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THE MÖSSBAUER EFFECT FOR AN IMPURITY NUCLEUS IN A CRYSTAL. I

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Using the solution of the problem of vibration of an impurity nucleus located at a lattice site in a crystal, we determine the probability for the Mössbauer effect on such an impurity nucleus. In addition to the change in mass, we also take account of the change in the force constants for the impurity site. The roles of the discrete and the quasicontinuous phonon spectra are analyzed. The case of a cubic crystal is considered in detail. The final formulas depend on the properties of the host lattice only via the frequency distribution function for the phonon spectrum. Expressions for the effect are given explicitly for the two limiting cases where the mass of the impurity atom is small or large compared to the mass of the atoms of the host lattice.

1. INTRODUCTION

So far, in treating the Mössbauer effect in solids, only the case of a regular crystal lattice has been studied.[1-4] It would be of great interest to analyze the probability of resonant emission (or absorption) of γ quanta when the radiator is a foreign nucleus in a host lattice. The solution of this problem is faced with considerable difficulties, mainly related to the need for determining the nature of the vibrations of the impurity atom in the crystal. Since the presence of the impurity atom destroys the translational symmetry, the nature of the difficulties which arise in the general case is obvious.

If the introduction of the impurity atom does not change the harmonic character of the forces, the solution of the problem of normal vibrations gives a spectrum which we know has, in general, the form of a set of energy bands which are equivalent to the bands in the ideal crystal, as well as a set of discrete levels. At first glance it may seem that, since the number of discrete levels is $\sim 1/N$ of the total number of normal modes (where N is the number of atoms in the crystal), they should be of no importance. But this is not the case. Actually the spatial localization of the oscillations corresponding to discrete levels has the consequence that a considerable part of the energy of these oscillations is associated with the motion of the impurity atom. On the other hand, for a nonlocalized vibration, the energy assignable to a single atom is of order $1/N$. Thus, in general, the contributions of the discrete levels and the quasi-continuous spectrum to the displacement of the impurity are of the same order.

Although the quasi-continuous spectrum is only slightly changed (the levels suffer a percentage displacement of order $1/N$), the amplitudes of the normal vibrations in this spectrum for the impurity atom may be considerably different from the corresponding amplitudes in the regular lattice. As we shall see later, finding these amplitudes is probably the main complication in the problem.

The problem of lattice vibrations when impurity atoms are present has been treated in many papers. Of these we should mention first the well-known series of papers by I. Lifshitz (especially [5]) and the work of Montroll and his co-workers.[6] Unfortunately in all the work on this problem the spectrum and the scattering of waves by the impurity center is analyzed in detail, but there is practically no analysis of the displacement of the impurity atom itself, especially in the three-dimensional case.

The present paper attempts to determine the probability for the Mössbauer effect on an isolated impurity atom in a lattice (small concentration of impurity). It is assumed that the impurity atom is at a lattice site. In addition to the change in mass, we also take into account the change in the force constants associated with the impurity site; the percentage change is assumed to be the same for all the constants.

2. PROBABILITY FOR THE MÖSSBAUER EFFECT

It is well known (cf., for example, [2,7]) that the normalized probability of recoilless resonance absorption (emission) by a nucleus located at the origin of coordinates in a crystal is given by the square of the matrix element

$$M = \langle\{n\}\,|\,e^{i\mathbf{k}\mathbf{u}}\,|\,\{n\}\rangle, \tag{2.1}$$

where **u** is the displacement of the particular atom, **k** is the wave vector of the γ quantum, and $\{n\}$ is the set of occupation numbers for the vibration spectrum of the crystal.

We resolve **u** into displacements $\mathbf{u}_1$ in the quasi-continuous spectrum and $\mathbf{u}_2$ in the discrete spectrum:

$$\mathbf{u} = \mathbf{u}_1 + \mathbf{u}_2 \tag{2.2}$$

and write the expansion of $\mathbf{u}_1$ in normal modes which we label with an index β:

$$\mathbf{u}_1 = \sum_\beta \mathbf{u}_{1\beta}. \tag{2.3}$$

We expand $\exp(i\mathbf{k}\cdot\mathbf{u}_{1\beta})$ in series, keeping the first three terms in the expansion ($\mathbf{u}_{1\beta} \sim 1/\sqrt{N}$). Using the fact that the oscillators are independent, we find for the probability of the Mössbauer effect

$$W = W_1 W_2; \tag{2.4}$$

$$W_1 = \exp\Big\{-\sum_\beta \overline{|\mathbf{k}\mathbf{u}_{1\beta}|^2}\Big\}, \tag{2.5}$$

$$W_2 = \overline{|\langle[n]\,|\,e^{i\mathbf{k}\mathbf{u}_2}|[n]\rangle|^2}, \tag{2.5'}$$

where $[n]$ is the set of occupation numbers referring to the discrete spectrum. The bar in (2.5) denotes an average over the equilibrium phonon distribution.

According to (2.4), W splits into a product of two probabilities, which determine the probabilities that there is no excitation in the quasi-continuous and the discrete spectrum, respectively.

3. VIBRATIONS OF THE IMPURITY ATOM

Consider a lattice with one atom in the unit cell and assume that there is an impurity atom at one of the lattice sites. The equation of motion has the form (with the impurity atom at the origin):

$$m_\mathbf{n}\ddot{u}^i_\mathbf{n} = -\sum_{\mathbf{n}'} A^{ik}(\mathbf{r}_\mathbf{n}, \mathbf{r}_{\mathbf{n}'})\, u^k_{\mathbf{n}'}, \quad m_\mathbf{n} = m(1 - \varepsilon\delta_{\mathbf{n}0}); \tag{3.1}$$

$$\varepsilon = (m - m')/m, \tag{3.2}$$

where m′ is the mass of the impurity atom, m the mass of the atoms of the host lattice. The rest of the notation is standard; we sum over repeated superscripts. Assuming that the percentage changes in all the force constants for the impurity site are the same, we have

$$A^{ik}(\mathbf{r}_\mathbf{n}, \mathbf{r}_{\mathbf{n}'}) = A^{ik}_0(\mathbf{r}_{\mathbf{n}'} - \mathbf{r}_\mathbf{n}), \quad n,\ n' \neq 0;$$

$$A^{ik}(0, \mathbf{r}_\mathbf{n}) = A^{ik}_0(\mathbf{r}_\mathbf{n})\,(1 - \gamma), \quad A^{ik}(\mathbf{r}_\mathbf{n}, 0) = A^{ik}_0(-\mathbf{r}_\mathbf{n})\,(1 - \gamma). \tag{3.3}$$

Here the index 0 denotes the force constants for the original regular lattice.

If we look for a solution of (3.1) in the form

$$u^i_\mathbf{n} = w^i_\mathbf{n}\, e^{-i\omega t}, \tag{3.4}$$

we find, using (3.3),

$$m\omega^2(1 - \varepsilon\delta_{\mathbf{n}0})\, w^i_\mathbf{n} = \sum_{\mathbf{n}'} A^{ik}_0(\mathbf{r}_{\mathbf{n}'} - \mathbf{r}_\mathbf{n})\, w^k_{\mathbf{n}'}$$

$$- \gamma\,\Big[\delta_{\mathbf{n}0}\sum_{\mathbf{n}'} A^{ik}_0(\mathbf{r}_{\mathbf{n}'})\, w^k_{\mathbf{n}'} + A^{ik}_0(-\mathbf{r}_\mathbf{n})\, w^k_0 - \delta_{\mathbf{n}0} A^{ik}_0(0)\, w^k_0\Big]. \tag{3.5}$$

If we set $\epsilon = \gamma = 0$ in (3.5), we get the system of equations for the regular lattice. The complete set of 3N orthonormal functions corresponding to the solution of this system has the form (cf., for example, [8])

$$N^{-1/2} e^i(\mathbf{f}, \alpha)\, e^{i\mathbf{f}\mathbf{r}_\mathbf{n}}, \quad \alpha = 1, 2, 3; \tag{3.6}$$

$$e^{i*}(\mathbf{f}, \alpha)\, e^i(\mathbf{f}, \alpha') = \delta_{\alpha\alpha'}, \quad \sum_\alpha e^i(\mathbf{f}, \alpha)\, e^k(\mathbf{f}, \alpha) = \delta^{ik}. \tag{3.6'}$$

The eigenvalues $\omega_0^2(\mathbf{f}, \alpha)$ and the projections of the unit vector $\mathbf{e}(\mathbf{f}, \alpha)$ for each **f** and each branch number α are determined by the system of equations

$$m\omega_0^2(\mathbf{f}, \alpha)\, e^i(\mathbf{f}, \alpha) = \sum_\mathbf{n} A^{ik}_0(\mathbf{r}_\mathbf{n})\, e^{i\mathbf{f}\mathbf{r}_\mathbf{n}}\, e^k(\mathbf{f}, \alpha). \tag{3.7}$$

The N values of the wave vector **f** in (3.6) are distributed uniformly over the reciprocal lattice space in accordance with the usual cyclic boundary conditions. [8]

We expand $w^i_\mathbf{n}$ in the functions (3.6):

$$w^i_\mathbf{n} = N^{-1/2}\sum_{\mathbf{f},\alpha} C(\mathbf{f}, \alpha)\, e^i(\mathbf{f}, \alpha)\, e^{i\mathbf{f}\mathbf{r}_\mathbf{n}} \tag{3.8}$$

and substitute (3.8) in (3.5). After some simple transformations we find

$$C(\mathbf{f}, \alpha)\,[\omega^2 - \omega_0^2(\mathbf{f}, \alpha)]$$

$$= N^{-1/2}\,\Big[\varepsilon\omega^2 w^i_0 e^{i*}(\mathbf{f}, \alpha) - \gamma\omega^2 a^i e^{i*}(\mathbf{f}, \alpha)$$

$$- \gamma\omega_0^2(\mathbf{f}, \alpha)\, w^i_0 e^{i*}(\mathbf{f}, \alpha) + \frac{\gamma}{m} A^{ik}_0(0)\, w^k_0 e^{i*}(\mathbf{f}, \alpha)\Big]; \tag{3.9}$$

$$a^i = \frac{1}{\sqrt{N}}\frac{1}{\omega^2}\sum_{\mathbf{f},\alpha} C(\mathbf{f}, \alpha)\,\omega_0^2(\mathbf{f}, \alpha)\, e^i(\mathbf{f}, \alpha), \tag{3.10}$$

$$w^i_0 = \frac{1}{\sqrt{N}}\sum_{\mathbf{f},\alpha} C(\mathbf{f}, \alpha)\, e^i(\mathbf{f}, \alpha). \tag{3.11}$$

If we set $\mathbf{n} = 0$ in (3.5), substitution of (3.8) gives

$$m(1 - \varepsilon)\,\omega^2 w^i_0 = m a^i\omega^2 - \gamma m a^i\,\omega^2.$$

Then

$$a^i = (1 - \varepsilon)\, w^i_0/(1 - \gamma). \tag{3.12}$$

If some of the frequencies in the perturbed spectrum are rigorously the same as frequencies in the unperturbed spectrum, then according to (3.9) and (3.12) the corresponding displacements of the impurity atom $\mathbf{w}_0$ are equal to zero. If there is a recoil at the moment of decay, these frequencies cannot be excited and consequently they contribute nothing to (2.4).

For all other frequencies in the perturbed spectrum we have from (3.8) and (3.9):

$$w_{\mathbf{n}}^l = w_0^k \frac{1}{N} \sum_{\mathbf{f},\,\alpha} \frac{e^l(\mathbf{f},\alpha)\, e^{i*}(\mathbf{f},\alpha)}{\omega^2 - \omega_0^2(\mathbf{f},\alpha)} \Big[\omega^2 \Big(\varepsilon - \gamma \frac{1-\varepsilon}{1-\gamma}\Big)\delta^{ik} - \gamma\omega_0^2(\mathbf{f},\alpha)\,\delta^{ik} + \frac{\gamma}{m} A_0^{ik}(0)\Big]\, e^{i\mathbf{f}\mathbf{r}_{\mathbf{n}}}.$$

We transform this expression, using the relation [cf. (3.6′)]

$$\sum_{\mathbf{f},\,\alpha} e^{i*}(\mathbf{f},\alpha)\, e^l(\mathbf{f},\alpha)\, e^{i\mathbf{f}\mathbf{r}_{\mathbf{n}}} = N\delta^{il}\,\delta_{\mathbf{n}0}.$$

Finally we get

$$w_{\mathbf{n}}^l(1 - \gamma\delta_{\mathbf{n}0}) = w_0^k \frac{\omega^2}{N} B^{ik} \sum_{\mathbf{f},\,\alpha} \frac{e^l(\mathbf{f},\alpha)\, e^{i*}(\mathbf{f},\alpha)}{\omega^2 - \omega_0^2(\mathbf{f},\alpha)}\, e^{i\mathbf{f}\mathbf{r}_{\mathbf{n}}}, \quad (3.13)$$

$$B^{ik} = \Big(\frac{\varepsilon-\gamma}{1-\gamma} - \gamma\Big)\delta^{ik} + \frac{\gamma}{m\omega^2} A_0^{ik}(0). \quad (3.14)$$

Let us set $\mathbf{n} = 0$. It is easy to show that then the tensor on the right side of (3.13) is real. Because of this the quantities $\mathrm{w}_0^{\mathrm{i}}$, which are the solution of the system of equations, can be taken to be real. We introduce the notation

$$\mathbf{w}_0 = \mathbf{j}w_0 \quad (3.15)$$

(where $\mathbf{j}$ is a unit vector). As a result we get a system of equations which enable us to determine the frequencies of the perturbed spectrum and the corresponding polarization vectors $\mathbf{j}$:

$$j^l = D^{lk}(\omega^2)\, j^k; \quad (3.16)$$

$$D^{lk} = \frac{\omega^2}{N(1-\gamma)} B^{ik} \sum_{\mathbf{f},\alpha} \frac{e^l(\mathbf{f},\alpha)\, e^{i*}(\mathbf{f},\alpha)}{\omega^2 - \omega_0^2(\mathbf{f},\alpha)}. \quad (3.17)$$

It can be shown that the functions (3.13) corresponding to different levels of the perturbed spectrum are orthogonalized according to the condition

$$\sum_{\mathbf{n}} m_{\mathbf{n}} w_{\mathbf{n}}^{l}(\omega_p)\, w_{\mathbf{n}}^{l}(\omega_{p'}) = 0 \text{ for } p \neq p'.$$

If we now write the total energy of the system, it splits in an obvious way into a sum of energies corresponding to the independent vibrations with frequencies ω_p. Using (3.6) and (3.16), we then have for the shifted frequencies,

$$T_p = \tfrac{1}{2} m\omega_p^2\, w_0^2(\omega_p) \times \Big[B^{ik} B^{st}\, j^k j^t\, \frac{\omega_p^4}{N} \sum_{\mathbf{f},\,\alpha} \frac{e^{i*}(\mathbf{f},\alpha)\, e^{s}(\mathbf{f},\alpha)}{(\omega_p^2 - \omega_0^2)^2} + 2\gamma - \gamma^2 - \varepsilon\Big]. \quad (3.18)$$

We multiply (3.16) by B^{ls}, differentiate both sides of the equation with respect to ϵ for fixed γ, and multiply the result by j^{s}. After some simple transformations we arrive at the relation

$$B^{ik} B^{st}\, j^k j^t \Big(\frac{\partial\omega_p^2}{\partial\varepsilon}\Big)_{\gamma} \frac{\omega_p^4}{N} \sum_{\mathbf{f},\,\alpha} \frac{e^{i*}(\mathbf{f},\alpha)\; e^{s}(\mathbf{f},\alpha)}{(\omega_p^2 - \omega_0^2)^2} = (\partial\omega_p^2/\partial\varepsilon)_{\gamma}(\varepsilon - 2\gamma + \gamma^2) + \omega_p^2.$$

Comparing this expression with (3.18), we find

$$T_p = \tfrac{1}{2} m\omega_p^2\, w_0^2(\omega_p)[(\partial \ln \omega_p^2 / \partial\varepsilon)_{\gamma}]^{-1}. \quad (3.19)$$

We find the values of w_0^2 by equating T_{p} to the energy $\hbar\omega_{\mathrm{p}}(\mathrm{n} + \frac{1}{2})$ of the normal mode:

$$w_0^2(\omega_p) = \frac{2\hbar(n + {}^1\!/_2)}{m\omega_p} \Big(\frac{\partial \ln \omega_p^2}{\partial\varepsilon}\Big)_{\gamma}. \quad (3.20)$$

We introduce the real normal coordinates

$$q_p = w_0 \sqrt{m}[(\partial \ln \omega_p^2 / \partial\varepsilon)_{\gamma}]^{-1/2} \cos\omega_p t.$$

The displacement of the impurity atom in the p-th normal mode is given by

$$\mathbf{u}_p = \mathbf{j}_p\, [(\partial \ln \omega_p^2/\partial\varepsilon)_{\gamma}]^{1/2}\, m^{-1/2}\, q_p. \quad (3.21)$$

Using (3.21) we can immediately find the expression for the probability that there is no excitation of phonons of the quasi-continuous spectrum during recoil [cf. (2.5)]:

$$W_1 = \exp\Big\{-\sum_p \frac{R}{\hbar\omega_p}(\varkappa\mathbf{j}_p)^2 \Big(\frac{\partial \ln \omega_p^2}{\partial\varepsilon}\Big)_{\gamma}(2\bar{n}(\omega_p) + 1)\Big\}. \quad (3.22)$$

Here R is the recoil energy, taken with the mass of the atom of the host lattice:

$$R = \hbar^2 k^2/2m, \quad \varkappa = \mathbf{k}/k. \quad (3.23)$$

The quantity $\bar{\mathrm{n}}$ denotes the equilibrium value corresponding to the temperature of the crystal.

We shall determine W_2 (2.5′) for an arbitrary relation between R and the energies of the discrete levels.* To find the matrix element, we can use the general expression obtained by Bloch and Nordsieck:[9]

$$\langle n_p|\exp\Big(i\sqrt{\frac{\omega_p}{\hbar}}\, a_p q_p\Big)|n_p\rangle = \exp(-a_p^2/4)\, n_p! \sum_{\nu=0}^{n_p} \frac{(-a_p^2/2)^{\nu}}{(n_p - \nu)!\,(\nu!)^2}. \quad (3.24)$$

Then, remembering (3.21), we find

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*We note that in the quasi-continuous spectrum $\partial \ln \omega_{\mathrm{p}}^2/\partial\varepsilon \sim 1/N$, whereas these quantities do not depend on N in the discrete spectrum.

$$W_2 = \exp\left\{-\sum_l \frac{R}{\hbar\omega_l}(\varkappa \mathbf{j}_l)^2\left(\frac{\partial \ln \omega_l^2}{\partial \varepsilon}\right)_\gamma\right\}$$
$$\times \prod_s \left[\sum_{\nu=0}^{n_s} \frac{n_s!}{(n_s-\nu)!\,(\nu!)^2}\left(-\frac{R}{\hbar\omega_s}(\varkappa \mathbf{j}_s)^2\left(\frac{\partial \ln \omega_s^2}{\partial \varepsilon}\right)_\gamma\right)^\nu\right]^2. \tag{3.25}$$

Here the summation extends over discrete levels only.

If the temperature is sufficiently low so that for the discrete frequencies $\bar{n} \ll 1$ (for $T/\Theta \ll 1$, this is surely the case), then expression (3.25) can be simplified considerably:

$$W_2 = \exp\left\{-\sum \frac{R}{\hbar\omega_l}(\varkappa \mathbf{j}_l)^2\left(\frac{\partial \ln \omega_l^2}{\partial \varepsilon}\right)_\gamma\right\}$$
$$\times \prod_s \left\{1-2\left[\frac{R}{\hbar\omega_s}(\varkappa \mathbf{j}_s)^2\left(\frac{\partial \ln \omega_s^2}{\partial \varepsilon}\right)_\gamma\right.\right.$$
$$\left.\left.-\frac{1}{2}\left(\frac{R}{\hbar\omega_s}\right)^2(\varkappa \mathbf{j}_s)^4\left(\frac{\partial \ln \omega_s^2}{\partial \varepsilon}\right)_\gamma^2\right]\bar{n}(\omega_s)\right\}. \tag{3.26}$$

If in addition

$$\frac{R}{\hbar\omega_s}(\varkappa \mathbf{j}_s)^2\left(\frac{\partial \ln \omega_s^2}{\partial \varepsilon}\right)_\gamma \ll 1,$$

then (3.26) goes over into an expression of the same form as (3.22).

Expressions (3.22) and (3.25)—(3.26) in principle solve the problem. But one should not be deceived by their simplicity, since a rigorous determination of $(\partial \ln \omega_s^2/\partial\epsilon)_\gamma$ and $\mathbf{j}_p$ requires the solution of the system (3.16).

4. INFLUENCE OF THE DISCRETE SPECTRUM ON THE MÖSSBAUER EFFECT

Now let us turn to Eq. (3.16). The tensor

$$T^{ll}(\omega^2) = \frac{1}{N}\sum_{\mathbf{f},\alpha}\frac{e^l(\mathbf{f},\alpha)\,e^{l*}(\mathbf{f},\alpha)}{\omega^2-\omega_0^2(\mathbf{f},\alpha)}$$

which appears in (3.17) must have the symmetry of the original crystal. We limit ourselves to the case of a cubic lattice. Then

$$T^{ll}(\omega^2) = \delta^{ll}\frac{1}{3N}\sum_{\mathbf{f},\alpha}\frac{1}{\omega^2-\omega_0^2(\mathbf{f},\alpha)}. \tag{4.1}$$

We substitute this value in (3.17) and get

$$D^{lk} = \frac{\omega^2}{3N(1-\gamma)}B^{lk}\sum_{\mathbf{f},\alpha}\frac{1}{\omega^2-\omega_0^2(\mathbf{f},\alpha)}. \tag{4.2}$$

The force constant $A_0^{lk}(0)$ appears in the expression (3.14) for B^{lk}. To determine this quantity we use Eq. (3.7) for the vibrations of the regular lattice. We multiply (3.7) by $e^{l*}(\mathbf{f},\alpha)$ and sum over f and α. Using (3.6′), we find

$$A_0^{ll}(0) = \frac{m}{N}\sum_{\mathbf{f},\alpha}\omega_0^2(\mathbf{f},\alpha)\,e^l(\mathbf{f},\alpha)\,e^{l*}(\mathbf{f},\alpha). \tag{4.3}$$

In the case of a cubic crystal

$$A_0^{ll}(0) = \delta^{ll}\,m\,\langle\omega_0^2\rangle, \tag{4.4}$$

where $\langle\ldots\rangle$ denotes an average over the phonon spectrum of the regular crystal.

We substitute (4.4) in (3.14). We insert the transformed expression for B^{lk} into (4.2). Substituting the resulting expression in (3.16), we get an equation for determining the displaced frequencies:

$$1 = \frac{\omega^2}{3N(1-\gamma)}\left[\frac{\varepsilon-\gamma}{1-\gamma}-\gamma\left(1-\frac{\langle\omega_0^2\rangle}{\omega^2}\right)\right]\sum_{\mathbf{f},\alpha}\frac{1}{\omega^2-\omega_0^2(\mathbf{f},\alpha)}. \tag{4.5}$$

Let us consider the case of the discrete frequencies. Since $\omega^2 \geq \omega_{0\,\mathrm{max}}^2$, on the right side of (4.5), for $N \to \infty$ we can change over from summation to integration. Introducing the normalized frequency distribution function $g(\omega_0^2)$, we get an equation for determining the threefold degenerate discrete frequency in the form

$$1 = \frac{1}{1-\gamma}\left[\frac{\varepsilon-\gamma}{1-\gamma}-\gamma\left(1-\frac{\langle\omega_0^2\rangle}{\omega^2}\right)\right]\omega^2\int_0^{\omega_0^2\,max}\frac{g(\omega_0^2)\,d\omega_0^2}{\omega^2-\omega_0^2}. \tag{4.6}$$

For $\gamma = 0$, Eq. (4.6) goes over into the equation obtained by I. Lifshitz.[5]

In the three-dimensional case, the integral appearing in (4.6) has a finite value for $\omega^2 = \omega_{0\,\mathrm{max}}^2$. Because of this, the discrete frequency appears only under the conditions

$$b(\omega_{0max}^2) > \left[\int_0^1 \frac{g(x)\,dx}{1-x}\right]^{-1}, \tag{4.7}$$

$$b(\omega^2) = \frac{1}{1-\gamma}\left[\frac{\varepsilon-\gamma}{1-\gamma}-\gamma\left(1-\frac{\langle\omega_0^2\rangle}{\omega^2}\right)\right] \tag{4.8}$$

(cf. the appendix). From (4.7) and (4.8) it follows that for $\gamma > 0$ (i.e., the force constants decrease when the impurity atom is introduced), discrete frequencies can appear only if the impurity atom is lighter than the host, which is surely so for $\epsilon > \gamma$. For $\gamma < 0$, the inequality (4.7) can under certain conditions also be satisfied for the case of a heavier atom.

Thus when condition (4.7) is satisfied, if we know the frequency distribution function $g(\omega_0^2)$ for the regular crystal, then from (4.6) we find $\omega^2(\gamma, \epsilon)$ and consequently $(\partial \ln \omega^2/\partial\epsilon)_\gamma$. Using (3.25) we immediately obtain W_2.

A case of great interest is that where b approaches unity and the discrete spectrum is quite high up. Such a situation is realized in particular for sufficiently light impurity atoms when $\gamma < \epsilon$. We expand the integrand on the right side of (4.6) in a series in powers of $(\omega_0/\omega)^2$, keeping only the first three terms. Solving the resulting equation, we get

$$\omega^2 \approx \langle\omega_0^2\rangle \frac{\varepsilon-\gamma}{1-\varepsilon}\left\{1+\frac{1-\varepsilon}{(\varepsilon-\gamma)^2}\right.$$

$$\left.\times\left[(\varepsilon-2\gamma+\gamma^2)\frac{\langle\omega_0^4\rangle}{\langle\omega_0^2\rangle^2}+\gamma(1-\gamma)\right]\right\}. \qquad (4.9)$$

For ϵ close to unity, only the first term is really important in (4.9). Then

$$\omega^2 \approx \langle\omega_0^2\rangle \frac{\varepsilon-\gamma}{1-\varepsilon}. \qquad (4.9')$$

Now we determine the derivative $(\partial \ln \omega^2/\partial\epsilon)_\gamma$. From (4.9) we have

$$\left(\frac{\partial \ln \omega^2}{\partial\varepsilon}\right)_\gamma \approx \frac{1-\gamma}{(1-\varepsilon)(\varepsilon-\gamma)}$$

$$\times\left\{1-\frac{1-\varepsilon}{(\varepsilon-\gamma)(1-\gamma)}\left[(\varepsilon-2\gamma+\gamma^2)\frac{\langle\omega_0^4\rangle}{\langle\omega_0^2\rangle^2}+\gamma(1-\gamma)\right]\right\}. \qquad (4.10)$$

We substitute (4.10) in (3.25) and determine the value of W_2 for $T \rightarrow 0$. Remembering that the j_l are mutually orthogonal, we find

$$W_2 \approx \exp\left\{-\frac{R'}{\hbar\langle\omega_0^2\rangle^{1/2}}\sqrt{\frac{m'}{m}}\frac{1-\gamma}{(\varepsilon-\gamma)^{3/2}}\right.$$

$$\times\left[1-\frac{(1-\varepsilon)(2\varepsilon-3\gamma+1)}{2(\varepsilon-\gamma)^2(1-\gamma)}\right.$$

$$\left.\left.\times\left((\varepsilon-2\gamma+\gamma^2)\frac{\langle\omega_0^4\rangle}{\langle\omega_0^2\rangle^2}+\gamma(1-\gamma)\right)\right]\right\}, \qquad (4.11)$$

where R′ is the recoil energy for the impurity nucleus. If the approximation (4.9′) is valid, we should drop the second term in the square brackets in (4.11).

From the form of (4.11) we can draw the important conclusion that with decreasing mass of the radiating atom, when ϵ tends toward unity, the exponent in the expression for the probability increases not like $1/m'$ but only like $1/\sqrt{m'}$. Physically this result is related to the fact that as m′ decreases the frequency of the localized levels increases and consequently the probability of excitation of these levels by recoil decreases.

As the temperature increases, W_2 falls off [cf. (3.25) and (3.26)], but much more slowly than W_1. The reason for this is that ω is above $\omega_{0\,\max}$ and the temperature excitation of these vibrations occurs for much higher values of T than does the excitation of the characteristic frequencies of the acoustic branches of the crystal. We note that at reasonable temperatures W_2 is somewhat anisotropic even in cubic crystals.

The first few even moments of the frequency appear in (4.11). An essential point is that to find these quantities we do not need to know the explicit form of $g(\omega_0^2)$ [i.e., we do not have to solve the system (3.7)]. In fact, from (4.4),

$$\langle\omega_0^2\rangle = A_0^{ii}(0)/3m.$$

It can also be shown that

$$\langle\omega_0^4\rangle = \frac{1}{3m^2}\sum_{\mathbf{n}} A_0^{ik}(\mathbf{r_n})\,A_0^{ik}(\mathbf{r_n}).$$

Thus the moments which we want are expressed in terms of simple combinations of the force constants. If we include interactions with only a limited number of neighbors, the latter are expressed in terms of measurable macroscopic quantities (e.g., the elastic moduli). We note that $\langle\omega_0^2\rangle$ can be determined directly from the deviation of the specific heat from its classical limit at high temperatures. For $T/\Theta \gg 1$,

$$c = 3k - \frac{k}{12}\frac{\hbar^2}{(kT)^2}\langle\omega_0^2\rangle.$$

If we use a definite model of the crystal right from the start, we can determine $W_2(\epsilon,\gamma)$ over the whole range of variation of ϵ and γ which is consistent with (4.7). We shall take the model of a simple cubic lattice and include only interactions with nearest neighbors. In this case (cf. [6,3])

$$g(\omega_0^2) = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty}\exp\left\{-i\rho\omega_0^2+i\frac{2\rho}{m}(\beta_1+2\beta_2)\right\}$$

$$\times J_0\left(\frac{2\rho\beta_1}{m}\right)J_0^2\left(\frac{2\rho\beta_2}{m}\right)d\rho, \qquad (4.12)$$

where β_1 and β_2 are the central and noncentral force constants, and $J_0(x)$ is a Bessel function. Substituting (4.12) in (4.6), we arrive at the equation

$$\frac{(1-\gamma)^2}{\varepsilon-\gamma-\gamma(1-\gamma)(1-\langle\omega_0^2\rangle/\omega^2)}$$

$$=\omega^2\int\limits_0^{\infty}\exp\left\{-\rho\omega^2+\frac{2\rho}{m}(\beta_1+2\beta_2)\right\}I_0\left(\frac{2\rho\beta_1}{m}\right)I_0^2\left(\frac{2\rho\beta_2}{m}\right)d\rho. \qquad (4.13)$$

Here $I_0(x)$ is the Bessel function of imaginary argument. If we set $\beta_1 = \beta_2$, then in finding $\omega^2(\epsilon,\gamma)$ we can use the results of the numerical computation[10] of the integral in (4.13) (as a function of ω^2).

5. INFLUENCE OF THE QUASI-CONTINUOUS SPECTRUM ON THE MÖSSBAUER EFFECT

To determine the shifted frequencies in the quasi-continuous spectrum, we must turn to Eq. (3.16) or, if we restrict ourselves to the case of cubic symmetry, to (4.5). Unfortunately, for this part of the spectrum we cannot immediately make the transition to the limit $N \to \infty$ in (4.5) and replace the summation by an integration. Let us fix some very large value of N. Taking the cyclic boundary conditions into account, we get a uniform three-dimensional net for the values of **f** in phase space. Now let us plot all the values of ω_0^2 corresponding to these discrete values (of **f** and α) on a scale of squares of frequency, in increasing order. Then the displaced frequencies ω^2 will be located in the intervals between successive different values of ω_0^2, and consequently $(\partial \ln \omega^2/\partial\epsilon)_\gamma \sim 1/N$. (Remember that the undisplaced frequencies, which coincide with ω_0^2, give no contribution to W_1.) We enumerate the different values of ω_0^2 and the corresponding displaced frequencies in increasing order, ω_{0m}^2, ω_m^2. We denote the degree of degeneracy of each level of the unperturbed spectrum by ϑ_m.

First let us consider the region of small values of ϵ and γ, which corresponds to the condition $|b|\omega^2/\omega_{0\max}^2 \ll 1$ for all ω^2 in the interval from 0 to $\omega_{0\max}^2$. We shall make the limiting transition in (4.5) by a method similar to that developed by I. Lifshitz.[5] To do this we write

$$\omega_p^2 = \omega_{0p}^2 + \Delta\omega_p^2 \tag{5.1}$$

and, using the fact that $\Delta\omega_p^2 \to 0$ for $|b|\omega^2/\omega_{0\max}^2 \to 0$, we transform the right side of (4.5), keeping only terms which are quadratic in the small parameter:

$$\frac{b(\omega_{0p}^2)\,\omega_{0p}^2\,\vartheta_p}{3N\,\Delta\omega_p^2} + \frac{b(\omega_{0p}^2)\,\omega_{0p}^2}{3N}\sum_{m\neq p}\frac{\vartheta_m}{\omega_{0p}^2-\omega_{0m}^2}$$
$$-\frac{b(\omega_{0p}^2)\,\omega_{0p}^2\,\Delta\omega_{0p}^2}{3N}\sum_{m\neq p}\frac{\vartheta_m}{(\omega_{0p}^2-\omega_{0m}^2)^2} = 1. \tag{5.2}$$

We introduce the notation

$$\frac{\omega_{0p}^2}{3N}\sum_{m\neq p}\frac{\vartheta_m}{\omega_{0p}^2-\omega_{0m}^2} = S_p, \quad \frac{\omega_{0p}^4}{(3N)^2}\sum_{m\neq p}\frac{\vartheta_p\,\vartheta_m}{(\omega_{0p}^2-\omega_{0m}^2)^2} = F_p. \tag{5.3}$$

Then, solving (5.2), we find

$$\Delta\omega_p^2 = \frac{b(\omega_{0p}^2)\,\omega_{0p}^2\,\vartheta_p}{3N}\left[1 + b(\omega_{0p}^2)\,S_p + b^2(\omega_{0p}^2)\,(S_p^2 - F_p)\right]. \tag{5.4}$$

From this,

$$\left(\frac{\partial \ln\omega_p^2}{\partial\varepsilon}\right)_\gamma = \frac{\vartheta_p}{3N(1-\gamma)^2}\left[1 + 2b(\omega_{0p}^2)\,S_p\right.$$
$$\left.+ 3b^2(\omega_{0p}^2)\,(S_p^2 - F_p)\right]. \tag{5.5}$$

Now we calculate the probability W_1 (3.22). Substituting (5.5) in the exponent and taking account of the cubic symmetry and the corresponding threefold degeneracy of each displaced level, we find

$$W_1 = \exp\left\{-\frac{R}{3N(1-\gamma)^2}\sum_p\frac{\vartheta_p}{\hbar\omega_{0p}}\left[1 + 2b(\omega_{0p}^2)\,S_p\right.\right.$$
$$\left.\left.+ 3b^2(\omega_{0p}^2)\,(S_p^2 - F_p)\right]\,(2\bar{n}(\omega_{0p}) + 1)\right\}. \tag{5.6}$$

Let $T = 0$. We transform the term linear in b in (5.6), using (5.3) and (4.8):

$$2\sum_p\frac{\vartheta_p}{\hbar\omega_{0p}}\,b(\omega_{0p}^2)\,S_p = \frac{2}{3N\hbar(1-\gamma)}\sum_p\sum_{m\neq p}\left\{\frac{\omega_0}{\omega_{0p}^2-\omega_{0m}^2}\left(\frac{\varepsilon-\gamma}{1-\gamma}-\gamma\right)\right.$$
$$\left.+\gamma\langle\omega_0^2\rangle\frac{1}{\omega_{0p}(\omega_{0p}^2-\omega_{0m}^2)}\right\}\vartheta_p\,\vartheta_m.$$

If we interchange the subscripts p and m in the curly brackets, the expression is left unchanged. Taking half the sum of the original and the new expressions, we get

$$\frac{1}{3N\hbar(1-\gamma)}\sum_p\sum_{m\neq p}\frac{\vartheta_p\,\vartheta_m}{\omega_{0p}+\omega_{0m}}\left\{\frac{\varepsilon-\gamma}{1-\gamma}-\gamma-\gamma\frac{\langle\omega_0^2\rangle}{\omega_{0p}\,\omega_{0m}}\right\}.$$

We substitute this result in (5.6). Now we go to the limit $N \to \infty$, remembering that in going to the limit

$$\frac{1}{3N}\sum_p\vartheta_p\ldots \to \int d\omega_0^2\,g(\omega_0^2)\ \ldots \tag{5.7}$$

We then have in the linear approximation in b,

$$W_1 = \exp\left\{-\frac{R}{\hbar(1-\gamma)^2}\left[\int_0^{\omega_{0\max}^2} dx^2\,\frac{g(x^2)}{x}\right.\right.$$
$$\left.\left.+\iint_0^{\omega_{0\max}^2}\frac{dx^2\,dy^2 g(x^2)\,g(y^2)}{x+y}\left(\frac{\varepsilon-\gamma}{(1-\gamma)^2}-\frac{\gamma}{1-\gamma}-\frac{\gamma}{1-\gamma}\frac{\langle\omega_0^2\rangle}{xy}\right)\right]\right\}. \tag{5.8}$$

For $\epsilon = \gamma = 0$, (5.8) goes over into the expression for the probability of the Mössbauer effect for an ideal cubic crystal at $T = 0$ (cf., for example, [1,2]). If only the mass is changed, the correction term in the exponent in (5.8) is proportional to ϵ and the sign of the change is uniquely related to the sign of ϵ. (When a lighter atom is introduced, W_1 is less than for the ideal lattice.)

It is easy to show that

$$\iint_0^{\omega_{0\max}^2} dx^2 dy^2\,\frac{g(x^2)\,g(y^2)}{x+y} < \int_0^{\omega_{0\max}^2} dx^2\,\frac{g(x^2)}{x}.$$

This inequality has the important consequence that, for small ϵ, W_1 always changes more slowly with ϵ than is the case when we go from an ideal lattice with atoms of mass m to one with atoms of mass m′, keeping the same frequency spectrum.

Now let us consider the case of arbitrary temperature. Using (5.7), we make the limiting transition in the original expression (5.6). In the quadratic approximation in b, we have

$$W_1 = \exp\left\{-\frac{R}{\hbar(1-\gamma)^2}\int_0^{\omega^2_{0max}} d\omega_0^2\,\frac{g(\omega_0^2)}{\omega_0}\Big[1 + 2b(\omega_0^2)\,S(\omega_0^2) + 3b^2(\omega_0^2)\left(S^2(\omega_0^2) - F(\omega_0^2)\right)\Big](2n(\omega)+1))\right\}. \tag{5.9}$$

Here $S(\omega_0^2)$ and $F(\omega_0^2)$ are continuous functions of the argument ω_0^2, corresponding to the limiting transition $N \to \infty$ in (5.3). We note that S is simply

$$S(\omega^2) = \omega^2 \int_0^{\omega_0^2\,max} d\omega_0^2\,\frac{g(\omega_0^2)}{\omega^2 - \omega_0^2}; \tag{5.10}$$

[$g(\omega_0^2)$ goes to zero at the ends of the interval, so that the integral, in the sense of a principal value, is defined for the whole interval $0 \le \omega^2 \le \omega^2_{0\,\mathrm{max}}$, including the boundaries.]

Now we proceed to consider arbitrary ϵ and γ. We introduce the notation

$$\omega^2_{0\;p+1} - \omega^2_{0p} = \delta\omega^2_{0p}, \quad \Delta\omega_p^2/\delta\omega^2_{0p} = z_p \tag{5.11}$$

and transform (4.5) to the form

$$\frac{b(\omega^2_{0p})\,\omega^2_{0p}\,\vartheta_p}{3Nz_p\,\delta\omega^2_{0p}} - \frac{b(\omega^2_{0p})\,\omega^2_{0p}\,z_p}{3N\,\delta\omega^2_{0p}} \times \sum_{m\neq p}\frac{\vartheta_m}{[(\omega^2_{0p}-\omega^2_{0m})/\delta\omega^2_{0p} + z_p]\,[(\omega^2_{0p}-\omega^2_{0m})/\delta\omega^2_{0p}]} = 1 - b(\omega^2_{0p})\,S_p. \tag{5.12}$$

It is not hard to see that the series in the second term on the left of (5.12) converges rapidly, and that only the levels in the immediate neighborhood of ω^2_{0p} are of any importance. For the overwhelming majority of levels, ϑ_m has the same value, determined by the symmetry of the crystal. The exceptions are those cases where the wave vector, to which the particular frequency corresponds, lies in a plane of symmetry or along a symmetry axis, or when there is a case of accidental degeneracy. It is clear that if we assume ϑ_m to be constant (and equal to ϑ_p) in the sum which appears in (5.12), in determining z_p we will make an error only for a negligible fraction of the displaced levels in any macroscopic frequency interval. Since the sum over all the displaced frequencies appears in the exponent in (3.22), this assumption does not affect the accuracy of our determination of W_1.

In order to find the explicit relation between z_p and ϵ, γ for computing the sum in (5.12), we make the assumption that the levels in the vicinity of any ω^2_{0p} are distributed equidistantly. Then*

$$z_p \sum_{m\neq p}\frac{1}{[(\omega^2_{0p}-\omega^2_{0m})/\delta\omega^2_{0p} + z_p]\,[(\omega^2_{0p}-\omega^2_{0m})/\delta\omega^2_{0m}]} = z_p \sum_{m\neq p}\frac{1}{(p-m+z_p)(p-m)} = -\pi\,\mathrm{ctg}\,\pi z_p + 1/z_p.$$

Substituting this result in (5.12), we find

$$\frac{b(\omega^2_{0p})\,\omega^2_{0p}\,\vartheta_p}{3N\delta\omega^2_{0p}}\,\pi\,\mathrm{ctg}\,\pi z_p = 1 - b(\omega^2_{0p})\,S_p. \tag{5.13}$$

From this we determine $(\partial z_p/\partial\epsilon)_\gamma$. Using the definition (5.11), we find

$$\left(\frac{\partial \ln \omega_p^2}{\partial\varepsilon}\right)_\gamma = \frac{\vartheta_p}{3N(1-\gamma)^2\,(1-b(\omega^2_{0p})\,S_p)^2}\left\{1 + \left[\frac{\pi b(\omega^2_{0p})\,\vartheta_p\,\omega^2_{0p}}{3N\delta\omega^2_{0p}\,(1-b(\omega^2_{0p})\,S_p)}\right]^2\right\}^{-1}. \tag{5.14}$$

When $N \to \infty$, S takes on the value (5.10), and

$$\vartheta_p/3N\delta\omega^2_{0p} \to g(\omega_0^2).$$

Using (5.7), we get the final expression for W_1 in a cubic crystal:

$$W_1 = \exp\left\{-\frac{R}{\hbar(1-\gamma)^2}\int_0^{\omega_0^2\,max} d\omega_0^2\,\frac{g(\omega_0^2)}{\omega_0} \times \frac{1}{[1-b(\omega_0^2)\,S(\omega_0^2)]^2 + [\pi b(\omega_0^2)\,\omega_0^2\,g(\omega_0^2)]^2}\,(2\bar{n}(\omega_0)+1)\right\}. \tag{5.15}$$

For small values of $|b|\omega^2/\omega^2_{0\,\mathrm{max}}$, (5.15) goes over into (5.9), if we determine the quantities in that equation by using (5.3) and assuming that the levels are equidistant. Then

$$F_p = \frac{\omega^4_{0p}}{(3N)^2}\left(\frac{\vartheta_p}{\delta\omega^2_{0p}}\right)^2 \sum_{m\neq p}\frac{1}{(p-m)^2} = \frac{\omega^4_{0p}}{(3N)^2}\left(\frac{\vartheta_p}{\delta\omega^2_{0p}}\right)^2 \frac{\pi^2}{3} \to \frac{\pi^2\omega_0^4}{3}\,[g(\omega_0{}^2)]^2.$$

If we know the frequency distribution function for the regular crystal, the calculation of (5.15) using (5.10) and (4.8) is easily done. Thus, knowing $g(\omega_0^2)$, we can compute W_1 and W_2 in general (cf. the preceding section) and thus determine the total probability for the Mössbauer effect for arbitrary ϵ and γ, which is simply a product of these two functions.

It is interesting to consider the case where the mass of the impurity atom is relatively small. Then ϵ is close to unity, and in general the dependence on m′ in (5.15) disappears. (We emphasize that the recoil energy in (5.15) is referred to the mass of the atoms of the host lattice.) If we use the expression (4.11) for W_2 (assuming that $\epsilon > \gamma$) then we get the result that when m′ is decreased (for fixed γ), the logarithm of the probability for the Mössbauer effect is proportional not to 1/m′ but to $1/\sqrt{m'}$. Thus there is a possibility in certain cases of considerably increasing the Mössbauer effect by embedding the

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*ctg = cot

atom in a heavier lattice, provided the regular lattices of the two types of atoms have almost the same characteristic frequencies of their phonon spectra. We should however point out that if there is a marked reduction of the force constants this picture may be considerably altered.

Let us now consider the opposite limiting case, where the mass of the impurity atom is relatively large and $\gamma \geq 0$. Writing $b(\omega^2)$ of (4.8) in the form

$$b = b_0 + b_1 \frac{\omega^2_{max}}{\omega^2}, \quad b_0 = 1 + \frac{\varepsilon - 1}{(1-\gamma)^2}, \quad b_1 = \frac{\gamma}{1-\gamma} \frac{\langle \omega_0^2 \rangle}{\omega^2_{0max}},$$

we have for this case, $b_0 < 0$, $|b_0| \gg 1$, b_1.

It can be shown that under these conditions the integrand in (5.15) is localized in the region of low frequencies and has a resonance shape. Using this, and remembering that in this region $g \sim \sqrt{\omega_0^2}$, we can carry out the integration explicitly $(T = 0)$:

$$W_1 = \exp\left\{-\frac{R}{\hbar\omega_{0\,max}} \frac{1}{(1-\gamma)^2} \left[\frac{\langle \omega^2_{0\,max}/\omega_0^2 \rangle}{|b_0|\,(1 + b_1 \langle \omega^2_{0\,max}/\omega_0^2 \rangle)}\right]^{1/2}\right\},$$

$$W_2 = 1. \tag{5.16}$$

For $\gamma = 0$, this expression reduces to

$$W_1 = \exp\left\{-\frac{R}{\hbar}\left\langle \frac{1}{\omega_0^2}\right\rangle^{1/2} |\varepsilon|^{-1/2}\right\}. \tag{5.17}$$

Thus, in a light lattice, with increasing mass of the radiator there is an increase in the Mössbauer effect, but the exponent falls off like $1/\sqrt{m'}$ and not like $1/m'$ (cf. note added in proof).

Since the vibrations of the heavy impurity atom are preferentially in the low frequency range, the effect falls off rapidly with increasing temperature. For $kT \gg \hbar \langle 1/\omega_0^2 \rangle^{-1/2} |\epsilon|^{-1/2}$, Eq. (5.15) goes over into the expression:

$$W_1 = \exp\left\{-\frac{R}{\hbar}\left\langle \frac{1}{\omega_0^2}\right\rangle^{1/2} |\varepsilon|^{-1/2} \left[1 + \frac{2kT}{\hbar} |\varepsilon|^{1/2} \left\langle \frac{1}{\omega_0^2}\right\rangle^{1/2}\right]\right\}. \tag{5.18}$$

APPENDIX

We shall derive condition (4.7), the condition for the existence of a solution of Eq. (4.6), and at the same time we shall prove uniqueness. Introducing the variables

$$x = \omega_0^2/\omega^2_{0\,max} \quad (0 \leqslant x \leqslant 1); \quad z = \omega^2_{0\,max}/\omega^2 \quad (0 \leqslant z \leqslant 1),$$

we write Eq. (4.6) in the form

$$b(z) = \Phi^{-1}(z), \quad \Phi(z) = \int_0^1 \frac{g(x)\,dx}{1 - xz};$$

$$b(z) = b_0 + \frac{\gamma}{1-\gamma}\langle x \rangle z, \qquad b_0 = 1 - \frac{1-\varepsilon}{(1-\gamma)^2}$$

(where we have introduced the notation $g(x) = \omega^2_{0max} g(\omega_0^2)$, so that

$$\int_0^1 g(x)\,dx = 1).$$

Since $1 \geq \epsilon > -\infty$, and $1 \geq \gamma$, $1 \geq b_0 > -\infty$. It is easy to show that over the whole range of variation of z,

$$d\Phi^{-1}/dz < 0, \quad d^2\Phi^{-1}/dz^2 < 0,$$

and that

$$\Phi^{-1}(0) = 1, \quad \Phi^{-1}(1) = \langle (1-x)^{-1} \rangle^{-1},$$

$$d\Phi^{-1}(0)/dz = -\langle x \rangle, \quad d\Phi^{-1}(1)/dz = -\infty.$$

Consequently the function $\Phi^{-1}(z)$ is a convex function which continually decreases with increasing z.

On the other hand, since $b(0) = b_0 \leq 1 = \Phi^{-1}(0)$, it is immediately clear that the straight line

$$b(z) = b_0 + (\gamma/(1-\gamma))\langle x \rangle z$$

has a single point of intersection with the curve $\Phi^{-1}(z)$ (for arbitrary γ), if

$$b(1) > \Phi^{-1}(1),$$

and has no point of intersection if this inequality is not satisfied.

Note added in proof (December 7, 1961). After this paper went to press, there appeared the paper of Shirley et al.,[11] which gives results of measurements of the Mössbauer effect on nuclei of Au^{197} embedded in light lattices of Fe, Co and Ni, at 4° K. For such a large difference in the atomic masses $(m'/m \sim 4)$, the change in the force constants can be neglected and the effect should be described by formula (5.17). A comparison showed that there is good agreement between the computed and experimental results.

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