

An Analysis of States in the Phase Space: the Anharmonic Oscillator

Sebastiano Tosto

ENEA Casaccia, via Anguillarese 301, 00123 Roma, Italy. E-mail: sebastiano.tosto@enea.it, stosto@inwind.it

The paper introduces a simple quantum model to calculate in a general way allowed frequencies and energy levels of the anharmonic oscillator. The theoretical basis of the approach has been introduced in two early papers aimed to infer the properties of quantum systems exploiting the uncertainty principle only. Although for clarity the anharmonic oscillator is described having in mind the lattice oscillations of atoms/ions, the quantum formalism of the model and approach have general character and can be extended to any oscillating system. The results show that the harmonic energy levels split into a complex system of anharmonic energy levels dependent upon the number of terms of the Hamiltonian that describes the anharmonicity.

1 Introduction

The anharmonic phenomena, well known in physics [1], regard a wide range of properties of practical and theoretical interest; e.g. in acoustics they account for large variations of sound velocity in solids [2], in optics for non-linear interaction of powerful light with lattice vibrations [3]. Moreover are known physical effects that lead to a behavior impossible in harmonic oscillators, like the “foldover effect” [4] and “superharmonic resonance” [5]; both are due to the dependency of the eigenfrequency of nonlinear oscillators on the amplitude and to the non-harmonicity of the oscillations. In solid state physics, non-linear effects occur when atoms consisting of a positively charged nucleus surrounded by a cloud of electrons are subjected to an electric field; the displacement of nucleus and electrons causes an electric dipole moment, whose interaction with the applied field is linear for small field intensities only [6].

The present paper aims to propose a quantum mechanical approach to tackle the problem of non-harmonic oscillations in a general way, i.e. regardless of the particular issue of specific interest, and in line with the concepts introduced in two papers [7, 8] concerning simple quantum systems, many-electron atoms/ions and diatomic molecules. The basic idea of these papers starts from a critical review of the concepts of positions and momenta of interacting particles in a quantum system, where the dynamical variables are perturbed in a complex way by mutual interactions and change within appropriate ranges of values in agreement with boundary conditions like the minimum total energy.

Consider for instance the hydrogenlike atoms. It is reasonable to regard radial momentum p_ρ and distance ρ between electron and nucleus as variables included within proper ranges of values; so it is certainly possible to write $0 < \rho \leq \Delta\rho$ and $0 < p_\rho \leq \Delta p_\rho$ if $\Delta\rho$ and Δp_ρ have arbitrary sizes, including even the chance of infinite sizes. The only basic hypothesis of the quoted papers was that in general any ranges of conjugate dynamical variables Δx and Δp_x have physical meaning of quantum uncertainty ranges, thus to

be regarded according to the basic ideas of quantum statistics; hence

$$\Delta x \Delta p_x = n\hbar, \quad (1.1)$$

with n arbitrary integer.

No hypothesis is necessary about Δx and Δp_x , which are by definition arbitrary, unknown and unpredictable. Eq. (1.1) was the unique assumption in [7, 8] and does so also in the model proposed here. Despite the apparently agnostic character of eq. (1.1), the results inferred in the quoted papers were in all cases completely analogous to that of the usual wave mechanics formalism; in particular it was found that the quantum numbers actually coincide with the numbers of allowed states in the phase space for the concerned systems. Eq. (1.1) only is enough to give the classical Hamiltonian, H_{cl} , the physical meaning of quantum Hamiltonian, H_q ; it simply requires considering the ranges of dynamical variables rather than the dynamical variables themselves, which are therefore disregarded since the beginning. For instance, in a one-dimensional problem like that of a mass constrained to oscillate along a fixed direction, it means that hold the positions

$$H_{cl}(x, p_x) \Rightarrow H_q(\Delta x, \Delta p_x) \Rightarrow H_q(\Delta p_x, n). \quad (1.2)$$

The uncertainty is regarded in this way as fundamental principle of nature rather than as mere consequence of commutation rules of quantum operators. The case of the harmonic oscillator, already introduced in [7], has central importance here; its quantum formulation according to eq. (1.1) and positions (1.2) is so short and simple that it is sketched in the next section 2 to make the present paper clearer and self-consistent.

The next section aims also to emphasize how the concepts so far introduced enable the quantum approach. For clarity the anharmonic oscillator is regarded in section 3 having in mind the lattice oscillations of atoms/ions, yet through a very general approach that can be extended to any quantum system. The discussion on the results of the model and the conclusion are reported in sections 4 and 5.

2 The harmonic oscillator

With the positions 1,2, the classical energy equation $E = p^2/2m + k_{har}(x - x_o)^2/2$ of the oscillating mass around the equilibrium position x_o reads $\Delta E = \Delta p^2/2m + k_{har}\Delta x^2/2$, having omitted for simplicity the subscript x ; owing to eq. (1.1), $E = E(\Delta p, n)$ is now because of n a random quantity within an energy range ΔE that corresponds to local uncertainty of dynamical variables within Δx and Δp . Both these latter and ΔE are assumed positive by definition. Then, one finds

$$\Delta E = \frac{\Delta p^2}{2m} + \frac{m(n\hbar\omega_{har})^2/2}{\Delta p^2}, \quad \omega_{har}^2 = \frac{k_{har}}{m}. \quad (2.1)$$

Eq. (2.1) has a minimum as a function of Δp , i.e.

$$\Delta p_{min} = \sqrt{mn\hbar\omega_{har}}, \quad \Delta E_{min} = n\hbar\omega_{har}, \quad (2.2)$$

being now n the number of vibrational states. Although for $n = 0$ there are no vibrational states, the necessity that $\Delta p \neq 0$ compels $\Delta E \neq 0$ and thus $\Delta E_0 = \Delta p_0^2/2m \neq 0$ with $\Delta p_0 = \Delta p_{min}(n = 0)$. In this particular case, the problem reduces to that of a free particle in the box, i.e. Δp_0 is related to the zero point energy. This requires $\Delta p_0 = \Delta p_{min}(n = 1)$, because the minimum quantum uncertainty of Δp can be nothing else but that of Δp_{min} for $n = 1$. The numerical correspondence between non-vibrational momentum range, Δp_0 , and first vibrational momentum range, $\Delta p_{min}(n = 1)$, means that at the zero point energy state the mass m is delocalized in a space range, $\Delta x_0 = \Delta x(n = 0)$, equal to that, $\Delta x(n = 1)$, pertinent to the lowest vibrational state. In other words, the oscillation amplitude at the ground energy level is the same as the delocalization range size of the particle with zero point energy only. Hence $\Delta p_0 = \sqrt{m\hbar\omega_{har}}$ defines $E_0 = \Delta p_0^2/2m = \hbar\omega/2$. The minimum of ΔE must be $\Delta E_{min} = E_{min} - \hbar\omega_{har}/2$; then, regarding $E_{min} = E_{har}$ as the harmonic energy level, the known result

$$E_{har} = n\hbar\omega_{har} + \frac{\hbar\omega_{har}}{2} \quad (2.3)$$

is obtained considering uncertainty ranges of eq. (1.1) only, and without any further hypothesis. Note that with $\Delta p = \Delta p_{har}$

$$\frac{\Delta p^2}{2m} = \frac{\omega_{har}^2 m n^2 \hbar^2}{2\Delta p^2} = \frac{n\hbar\omega_{har}}{2},$$

in agreement with the virial theorem as E_{min} is given by the sum of kinetic and potential terms, whereas the zero point term has kinetic character only. Also note in this respect that Δp_{min} and Δp_0 are merely particular range sizes, among all the ones allowed in principle, fulfilling the condition of minimum E_{min} and E_0 .

These results do not contradict the complete arbitrariness of Δp and Δx , since in principle there is no compelling reason to regard the particular ranges of eqs. (2.2) in a different way with respect to all the other ones allowed by eq. (1.1); rather the results merely show the preferential propensity of

nature for the states of minimum energy. In effect it is not surprising that the energy calculated with extremal values of dynamical variables in the ranges of eq. (2.1) does not coincide, in general, with the most probable energy. In conclusion, this example highlights that the physical properties of a quantum system can be inferred without solving any wave equation simply replacing the local dynamical variables with the respective quantum uncertainty ranges: the key problem becomes then that of counting correctly case by case the appropriate number of allowed states, as shown in [7,8] for more complex quantum systems.

It appears that, once accepting the eq. (1.1) and the consequent positions 1,2, have actual physical meaning the uncertainty ranges rather than the dynamical variables themselves; these latter are considered here random, unknown and unpredictable within the respective ranges and thus are disregarded since the beginning when formulating the physical problem. Just this is the essence of eq. (2.1). Eventually note that the vibrational quantum number n appears to be here the number of quantum states allowed to the oscillator. Since the present approach gives sensible results for harmonic oscillations, there is no reason to exclude that the same holds for anharmonic oscillations as well. The next paragraph aims to generalize the kind of approach just introduced to the case of anharmonic oscillations.

3 The anharmonic oscillator

The classical Hamiltonian reads now

$$E = p^2/2m + \sum_{i=2}^N a'_i(n\hbar)^{-i}(x - x_o)^i, \quad (3.1)$$

being N the arbitrary number of terms of the series including quadratic and anharmonic terms and a'_i proper coefficients assumed known; indeed the values of these coefficients characterize distinctively the specific kind of oscillating system. The signs of a'_3 and a'_4 are taken here negative [9]; the former expresses the asymmetry of the mutual repulsion between atoms or ions, e.g. in a metallic lattice, the latter describes the softening of the vibration at large amplitudes. The higher order terms allow to describe these effects in a more general way, so their sign and values must agree with the idea that the global consequence of anharmonicity is to lower the potential energy of oscillation; indeed the potential energy reads $a'_2(x - x_o)^2 f(x)$, i.e. it consists of a quadratic term with x -dependent correction factor $f(x) = 1 + \sum_{i=3}^N (a'_i/a'_2)(x - x_o)^{i-2} < 1$. By analogy with the harmonic case, the coefficient of the quadratic term, anyway related to the force constant k_{an} , is reasonably expected to have still the form $m(n\hbar\omega_{an})^2/2$ with oscillation frequency defined now by $\omega_{an}^2 = k_{an}/m$. Moreover the dependence of this term on ω_{an} suggests that in general $a'_i = a'_i(\omega_{an})$ are to be expected as well.

The following discussion aims to guess this dependence and the relationship between ω_{an} and ω_{har} through the same

approach shown previously; so, as done in section 2, we aim to calculate ΔE_{\min} and infer next the anharmonic vibrational levels E_{an} and zero point energy E_0 , being clearly $\Delta E_{\min} = E_{\min} - E_0$ and $E_{an} = E_{\min}$.

According to the position (1.2) and eq. (1.1), the quantum energy equation corresponding to eq. (3.1) reads

$$\Delta E = \frac{\Delta p^2}{2m} + \sum_{i=2}^N \frac{a'_i}{\Delta p^i}. \quad (3.2)$$

This equation, minimized with respect to the range Δp , yields

$$\Delta p_{\min} = m \sum_{i=2}^N i a'_i \Delta p_{\min}^{-(i+1)}, \quad (3.3)$$

being

$$\Delta E_{\min} = \Delta E(\Delta p_{\min}), \quad \Delta p_{\min} = \Delta p_{\min}(\omega_{an}).$$

For assigned coefficients a'_i , the first equation admits in general $N + 2$ solutions Δp_{\min} , some of which can be however imaginary. Being the momentum uncertainty range Δp real positive by definition, let $I' \leq N + 2$ be the number of positive real roots; so I' possible values of Δp_{\min} describe the allowed momentum ranges of the oscillating particle that fulfil the minimum condition. A further limitation to these values is that the series must converge. Disregard also the values of Δp_{\min} that with the given a'_i possibly do not fulfil the inequality $|(i + 1)a'_{i+1}\Delta p_{\min}^{-(i+2)}| \ll |ia'_i\Delta p_{\min}^{-(i+1)}|$ inferred from eq. (3.2), i.e.

$$|a'_{i+1}| \ll |a'_i\Delta p_{\min}|. \quad (3.4)$$

Then $I \leq I'$ is the number of real roots of physical interest to be considered in the following. Trivial manipulations of eq. (3.2) to eliminate m with the help of eq. (3.3) yield

$$\Delta E = \frac{1}{2} \left(\frac{\Delta p}{\Delta p_{\min}} \right)^2 \sum_{i=2}^N \frac{ia'_i}{\Delta p_{\min}^i} + \sum_{i=2}^N \frac{a'_i}{\Delta p^i}. \quad (3.5)$$

To extract the allowed physical information from this equation one should minimize with respect to Δp and then proceed as shown in the harmonic case. Actually this minimum condition has been already exploited to infer eq. (3.3) itself, which suggests that eq. (3.5) should not need being minimized once more. To understand this point replace Δp with Δp_{\min} in eq. (3.5) and consider first the resulting equation $\Delta E(\Delta p_{\min}) = \sum_{i=2}^N (1 + i/2)a'_i\Delta p_{\min}^{-i}$ in the harmonic case; then $N = 2$, i.e. $a'_{i>2} = 0$, yields $3a'_2\Delta p_{\min}^{-2}/2$. By comparison with eq. (2.1) this result takes a more familiar form replacing a'_2 with $a_2\Delta p_{\min}^4/m$ where a_2 is a dimensionless proportionality coefficient linking a'_2 and Δp_{\min} ; in this way one obtains

$$\Delta E(\Delta p_{\min}) = \frac{3a_2\Delta p_{\min}^2}{2m},$$

which has the same form of eqs. (2.2) a proportionality factor apart. As expected, an immediate connection with the harmonic case is possible uniquely on the basis of the condition 3,3 without introducing explicitly neither ω_{har} nor the equations of Δp_{har} and ΔE_{har} . Express thus in general the coefficients a'_i as a function of Δp_{\min} as follows

$$a'_i = \frac{\Delta p_{\min}^{i+2}}{m} a_i, \quad \sum_{i=2}^N i a_i = 1, \quad 1 \leq j \leq I \quad (3.6)$$

where a_i are new constants that fulfil the boundary condition expressed by the second equation, straightforward consequence of eq. (3.3). Note that a'_i are uniquely defined for the specific oscillating system, whereas the appropriate notation of the various a_i should be $a_i^{(j)}$ to emphasize that a set of these coefficients is defined by each solution $\Delta p_{\min}^{(j)}$ of physical interest calculated through eq. (3.3). This would also compel indicating in eq. (3.5) $\Delta E^{(j)}$ and then $\Delta E_{\min}^{(j)}$. To simplify the notations the superscript (j) will be omitted, stressing however once for all that if $N > 2$ then eq. (3.5) actually represents anyone among I admissible equations. Replacing a'_i into the energy equation (3.5), one finds

$$\Delta E = \left(\left(\frac{\Delta p}{\Delta p_{\min}} \right)^2 \frac{1}{2} + \sum_{i=2}^N a_i \left(\frac{\Delta p_{\min}}{\Delta p} \right)^i \right) \frac{\Delta p_{\min}^2}{m}.$$

This suggests putting

$$q \frac{\Delta E}{\Delta E_{\min}} = \frac{1}{2} \left(\frac{\Delta p}{\Delta p_{\min}} \right)^2 + \sum_{i=2}^N a_i \left(\frac{\Delta p_{\min}}{\Delta p} \right)^i, \quad (3.7)$$

$$\Delta E_{\min} = q \frac{\Delta p_{\min}^2}{m}, \quad a_2 = \frac{1}{2} \left(1 - \sum_{i=3}^N i a_i \right).$$

The proportionality factor q aims to fulfil the reasonable condition $\Delta E = \Delta E_{\min}$ for $\Delta p = \Delta p_{\min}$ and express in a general way the expected link between ΔE_{\min} and $\Delta p_{\min}^2/m$. Trivial calculations yield

$$q = 1 + \sum_{i=3}^N (1 - i/2)a_i. \quad (3.8)$$

Of course q must be intended here as $q^{(j)}$ likewise as $a_i^{(j)}$. Whatever a_i might be, eq. (3.7) does not need being minimized; it simply expresses as a function of $\Delta p/\Delta p_{\min}$ the energy deviation from the harmonic condition for assigned values of the coefficients $a'_{i \geq 2} \neq 0$. Eq. (3.7) and a_2 are uniquely defined in the particular case $a_{i>2} = 0$ only, which corresponds to $q = 1$ as well. Moreover the form of the second equation, analogous to that of eqs. (2.2), suggests that Δp_{\min} and ΔE_{\min} must be also equal or proportional to the respective harmonic quantities Δp_{har} and ΔE_{har} . So putting

in general $\Delta E_{\min} = w^2 \Delta E_{har}$ and $\Delta p_{\min} = w \Delta p_{har}$, with w proportionality factor, one finds

$$\frac{q}{w^2} \frac{\Delta E}{\Delta E_{har}} = \frac{1}{2w^2} \left(\frac{\Delta p}{\Delta p_{har}} \right)^2 + \sum_{i=2}^N a_i w^i \left(\frac{\Delta p_{har}}{\Delta p} \right)^i, \quad (3.9)$$

$$\omega_{an} = w^2 \omega_{har}.$$

Likewise q , also w must be intended in general as $w^{(j)}$. So eqs. (3.9) define I anharmonic frequencies $\omega_{an}^{(j)} \neq \omega_{har}$, here designated shortly ω_{an} , corresponding to the unique harmonic frequency ω_{har} ; i.e. the various ΔE_{\min} describe the splitting of each n -th vibrational energy level $n\hbar\omega_{har}$. The anharmonic potential of eq. (3.9) is expected to depend upon ω_{an} through the dimensionless coefficients a_i , by analogy with the dependence of the harmonic term upon ω_{har}^2 . Thus, to complete the task of the present section it is necessary: (i) to define the factor w of eq. (3.9); (ii) to highlight the analytical form of the functions $a_i = a_i(\omega_{an})$; (iii) to express the potential energy of equation (3.9) as a function of ω_{an} through these coefficients.

Rewrite to this purpose the coefficients of eq. (3.2) as shown in following series

$$q\Delta E = \frac{1}{2} \frac{\Delta p^2}{m} + \sum_{i=2}^N a_i'' \frac{m^{i/2} (n\hbar\omega_{an})^{i/2+1}}{\Delta p^i}, \quad (3.10)$$

where the powers of $n\hbar\omega_{an}$ and m have been determined by dimensional consistency of the various terms with both ΔE and Δp^i . Minimizing with respect to Δp and equating to zero, one finds

$$R_E = \frac{1}{2} R_p^2 + \sum_{i=2}^N a_i'' R_p^{-i}, \quad (3.11)$$

where

$$R_E = q \frac{\Delta E}{\Delta E_{har}}, \quad R_p = \frac{\Delta p}{\Delta p_{har}}, \quad a_i'' = a_i w^{i+2}.$$

With the coefficients a_i'' and a_i linked by the last position, eq. 3.(11) is identical to eq. (3.9); this consistency supports therefore the positions of both eqs. (3.6) and (3.10). To specify w put first $N = 2$ in eq. (3.9); minimizing $R_p^2/2w^2 + a_2 w^2/R_p^2$ with respect to R_p yields $R_p^4 = 2a_2 w^4$. Since the minimum of R_p can be nothing else but 1 by definition, $w = (2a_2)^{-1/4}$ yields $w = 1$, whereas in this particular case $a_2 = 1/2$. As expected, eq. (3.9) is thus uniquely defined for $a_{i>2} = 0$ only. Note that the coefficient of the quadratic term of eq. (3.10) reads $a_2'' m (n\hbar\omega_{an})^2$; if the result $w = (2a_2)^{-1/4}$ previously obtained for $N = 2$ still holds for any N with a_2 given now by the last eq. (3.7), then $a_2'' = a_2 w^4$ yields $a_2'' = 1/2$ and thus the expected form $m(n\hbar\omega_{an})^2/2$ formerly quoted whatever $a_{i>2}$ might be.

This consideration encourages one to conclude with the help of eq. (3.7)

$$w^2 = (2a_2)^{-1/2} = \left(1 - \sum_{i=3}^N ia_i \right)^{-1/2},$$

$$a_i'' = a_i \left(1 - \sum_{i=3}^N ia_i \right)^{-i/4-1/2}.$$

Replacing a_i'' in eq. (3.10) one finds

$$\Delta E = \frac{1}{2q} \frac{\Delta p^2}{m} + \sum_{i=2}^N q^{-1} a_i \frac{m^{i/2} (n\hbar\omega_{har})^{i/2+1}}{\Delta p^i} \left(1 - \sum_{i=3}^N ia_i \right)^{-\frac{3}{4}(i+2)}. \quad (3.12)$$

This is the sought generalization of eq. (2.1) when $a'_{i>2} \neq 0$; the positions so far introduced link eq. (3.2) with the harmonic case. Moreover eq. (3.9) yields

$$\omega_{an} = \left(1 - \sum_{i=3}^N ia_i \right)^{-1/2} \omega_{har}. \quad (3.13)$$

With the given choice of w^2 , therefore, $a_{i \geq 3} = 0$ yield not only $\omega_{an} = \omega_{har}$ but also $\Delta p_{\min} = \Delta p_{har}$ and $\Delta E_{\min} = \Delta E_{har}$. Hence

$$\Delta E_{\min} = n\hbar\omega_{an} = \left(1 - \sum_{i=3}^N ia_i \right)^{-1/2} n\hbar\omega_{har}, \quad (3.14)$$

$$\Delta p_{\min} = \sqrt{mn\hbar\omega_{an}} = \left(1 - \sum_{i=3}^N ia_i \right)^{-1/4} \sqrt{mn\hbar\omega_{har}}.$$

As concerns the zero point energy E_0 hold the considerations of the previous section, i.e. $\Delta E_{\min} = E_{\min} - E_0$; moreover also now for $n = 0$ the minimum of eq. (3.12) reduces to $\Delta p_0^2/2qm$, with $\Delta p_0^2 = \Delta p_{\min}^2 (n = 0)$. As explained before, even in lack of vibrational states $\Delta p_{\min} \neq 0$ compels putting $\Delta p_0 = \Delta p_{\min}^{(0)}$ ($n = 1$) by virtue of eq. (3.14) so that $E_0 = \left(1 - \sum_{i=3}^N ia_i^{(0)} \right)^{-1/2} \hbar\omega_{har}/2q$; since in general are allowed several values of Δp_{\min} , the notation emphasizes that one must consider here the set of values of $a_i^{(j)}$ corresponding to the smallest among the various $\Delta p_{\min}^{(j)}$.

In conclusion, since the anharmonic energy and momentum must correspond to the respective ΔE_{\min} and Δp_{\min} , it is possible to summarize the previous results, with full notation for clarity, as follows with the help of eq. (3.8)

$$E_{an}^{(j)} = \left(1 - \sum_{i=3}^N ia_i^{(j)} \right)^{-1/2} n^{(j)} \hbar\omega_{har} + \frac{1}{2} \left(1 + \sum_{i=3}^N (1-i/2) a_i^{(0)} \right)^{-1} \left(1 - \sum_{i=3}^N ia_i^{(0)} \right)^{-1/2} \hbar\omega_{har}, \quad (3.15)$$

with

$$1 \leq j \leq I,$$

$$\Delta p_{an}^{(j)} = \left(1 - \sum_{i=3}^N ia_i^{(j)} \right)^{-1/4} \sqrt{mn^{(j)}\hbar\omega_{har}},$$

$$\omega_{an}^{(j)} = \left(1 - \sum_{i=3}^N ia_i^{(j)} \right)^{-1/2} \omega_{har},$$

$$a_i^{(j)} = \frac{ma_i'}{(\Delta p_{min}^{(j)})^{i+2}}.$$

4 Discussion

The strategy of the papers [7, 8] to exploit via eq. (1.1) the classical Hamiltonians of the system of interest was outlined in section 2 and then extended in section 3 to the anharmonic case. The first task of the discussion aims to clarify the classical and quantum ways to regard the harmonic and anharmonic oscillation. The classical potential energy of eq. (3.1), $U_{cl} = U_{cl}(x - x_o)$, concerns a withholding force progressively increasing as a function of $x - x_o$ while the oscillation turns gradually from harmonic into anharmonic behaviour. Moreover if momentum and position of m are both exactly known, U_{cl} can be defined with arbitrary accuracy simply increasing the number of terms of the series.

This description is clearly inadequate for the potential energy, $U_q = U_q(\Delta p, n)$, of the quantum eq. (3.2); in principle the exact elongation of m with respect to the rest position and the corresponding momentum are not jointly specifiable, i.e. the limit $\Delta x \rightarrow 0$ could not be described by finite values of Δp_{min} . Indeed $\Delta p_{min} \rightarrow \infty$ compels $\Delta p \rightarrow \infty$ that yields $\Delta E = \Delta p^2/2m$ regardless of a_i' ; this limit corresponds to the classical case of a free particle in a one-dimensional box, of no interest here, rather than to the harmonic limit expected for $\Delta x \rightarrow 0$. Eventually the quantum uncertainty compels regarding in a different way also the number of terms of U_{cl} and of U_q : in the former case N is in principle arbitrary, being significant its actual ability to provide a description as detailed as possible of the local state of motion of m , in the latter case does not, being instead significant its actual ability to introduce the allowed physical information into the system.

If for instance the model aims to describe softening and asymmetry effects only, then are justified terms like Δx^i with powers and signs [9] pertinent to these effects only. Solving eq. (3.1) requires exploiting the functional relationship U_{cl} upon Δx through numerical methods, solving eq. (3.2) requires instead a different reasoning because the anharmonic effects inherent the various Δx^i are related to the respective Δp^{-i} through eq. (1.1) only: the previous results show that a general physical principle, the minimum energy, is enough to this purpose. According to the classical eq. (3.1) the harmonicity requires $a'_{i \geq 3} \Delta x^i \ll a'_2 \Delta x^2$ in agreement with the convergence condition (3.4); the quantum eq. (3.2) requires $a'_{i \geq 3} \Delta p^{-i} \ll a'_2 \Delta p^{-2}$, which is still a statement of "small" oscillation amplitudes since $a'_i \Delta p^{-i} \propto a'_i \Delta x^i$. Both definitions

are thus equivalent, yet the latter is more interesting because it involves eq. (1.1) and allows further considerations on the classical and quantum concepts of harmonicity. Eq. (3.4) and the first eq. (3.3) yield for $i \geq 3$

$$a'_{i \geq 3} \Delta p^{-i} \ll a'_2 \Delta p^{-2} \Rightarrow a_i \left(\frac{\Delta p_{min}}{\Delta p} \right)^i \ll a_2 \left(\frac{\Delta p_{min}}{\Delta p} \right)^2.$$

Noting that Δp is arbitrary by assumption and that $\Delta p_{min} \leq \Delta p$ by definition, it turns out that the second inequality can be merely fulfilled by $\Delta p/\Delta p_{min} \gg 1$ regardless of the values of the ratios a_2/a_i and a'_2/a'_i . Since in principle a'_i only are required to fulfil the convergence condition (3.4), whereas the values of a_i are ineffective in this respect because their values are consequently defined in the successive eq. (3.6) only, the conclusion is that small oscillation amplitudes do not require necessarily vanishing $a_{i > 2}$. According to eq. (3.13), however, just these latter define w that in turn control ω_{an} and thus the splitting of energy levels. The fact that in general $w \equiv w^{(j)} \neq 1$ even for small oscillations supports the idea that the quantum harmonicity is a particular case, but not a limit case, of the quantum anharmonicity; in other words, an oscillating quantum system does not change gradually from harmonic to anharmonic behaviour.

This conclusion is confirmed also considering the dependence of the constants w on a_i . In eq. (3.6) large values of Δp_{min} entail small a_i and thus w such that the corresponding allowed frequencies ω_{an} are expected to have values similar to ω_{har} ; the contrary holds for small values of Δp_{min} , to which correspond larger values of w and therefore larger gaps $\omega_{an} - \omega_{har}$.

Hence, when considering the totality of allowed frequencies consistent with the different sizes of all ranges Δp_{min} , even small values of a'_i classically compatible with the harmonic condition entail anyway relevant splitting and gap of energy levels with respect to ω_{har} typical of the anharmonicity; otherwise stated, the quantum harmonicity requires $a'_{i \geq 3} = 0$ exactly. The harmonic ground level is a reference energy rather than an attainable limit energy because fails the classical expectation of anharmonic frequencies progressively deviating from ω_{har} along with a'_i ; the last eq. (3.7) shows indeed that even the first quadratic coefficient a_2 of potential energy differs from the corresponding harmonic coefficient unless $a_{i \geq 3} = 0$. It is also significant the fact that the unique ω_{har} , classically defined in eq. (2.1) through the force constant k_{har} of Hooke law only, never corresponds to a unique ω_{an} whatever $a'_{i \geq 3} \neq 0$ might be; this latter, although formally introduced in the early eq. (3.3) as $\omega_{an}^2 = k_{an}/m$, has quantum character after being subsequently redefined by eq. (3.9) through the multiplicity of values of w .

It is however worth noting in this respect a further chance to define the oscillation frequency in a mere quantum way through an uncertainty equation having a form seemingly different but conceptually equivalent to eq. (1.1). Introduce the

time range Δt necessary to displace m by Δx with finite average velocity v_x ; defining then $\Delta t = \Delta x/v_x$ and $\Delta E = \Delta p v_x$, eq. (1.1) takes a form that introduces new dynamical variables t and E having random, unpredictable and unknown values within the respective uncertainty ranges defined by the same $n\hbar$. Of course Δt and ΔE are completely arbitrary, as they must be, likewise Δx and v_x . Thus, with the constrain of equal n , eq. (1.1) reads equivalently as

$$\Delta E \Delta t = n\hbar, \quad \Delta t = t - t_o, \quad (4.1)$$

being the constant t_o the arbitrary origin of time coordinates. Eq. (4.1) is not a trivial copy of eq. (1.1): it introduces new information through v_x and shows that during successive time steps Δt the energy ranges ΔE change randomly and unpredictably depending on n . Of course the eq. (1.1) could have been inferred itself in the same way from eq. (4.1), i.e. regarding this latter as the fundamental statement. Relating eqs. (1.1) and (4.1) via the same arbitrary integer n , whatever it might be, means describing the oscillation of m through energy and time uncertainty ranges. This is equivalent to say that the time coordinate is regarded in an analogous way as the space coordinate hitherto concerned.

To show the consequences of this assertion, consider that $1/\Delta t$ has in general physical dimensions of frequency; then eq. (4.1) can be rewritten as $\Delta E_n = n\hbar\omega^\S$, being ω^\S a function somehow related to any frequency ω . If in particular ω^\S is specified to be just the previous frequency ω_{har} , whatever the value of this latter might be, eq. (4.1) reads

$$\Delta E_n = n\hbar\omega_{har}. \quad (4.2)$$

The notation emphasizes that the particular case $\omega^\S \equiv \omega_{har}$ enables a direct conceptual link with eq. (2.3), i.e. it concerns the harmonic; having found that n is according to eq. (1.1) the number of vibrational states of the oscillator and $n\hbar\omega_{har}$ their energy levels, then without need of minimizing anything one infers that ΔE_n is again the energy gap between the n -th excited state of the harmonic oscillator and its ground state of zero point energy; the condition of minimum energy and Δp_{min} are now replaced by the specific meaning of Δt .

This conclusion shows that a particular property of the oscillating system is correlated to a particular property of the uncertainty ranges, thus confirming the actual physical meaning of these latter. So E_n falling within ΔE_n are still now random, unpredictable and unknown because of n . While ω_{har} was formerly defined by the formal position 2,1, now eq. (4.1) reveals its actual quantum meaning due to its direct link with the time uncertainty Δt .

This last result is significant for the present discussion: it justifies the different outcomes of the quantum approach with respect to the classical expectation in terms of uncertainty about the dynamical variables of m only; thus, as shown in [7, 8], this result disregards any phenomenological/classical hint to describe the system. In other words, instead of thinking to

a withholding spring bound to a mass moving back and forth, the oscillation can be imagined in a more abstract way. It is enough to introduce an arbitrary energy range ΔE_n to which corresponds a respective quantum frequency $1/\Delta t_n$; then the form of eq. (1.1) is suitable to introduce an appropriate potential energy with elongation extent described by a unique quadratic term or by a series of terms, whose coefficients are respectively expressed as a function of ω_{har} or ω_{an} like in eqs. (2.1) or (3.10).

The worth of this conclusion is due to the generality of the resulting concept of oscillation, which skips any information on actual kind of motion of m , particular property of the oscillating mass, specific nature of the withholding force and hypothesis on the allowed range of frequencies. Both time and space uncertainties allow thus to describe an oscillating system in a fully quantum way, without writing and solving its wave equation. The previous results highlight the link of the allowed frequencies to the terms of U_q , see in particular the remarks about eqs. (3.5) and 3,13. A consequence of this point of view is that replacing U_{cl} with U_q compels the existence of several momentum uncertainty ranges Δp_{min} and thus of as many ω_{an} even when one would expect a mere perturbation of the unique ω_{har} : the physical information provided by the quadratic term only is uniquely defined, instead the various values of Δp_{min} and ω_{an} for $N > 2$ in eq. (3.2) reveal according to the last eq. (3.7) multiple anharmonic effects that influence also the quadratic term. The quantum uncertainty is therefore crucial in describing the oscillation.

For instance let us show that, at least for certain frequencies, the anharmonic oscillator appears to be a system intrinsically unstable. Let i be the index of any high order term of the series such that $a'_i/\Delta p^i \ll a'_2/\Delta p^2$ is true by definition because of the convergence condition; so $a'_i/\Delta p^i$ represents a small contribution to the total energy of oscillation. Let $\delta a'_i/\Delta p^i$ be its value altered by the change of the coefficient a_i because of an external perturbation acting on the oscillator; if for instance an impurity diffuses through the lattice in proximity of the given oscillating atom/ion, the stress field around this impurity or its possible charge field reasonably modify the local repulsion between atoms/ions or the softening effects at large oscillation amplitudes, as a consequence of which the anharmonic coefficients a'_3 and/or a'_4 are expected to change.

Let us exemplify any perturbation like this through a suitable change of some a'_i of the i -th energy terms in eq. (3.2); here however we consider for simplicity one term only to describe the local effect. The proof that some Δp_{min} and resulting ΔE_{min} are strongly affected even by a very small change of any $a'_{i>2}$ is easy in the particular case where the series describing the potential energy converges very quickly. Differentiating eq. (3.6) one finds

$$\delta a'_i = a'_i \left((i+2) \frac{\delta \Delta p_{min}}{\Delta p_{min}} + \frac{\delta a_i}{a_i} \right).$$

Fix the value of $\delta a'_i$; if the local perturbation of the lattice affects a'_i in such a way that $\delta a'_i \gg a'_i$, i.e. it alters significantly a_i , then the quantity in parenthesis is very large. If this happens while holds for $\delta a'_i$ also the condition $\delta a'_i/\Delta p^i \ll a'_i/\Delta p^2$, still possible because no hypothesis has been made on the strength of the perturbation, then considering that the quadratic term provides the most essential contribution to the total potential energy the result is: even a small perturbation $\delta a'_i/\Delta p^i$ of the whole oscillation energy is able to change significantly both Δp_{\min} and a_i that define ω_{an} , see eqs. (3.13) to (3.15). The altered size of the range Δp_{\min} , actually verified by preliminary numerical simulations carried out with coefficients a'_i arbitrarily chosen to match the aforesaid condition, means in particular that the whole energy of the system admits not only a different ω_{an} allowed to the oscillator but also a larger range of corresponding momenta p_{\min} allowed to m ; this does not exclude even the chance of chaotic motion related to a random sequence of values ω_{an} during a weak perturbation transient due to the diffusing impurity.

The reason of such instability rests once again on the different way of regarding the oscillation amplitudes in classical and quantum physics. The former admits the limit $\Delta x \rightarrow 0$ regardless of Δp , the latter does not; so the quantum oscillation range of physical interest cannot be arbitrarily small or change arbitrarily without violating the crucial condition of minimum energy. Indeed the oscillation range sizes corresponding to the vibrational levels are quantized themselves

$$\Delta x_{\min} = \sqrt{\frac{n\hbar}{\omega_{an}m}}, \quad \Delta x_0 = \sqrt{\frac{\hbar}{\omega_{an}^{(0)}m}}.$$

At this point it is worth remembering what has been previously emphasized, i.e. that the sizes of the ranges Δx and Δp are unspecified and indefinable; Δx_{\min} and Δp_{\min} are merely particular values showing the propensity of nature to fulfil the condition of minimum energy, however without contradicting the assumption that the uncertainty ranges are in principle completely arbitrary. So oscillation ranges that do not fulfil the former condition are certainly possible but unstable because of mere quantum reasons, i.e. they do not correspond to momentum range sizes that minimize the oscillation energy levels.

This conclusion is important because its validity follows uniquely from the assumption of convergence of the potential series only, i.e. it concerns a realistic condition effectively possible for the oscillator rather than an unusual and improbable limit case. Also, this result holds whatever the origin of the anharmonicity might be and confirms the physical diversity of harmonic and anharmonic quantum systems. Note however that the former is actually an ideal abstraction only; what can be expected in practice is a strong or weak anharmonicity, unless some specific physical reason requires just a potential energy with quadratic term only. So the results of the present approach should be regarded as the realistic be-

haviour of any oscillating system, rather than a sophisticated improvement of the naive harmonic behaviour; now this latter appears thus in general reductive and incomplete, rather than merely approximate. Yet eq. (3.15) shows that the zero point energy is formally analogous in both cases, a numerical difference apart: the only difference between the harmonic and anharmonic cases is that instead of considering the unique $\hbar\omega_{har}/2$ one must select the smallest $\omega_{an}^{(j)}$ to calculate $\hbar\omega_{an}^{(0)}/2$.

Note eventually that easy considerations allow to generalize the concept of perturbed oscillator in the conceptual frame of the present model. So far the present approach aimed to introduce the terms a_3 and a_4 to account for the anharmonicity, so that eqs. (3.2) to (3.15) tacitly assume an isolated oscillating system. Simple considerations however allow to further generalize the physical meaning of eq. (3.2) taking advantage of the fact that the present model works with a number of high order terms in principle arbitrary. In particular coefficients and number of terms could be exploited to describe even an oscillating system perturbed by an external force, for instance due to the interaction with other oscillators; indeed this force can be certainly described as a series development having the form $\sum a'_i \Delta x^i$ if it is related, in the most general case non-linearly, to the displacement extent of the oscillating mass. Of course i can be even negative if the force vanishes at infinite distance. So, whatever the nature of the perturbation might be, this means that the potential energy of the system changes by an additional amount $-\sum a'_i (1+i)^{-1} \Delta x^{i+1}$ to be summed up with the corresponding terms of eq. (3.1). In any case, however, adding an arbitrary number of such energy terms to those intrinsically characterizing the oscillator does not change in principle the approach so far exposed, except of course the numerical value of the various a_i of eq. (3.9), which are now replaced by the sum $a''_i + a'_i$ for each i -th power of oscillation elongation. So nothing hinders to regard the energy range ΔE_{an} of this equation as $\Delta E_{an+pert}$ still normalized to that of an isolated harmonic oscillator; it is enough that the coefficients a'_i up to the N -th order are still known, i.e. defined by the particular kind of oscillating system and external perturbation, yet without necessarily assuming any constrain on their signs, now determined by the sum of both effects. Even in the case where the force is described by terms like $a'/\Delta x^i$ one would find an equation like (3.2) containing however terms like $a'_k \Delta p^k$ with $k > 2$. Also in this case, minimizing with respect to Δp would yield an appropriate number of roots Δp_{\min} and thus prospective conclusions in principle completely analogous to that previously carried out. In the present case holds therefore the following position

$$\omega_{an+pert} \cong \omega^2 \omega_{har}.$$

As expected, the previous scheme of vibrational levels is modified the external perturbation that affects w . This last result confirms the very general character of the way to describe any oscillating system simply with the help of the fundamental eq. (1.1).

5 Conclusion

The computational scheme introduced in the present paper is very simple: the most important achievements hitherto exposed do not require numerical calculations, but are consequence of general considerations on basic concepts of quantum mechanics. The general character of the approach, e.g. due to the arbitrary number N of anharmonic terms, and the possibility of extension to the case of a perturbed oscillator, propose the model as a useful tool in a broad variety of physical problems.

Submitted on June 13, 2011 / Accepted on June 16, 2011

References

1. Landau L.D., Lifshitz E.M., *Mecanica*, (1969), Editions MIR, Moscou, p. 118 and ff.
2. Hoehli U.T. Acoustic anharmonicity and the ΔE effect in tetragonal $SrTiO_3$. *Solid State Communications*, 1973, v. 13, no. 9, 1369–1373.
3. Piekara A.H., Ratajska B. Nonlinear interaction of a powerful light beam with crystal lattice vibrations. *Applied Optics*, 1978, v. 17, no. 5, 689–690.
4. Petrovsky A.B. Foldover ferromagnetic resonance and damping in permalloy microstrips. *Physics Letters A*, 1968, v. 27, 220–221.
5. Abdel-Rahman E.M., Nayfeh A.H. Superharmonic resonance of an electrically actuated resonant microsensors. *Proceedings of the International Conference on Nanotechnology, Nanotech*, 2003, v. 2, 440–443.
6. Berrondo M., Recamier J. Resonances and anti-bound states in a Morse potential. *Journal of Chemical Physics Letters*, 2011, v. 503, no. 1–3, 180–184.
7. Tosto S. An analysis of states in the phase space: the energy levels of quantum systems. *Il Nuovo Cimento B*, 1996, v. 111, no. 2, 193–215.
8. Tosto S. An analysis of states in the phase space: the diatomic molecules. *Il Nuovo Cimento D*, 1996, v. 18, no. 12, 1363–1394.
9. Kittel C. *Introduction to Solid State Physics*. Third Edition, J. Wiley and Sons, New York, 1967, p. 184.