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Comments on the anharmonic oscillator model

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Abstract. A good and helpful definition of the transition point between the harmonic and anharmonic regimes of the anharmonic oscillators is given. It is shown that there exist some expectation values which are more useful than the energy to define the aforesaid regimes.

I. Introduction

The $2k$-anharmonic oscillators

$$H=\tfrac{1}{2}(p^2+x^2)+\lambda x^{2k}; \qquad p=-i\frac{d}{dx}; \qquad \lambda, k>0, \tag{1}$$

play an important role in field theory and molecular physics. It is of great importance to know the analytic structure of the eigenvalues E_n of H in terms of n (quantum number), λ and k. One of the main features of this model is the divergence of the λ-power perturbation series

$$E_n=\sum_{i=0}^{\infty} E_n^{(i)}\lambda^i, \tag{2}$$

for all λ-values (1, 2). For this reason, the model is very interesting from the perturbation theory viewpoint.

When λ is large enough, the eigenvalues E_n can be expanded as

$$E_n=\lambda^{1/(k+1)}\sum_{i=0}^{\infty} e_n^{(i)}\lambda^{-2i/(k+1)}. \tag{3}$$

This result follows immediately from the Symanzik's theorem (1) and the power series (3) is known to be convergent for $k=2$ (1). Unfortunately, the coefficients $e_n^{(i)}$ are unknown.

An important task is to find the range of (λ, n)-values for which the $2k$-anharmonic oscillator behaves like an harmonic oscillator of like a pure $2k$-oscillator ($H=p^2/2+x^{2k}$); i.e. the so called harmonic and anharmonic regimes, respectively (3–8). Since the λ-powers series (2) is divergent, it is necessary to resort to summation techniques such as Padé or Padé–Borel methods (1) in order to obtain accurate eigenvalues. It was found that the Padé approximants built from this series are very reliable in the harmonic regime (1–4), so it is mandatory to know the harmonic regime extension as accurately as possible. But the eigenvalues obtained in this way do not behave like (3) in the large λ-regime. This failure can be removed by means of variationally renormalized perturbation methods (9–16).

This paper is concerned with the definition of the harmonic and anharmonic regimes. There are several proposals in the current literature. For example, Hioe et al. (3, 4) found that both regimes can be defined in terms of the variable

$$\xi = \lambda(n+\tfrac{1}{2})^{k-1}. \tag{4}$$

Harmonic and anharmonic regimes are determined by the conditions $\xi \ll 1$ and $\xi \gg 1$, respectively. The range of ξ-values between these extreme zones is usually called boundary layer (3, 4).

Banerjee et al. (5) and Banerjee (6) proposed an even better way to define the harmonic and anharmonic regimes. They modified the wavefunction that had been employed by Biswas et al. (17) to approximate the eigenstates of (1) in order to introduce a scaling factor η in the form

$$\Psi_n(\lambda, x) = \exp(-\eta x^2) \sum_i a_i x^i. \tag{5}$$

Since the proper dependence of η on n and λ was found to be

$$\eta(n, \lambda) = \tfrac{1}{2} + \text{const. } \xi^{1/(k+1)}, \tag{6}$$

they concluded that the harmonic and anharmonic regimes should be defined by means of the conditions $\xi^{1/(k+1)} \ll \frac{1}{2}$ and $\xi^{1/(k+1)} \gg \frac{1}{2}$, respectively.

The variable α used by Kesarwani and Varshni (7, 8)

$$0 < \alpha = \lambda^{2/3}/(1+\lambda^{2/3}) < 1, \tag{7}$$

is not useful to define the harmonic anharmonic regimes of the 4-anharmonic oscillator for it does not take into account the well-known shift of the boundary layer to small λ-values when n increases.

Though the proper variable (ξ or $\xi^{1/(k+1)}$) that describes the transition between the harmonic and anharmonic regimes is known, the boundary layer is placed rather arbitrarily. The first criterium to define the regimes was based on the energy (3, 4).

In the present paper we show that there exist some expectation values which are more useful than the energy to define the aforesaid regimes because their plots (vs $\log \lambda$) exhibit three different zones which can be easily related with the harmonic and anharmonic regimes and with the boundary layer. Besides, they also possess a well-defined transition point between the two limits. For example, any expectation value of the form $\langle x^{2s} \rangle$, $s = 1, 2, \ldots$ have these properties.

II. Definition of regimes

For simplicity we will consider $s = 1$ and $s = k$ only. These expectation values can be written as a function of the energy and its first derivative by means of the virial and Hellmann–Feynam theorems

$$\langle x^2 \rangle = E - (k+1)\lambda \frac{\partial E}{\partial \lambda}, \tag{8}$$

$$\langle x^{2k} \rangle = \frac{\partial E}{\partial \lambda}. \tag{9}$$

Throughout this paper we use standard quantum-mechanical notation and we omit any reference to the dependence of the expectation values and the energy on n, λ and k, when it is possible, in order to simplify the notation.

The normalized quantity

$$X_n(\lambda, k) = \langle n \,|x^2|\, n\rangle(\lambda, k)/(n+\tfrac{1}{2}), \tag{10a}$$

is very useful because it is a bounded monotonic decreasing function of λ

$$X(\lambda = 0) = 1 > X(\lambda) > X(\lambda \to \infty) = 0. \tag{10b}$$

for any n- and k-value.

We have computed accurate enough E- and $\langle x^{2k} \rangle$-values from $\lambda = 0$ to $\lambda = 10^4$ by means of the Rayleigh–Ritz variational method together with an appropriate trigonometric basis set (18). The expectation values of p^2 and x^2 can be easily obtained from the well-known virial theorem.

Figures I and II show the plots X vs log (2λ) for several n- and k-values. Due to the shape of these curves it is very easy to identify three different zones: the harmonic regime ($X \simeq 1$), the anharmonic regime ($X \simeq 0$) and the boundary layer. The main feature of these plots is that they exhibit a well-defined transition point between the two regimes: an inflexion point λ_i

$$\{\partial^2 X/\partial(\log \lambda)^2\}(\lambda = \lambda_i) = 0. \tag{11}$$

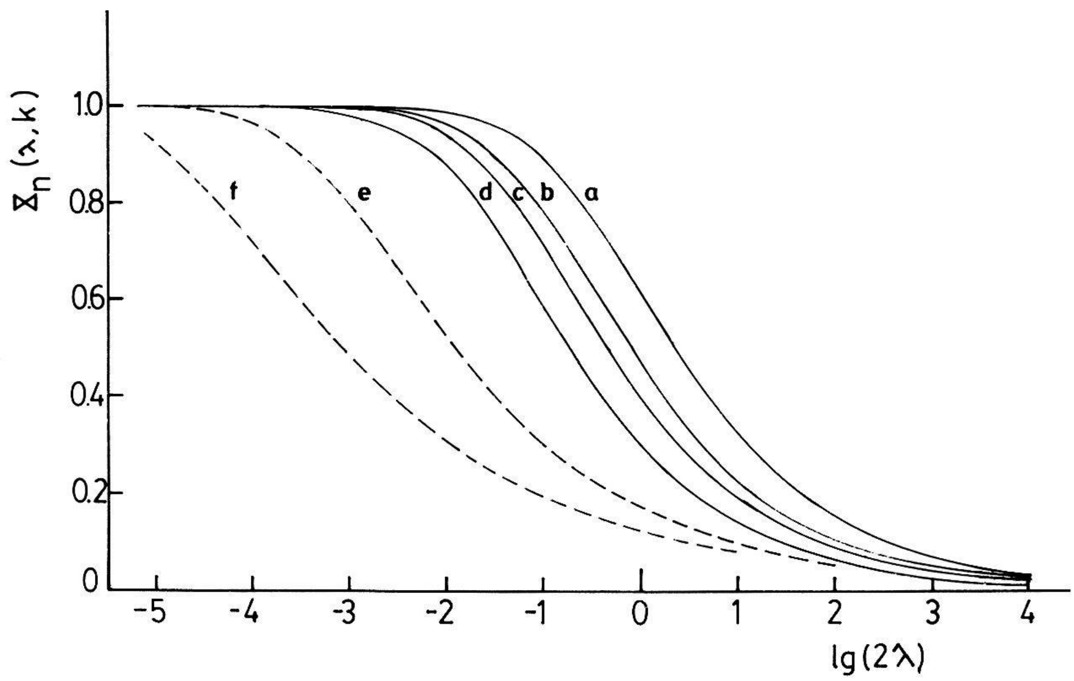

Figure I.
X_n versus log (2λ) for several n and k values: a: $k=2$, $n=0$, b: $k=2$, $n=2$, c: $k=2$, $n=4$, d: $k=2$, $n=10$, e: $k=3$, $n=10$, f: $k=4$, $n=10$.

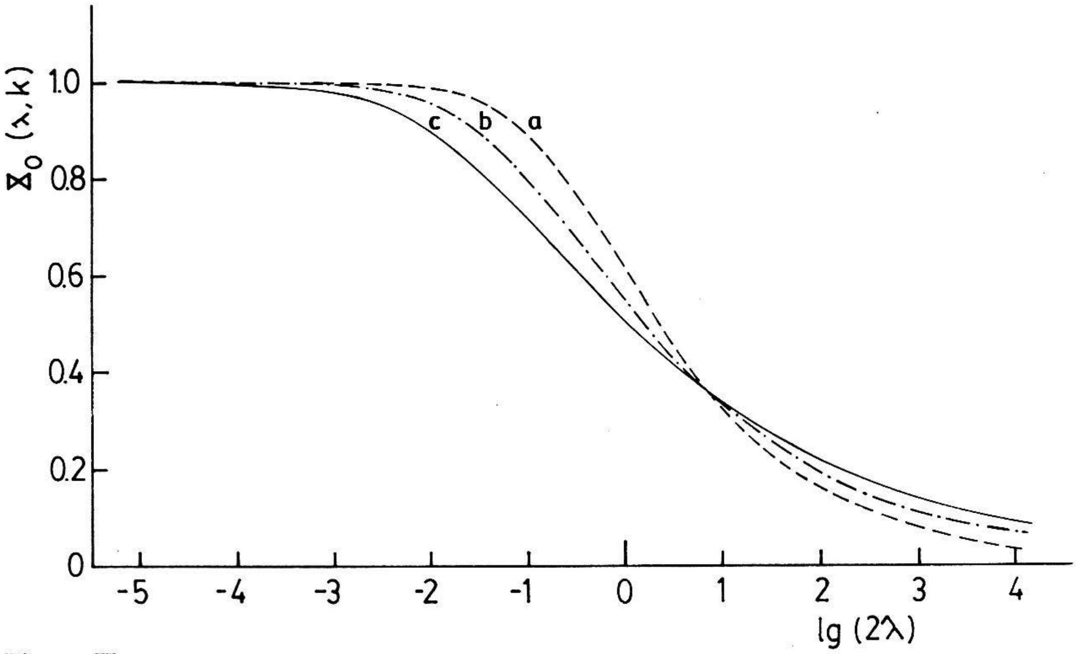

Figure II.
X_0 versus $\log(2\lambda)$ for $k = 2$ (a), $k = 3$ (b) and $k = 4$(c).

This condition can be easily written in terms of the energy

$$-k(\partial E/\partial\lambda)(\lambda=\lambda_i)+k\lambda_i(\partial^2 E/\partial\lambda^2)(\lambda=\lambda_i)=-(k+1)\lambda_i^2(\partial^3 E/\partial\lambda^3)(\lambda=\lambda_i). \quad (12)$$

It is a very interesting fact that λ_i lies within the boundary layer as defined by Hioe et al. (4). But the plots E vs $\log\lambda$ do not exhibit three well-differentiated zones such as those shown in Figures I and II. The inflexion point λ_i can be roughly approximated through the condition $X = \frac{1}{2}$.

We said before that $\xi^{1/(k+1)}$ is better than ξ in order to define the regimes. This can be seen in Table I where we show that the quantity $\xi_i^{1/(k+1)}(\xi_i = \lambda_i(n+\frac{1}{2})^{k-1})$ is almost independent on k when $n = 10$. Since ξ_i is almost independent on n too, then it follows that ξ_i fulfils the condition

$$\tfrac{1}{2} < \xi_i^{1/(k+1)} < 1, \quad (13)$$

for all states of any $2k$-anharmonic oscillator.

Another very striking fact is that the three curves in Fig. II cross each other approximately in only one point (λ_c) which lies in the anharmonic regime. Similar results were obtained by Hioe et al. (4) and Banerjee (6) with regard to the energy eigenvalues. Using WKB arguments, Banerjee (6) found the level crossing condition for the $2k$- and $2k'$-anharmonic oscillators in the large quantum

Table I
Inflexion points for 4-, 6-, and 8-anharmonic oscillator ($n = 10$).

k	λ_i	$\xi_i^{1/(k+1)}$
2	$2.51\ 10^{-2}$	0.641
3	$1.58\ 10^{-3}$	0.646
4	$8.89\ 10^{-5}$	0.635

number regime to be

$$\lambda_c' = f(k, k')(n+\tfrac{1}{2})^2, \tag{14}$$

where $f(k, k')$ is a function that changes very slowly with k and $k'(f(k, k') \simeq 1)$. Following Banerjee's arguments (6) and supposing $f(k, k') \simeq 1$, it is very easy to relate λ_c with λ_c'. The result is:

$$\lambda_c \simeq \left(\frac{k+1}{k'+1}\right)^{1/2} \lambda_c'. \tag{15}$$

We stated before that all expectation values $\langle x^{2s}\rangle$ $(s = 1, 2, \ldots)$ are more useful than the energy eigenvalues to define the regimes. In fact, all these quantities behave like $\langle x^2\rangle$. We cannot prove that the inflexion points (λ_{is}) and the crossing points (λ_{cs}) for any s-value lie close to those of $\langle x^2\rangle$ but we have found that this is so for the case $s = k$. The λ_{ik}- and λ_{ck}-values were calculated through the numerical technique described before. In this case the inflexion points

$$\{\partial^2\langle x^{2k}\rangle/\partial(\log\lambda)^2\}(\lambda = \lambda_{ik}) = 0. \tag{16}$$

lead to the following energy condition (cf. equation (9))

$$(\partial^2 E/\partial\lambda^2)(\lambda = \lambda_{ik}) = -\lambda_{ik}(\partial^3 E/\partial\lambda^3)(\lambda = \lambda_{ik}). \tag{17}$$

Even more interesting than the expectation values of x^{2s} are several scaling independent quantities such as

$$A = \langle x^2\rangle\langle p^2\rangle, \tag{18}$$

$$B = \langle x^{2k}\rangle/\langle x^2\rangle^k, \tag{19}$$

which also remain finite for any λ-value. The behaviors of A and B are closely related, as we will see below.

From the virial and Hellmann–Feynman theorems it follows immediately that

$$\langle p^2\rangle = E + (k-1)\lambda\frac{\partial E}{\partial\lambda}. \tag{20}$$

Introducing (8), (9) and (20) into (18) and (19) and then differentiating the result with respect to λ, we obtain

$$\frac{\partial A}{\partial\lambda} = -2\lambda\langle x^2\rangle^{k+1}\frac{\partial B}{\partial\lambda}. \tag{21}$$

Second derivatives also relate each other through a simple expression:

$$\frac{\partial^2 A}{\partial\lambda^2} = -2\frac{\partial B}{\partial\lambda}\frac{\partial}{\partial\lambda}(\lambda\langle x^2\rangle^{k+1}) - 2\lambda\langle x^2\rangle^{k+1}\left(\frac{\partial^2 B}{\partial\lambda^2}\right). \tag{22}$$

If A has a maximum (minimum) at $\lambda = \lambda_0$, then B will have a minimum (maximum) at the same point. Besides, if A is a monotonic increasing (decreasing) function of λ, then B will be monotonic decreasing (increasing). For each pair (n, k) the inflexion points of A and B have to occur at different λ-values, as it is shown in (22). Notwithstanding, numerical calculation shows that they lie close together because the first term in the right hand side of equation (22) is small near these inflexion points.

Table II
State types for 4-, 6-, and 8-anharmonic oscillator.

k	Type I	Type II A	Type II B	Type III
2	$n \leqq 1$	—	$n = 2$	$n \geqq 3$
3	$n \leqq 1$	—	$n = 2, 3$	$n \geqq 4$
4	$n \leqq 1$	$n = 2$	$n = 3, 4$	$n \geqq 5$

The inflexion points of all quantities we have studied numerically (i.e. $\langle x^2 \rangle$, $\langle x^{2k} \rangle$, A and B) lie within a small zone contained in the boundary layer defined by Hioe et al. (3, 4). Then, we can conclude that the boundary layer is almost independent on the quantity used to define it. Nevertheless, it must be kept in mind that the behaviour of some unbounded observables (e.g. the energy) does not show the three different zones clearly.

The functions A and B allow us to classify the states of any $2k$-anharmonic oscillator among three different groups:

Type I: A is a monotonic increasing function.

Type II A: A has a maximum, $A(\lambda = 0) > A(\lambda \to \infty)$ and $B(\lambda = 0) > B(\lambda \to \infty)$.

Type II B: A has a maximum, $A(\lambda = 0) > A(\lambda \to \infty)$ and $B(\lambda = 0) < B(\lambda \to \infty)$.

Type III: A is a monotonic decreasing function.

Our numerical calculation suggests that any state of any $2k$-anharmonic oscillator belongs to one of these classes. Results are given in Table II for the cases $k = 2, 3, 4$ from which some general conclusions can be obtained for all $2k$-anharmonic oscillators. States $n = 0$ and $n = 1$ are always of Type I and those with large quantum numbers belong to Type III. (In both cases the states possess only one inflexion point) Type II states seem to be transition states between these two limits and their number increases as k grows. At this moment we are unable to prove these assertions rigorously but we are working on this subject and results will be given elsewhere in a forthcoming paper.

The inflexion points of the functions A and B are useful to define the transition between the harmonic and anharmonic regimes because they shift as those inflexion points of $\langle x^2 \rangle$ and $\langle x^{2k} \rangle$. Furthermore, the plots A vs $\log \lambda$ possess a very interesting physical meaning; i.e. they show the change of the uncertainty coordinate-momentum products $\Delta x \, \Delta p$ with $\lambda (\Delta x = \langle x^2 \rangle; \Delta p = \langle p^2 \rangle)$.

III. Conclusions

In this paper we have shown that functions like $\langle x^{2s} \rangle$ $(s = 1, 2, \ldots)$, A and B are very useful to define the harmonic and anharmonic regimes in $2k$-anharmonics oscillators. In fact, their plots (vs $\log \lambda$) exhibit two flat zones which can be associated with the aforesaid regimes and an intermediate zone (with higher slopes) which is easily related with the boundary layer. On the contrary, the energy, that was employed previously by other authors to define these regimes (3, 4), is a monotonic increasing function which does not plainly show different zones. Besides, each of the functions we propose here possesses an inflexion point that seems to define the transition between both regimes in a very natural manner and that lies within the boundary layer defined by Hioe et al. (3, 4). In addition to this, the inflexion points shift accordingly with the variable $\xi^{1/(k+1)}$ which was proved to be very powerful to describe the change from one regime to the other (5, 6).

Since the inflexion points of all aforementioned functions lie close together within the boundary layer, we can deduce that the regimes are a characteristic of the system as a whole (i.e. of the $2k$-anharmonic oscillator) and not, as it could be supposed, of some particular function of λ (the energy, for example). Also, we have found that the plots $\langle x^2 \rangle$ vs $\log \lambda$ for different k-values cross each other almost at the same λ-point in the anharmonic regime. This behaviour, which is also showed by the other plots $\langle x^{2s} \rangle$ vs $\log \lambda$, was previously found by other authors (4, 6) in the energy vs $\log \lambda$ curves. Our results confirm that the crossings like the inflexion points, are a characteristic of the system as a whole.

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