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Zero-point oscillations and Mössbauer effect

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The peculiar properties of the Mössbauer effect provide an important test, and possibly a challenge, to Quantum Physics. The zero-point momentum reservoir of the mechanical oscillators forming a crystal lattice is indicated, in the present paper, as the possible way out from apparent contradictions of the observed features with both momentum conservation and the uncertainty principle.

Keywords: Mössbauer, zero-point, elastic interaction, nuclear decay

1. Introduction

The Mössbauer effect (ME), as is well known, is an elastic process involving photon emission/absorption without transfer of energy to the internal degrees of freedom of the lattice where the emitting/absorbing nucleus is inserted. Its main properties are the following:

A. The ME occurs without observable recoil of the nuclei, in *apparent* contradiction with momentum conservation. No shift, indeed, is observed, with respect to the energy E_γ of the excited nuclear state, in the emission (or absorption) lines.

B. The ME occurs without Doppler broadening of the observed spectral lines, whose *actual* linewidth Γ_{obs} is very close to the *natural* minimum value $\Gamma_o \cong \hbar/\tau$ (where τ is the mean life-time of the excited nuclear state) due to the uncertainty principle. The *apparent* immobility of the nuclei largely exceeds the limits imposed by the uncertainty principle itself [1].

C. The Mössbauer peak is strongly enhanced close to 0 K. The complete emission spectrum includes, besides the narrow and unshifted line of Mössbauer radiation, a non-Mössbauer bulk, whose maximum is endowed with an ordinary thermal Doppler broadening and is shifted with respect to the Mössbauer peak by an amount equal to the quantity $E_{\text{R}} = E_\gamma^2/2Mc^2$, representing the recoil energy received by a free atom with the same mass M of the atoms of the lattice.

D. The ME *does not* occur [2,3] in gases, in liquids and in solids with insufficiently rigid interatomic bonds. The ME progressively vanishes by reducing the dimensions of the solid below 0.1 μm^3, i.e., for crystals containing less than, say, 10^8 atoms.

E. The ME affects (under the same initial conditions) only a fraction of the nuclei of the lattice, which is provided by the well-known Debye–Waller (D–W) "form factor" f, given, for a temperature close to 0 K, by the expression [4]

$$f = \exp\left[-3\frac{E_R}{2k_B T_D}\right], \tag{1a}$$

where k_B is the Boltzmann constant and T_D is the Debye temperature of the lattice, while for $T \gg T_D/2$

$$f = \exp\left[\frac{-6E_R T}{k_B T_D^2}\right]. \tag{1b}$$

These properties are obviously interrelated. Concerning property A, for instance, it is quite natural to think that the "missing" momentum must be absorbed, by means of some kind of coalescence, by the whole crystal. We may therefore perform a rough evaluation of the minimum number of atoms allowing a process with an undetectable line-shift. Recalling, in fact, that the limit of detectability of a Mössbauer spectroscope is better than 10^{-10} eV, we would have, in the case of Fe^{57}, $E_R \approx 10^{-2}$ eV for a single atom, and should assume an aggregation of at least 10^8 atoms (thus leading to property D) in order to build up an effective recoiling mass emitting a radiation endowed with an undetectable shift.

But the question remains: What is the nature of this coalescence?

We shall discuss in the present paper the level of understanding of the ME reached so far.

According to Lipkin [5], indeed, *"Form factor physics provides an excellent introduction to wave-particle duality, complementarity and uncertainty principle because the emitted, absorbed and scattered radiation can be described as either a classical wave or a beam of particles (...). The ME is a particularly simple example (...): it is an ideal subject for students of an introductory course of Quantum Mechanics" (...). Its basic features are perfectly clear (...). The basic physics underlying the ME (...) is all elementary Quantum Mechanics, and should have been understood years before the effect was discovered".*

Analogously, according to Chumakov [6] there exists *"no single experimental result which would contradict the presently accepted mathematical description of the ME. (...) The majority of questions arises because in any simplified approach one loses something. For instance, in the wave-like approach one cannot get the idea of the probability and relative populations of the sidebands depending on temperature, and so on".*

Our personal opinion is that, on the contrary, the co-existence of the wave-like and particle-like models does not reflect the spirit of the complementarity principle. According to this principle, in fact, the wave-like and particle-like models should be invoked for the description of *different* and complementary aspects of physical reality, excluding therefore any *double-face* explication of the same physical feature. Any superposition, indeed, would represent much more a point of weakness than a point of force.

There is, moreover, a certain tendency of each one of the two models (the wave-like and the particle-like one) to commit the explanation of the most delicate points to the other one; so that the basic features of ME remain somewhat obscure.

The standard attitude towards Quantum Mechanics has probably induced many people to an indiscriminate reliance on formalism, even when mere models (requiring every possible explication) and not only the basic axioms are involved. If, however, momentum conservation and the uncertainty principle appear to be in discussion, a further consideration is opportune. Our idea is that the large amount of experimental results allowed by the exploitation of the ME provides a largely unexplored display of tests of Quantum Physics, whose implications and interpretation deserve a careful analysis. The aim of the present paper is to give a contribution to such a far-leading task.

2. The wave-like approach

According to the wave-like approach [7–9] the excited nuclei emit coherent wave-trains (whose frequency we shall call ν_o) with an average time-length of the order of the life-time $\tau\,(\approx 10^{-6} \div 10^{-8}$ s, in the case of γ radiation) of the excited nuclear state. Since such a time is quite longer than the oscillation period ($\approx 10^{-19} \div 10^{-20}$ s) of the emitted waves, it appears plausible to treat the emitting nucleus as a continuous source of monochromatic, classical-like radiation, linked with a mechanical oscillator inserted in a three-dimensional lattice composed of N identical oscillators. The continuous electromagnetic wave-train emitted by the excited nucleus is assumed to be modulated by each one of the mechanical oscillations of the crystal, thus leading to the formation, along each space direction, of N sets of modulation lines centered at ν_o. Recalling that the ME is characterized by a line spectrum without Doppler broadening, the probability of such a process is evaluated by looking for the un-modulated part of the spectrum, i.e., for the (D–W) energy fraction f emitted exactly at the frequency ν_o. The modulated part should therefore represent the energy fraction corresponding to the ordinary radiation, emitted with the usual Doppler effect.

It may be observed, however, that the non-Mössbauer bulk, if it were due to a modulation process, should be symmetrically centered at the Mössbauer (unshifted) peak, and not shifted by E_R as it turns out to be (property C of section 1). The wave-like picture appears therefore to be contradicted by the basic properties of the observed (entire) spectrum.

Let us notice, moreover, that the wave-like model involves a semi-classical process which could be apt to describe the modulation of an ordinary, low frequency and high intensity electromagnetic wave-train, containing a large amount of photons. Because, however, of the very nature of the ME, every wave-train emitted by a nucleus can be coherent only with itself, and can only contain *a single photon* at a time [8]. The modulation predicted by the undulatory model should therefore be impressed on each mono-photonic wave-train, which would virtually contain both the (coherent) Mössbauer line and the incoherent part of the entire γ emission spectrum. The same photon, in other words, should be statistically distributed between the coherent and the incoherent part of a single wave-train!

As a further comment to the wave-like model, let us consider the case of the *reflection* of a wave-train of Mössbauer radiation (with a typical time-length $\tau \approx 10^{-7}$ s) by the resonant nuclei of a lattice. If, as is generally assumed [10], such a reflection occurs in the terms of classical electromagnetism, it implies the formation of a stationary field (due to the sum of incident and reflected waves), where the "nodes" of the electric field in correspondence of the reflecting nuclei cause a vanishing probability of any absorption process. Should the well ordered structure of such a stationary field disappear, a total resonant *absorption* of the wave-train would occur. The *reflection* process requires therefore a stationary field lasting for the entire time τ, giving strong elements of reality to the wave associated to the (not yet revealed) photon. But how can the resonance be preserved for such a long time with an absorbing nucleus mechanically vibrating with the reticular frequencies, up to 10^{13} Hz? A resonant absorbing nucleus, in fact, is subject, during the time $\tau \approx 10^{-7}$ s, to almost 10^{6} oscillations, which should cause a Doppler shift destroying the resonance itself.

3. The particle-like approach

The particle-like model of the ME conceives such an effect as a sudden *ground state* $\rightarrow$ *ground state* transition of the mechanical oscillator containing the emitting nucleus [11,12]: a transition occurring with a probability given, once more, by the D–W factor. Such a factor, indeed, may be obtained in many different semi-empiric ways, none of which turns out to be completely convincing.

The particle-like model was treated in its most exhaustive form by Lipkin [5,11], whose approach develops in two successive stages:

The *first stage* treats the case of a single, unidimensional oscillator, moving in an external harmonic potential and perturbed by the emission process. According to Lipkin "*This simple model already contains the basic features of the ME*" [5];

The *second stage* extends the treatment to a set of coupled oscillators, in terms of the so-called normal variables, which naturally lend themselves to the overall description of the small oscillations of the entire crystal (viewed as a unique physical system) around its equilibrium configuration. A bi-univocal correspondence is also established between these variables and the mechanical eigen-frequencies of the crystal.

According to Lipkin, the emission process cannot, on the one hand, draw energy from the ground state mechanical oscillations of the atom, and is not able, on the other hand (for the fraction undergoing ME), to bring the atom from the lowest (mechanical) energy level to higher ones, because "*the oscillator energy level spacing is large compared with the free recoil energy*" [11]. The observed lack of Doppler effect is therefore due to the fact that any frequency shift $\Delta\nu$ would be associated to an illicit (positive or negative) energy exchange $\Delta E = h\,\Delta\nu$. While, in conclusion, according to Lipkin, the atom does oscillate with its zero-point energy, thus satisfying the uncertainty principle, such a state of motion cannot be revealed by a corresponding Doppler shift of the radiation itself.

One major objection to Lipkin's approach concerns the first stage of his treatment. involving a single harmonic oscillator. We may observe, in fact, that such an oscillator its usual acceptation, has at its disposal an unlimited momentum absorber (behaving like a rigid object of macroscopic dimensions): the force field corresponding to the harmonic potential where the oscillator is placed.

In the case of a *classical* oscillator, any impulse applied to the oscillating mass is transferred to the external potential in a time of the order of the oscillation period.

In the *quantum* case, on the other hand, when the perturbation energy is not sufficient to cause a transition to a different level, the relevant momentum is instantaneously absorbed by the external potential, which is therefore implicitly assumed to be infinitely rigid: an unphysical abstraction which may be accepted only for didactic aims. The proof of such an unphysical character is given by the fact that no ME is practically possible for a single oscillator.

In the second stage of Lipkin's treatment, involving a lattice (i.e., a macroscopic aggregate of oscillators), the tacit assumption is that such an aggregate should generate a potential analogous to that of the single oscillator, at least for the property of *instantaneously* absorbing the recoil momentum.

This picture, however, does not appear to be physically realistic: the impulse due to the emitted quantum may generate at most an acoustic perturbation, which cannot grant a suitable reaction of the medium within the sudden emission time.

The experimentally observed rigid behaviour of crystals subject to elastic processes has apparently suggested to *assume*, rather than to *explain*, the rigidity of the elastic potential. Such a rigidity, however, is not implicit in the postulates of Quantum Mechanics: it is a property, on the contrary, which any model should expressly justify.

We observe, moreover, that the large energy level spacing invoked by Lipkin in order to exclude the oscillator excitation above the ground state may be correct for the afore-mentioned, highly idealized single oscillator, but does not reflect the case of a crystal, where each atom is subject to a large spectrum of oscillations.

4. The zero-point coalescence

Let us recall here that a crystal (composed of N atoms) is submitted, in the limit of linear elasticity, to a spectrum of $3N$ mechanical oscillations, with frequencies $\omega_j \equiv \omega(\mathbf{k}_j)(j = 1, \ldots, 3N)$. At thermal equilibrium, the average number of phonons is given, for any normal mode of oscillation, by Planck's distribution function

$$\bar{n}(\mathbf{k}_j) = \frac{1}{\exp(\hbar\omega(\mathbf{k}_j)/k_\mathrm{B}T) - 1}. \qquad (2)$$

The frequencies of such a spectrum range between a *minimum* value ω_{min}, corresponding to wavelengths of the order of the crystal linear dimensions, and a *maximum* value

$\omega_{max} = \omega_D$ (where $\omega_D \approx 10^{13} \div 10^{14}$ Hz is the Debye frequency of the lattice), corresponding to a wavelength equal to twice the equilibrium interatomic spacing, and determined by the atomic mass and by the elastic constants of the interatomic forces.

At low enough temperatures, the high frequency *thermal* oscillations cannot be excited: when the crystal is close to 0 K, in fact, the only possible mechanical oscillations, at *any* spectral frequency, are the zero-point ones, in agreement with the uncertainty principle.

On these grounds, each atom of a crystal perceives the fact of belonging *to the whole lattice* through its oscillation spectrum. While, however, the *thermal* oscillation spectrum cannot involve, for $T < T_D$, the full set of eigen-frequencies (being limited to the lowest ones), the entire frequency spectrum is always active in the *zero-point* oscillation motions. The zero-point oscillations are therefore the only, complete source of information, acquainting each atom with the characteristics of the lattice to which it belongs – including its irregularities, which strongly affect the spectral structure of the crystal [13].

According to Debye's theory [14], the spectral density of the mechanical oscillations of an isotropic solid (regarding the crystal, and therefore the frequency spectrum, as a continuum with frequency-independent elastic constants) is well approximated by the expression

$$D(\omega) = \frac{9N\omega^2}{(\omega_D)^3}. \tag{3}$$

Since the zero-point oscillation energy of each normal mode ω_j (involving all the atoms of the lattice) is equal to $\hbar\omega_j/2$, the continuous approximation provided by eq. (3) leads therefore to a total zero-point energy of the entire crystal given by

$$E_0 \cong \frac{1}{2}\int_0^{\omega_D} \hbar\omega D(\omega)\,\mathrm{d}\omega = \frac{9}{8}N\hbar\omega_D, \tag{4}$$

where we assumed $\omega_{min} \cong 0$, thus implicitly assuming a crystal of infinite dimensions. The total zero-point energy of every atom is, therefore, at most

$$E_0^{(at)} \cong \frac{9}{8}\hbar\omega_D. \tag{5}$$

Within this quantum level, constituting a sort of *coalescence* of the matter, lays a complete information about the crystal structure, without the need of any exchange of atom-lattice messages, which could only travel at the speed of sound.

5. The zero-point reservoir

We will not try here to understand the nature (which is and remains a stimulating challenge) of the quantum coalescence underlying the elastic phenomena of a crystal and, some way or other, the entire Solid State Physics. We will limit ourselves to stress its physical implications. While, indeed, describing the behaviour of a lattice as a system of harmonic oscillators is a way (may be the only possible way) to translate into a formal language the experimental evidence, such a behaviour implies a set of physical features which cannot be ignored, and whose identification may help to take up the gauntlet.

Having this in mind, let us consider a sudden perturbation (such as, for instance, the highly localized emission/absorption of a γ particle by a nucleus), with energy and momentum below the zero-point phonon level.

In order to conciliate the experimental evidence with both momentum conservation and the uncertainty principle it appears quite natural to assume that the "sea" of zero-point energy of the crystal tends to preserve its original spectrum, whenever an exact and instantaneous momentum compensation may be obtained by means of a transient, non-dissipative re-distribution of the energy spectrum below the level allowed by the uncertainty principle itself.

Considering, in particular, the perturbation due to a Mössbauer process, let us quote, on this matter, Lipkin's words: "*An essential feature of the ME is the zero-point motion of large momentum, which can absorb the momentum transfer involved in the emission of the γ ray*" [5].

Taking this as a starting point, we observe that if a zero-point *energy* spectrum pertains to the crystal, and therefore an average zero-point kinetic energy $\langle E_{k0}\rangle = E_0^{(at)}/2$ pertains to each one of its atoms, a ground state *momentum* spectrum must also exist, whose absolute mean-square value, for each atom, is given by $\langle P_0^2\rangle = 2M\langle E_{k0}\rangle$. In this frame, and for very large values of N, the set of $3N$ mechanical oscillations of the crystal may provide (although remaining in the ground state) a reservoir of momentum with different intensities and *in almost any possible direction*, because the wave vector $\mathbf{k}_j$ ranges over $3N$ values in the first Brillouin zone of the lattice [15]. The large number of atoms required in order to meet an oscillation able to balance the momentum due to the emitted (or absorbed) photon is in agreement with property D of section 1.

It is seen in particular, from eq. (5), that $\langle P_0^2\rangle$ increases with increasing ω_D, i.e., when the stiffness of the interatomic bonds is increased.

If E_γ is the energy of the emitted/absorbed photon, the corresponding momentum $P_\gamma = E_\gamma/c$ may be exactly and instantaneously balanced by the momentum P_ω provided by the zero-point reservoir when

$$\frac{(P_\omega)^2}{2M} = \frac{(E_\gamma/c)^2}{2M} < E_0^{(at)} \cong \frac{9}{8}\hbar\omega_D. \tag{6}$$

The term $(E_\gamma/c)^2/(2M)$ is seen to coincide with the free recoil energy E_R. The radiation momentum may be therefore balanced below a maximum energy value of the emitted (or absorbed) quantum

$$E_{\gamma\,\max} \cong c\sqrt{\frac{9}{4}\hbar\omega_D M}. \tag{7}$$

Values slightly larger than $E_{\gamma\,\max}$ could also be compensated according to the quantum statistics of the process.

Referring, for simplicity sake, to a one-dimensional lattice, let $\Phi_0(p_1, \ldots, p_N)$ be its wave function in momentum space, and $p_1, \ldots, p_N$ the momenta of the single atoms. The probability for the mth atom to have momentum p_m *after* the recoil must be equal to the probability for it to have momentum $p_m - P_\gamma$ *before* the recoil. The probability P_{00} of a transition ground state $\rightarrow$ ground state induced by the γ emission/absorption is therefore given by

$$P_{00} = \left| \int \mathrm{d}p_1 \ldots \mathrm{d}p_N \, \Phi_0^*(p_1, \ldots, p_N) \Phi_0(p_1, \ldots, p_m - P_\gamma, \ldots, p_N) \right|^2. \quad (8)$$

By assuming a suitable Gaussian form for Φ_0 (a choice which corresponds to *assigning* rather than to *finding* a solution) it is possible to obtain from eq. (8), as is done in [12], a D–W expression, which lays however beyond the aims of the present paper. The point of interest here is that, in the frame of our hypothesis of the self-preserving character of the zero-point energy spectrum, the virtual oscillations of the spectrum must borrow from the momentum spectrum (within the extremely short time allowed by the uncertainty principle) the exact momentum value allowing a zero-energy exchange of the emitted/absorbed photon. According to eq. (1b), the main part of the momentum reservoir effective for the required compensation is given, up to temperatures of the order of T_D, by the high energy tail of the oscillation spectrum, of which $\langle P_0^2 \rangle$ represents the extension.

Such a process avoids the excitation of phonon levels lower than E_R and allows the elastic properties of the ME, including the absence of Doppler effect.

This view is supported by the analogy with the case of *superconductivity*, determined by the interaction of the atoms (within the coherence length) with the conduction electrons by means of the zero-order lattice oscillations, whose spectrum is distorted without altering the total energy of the system. The Cooper pairs creation [16] may be described by assuming that in the absence of thermal phonons (i.e., close to 0 K) a first electron polarizes the lattice, without any phonon generation, limiting itself to distort the zero-point phonon spectrum. A second electron interacts then with such a polarization (i.e., with the zero-point spectral distortion due to the first one), giving rise to a perfectly elastic (i.e., non-dissipative) coupling. The ME appears to be profoundly analogous to this phenomenology, although it involves frequencies ($\approx 10^{13}$ Hz) larger by two orders of magnitude with respect to those of superconductivity. From eq. (2) it is seen that, for the superconductivity frequencies ($\approx 10^{11}$ Hz), a sufficiently low number of thermal phonons is present close to 0 K. In the case of the ME, on the other hand, even slightly above T_D there exists a fraction of atoms (vibrating close to ω_D, i.e., at the maximum possible frequencies) not submitted to thermal oscillations, and therefore able to sustain an elastic process.

Just like superconductivity, the ME must not encounter thermal phonons at the involved frequencies (whatever they may be), as shown by the temperature dependence of the D–W factor (1b). And, just like superconductivity, the ME is associated with a temporary and non-dissipative distortion of the zero-point energy spectrum.

When emissions occur (within the same lattice) *not submitted* to ME, both Doppler broadening and recoil are present in the radiation spectra, since mechanical phonons are then generated, causing a sudden impulse on the emitting nucleus. In this case, high energy phonons turn out to be the most probably excited ones. The quantum coalescence is not invoked in this case, and no apparent contradiction with the uncertainty principle is present.

6. Other elastic processes

We observe that in phenomena involving – contrary to the case of the ME and to the D–W statistics – low momentum photons (e.g., in the emission, reflection or absorption of optical radiation [17]), a strong temperature dependence is found, which confines to temperatures very close to 0 K the probability of occurring in an elastic way. In this case, indeed, a momentum compensation can only be granted by zero-point oscillations at the lowest frequencies: frequencies which, however, can easily turn out to be already excited by thermal phonons.

Another interesting elastic process (correctly described, once more, by a D–W expression) is the reflection of low energy neutrons by the atoms of a crystal. Also in this case the only mechanism we may imagine to be able to warrant an elastic behaviour is provided by the self-preserving character of the zero-point energy spectrum proposed in the present paper. The monochromaticity, however, of a neutron beam cannot be revealed with the high precision allowed by the Mössbauer γ-rays. The ME remains therefore the only valid indication supporting our hypothesis.

7. Conclusions

The peculiar properties of the ME have always provided a stimulating challenge for their physical interpretation: a task where both the current wave-like and particle-like models lay themselves open to serious objections.

The natural zero-point oscillations, through the role of their momentum spectrum, may warrant the self-preserving character of the zero-point structure of the lattice by balancing the sudden impulse of the emission/absorption process while avoiding, according to the D–W distribution, the excitation of acoustic phonons, which would destroy the elastic character of the process.

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