{e^{-i\mu\hbar\omega_2}-e^{-i\mu\hbar\omega_1}}{\mu}\right)d\mu+O(D_0{}^4). \tag{20}$$

The first term is the absorption cross section for proc-

[9] E. W. Montroll, Am. Math. Monthly **61**, 46 (1954).

esses other than LM excitation. The second term represents processes in which only one LM can be excited. Higher orders permit the excitation of more than one for a given frequency in the LM band, and are negligible at $T=0$. The cross section for an $\mathcal{E}=4.3\times10^{-2}$ eV photon is calculated in Appendix III for LM excitation and continuum excitation.

V. SUMMARY

The LM spectrum of the disordered simple cubic crystal was related in Eq. (17), to the squared frequency distribution of the perfect crystal, the function $p(\omega^2)$ determining the shape of the spectrum. From (8) and (16) the width of this spectrum is determined since (16) can have an imaginary part only when f^2p lies between 0 and 1. The lower bound is the Montroll localized mode frequency, f_0, and the upper end of the band is reached when $f^2p=1$, because of the dependence upon the squared frequency distribution. From (15) one can see that the band narrows down to f_0 as the concentration q is reduced or as the mass parameter κ approaches its least permitted value for which a LM can appear.[2] The value $\kappa=0.4$ was chosen to make reasonable the appearance of such modes in a real crystal. The resulting band has a width at half-maximum[10] of 10^{-4} eV.

Although the absorption cross section for LM excitation in the case of a single absorbing light impurity is large, about[4] 10^4 b, the widening of the vibrational line produced by concentrations of such nuclei, reduces the cross section to the order of a barn. Diluting the concentration as a means of narrowing the bandwidth would probably not increase the cross section, because the anharmonic attenuation of the LM's produces a comparable widening of the band, 10^{-4} or 10^{-3} eV.[5] The ratio of LM band excited absorption to continuum excited absorption is 10^3, neglecting the anharmonic widening of the LM states. Even without phonon interactions, the background of atomic absorption, 10^3 b, prevents the use of absorbers of sufficient thickness for a detectable dip in the transmission through them. A 1 mm absorber reduces by $1/e$ of its initial value, the intensity of transmitted 14.4 keV photons. The absorber, assumed to have a concentration of 10^{20} Fe^{57} nuclei, in a host crystal of atomic mass, ~95, has an LM cross section of 0.36 b, which causes only a 0.01% dip in the transmitted intensity.

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APPENDIX I

The LM contribution to the displacement is

$$u_0^\alpha(\mathbf{R})=\epsilon_0^\alpha u_0^\alpha(0)\frac{(M-M')\omega_0^\alpha}{\sum\gamma_i}\mathcal{G}(\mathbf{R})\left(\frac{\hbar}{2\omega_0}\right)^{1/2}\times(a_0+a_0^\dagger), \quad (21)$$

where $\mathbf{R}$ is the lattice vector; ϵ_0^α, the α component of the LM polarization and $\mathcal{G}(\mathbf{R})$ is the Montroll Green's function. The normality of the transformation to normal coordinates requires

$$16M'[u_0^\alpha(0)]^2\kappa f^4\left[\mathcal{G}^2(0)+\sum_{\mathbf{k}\neq0}\frac{M}{M'}\mathcal{G}^2(\mathbf{R})\right]=1. \quad (22)$$

For $\kappa=0.4$, $f_0^4=1.063$ and with $\alpha=1$

$$\mathcal{G}^2(\mathbf{R})=(9/4)I^\alpha(\mathbf{R};1;\beta_0). \quad (23)$$

Since f^4I is a decreasing function of f in the LM band, f_0 is chosen to calculate $u_0^\alpha(0)$. The band is sufficiently narrow to permit the use of $u_0^\alpha(0)$, underestimated in this manner, for all the LM frequencies. The sum in (22) is found from the Green's function tables for $|\mathbf{R}|\leq\sqrt{14}$ and from an asymptotic expression when $|\mathbf{R}|>\sqrt{14}$:

$$u_0^\alpha(0)\approx0.69/\sqrt{M'}.$$

Because f_0 satisfies $4\kappa f_0^2\mathcal{G}(0)=1$, we may write

$$u_0^\alpha(\mathbf{R})=\epsilon_0^\alpha(0.69)\frac{\mathcal{G}(\mathbf{R})}{\mathcal{G}(0)}\left(\frac{\hbar}{2M'\omega_0}\right)^{1/2}(a_0+a_0^\dagger). \quad (24)$$

The amplitude of the LM is of order 1, whereas that of a propagating mode is of order $1/\sqrt{N}$. From the estimate above of $u_0^\alpha(0)$, we find for D_0^2, $D_0^2=[u_0^\alpha(0)]^2\times(\mathbf{p}^2/6M'\hbar\omega_0)=7\times10^{-3}$ for the 14.4-keV photons of Fe^{57} in an isotropic crystal.

APPENDIX II

Let

$$v|0\rangle=\exp[iD_0(a_0+a_0^\dagger)]|0\rangle. \quad (25)$$

Since $[a_0,a_0^\dagger]=1$, the identity,[11] $e^{x+y}=e^{-\frac{1}{2}[x,y]}e^x\cdot e^y$, where the commutator $[x,y]$ is a c number, may be used to factor (25);

$$v|0\rangle=e^{-(D_0^2/2)}e^{iD_0a^\dagger}e^{iD_0a_0}|0\rangle. \quad (26)$$

Expanding the last factor on the right, we have

$$v|0\rangle=e^{-D_0^2/2}e^{iD_0a_0^\dagger}|0\rangle, \quad (27)$$

[10] A. A. Maradudin, P. Mazur, E. W. Montroll, and G. H. Weiss, Rev. Mod. Phys. **30**, 175 (1958). This article contains a simple, probability argument for the width of the LM impurity band. The estimate for the parameters chosen in the present paper is an order of magnitude larger, about 10^{-3} eV; possibly, their estimate is larger because it permits smaller pair separations than a lattice constant.

[11] H. F. Baker, Proc. Math. Soc. (London) **3**, 24 (1905); F. Hausdorff, *Die Symbolische Exponentialformel in Gruppentheorie, Berichte der Saechsischen Akademie der Wissenschaften* (Math. Phys. Kl., Leipzig, 1906), Vol. 58, pp. 19–48 (1906).

or

$$v|0\rangle=e^{-D_0^2/2}\sum_{r=0}^{\infty}\frac{(iD_0)^r}{r!}\sqrt{r!}\,|r\rangle.$$

The expectation value becomes

$$\langle 0|v^+e^{-i\mu\hbar\omega_0 a_0^\dagger a_0}v|0\rangle$$

$$=e^{-D_0^2}\sum_{r,s=0}^{\infty}\frac{(i)^r(-i)^sD_0^{r+s}}{(r!s!)^{1/2}}e^{-i\mu\hbar\omega_0 r}\langle s|r\rangle \quad (28)$$

and by the orthonormality of the phonon states the expectation value simplifies to

$$\langle\ \rangle_{0,0}=e^{-D_0^2}\sum_{r=0}^{\infty}\frac{D_0^{2r}}{r!}e^{-i\mu\hbar\omega_0 r} \quad (29)$$

or

$$\langle\ \rangle_{0,0}=e^{-D_0^2}\exp[D_0^2e^{-i\mu\hbar\omega_0}].$$

APPENDIX III

The function $g(\mu,0)$ in (20) is obtained by using a Debye spectrum to pass from the spectral sum, shown in Eq. (3), to an integral.

$$g_D(\mu,0)=\frac{3R'(1-\kappa)}{(\hbar\omega_D)^3}$$

$$\times\left[\frac{i\hbar\omega_De^{-i\hbar\omega_D\mu}}{\mu}+\frac{e^{-i\mu\hbar\omega_D}-1}{\mu^2}-\frac{(\hbar\omega_D)^2}{2}\right]. \quad (30)$$

$R'=P^2/2M'=0.19\times10^{-2}$ eV for Fe^{57}. A Debye temperature of 490°K (4.22×10^{-2} eV), as determined by the Mössbauer effect is chosen. For convenience call

$$\delta=\frac{3R'(1-\kappa)}{(\hbar\omega_D)^3}\approx45.4,$$

$$A=\frac{\sigma_0'\Gamma}{2\hbar\omega_D}\exp[-D_0^2-\delta(\hbar\omega_D)^2/2]\approx7.72\times10^{-2},$$

$$B=\frac{\sigma_0'\Gamma}{2\hbar\Delta\omega}D_0^2\exp[-D_0^2-\delta(\hbar\omega_D)^2/2]\approx1.14\times10^{-1}.$$

From (20)

$$\bar{W}(\mathcal{E},0)$$

$$=A\int_0^{\infty}\left(\exp\left\{-\frac{x\Gamma}{2\hbar\omega_D}+\frac{\delta(\hbar\omega_D)^2}{x^2}(x\sin x+\cos x-1)\right\}\right)$$

$$\times\left\{\cos\left[x\frac{\mathcal{E}}{\hbar\omega_D}+\frac{\delta(\hbar\omega_D)^2}{x^2}(x\cos x-\sin x)\right]\right\}dx$$

$$+B\int_0^{\infty}\left\{\exp\left[-\frac{x\Gamma}{2\hbar\omega_D}+\frac{\delta(\hbar\omega_D)^2}{x^2}(x\sin x+\cos x-1)\right]\right\}$$

$$\times\left\{\sin\left[x\left(\frac{\hbar\omega_2-\mathcal{E}}{\hbar\omega_D}\right)-\frac{\delta(\hbar\omega_D)^2}{x^2}(x\cos x-\sin x)\right]\right.$$

$$\left.+\sin\left[x\left(\frac{\mathcal{E}-\hbar\omega_1}{\hbar\omega_D}\right)+\frac{\delta(\hbar\omega_D)^2}{x^2}(x\cos x-\sin x)\right]\right\}\frac{dx}{x}. \quad (31)$$

Choosing the value $\mathcal{E}=4.30\times10^{-2}$ eV, halfway between ω_1 and ω_2, we may approximate $\bar{W}(E,0)$ by dividing the range of integration into two intervals, (0,0.1) and (0.1, ∞). In the first interval the trigonometric contributions to the exponential factor and to the cosine and sine factors may be expanded. In the second interval Laplace transforms are used to advantage.

The integral whose coefficient is A in (31), gives the contribution to $\bar{W}$ from absorption without LM excitation. Its value is determined in the first range of integration (32). Absorption by means of LM excitation is measured by the integral with coefficient B, which is determined in the second interval (0.1, ∞) by a Laplace transform.

$$A\left[(1.04)\int_0^{0.1}\cos(0.993)x\,dx\right.$$

$$\left.-(0.01)\int_0^{0.1}x^2\cos(0.993)x\,dx-\int_0^{0.1}\cos(1.02)x\,dx\right]$$

$$\approx7.72\times10^{-2}[4\times10^{-3}]\approx0.31\text{ mb}, \quad (32)$$

$$B\,\mathrm{LT}\left\{\frac{2\sin(0.0024)x}{x}\right\}_{s=5.4\times10^{-8}}$$

$$\approx1.14\times10^{-1}\pi\approx0.36\text{ b}. \quad (33)$$

The ratio of LM absorption to continuum absorption is, therefore, about 10^3, at $T=0$.

Altering Γ to include the anharmonic width of the LM phonons, we find from (33), for $\Gamma'=10^{-4}$ eV,

$$s'=\frac{\Gamma'}{2\hbar\omega_D},\quad \bar{W}_{\mathrm{LM}}=B\,\mathrm{LT}\left\{\frac{2\sin(0.0024)x}{x}\right\}_{s'}\approx0.125\text{ b},$$

and

$$\bar{W}_{\mathrm{LM}}/\bar{W}_{\mathrm{CONT}}\approx4\times10^2.$$