

The Mössbauer effect explained

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(Received 14 July 1997; accepted 22 December 1997)

Direct integration of Schrödinger's equation yields the transition probability for the Mössbauer effect, assuming that the bound nucleus receives a sudden impulse of momentum from a gamma particle. Generalization from two coupled oscillators to a linear chain introduces the discrete Fourier transform, in real variables. This chain of coupled oscillators can be used to suggest how very low order collective modes can remain unexcited by the impact. © 1998 American Association of Physics Teachers.

I. INTRODUCTION

R. L. Mössbauer was awarded the Nobel Prize for his 1958 discovery of recoilless resonant nuclear absorption by a photon.¹⁻⁸ A common example occurs when ⁵⁷Co decays to ⁵⁷Fe, emitting a 14.4-keV gamma particle with remarkably narrow linewidth, corresponding to an energy of 4.7×10^{-9} eV. Such a small change of energy is consistent with a Doppler shift of only 0.02 cm/s, and is much smaller than the recoil energy of 2×10^{-3} eV resulting from the absorption or emission of the photon by a free nucleus. The Mössbauer effect is recoilless emission or absorption, in which the energy shift associated with recoil (2×10^{-3} eV in the case of ⁵⁷Fe) is absent because the nucleus is bound by the lattice.

Here we present a simple derivation of how the Mössbauer effect⁴ permits the absorption of a gamma ray without recoil. A free particle at rest acquires $\hbar^2 k^2/2m$ of kinetic energy if a force imparts an impulse of momentum equal to $\hbar k$. If the struck particle is a nucleus bound in a crystal lattice, the momentum can be absorbed with no change in energy. How does this happen? Direct integration of Schrödinger's equation (with the kinetic energy term neglected) shows that the oscillator usually remains in the ground state whenever $\hbar^2 k^2/2m \ll \hbar \omega$, where $\hbar \omega$ is the excitation energy of the oscillator. This is intuitively reasonable: The oscillator is not excited if the energy required to reach the next quantum state is larger than what might be called the "available kinetic energy" associated with an impulse. However, this leaves an important question unanswered: Collective (phonon) modes can have excitation energies much less than $\hbar^2 k^2/2m$. Why are they not excited by the impulse? This can be answered qualitatively by first using a familiar and intuitive change of variables to analyze two coupled oscillators. The discrete real Fourier transform then allows generalization to a linear chain of arbitrary length. While the assumption of a one-dimensional linear chain yields results that differ from the three-dimensional case, this analysis yields an intuitive understanding of how low order modes escape excitation by the impact of a gamma ray on a nucleus. The Appendix presents an alternative model in which the nucleus receives its impulsive via a collision with another particle, instead of via an impulse force "suddenly" applied at $t=0$.

II. SINGLE NUCLEUS

A particle of mass m suddenly receives an impulse of momentum $\hbar k$ at $t=0$. The impulse is modeled as a very

large force, F , acting for a very short time, τ . Since the force is large, we can neglect the kinetic energy in Schrödinger's equation and integrate, noting that the potential is $V(x) = -xF$,

$$i\hbar \frac{\partial \psi}{\partial t} = -xF\psi - \frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \approx -xF\psi. \quad (1)$$

Integration with respect to time yields

$$\psi(x, \tau) = \psi(x, 0) e^{iFx\tau/\hbar} = \psi(x, 0) e^{ikx}, \quad (2)$$

where $\hbar k = F\tau$ is the applied impulse. It is interesting that the Fourier transform $\psi(q) = \int \psi(x) e^{-iqx} dx$ is converted into $\psi(q-k)$ by the impulse, meaning that the wave function is shifted in momentum space by the applied impulse.

Denote the normalized energy states of the harmonic oscillator as $u_j(x)$, where j is a non-negative integer. By a fundamental postulate of quantum mechanics, the probability that the collision leaves the wave function in the j th excited state is obtained by taking the inner product of $\psi(x, \tau)$ with $u_j(x)$. For example, if the particle is in the ground state prior to collision, then $\psi(x, 0) = u_0(x)$. Thus

$$P_j = \left| \int u_0(x) e^{ikx} u_j^*(x) dx \right|^2 \quad (3)$$

is the probability that the collision converts a ground state into the j th excited state. In the event that $P_0 \approx 1$, we may expand the exponential to obtain an approximate expression for $P_E = P_0 - 1$, the probability of putting the nucleus into one of the excited states:

$$P_E = 1 - P_0 \approx \frac{1}{2} k^2 \langle x^2 \rangle, \quad (4)$$

where x is referenced to a point where $\langle x \rangle = 0$. Let σ be the spring constant, so that $\omega = (\sigma/m)^{1/2}$ is the oscillator's frequency. Noting that total energy, $\hbar \omega/2$, arises from equal contributions of kinetic energy $\langle p^2 \rangle/2m$ and potential energy $\sigma \langle x^2 \rangle/2$, a more illuminating form for P_E is obtained:

$$P_E \approx \frac{k^2 \langle x^2 \rangle}{2} = \frac{\hbar^2 k^2}{2m} \bigg/ \hbar \omega \quad (5)$$

(provided $P_E \ll 1$). Equation (5) has a simple interpretation: No transfer of energy from an impulse takes place if the energy required to reach the next eigenstate, $\hbar \omega$, is larger

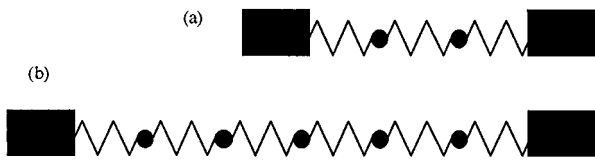


Fig. 1. Coupled harmonic oscillators showing (a) $N=2$ and (b) $N=5$.

than the kinetic energy, $\hbar^2 k^2/2m$, acquired when a free particle at rest is subject to the impulse $\hbar k$.

The reader may find it difficult to reconcile this simple discussion of a ‘‘sudden’’ impulse with a collision involving a photon of very well-defined wavelength. By Heisenberg’s uncertainty principle, such a photon has a very long coherence time, and cannot be made to strike the nucleus at time $t=0$. Insight into this question is developed in the Appendix, where an alternative means of applying the impulse to the oscillator is presented.

III. TWO COUPLED OSCILLATORS

The previous discussion explains why the nucleus does not recoil against its nearest neighbors. But long wavelength collective modes have very closely spaced energy levels. How do they avoid excitation by the impulse? To investigate this, we consider a chain of harmonic oscillators, coupled together as in Fig. 1. The case $N=2$ is modeled by Schrödinger’s equation for two variables:

$$\begin{aligned} \psi &= \psi(x_1, x_2), \\ i\hbar \frac{\partial \psi}{\partial t} &= \frac{-\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial x_1^2} + \frac{\partial^2 \psi}{\partial x_2^2} \right) + \frac{\sigma}{2} x_1^2 \psi \\ &\quad + \frac{\sigma}{2} x_2^2 \psi + \frac{\sigma}{2} (x_1 - x_2)^2 \psi. \end{aligned} \quad (6)$$

The change of variables,

$$\xi_1 = \frac{x_1 + x_2}{\sqrt{2}}, \quad \xi_2 = \frac{x_1 - x_2}{\sqrt{2}}, \quad (7)$$

is known to ‘‘decouple’’ two coupled pendulums in the classical case. Using identities such as $\sqrt{2} \partial/\partial x_1 = \partial/\partial \xi_1 + \partial/\partial \xi_2$, this converts Schrödinger’s equation into a simpler (i.e., separable) form:

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial \xi_1^2} + \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial \xi_2^2} + \frac{\sigma_1}{2} \xi_1^2 \psi + \frac{\sigma_2}{2} \xi_2^2 \psi, \quad (8)$$

where $\sigma_1 = \sigma$ and $\sigma_2 = 3\sigma$.

From (8), we see that in these ‘‘normal mode’’ ξ variables, Schrödinger’s equation separates into two independent harmonic oscillator equations, allowing us to write ψ as a product $\psi_1(\xi_1)\psi_2(\xi_2)$. While these decoupled oscillators don’t really exist in a physical sense, they exist mathematically. And mathematically speaking, we shall see that each decoupled oscillator independently receives its share of ‘‘effective impulse’’ as a single nucleus is struck. This ‘‘effective impulse’’ is not momentum in the sense of mass times velocity. The choice of the $\sqrt{2}$ in (7) is arbitrary, but deliberately chosen in order that the ‘‘mass’’ of these normal mode oscillators equals the mass of the particles, m .

Let x_1 represent the particle that receives the impulse $\hbar k$. Since $dx_1 dx_2 = d\xi_1 d\xi_2$, we can write the matrix element in (3) as

$$\begin{aligned} &\int \psi(x_1, x_2) e^{ikx_1} \psi^*(x_1, x_2) dx_1 dx_2 \\ &= \left\{ \int \psi_1(\xi_1) e^{iK_1 \xi_1} \psi_1^*(\xi_1) d\xi_1 \right\} \\ &\quad \times \left\{ \int \psi_2(\xi_2) e^{iK_2 \xi_2} \psi_2^*(\xi_2) d\xi_2 \right\}, \end{aligned} \quad (9)$$

where we have defined $K_1 = K_2 = k/\sqrt{2}$ so that $kx_1 = K_1 \xi_1 + K_2 \xi_2$. Note that $K_1^2 + K_2^2 = k^2$. This is a special case of the general result for a one-dimensional chain of N coupled oscillators, $\sum K_j^2 = k^2$, to be discussed in Sec. IV. Note that the ‘‘effective’’ impulse for each normal mode, $\hbar K_j$, is smaller than the impulse, $\hbar k$, applied to a single atom. This is the mechanism by which low energy modes avoid excitation by the impulse: The ‘‘effective momentum’’ must be shared in such a way that each normal mode gets a fraction of the impulse.

IV. N COUPLED OSCILLATORS

The previous change of variables (7) is actually a special case of the discrete Fourier transform for N real variables, which also transform into the normal mode coordinates, ξ_j , associated with classical physics:

$$\begin{aligned} x_n &= \sqrt{\frac{2}{N+1}} \sum_{j=1}^N \xi_j \sin\left(\frac{j\pi n}{N+1}\right), \\ \xi_j &= \sqrt{\frac{2}{N+1}} \sum_{n=1}^N x_n \sin\left(\frac{j\pi n}{N+1}\right). \end{aligned} \quad (10)$$

Here x_0 and x_{N+1} are not quantum variables, but are simply defined as zero, establishing boundary conditions for the normal modes. The inverse transform is verified using

$$\begin{aligned} \sum_{j=1}^N \sin\left(\frac{j\pi n}{N+1}\right) \sin\left(\frac{k\pi n}{N+1}\right) &= \frac{N+1}{2} \delta_{jk}, \\ \sum_{j=1}^N \sin\left(\frac{j\pi n}{N+1}\right) \cos\left(\frac{k\pi n}{N+1}\right) &= 0. \end{aligned} \quad (11)$$

Other useful identities are $\sum x_n^2 = \sum \xi_j^2$ and $\sum \partial^2/\partial x_n^2 = \sum \partial^2/\partial \xi_j^2$. The latter is obtained using the chain rule of multivariable calculus:

$$\frac{\partial}{\partial x_n} = \sum_{j=1}^N \frac{\partial \xi_j}{\partial x_n} \frac{\partial}{\partial \xi_j} = \sqrt{\frac{1}{N+1}} \sum_{j=1}^N \sin\left(\frac{n\pi j}{N+1}\right) \frac{\partial}{\partial \xi_j}.$$

Schrödinger’s equation,

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \sum_{n=1}^N \frac{\partial^2 \psi}{\partial x_n^2} + \frac{\sigma}{2} \sum_{n=0}^N (x_n - x_{n+1})^2 \psi \quad (12)$$

becomes a separable equation,

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \sum_{n=j}^N \frac{\partial^2 \psi}{\partial \xi_j^2} + \frac{1}{2} \sum_{n=0}^N \sigma_j \xi_j^2 \psi, \quad (13)$$

where the effective spring constant for each mode is

$$\sigma_j = 2\sigma \left[1 - \cos\left(\frac{j\pi}{N+1}\right) \right]. \quad (14)$$

Next we rewrite the term $\exp(ikx_p)$ by direct substitution for x_p ($1 \leq p \leq N$) where p labels the single nucleus that absorbs the impulse $\hbar k$:

$$\begin{aligned} \exp(ik_0 x_p) &= \exp\left(ik_0 \left\{ \sqrt{\frac{2}{N+1}} \sum_{j=1}^N \xi_j \sin\left(\frac{j\pi p}{N+1}\right) \right\} \right) \\ &= \prod_{j=1}^N \exp(ik_j \xi_j), \end{aligned} \quad (15)$$

where the “effective” momentum received by the j th normal mode,

$$\hbar K_j = \left\{ \sqrt{\frac{2}{N+1}} \sin\left(\frac{j\pi p}{N+1}\right) \right\} \hbar k_0, \quad (16)$$

is typically smaller than $\hbar k$ by a factor \sqrt{N} . Define $\hbar \omega_j$ as the characteristic energy of the j th mode. Taylor expanding (14) for low order modes ($j \ll N$) yields $\omega_j \approx j\pi\omega/N$, where $\hbar\omega = \hbar(\sigma/m)^{1/2}$ is the characteristic energy of a single mass–spring system described in Sec. II. Using (5), the probability of exciting a low order mode is

$$P_E(j) \approx \frac{\hbar^2 K_j^2}{2m} / \hbar \omega_j \approx \frac{1}{j\pi} P_E, \quad (17)$$

where P_E is the probability for a single mass–spring system given by (5), and we have assumed both $j \ll N$ and $P_E \ll 1$.

Equation (17) explains how very low energy phonons might escape excitation by an impulse applied to a single atom. But it does not explain how all the phonons escape excitation. In fact, (17) predicts that the Mössbauer effect does not happen because after summing over all lower order modes, we find that

$$\frac{1}{1} + \frac{1}{2} + \frac{1}{3} + \dots \approx \ln(n_{\max}) \quad (18)$$

for some $n_{\max} < N$.

This logarithmic divergence is relatively weak (the logarithm of a large number is not very large). In three dimensions, the sum does not diverge. One reason is that low order modes occupy a smaller amount of phase space in three dimensions. The density of modes in three dimensions is $g(q) \propto q^2$, while it is independent of q in one dimension (q is the phonon wave number). Suppose that the one-dimensional chain of this calculation were actually imbedded in a three-dimensional crystal, with the applied impulse being parallel to the chain. The shear forces between atoms would excite normal modes other than those calculated in this paper. This would certainly dilute the “effective” momentum applied to each normal mode. Thus we know that (17) and (18) represent an over-estimate of the probability of energy transfer. For another discussion of three versus one-dimensional crystals, see Ref. 4.

ACKNOWLEDGMENT

This work is partially sponsored by P.E.T.E. (Partners for Excellence in Teacher Education): NSF Grant No. DUE-9453612.

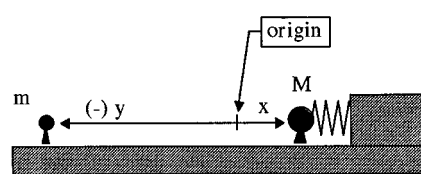


Fig. 2. Sketch of geometry for a model of two colliding particles in one dimension. The particles are “hard” in that they do not pass through each other.

APPENDIX: ALTERNATIVE MODEL FOR A “SUDDEN” IMPULSE

The calculation of Sec. II forces the reader to imagine that a photon of known momentum is made to strike the nucleus at a certain time, in apparent violation of Heisenberg’s uncertainty principle, as applied to the photon’s wavelength and position. We shall refer to this calculation of (2) as the “sudden” approximation. In this section, we model the incoming gamma ray as a free quantum particle striking a bound quantum particle. While the free particle is treated nonrelativistically, it is represented by a plane wave with exact momentum and unknown position. In this section, we will obtain an equation that looks like (2), in spite of the fact that we do not know when the collision takes place.

Consider a system that is strictly one dimensional, with the two particles being unable to pass through each other. The situation is similar to the case of two carts on an air track, as sketched in Fig. 2. To make an analogy with a two-dimensional scattering problem, we denote the free particle of mass m by the coordinate “ y ,” and the bound particle of mass M by the coordinate “ x .” As is the case of a particle in an infinite square well, we demand that $\psi(x, y) = 0$ at $y = x$. The Hamiltonian for $y < x$ is

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2} + \frac{\sigma}{2} x^2. \quad (19)$$

The lines of constant potential for this system can be represented in Fig. 3, where both particles are described by a single wave function that obeys a wave equation with properties similar to that of Schrödinger’s equation. The “ y ”

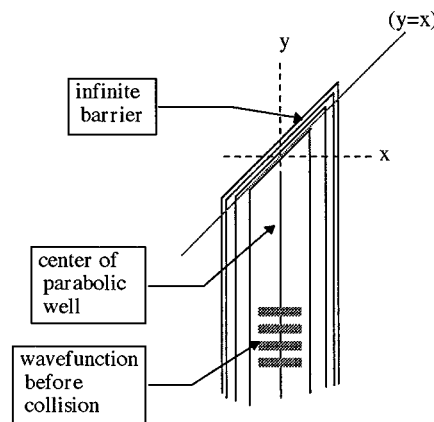


Fig. 3. Two-dimensional analog associated with the two-particle one-dimensional problem. The lines are equipotentials of potential. The infinite force preventing the incoming particle from passing the bound particle is actually represented by closely spaced lines.

particle is incident (free), and sketched in the figure as a wave packet just about to impinge on the bound “ x ” particle, located at $y=0$. The absence of node lines in the “ x ” direction indicates that the oscillator is in the ground state before the collision. After colliding, the wave packet will reverse direction, having suffered disruptions at the slanted potential barrier that cause ripples to appear in the x direction, representing the fact that the post-collision oscillator has a finite probability of being excited.

We shall now seek coefficients C_j such that

$$\psi(x,y) = u_0(x)\exp(ik_0y) + \sum_{j=0}^{\infty} C_j u_j(x)\exp(-ik_jy) \quad (20)$$

matches the boundary condition $\psi=0$ at $x=y$. The first term in (20) is the ingoing wave, and the sum represents outgoing waves, with $u_n(x)$ being normalized oscillator wave functions. Defining $\omega = (\sigma/M)^{1/2}$ and j as the harmonic oscillator quantum number, we have the condition that the momenta of outgoing waves obey

$$E = \frac{\hbar^2}{2m} k_j^2 + (j+1/2)\hbar\omega. \quad (21)$$

This ensures that (20) represents an energy eigenstate with some arbitrary energy E . To find C_j (for $j=0,1,2,\dots$) we set $y=x$ (demanding that ψ vanish there), and multiply (20) by $u_n(x)\exp(ik_nx)$ and integrate over x :

$$0 = \int u_0(x)e^{i(k_0+k_n)x}u_n(x)dx + \sum_{j=0}^{\infty} M_{nj}C_j, \quad (22)$$

where

$$M_{nj} = \int u_n(x)e^{i(k_n-k_j)x}u_j(x)dx = \int u_n(x)e^{i\Delta kx}u_j(x)dx \quad (23)$$

and we have defined $\Delta k = |k_n - k_j|$. The sign convention is that k_j is always positive, so that $\Delta k=0$ corresponds to equal but opposite momenta for the incoming and outgoing free particle channels.

At this point, we need to make the approximation that the incoming (free) particle is very fast and very light, corresponding to the limit that m/M vanishes. As is well known from non-quantum mechanics, a very light particle suffers little change in speed from a collision with a slow-moving heavy particle. This approximation causes the matrix M_{nj} to become the Kroniker (identity) matrix δ_{nj} . A rigorous mathematical justification for this claim starts with (21): Since all transition channels are associated with the same net energy E , one can relate Δk to the change in the bound particle's energy, denoted as $\Delta E_b = \hbar\omega|n-j|$:

$$\frac{\Delta E_b}{E_f} \approx 2 \frac{\Delta k}{k}, \quad (24)$$

where $E_f = \hbar^2 k^2/2m$ is the energy of the free particle. E_f can be made arbitrarily large by a sufficiently small choice of m/M , so that Δk can be made arbitrarily small for a given value of k . By (24), this implies that the energy of the incoming free particle must greatly exceed the available energies of the bound particle ($E_f \gg \Delta E_b$).

Henceforth we carry this approximation to the limit, so that $\Delta k=0$ in (23), causing the matrix M_{nj} to become the Kroniker (identity) matrix δ_{nj} . The wave function becomes, in this limit:

$$\psi(x,y) = u_0(x)\exp(ik_0y) - \sum_{n=0}^{\infty} |n\rangle\langle n|e^{2ik_0y}|0\rangle \times \exp(-ik_ny), \quad (25)$$

where we have used Dirac notation,

$$\langle n|e^{2ik_0y}|0\rangle = \int u_n(x)e^{i2k_0x}u_0(x)dx. \quad (26)$$

Equation (25) expresses the idea of (3) in a slightly different form: Instead of the “final state” of the sudden approximation leading to (3), we have an outgoing wave. The use of Dirac notation puts the completeness of harmonic oscillator wave functions, $\phi(x) = \sum\{u_n(s)\phi(s)ds\}u_n(x)$, into the unforgettable form, $|\phi\rangle = |n\rangle\langle n|\phi\rangle$, so that the energy eigenstate becomes:

$$\psi(x,y) = u_0(x)\exp(ik_0y) - \exp(2ik_0x)u_0(x) \times \exp(-ik_0y). \quad (27)$$

It is instructive to inspect (27) for comparison with the derivation of (2), which was based on a sudden impulse on a single particle. In (27), the extra factor of 2 in $\exp(2ik_0x)$ arises from the fact that the incoming particle imparts twice the impulse as it rebounds. The negative sign before the second term on the right-hand side arises from the inversion of the incoming particle's wave function at the barrier as $\exp(ik_0y)$ converts to $-\exp(-ik_0y)$ after the collision.

Perhaps the most fascinating difference between (27) and (2) is the need to make the approximation $m/M \ll 1$ in order to obtain (27). One might have thought that any collision between two “hard” particles produces the “sudden” prescription (2) for transforming the wave function. This is apparently not the case. One complication is the possibility of multiple collisions when the case $M \approx m$ is treated classically. A more important question is whether a “sudden” impact can occur between quantum particles with small relative velocity. Fortunately, in the Mössbauer effect, the assumption $m/M \ll 1$ seems reasonable because the collision is between a photon and a nucleus.

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