Log-anharmonic oscillator and its large—$N$ solution

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Abstract

Anharmonic oscillator is considered using an unusual, logarithmic form of the anharmonicity. The model is shown connected with the more conventional power-law anharmonicity $\sim |x|^\alpha$ in the limit $\alpha \to 0$. An efficient and user-friendly method of the solution of the model is found in the large—$N$ expansion technique.
1 Introduction

The popularity of one-dimensional Schrödinger equations with a wide family of anharmonic-oscillator interactions

\[ V^{(AHO)}(x) = \omega^2 x^2 + \lambda V_I(x) \]  

found its motivation in the phenomenological appeal of the model (say, in the context of atomic and molecular physics [1]) as well as in the methodical relevance. Thus, one finds that the radius of convergence of the most common Rayleigh-Schrödinger perturbation-series representation of the bound-state energies appears to be zero even after one of the most elementary power-law choices of perturbations \( V_I(x) \sim x^n \) with, typically, quartic anharmonicity at \( n = 4 \) [2]. Such an obstacle forces one to search for a more sophisticated method of the evaluation and prediction of the experimental measurements: several nice, compact and comparatively elementary outlines of the problem may be found, e.g., in dedicated proceedings [3].

In the early nineties the study of the one-dimensional anharmonic oscillators found another specific motivation in the context of quantum field theory where the choice of \( V_I(x) \sim x^\alpha \) with a non-integer exponent \( \alpha \notin \mathbb{N} \) provided an innovative insight in the mechanism of the spontaneous symmetry-breaking phenomena [4] or in the robust nature of supersymmetry [5]. The idea (called, sometimes, delta-expansion technique [6]) was based on the truncated Taylor-series approximation of the general power of the coordinate or, in the field-theory context, of the field,

\[ |\phi|^\alpha = e^{\alpha \ln |\phi|} = 1 + \alpha \ln |\phi| + \frac{1}{2} \alpha^2 \ln^2 |\phi| + \ldots. \]  

The latter trick opened a way towards the efficient perturbation-expansion study of the three-parametric family

\[ \left[-\frac{d^2}{dx^2} + \omega^2 x^2 + \lambda |x|^\alpha \right] \psi_n(x) = E_n \psi_n(x), \quad n = 0, 1, \ldots \]  

of the anharmonic-oscillator Schrödinger equations in the three alternative, phenomenologically different dynamical regimes. In Ref. [7] we studied such a possibility in detail, distinguishing between the three versions of Eq. (3) where (a) \( \alpha \approx 2 \), (b) \( \alpha \approx 0 \) and (c) \( \alpha \approx -2 \).

The first option (a) may be interpreted as making the spring constant slightly coordinate-dependent, \( \omega^2 \rightarrow \omega^2(x) = \omega^2 |x|^{\alpha-2} \). Naturally, in all of the three cases (as well as in their mutual combinations [7]) one arrives at the perturbative Schrödinger equation of interest by employing and, \textit{mutatis mutandis}, approximatively truncating the respective infinite Taylor-series versions (2) of the interaction.

In our present letter our attention will be concentrated upon the most elementary option (b). In this case one can neglect the \( \mathcal{O}(\alpha^2) \) corrections, abbreviate \( \lambda \alpha = -2g^2 \), shift the origin of
the energy scale and arrive at a remarkably elementary logarithmically anharmonic Schrödinger equation

\[
\left[-\frac{d^2}{dx^2} + \omega^2 x^2 - 2g^2 \ln |x| \right] \psi_n(x) = E_n \psi_n(x), \quad x \in (-\infty, \infty), \quad n = 0, 1, \ldots
\]  \hspace{1cm} (4)

Once we arrived at the bound-state problem (4) we realized (cf. section 2 below) that the choice of a small exponent \( \alpha \) in the anharmonicity of Eq. (3) (and, in particular, of its leading-order logarithmic approximation) combines several features of the interaction endowing the underlying Schrödinger Eq. (4) with an independent, purely mathematical appeal. The most characteristic feature of the interaction is found to lie in the presence of a central barrier which is softer than usual. In contrast to the customary centrifugal barrier \( \sim \ell(\ell+1)/x^2 \) (which is strictly impenetrable so that it forces us to restrict the admissible coordinates to a half-line), the present logarithmic soft barrier \( V_1^{(\log)}(x) = -2g^2 \ln |x| \) remains penetrable so that the motion of a hypothetical particle may proceed along the whole real line of \( x \in (-\infty, \infty) \).

A semi-quantitative analysis of the basic qualitative features and consequences of the underlying processes of the tunneling through the logarithmic singularity in the origin has been performed in our preceding paper [8]. In the generic case we were only able to construct a purely numerical solution. Moreover, for the sake of simplicity of this solution we replaced the asymptotically dominant confining force \( \sim \omega^2 x^2 \) by an infinitely deep square-well approximation (i.e., after a re-scaling, by the Dirichlet boundary conditions at \( x = \pm 1 \)).

Near the minimum, such a replacement changed the nature of the force significantly, especially in the strong-repulsion dynamical regime. Our present paper will fill the gap. In section 3 we shall return to the untruncated and smooth potential in the perturbed harmonic oscillator regime. Using the less usual perturbation-series formalism of the so called large\(-N\) expansions we shall show that a consistent picture of the coupling-dependence of the bound states becomes provided in the form which may be characterized as semi-numerical.

In our last section 4 we will summarize our message and emphasize the very satisfactory numerical convergence of our present large\(-N\) results.

2 The context of quantum mechanics

2.1 Special role of the small exponents \( \alpha \)

Equation (3) represents quantum system, the mathematical friendliness, probabilistic interpretation and/or physical applications of which can be different for different parameters \( \omega, \lambda \) and \( \alpha \). For example, for a rather artificial choice of negative \( \alpha = -2 \), the oscillator has to be defined, on
the half-axis of \( x \in (0, \infty) \), as exactly solvable at any \( \lambda > -1/4 \) \(^9\). In the context of physics, on the contrary, the choices of the large and positive \( \alpha = 4 \) or \( \alpha = 6 \) define the most popular anharmonic oscillators living on the whole real line of \( x \in (-\infty, \infty) \). These oscillators are important in quantum chemistry \(^{10}\) as well as in quantum field theory \(^{11}\). One of the reasons is that they remain tractable, at any sufficiently weak coupling \( \lambda > 0 \), by the standard Rayleigh-Schrödinger perturbation theory (cf. \(^{12}\), p. 80).

The main qualitative change of the shape of the potential occurs in the limit \( \alpha \to 0 \). The sharply spiked shape (and, for \( \lambda > 0 \), the double-well shape) of the potentials with negative exponents gets smeared at \( \alpha = 0 \). For the small and positive \( \alpha \) the spike becomes bounded and inessential. Ultimately, it disappears completely beyond \( \alpha = 1 \). In the vicinity of the vanishing exponent \( \alpha \) one may expect the emergence of phenomena which would depend upon the sign of \( \alpha \). The existence of such a boundary, emphasized in \(^{7}\), served as an additional motivation of our interest in Eq. (4).

2.2 Large\(−N\) expansions

The mathematical essence of large\(−N\) method (cf., e.g., its compact review in Ref. \(^{13}\) or a small sample of applications in Refs. \(^{14}\)) can be most easily explained using Eq. (3) in the impenetrable-barrier limit \( \alpha \to -2 \). Then, Schrödinger equation

\[
H(N) |\psi_n(N)\rangle = E_n(N) |\psi(N)\rangle, \quad n = 0, 1, \ldots
\]

may be considered with elementary Hamiltonian

\[
H(N) = H^{(HO)}(N) = -\frac{d^2}{dx^2} + V^{(HO)}(x), \quad V^{(HO)}(x) = x^2 + \frac{N(N + 1)}{x^2}, \quad x \in (0, \infty)
\]

and with a large and real though not necessarily integer \( N \). Our effective potential \( V^{(HO)}(x) \) then acquires a unique minimum at

\[
x_{(min)} = R = R(N) = [N(N + 1)]^{1/4} \gg 1.
\]

We may replace parameter \( N \gg 1 \) by its elementary function \(^{7}\). This simplifies the approximation of the potential near its absolute minimum,

\[
V^{(HO)}(R + \xi) = V^{(HO)}(R) + 4 \xi^2 - \frac{4}{R} \xi^3 + O(\xi^4/R^2).
\]

Any higher-precision amendments of this formula may be also considered. Up to the asymptotically vanishing corrections one obtains the low-lying spectrum of Eq. (5) + (6) in equidistant form

\[
E_n^{(HO)} = 2R^2 + 2(2n + 1) + O(1/R), \quad n = 0, 1, \ldots
\]
Within the error bars this result *precisely* coincides with the known exact formula for energy levels $E_n^{(HO)} = 4n + 2N + 3$ where $n = 0, 1, \ldots$.

For some more general potentials or Schrödinger equations (studied, e.g., in Refs. [15, 16, 17]), the essence of the success or failure of the whole approach remains the same. The potential has to develop a deep minimum at a suitable large parameter (mostly called, in the literature, $N$). Provided that symbol $R$ denotes the position of the minimum, even the inspection of our most elementary illustrative example (8) + (9) reveals that an amended, more explicative name of the technique could read $1/R$-expansion method.

### 3 Log-anharmonic oscillator in the large-$N$ approach

The potential in Eq. (4) is, at small $|x|$, dominated by an unbounded repulsive spike. In Ref. [8] we showed that such a form of the left-right symmetric barrier is soft, i.e., that it admits tunneling. We restricted attention to the small vicinity of the origin and we simulated the effects of the asymptotic confinement using a square-well potential $V_\infty(x)$. Indeed, such a simplification went partially against the spirit of our original physical motivation. For this reason we are now returning to Eq. (4) in which the *a priori* constraints imposed upon the potential at large $x$ are smoother, analytic and more natural.

#### 3.1 Non-numerical preliminaries

The overall strategy of our present study of the coexistence of the logarithmic spike with the harmonic-oscillator asymptotics of the interaction will be based on two assumptions. Firstly, we shall accept the results of the comparatively self-contained description of the system in the weak-coupling setting as given in Ref. [8]. Thus, we shall only be interested here in the strong-coupling dynamical regime in which either $\omega$ is small or $g$ is large, or both. After a transfer of interest to the strong-coupling-related phenomena we shall try to clarify the limitations imposed upon the admissible parameters by the softness of the barrier.

We will *not* assume that the applicability of the large-$N$ expansion technique is guaranteed *a priori*. In fact, whenever the central barrier admits a perceivable tunneling one *must* expect that such a method of the construction of bound states could encounter its natural limitation of validity (cf. also paragraph 3.3 below).

Our present verification and confirmation of the applicability of the large-$N$ expansion techniques to the specific double-well potential of Eq. (4) will have two components. First, we shall develop an appropriate (i.e., harmonic-oscillator, exactly solvable, leading-order) approximation of the low-lying-spectrum of the system in question. Second, a less common test of the method
will be performed. We shall verify (or, depending on the parameters, disprove) that for the low-lying set of bound states the approximate harmonic-oscillator potential is a good approximation, i.e., that its shape more or less coincides with its full-fledged exact physical predecessor near its minimum.

Although such a test seems to be based on intuitive criteria, it can also be given a more constructive form via the evaluation of higher-order corrections. We will check that in certain strong-coupling dynamical regime the tunneling through the soft logarithmic barrier is truly suppressed, indeed. We will demonstrate that for any pre-selected set of the low-lying (and, in principle, exponentially damped) wave-functions $\psi_n(x)$ their numerical size becomes negligible before the coordinate gets any close to the origin.

In the non-numerical, analytic part of our analysis the shape of our potential will be taken into account on both of the half-axes. Thus, say, at $x \in (0, \infty)$ we have

$$V(x) = \omega^2 x^2 - 2g^2 \ln x, \quad V'(x) = 2 \omega^2 x - 2g^2 / x, \quad V''(x) = 2 \omega^2 + 2g^2 / x^2, \quad \ldots$$  \hspace{1cm} (10)

We can easily localize the minimum of the potential at $x = x_{\text{min}} = R = g / \omega$, yielding

$$V(R) = \omega^2 R^2 - 2g^2 \ln R = (-2 \ln g + 1 + 2 \ln \omega) \ g^2, \quad V'(R) = 0, \quad V''(R) = 4 \omega^2, \quad \ldots$$  \hspace{1cm} (11)

Then, the strong-coupling regime may be characterized by the property $R = g / \omega \gg 1$. The harmonic-oscillator expansion (8) finds its truncated logarithmic-anharmonicity-related Taylor series analogue in formula

$$V(R + \xi) = V(R) + 2 \omega^2 \xi^2 + O(\xi^3 / R).$$  \hspace{1cm} (12)

This yields our ultimate large-$N$ alias $1/R$–expansion prediction

$$E_n = V(R) + \sqrt{2} (2n + 1) \omega + O(1/R), \quad n = 0, 1, \ldots$$  \hspace{1cm} (13)

of spectrum of the low-lying bound states.

Table 1: A sample of the low-lying energy-level shifts $\varepsilon_n = E_n - V(R)$ for potential (10). The couplings $\omega = 0.001$ and $g = 1.0$ are the same as in Fig. 1 below.

| method      | n=0      | n=1      | n=2      | n=3      |
|-------------|----------|----------|----------|----------|
| large-$N$   | 0.00141421 | 0.00424264 | 0.00707107 | 0.00989949 |
| numerical   | 0.00141432 | 0.00424309 | 0.00707218 | 0.00990161 |
| difference  | -0.00000011 | -0.00000045 | -0.00000111 | -0.00000212 |
3.2 Numerical considerations

As we already indicated, there are two criteria for the applicability of the approximate spectral formula (13). The first condition requires the smallness of $1/R$. This can be satisfied by our choice of parameters. Beyond this extreme, we could also localize the boundaries of validity of the approximations via an explicit perturbative evaluation of corrections or, alternatively, by the comparison of the approximations with the results of a suitable numerical method. Table 1 offers a small sample of such a test.

| $V(x)$ | $E_2$ | $E_1$ | $E_0$ |
|--------|-------|-------|-------|
| ±12.81 | ±12.80 | 950   | 1000  | 1050  |

Figure 1: Logarithmically anharmonic potential (10) and its almost identical large-$R$ harmonic-oscillator approximation (12) at $\omega = 1/1000$ and $g = 1$. Horizontal lines mark the first three energy levels. The picture also displays the shapes of the related wave functions.

The second condition asks for a guarantee of suppression of the tunneling. This seems to be a purely numerical check. Still, a key to such a check is analytic. It lies in the availability of the harmonic-oscillator bound states in closed form. For the ground state we have

$$\psi_0(x) \sim \exp[-\sqrt{2}\omega (x - R)^2/2].$$

From this formula we can deduce that at a numerical cut-off $\xi_{\text{max}} = R - x_{\text{min}}$ the wave function must be already negligible, i.e., we must have

$$\omega \xi_{\text{max}}^2 \gg \sqrt{2}.$$

It is sufficient to pick up any boundary of the numerically relevant vicinity of $x = R$,

$$\xi_{\text{max}} \gg \sqrt{2}/\sqrt{\omega}.$$

In addition we need that $x_{\text{min}}$ remains positive, i.e.,

$$\xi_{\text{max}} \ll R. \quad (14)$$
Putting the two constraints together we arrive at our ultimate safe-approximation constraint

\[ g \gg \sqrt{\omega}. \]

For illustration let us recall Figure 1 in which we choose \( \omega = 0.001 \) and \( g = 1 \). The picture demonstrates that the difference between the exact and approximate potentials is really small, more or less comparable with the thickness of the drawing lines. Secondly, with \( R = g/\omega = 10^3 \), the three lowest-lying (viz., \( n = 0, n = 1 \) and \( n = 2 \)) bound-state wave functions can be considered practically vanishing at our tentative choice of boundaries \( \xi_{max} = 85 \), i.e., already perceivably below our generic estimate (14).

Let us add that just the logarithmic corrections will enter a not too different asymptotic estimate

\[
\psi_n(x) \sim \exp\left[-\sqrt{2} \omega \frac{(x-R)^2}{2} + \mathcal{O}(\ln |x-R|)\right], \quad |x-R| \gg 1/\sqrt{\omega}
\]

valid for the first few excited states. Fig. 1 indicates that the growth of the excitation quantum number \( n \) should be accompanied, in practical calculations, also by a certain not too quick growth of the safe-estimate value of \( \xi_{max} = \xi_{max}(n) \).

### 3.3 Consequences

Our preceding considerations have shown that in the strong-coupling regime with \( R \gg 1 \) and for the low-lying states of our log-anharmonic oscillator with the first few quantum numbers \( n = 0, 1, \ldots \) the tunneling between the left and right half-axes of \( x \) in Eq. (4) is suppressed because the wave functions are very well approximated by their harmonic-oscillator approximants. These approximants are all exponentially small long before the coordinate \( x \) gets any close to the origin at \( x = 0 \), i.e., they are exponentially small in the displacement variable \( \xi^2 = \mathcal{O}(R^2) \) (cf. Fig. 1). The low-lying spectrum of energies remains almost exactly doubly degenerate.

In other words, the experimental detection of the effect of the tunneling would only be possible for the highly excited states or for the much smaller values of the ratio of couplings \( R = g/\omega \). In particular, the decrease of \( R \) would imply the necessity of the study and incorporation of the higher-order terms in the large\( - N \) expansions. Strictly speaking, the technique ceases to be comfortable and/or sufficiently efficient. Still, the non-numerical nature of the leading-order harmonic-oscillator large\( - N \) approximants preserves its appeal, in spite of the expected necessity of the inclusion of the higher-order corrections.

The emergence of such a scenario is illustrated in Figs. 2 and 3. Non-numerically, the onset of such a necessity may be characterized by the decrease of the \( x = 0 \) intersection of the two
Figure 2: The emergence of undesirable overlaps of the two harmonic-oscillator potentials (12) (thin curves), i.e., a threat of the failure of the large–$N$ approach for the double well potential (10) (thick curve) at the insufficiently large $R = 1$ for $\omega = 1$ and $g = 1$.

Figure 3: The emergence of the significant overlaps of the left and right harmonic-oscillator wave functions at $\omega = 1$, $g = 1$ and $R = 1$ for $n = 0$, $n = 1$ and $n = 3$ indicates that the degeneracy of the leading-order horizontal-line energy levels will break down due to the tunneling. (viz., left and right) auxiliary potentials (12) at the height which becomes comparable with the estimated bound-state energy (viz., close to $E_0$ in Fig. 2).

In the small–$R$ dynamical regime of Fig. 2 one encounters the tunneling effect, i.e., an increase of the overlaps between the left and right approximate wave functions (cf. Fig. 3). Their even- and odd-parity linear combinations will become perceivably different, so that the double degeneracy of the spectrum will be lost. Still, the split will remain small in the ground state which feels the thickness of the infinitely high central barrier.

A decisive loss of the applicability of the large–$N$ method may be now illustrated by Fig. 4 in which $R = 1/10$ is really small. The analytic large–$N$ estimates will fail, for several reasons. Firstly, the infinitely high central barrier will become so thin (in fact, invisible in Fig. 4) that the
The double-well structure of the full potential is hardly felt by its wave functions, exact or approximate. This observation reflects the “soft” nature of the central logarithmic spike.

The availability of the approximate energies enables us to see that the higher excitations will only “feel” the logarithmic singularity perceptibly less than their lower-lying predecessors. Thus, the even-odd-parity degeneracy becomes almost completely removed.

The superpositions of the higher-order $O(1/R)$ corrections cease to be negligible and seem to act in the single direction. Indeed, in Fig. 4 we clearly see that the left and right harmonic-oscillator wells prove rather narrow so that the large−$N$ approximation now obviously overestimates the low-lying energy spectrum in systematic manner.

4 Concluding remarks

Asymptotically confining components $V_\infty(x)$ of phenomenological potentials are often combined with a short-range repulsive and impenetrable barrier, say, $V_0(x) = N(N + 1)/x^2$. The large−$N$ expansion techniques are then known to work because the barrier does not admit any tunneling. A softened, logarithmic central repulsion $V_0(x) = -N(N + 1) \ln |x|$ has been considered here, therefore, as a new and challenging model in which the tunneling is allowed.

In the context of mathematics we demonstrated that, in principle, the applicability of the large−$N$ method can survive in multiple applications of such a type. Their specific feature has been found in the fact that the precision of the approximation may become sensitive to the choice of the asymptotic interaction component $V_\infty(x)$ in practice. This observation is closely correlated with the underlying motivations in phenomenology. In our preceding paper [8], for example, we were interested in the similar picture of physics along the lines of considerations inspired, e.g., by
We studied there a closely related logarithmic-interaction model which was, incidentally, non-analytic and, hence, unsuitable for the large−N mathematical study. Thus, in our present paper we turned attention to an amended, fully analytic phenomenological model.

The impact of our results upon the understanding of Schrödinger equations with logarithmic singularities might be further enhanced, in the future, via a replacement of our present logarithmic interaction term $\sim \ln x$ by its almost equally elementary power-law-screening modifications $\sim x^{\text{const}} \ln x$ and/or by the more-term superpositions. All of these models will share most of the technical merits of the elementary $V \sim \ln x$. Typically, the next-to-trivial one-parametric potential $V_c(x) = x^2(\ln x - c)$ will possess the easily-derived Taylor-series representation near its closed-form double-well minima at $\pm R$ with $R = \exp(c - 1/2)$. Thus, one can conjecture that the present systematic large-$N$ approximation technique becomes applicable, without essential changes, whenever the relevant quantity $R$ appears sufficiently large.

The smooth nature of our present, most elementary log-anharmonic model gave us a decisive methodical advantage due to its non-numerical large−$N$ tractability. This observation is to be read as the main message delivered by our present paper. It is necessary to add that the main mathematical part of the task is to be seen in the details. For example, in the light of the definition of $g^2 = -\lambda \alpha / 2$ we imagined that the assumption of a simultaneous smallness of $\alpha$ and $g^2$ would imply that one stays in the small-perturbation regime of our preceding paper [8] whenever the range of $\lambda$ remains bounded.

We turned attention to the genuine strong-coupling dynamical regime where $\lambda \gg 1$ is large. Naturally, this reopened the questions of convergence as well as of an appropriate account of the higher-order corrections in $\alpha$. Indeed, whenever the exponent $\alpha$ of the general power-law anharmonicity in Eq. (3) ceases to be small, one must take into consideration also the influence of the originally neglected terms in Taylor series (2). Fortunately, the task is not prohibitively difficult. The incorporation of the corrections merely leads to a replacement of our most elementary Schrödinger Eq. (4) by its appropriately generalized forms.

For illustration one can consider the single-anharmonicity problem

$$\left[ -\frac{d^2}{dx^2} + \omega^2 x^2 - 2g^2 (\ln |x|)^p \right] \psi_n(x) = E_n \psi_n(x), \quad x \in (-\infty, \infty), \quad n = 0, 1, \ldots$$

containing a new, variable integer $p = 1, 2, \ldots$. One finds that the overall principles of the implementation of the large−$N$ method at $x > 0$ remain unchanged. The $p \neq 1$ update of Eq. (10) reads

$$V(x) = \omega^2 x^2 - 2g^2 (\ln x)^p, \quad V'(x) = 2\omega^2 x - 2pg^2 (\ln x)^{p-1}/x,$$

$$V''(x) = 2\omega^2 - 2p(p-1)g^2 (\ln x)^{p-2}/x^2 + 2pg^2 (\ln x)^{p-1}/x^2, \ldots.$$
Its form implies that the decisive technical step of the localization of the position of the absolute minimum of the potential at $x = R$ remains unchanged. Using relation $V'(R) = 0$ we get

$$R^2 = \frac{pg^2}{\omega^2} (\ln R)^{p-1}. \quad (17)$$

Whenever $p \neq 1$, this is an implicit and, in general, ambiguous definition. Still, once we restrict attention to the quantum systems with a sufficiently large ratio between coupling constants $g/\omega$ we only have to pick up the maximal root $R$. This yields, as before, the absolute minimum of the potential in the strong-coupling dynamical regime (let us leave the necessary lengthy but straightforward discussion to interested readers).

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