

applied field, and, in consequence, the coupling between the rare-earth and iron sublattices, though basically of antiferromagnetic sign, makes the moment of these sublattices parallel rather than antiparallel.¹³

In closing, we should emphasize that the present paper makes no pretense of including anisotropy, and it can be regarded rather as an attempt to see how far one can push the theory with a purely isotropic model. Of course, the effects of anisotropy are particularly

important at low temperatures. The theory usually does not appear to work too well at low temperatures if the correction for anisotropy is made in the usual way by introducing an anisotropy field. The question of how far it is warranted to include the anisotropic part of the crystalline potential simply through this artifice is a subject into which we do not want to enter here.

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¹³ V. Jaccarino, B. T. Matthias, M. Peter, H. Suhl, and J. H. Wernick, *Phys. Rev. Letters* **5**, 251 (1960); G. Goldring, M. Schieber, and Z. Vager, *J. Appl. Phys.* **31**, 2057 (1960); W. P. Wolf, *ibid.* **32**, 742 (1961).

Debye-Waller Factor in Mössbauer Interference Experiments

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A simple calculation is presented of the effects of lattice dynamics on interference between Mössbauer processes and corresponding atomic processes, i.e., between Mössbauer and Rayleigh scattering, or between internal conversion of Mössbauer radiation and the photoelectric effect. When the energy of the emitted γ ray or electron is not measured, it is necessary to sum over all possible final states of the lattice. The interference contribution is found to be attenuated by the same "Debye-Waller" factor as the ordinary Mössbauer contribution, depending only upon the momentum of the incident γ ray. If the energy of the emitted γ ray is measured (e.g., by a Bragg scattering experiment), the atomic contribution is attenuated by the usual x-ray Debye-Waller factor, depending upon the momentum transfer, the Mössbauer contribution by the square of the usual Mössbauer factor, and the interference term by the geometric mean of the atomic and Mössbauer factors.

IT is now generally known¹⁻³ that the effects of lattice dynamics in Mössbauer experiments are expressed very simply in terms of the fraction f of gamma rays emitted from the source without energy loss due to recoil. This is the Debye-Waller factor⁴

$$f = |\langle i | \exp(-i\mathbf{k} \cdot \mathbf{X}_L) | i \rangle|^2, \quad (1)$$

where $|i\rangle$ is the initial state of the lattice, $\hbar\mathbf{k}$ is the momentum of the gamma ray, and \mathbf{X}_L is the coordinate of the nucleus emitting the gamma ray. Interest has recently been expressed in interference between atomic effects and the Mössbauer effect; e.g., between Rayleigh and Mössbauer scattering,⁵ or between atomic photoelectric absorption and Mössbauer absorption followed by emission of a conversion electron.⁶ The purpose of this note is to point out that the effect of

the lattice dynamics on the interference term is given by the *same factor* f which appears in the direct Mössbauer term.

Let us consider the scattering of a gamma ray of momentum $\hbar\mathbf{k}_1$ into a state of momentum $\hbar\mathbf{k}_2$ by an atom whose motion in the lattice is described by the coordinate \mathbf{X}_L . Let M be the probability amplitude for the process due to the Mössbauer effect, and let A be the amplitude for Rayleigh scattering by the atomic electrons. Then the scattering cross section will be given by

$$\sigma \propto \{|A|^2 + |M|^2 + 2C \operatorname{Re}(A^*M)\}, \quad (2)$$

where C is a factor expressing the degree of coherence of the two elementary processes. This factor C is independent of the lattice and is not considered further here.

We wish to investigate the effect of the lattice dynamics upon Eq. (2). From ordinary Mössbauer and Rayleigh scattering we know that the direct Mössbauer term $|M|^2$ is proportional to f , and that the direct Rayleigh term $|A|^2$ is independent of the lattice dynamics. The dependence of the interference term upon the lattice is not evident, *a priori*.

The coherence properties of the final lattice states

¹ *Proceedings of Illinois Conference on the Mössbauer Effect*, edited by H. Frauenfelder and H. Lustig (University of Illinois Urbana, Illinois, 1960).

² H. J. Lipkin, *Ann. Phys.* **9**, 332 (1960).

³ C. Tzara and R. Barloutaud, *Phys. Rev. Letters* **4**, 405 (1960).

⁴ I. Waller, *Ann. Physik* **79**, 261 (1926); W. Marshall and J. P. Schiffer, Atomic Energy Research Establishment Report, 1959 (unpublished).

⁵ P. J. Black and P. B. Moon, *Nature* **188**, 481 (1960).

⁶ L. J. Tassie (to be published). See also reference 1, p. 25.

must first be investigated. Although the Mössbauer resonance condition requires that the gamma ray be *absorbed* (either really or virtually) without excitation of lattice vibrations, no such restrictions exist for the re-emission process. Thus the lattice can be left after the scattering in a final state $|f\rangle$ which is different from the initial state. The same is true for Rayleigh scattering, where there is no resonance condition. However, interference can only occur between two amplitudes, Mössbauer and Rayleigh, describing processes in which the lattice is left *in the same final state* $|f\rangle$. We must therefore define atomic and Mössbauer scattering amplitudes $A(\mathbf{k}_1, \mathbf{k}_2, i, f)$ and $M(\mathbf{k}_1, \mathbf{k}_2, i, f)$ for scattering in which the lattice goes from a definite state $|i\rangle$ to a definite state $|f\rangle$ during the transition.

Because lattice forces are weak in comparison with atomic and nuclear forces, the perturbation of internal atomic and nuclear structure by the lattice can be neglected, and the internal and lattice degrees of freedom can be separated. The scattering amplitudes can therefore be separated into a factor A_{at} (or M_{nuc}) depending upon the elementary atomic (or nuclear) process, and a lattice factor describing the transfer of momentum to the atom \mathbf{X}_L in the lattice. The latter is simply the matrix element of the operator $\exp[i\Delta\mathbf{k}\cdot\mathbf{X}_L]$ between appropriate lattice states, where $\Delta\mathbf{k}$ is the appropriate momentum transfer.² Thus,

$$A(\mathbf{k}_1, \mathbf{k}_2, i, f) = A_{\text{at}} \langle f | \exp[i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{X}_L] | i \rangle, \quad (3a)$$

$$M(\mathbf{k}_1, \mathbf{k}_2, i, f) = M_{\text{nuc}} \langle f | \exp(-i\mathbf{k}_2 \cdot \mathbf{X}_L) | i \rangle \times \langle i | \exp(i\mathbf{k}_1 \cdot \mathbf{X}_L) | i \rangle. \quad (3b)$$

In the atomic case, the total momentum transfer $(\mathbf{k}_1 - \mathbf{k}_2)$ is given to the lattice during the scattering process. Whether or not this is considered as a two-step process involving virtual absorption and re-emission is irrelevant, as there is no resonance in the intermediate state. The sum over all intermediate virtual states can be performed directly by closure to yield the result (3a), neglecting the variation of the energy denominator which is very large compared to lattice energies. This is not true for the Mössbauer case, as the resonance in the intermediate state is so narrow that only a single lattice state is relevant, namely the initial state. In the Mössbauer case, the lattice remains in the initial state during the absorption of \mathbf{k}_1 and goes to the final state in the emission of \mathbf{k}_2 .

The total amplitude for the process is just the sum of the two terms of (3). The total cross section is obtained by squaring the total amplitude and summing over all lattice final states $|f\rangle$, since the lattice final

state is not measured. Thus,

$$\begin{aligned} \sigma \propto \sum_f |A_{\text{at}}|^2 & \langle f | \exp[i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{X}_L] | i \rangle^2 \\ & + |M_{\text{nuc}}|^2 \langle f | \exp(-i\mathbf{k}_2 \cdot \mathbf{X}_L) | i \rangle^2 \langle i | \exp(i\mathbf{k}_1 \cdot \mathbf{X}_L) | i \rangle^2 \\ & + 2C \operatorname{Re}\{A_{\text{at}}^* M_{\text{nuc}} \langle i | \exp[i(\mathbf{k}_2 - \mathbf{k}_1) \cdot \mathbf{X}_L] | f \rangle \\ & \times \langle f | \exp(-i\mathbf{k}_2 \cdot \mathbf{X}_L) | i \rangle \langle i | \exp(i\mathbf{k}_1 \cdot \mathbf{X}_L) | i \rangle\}. \quad (4) \end{aligned}$$

The summation over final states $|f\rangle$ is simple matrix multiplication. The result, obtained by closure is

$$\sigma \propto \{|A_{\text{at}}|^2 + |M_{\text{nuc}}|^2 f(\mathbf{k}_1) + 2C \operatorname{Re}(A_{\text{at}}^* M_{\text{nuc}}) f(\mathbf{k}_1)\}, \quad (5)$$

where $f(\mathbf{k}_1)$ is the ordinary Mössbauer fraction, Eq. (1) for momentum \mathbf{k}_1 . We now note the following points:

(1) The derivation of Eq. (5) does not depend specifically upon the nature of the processes of Rayleigh and Mössbauer scattering. It is valid for any process in which a particle of momentum $\hbar\mathbf{k}_1$ is absorbed by an atom in a lattice and a particle of momentum $\hbar\mathbf{k}_2$ is emitted. It is therefore also valid for the case where a conversion electron is emitted.

(2) The interference term is attenuated by exactly the same lattice factor $f(\mathbf{k}_1)$ as the direct Mössbauer term.

(3) The attenuation is independent of the emitted momentum \mathbf{k}_2 . This surprising effect is particularly interesting in the case of the conversion electron, where \mathbf{k}_2 is large because of the electron mass, and $f(\mathbf{k}_2)$ would be very small.

It is also of interest to note that Eq. (4) can describe lattice effects in coherent "Bragg" scattering from many atoms in a single crystal. For this case Eq. (4) should not be summed over all final state $|f\rangle$; rather $|f\rangle$ should be set equal to $|i\rangle$, since there is constructive interference at the Bragg angle only if the outgoing gamma ray has the same wavelength as the emitted one; i.e., if there is no energy transfer to the lattice. For this case, we obtain

$$\begin{aligned} \sigma_{\text{Bragg}} \propto & \{|A_{\text{at}}|^2 f(\mathbf{k}_1 - \mathbf{k}_2) + |M_{\text{nuc}}|^2 \{f(\mathbf{k}_1)\}^2 \\ & + 2C \operatorname{Re}(A_{\text{at}}^* M_{\text{nuc}}) [f(\mathbf{k}_1 - \mathbf{k}_2)]^{\frac{1}{2}} f(\mathbf{k}_1)\}. \end{aligned}$$

The direct atomic term has the familiar Debye-Waller factor for Bragg scattering, depending upon the momentum transfer. The direct Mössbauer term has the *square* of the usual factor. The interference term has the geometric mean of the two direct factors, as is to be expected when there is only a single final state.

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