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Quantum rigidity of microscopic bonds

R. Giovanelli, A. Orefice *

Università di Milano, DI.PRO.VE., Via Celoria, 2, 20133 Milano, Italy

Abstract

Exact solutions of the Schrödinger equation exist in the case of a linear oscillator submitted to a strong force exerted for a time much shorter than the oscillation period, and lead to transition probabilities admitting an enhancement (in suitable conditions) of the relative number of elastic processes with increasing perturbing energy. When, however, the oscillator is an atom belonging to a crystal lattice, elastic processes present new and interesting rigidity properties, which could be explored by means of slow neutron scattering and nano-technologies.
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1. Introduction

The basic interest, in solid state physics, of impulsive and highly localized quantum processes was not particularly appreciated until it was experimentally discovered that a localized and sudden event (such as the emission, absorption and scattering of X and γ quanta, or electrons, or neutrons, or light neutral atoms) affecting a single atom of a crystal lattice may occur without any energy exchange at all, thus suggesting a perfectly rigid behaviour of the whole lattice. The most impressive case (but by no means the only one) is provided by the Mössbauer Effect (ME). During his experiments on the nuclear resonant absorption of the γ-rays emitted in many decays of excited nuclei [1] Mössbauer observed, indeed, that a fraction of the emitted photons exhibited an increased absorp-

tion when, because of the cooling applied both to the source and to the absorber, no effect at all was to be expected. This result was accompanied by a set of surprising properties which may be summarized as follows:

(A) The observed effect occurs in a phononless (elastic) way, i.e., without exciting any one of the eigen-modes of mechanical oscillation of the lattice.

(B) No shift is observed (with respect to the energy of the excited nuclear state) in the emission/absorption lines when the linear dimensions of the solid are above, say, 0.5 μm (corresponding to an aggregate of about 10^8 atoms). This amounts to say that, in a fraction of cases (and contrary to the remaining cases), there is no appreciable recoil of the emitting/absorbing nucleus.

(C) No Doppler broadening is exhibited by the spectral lines, whose observed line-width Γ_{obs} is very close to the natural value $\Gamma_0 \cong \hbar/\tau$ (where τ is

* Corresponding author.
E-mail address: adriano.orefice@unimi.it (A. Orefice).

the mean life-time of the excited nuclear state) due to the uncertainty principle.

These features join in common, as we mentioned above, a great number of sudden and localized elastic processes where a whole aggregate of microscopic oscillators behaves, in a fraction of cases, like a unique rigid body [2]. Both wave-like and particle-like models were devised in order to predict such a fraction. In the wave-like approach, for instance, each excited nucleus is assumed to emit (or to scatter) an electromagnetic wave (or a de Broglie matter wave) which is frequency-modulated by the mechanical oscillation spectrum characterizing the crystal lattice. The fraction of recoilless nuclei is then obtained in the so-called Debye–Waller (DW) form [3,4] by simply expressing, in terms of the mean-square displacement of the nuclei, the unmodulated part of the spectrum.

It is our opinion that the rigidity exhibited in the recoilless fraction of cases still constitutes an open problem, which is often overlooked in different ways. We recall, for example, that it is currently associated to the role of the so-called reciprocal vector G. Since the very beginning of classical crystallography, indeed, this quantity (defined as the product of two suitable vectors characterizing each reticular plane of a crystal) was employed [5] for the description of visible light reflection from such a plane. When, successively, experiments concerning X-rays were performed, the use of the vector G was maintained [6], as if the recoil due the radiation could still be neglected. The rigidity suggested by the experimental results was, more or less explicitly, attributed to the vector G by assuming it as something more than a mere abstraction: in all scattering events, for instance, the quantity $\hbar G$ is assumed [7] to contribute in an essential way to the overall momentum balance. It is clear, however, that such a vector (anchored to ptolemaic-looking crystal planes) provides a useful geometrical idealization, but cannot be understood as an effective physical reality in itself.

We also recall that, in the particle-like description of a quantum system endowed with a discrete set of bound eigen-states (labelled with the index $m = 0, 1, 2, \ldots$), the expression of the overall probability of $m \rightarrow m$ transitions (leaving the system in a final state coinciding with the initial one) was found to present itself, from both a logical and formal point of view,

as a generalization of the DW form factor [8]. This observation induced many researchers to believe that the complete theoretical interpretation of the observed phenomena had been found. According to Ref. [8b], for example, *"The simple model of an atom moving in an external harmonic potential already contains the basic features of the ME (...). The basic physics underlying the ME (...) is all elementary Quantum Mechanics, and should have been understood years before the effect was discovered"*.

As we shall see in the present Letter, however, the matter is not so simple, for at least two reasons. The first one is that both the wave-like and the particle-like theories were developed in the limit of weak perturbations, while the processes considered in the present Letter do not always lend themselves to this simplification. The description, for instance, of highly energetic $m \rightarrow m$ transitions with $m > 0$ (whose role could be appreciable for lattices at relatively high temperatures) is completely unattainable by a perturbative approach. The second one, as we shall point out in the following, is that a theory predicting the recoilless fraction of nuclei is a necessary but not sufficient condition for the interpretation of the experimental results. The behaviour observed in elastic processes undergone by single atoms belonging to a macroscopic lattice has often induced, indeed, to attribute to the potential acting between the atoms of a crystal lattice a rigidity which is certainly not implicit in the postulates of Quantum Mechanics.

We shall see in Sections 2 and 3 that exact, nonperturbative analytical expressions (corresponding to realistic values of the physical parameters in many nuclear elastic processes) may be found for the transition probabilities of a single harmonic oscillator. We shall consider then, in Section 4, the case of localized impulsive processes undergone by an oscillator belonging to a more or less complex material aggregate. We shall stress, in Section 5, that the transmission of energy and momentum from an atom (involved in a sudden elastic process) to the whole aggregate to which it belongs appears to present peculiar properties, which we propose, in Section 6, to explore by means of crucial experiments, nowadays allowed by slow neutron scattering and nano-technologies. The present lack of experimental tests of *phononless* quantum elastic processes is due to the fact that the main current interest concerns the analysis (typically performed by

means of neutron scattering) of the *phononic* spectrum of crystal lattices.

2. Exact analytical solutions of the Schrödinger equation

As it was very well stated by Chester [9] *"there are no ideal harmonic oscillators. But this idealization capture the essential behaviour of many real systems. It is a computationally tractable model for what is encountered in nature"*. Let us consider, in this spirit, the case of a unidimensional harmonic oscillator of mass M, submitted to a space-independent force $F(t)$ of arbitrary strength. Such a force could represent, for instance, either a long range interaction, or a sudden absorption, emission or scattering process. The *classical* differential equation for this problem is obviously of the following form:

$$M\ddot{x}_c + kx_c = F(t). \tag{1}$$

Exact (non-perturbative) solutions of the Schrödinger equation corresponding to the quantum version of this problem,

$$-\frac{\hbar^2}{2M}\frac{\partial^2\psi}{\partial x^2} + \left[\frac{1}{2}kx^2 - xF(t)\right]\psi = i\hbar\frac{\partial\psi}{\partial t}, \tag{2}$$

were obtained almost half a century ago by Kerner [10] in a paper which did not obtain the diffusion it deserved. We shall give here a somewhat modified version of such a procedure.

Starting from a *quantum* stationary state of the oscillator for $F(t) = 0$, its energy

$$W_m = \left(m + \frac{1}{2}\right)\hbar\omega_c,$$

with $\omega_c = \sqrt{k/M}$ and $m = 0, 1, 2, \ldots,$ (3)

is assumed to be exactly known, so that the time at which this energy has been measured is totally indetermined. The closest *classical* case is that of an oscillator with a known total energy $E_{TOT} = W_m$ and a completely indetermined space position within the range $\pm x_0$, with $x_0 = \sqrt{2E_{TOT}/k}$. The classical probability dP for the oscillator to be found in the space interval dx is given by the relation

$$\frac{dP}{dx} = \frac{1}{\pi\sqrt{x_0^2 - x^2}}. \tag{4}$$

In the quantum case, the possible stationary probability distributions are given by

$$\left(\frac{dP}{dx}\right)_m = N_m^2 H_m^2(\alpha x)e^{-\alpha^2 x^2} \quad (m = 0, 1, 2, \ldots), \tag{5}$$

where

$$N_m = \sqrt{\frac{\alpha}{2^m m!\pi^{1/2}}}, \qquad \alpha = \sqrt{\frac{M\omega_c}{\hbar}}, \tag{6}$$

and the functions H_m are Hermite polynomials. In any case, as long as no force is applied, the center of the probability distribution is placed at $x_c = 0$, with $\dot{x}_c = 0$. The basic idea is now to "couple" the quantum solution, when an arbitrary force $F(t)$ is applied, to the corresponding *classical trajectory* $x_c(t)$ *of such a center*, obtained from Eq. (1). This "coupling" is obtained by passing from the space variable x to the variable $\xi = x - x_c(t)$, and looking for solutions of Eq. (2) in the quite general form

$$\psi(x, t) = \Phi(\xi, t)\exp[ig(\xi, t)], \tag{7}$$

where the function $g(\xi, t)$ remains to be fixed.

Starting then from Eq. (2), we obtain an equation of the form

$$-\frac{\hbar^2}{2M}\frac{\partial^2\Phi}{\partial\xi^2} + A(\xi, t)\frac{\partial\Phi}{\partial\xi} + B(\xi, t)\Phi = i\hbar\frac{\partial\Phi}{\partial t}. \tag{8}$$

As far as the coefficient $A(\xi, t)$ is concerned, it turns out to be given by the relation

$$A(\xi, t) = i\hbar\dot{x}_c(t) - i\frac{\hbar^2}{M}\frac{\partial g}{\partial\xi}, \tag{9}$$

and it is expedient to assume the function $g(\xi, t)$ in a form allowing to make this coefficient vanish, i.e.,

$$g(\xi, t) = \frac{M}{\hbar}\left[\dot{x}_c(t)\xi + Q(t)\right], \tag{10}$$

where $Q(t)$ is an arbitrary function of time alone. By means of the choice

$$Q(t) = x_c(t)\dot{x}_c(t), \tag{11}$$

and by means of a repeated use of Eq. (1), the coefficient $B(\xi, t)$ takes up, in its turn, the simple form

$$B(\xi, t) = \frac{k\xi^2}{2} + \delta(t),$$

with $\delta(t) = \frac{M\dot{x}_c^2}{2} - \frac{kx_c^2}{2}$. (12)

Eq. (8), in conclusion, turns out to be written in the form

$$-\frac{\hbar^2}{2M}\frac{\partial^2\Phi}{\partial\xi^2} + \left[\frac{k\xi^2}{2} + \delta(t)\right]\Phi = i\hbar\frac{\partial\Phi}{\partial t}, \qquad (13)$$

a well-known equation (analogous to the one of the harmonic oscillator) which may be treated, as usual, by variable separation, looking for a solution of the form $\Phi(\xi, t) = X(\xi)T(t)$. Going back, then, to the x-variable and to the wave function ψ given by Eq. (7) we obtain, for Eq. (2), the general solution

$$\psi = \psi_m(x, t)$$

$$= N_m \exp\left\{\frac{i}{\hbar}\left[Mx\dot{x}_c(t) - \int_0^t \delta(t)\,dt - W_m t\right]\right\}$$

$$\times H_m\{\alpha[x - x_c(t)]\}\exp\left\{-\frac{\alpha^2}{2}[x - x_c(t)]^2\right\}$$

$$\qquad (14)$$

with $m = 0, 1, 2, \ldots$. As long as $F(t) = 0$, the (classical) coordinate $x_c(t)$ of the center of the probability distribution remains equal to zero together with its time derivative $\dot{x}_c(t)$ and, as shown by Eq. (14), the harmonic oscillator remains in the standard stationary m-state. When, however, a force $F(t) \neq 0$ is applied, the solution (14) evolves in strict association with the classical motion $x_c(t)$, whose general form is provided, for instance, in Ref. [11]. Eq. (14) shows then, in Kerner's words [10], that "*the oscillator dances a quantum dance centered at the instantaneous classical position*".

The general solution (14) may be expressed in terms of the standard orthonormal set of eigen-solutions of the unperturbed quantum oscillator

$$u_n(x, t) = N_n \exp\left(-\frac{i}{\hbar}W_n t\right)H_n(\alpha x)e^{-\frac{\alpha^2}{2}x^2}$$

$$(n = 0, 1, 2, \ldots) \qquad (15)$$

in the form

$$\psi_m(x, t) = \sum_{n=0}^{\infty} A_{mn}(t)u_n(x, t). \qquad (16)$$

We have in fact, after straightforward calculations:

$$A_{mn}(t) = \int_{-\infty}^{\infty} \psi_m u_n^* \, dx$$

$$= \frac{N_m N_n}{\alpha}\exp\left\{-\frac{\varepsilon(t)}{2} + \frac{i}{\hbar}\left[(W_n - W_m)t\right.\right.$$

$$\left.\left. - \int_0^t \delta(t)\,dt + \frac{Mx_c\dot{x}_c}{2}\right]\right\}G_{mn},$$

$$\qquad (17)$$

where the asterisk labels a complex conjugation, the term

$$\varepsilon(t) = \frac{1}{\hbar\omega_c}\left(\frac{kx_c^2}{2} + \frac{M\dot{x}_c^2}{2}\right) \qquad (18)$$

represents the total energy reached by the *classical oscillator* at the time t, divided by the quantum energy $\hbar\omega_c$; the term

$$G_{mn} = \int_{-\infty}^{\infty} d\rho \exp(-\rho^2)H_m[\rho + y]H_n[\rho + z] \qquad (19)$$

is a tabulated integral (see, for instance, [12]) which may be expressed in terms of associate Laguerre polynomials:

$$G_{mn} = \begin{cases} 2^n\pi^{1/2}m!y^{n-m}L_m^{n-m}(-2yz) \\ \quad (n \geq m), \\ 2^m\pi^{1/2}n!z^{m-n}L_n^{m-n}(-2yz) \\ \quad (n < m), \end{cases} \qquad (20)$$

and

$$z = \frac{\alpha x_c(t)}{2} + i\frac{M\dot{x}_c(t)}{2\alpha\hbar}, \qquad y = -z^*,$$

$$-2yz = \varepsilon(t), \qquad |y|^2 = |z|^2 = \frac{\varepsilon(t)}{2}. \qquad (21)$$

According to Eq. (17) the oscillator, starting from an unperturbed stationary state m with $x_c(t = 0) = \dot{x}_c(t = 0) = 0$, develops, under the influence of the force $F(t)$, the probability

$$P_{mn}(t) = |A_{mn}(t)|^2$$

$$= \frac{m!}{n!}[\varepsilon(t)]^{n-m}\left|\exp\left(-\frac{\varepsilon(t)}{2}\right)L_m^{n-m}[\varepsilon(t)]\right|^2 \qquad (22)$$

(assuming $n \geq m$) of being found at the time t in any state n (possibly, but not necessarily, coinciding with the initial one, m). Such a probability is seen to depend in an essential way on the total energy attained by the oscillator in the corresponding classical case. The probability P_{nm} of the reverse transition turns out to coincide with P_{mn}. In particular, the probability of

remaining in the initial state m is found by taking $n = m$ in Eq. (22), so that

$$P_{mm}(t) = e^{-\varepsilon(t)} \left| L_m[\varepsilon(t)] \right|^2, \tag{23}$$

since the *associate* Laguerre polynomial L_m^0 reduces to a standard Laguerre polynomial L_m. It must be stressed that, in the present non-perturbative theory, the energy ratio $\varepsilon(t)$, provided by Eq. (18), was never assumed to be a small quantity.

3. Sudden elastic processes undergone by a single oscillator

The general solution (14) may be applied to the particular case of an impulsive strong perturbation undergone by a single oscillator, by assuming that a constant force F of arbitrary strength is exerted for a very short time $\tau \ll 2\pi/\omega_c$, as it is quite plausible in view of emission, absorption or scattering processes. The total energy, E_c, delivered to a *classical* oscillator starting from $x_c(t = 0) = \dot{x}_c(t = 0) = 0$, is given by

$$E_c = \frac{(F\tau)^2}{2M}. \tag{24}$$

Assuming, for simplicity sake, that the oscillator, submitted to such a shock, has no time to substantially change its initial position $x_c = 0$, we may employ the solution (14) with

$$x_c(t) = \sqrt{\frac{2E_c}{k}} \sin \omega_c t, \tag{25}$$

$$\dot{x}_c(t) = \sqrt{\frac{2E_c}{M}} \cos \omega_c t, \tag{26}$$

$$\int_0^t \delta(t)\,dt = \frac{E_c}{2\omega_c} \sin 2\omega_c t, \tag{27}$$

and make use of the transition probability (22), with $\varepsilon = \frac{E_c}{\hbar\omega_c}$. The effect of the shock is that of inducing a classical-looking oscillation of the probability distribution (see Ref. [13] for the simple case $m = 0$).

Such an oscillating distribution is a superposition of all the stationary states of the unperturbed oscillator. The probability, in particular, for the oscillator, of remaining in its initial state m is obtained from
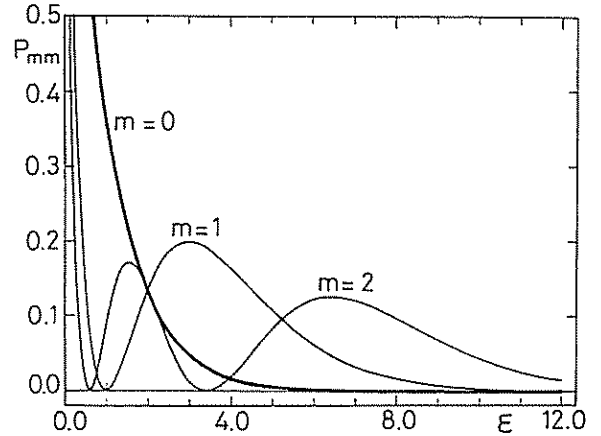

Fig. 1. The probability P_{mm} of a sudden process leaving the oscillator in its initial state m is plotted (for $m = 0, 1, 2$) versus the energy ratio $\varepsilon \equiv \frac{E_c}{\hbar\omega_c}$.

Eq. (23) in the form

$$P_{mm} = \exp\left(-\frac{E_c}{\hbar\omega_c}\right) \left| L_m\left(\frac{E_c}{\hbar\omega_c}\right) \right|^2. \tag{28}$$

By plotting the function P_{mm} versus $\varepsilon \equiv \frac{E_c}{\hbar\omega_c}$ (see Fig. 1) it may be verified that it exhibits, for $\varepsilon > 1$, a set of m maxima which no perturbative approach (with $\varepsilon \ll 1$) may predict, although values of ε even much greater than unity may be currently encountered in the family of elastic processes we are considering here. Very large values of the energy ratio ε may be reached, in fact, in the case of neutron scattering from a crystal lattice; and considerably large values of such a parameter may be attained even in the case of the Mössbauer Effect. Making use, for instance, of the parameters corresponding to the γ emission occurring in excited Zn^{67} ($M \cong 1.11 \times 10^{-22}$ g), where the energy of the emitted quantum amounts to $E_\gamma \cong 93.26$ keV, the free recoil energy is given by $E_c = E_\gamma^2/2Mc^2 \cong 6.99 \times 10^{-2}$ eV, and (assuming for ω_c the relevant Debye frequency) $\hbar\omega_c \cong 2.01 \times 10^{-2}$ eV, we obtain $\varepsilon \cong 3.47$.

In the case of the first, and most energetic, γ emission from excited nuclei of Fe^{57} (where $M \cong 9.46 \times 10^{-23}$ g, $E_\gamma \cong 136.32$ keV, $E_c \cong 1.75 \times 10^{-1}$ eV; $\hbar\omega_c \cong 3.62 \times 10^{-2}$ eV) we obtain $\varepsilon \cong 4.8$. Let us observe, however, that in the second, and less energetic, γ emission from Fe^{57} (which is the most commonly employed in Mössbauer diagnostics) we

have $E_\gamma \cong 14.412 \, \text{keV}$, $E_c \cong 1.95 \times 10^{-3} \, \text{eV}$ and $\varepsilon \cong 0.054$, thus allowing a simple perturbative approach. It must be noticed that the maxima of the function P_{mm} may be physically reached only by means of a strong shock occurring in a time much shorter than the "relaxation time" of the oscillator. A slower interaction would in fact progressively reduce to zero the existing population of excited states.

It is worthwhile to recall here that in Ref. [14] the behaviour of single orbital electrons was approximated by means of unidimensional harmonic oscillators, as allowed by the small ratio between the electron and nuclear mass. The Schrödinger time-dependent equation was shown to lead to different possible energy transitions, and the probability, for the electron, of remaining in its initial state was seen to be enhanced in the case of a strong and sudden force, both in the case of usual atoms and for Rydberg artificial atoms, submitted to the electric field of an intense laser beam. This enhancement was also confirmed by experimental tests, without remarking, however, that it corresponded to the maxima of the function P_{mm} provided by Eq. (28), and therefore to an elastic process.

Let us also recall that Ref. [15] presented the experimental results of the application of a strong and ultra-short electric field due to a laser beam injected into a diatomic gas. The probability of molecular dissociation was shown to decrease with increasing intensity of the beam, a fact which may be attributed to the presence (at high enough values of the energy ratio ε, and for $m > 1$) of maxima in the function P_{mm} describing the probability of elastic scattering events.

4. Sudden elastic processes in crystal lattices

Let us pass now to the case of sudden and localized elastic processes undergone by atoms belonging to a crystal lattice, composed of N atoms. Each atom of such a crystal is subject to mechanical oscillations distributed according to a spectrum of $3N$ eigenfrequencies, ranging between a minimum value, ω_{min}, corresponding to wavelengths of the order of the crystal linear dimensions, and a maximum value ω_D (the "Debye frequency"), corresponding to wavelengths equal to twice the equilibrium interatomic spacings. In the so-called *Debye model* the spectral distribution function of the eigen-frequencies of the lattice is ap-

proximated as a continuum by means of a function $f(\omega)$ proportional to ω^2 (according to the Rayleigh–Jeans calculation) in the form

$$f(\omega) = 3 \frac{\omega^2}{\omega_D^3} \tag{29}$$

such that $\int_0^{\omega_D} f(\omega) \, d\omega = 1$, having assumed $\omega_{\text{min}} \cong 0$.

In the *thermal* oscillation spectrum, the average number of phonons with eigen-frequency ω is given (at temperature T) by the expression

$$\bar{n}(\omega, T) = \frac{1}{\exp(\hbar\omega/k_B T) - 1} \equiv \frac{1}{\exp\left(\frac{\omega/\omega_D}{T/T_D}\right) - 1}, \tag{30}$$

where k_B is the Boltzmann constant and $T_D = \hbar\omega_D/k_B$ is the "Debye temperature".

Clearly enough, the function $\bar{n}$ tends to zero in the limit $T/T_D \to 0$. Below the temperature T_D the average phonon density is restricted therefore to a rather narrow low-frequency range. The entire spectrum, on the contrary, is always present and active in the *zero-point* (phononless) motions. In stationary conditions the zero-point background has therefore the possibility of acquainting each atom of the crystal with the characteristics of the whole lattice to which it belongs, including its irregularities, which strongly affect the spectral structure of the crystal oscillations.

Coming now to the case of elastic processes, i.e., of events leaving the lattice in its initial energy state, we shall make the assumption that the energy levels m are low enough to allow a harmonic approximation of the oscillations, and introduce, for the atom involved in the emission, absorption or scattering process, the probability P_m of been found in the mth energy level of mechanical oscillation at the eigen-frequency ω [16]:

$$P_m\left(\frac{\omega}{\omega_D}; \frac{T}{T_D}\right) = \frac{\bar{n}^m}{(1 + \bar{n})^{m+1}}. \tag{31}$$

where the function $\bar{n}(\omega/\omega_D; T/T_D)$ is provided by Eq. (30). Therefore, $P_m \to 0$ when $\omega/\omega_D \to 0$.

The probability P_{mm} of an elastic process (i.e., of a process leaving an oscillator in its initial energy level m) is provided, in its turn, by our Eq. (28) with $\omega_c = \omega$, and may be written in the form

$$P_{mm}\left(\frac{\omega}{\omega_D}; \varepsilon_D\right) = \exp\left(-\frac{\varepsilon_D}{\omega/\omega_D}\right) \left| L_m\left(\frac{\varepsilon_D}{\omega/\omega_D}\right) \right|^2. \tag{32}$$

where

$$\varepsilon_D = \varepsilon \frac{\omega}{\omega_D} = \frac{E_c}{\hbar \omega} \frac{\omega}{\omega_D} = \frac{E_c}{\hbar \omega_D} \qquad (33)$$

and E_c is the free recoil energy defined in Eq. (24).

Making use, now, of Eq. (29), we may finally write the probability P_{el} of an elastic process (undergone by any atom of the crystal lattice, and leaving the crystal in its initial energy state) in the compact form

$$P_{el}\left(\tfrac{T}{T_D}; \varepsilon_D\right) = \int_0^1 d(\omega/\omega_D)\, F\left(\tfrac{\omega}{\omega_D}; \tfrac{T}{T_D}; \varepsilon_D\right), \qquad (34)$$

where ω/ω_D is the integration variable, and

$$F\left(\tfrac{\omega}{\omega_D}; \tfrac{T}{T_D}; \varepsilon_D\right)$$
$$= 3\left(\frac{\omega}{\omega_D}\right)^2 \sum_{m=0}^{\infty} P_m\left(\tfrac{\omega}{\omega_D}; \tfrac{T}{T_D}\right) P_{mm}\left(\tfrac{\omega}{\omega_D}; \varepsilon_D\right) \qquad (35)$$

with P_{mm} given by Eq. (32). It is seen that, because of Eqs. (30) and (31), the lowest eigen-frequencies of the oscillation spectrum give almost no contribution to the probability of elastic processes. In the limit $\varepsilon_D \to 0$ the function P_{mm} provided by Eq. (32) may be approximated in the form

$$P_{mm}(\omega/\omega_D; \varepsilon_D) = e^{-\varepsilon}\left|L_m(\varepsilon)\right|^2$$
$$\approx \exp\left[-(1+2m)\varepsilon\right] \qquad (36)$$

(with $\varepsilon = \frac{\varepsilon_D}{\omega/\omega_D}$), which, introduced into Eq. (35), leads to an expression holding in the weak interaction limit, as long as the role of the m maxima of the function P_{mm} is negligible. The use of the full expression (32) is required, however, in strong and sudden processes, when these high energy maxima become physically accessible and significant. For comparison, the Debye–Waller fraction may be expressed, in one of its most simple forms, as

$$P_{DW}\left(\tfrac{T}{T_D}; \varepsilon_D\right) = \begin{cases} \exp\left(-\dfrac{3}{2}\varepsilon_D\right) \\ \qquad \text{for } T \approx 0\text{ K,} \\ \exp\left(-6\varepsilon_D \dfrac{T}{T_D}\right) \\ \qquad \text{for } \dfrac{T}{T_D} \gg \dfrac{1}{2}. \end{cases} \qquad (37)$$

In Figs. 2–4 we plot versus T/T_D the function $P_{el}(T/T_D; \varepsilon_D)$ provided by Eq. (34), with P_{mm} given
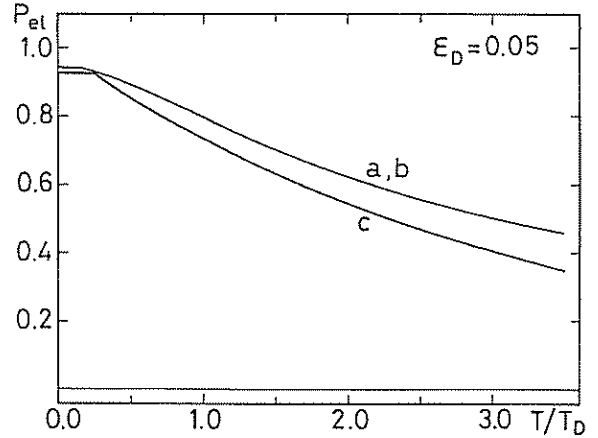

Fig. 2. Plot versus T/T_D (for $\varepsilon_D = 0.05$, with ε_D defined in Eq. (33)) of the probability of a process leaving the crystal lattice in its initial energy state, under the action of a sudden shock undergone by one of its atoms. Curve a represents the "exact" function P_{el} given by Eq. (34); curve b represents its weak interaction limit; curve c represents the Debye–Waller approximation given by Eq. (37).
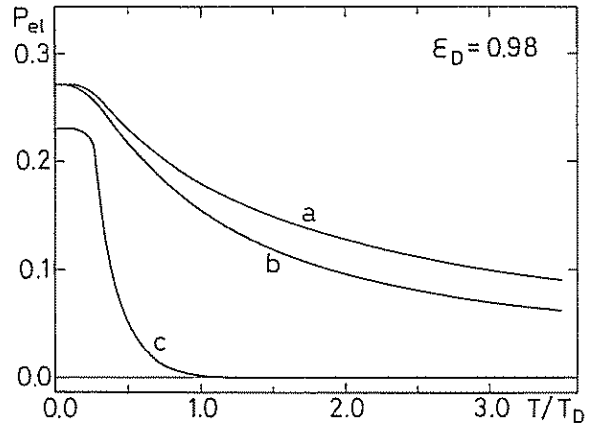

Fig. 3. The same as in Fig. 2, with $\varepsilon_D = 0.98$.

both by Eq. (32) (curves a) and by its weak interaction limit (36) (curves b), for different values of the parameter ε_D defined in Eq. (33). The DW probability factor (37) is represented, in its turn, in curves c, for the same values of ε_D.

Fig. 2 refers to a very low value of ε_D ($\varepsilon_D = 0.05$, corresponding to the lower energy emission in Fe[57]), and shows that, in this energy range, the curves a and b almost coincide, and the DW curve c itself is not very different from a and b.
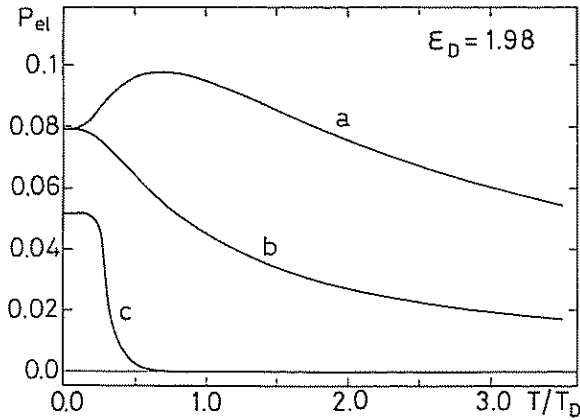
Fig. 4. The same as in Fig. 2, with $\varepsilon_D = 1.98$

In Fig. 3, obtained with $\varepsilon_D = 0.98$, the curves a and b are quite close to one another, showing that the energy range affected by the role of the maxima of P_{mm} is not yet reached. The DW curve c, however, remains quite lower than the others, clearly showing that its validity is limited, for any temperature, to very low values of ε_D.

In Fig. 4, obtained with $\varepsilon_D = 1.98$, the "exact" curve a strongly diverges from the approximated curve b, exhibiting a maximum due to the increasing role (with increasing temperature) of the excited states with $m > 0$. The DW curve c remains, of course, quite lower.

5. Momentum and energy transmission in crystal lattices

The knowledge of the non-perturbative expression of the transition probabilities is, in any case, a necessary but not sufficient condition for an answer to the problem of the propagation (even to the closest atoms) of the momentum due to a sudden process undergone by an atom belonging to an aggregate of mechanical oscillators.

Let us observe that in *Classical Mechanics* the possibility that a sudden shock, reversing the momentum p_x of the oscillator into $-p_x$ (and therefore leaving its kinetic energy unchanged) does indeed exist, but is endowed with a vanishing probability. In the case of *Quantum Mechanics*, on the other hand, there exists a finite probability, for a single ideal oscillator, of "tak-

ing in" the momentum due to the shock while remaining in the same initial energetic state. This finite quantum probability is granted, indeed, by the momentum spread (ranging between $p_x = \pm\infty$) pertaining to each stationary state: in the ground state, for instance, we have from Eq. (15)

$$
\begin{aligned}
u_0(x,t) &= \sqrt{\frac{\alpha}{\pi^{1/2}}} \exp\left(-i\frac{\omega_c t}{2} - \frac{\alpha^2}{2}x^2\right) \\
&= \frac{\exp\left(-i\frac{\omega_c t}{2}\right)}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk_x \frac{\exp\left(-\frac{k_x^2}{2\alpha^2}\right)}{\sqrt{\pi^{1/2}\alpha}} e^{ik_x x} \quad (38)
\end{aligned}
$$

with $k_x = p_x/\hbar$. The momentum due to the shock is effectively "taken in", however, as well as in the classical (and highly improbable) energy-preserving case, by the external potential itself, behaving like an unlimited and instantaneous momentum absorber.

In the case of a material aggregate of oscillators, on the other hand, the critical role, and the peculiar properties, of momentum transmission occurring in elastic events may be adequately described by the following brief review of the experimental evidence.

- Let us consider, to begin with, Compton's papers [17] on his famous experiment of X-ray scattering by the atoms of a graphite crystal. The observed scattered radiation spectrum includes, as is well known, two different peaks:
  - *the first peak* (corresponding to the standard Compton effect), when plotted versus wavelength, is *upshifted* with respect to the incident radiation, and is currently explained as a photon scattering (conserving both energy and momentum in each single microscopic event) by the most external, and almost free, orbital electrons;
  - *the second peak*, in its turn, is *unshifted* and centered around the incident wavelength itself, and is attributed to strongly bound orbital electrons, which the impinging photons may be unable to excite to the next energy level. In this second case the entire atom behaves like a unique rigid body, with an effective scattering mass thousands of times larger than the electron mass.
- When an incident particle is scattered by a *diatomic molecule*, it often behaves, once more, as

a rigid body (see, for instance, [18,19]), preserving its initial internal energy level. After having mixed, for instance, a diatomic gas with a rarefied, mono-atomic one at a higher temperature, the thermalization time of the two gases (revealed by a "rapid" bolometer) is seen to be much shorter than the excitation time (revealed by infrared spectroscopy) of the vibrational internal levels of the diatomic molecules. This is a clear proof that a diatomic molecule colliding with a mono-atomic one has a high probability of recoiling as a whole, i.e., of exhibiting a perfectly rigid behaviour.

- Analogous features were described in Ref. [20] in the case of 4-*atomic molecules*.
- Passing now to the case of *an aggregate* of a very large number ($\approx 10^8$) of atoms, let us consider, for instance, the nuclear scattering of thermal neutrons ($v \approx 10^6$ cm/s) by a crystal composed of light nuclei, such as, for instance, beryllium. It may be verified with a high degree of precision that a part of the colliding neutrons does not lose any energy at all, thus interacting with the whole mass of the lattice. As we know, the neutron crossing time Δt through the region defined by the range of the nuclear forces ($\approx 10^{-13}$ cm) may be estimated (see, for instance, [21]) around 10^{-19} s. Although a mechanical "message" between an atom and the rest of the lattice can only travel at sound's speed, let us admit for a moment (as proposed in Ref. [22]) an electromagnetic nature of such a "message". In the time Δt an electromagnetic signal may only cover a distance of the order of 3×10^{-9} cm, even lower than the average spacing between two atoms in a molecule or in a crystal lattice, which is around 1 Å. Not even an electromagnetic message may allow, therefore, the transmission (even to the closest atoms of the lattice) of the force required to provide the rigidity implied by the absence of any recoil.

6. Discussion

There exists, as we have seen, a wide display of experimental results based on nuclear absorption, emission and scattering processes occurring at single atoms of material aggregates ranging from small to very large total mass, showing that these processes (in a predictable fraction of cases) do not excite any internal oscillation mode: neither of the single involved atom, nor of the whole lattice.

When the total mass of the aggregate is small enough, its recoil, due to the mechanical shock, appears to occur with an instantaneous transmission of energy and momentum to its barycenter. When, on the other hand, the total mass is large enough, these elastic processes occur without any energy variation, as if the solicited oscillators had instantaneously shared the shock with a standing, unlimited momentum absorber. In any case, the relevant spectral lines show that the emitted (or scattered) particles or quanta "know", in their apparently instantaneous interaction, the mass of the whole aggregate to which the emitting (or scattering) atom belongs. It seems, in other words, that the "information" level granted by the zero-point oscillation spectrum in *stationary conditions* could be maintained "in real time" in *transient conditions*. We recall, in this connection, that energy exchanges below the zero-point level appear to be present in the excitation of the so-called "bcc crystals" of He^4 [23] during neutron scattering experiments.

Although we recall that Wheeler and Feynman [24] have devised a mechanism (based on advanced and retarded waves) of information/confirmation exchange of messages, allowing an *apparently* instantaneous sharing of physical "knowledge" between the particles of a complex quantum system, we observe (before invoking these extreme theoretical approaches) that there are several points of the present paper which could be fruitfully explored by means of the recent development of nano-technologies.

The intermediate case, for instance, of impulsive processes occurring in nano-tubes of 10^3–10^4 atoms the so-called "cylindrical fullerenes", providing a powerful experimental tool for the analysis of unidimensional quantum processes [25] could be studied with slow neutron scattering experiments. The phonons created in the inelastic fraction of scattering events may be detected by means of microscopic superconductive Josephson junctions [26], thus allowing to discriminate elastic (phononless) from inelastic (phononic) events, in coincidence with the revelation of single scattered neutrons and with the measurement of their energy.

Concerning possible (elastic) $m \to m$ transitions with $m > 0$, we may imagine experiments of slow neutron scattering by a fullerene-like cluster [27,28] (composed of $\approx 10^2$ atoms) suspended in a cavity by optical levitation [29–32]. An infrared, photon by photon measurement of the temperature of the cluster could reveal the spectrum of the excited vibrational modes of the cluster. These modes should be rather easily identified because of their small number, due to the high symmetry level of the cluster structure. In the meantime, the transitions between these modes (induced by a monochromatic slow neutron beam, with energy of the order of 10^{-2}–10^{-1} eV) could be revealed both by the time-resolved evolution of the cluster infrared radiation spectrum itself and by the measurement of the energy variations between incoming and outgoing neutrons, performed by means of a spin-echo neutron spectrometer, nowadays able to evidence variations even lower than 10^{-8} eV [33]. By varying the energy of the injected neutrons, and by measuring the corresponding radiation spectra, one could verify the energy dependence of the transition probabilities.

The same experimental setup could allow the optical measurement of the mechanical recoil of the cluster itself, when a photon-by-photon analysis a of the time-resolved emission spectrum reveals that no excitation of internal oscillation levels has occurred. This would provide a direct evidence of the (possibly instantaneous) transmission of energy and momentum to the center of mass of the cluster.

It is clear, in conclusion, that phononless features such as the ones prospected in Fig. 4, and characterized by quite low probabilities, may be observed only by means of *ad hoc* experiments, up to now neglected because of their little applicative interest. This does not means, however, that these *ad hoc* experiments cannot be performed in the frame of present time technology.

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