



HAL
open science

Calculation of the characteristic functions of anharmonic oscillators

Ulrich D. Jentschura, Jean Zinn-Justin

► **To cite this version:**

Ulrich D. Jentschura, Jean Zinn-Justin. Calculation of the characteristic functions of anharmonic oscillators. *Applied Numerical Mathematics*, 2010, 60 (12), pp.1332-1341. 10.1016/j.apnum.2010.03.015 . cea-02895309

HAL Id: cea-02895309

<https://cea.hal.science/cea-02895309>

Submitted on 9 Jul 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Calculation of the Characteristic Functions of Anharmonic Oscillators

Ulrich D. Jentschura

*Department of Physics, Missouri University of Science and Technology
Rolla, Missouri, MO65409, USA*

Jean Zinn-Justin

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

Abstract The energy levels of quantum systems are determined by quantization conditions. For one-dimensional anharmonic oscillators, one can transform the Schrödinger equation into a Riccati form, i.e., in terms of the logarithmic derivative of the wave function. A perturbative expansion of the logarithmic derivative of the wave function can easily be obtained. The Bohr–Sommerfeld quantization condition can be expressed in terms of a contour integral around the poles of the logarithmic derivative. Its functional form is $B_m(E, g) = n + \frac{1}{2}$, where B is a characteristic function of the anharmonic oscillator of degree m , E is the resonance energy, and g is the coupling constant. A recursive scheme can be devised which facilitates the evaluation of higher-order Wentzel–Kramers–Brillouin (WKB) approximants. The WKB expansion of the logarithmic derivative of the wave function has a cut in the tunneling region. The contour integral about the tunneling region yields the instanton action plus corrections, summarized in a second characteristic function $A_m(E, g)$. The evaluation of $A_m(E, g)$ by the method of asymptotic matching is discussed for the case of the cubic oscillator of degree $m = 3$.

MSC numbers 34E20, 81Q20, 81S99

Keywords Singular perturbations, turning point theory, WKB methods;
Semiclassical techniques including WKB and Maslov methods;
General quantum mechanics and problems of quantization

1 Introduction

The cubic anharmonic oscillator, defined by the Hamiltonian,

$$h_3(g) = -\frac{1}{2} \frac{\partial^2}{\partial q^2} + \frac{1}{2} q^2 + \sqrt{g} q^3, \quad (1)$$

is a paradigmatic example of a quantum mechanical problem which gives rise to complex resonance energies. A particle initially trapped in the region $q \approx 0$ may tunnel through the classically forbidden well and escape toward $q \rightarrow -\infty$. For positive coupling $g > 0$, the energies can be determined numerically by the method of complex scaling[2, 24]. One scales the coordinate as $q \rightarrow q e^{i\theta}$ for the cubic oscillator, which results in the Hamiltonian

$$H_c(\theta) = e^{-2i\theta} \left(-\frac{1}{2} \frac{\partial^2}{\partial q^2} + \frac{1}{2} q^2 e^{4i\theta} + \sqrt{g} q^3 e^{5i\theta} \right). \quad (2)$$

If one diagonalizes this complex operator in the basis of harmonic oscillator wavefunctions $\{\phi_n(g)\}_{n=0}^{N_{\max}}$, for large enough N_{\max} , one can numerically determine the (complex) resonance energies of the original cubic Hamiltonian (1). As discussed in Refs. [1, 24], these resonance energies are independent of θ , provided we choose θ sufficiently large so that the rotated branch passes the position of the resonance under investigation. The numerical variation of the resonance energies of the cubic oscillator,

$$\epsilon_n^{(3)}(g) = \text{Re} \left(\epsilon_n^{(3)}(g) \right) + i \text{Im} \left(\epsilon_n^{(3)}(g) \right), \quad (3)$$

as a function of g under a suitable increase of N_{\max} can be used to estimate the numerical uncertainty of the numerical results for the complex resonance energies [16]. Throughout this article, we keep the superscript “3” of the resonance energy $\epsilon_n^{(3)}(g)$ of the cubic oscillator in order to remain consistent with the notation of a brief Letter (see Ref. [18]), in which part of the results presented here have already been indicated.

For reasons which will be explained below, we associate the resonance energy (with a negative imaginary part) with a value of the coupling parameter g that has an infinitesimal positive imaginary part, whereas a coupling with an infinitesimal negative imaginary part is associated with an antiresonance, that has a positive imaginary part. The resonance energies of the cubic potential as a function of g have a branch cut along the positive real axis, and fulfill the dispersion relation [3, 5],

$$\epsilon_n^{(M)}(g) = n + \frac{1}{2} + \frac{g}{\pi} \int_0^\infty ds \frac{\text{Im} \epsilon_n^{(M)}(s + i0)}{s(s-g)}. \quad (4)$$

We note that the spectrum of resonances is invariant under the transformation $\sqrt{g} \rightarrow -\sqrt{g}$ in Eq. (1), which can be compensated by a parity transformation $q \rightarrow -q$ (the latter leaves the spectrum manifestly invariant).

For weak positive coupling $g = |g| \rightarrow 0$ (with $\text{Im} g > 0$), the imaginary part of the resonance energies is determined by a nonanalytic factor, which reads [16]

$$\text{Im} \epsilon_0^{(3)}(g + i0) \sim -\frac{2^{3n}}{n! \sqrt{\pi}} g^{-n-1/2} \exp\left(-\frac{2}{15g}\right) \quad \text{for} \quad g = |g| \rightarrow 0, \quad \text{Im} g > 0. \quad (5)$$

For large positive coupling $g = |g| \rightarrow \infty + i0$, the first three resonance energies possess the following asymptotics [see Eq. (17) and Table II of Ref. [16]],

$$\begin{aligned} \epsilon_0^{(3)}(g + i0) &\sim g^{1/5} (0.617\ 160\ 050 - i0.448\ 393\ 023) & \text{for} \quad g = |g| \rightarrow \infty + i0, \\ \epsilon_1^{(3)}(g + i0) &\sim g^{1/5} (2.193\ 309\ 731 - i1.593\ 532\ 797) & \text{for} \quad g = |g| \rightarrow \infty + i0, \\ \epsilon_2^{(3)}(g + i0) &\sim g^{1/5} (4.036\ 380\ 020 - i2.932\ 601\ 744) & \text{for} \quad g = |g| \rightarrow \infty + i0. \end{aligned} \quad (6)$$

All of the above results have a complex argument of $-\pi/5$, as they should. For intermediate g , a large number of resonance energies can be determined numerically by a suitable basis-set method and be used in order to construct a complex-scaled time propagation algorithm for a quantum mechanical wave packet (see Sec. III of Ref. [16]).

A second available method for the calculation of resonance energies consists in the resummation of the divergent perturbation theory in complex directions of the parameters. The perturbative coefficients $\epsilon_{n,K}^{(3)}$ in the perturbation series

$$\epsilon_n^{(3)}(g) \sim \sum_{K=0}^{\infty} \epsilon_{n,K}^{(3)} g^K, \quad g \rightarrow 0, \quad (7)$$

which describe the n th resonance energy of the cubic oscillator, diverge factorially for large perturbation theory order K . Indeed, for large K , the leading asymptotics read (see, e.g., Ref. [18]),

$$\epsilon_{n,K}^{(3)} \sim -\frac{2^{2n-1/2-K} 15^{n+K+1/2}}{\pi^{3/2} n!} \Gamma\left(n + K + \frac{1}{2}\right), \quad K \rightarrow \infty. \quad (8)$$

With the exception of the coefficient of order zero, which reads $\epsilon_{n,0}^{(3)} = n + 1/2$, all $\epsilon_{n,K}^{(3)}$ are negative for $K \geq 1$. For $g > 0$, the series (7) is formally not Borel summable. However, numerical evidence [10, 12, 15, 16] suggests that

the Borel–Padé summation method with the Laplace–Borel integration being carried out along complex contours, as given by Eqs. (196)–(198) of Ref. [10], provides useful numerical approximants to the resonance energies. The method has been put on rigorous mathematical grounds recently [6] in the framework of distributional Borel summability [8, 9]. When the integration contour C_{+1} in the conventions of Ref. [10] is employed, a negative sign is obtained for the imaginary part of the resonance energy. The accuracy obtainable using complex Borel summation of the weak-coupling expansion (7) is restricted by numerical oscillations in the values of the complex Borel–Padé transforms as the order of the Padé transformation is increased. These oscillations cannot be overcome even if extended-precision arithmetic is used in intermediate steps of the calculation. These oscillations have been described in Refs. [16, 21] for the complex Borel–Padé resummation method. Indeed, it has been observed in [16] that, at a relatively moderate coupling $g = 0.6$, the ground-state energy of the cubic oscillator as determined by resummation cannot be calculated to better accuracy than

$$\epsilon_0^{(3)}(g = 0.6) = 0.554(1) - 0.351(6) i \quad (9)$$

by Borel resummation. The oscillations, which are described by the numerical uncertainty in the last digit reported in result of Eq. (9), cannot be overcome when the (Borel) transformation order is increased and appear to represent a fundamental limit of the convergence of resummed weak-coupling perturbation theory in the case of a moderate and large (modulus of the) coupling parameter g . A more accurate result obtained by complex scaling (2) for the same coupling parameter is

$$\epsilon_0^{(3)}(g = 0.6) = 0.554053519 - 0.351401778 i. \quad (10)$$

The applicability of the weak-coupling expansion for the cubic oscillator resonance energies thus is found to be severely limited in the domain of moderate and large coupling, even if the perturbative expansion is *a posteriori* enhanced by a summation method acting in the complex plane. Likewise, the leading-order analytic result (5) cannot be applied to the domain of moderate and large coupling g . In this article, we explore the question whether one can find higher-order analytic formulas for the corrections to the leading result (5) for the decay width of the ground-state resonance energy (and, possibly, an arbitrary excited resonance energy) of the cubic oscillator, and if yes, how large the correction terms are.

Indeed, in Ref. [18], an analysis has been presented which allows us to calculate higher-order correction terms to the resonance energies for even and odd anharmonic oscillators of arbitrary degree, and to formulate modified Bohr–Sommerfeld quantization conditions for anharmonic oscillators such as the cubic one. Here, we provide a few more details of the analysis that leads to the results of Ref. [18], with a special emphasis on the cubic potential. To this end, we review in Sec. 2 the calculation of higher-order perturbative (in g) approximants to the wave function for the cubic potential. In Sec. 3, the calculation of higher-order corrections to the WKB approximation of the wave function is reviewed. The modified quantization condition pertaining to the cubic oscillator is described in Sec. 4, with a few new results for higher-order terms reserved for Sec. 5. Finally, conclusions are drawn in Sec. 6.

2 Perturbative expansion

The Schrödinger equation corresponding to the Hamiltonian given in Eq. (1) reads

$$\left(-\frac{1}{2} \frac{\partial^2}{\partial q^2} + \frac{1}{2} q^2 + \sqrt{g} q^3 \right) \varphi = E \varphi. \quad (11)$$

If we transform the coordinate according to $q \rightarrow q/\sqrt{g}$, we obtain

$$\left(-\frac{g^2}{2} \frac{\partial}{\partial q^2} + \mathcal{V}(q) \right) \varphi = g E \varphi, \quad \mathcal{V}(q) = \frac{1}{2} q^2 + q^3. \quad (12)$$

We may transform to the Riccati equation by setting

$$\frac{\varphi'(q)}{\varphi(q)} = -\frac{s(q)}{g}, \quad \frac{\varphi''(q)}{\varphi(q)} = \frac{s^2(q)}{g^2} - \frac{s'(q)}{g}, \quad (13)$$

The Riccati form of the Schrödinger equation then reads,

$$g s'(q) - s^2(q) + \mathcal{U}^2(q) = 0, \quad \mathcal{U}(q) = \sqrt{2[\mathcal{V}(q) - gE]}. \quad (14)$$

The zeroth-order term is

$$s(q) \approx s_0(q) = u(q) = \sqrt{2\mathcal{V}(q)}. \quad (15)$$

The following recursion yields higher-order approximants (in g) for the logarithmic derivative of the wave function,

$$s(q) = \sum_{K=0}^{\infty} g^K s_K(q), \quad s_0(q) = u(q), \quad s_1(q) = \frac{u'(q) - 2E}{2u(q)},$$

$$s_K(q) = \frac{1}{2u(q)} \left(s'_{K-1}(q) - \sum_{l=1}^{K-1} s_{K-l}(q) s_l(q) \right), \quad K \geq 2. \quad (16)$$

We can divide $s(q)$ into a symmetric and an antisymmetric component under the simultaneous interchange $g \rightarrow -g$, $E \rightarrow -E$,

$$s(q) = s_+(q) + s_-(q) = s_+(q, E, g) + s_-(q, E, g), \quad s_{\pm}(q, -E, -g) = \pm s_{\pm}(q, E, g). \quad (17)$$

From the following system of equations,

$$g s'_-(q) - s_+(q)^2 - s_-(q)^2 + \mathcal{U}^2(q) = 0, \quad (18a)$$

$$g s'_+(q) - 2s_+(q)s_-(q) = 0, \quad (18b)$$

we can eliminate the antisymmetric component by setting

$$s_-(q) = \frac{g}{2} \frac{s'_+(q)}{s_+(q)}. \quad (19)$$

The Bohr–Sommerfeld quantization condition reads

$$-\frac{1}{2\pi i g} \oint_C dz s_+(z) = n + \frac{1}{2}, \quad (20)$$

where C is a contour that encloses the zeros of the function $s_+(z)$ in the anticlockwise (mathematically positive) direction, and n is the quantum number of the level. The function $B_3(E, g)$, defined by

$$B_3(E, g) \equiv -\frac{1}{2\pi i g} \oint_C dz s_+(z), \quad (21)$$

[we recall the implicit dependence of $s_+(z)$ on g and E] provides for a universal means of determining the perturbative expansion for an arbitrary excited level of the cubic potential, by means of the perturbative quantization condition $B_3(E, G) = n + \frac{1}{2}$. A calculation leads to the result

$$B_3(E, g) = E + g \left(\frac{7}{16} + \frac{15}{4} E^2 \right) + g^2 \left(\frac{1365}{64} E + \frac{1155}{16} E^3 \right) + g^3 \left(\frac{119119}{2048} + \frac{285285}{256} E^2 + \frac{255255}{128} E^4 \right) + \mathcal{O}(g^4). \quad (22)$$

3 WKB expansion and contour integral

The WKB expansion is an expansion in g at gE fixed, i.e., it implies large values of E . We use this expansion in order to derive, roughly speaking, higher-order corrections to the instanton action which can later be used in order to derive higher-order corrections to resonance energies E of levels whose principal quantum number is *not* large (this is based on a rather fortunate enhancement of the applicability regions of certain expansions, as explained

below). The instanton configuration for the cubic potential has been discussed in Ref. [17], with a graphical representation being given in Fig. 3(b) of [17]. In order to achieve an instanton configuration pertaining to positive values of the coordinates, we scale the coordinate as $q \rightarrow -q/\sqrt{g}$. We start from

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial q^2} + \frac{1}{2}q^2 + gq^3\right)\phi = E\phi \quad (23)$$

and transform according to $q \rightarrow -q/\sqrt{g}$, which gives

$$\left(-\frac{g^2}{2}\frac{\partial}{\partial q^2} + \mathcal{W}(q)\right)\phi = gE\phi, \quad \mathcal{W}(q) = \frac{1}{2}q^2 - q^3. \quad (24)$$

We note that $\mathcal{W}(q)$ differs from $\mathcal{V}(q)$ in the sign of the cubic term. Setting

$$\frac{\phi'}{\phi} = -\frac{S(q)}{g}, \quad (25)$$

where the logarithmic derivative is denoted $S(q)$ instead of $s(q)$, we obtain

$$gS'(q) - S^2(q) + \mathcal{T}(q) = 0, \quad \mathcal{T}(q) = \sqrt{2[\mathcal{W}(q) - gE]}. \quad (26)$$

The zeroth-order term is different as compared to the perturbative expansion,

$$S(q) \approx S_0(q) = \sqrt{2[\mathcal{W}(q) - gE]}. \quad (27)$$

A recursion in g can be defined,

$$S(q) = \sum_{K=0}^{\infty} g^K S_K(q), \quad S_0(q) = \mathcal{T}(q), \quad S_1(q) = \frac{S'_0(q)}{2S_0(q)},$$

$$S_K(q) = \frac{1}{2S_0(q)} \left(S'_{K-1}(q) - \sum_{l=1}^{K-1} S_{K-l}(q) S_l(q) \right). \quad (28)$$

Like the perturbative expansion, the WKB expansion of the logarithmic derivative of the wave function can be calculated recursively in ascending powers of g , and we can also distinguish between even and odd components under the symmetry operator $g \rightarrow -g$, $E \rightarrow -E$,

$$S(q) = S_+(q) + S_-(q) = S_+(q, E, g) + S_-(q, E, g), \quad S_{\pm}(q, -E, -g) = \pm S_{\pm}(q, E, g). \quad (29)$$

The contour integral about the cut of the function $S_+(q)$ leads to a more complex structure as compared to the right-hand side of Eq. (20). It reads

$$\frac{1}{g} \oint_{\mathcal{C}} dz S_+(q) = A_3(E, g) + \frac{1}{2} \ln(2\pi) - \ln \left[\Gamma \left(\frac{1}{2} - B_3(E, g) \right) \right] + B_3(E, g) \ln \left(-\frac{g}{8} \right). \quad (30)$$

Here, \mathcal{C} is a contour that encloses the cut of the WKB expansion of the logarithmic derivative of the wave function in the clockwise sense. We thus have to calculate the integral

$$T = \frac{1}{g} \oint_{\mathcal{C}} dq S_+(q) \approx \frac{1}{g} \oint_{\mathcal{C}} dq [S_0(q) + g^2 S_2(q) + g^4 S_4(q)] = T_0 + T_2 + T_4, \quad (31)$$

Here, the WKB approximants $S_0(q)$, $S_2(q)$ and $S_4(q)$ are defined in Eq. (28), and the integrals T_0 , T_2 and T_4 correspond to the contour integrals of the WKB approximants of the respective order. The zeroth-order term is

$$T_0 = \frac{1}{g} \oint_{\mathcal{C}} dq S_0(q) \quad (32)$$

which involves the zeroth-order WKB approximant

$$S_0(q) = \sqrt{2\mathcal{W}(q) - gE} = \sqrt{q^2 - 2q^3 - gE}. \quad (33)$$

If we define the square root function to have its branch cut along the positive real axis, then the above expression has its branch cut (in the limit $gE \rightarrow 0$) from $q = 0$ to $q = \frac{1}{2}$. Directly above the cut, the value of the square root is positive, while directly below, it is negative. As the contour encircles the cut in the clockwise direction, we have an integration interval from zero to $\frac{1}{2}$ above the real axis, while below the real axis, we go from $\frac{1}{2}$ to zero. With this definition, the contour integral is

$$T_0 = \frac{1}{g} \oint_C dq \sqrt{q^2 - 2q^3 - gE} = \frac{2}{g} \operatorname{Re} \int_0^{1/2} dq (q^2 - 2q^3 - gE)^{1/2}. \quad (34)$$

For $gE > 0$, the cut of the WKB approximant does not extend along the full interval $(0, \frac{1}{2})$ any more. However, by specifying the real part of the final result, we pick up only those terms which are due to the cut.

The method of asymptotic matching (see Ch. 7.4 of Ref. [4]) can be used in order to evaluate (34). It involves an overlapping parameter ϵ , that is also used in Lamb shift calculations [11, 14, 20] in order to separate the low-energy from the high-energy contribution to the bound-electron self-energy. The overlapping parameter fulfills

$$0 < gE \ll \epsilon. \quad (35)$$

We then separate the integration interval into three parts, the first of which extends from $(0, \epsilon)$, the second, from $(\epsilon, \frac{1}{2} - \epsilon)$, and the third complementing interval finally reads $(\frac{1}{2} - \epsilon, \frac{1}{2})$.

The method of evaluation depends on the particular integration interval. For the interval $(0, \epsilon)$, we have to be careful to avoid divergences for very small $q = 0$. We have to keep the expression $\sqrt{q^2 - 2gE}$ within $S_0(q)$ in unexpanded form. However, we can expand the expression $\sqrt{q^2(1-2q) - 2gE} = \sqrt{q^2 - 2gE - 2q^3}$ in the q^3 term, then do the q integration, subsequently expand the result in gE , and finally in ϵ up to order ϵ^0 , keeping all divergent terms [11, 14, 20]. This leads to the result

$$\begin{aligned} I_1 = \operatorname{Re} \int_0^\epsilon dq (q^2 - 2q^3 - gE)^{1/2} &= (gE) \left[-\frac{1}{2} - \frac{1}{2} \ln \left(\frac{2\epsilon^2}{gE} \right) \right] + (gE)^2 \left[\frac{47}{16} + \frac{1}{4\epsilon^2} + \frac{3}{2\epsilon} - \frac{15}{8} \ln \left(\frac{2\epsilon^2}{gE} \right) \right] \\ &+ (gE)^3 \left[\frac{13327}{192} + \frac{1}{8\epsilon^4} + \frac{5}{6\epsilon^3} + \frac{35}{8\epsilon^2} + \frac{105}{4\epsilon} - \frac{1155}{32} \ln \left(\frac{2\epsilon^2}{gE} \right) \right] \\ &+ (gE)^4 \left[\frac{6364777}{3072} + \frac{5}{48\epsilon^6} + \frac{7}{8\epsilon^5} + \frac{315}{16\epsilon^4} + \frac{385}{16\epsilon^3} + \frac{15015}{128\epsilon^2} + \frac{45045}{64\epsilon} - \frac{255255}{256} \ln \left(\frac{2\epsilon^2}{gE} \right) \right] + \mathcal{O}(gE)^5. \end{aligned} \quad (36)$$

For the interval $(\epsilon, \frac{1}{2} - \epsilon)$, we can expand in gE to any power, because all divergences near $q = 0$ or $q = 1/2$ are cut off by the overlapping ϵ parameter. The result reads

$$\begin{aligned} I_2 = \operatorname{Re} \int_\epsilon^{1/2-\epsilon} dq (q^2 - 2q^3 - gE)^{1/2} &= \frac{1}{15} + (gE) \left[\frac{1}{2} \ln \left(\frac{\epsilon^2}{4} \right) \right] + (gE)^2 \left[\frac{47}{8} - \frac{1}{4\epsilon^2} - \frac{3}{2\epsilon} - \frac{2\sqrt{2}}{\sqrt{\epsilon}} + \frac{15}{8} \ln \left(\frac{\epsilon^2}{4} \right) \right] \\ &+ (gE)^3 \left[\frac{23189}{192} - \frac{1}{8\epsilon^4} - \frac{5}{6\epsilon^3} - \frac{35}{8\epsilon^2} - \frac{105}{4\epsilon} - \frac{4\sqrt{2}}{3\epsilon^{3/2}} - \frac{40\sqrt{2}}{\epsilon^{1/2}} + \frac{1155}{32} \ln \left(\frac{\epsilon^2}{4} \right) \right] + (gE)^4 \left[\frac{5241655}{1536} - \frac{5}{48\epsilon^6} \right. \\ &\left. - \frac{7}{8\epsilon^5} - \frac{315}{64\epsilon^4} + \frac{385}{16\epsilon^3} - \frac{15015}{128\epsilon^2} - \frac{45045}{64\epsilon} - \frac{2\sqrt{2}}{\epsilon^{5/2}} - \frac{140\sqrt{2}}{\epsilon^{3/2}} - \frac{1120\sqrt{2}}{\epsilon^{1/2}} + \frac{255255}{256} \ln \left(\frac{\epsilon^2}{4} \right) \right] + \mathcal{O}(gE)^5. \end{aligned} \quad (37)$$

The result from the interval I_3 compensates the divergences of fractional order in ϵ from I_2 ,

$$I_3 = \text{Re} \int_{1/2-\epsilon}^{1/2} dq (q^2 - 2q^3 - gE)^{1/2} = (gE)^2 \left[\frac{2\sqrt{2}}{\epsilon^{1/2}} \right] + (gE)^3 \left[\frac{4\sqrt{2}}{3\epsilon^{3/2}} + \frac{40\sqrt{2}}{\epsilon^{1/2}} \right] \\ + (gE)^4 \left[\frac{2\sqrt{2}}{\epsilon^{5/2}} + \frac{140\sqrt{2}}{3\epsilon^{3/2}} + \frac{1120\sqrt{2}}{\epsilon^{1/2}} \right] + \mathcal{O}(gE)^5. \quad (38)$$

In the result for T_0 ,

$$T_0 = \frac{2}{g} (I_1 + I_2 + I_3), \quad (39)$$

the overlapping parameter ϵ cancels, and we obtain

$$T_0 = \frac{2}{15g} + \left\{ -E + E \ln \left(\frac{gE}{8} \right) \right\} + g \left[-\frac{141}{8} E^2 - \frac{15}{4} E^2 \ln \left(\frac{gE}{8} \right) \right] \\ + g^2 \left[\frac{3043}{8} E^3 + \frac{1155}{16} E^3 \ln \left(\frac{gE}{8} \right) \right] + g^3 \left[\frac{5616029}{512} E^4 + \frac{255255}{128} E^4 \ln \left(\frac{gE}{8} \right) \right]. \quad (40)$$

The second term reads

$$T_2 = g \oint_{\mathcal{C}} dq S_2(q) = -\frac{1}{24E} + g \left[\frac{41}{16} + \frac{7}{16} \ln \left(\frac{gE}{8} \right) \right] \\ + g^2 \left[\frac{16431}{128} E + \frac{1365}{64} E \ln \left(\frac{gE}{8} \right) \right] + g^3 \left[\frac{862501}{128} E^2 - \frac{285285}{256} E^2 \ln \left(\frac{gE}{8} \right) \right]. \quad (41)$$

The third term is

$$T_4 = g^3 \oint_{\mathcal{C}} dq S_4(q) = \frac{7}{2880 E^3} - \frac{7g}{768 E^2} + \frac{539g^2}{1024 E} + g^3 \left[\frac{27101039}{611440} + \frac{119119}{2048} \ln \left(\frac{gE}{8} \right) \right]. \quad (42)$$

The total result of the contour integral of the WKB expansion is $T = T_0 + T_2 + T_4$, where

$$T = \frac{7}{2880 E^3} - \frac{1}{24E} + \frac{2}{15g} + \left\{ -E + E \ln \left(\frac{gE}{8} \right) \right\} + g \left[-\frac{7}{768 E^2} + \frac{41}{16} + \frac{141}{8} E^2 + \left(\frac{7}{16} + \frac{15}{4} E^2 \right) \ln \left(\frac{gE}{8} \right) \right] \\ + g^2 \left[\frac{539}{1024 E} + \frac{16431}{128} E + \frac{3043}{8} E^3 + \left(\frac{1365}{64} E + \frac{1155}{16} E^3 \right) \ln \left(\frac{gE}{8} \right) \right] \\ + g^3 \left[\frac{27101039}{611440} + \frac{862501}{128} E^2 + \frac{5616029}{512} E^4 + \left(\frac{119119}{2048} + \frac{285285}{256} E^2 + \frac{255255}{128} E^4 \right) \ln \left(\frac{gE}{8} \right) \right] + \mathcal{O}(g^4). \quad (43)$$

The perturbative counterterms read

$$P = \frac{1}{2} \ln(2\pi) - \ln \left[\Gamma \left(\frac{1}{2} - B_3(E, g) \right) \right] + B_3(E, g) \ln \left(-\frac{g}{8} \right) = \frac{7}{2880 E^3} - \frac{1}{24E} + \left\{ -E + E \ln \left(\frac{gE}{8} \right) \right\} \\ + g \left[-\frac{7g}{768 E^2} + \frac{5}{32} + \left(-\frac{7}{16} + \frac{15}{4} E^2 \right) \ln \left(\frac{gE}{8} \right) \right] \\ + g^2 \left[\frac{539}{1024 E} + \frac{65}{16} E + \frac{225}{32} E^3 + \left(\frac{1365}{64} E + \frac{1155}{16} E^3 \right) \ln \left(\frac{gE}{8} \right) \right] \\ + g^3 \left[\frac{319081}{8192} + \frac{175325}{1024} E^2 + \frac{33525}{128} E^4 + \left(\frac{119119}{2048} + \frac{285285}{256} E^2 + \frac{255255}{128} E^4 \right) \ln \left(\frac{gE}{8} \right) \right]. \quad (44)$$

where the result of $B_3(E, g)$ from Eq. (22) has been used, as well as the asymptotic expansion

$$\ln \Gamma \left(\frac{1}{2} + z \right) = z \{ \ln(z) - 1 \} + \frac{1}{2} \ln(2\pi) - \frac{1}{24z} + \frac{7}{2880 z^3} + \dots \quad (45)$$

Note that the logarithm $\ln(gE/8)$ is obtained as the combination of $B_3(E, g) \ln(-g/8) \approx E \ln(-g/8)$ and from the asymptotic expansion of the expression $-\ln \Gamma(\frac{1}{2} - B_3(E, g)) \approx E \ln(-E)$. Finally, the instanton function $A_3(E, g)$ for the cubic potential is found to read

$$A_3(E, g) = T - P = \frac{2}{15g} + g \left(\frac{77}{32} + \frac{141}{8} E^2 \right) + g^2 \left(\frac{15911}{128} E + \frac{11947}{32} E^3 \right) \quad (46)$$

$$+ g^3 \left(\frac{49415863}{122880} + \frac{6724683}{1024} E^2 + \frac{5481929}{512} E^4 \right) + \mathcal{O}(g^4). \quad (47)$$

This result for the instanton function is the basis for the calculation of higher-order corrections to the decay width of the resonance energies, as will be explained in the following.

4 Modified quantization condition

For $g < 0$, the interaction Hamiltonian $\sqrt{g} q^3 = \pm i |\sqrt{g}| q^3$ is \mathcal{PT} -symmetric, and its spectrum is purely real. In view of Eqs. (20) and (21), we then have the purely perturbative quantization condition

$$B_3(E, g) = n + \frac{1}{2} \Leftrightarrow \frac{1}{\Gamma(\frac{1}{2} - B_3(E, g))} = 0, \quad g < 0. \quad (48)$$

Let us now study how this condition needs to be modified in case instantons exist, i.e., for $g > 0$. We start from the unperturbed harmonic oscillator

$$\mathcal{H} = -\frac{1}{2} \frac{\partial^2}{\partial q^2} + \frac{1}{2} q^2. \quad (49)$$

In this form, we naturally identify

$$\frac{1}{\Gamma(\frac{1}{2} - E)} = \det(\mathcal{H} - E) \quad (50)$$

as the spectral determinant. The effect of the instanton is to add an infinitesimal imaginary part to the energy of the bound state,

$$E \approx \mathcal{E} \equiv n + \frac{1}{2} + i \operatorname{Im} \mathcal{E}. \quad (51)$$

Indeed, the definition of resonance energies via complex scaling and the proof of their existence can be found in Ref. [7]. Expanding in the nonperturbatively small (in g) imaginary part of the energy, we obtain

$$\frac{1}{\Gamma(\frac{1}{2} - \mathcal{E})} \approx -(-1)^{n+1/2} n! \operatorname{Im} \mathcal{E}. \quad (52)$$

For the cubic oscillator, we approximate the right-hand side of Eq. (52) as

$$\operatorname{Im} \mathcal{E} \approx \operatorname{Im} \epsilon_n^{(M)}(g) \approx -\frac{2^{3n}}{n! \sqrt{\pi}} g^{-n-1/2} \exp\left(-\frac{2}{15g}\right) \approx -\frac{1}{n! \sqrt{8\pi}} \left(\frac{8}{g}\right)^{B_3(E, g)} \exp(-A_3(E, g)). \quad (53)$$

We now generalize the left-hand side of Eq. (52) as $1/\Gamma(\frac{1}{2} - B_3(E, g))$ and approximate the right-hand side of Eq. (52) by the right-hand side of Eq. (53), and obtain

$$\frac{1}{\Gamma(\frac{1}{2} - B_3(E, g))} = \frac{1}{\sqrt{8\pi}} \left(-\frac{8}{g}\right)^{B_3(E, g)} \exp[-A_3(E, g)], \quad g > 0, \quad (54)$$

which is our conjecture for the resonance energies of the cubic anharmonic oscillator in the “unstable” regime of positive coupling parameter $g > 0$. When the logarithm of both sides of Eq. (54) is taken, we recover the structure of the terms on the right-hand side of Eq. (30).

In Sec. 3, we have calculated the function $A_3(E, g)$ in the WKB limit $g \rightarrow 0$, with gE fixed. In order to derive the result (46) for the function $A_3(E, g)$, we had to expand the function $B_3(E, g)$ in the limit of large E , which

implies [according to Eq. (45)] the approximation $-\ln \Gamma(\frac{1}{2} - B_3(E, g)) \approx E \ln \Gamma(-E)$. *A priori*, this expansion is not applicable when $E \approx n + \frac{1}{2} + \delta$, where δ summarizes the perturbative and nonperturbative corrections (in g). We have calculated the instanton function $A_3(E, g)$ in an “unphysical” domain of large quantum numbers n (large E), “away” from the first few resonance energies. However, the result (46) is written in terms of an expansion whose terms actually decrease for typical values of E for the first few resonance energies, where E is close to a small half-integer. We can thus make an—in some sense fortunate—observation: While the expansion (45) for the logarithm of the Γ function is not applicable to the physical domain of $E = n + \frac{1}{2} + \delta$, the obtained expansion for the $A_3(E, g)$ function is applicable in both the “unphysical” WKB domain of gE fixed, and $g \rightarrow 0$, thus $E \rightarrow \infty$, as well as the physical domain of $E \approx n + \frac{1}{2}$, and $g \rightarrow 0$. We can thus use the modified quantization condition (54) in the regime of low principal quantum numbers, which is of prime interest.

This unified result, which gives immediate and systematic access to the higher-order corrections, should be compared to other approaches (Refs. [13, 19, 22, 23], which also strive to go beyond the simple leading-order results for the decay rates of the resonances. One approach [13, 19] uses variationally improved perturbation theory which leads to a numerical improvement over the simple summation of the first few perturbative terms in the strong-coupling domain, but does not lead to a systematic prescription for calculation of higher-order coefficients in the “resurgent” expansion. The other approach [22, 23] is based on a set of quantization conditions derived as variations of the Bohr–Sommerfeld condition.

5 Results

Based on the results presented in Eqs. (22), (46) and (54), it is easy to derive higher-order corrections to the imaginary part of the first few resonance energies of the cubic potential, by entering into the condition (54) with an ansatz

$$\text{Im } \epsilon_n^{(3)}(g) = -\frac{2^{3n}}{n! \sqrt{\pi}} g^{-n-1/2} \exp\left(-\frac{2}{15g}\right) (1 + a_n g + b_n g^2 + \dots), \quad \text{for } g > 0, \quad (55)$$

and equating coefficients. The higher-order coefficients, for the lowest four states, read

$$\text{Im } \epsilon_0^{(3)}(g) = -\frac{\exp\left(-\frac{2}{15g}\right)}{\sqrt{\pi} g} \left\{ 1 - \frac{169}{16} g - \frac{44507}{512} g^2 - \frac{86071851}{40960} g^3 - \frac{189244716209}{2621440} g^4 + \mathcal{O}(g^5) \right\}, \quad (56a)$$

$$\text{Im } \epsilon_1^{(3)}(g) = -\frac{8 e^{-2/(15g)}}{\sqrt{\pi} g^{3/2}} \left\{ 1 - \frac{853}{16} g + \frac{33349}{512} g^2 - \frac{395368511}{40960} g^3 - \frac{1788829864593}{2621440} g^4 + \mathcal{O}(g^5) \right\}, \quad (56b)$$

$$\text{Im } \epsilon_2^{(3)}(g) = -\frac{32 e^{-2/(15g)}}{\sqrt{\pi} g^{5/2}} \left\{ 1 - \frac{2101}{16} g + \frac{1823341}{512} g^2 - \frac{1085785671}{40960} g^3 - \frac{4272925639361}{2621440} g^4 + \mathcal{O}(g^5) \right\}, \quad (56c)$$

$$\text{Im } \epsilon_3^{(3)}(g) = -\frac{256 e^{-2/(15g)}}{3\sqrt{\pi} g^{7/2}} \left\{ 1 - \frac{3913}{16} g + \frac{8807869}{512} g^2 - \frac{1571666861}{40960} g^3 - \frac{3214761534593}{2621440} g^4 + \mathcal{O}(g^5) \right\} \quad (56d)$$

For the coefficient of relative order g , a general result (for any n) has been indicated in Eq. (22) of Ref. [1]. For $n = 2$, Eq. (22) of Ref. [1] gives a correction term of $-2041g/16$ instead of $-2101g/16$ for the state with $n = 2$, and a correction term of $-10543g/48$ instead of $-3913g/16$ for the state with $n = 3$. With the help of the dispersion relation (4), these coefficients can be related to the corrections to the leading factorial asymptotics (8) of the perturbative coefficients of relative order $1/K$. We have checked our calculation against numerical values of the perturbative coefficients of up to 60th order, which can easily be determined on the basis of the relation $B_3(E, g) = n + 1/2$.

6 Conclusions

The calculation of higher-order corrections to the decay widths of quantum states in unstable potentials is a challenging problem. Analytic approximations are useful in that regard, if they contain a sufficient number of correction terms which also permit an estimate of the truncation error. As shown in Secs. 4 and 5, the calculation of higher-order corrections to the decay widths of resonances of the cubic anharmonic oscillator, is based on two characteristic functions, namely, the

$$\text{perturbative function} \quad B_3(E, g) = E + \mathcal{O}(g) \quad \text{defined in Eq. (21) and evaluated in Eq. (22)} \quad (57)$$

and on the

$$\text{instanton function} \quad A_3(E, g) = \frac{2}{15g} + \mathcal{O}(g) \quad \text{defined in Eq. (30) and evaluated in Eq. (46)}. \quad (58)$$

The first of these functions is given by an evaluation of a contour integral about the poles of the perturbative approximation to the logarithmic derivative of the wave function (see Sec. 2). The second function, $A_3(E, g)$, is determined by a contour integral about the cut of the WKB approximation of the wave function (see Sec. 3).

The modified Bohr–Sommerfeld quantization condition (4) then gives us access to the higher-order corrections to the imaginary part of the resonance energies. These are given, for the first few resonances of the cubic potential, in Sec. 5. The full solution of the modified quantization condition has the structure of a generalized nonanalytic expansion, or “resurgent” expansion,

$$\epsilon_n^{(3)}(g) = \sum_{J=0}^{\infty} \left[\frac{i}{n! \sqrt{8\pi}} \left(\frac{8}{g} \right)^{n+\frac{1}{2}} \exp\left(-\frac{2}{15g}\right) \right]^J \sum_{L=0}^{L_{\max}} \ln^L \left(-\frac{8}{g} \right) \sum_{K=0}^{\infty} \Xi_{J,L,K}^{(3,n)} g^K, \quad g > 0, \quad (59)$$

where

$$L_{\max} = \max(0, J - 1). \quad (60)$$

The perturbative coefficients $\epsilon_{n,K}^{(3)}$ are equal to the $\Xi_{0,0,K}^{(3,n)}$ coefficients. The coefficients entering Eq. (56) are the $\Xi_{1,0,K}^{(3,n)}$ coefficients.

The coefficients $\Xi_{1,0,1}^{(3,n)}$ multiply the correction of relative order g to the one-instanton ($J = 1$) effect and are given in Eq. (56) for $n = 0, 1, 2, 3$. They grow quite drastically in magnitude with the principal quantum number. In the notation of Eq. (55), we have for the state with $n = 3$ a coefficient of $a_3 = -244.563$. This means that the correction term of order g halves the total result for the decay width of the third excited state of the cubic potential already at a minuscule coupling parameter of $g \approx 0.002$. It is quite interesting to see that numerically approximations to such a fundamental physical quantity as the resonance energies of the cubic anharmonic oscillator require a considerable effort in their evaluation. Here, our aim was to carefully explain the calculational approach necessary in order to gain access to the higher-order corrections, which are numerically significant.

Acknowledgments

The authors gratefully acknowledge support from the National Science Foundation (Grant PHY–8555454) and from the Missouri Research Board.

References

- [1] G. Alvarez, Coupling-constant behavior of the resonances of the cubic anharmonic oscillator, Phys. Rev. A 37 (1988) 4079–4083.

- [2] E. Balslev, J. C. Combes, Spectral properties of many-body Schrödinger operators with dilation-analytic interactions, *Commun. Math. Phys.* 22 (1971) 280–294.
- [3] C. M. Bender, G. V. Dunne, Large-order perturbation theory for a non-Hermitian \mathcal{PT} -symmetric Hamiltonian, *J. Math. Phys.* 40 (1999) 4616–4621.
- [4] C. M. Bender, S. A. Orszag, *Advanced Mathematical Methods for Scientists and Engineers*, McGraw-Hill, New York, NY, 1978.
- [5] C. M. Bender, E. J. Weniger, Numerical evidence that the perturbation expansion for a non-Hermitian \mathcal{PT} -symmetric Hamiltonian is Stieltjes, *J. Math. Phys.* 42 (2001) 2167–2183.
- [6] E. Caliceti, Distributional Borel summability of odd anharmonic oscillators, *J. Phys. A* 33 (2000) 3753–3770.
- [7] E. Caliceti, V. Graffi, M. Maioli, Perturbation theory of odd anharmonic oscillators, *Commun. Math. Phys.* 75 (1980) 51–66.
- [8] E. Caliceti, V. Grecchi, M. Maioli, The Distributional Borel Summability and the Large Coupling ϕ^4 Lattice Fields, *Commun. Math. Phys.* 104 (1986) 163–174.
- [9] E. Caliceti, V. Grecchi, M. Maioli, Stark Resonances: Asymptotics and Distributional Borel Sum, *Commun. Math. Phys.* 157 (1993) 347–357.
- [10] E. Caliceti, M. Meyer-Hermann, P. Ribeca, A. Surzhykov, U. D. Jentschura, From useful algorithms for slowly convergent series to physical predictions based on divergent perturbative expansions, *Phys. Rep.* 446 (2007) 1–96.
- [11] R. P. Feynman, Space–Time Approach to Quantum Electrodynamics, *Phys. Rev.* 76 (1949) 769–789.
- [12] V. Franceschini, V. Grecchi, H. J. Silverstone, Complex energies from real perturbation series for the LoSurdo-Stark effect in Hydrogen by Borel-Padé approximants, *Phys. Rev. A* 32 (1985) 1338–1340.
- [13] B. Hamprecht, H. Kleinert, Tunneling amplitudes from perturbation expansions, *Phys. Lett. B* 564 (2003) 111–114.
- [14] U. Jentschura, K. Pachucki, Higher-order binding corrections to the Lamb shift of $2P$ states, *Phys. Rev. A* 54 (1996) 1853–1861.
- [15] U. D. Jentschura, Resummation of nonalternating divergent perturbative expansions, *Phys. Rev. D* 62 (2000) 076001.
- [16] U. D. Jentschura, A. Surzhykov, M. Lubasch, J. Zinn-Justin, Structure, time propagation and dissipative terms for resonances, *J. Phys. A* 41 (2008) 095302.
- [17] U. D. Jentschura, A. Surzhykov, J. Zinn-Justin, Generalized nonanalytic expansions, \mathcal{PT} -symmetry and large-order formulas for odd anharmonic oscillators, *SIGMA (Symmetry, Integrability and Geometry: Methods and Applications)* 5 (2009) 005.
- [18] U. D. Jentschura, A. Surzhykov, J. Zinn-Justin, Unified Treatment of Even and Odd Anharmonic Oscillators of Arbitrary Degree, *Phys. Rev. Lett.* 102 (2009) 011601.
- [19] R. Karrlein, H. Kleinert, Precise variational tunneling rates for anharmonic oscillator with $g < 0$, *Phys. Lett. A* 187 (1994) 133–139.
- [20] K. Pachucki, Higher-Order Binding Corrections to the Lamb Shift, *Ann. Phys. (N.Y.)* 226 (1993) 1–87.
- [21] A. Surzhykov, M. Lubasch, J. Zinn-Justin, U. D. Jentschura, Quantum dot potentials: Symanzik scaling, resurgent expansions and quantum dynamics, *Phys. Rev. B* 74 (2006) 205317.
- [22] A. Voros, Airy function—exact WKB results for potentials of odd degree, *J. Phys. A* 32 (1999) 1301–1311.

- [23] A. Voros, Exact resolution method for general 1D polynomial Schrödinger equation, *J. Phys. A* 32 (1999) 5993–6007.
- [24] R. Yaris, J. Bendler, R. A. Lovett, C. M. Bender, P. A. Fedders, Resonance calculations for arbitrary potentials, *Phys. Rev. A* 18 (1978) 1816–1825.