Unified Treatment of Even and Odd Anharmonic Oscillators of Arbitrary Degree

Ulrich D. Jentschura,[1,2,*] Andrey Surzhykov,[2,3] and Jean Zinn-Justin[4]

[1]*Department of Physics, Missouri University of Science and Technology, Rolla Missouri 65409-0640, USA*

[2]*Max-Planck-Institut für Kernphysik, Postfach 103980, 69029 Heidelberg, Germany*

[3]*Physikalisches Institut der Universität, Philosophenweg 12, 69120 Heidelberg, Germany*

[4]*CEA, IRFU, and Institut de Physique Théorique, Centre de Saclay, 91191 Gif-Sur-Yvette, France*

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We present a unified treatment, including higher-order corrections, of anharmonic oscillators of arbitrary even and odd degree. Our approach is based on a dispersion relation which takes advantage of the $\mathcal{PT}$ symmetry of odd potentials for imaginary coupling parameter, and of generalized quantization conditions which take into account instanton contributions. We find a number of explicit new results, including the general behavior of large-order perturbation theory for arbitrary levels of odd anharmonic oscillators, and subleading corrections to the decay width of excited states for odd potentials, which are numerically significant.

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Introduction.—One-dimensional anharmonic oscillators are quite basic. Because of their enormous phenomenological significance, they occupy a unique position within quantum theory [1–5]. They are treated at various levels of sophistication in nearly every textbook on quantum mechanics. Here, we use the Hamiltonians of even oscillators in the convention

$$H_N(g) = -\frac{1}{2}\partial_q^2 + \frac{1}{2}q^2 + g q^N, \qquad (N \text{ even}), \qquad (1)$$

and odd oscillators as follows,

$$h_M(g) = -\frac{1}{2}\partial_q^2 + \frac{1}{2}q^2 + \sqrt{g} q^M. \qquad (M \text{ odd}). \qquad (2)$$

For $g < 0$, the potential of an even oscillator has a double-hump structure, and it is intuitively clear that the particle can tunnel through the barrier(s). This is manifest in the energy levels because they develop a nonvanishing imaginary part as we vary the coupling from positive g to negative g in the complex plane. The smaller we choose the modulus of g, the bigger the humps, the longer the tunneling time of the particular, and the smaller is the decay width of the state (i.e., the smaller is the modulus of the imaginary part of the resonance energy). The resonance energies are manifestly complex, and their imaginary parts also involve nonanalytic exponentials.

Given the large amount of work already invested by the physics community into the study of anharmonic oscillators, it is perhaps surprising that two very basic questions regarding the above mentioned anharmonic oscillators have not yet been fully addressed in the literature: (i) What are the higher-order corrections to the nonperturbative behavior of the resonance energies, and how are the real and the imaginary part of the resonance energy described by a (possibly) nonanalytic, generalized expansion in g? Which mathematical structures (exponentials, logarithms, ...) form part of such an expansion? (ii) What is the general large-order behavior of perturbation theory for an arbitrary energy levels of an odd oscillator of arbitrary degree?

Indeed, to answer the above questions, we rely in part on the work of Bender and Wu who, in 1971 (see Ref. [2]), solved question (ii) for even anharmonic oscillators, and on the concept of $\mathcal{PT}$ symmetry [6–9] for the formulation of a dispersion relation for the resonance energies of odd oscillators. Another essential ingredient of our analysis is generalized quantization conditions which allow us to describe instanton contributions and which go beyond the ordinary Bohr-Sommerfeld formalism.

Instanton actions.—We consider even anharmonic oscillators of degree N in the convention (1) with energy eigenvalues $E_n^{(N)}(g)$, and odd Hamiltonians in the convention (2) with complex resonance energies are $\epsilon_n^{(M)}(g)$. Formulating the problem of the determination of energy levels in terms of a Euclidean path integral [10], it becomes clear that instanton configurations should be analyzed, and we start with the case of even oscillators. Here, the instanton configuration exists for negative g, and we thus scale $q(t) = (-g)^{-1/(N-2)}\xi(t)$. The Euclidean action reads

$$S[\xi] = (-g)^{-(2/N-2)} \int dt \left(\frac{1}{2}\dot{\xi}^2 + \frac{1}{2}\xi^2 - \xi^N\right). \qquad (3)$$

The instanton configurations are (N even)

$$q_{\rm cl}^{\pm}(t) = \pm(-g)^{-(2/N-2)}\{1 + \cosh[(N-2)(t-t_0)]\}^{-(1/N-2)}. \qquad (4)$$

Here, t_0 is a collective coordinate. For odd anharmonic oscillators, we transform $q(t) = -g^{-1/(2M-4)}\chi(t)$ and obtain the Euclidean action (M odd)

$$S'[\chi] = g^{-(1/M-2)} \int dt \left(\frac{1}{2}\dot{\chi}^2 + \frac{1}{2}\chi^2 - \chi^M\right). \qquad (5)$$

The instanton $q(t) = q_{\rm cl}(t)$ is unique because the potential has lost the invariance under parity (see Fig. 1),

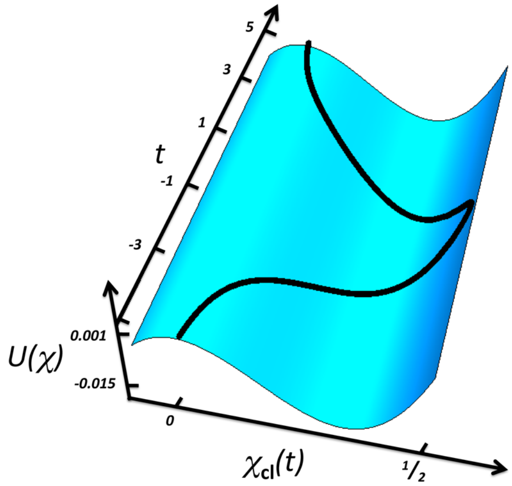

FIG. 1 (color online). Instanton configuration for the cubic potential. The plot shows the instanton worldline $\chi_{\rm cl}(t) = [\cosh(t) + 1]^{-1}$ immersed in the scaled potential $U(\chi) = \chi^3 - \frac{1}{2}\chi^2$.

$$q_{\rm cl}(t) = g^{-(1/M-2)}\{1 + \cosh[(M-2)(t-t_0)]\}^{-(1/M-2)}. \tag{6}$$

Inserting the solutions $q_{\rm cl}^{\pm}(t)$ and $q_{\rm cl}(t)$ into Eqs. (3) and (5), we obtain the classical Euclidean instanton actions

$$S[q_{\rm cl}^{\pm}] = (-g)^{-(2/N-2)}\mathcal{A}(N),$$
$$S'[q_{\rm cl}] = g^{-(1/M-2)}\mathcal{A}(M), \tag{7a}$$
$$\mathcal{A}(m) = 2^{2/(m-2)}B\left(\frac{m}{m-2}, \frac{m}{m-2}\right), \tag{7b}$$

where $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the Euler Beta function.

Dispersion relations.—An evaluation of the quantum fluctuations about the instanton configurations according to Ref. [10] reveals that the imaginary part of the nth resonance energy $E_n^{(N)}(g)$, for potentials of even order N, is given by [in leading order, corrections are of relative order $g^{2/(N-2)}$]

$$\mathrm{Im}\,E_n(N, g<0) = -\frac{1}{n!\sqrt{2\pi}}\left(-\frac{2\mathcal{C}(N)}{(-g)^{2/(N-2)}}\right)^{n+1/2} \times \exp[-(-g)^{-2/(N-2)}\mathcal{A}(N)], \tag{8}$$

with $\mathcal{C}(m) = 2^{2/(m-2)}$. For odd potentials in the normalization given by Eq. (2) and for positive coupling, ignoring corrections of relative order $g^{1/(M-2)}$,

$$\mathrm{Im}\,\epsilon_n^{(M)}(g>0) = -\frac{1}{2n!\sqrt{2\pi}}\left(\frac{2\mathcal{C}(M)}{g^{1/(M-2)}}\right)^{n+1/2} \times \exp[-g^{-1/(M-2)}\mathcal{A}(M)]. \tag{9}$$

The subtracted dispersion relation [2,3,11] for the energies $E_n(N, g)$ of the even anharmonic oscillators of degree N is

$$E_n^{(N)}(g) = n + \frac{1}{2} - \frac{g}{\pi}\int_{-\infty}^{0} ds\,\frac{\mathrm{Im}E_n^{(N)}(s+i0)}{s(s-g)}. \tag{10}$$

Using the formula (8) and the dispersion relation (10), one may calculate [2] the large-order perturbative expansion for the ground-state energy of the nth level of an anharmonic oscillator of order N, where we use the perturbative coefficients in the form $E_n^{(N)}(g) \sim \sum_K E_{n,K}^{(N)} g^K$. For an arbitrary level of an even oscillator of arbitrary degree, we thus rederive [2]

$$E_{n,K}^{(N)} \sim \frac{(-1)^{K+1}(N-2)}{\pi^{3/2}n!2^{K+1-n}}\Gamma\left(\frac{N-2}{2}K + n + \frac{1}{2}\right) \times \left[B\left(\frac{N}{N-2}, \frac{N}{N-2}\right)\right]^{-(N-2/2)K-n-(1/2)}, \tag{11}$$

which is valid up to corrections of relative order K^{-1}. For odd Hamiltonians $h_M(g)$ which involve a perturbation of the form $\sqrt{g}q^M$, we have only one branch cut in the energy [7]. The $\mathcal{PT}$ symmetry for purely imaginary coupling leads to the following dispersion relation [7,12],

$$\epsilon_n^{(M)}(g) = n + \frac{1}{2} + \frac{g}{\pi}\int_0^{\infty} ds\,\frac{\mathrm{Im}\epsilon_n^{(M)}(s+i0)}{s(s-g)}. \tag{12}$$

Based on the dispersion relation (12) and on the general result for the imaginary part of the resonance energy for an odd anharmonic oscillator given in Eq. (9), we are now in the position to write down the large-order behavior of the perturbative coefficients of an arbitrary level of an odd anharmonic oscillator of arbitrary degree. Specifically, for a resonance $\epsilon_n^{(M)}(g) \sim \sum_K \epsilon_{n,K}^{(M)} g^K$, we find ($M$ odd, $M \geq 3$)

$$\epsilon_{n,K}^{(M)} \sim \frac{2-M}{\pi^{3/2}n!2^{2K+1-n}}\Gamma\left((M-2)K + n + \frac{1}{2}\right) \times \left[B\left(\frac{M}{M-2}, \frac{M}{M-2}\right)\right]^{-(M-2)K-n-(1/2)}. \tag{13}$$

Subleading corrections.—In order to go beyond the leading-order results, further considerations are needed. While details of the derivation will be presented in [13], we would like to give here the essential ingredients of our formalism. First of all, we scale the coordinate in the Hamiltonians (1) and (2) as $q \to g^{-(2[[m/2]]-m+2/m-2)}q$, where $[[X]]$ is the integer part of X (m stands for a general integer). We then transform the Schrödinger to the Riccati equation by setting $\varphi'(q)/\varphi(q) = -S(q)g^{-(2[[m/2]]-m+2/m-2)}$, and we denote by $S_+(q)$ the component of $S(q)$ which is even under the operation $(g, E) \to (-g, -E)$. For S_+, we calculate the Wentzel-Kramers-Brioullin (WKB) expansion for $S(q)$ for given g and energy E, using the algorithm described for a general potential in Sec. of Ref. [14], by expanding the solution in fractional powers of g while keeping the quantity $g^{(2[[m/2]]-m+2/m-2)}E$ fixed. A recursive procedure for the construction of the WKB expansion of $S_+(z, g, E)$ has been outlined in Eqs. (3.40)–(3.42) of Ref. [14]. We then integrate the WKB expansion of the function $S_+(q)$ around its cuts using an approach based on Mellin transforms as outlined in Appendix F.3 of Ref. [15] for general potentials (the integration contour $\mathcal{C}'$ around the cuts is chosen in accordance with Eq. (3.52) of Ref. [14]) and conjecture the following form for the result of the contour integral,

$$g^{-(2[[m/2]]-m+2/m-2)} \oint_{C'} dz \mathcal{S}_+(q) = A_m(E,g) + \ln(2\pi) - \ln\Gamma\left(\frac{1}{2} - B_m(E,g)\right) + B_m(E,g)\ln\left(-\frac{g}{2\mathcal{C}(m)}\right). \quad (14)$$

From the right-hand side, under a suitable separation of real and imaginary parts, one can directly read off the two functions $B_m(E,g)$ and $A_m(E,g)$, which we refer to as the "perturbative function" and the "instanton function," respectively. We here indicate for completeness the first few terms of $B_m(E,g)$ for the oscillators with $M = 3$, 7 and $N = 4$, 6,

$$B_3(E,g) = E + g\left(\frac{7}{16} + \frac{15}{4}E^2\right) + \mathcal{O}(g^2), \quad (15a)$$

$$B_4(E,g) = E - g\left(\frac{3}{8} + \frac{3}{2}E^2\right) + \mathcal{O}(g^2), \quad (15b)$$

$$B_6(E,g) = E - g\left(\frac{25}{8}E + \frac{5}{2}E^3\right) + \mathcal{O}(g^2), \quad (15c)$$

$$B_7(E,g) = E + g\left(\frac{180675}{2048} + \frac{444381}{512}E^2 + \frac{82005}{128}E^4 + \frac{3003}{32}E^6\right) + \mathcal{O}(g^2). \quad (15d)$$

The leading term of the A functions contains the instanton action as given in Eq. (7): $A_N(E,g) = \mathcal{A}(N) \times (-g)^{-2/(N-2)} + \mathcal{O}(g^{2/(N-2)})$ for even potentials and $A_M(E,g) = \mathcal{A}(M) g^{-1/(M-2)} + \mathcal{O}(g^{1/(M-2)})$ for odd potentials, respectively. Higher-order terms read

$$A_3(E,g) = \frac{2}{15g} + g\left(\frac{77}{32} + \frac{141}{8}E^2\right) + \mathcal{O}(g^2), \quad (16a)$$

$$A_4(E,g) = -\frac{1}{3g} - g\left(\frac{67}{48} + \frac{17}{4}E^2\right) + \mathcal{O}(g^2), \quad (16b)$$

$$A_6(E,g) = \frac{\pi}{2^{5/2}(-g)^{1/2}} - g\left(\frac{221}{24}E + \frac{17}{3}E^3\right) + g^2\left(\frac{2504899}{7680}E + \frac{45769}{96}E^3 + \frac{17527}{160}E^5\right) + \mathcal{O}(g^3), \quad (16c)$$

$$A_7(E,g) = \frac{5^{1/4}\Gamma(\frac{1}{5})\Gamma(\frac{2}{5})}{2^{3/5}9\pi\sqrt{\phi}g^{1/5}} + g^{1/5}\frac{5^{1/4}\Gamma^2(\frac{3}{5})\Gamma(\frac{4}{5})}{2^{7/5}\pi\sqrt{\phi}}\left(\frac{5}{8} + \frac{9}{10}E^2\right) + \mathcal{O}(g^{2/5}). \quad (16d)$$

The function $A_7(E,g)$ involves the square root of the golden ratio $\phi = (\sqrt{5}+1)/2$. The result for the sextic oscillator ($N = 6$) is at variance with expectation because one would have assumed the presence of a term of order $g^{2/(N-2)} = g^{1/2}$, but it cancels, accidentally.

In terms of the A and B functions, we can now write down our conjectures for the generalized quantization conditions. For the "stable" cases (odd oscillator, imaginary coupling and even oscillator, positive coupling), we simply conjecture them to read (we indicate two equivalent forms)

$$1\Big/\Gamma\left[\frac{1}{2} - B_m(E,g)\right] = 0, \qquad B_m(E,g) = n + \frac{1}{2}, \quad (17)$$

where m can be even or odd. This form of the condition generalizes the result $1/\Gamma(\frac{1}{2} - E) = \det(H - E) = 0$ for the Fredholm determinant of the harmonic oscillator Hamiltonian H. In the presence of instanton configurations, the resonance energy is slightly displaced from the energy that would otherwise lead to a pole of the Γ function according to Eq. (17). The displacement of E is by a nonperturbative correction which can be evaluated exactly in leading order [see Eqs. (8) and (9)]; this means that the zero on the right-hand side of $1/\Gamma[\frac{1}{2} - B_m(E,g)] = 0$ has to be replaced by the nonperturbatively small imaginary part of the resonance energy. A comparison of the resulting equation to the leading terms of the functions $A_m(E,g)$ and $B_m(E,g)$ which emerge from the evaluation of the contour integral of the WKB expansion (14) then, in turn, naturally leads to the following conjectures for even potentials ($g < 0$) and odd potentials ($g > 0$), respectively,

$$\frac{\Gamma[\frac{1}{2} - B_N(E,g)]}{\sqrt{2\pi}e^{A_N(E,g)}}\left(-\frac{2\mathcal{C}(N)}{(-g)^{(2/N-2)}}\right)^{B_N(E,g)} = 1, \quad (18a)$$

$$\frac{\Gamma[\frac{1}{2} - B_M(E,g)]}{\sqrt{8\pi}e^{A_M(E,g)}}\left(\frac{2\mathcal{C}(M)}{g^{(1/M-2)}}\right)^{B_M(E,g)} = 1. \quad (18b)$$

In order to solve the perturbative quantization condition (17), we enter with an ansatz $E = E_0 + gE_1 + g^2E_2 + \ldots$ and compare coefficients in each order in g. In order to solve (18), our ansatz also has involved nonanalytic terms as implied by the instanton contributions, and we then expand systematically in powers of g and simultaneously in powers of the nonanalytic factor $\exp(-A/|g|^p)$ (with A and p suitably chosen). This ansatz naturally leads to the triple expansions [with constant coefficients $\Xi^{(m,n)}_{J,L,K}$ and $L_{\max} \equiv \max(0, J-1)$],

$$E^{(N)}_n(g<0) = \sum_{J=0}^{\infty}\left[\left(\frac{2\mathcal{C}(N)}{(-g)^{2/(N-2)}}\right)^{n+(1/2)}\frac{i\exp(-\frac{\mathcal{A}(N)}{(-g)^{2/(N-2)}})}{n!\sqrt{2\pi}}\right]^J \times \sum_{L=0}^{L_{\max}}\ln^L\left(-\frac{2\mathcal{C}(N)}{(-g)^{2/(N-2)}}\right) \times \sum_{K=0}^{\infty}\Xi^{(N,n)}_{J,L,K}(-g)^{2K/(N-2)}, \quad (19a)$$

$$\epsilon^{(M)}_n(g>0) = \sum_{J=0}^{\infty}\left[\left(\frac{2\mathcal{C}(M)}{g^{1/(M-2)}}\right)^{n+(1/2)}\frac{i\exp(-\frac{\mathcal{A}(M)}{g^{1/(M-2)}})}{n!\sqrt{8\pi}}\right]^J \times \sum_{L=0}^{L_{\max}}\ln^L\left(-\frac{2\mathcal{C}(M)}{g^{1/(M-2)}}\right)\sum_{K=0}^{\infty}\Xi^{(M,n)}_{J,L,K}g^{K/(M-2)}. \quad (19b)$$

The above triple expansion is involved and in need of an interpretation [we concentrate on the "even case" (19a)]. The term with $J = 0$ recovers the basic, perturbative expansion which has only integer powers in g. Therefore, $\Xi^{(N,n)}_{0,0,K(N-2)/2} = (-1)^K E^{(N)}_{n,K}$. The term with $J = 1$ recovers the leading contribution in the expansion in powers of $\exp[-\mathcal{A}(N)/(-g)^{2/(N-2)}]$ to the imaginary part of the resonance energy, but including perturbative corrections which can be expressed in terms of a fractional power series in g multiplying the nonanalytic exponential. The first few terms of this series are given below for the first excited state of the cubic potential. The term with $J = 2$ involves a logarithm of the form $\ln(-\frac{2\mathcal{C}(N)}{(-g)^{2/(N-2)}})$. The explicit imaginary parts of the logarithms cancel against the imaginary parts of Borel sums carried out in complex directions [16] of perturbation series that occur in lower-order (in J) contributions. Indeed, the Laplace-Borel integrations have to be carried out in a manner consistent with the analytic continuation of the logarithms [15,17].

The above formulas allow, in principle, the determination of corrections of arbitrary order to the resonance energies of oscillators of arbitrary degree. Our first example concerns the corrections to the excited-state energy of the cubic,

$$\mathrm{Im}\,\epsilon^{(3)}_1(g) = -\frac{8e^{-2/(15g)}}{\sqrt{\pi}g^{3/2}}\left\{1 - \frac{853}{16}g + \frac{33349}{512}g^2 + \ldots\right\}, \tag{20}$$

which have numerically large coefficients. The second result concerns the correction to the large-order growth of the perturbative coefficients for the ground state of the seventh-degree potential,

$$\epsilon^{(7)}_{0,K} = -\frac{5\Gamma(5K+\frac{1}{2})}{2^{2K+1}\pi^{3/2}}\left(\frac{18\pi\sqrt{\phi}}{5^{1/4}\Gamma(\frac{1}{5})\Gamma^2(\frac{2}{5})}\right)^{5K+1/2} \times\left\{1 - \frac{2^{1/2}17\pi}{5^{1/4}\phi^{3/2}450K} + \ldots\right\}. \tag{21}$$

Note that the absence of the $g^{1/2}$ correction from the result (16c) implies the peculiar absence of a $1/K$ correction to the leading factorial growth of perturbative coefficients for the sixth-degree potential.

Conclusions.—The general nonanalytic expansions (19) for the resonance energies of even and odd oscillators are triple expansions in terms of nonanalytic exponentials, logarithmic factors, and fractional power series. They follow from the generalized quantization conditions (18a) and (18b). The general leading-order behavior of perturbation theory for arbitrary levels of odd oscillators is given in Eq. (13). These results allow us to describe the widths of arbitrary resonances accurately by higher-order analytic formulas. E.g., the first two corrections terms given in (20) are indispensable for obtaining satisfactory agreement of the analytic formula for the first excited cubic resonance energy with numerical calculations, even at small $g \approx 0.01$.

In a wider context, the following applications of our results can be envisaged: in field theory (large-order estimates), the perturbations about the instanton configurations have usually been neglected in the calculation of n-point functions which enter the renormalization-group equations; our results indicate that numerically large corrections may enter already on the level of model calculations, and it may thus be worthwhile to revisit the subject. Our analysis may also be helpful for the analytic description of resonances in quantum dot potentials which approximate the cubic anharmonic oscillator and are important for quantum computing; from our analysis, it is obvious that in a general potential, allowance should be made for higher-order correction terms in the description of the width {a functional form $\exp(-A/|g|^p)[1 + Bg + Cg^2 + \ldots]$ with nonvanishing B and C seems to be indispensable}. From a more fundamental point of view, we can say that in potentials which allow for tunneling of the particle, our analysis suggests that the familiar Bohr-Sommerfeld-Wilson quantization condition $\oint p dq = 2\pi n\hbar$ still holds, but only if we assume a rather complicated analytic form for the left-hand side of this quantization condition [see Eq. (14)].

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*ulj@mst.edu

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