Physics of the Mössbauer Effect

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This paper considers from a simple physical point of view the Mössbauer effect, i.e., the "recoilless emission" of gamma rays from a nucleus bound in a crystal lattice. It begins with a discussion of the kinematics of gamma-ray emission from such a nucleus. The idealized case of a massive "lattice" characterized by a single frequency and the more realistic one and three-dimensional models are treated. We point up the fact that in the Mössbauer effect the lattice as a whole (the lattice center of mass) always recoils after photon emission, so that the term "recoilless emission" is in one sense misleading. We emphasize that the essence of the Mössbauer effect is not photon emission without recoil, but rather is photon emission without transfer of energy to internal degrees of freedom of the lattice. Using the basic ideas of quantum mechanics, namely, the rules for the manipulation of probability amplitudes (the so-called "transformation theory"), we calculate the probability for recoil without excitation of internal degrees of freedom, i.e., the Mössbauer f factor, on the assumption that the individual photon emissions, and consequent lattice recoil, are instantaneous. In Appendix A we discuss this question of instantaneous emission in some detail, and show how it is not in contradiction with the fact that the nuclear transition that leads to the gamma-ray emission has a finite half-width. In Appendix B those rules of transformation theory that are used in the body of the paper are summarized.

INTRODUCTION

THE aim of this paper is to discuss the Mössbauer effect in a way which highlights the basic physical features as clearly as possible and which, hopefully, clarifies various misconceptions that seem to exist about it. We assume then that the reader has some familiarity with the general features of the effect; if not, we refer him to any of several excellent references and review articles.[1] We however set the stage briefly by recalling that the effect has to do with the properties of photons emitted in nuclear transitions. Consider a free nucleus which has two states of internal energy E_2 and E_1. If a photon is emitted in a transition between those states the photon energy is *not* given by E_2-E_1, but is less by a small but significant amount R, called the recoil energy. This is just the kinetic energy which is perforce transmitted to the emitting nucleus as a consequence of energy and momentum conservation between the nucleus and emitted photon. If however the nucleus is bound in a crystal there can be a substantial probability for emission of a photon *without* this recoil energy shift. This is the "Mössbauer effect," sometimes also called "recoilless emission" although this terminology is occasionally used loosely, as we see later.

KINEMATICS OF PHOTON EMISSION

A. Free Nucleus

We begin then by analyzing energy and momentum conservation when a photon is emitted as a result of a transition between two states E_2 and E_1 of a nucleus, assumed of mass m. Such a nucleus is an isolated "system"; before emission the system simply consists of the nucleus itself, at rest; after emission the system consists of the nucleus with a velocity v, plus a photon of frequency ν (and hence momentum $h\nu/c$). Since the momentum and energy of the isolated system must be the same before and after the emission we get

$$\text{Momentum:}\quad 0=h\nu/c+mv \tag{1}$$
$$\text{Energy:}\quad E_2=E_1+h\nu+1mv^2/2.$$

[1] Among other good introductory articles, one may refer to: H. Lustig, Am. J. Phys. **29**, 1 (1961); R. L. Mössbauer, Science **137**, 731 (1962); G. K. Wertheim, *The Mössbauer Effect* (Academic Press Inc., New York and London, 1964). An extensive list of general references is given in Resource Letter ME-I on the Mössbauer Effect, Am. J. Phys. **31**, 1 (1963).

These two equations then yield

$$h\nu = E_0 - (h\nu)^2/2mc^2. \tag{2}$$

Thus the photon energy is less than $E_2 - E_1$ by the recoil energy R,

$$R = (h\nu)^2/2mc^2. \tag{3}$$

That is, not all the energy available in the transition goes to the photon, but some appears as kinetic energy of the nucleus.

B. Einstein "Lattice"

Since the Mössbauer effect can take place when an emitting nucleus is bound to a lattice, we should begin by working out the kinematics of gamma-ray emission by such a nucleus in a lattice. This is not very difficult, but we can make life easier for ourself and still extract the essential result by beginning with a simpler system.

Let us then schematize the lattice in the way sketched in Fig. 1, by imagining that instead of it, we have a nucleus of mass m bound to another mass M; this latter mass represents all the other nuclei in the lattice and is therefore enormous; $M \approx 10^{23} m$. This "lattice" is characterized by a single frequency ω; it is essentially the Einstein model for the true lattice. Now, as before, let us imagine that the nucleus emits a gamma ray in the transition between the levels of energies E_2 and E_1, and again apply the conservation laws to the system. Before emission the system consists of the two masses M and m at rest, with the nucleus in energy state E_2. After emission it consists of the two masses M and m with velocities, $\dot{x}_1 \equiv v_1$, $\dot{x}_2 \equiv v_2$, the nucleus in state E_1, and an emitted photon of frequency ν. The equations of momentum and energy balance are then, writing the potential energy of the spring as $(q/2)(x_2 - x_1 - a)^2$, where a is its unstretched length,

$$0 = Mv_1 + mv_2 + (h\nu/c),$$

$$E_2 = E_1 + h\nu + (Mv_1^2/2) + (mv_2^2/2) + (q/2)(x_2 - x_1 - a)^2.$$

These equations become more useful when they are expressed in terms of relative and center of mass coordinates x and X defined by

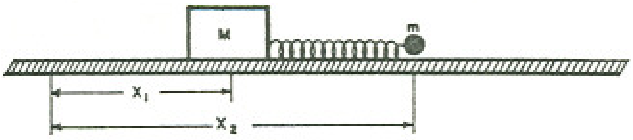

FIG. 1. Schematic sketch of the Einstein model. The Mössbauer nucleus of mass m is bound to the "lattice" of mass M ($M \gg m$) by a single "spring," i.e., with a single characteristic frequency.

$$x = x_2 - x_1,$$
$$X = (Mx_1 + mx_2)/(M+m).$$

A little algebra then shows that they become

$$0 = M_t V + (h\nu/c), \tag{5}$$

$$E_0 = h\nu + (M_t V^2/2) + (\mu/2)v^2 + (q/2)(x-a)^2, \tag{6}$$

where $\dot{x} = v$, $\dot{X} = V$, and the "total mass" M_t and the "reduced mass" μ are

$$M_t = M + m, \quad \mu = mM/(m+M).$$

If now we put Eq. (5) into (6) we get an equation which is the analog of Eq. (2) for emission from a free nucleon, viz.

$$h\nu = E_0 - [(h\nu)^2/2M_t c^2] - E_{\text{int}}, \tag{7}$$

where we have defined the "internal energy" E_{int} as

$$E_{\text{int}} = (\mu/2)v^2 + (q/2)(x-a)^2. \tag{8}$$

E_{int} is the energy of relative motion of the system, i.e., it is that part of the energy which depends only on the relative coordinate x.

The possibility of the Mössbauer effect begins to emerge when one compares Eqs. (2) and (7). The crucial difference is that M_t and not m appears in the second term on the right-hand side, that is, in the term we have previously called the "recoil energy." Since M_t is enormous, this term is negligible and to an extremely good approximation,

$$h\nu \approx E_0 - E_{\text{int}}. \tag{9}$$

Now if it were possible for E_{int} to be zero, we would have

$$h\nu \approx E_0, \tag{10}$$

and this is just a mathematical statement of the Mössbauer effect, i.e., it describes a transition between nuclear states in which the full energy difference available is given to the photon.

C. Periodic Lattice

Before discussing the conditions under which this possibility is realized, let us show how a similar result applies for a real lattice. We can then continue to use the Einstein model with some assurance that it is not oversimplified. Consider, for example, a one-dimensional lattice (the extension to three dimensions is trivial), of N nuclei of mass m, with coordinates $x_1, x_2, \cdots, x_N$. We can then introduce the center of mass coordinate X, defined by

$$X = \sum x_i / N$$

and $N-1$ other relative (or internal) coordinates, i.e., linear combinations of the x_i which are functions of the coordinate differences only. For example we can introduce the so-called Jacobi coordinates, $\xi_1 \cdots \xi_{N-1}$ defined by

$$\xi_n = [(x_1 + x_2 + \cdots + x_n)/n] - x_{n+1}, \qquad n = 1, 2, \cdots, N-1.$$

If now we suppose a photon is emitted by one of the nuclei, and work out the kinematics we get an equation like (7), in which, however, the total mass M_t is now just $M_t = Nm$, and in which E_{int} is a function, possibly complicated, of the $N-1$ interval variables only. Again for N large, M_t is large and we get back to an excellent approximation Eq. (9). If then E_{int} can be zero, or in other language, if no internal lattice vibrations (phonons) are excited we have the possibility of "recoilless emission," i.e., of the Mössbauer effect.

Now we are in a position to comment briefly on the term "recoilless emission." As has been indicated, in a sense this is a misnomer, because in fact the system as a whole always, and necessarily, recoils upon emission of the gamma ray. Thus the term must be understood as meaning that in the Mössbauer effect no *energy* is transmitted to internal motions, and it is only in this sense that the transition is recoilless. Unfortunately there are many statements in the literature to the effect that "The Mössbauer effect consists in the emission (or resonant absorption) by a nucleus in a solid of a gamma-quantum with an energy which is precisely equal to the energy of the transition, because the recoil momentum is transferred to the crystal as a whole." This is incorrect. *Whenever* a gamma ray is emitted by a nucleus, whether or not there is a Mössbauer effect, the recoil momentum is transferred to the crystal as a whole, in the sense that it is taken up by the center of mass momentum. The difference between Mössbauer and non-Mössbauer transitions lies in whether or not the internal energy of the crystal changes. It should also be stated that this distinction is clearly understood and clearly stated by Mössbauer himself.[2]

We return now to the Einstein model and to the question of the circumstances under which E_{int} in Eq. (9) can be zero. In classical mechanics it is fairly clear on intuitive grounds that this cannot be so; if, for example, referring to Fig. 1, the mass m suffers a sudden momentum impulse, we would expect that classically the internal energy will necessarily change. We amplify this later. The point we want to make now is that quantum mechanically, the story is different. For in quantum mechanics the internal energy is quantized and the allowed values are just the oscillator eigenvalues, which are

$$E_{\text{osc}} = (n + \tfrac{1}{2})\hbar\omega. \qquad (10)$$

Actually, the zero-point energy $\frac{1}{2}\hbar\omega$ which occurs in this equation remains unchanged in a transition between two states and since we are only interested in such transitions it plays no role in our argument. For our purposes then we can take the internal energy as

$$E_{\text{int}} = n\hbar\omega.$$

If, in quantum mechanics then, for the system initially in the ground state ($n=0$), there is a finite probability for the system still to be in the ground state after photon emission, the Mössbauer effect will be possible. Our next step then is to calculate this probability, and show that it is indeed different from zero.

THE PROBABILITY OF "RECOILLESS EMISSION"

A. Einstein Model

Let us now investigate the probability for recoilless emission, and begin by considering the

[2] R. L. Mössbauer and D. H. Sharp, Rev. Mod. Phys. 36, 410 (1964).

"Einstein model" of Fig. 1. But before we treat it quantum mechanically, it is useful to discuss it classically in a little more detail, and as a prerequisite to that, clarify what we mean by a classical discussion.

We are interested in what happens just after the mass m emits a gamma ray of frequency ν, thereby imparting to the system a recoil momentum $p_0 = h\nu/c$. Now, in one sense, the classical limit is that in which $h \to 0$, and in which therefore, there is no recoil momentum, and hence no problem. This is not the limit we wish to consider. Rather, let us continue to assume that the gamma ray does transmit a momentum to the system, i.e., gives it a sudden "kick." Then the aim of our discussion is to highlight the difference between the classical and quantum mechanical response of the system to this momentum kick. It is worth underlining the assumption that the effect of the photon is to transfer momentum suddenly, or instantaneously, since this is a point that has engendered much discussion and confusion in the literature, and which needs some explanation. In particular, the fact that the nuclear state has a finite lifetime has been thought by some to preclude an instantaneous momentum transfer. This is not correct. We, however, defer a more complete discussion of this assumption to an Appendix, since it is too tangential to be appropriate here, and in what immediately follows we simply work out some of its consequence.

What is then the difference between the response of the system of Fig. 1 considered classically and considered quantum mechanically? The answer is, rephrasing our previous remarks, classically, one cannot transfer an impulsive momentum to the nucleus without changing the internal energy of the system; quantum mechanically, one can. This is central to the Mössbauer effect, as Lipkin has clearly recognized.[3] Let us see how this comes about, in the Einstein model treated classically. We assume then that the nucleus of mass m has suffered an impulsive momentum "kick" upon the emission of a photon, and we further assume for the sake of definiteness that the gamma-ray is emitted to the right. Then we know, that somehow the "system as a whole" moves to the left. But we must look carefully at what we mean by "system as a whole." Consider the instant, call it $t=0$, just after the gamma ray has been emitted. Will the mass M have a finite velocity at this time? The answer, of course, is no. It takes a finite time for the spring to transmit a force, and only if the spring were infinitely stiff, i.e., only if the system (Mass m+spring+Mass M) comprised a rigid body would the mass M have a finite velocity at $t=0$. On the other hand, the nucleus of mass m does recoil instantly, so we can say that at $t=0$ its momentum is just equal in magnitude to the photon momentum. Thus the velocities at $t=0$ are

$$\dot{x}_1 = 0, \quad m\dot{x}_2 \equiv mv_0 = -(h\nu/c). \tag{11}$$

Now the motion of the center of the mass X and of the internal coordinate x are independent, so the total energy of the system is just the sum of the center-of-mass energy E_{cm}, and of the internal energy, E_{int}. Moreover the total energy of the system is just its value at $t=0$, namely $\frac{1}{2}mv_0^2$. Using these facts and Eq. (11) it is then easy to work out that E_{cm} and E_{int} are given by

$$E_{\mathrm{cm}} = \tfrac{1}{2}[m^2/(M+m)]v_0^2,$$
$$E_{\mathrm{int}} = \tfrac{1}{2}[mM/(m+M)]v_0^2.$$

Thus if one transfers a finite momentum to the system, making v_0 different from zero, the internal energy is necessarily different from zero. One cannot transfer momentum classically without adding to the internal energy.

Now let us turn to the quantum mechanical discussion, where our questions must be phrased differently. Unlike the case in classical mechanics, we cannot predict the unique subsequent motion of the system when the nucleus is given a sudden momentum kick. All we can do is predict the relative frequency (probability) with which it will have different energy values (states). The question we want to ask then is this: What is the probability that the system of Fig. 1 remains in the ground state, the nucleus having emitted a photon of momentum $h\nu/c$, and therefore having initially acquired for itself, as in the classical discussion above, a momentum $[-(h\nu/c)]$?

[3] H. Lipkin, Ann. Phys. (N. Y.) **18**, 182 (1962).

Now, it is familiar that in quantum mechanics one does not claculate probabilities directly, but rather calculates probability amplitudes whose squared magnitudes then give the probabilities themselves. For example, in a one-dimensional problem the ground-state wavefunction, $\psi_0(x)$ is the probability amplitude for finding the particle between x and $x+dx$ since its squared magnitude gives just that probability. Similarly $\phi_0(p)$, the analogous momentum space function, is the probability amplitude for finding the momentum between p and $p+dp$. Thus probabilistic quantum theory, which works with probability amplitudes, differs in an essential way from classical probability theory, which adds and multiplies probabilities themselves. But despite this difference there are also similarities. Specifically, there is a rule in classical probability theory for calculating the probability of an event, whose occurrence is contingent on the occurrence of other events. Suppose y is an "event" of some kind; for example, y may be the event which consists of getting a total of seven when two dice are thrown. Suppose x is an event of a similar kind, and that the probability of the occurrence of y depends upon whether x has occurred or not. We call the numerical value of this contingent probability, the "probability of (y, given x)." Then the rule is:

$$\text{Probability of } y = \sum_x, \int \begin{pmatrix}\text{Probability of}\\ (y, \text{given } x)\end{pmatrix} \cdot \begin{pmatrix}\text{Probability}\\ \text{of } x\end{pmatrix}. \quad \text{(R.1)}$$

Here the notation $\sum, \int$ means to sum or integrate over all the possible values of x, according as these are discrete or continuous.

There is a similar rule in quantum mechanics; it differs from the above rule in that it deals with probability amplitudes instead of probabilities, and in that the events it refers to are measurements, or rather the possible results (eigenvalues) of measurements, of quantum mechanical observables. The rule is discussed in textbooks under the name "transformation theory." Here we simply state it and apply it to the Mössbauer effect, leaving a more detailed discussion to an Appendix. The rule is just this:

$$\begin{matrix}\text{Probability}\\ \text{amplitude for } y\end{matrix} = \sum_x, \int \begin{pmatrix}\text{Probability amplitude}\\ \text{for } (y, \text{given } x)\end{pmatrix}^* \times \begin{pmatrix}\text{Probability ampli-}\\ \text{tude for } x\end{pmatrix}. \quad \text{(R.2)}$$

The asterisk (*) on the right-hand side stands for complex conjugate; the probability amplitudes of quantum mechanics are complex in general. Except for this the similarity of (R.2) to the classical rule is obvious.

Now let us apply this rule to find the probability amplitude, call it P_{00}, for the Einstein lattice of Fig. 1 to remain in the ground state after emitting a photon of momentum $p_0 = h\nu/c$, assuming of course that it was in the ground state to begin. It is convenient now to think of the mass M as being infinitely heavy, so that we don't have to be concerned with center of mass motion which would just obscure the issue in the present context: as we have seen there is no qualitative difference between M being very large and being strictly infinite.

We apply then the rule (R.2), pointing out the obvious, that the ground state referred to is, or course, the oscillator ground state. We have:

$$P_{00} = \begin{bmatrix}\text{Probability ampli-}\\ \text{tude for nucleus}\\ \text{to be in oscillator}\\ \text{ground state}\\ \text{after recoil}\end{bmatrix} = \sum_p, \int \begin{bmatrix}\text{Probability amplitude}\\ \text{for nucleus being in}\\ \text{oscillator ground}\\ \text{state when it has}\\ \text{momentum } p\end{bmatrix}^* \times \begin{bmatrix}\text{Probability ampli-}\\ \text{tude for nucleus}\\ \text{having momen-}\\ \text{tum } p \text{ after recoil}\end{bmatrix}. \quad \text{(R.3)}$$

What then are the probability amplitudes that enter the right-hand side of rule (R.3)? First, the probability amplitude for the nucleus to be in the ground state when it has momentum p is simply the ground-state wavefunction $\phi_0(p)$. Moreover, since the nucleus gets an additional momentum p_0 (in addition to its zero-point momentum), on recoiling from the photon, the probability amplitude for having momentum p

after recoil is just:

Probability amplitude for nucleus to have momentum p after recoil	=	Probability amplitude for nucleus to have had momentum $p-p_0$ before recoil.

Therefore, the probability amplitude for the nucleus to have had momentum $p-p_0$ before recoil is, since it was in the ground state before recoil, just $\phi_0(p-p_0)$. Thus, rule (R.3) applied to the present case is just

$$P_{00}=\int \phi_0^*(p)\phi_0(p-p_0)dp$$

and the Mössbauer f factor, the probability that the system remains in the ground state is

$$f\equiv|P_{00}|^2=\left|\int \phi_0^*(p)\phi_0(p-p_0)dp\right|^2.$$

This result, although simple enough, is not in the form one usually sees. To get to this form we introduce the ground-state space wavefunction $\psi_0(x)$, of which $\phi_0(p)$ is the Fourier transform

$$\phi_0(p)=\frac{1}{(2\pi)^{\frac{1}{2}}}\int \psi_0(x)e^{ipx/\hbar}dx.$$

If we put this into the expression above for P_{00} we get

$$P_{00}=\frac{1}{2\pi}\int\int\int \psi_0^*(x')$$
$$\times e^{ipx'/\hbar}\psi_0(x)e^{i(p-p_0)x/\hbar}dpdx'dx.$$

The p integration yields a δ function of $(x'-x)$ and we have

$$P_{00}=\int \psi_0^*(x)e^{ip_0x/\hbar}\psi_0(x)dx. \tag{12}$$

The f coefficient of Mössbauer is then the more common expression

$$f=\left|\int \psi_0^*(x)e^{ip_0x/\hbar}\psi_0(x)dx\right|^2. \tag{13}$$

The ground-state wavefunction $\psi_0(x)$ is

$$\psi_0(x)=\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\exp(-m\omega x^2/2\hbar).$$

If we evaluate Eq. (13) using this wavefunction we get

$$f=e^{-R/\hbar\omega}, \tag{14}$$

where R is the recoil energy defined by Eq. (3). We see that if R is of the same order as $\hbar\omega$, the oscillator quantum energy, the probability for the Mössbauer effect is substantial.

B. One and Three-Dimensional Lattices

The discussion of the last section was for a rather idealized problem, in which all the 10^{23} degrees of freedom and 10^{23} frequencies of the original problem were replaced by a single degree of freedom and a single frequency. Thus the existence of the effect depended on the fact that the energy of an Einstein oscillator is quantized, and more precisely on the fact that the quantized level spacing $\hbar\omega$ is of the order of R, the recoil energy. If $\hbar\omega$ were very small we would have had

$$f=e^{-R/\hbar\omega}\approx e^{-R/0}=0,$$

and there would have been no Mössbauer effect. Now in an actual solid, or even in a more accurate model such as the Debye model, one does have energy eigenvalues for vibration that are arbitrarily small. It is natural then to ask whether in this case the effect vanishes, "whittled away" by recoil energy loss to low-energy vibrational quanta.

There are various arguments in the literature that purport to show why this does not happen. For example, there is a classical argument,[4] the gist of which seems to be that since it is a single nucleus which emits the gamma ray and tends to excite the lattice by its recoil, it will mainly excite high-lattice frequencies since such a recoil is a sharply local disturbance demanding high Fourier components for its description. This statement is true, and it shows perhaps why the low-frequency modes are not easily excited, but

[4] H. Frauenfelder, *The Mössbauer Effect* (W. A. Benjamin, New York, 1962), pp. 22.

in our mind it leaves unanswered the question of why the Mössbauer effect is not then destroyed by the loss of energy to higher frequency phonons. In our opinion, any classical argument which purports to explain fine features of the effect must be specious, since we have seen that the effect has a strong and essential quantum-mechanical basis. We return then to this point after we work out some details of the quantum mechanics of the Mössbauer effect in a lattice.

Let us begin with the one-dimensional lattice; the extension to three-dimensions is then trivial and consists mainly of making scalars into vectors. Consider then a lattice consisting of N masses (nuclei) on a line, with harmonic forces acting between mass pairs. Let the coordinates of these masses be $x_1, x_2, \cdots, x_N$ and let x_1 be the coordinate[5] of the "Mössbauer nucleus." Suppose now the system is in its ground state, with a wavefunction $\psi_0(x_1, x_2, \cdots, x_N)$ and suppose as before that the "Mössbauer nucleus" emits a gamma ray, thereby suffering an instantaneous recoil momentum kick. We want to find the probability that the system will still be found in the ground state after gamma-ray emission; in fact it is useful to generalize this a little and find the probability that the system ends up in a specified final state F, wavefunction $\psi_F(x_1, x_2, \cdots, x_N)$, with the ground state as a special case. In this way we later are able to compare the relative probabilities of multiphonon processes.

The argument we use is basically similar to that for the Einstein model except that the notation gets more complicated since we are dealing with not one but N masses. Consider then the momentum distribution of the masses in the final state, i.e., after recoil. It is given by the squared magnitude of a probability amplitude, that we call $\phi_F(p_1, \cdots p_N)$; this is of course just the momentum space wavefunction,

$$\phi_F(p_1\cdots p_N)$$
$$=1/(2\pi)^{N/2}\int\cdots\int\psi_F(x_1,\cdots x_N)$$
$$\times e^{i(p_1x_1+\cdots+p_Nx_N)/\hbar}dx_1\cdots dx_N.$$

[5] There is no real loss of generality in letting x_1 be the coordinate of the Mössbauer nucleus, since the wavefunction satisfies periodic boundary conditions which essentially make every nucleus equivalent to every other one.

Consider now the probability amplitude for the first mass to have momentum p_1 after recoil, and for the other masses to have momentum $p_2\cdots p_N$. As we have argued for the Einstein model, since the first mass gets a momentum p_0 by the recoil process, the probability amplitude for its having p_1 after recoil, is the same as that for having had p_1-p_0 before recoil, and the probability amplitude in question is just

$$\phi_0(p_1-p_0,\ p_2,\cdots,\ p_N).$$

Now the probability amplitude for the system to be in the state F with momenta $p_1,\cdots, p_N$ is just the excited state wavefunction

$$\phi_F(p_1,\cdots,\ p_N).$$

Applying then the rule (R.2) as before, the total probability amplitude P_{0F} that the system end up in the final state F, is got by integrating over all values of individual momenta, $p_1\cdots p_N$, and is just

$$P_{0F}=\int\cdots\int\phi_F^*(p_1,p_2\cdots p_N)\phi_0$$
$$\times(p_1-p_0,\ p_2\cdots p_N)dp_1\cdots dp_N. \quad (15)$$

If we introduce the space wavefunction ψ_F defined above, and ψ_0 defined analogously, we are led to the usual expression for the probability amplitude P_{0F}

$$P_{0F}=\int\cdots\int\psi_F^*(x_1\cdots x_N)$$
$$\times e^{ip_0x/\hbar}\psi_0(x_1\cdots x_N)dx_1\cdots dx_N. \quad (16)$$

The probability that the system ends up in final state ψ_F is of course just the squared magnitude of this quantity.

Now we discuss the evaluation of the integral of Eq. (16). We assume, as is customary, a lattice with periodic boundary conditions and we recall that for such a lattice of N degrees of freedom there are N natural frequencies $\omega_1\cdots\omega_N$. These are usually expressed by writing $\omega=\omega(k)$ where the quantum or wavenumber k can take on the N different values, $0,\ 2\pi/N,\ 4\pi/N,\cdots,$ $(N-1)2\pi/N$. We put a superscript on k to differentiate among these N possibilities.

$$k^{(l)}=2\pi l/N.$$

Now for each $k^{(l)}$ and corresponding ω_l there is a normal coordinate y_l so defined that classically y_l satisfies the equation of motion of a simple harmonic oscillator. The transformation from the coordinates x_n to these normal coordinates is given by

$$x_n = \frac{1}{(N)^{\frac{1}{2}}} \sum_{l=1}^{N} a_{ln} y_l, \quad a_{ln} = \exp[ik^{(l)}n]. \tag{17}$$

In quantum mechanics, the transformation Eq. (17) separates the Schrödinger equation so that the wavefunction for the lattice can be written as the product of N harmonic oscillator wavefunctions. Each one of these is characterized by its frequency ω and by the usual harmonic oscillator quantum number n. We call these wavefunctions $u_{n,\omega}(y)$. Specifically, for $n=0$ and $n=1$

$$u_{0,\omega}(y) = (m\omega/\pi\hbar)^{\frac{1}{4}} e^{-m\omega y^2/2\hbar} \tag{18}$$
$$u_{1,\omega}(y) = (1/\sqrt{2}) y (m\omega/\pi\hbar)^{\frac{1}{4}} e^{-m\omega y^2/2\hbar}.$$

These wavefunctions are part of a complete set of eigenfunctions; hence they can be assumed to be orthonormal. In terms of them the ground state wavefunction ψ_0 is the product

$$\psi_0 = u_{0,\omega_1}(y_1) \cdots u_{0,\omega_N}(y_N). \tag{19}$$

The final state wavefunction is given by an analogous function, except that one or more of the oscillators may be in an excited state. We consider specifically the case when, say, the s'th oscillator is in its first excited state. In other language: a phonon of frequency ω_s is excited. For this case

$$\psi_F = u_{0,\omega_1}(y_1) u_{0,\omega_2}(y_2) \cdots u_{1,\omega_s}(y_s) \cdots u_{0,\omega_N}(y_N). \tag{20}$$

Now we use these wavefunctions to calculate the probabilities that the system ends up after emission in a given final state. Consider first P_{00} the probability amplitude for the system to remain in the ground state. If we put Eq. (19) into (16) we get for this, (the Jacobian of the transformation from the x's to the y's is unity)

$$P_{00} = \int \cdots \int |u_{0,\omega_1}(y_1) \cdots u_{0,\omega_N}(y_N)|^2 \times \exp\left[\frac{ip_0}{\hbar(N)^{\frac{1}{2}}} \sum a_{1l} y_l\right] dy_1 \cdots dy_N. \tag{21}$$

This last integral is in fact the product of N integrals, a typical one of which, say the q'th, is

$$\int |u_{0,\omega_q}(y_q)|^2 \exp\left[\frac{ip_0 a_{1q} y_q}{\hbar(N)^{\frac{1}{2}}}\right] dy_q = \exp\left[-\frac{p_0^2 |a_{1q}|^2}{2m\hbar\omega_q N}\right].$$

In the limit of N infinite this typical integral becomes the normalization integral and is unity; by the same token for N large but finite it becomes unity to within terms of order $1/N$. Returning then to Eq. (21), the N-fold integral that appears there breaks up into a product of N terms, each unity to within terms of $1/N$ and to evaluate it we must then look carefully at the mathematics of this in the limit of large N; we cannot go further by intuition. We defer this for the moment, however, to return to the question of calculating the probability of a transition in which one normal mode, say the s'th of frequency ω_s is excited. We must then calculate P_{0F} defined by (Eq. (16). If we insert into it the expressions (19) and (20) for ψ_F and ψ_0, we are led to an N-fold integral which is much like that for P_{00} except that the integral over y_s is now

$$\int u_{1,\omega q}^*(y_q) u_{0,\omega_s} y(s) \exp\left[\frac{ip_0 a_{1s} y_s}{\hbar(N)^{\frac{1}{2}}}\right] dy_s = \frac{ip_0 a_{1s}}{\hbar}\left(\frac{2}{N}\right)^{\frac{1}{2}} \exp\left[\frac{-p_0^2 |a_{1s}|^2}{2m\hbar\omega_s N}\right].$$

The other $N-1$ integrals lead to essentially the same result as (21), so we can say that the probability amplitude for exciting a *given* one-phonon mode is of the order of $1/(N)^{\frac{1}{2}}$ times that for staying in the ground state, and the probability itself is of the order $1/N$ as large. On the other hand, there are N such modes so the *total probability* of one-phonon excitation, i.e., of exciting one or the other of the N phonons, can be of the same order of magnitude as that for zero-phonon excitation, as far as factors of order N are concerned. Of course, the exact relative probabilities for no-phonon and one-phonon excitation depends on the details of the particular lattice and Mössbauer nucleus one is considering. The point of the above argument is to make clear why the total one-phonon contribution is not overwhelming for large N, first impressions perhaps to the contrary.

Now let us consider the extension of these results to three dimensional lattices. The general outline of the results is the same except that there are now $3N$ different frequencies. This is expressed by writing ω as a function of a vector $\mathbf{k}$ where $\mathbf{k}$ ranges over $3N$ values in the first Brillouin zone of the lattice. But given this difference, the introduction of normal coordinates $\mathbf{r}_i$ and the conversion of the integrals for P_{0F} into $3N$ single integrals closely parallels the one-dimensional case. We do not give the mathematical details of the evaluation of P_{00} and P_{0F}. Suffice it to say that to do these integrals one must know the frequency spectrum $\omega(\mathbf{k})$. This spectrum, known in principle, is but poorly known in practice, so what is usually done is to assume a Debye model in which $n(\omega)$ the number of frequencies with magnitudes between ω and $\omega+d\omega$ is given by

$$n(\omega)=\begin{cases} 3N\omega^2/\omega_D^3, & \omega<\omega_D \\ 0 \quad , & \omega>\omega_D \end{cases}. \tag{22}$$

With this approximation P_{00} can be evaluated and on squaring it one gets the probability for "recoilless emission," usually designated by f.

$$f\equiv|P_{00}|^2=e^{-3R/2\hbar\omega}\ . \tag{23}$$

This is similar to the result with the Einstein model. The reason is that the distribution of Eq. (22) weights high frequencies fairly heavily, peaking at the Debye frequency ω_D so that one does not find much difference between using it and using a single frequency. Similarly the probability $\mathcal{P}_{0F}$ for exciting a single mode of frequency ω_s (one-phonon process) turns out to be smaller than f by a factor involving $1/N$.

$$\mathcal{P}_{0F}=|P_{0F}|^2=Rf/N\hbar\omega_s. \tag{24}$$

Since the frequencies are so closely spaced however, they cannot usually be distinguished experimentally, and the quantity of interest is not Eq. (24) but the probability of exciting any of the modes with frequencies lying between ω and $\omega+d\omega$. Calling this probability $\mathcal{P}_{0\omega}(\omega)$ one gets, on combining Eq. (24) with the Debye distribution

$$\mathcal{P}_{0\omega}(\omega)d\omega=3Rf\omega d\omega/\hbar\omega_0^3.$$

DISCUSSION

In this section we discuss briefly several topics which are relevant to the Mössbauer effect, but which have not found an appropriate place in the preceding sections. First, we point out that we have confined our attention to the effect at zero temperature, since the statistical considerations that nonzero temperature would bring in are well understood and hence extraneous to our aim of getting at the basic physics of the Mössbauer effect. Secondly, we have considered the Mössbauer effect to be the "recoilless emission" of gamma rays, but there is a certain amount of arbitrariness here. This is, one might consider the Mössbauer effect to be the resonant scattering phenomenon originally observed by Mössbauer, which scattering involves both the emission and subsequent absorption of gamma rays. But to consider this two part process as a whole simply confuses the basic emission process we have tried to understand, without any compensating advantages. That is, in the usual methods for calculating this scattering process as a whole, one finds an expression for the cross section which involves the nuclear half-life gamma γ in a time integration,[6] and with this half-life appearing so naturally in the theory it becomes difficult to put it in proper perspective and assign it its correct role. In particular, it is then harder to reconcile its presence with the concept of instantaneous emission. It is easier then to do as we have done and concentrate on understanding the one-stage process of emission, in which case the significance of γ is clearer.

It should be emphasized once again that the Mössbauer effect is essentially a quantum mechanical phenomenon. There are derivations of the effect which look upon it as the emission of an electromagnetic wave by a nucleus which vibrates with the lattice, and which therefore in a sense frequency modulates the wave. But these derivations simply assume that the emission of the wave leaves the lattice unperturbed, and so take as a mere assumption the basic physical process which is at the heart of the Mössbauer effect, without throwing any real light on it. In this sense these derivations must be considered unsatisfactory. We have discussed the Möss-

[6] Reference 4, p. 195, Eq. (2).

bauer effect using the harmonic model of the lattice. Some authors have questioned the effect of introducing the anharmonic forces which certainly exist. If anharmonic forces are introduced the phonons cease to be true eigenstates of the system; in a way of speaking they "have a lifetime." Will this fact of the phonon lifetime spoil the Mössbauer effect? It can be seen immediately that this will not be so. For although from one point of view the anharmonic forces do endow the phonon with a lifetime, from another point of view we need not be concerned with this at all. For we simply observe that whatever the anharmonic forces may be, there is, in principle, an exact set of wavefunctions for them. When these wavefunctions are used in the expression (16) they certainly give a finite f factor, although this may be quite different in magnitude from that with purely harmonic forces. Thus nothing in principle is changed by the phonon lifetime.

APPENDIX A

On Instantaneous Momentum Transfer

As has been previously mentioned, the assumption we have adopted, of instantaneous momentum transfer in the recoil process, has generated some controversy in the literature. The point at issue is this. The nuclear state has a lifetime τ, which happens to be long compared to the time of lattice oscillations. Some authors then insist that this implies that momentum is not transferred instantaneously, but only over a time of the order of the nuclear lifetime, thereby providing "sufficient time for the recoil momentum to be transferred to the lattice via the binding forces during the scattering process." Our point of view is, of course, the opposite. We hold that τ has nothing to do with the time needed for momentum transfer, which can be taken to be instantaneous. Now, the case for instantaneous emission has been made strongly and at length by Lipkin,[3] so we do not repeat his arguments here but rather concentrate on trying to reconcile the difference of opinion that appears to exist.

We hold that the difference of opinion comes about because of a confusion between the two different time-scales that may pertain to the statistics of a large number of events. These are:

The time that characterizes the statistical distribution.

The time that characterizes each event.

Since it is essential that the distinction between these two times be clear, let us separate it from the *mystique* of quantum mechanics, and illustrate it by a homely example. Suppose we consider as events the automobile collisions that take place in a city between, say, noon and midnight. These are statistically distributed as a function of time, with a peak perhaps at five o'clock and with, for the sake of argument, a certain half-width T around this time. In addition to the halfwidth there is a time which characterizes the "duration of an individual collision," call it the mean collision time t_0; it is clearly much shorter than T, and for our purpose we can idealize it as being instantaneous. We have then a statistical distribution (half-width T) of instantaneous events. It is our claim that we have just this in the quantum mechanics of the Mössbauer effect, viz., a statistical distribution of events (γ-ray emission) characterized by a mean life τ, but with instantaneous individual events. That is, τ refers to the *distribution* and there is no sense in which it characterizes an individual event.

That is the statement of the conflict of opinion. In order to understand it better, however, let us follow some of the arguments that have led up to it. Those authors that look dubiously on the assumption of instantaneous recoil usually start with a question which the different authors formulate somewhat differently but whose essence can be paraphrased and summarized something like this: If the Mössbauer nucleus recoils instantaneously, the disturbance that it creates will propagate through the lattice with velocity of sound so that it will take a long time (many times the nuclear mean life τ) before the sound wave samples the edge of the crystal. On the other hand, the photon presumably is well defined from the moment of its assumed instantaneous emission; that is, it either has at that moment the full energy of the nuclear transition (zero-phonon process) or an energy corresponding to a one-phonon, two-phonon process, etc. These photon energies are characteristic of the phonons, which is to say they are characteristic of the details of the whole crystal structure. How then can the photon know instantly the details of the distant part of the crystal, long before these parts have been "sampled," so to speak, by the sound wave created by the initial recoil?

As soon as the question is phrased in this way we should be put on a certain alert. For it implies that we are looking at this quantum mechanical process in considerable space–time detail and, of course, in quantum mechanics this is frequently not permissible. Also, the argument overlooks one essential point, which in our mind resolves the difficulty. The point is that the Mössbauer nucleus does not recoil from rest, but is characterized at the moment of recoil by the momentum distribution of the crystal in which it finds itself. This distribution is given by the ground state wavefunction of the crystal, which wavefunction is determined by the crystal as a whole. Thus the photon "knows that it is in a crystal" because it is emitted from a nucleus that "knows it is in a crystal." The paradox about having to wait for the sound wave to travel to the edge of the crystal disappears.

We can elaborate on this, and also give ourselves the opportunity of disagreeing with some of the literature if we consider briefly the possibility of the Mössbauer effect in a different system from a lattice. Consider then not a Mössbauer nucleus bound in a lattice, but a Mössbauer nucleus in a "billiard-ball gas" of other nuclei. Now, various opinions in the literature to the contrary, it seems to us that a gas shows a Mössbauer effect in principle, i.e., it has a finite f factor although if the gas is very dilute this may be impractically small from the experimental point of view. The argument is simple; the f factor is given by the integral Eq. (16) and there is no reason for this to be identically zero. In fact, one knows experimentally that there can be a Mössbauer effect in a liquid; and one would not expect qualitative differences between liquids, gases, and dilute gases. To our mind the difference is quantitative, in that the f factor for a gas undoubtedly is small, depending on its dilution, but there is no reason for it to be identically zero.

Consider then a billiard-ball gas of nuclei in which there is a Mössbauer nucleus that emits a gamma ray and recoils. Suppose there is some mean collision time t_0, for collisions between two nuclei. If we assume, as we have done, that the emission is instantaneous then it is hard to see (if we fall in the trap of thinking too classically) how a Mössbauer effect is possible. For the Mössbauer effect can only exist, as we have seen, if the photon recoil momentum is transferred via collisions to the system as a whole. But how can the photon from the Mössbauer nucleus know that the nucleus collides with other nuclei, if the photon is emitted in a time much less than the collision time? The dilemma here is essentially identical to that for the lattice, and is resolved in much the same way. The single nucleus is not like a free nucleus. Rather, it is characterized by the momentum distribution of a nucleus in a gas. Thus, one doesn't have to allow time for the Mössbauer recoil nucleus to collide with the next and that with the next, in order for it to "know" that it is in a billiard-ball gas. It knows that instantaneously, because of its built-in momentum distribution, which is characteristic of that gas, and nothing else. Thus one need not make the attempt, doomed to failure, of following the path of the transfer of energy and momentum through the crystal.

The question of the instantaneous emission has also been phrased in terms of a Gedanken experiment. Suppose one tries to measure the Mössbauer effect in a crystal, using an apparatus that can determine the emission time of the photon, within very short time intervals, say 10^{-20} sec. Will there still be a Mössbauer effect? According to those authors who hold that momentum is not transferred instantaneously, the effect is necessarily destroyed since there is not enough time for the momentum of the recoil nucleus to be transferred to the lattice. Our point of view is somewhat more complicated: The Mössbauer effect is in one sense destroyed, in another not. Now a convincing exposition of this viewpoint presupposes an understanding of the so-called energy-time uncertainty relations, and as the recent work of Aharonov and Bohm[7] shows, this has been rather widely misunderstood. What we do then is divorce the energy-time uncertainty principle from the Mössbauer effect for the moment, and discuss it separately. Then we are in a position to apply it to the effect.

We want to discuss the measurement of energy in a short-time interval. Suppose then that we have an assemblage of nuclei, which nuclei we assume are infinitely heavy, to do away with problems of recoil. Let these nuclei emit gamma rays with an energy spectrum characterized by a width γ at half-maximum. Suppose we measure this spectrum first using an apparatus which simply determines the energy distribution of the photons, but tells nothing about the time of their emission. Then we get the usual intensity distribution[8] $I(\omega)$ in photon frequency

$$I(\omega)d\omega=\frac{\gamma}{2\pi}\frac{\hbar\omega d\omega}{(\omega-\omega_0)^2+\frac{1}{4}\gamma^2}. \tag{A.1}$$

Next, suppose that we have an apparatus which not only can detect photons, but also can tell us how many decay in an interval T, i.e., an apparatus which sorts out the number of decays between times zero and T, between T and $2T$, between $2T$ and $3T$, etc. Then the intensity distribution $I(\omega)$ is not given by the above formula but is proportional to[8]

$$\frac{1+e^{-\gamma T}-2e^{-\gamma T/2}\cos(\omega-\omega_0)T}{(\omega-\omega_0)^2+\frac{1}{4}\gamma^2}. \tag{A.2}$$

Why is there a difference in these two cases, reflected in the difference between (A.1) and (A.2)? It comes about, we hold, because we are dealing in these two cases with two different quantum mechanical systems and hence with two different Hamiltonians. That is, we must consider that the Hamiltonian of the system is the Hamiltonian of the nucleus plus that of the radiation field plus that of the apparatus, with appropriate interactions among all these partial Hamiltonians. Now the apparatus which can measure decays to within a time interval T clearly works differently from one that cannot, so we must assume its Hamiltonian is also different. Then it is not surprising that some properties of the total system (e.g., the gamma-ray spectrum) are also different from these two cases. This situation is thus different from the case one frequently encounters in quantum mechanics where the measuring apparatus acts impulsively, and a more obvious distinction between system and apparatus can be made. Here the measurement is not made impulsively, and one must consider that what one is tempted to call the apparatus must in fact be considered as part of the total system, and that the "cut" between system and apparatus must be made at some stage closer to the observer.

Now we come back to the original question. Will the Mössbauer effect take place if one measures the time distribution of the photons to within very short time intervals? As we have indicated, the answer is yes or no, depending on what one means by Mössbauer effect. If one means by it the emission of a photon by a nuclear gamma ray, with no excitation of internal energy of the lattice then there will be no difference in principle between the two systems with the two different apparatuses. In each case we have instantaneous emission of photons, (although of course the time spectra and energy distributions are different for the two systems) and the possibility of "recoilless emission," i.e., the possibility of emission without excitation of phonons. Practically, of course, this distribution may be so altered for the second case, depending on the

[7] Y. Ahoronov and D. Bohm, Phys. Rev. 122, 1649 (1961).

[8] C. S. Wu, Y. K. Lee, N. Bencer-Koller, and P. Sims, Phys. Rev. Letters 9, 432 (1960).

value of T, that the characteristic macroscopic features of the effect may well disappear; for example, the lines in emission and absorption may be so broadened that they overlap; the characteristic Doppler velocities are altered, etc., etc. In this sense the Mössbauer effect is quite different, and if conditions are extreme might be said to be destroyed, but the basic microscopic processes which underlie it, and which might well be called the Mössbauer effect, persist.

APPENDIX B

Transformation Theory: The Relations of Probability Amplitudes

In this Appendix, a brief review of the so-called transformation theory of quantum mechanics is presented. It is obviously not meant to be complete, but goes into only enough detail to enable the reader to understand the development of the text.

To begin, consider for simplicity a one-dimensional system, which can exist in different energy states E_n with corresponding eigenfunctions $\psi_n(x)$. Since the index n labels an energy eigenstate this eigenfunction implicitly refers to an energy and explicitly to position. Now in what follows, it is important to have as simple and general a notation as possible; moreover, we are interested in general properties of this wavefunction which hold for any energy state. The index n then is superfluous for our purposes, and it is more convenient to bring out explicitly the fact that this is an energy eigenfunction. Thus, we might simply call the wavefunction $\psi(E,x)$. But even the ψ can be done away with if, for example, we agree to write angular brackets $\langle\ \rangle$ to mean a wavefunction, and simply denote a general wavefunction like $\psi_n(x)$ by $\langle E|x\rangle$

$$\psi_n(x) \rightarrow \langle E|x\rangle.$$

We recall that this wavefunction has the meaning that its absolute magnitude squared is the probability that the particle is between x and $x+dx$.

$$\begin{pmatrix}\text{Probability of particle being}\\ \text{between } x \text{ and } x+dx\end{pmatrix} = |\langle E|x\rangle|^2.$$

Thus since $\langle E|x\rangle$ is something whose squared magnitude gives a probability, it is called a probability amplitude.

Take another well-known example, the momentum space wavefunction for the n'th energy eigenstate; call it $\phi_n(p)$. For this case also it is convenient to have a notation that emphasizes the fact that this refers simultaneously to momentum and to any energy eigenstate. Accordingly, we write

$$\phi_n(p) \rightarrow \langle E|p\rangle.$$

Here $\langle E|p\rangle$ can also properly be called a probability amplitude since its interpretation is

$$\begin{bmatrix}\text{Probability of particle having}\\ \text{momentum between } p\\ \text{and } p+dp\end{bmatrix} = |\langle E|p\rangle|^2.$$

Consider one final example, a particle with a known momentum p. Its wavefunction is simply a plane wave,

$$\frac{1}{(2\pi)^{\frac{1}{2}}} e^{ipx/\hbar}.$$

This wavefunction refers to both p and x simultaneously, and in line with the discussion above we make this explicit by designating it by $\langle p|x\rangle$

$$\frac{e^{ipx/\hbar}}{(2\pi)^{\frac{1}{2}}} \rightarrow \langle p|x\rangle.$$

Again $\langle p|x\rangle$ can be called a probability amplitude since its physical interpretation is:[9]

$$\begin{bmatrix}\text{Relative probability of particle}\\ \text{being in } dx \text{ when in}\\ \text{momentum eigenstate } p\end{bmatrix} = |\langle p|x\rangle|^2.$$

The three probability amplitudes given above have this in common: they all involve two quantum mechanical quantities which do not commute and which therefore cannot have simultaneous eigenvalues, but they all enable us to calculate the probability distribution of eigenvalues of the second observable, if we know the first observable is in a given eigenstate.

Now, in the set p, E, x there are in fact six ordered pairs of two variables that we can form. There are the three we have already discussed, $\langle E|x\rangle$, $\langle E|p\rangle$, $\langle p|x\rangle$. But there are in addition three others we might have considered, namely, $\langle x|E\rangle$, $\langle p|E\rangle$, $\langle x|p\rangle$. It is natural then to ask whether these latter pairs have probability amplitudes associated with them. The answer is yes; moreover their meaning is similar in that the first variable again refers to the eigenvalue of one observable, and the second to the probability distribution of a second. For example, the probability amplitude $\langle x|E\rangle$ is that for finding the distribution of energy eigenvalues if one knows the particle is at x.

The examples above are only special cases of the general kind of probability amplitude that quantum mechanics deals with. More generally then, suppose one has two quantum mechanical observables; call them α and β. Suppose that

Observable α has eigenvalues $a_1, a_2, a_3\cdots$,
Observable β has eigenvalues $b_1, b_2, b_3\cdots$.

We then ask: if α is known to have a definite eigenvalue (i.e., to be in a definite eigenstate) what is the relative probability of getting the results $b_1, b_2, b_2\cdots b_n\cdots$ for β. The answer is given by the squared magnitude of a probability amplitude which we can call $\langle\alpha|\beta\rangle$

$$\begin{bmatrix}\text{Probability of getting one of}\\ \text{eigenvalues of } \beta \text{ when}\\ \text{system is an eigenvalue of } \alpha\end{bmatrix} = |\langle\alpha|\beta\rangle|^2.$$

Two further questions now arise naturally. How does one find these probability amplitudes in general? Are there relations among the different probability amplitudes so

[9] Since this wavefunction is not normalizable it can only be interpreted in terms of relative probability.

that if one is known others can be found from it? We summarize the answers to these questions.

As is well known, one can find these probability amplitudes by solving eigenvalue equations; for example, $\psi_n(x)\equiv\langle E|x\rangle$ is found by solving the Schrödinger equation

$$H_{\text{operator}}\psi_n(x)=E_n\psi_n(x).$$

The momentum space wavefunction $e^{ip_0x/\hbar}$ is found by solving

$$p_{\text{operator}}\psi(x)=-i\hbar\partial/\partial x\psi(x)=p_0\psi(x).$$

However, once one has found two of these probability amplitudes a third can be found by a basic rule of quantum mechanics: given the probability amplitude, say $\langle\alpha|\xi\rangle$ for two quantum mechanical observables, and given also the probability amplitude, say $\langle\xi,\beta\rangle$ for ξ and some other variable β, then the joint probability amplitude $\langle\alpha|\beta\rangle$ for α and β is

$$\langle\alpha|\beta\rangle=\sum_\xi\langle\alpha|\xi\rangle^*\langle\xi|\beta\rangle, \tag{B.1}$$

or if ξ takes on continuous values

$$\langle\alpha|\beta\rangle=\int\langle\alpha|\xi\rangle^*d\xi\langle\xi|\beta\rangle.$$

This is the basic rule referred to in the text, in the derivation of the Mössbauer f factor. As we have noted, it is similar, in a sense, to the classical rule, stated in the text as rule (R.2) for calculating dependent probabilities,

$$(\text{Probability of } x)=\sum_y,\int[\text{Probability of } (x,\text{ given } y)]\cdot(\text{Probability of } y).$$

The crucial difference between (B.1) and the classical rule is, of course, that in the quantum mechanical case one multiplies not probabilities but probability amplitudes, and it is this that gives rise to the characteristic quantum mechanical "interference" effects.

A final important characteristic of the probability amplitudes is that,

$$\langle\alpha|\beta\rangle=\langle\beta|\alpha\rangle^*$$

or, in terms of probabilities

$$|\langle\alpha|\beta\rangle|^2=|\langle\beta|\alpha\rangle|^2. \tag{B.2}$$

As an example of the rule (B.1), we note that the common expression for the wavefunction in momentum space

$$\phi_n(p)=\frac{1}{(2\pi)^{\frac{1}{2}}}\int\psi_n(x)e^{ipx/\hbar}dx$$

is just a special case of it. That is, this equation can be written in our new notation as

$$\langle E|p\rangle=\int\langle E|x\rangle dx\langle x|p\rangle.$$

As an example of the rule (B.2) we may point out that $|\psi_n(x)|^2$ not only gives the probability of a particle being at x if one knows the energy is E_n, but also gives the probability that it will have energy E_n if one knows the particle is at x. To make this even more concrete suppose we have a particle in a box, i.e., confined to $0<x<L$. Then

$$\psi_n(x)=\frac{1}{(L)^{\frac{1}{2}}}\sin\frac{n\pi x}{L}\quad n=1,2,3,\cdots.$$

The relative probabilities then that upon measurement the particle will have energy eigenvalues $E_1, E_2, E_3,\cdots$ if one knows it is at, say $x=x_0$ are:

$$(\text{Relative probability of finding eigenvalue } E_n)=|\sin(n\pi x_0/L)|^2.$$