Exponentially small corrections in the asymptotic expansion of the eigenvalues of the cubic anharmonic oscillator

2000 J. Phys. A: Math. Gen. 33 5171

(http://iopscience.iop.org/0305-4470/33/29/302)

J. Phys. A: Math. Gen. **33** (2000) 5171–5182. Printed in the UK PII: S0305-4470(00)12643-5

Exponentially small corrections in the asymptotic expansion of the eigenvalues of the cubic anharmonic oscillator

Gabriel Álvarez and Carmen Casares

Departamento de Física Teórica II, Facultad de Ciencias Físicas, Universidad Complutense, 28040 Madrid, Spain

Received 14 March 2000, in final form 25 May 2000

Abstract. The asymptotic expansion of the eigenvalues of the cubic anharmonic oscillator is studied in a region of the coupling constant plane in which there is a sequence of exponentially small subseries beyond the standard Rayleigh–Schrödinger perturbation theory (RSPT) power series. We give a simple algorithm for the calculation of these subseries (to any desired order) in terms of the RSPT coefficients expressed as polynomials in the quantum number, and illustrate our results with numerical Borel–Padé summations of the expansion up to third exponentially small order.

1. Introduction

It seems that the initial interest in the eigenvalues of the cubic anharmonic oscillator

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}x^2 + gx^3 \tag{1}$$

came from the study of the Yang–Lee singularities of the Ising model [1–3] by renormalization group methods, which led Bessis and Zinn-Justin to conjecture that, for purely imaginary values of the coupling constant g, the spectrum of the operator (1) is real. Physical intuition also suggests that for nonzero real values of g the bound states of the harmonic oscillator become resonances, and Yaris *et al* [4] used the cubic anharmonic oscillator as a model to argue heuristically that the complex-dilation method [5] is applicable to potentials that do not vanish at infinity, and yields correctly both the real and the imaginary parts of the complex eigenvalues. Yet a mathematically rigorous discussion of the problem from the functional-analytic point of view is not straightforward because the action of the operator (1) on the space of infinitely differentiable functions of compact support admits infinitely many self-adjoint extensions [6]. This is the quantum analogue of the fact that a classical particle not confined to the potential well reaches minus infinity in a finite amount of time, and requires 'further instructions' to proceed. The essential result was given by Caliceti *et al* [7]: for $\operatorname{Im} g > 0$ the spectrum of the operator (1) consists of isolated eigenvalues of finite multiplicity that can be continued analytically to $\operatorname{Im} g = 0$, where they correspond to the solutions of the differential equation

$$-\tfrac{1}{2}\psi''(x) + (\tfrac{1}{2}x^2 + gx^3 - E)\psi(x) = 0 \tag{2}$$

that are exponentially decreasing at plus infinity and satisfy a Gamow–Siegert [8] purely outgoing wave boundary condition at minus infinity. Furthermore, for sufficiently small values of $|g|$ and $0 < \arg g < \pi$, the Rayleigh–Schrödinger perturbation theory (RSPT) power series

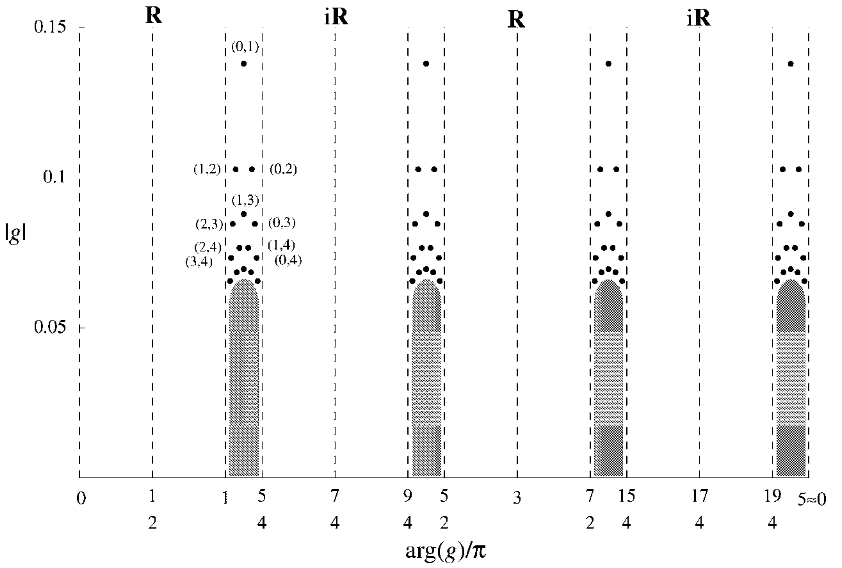

Figure 1. Schematic representation of the Riemann surface of the eigenvalues of the cubic anharmonic oscillator. The origin is a global $g^{2/5}$ singularity, and the arguments have to be understood modulo 5π. The dots mark the lowest Bender–Wu branch points; in the first of the four families they are labelled by the unperturbed quantum numbers of the levels that cross. The shaded areas represent the higher branch points, which cluster at the origin. The $\boldsymbol{R}$ and $\mathrm{i}\boldsymbol{R}$ labels mark the values of $\arg g$ for which the eigenvalues are real and purely imaginary, respectively.

is asymptotic and Borel summable to these resonances. Note that, for purely imaginary values of the coupling constant (i.e. $\arg g = \frac{\pi}{2}$), we have the typical alternating sign pattern of the Borel summable series with real Borel sum, while for real values of g the coefficients of the RSPT series have the same sign and the Borel transform develops a singularity on the positive real axis that prevents summability.

The conjecture of Bessis and Zinn-Justin has been reconsidered recently in the more general setting of PT-symmetric Hamiltonians by Delabaere and Pham [9], who rederived the small $|g|$ version of the result using the 'exact WKB method' [10, 11], and by Bender and Dunne [12], who also gave numerical evidence of the Padé summability of the RSPT series for purely imaginary values of the coupling constant.

Summing up, there are analytic proofs and numerical algorithms for the Borel summability of the RSPT series in the coupling constant region $0 < \arg g < \pi$. These results, however, dealt only with the behaviour of the eigenvalues in limited regions of the coupling constant, and a global description (analogous to the work of Bender and Wu on the quartic oscillator [13]) was still lacking. The main idea is that the different eigenvalues are the values that a single analytic function takes on different sheets of a Riemann surface characterized by the position of its singularities (the Bender–Wu branch points), at which level crossing occurs. In 1995 Alvarez [14] applied numerical and semiclassical methods to study the full analytic configuration of the eigenvalues of the cubic anharmonic oscillator, which is illustrated in figure 1. There are four families of square root branch points, each of which can be labelled by the quantum numbers of the two unperturbed levels that cross. The origin, which behaves as a $g^{2/5}$ global singularity in the sense defined by Simon [15], is a limit point of the four families of branch points. Therefore the Riemann surface consists of an infinite number of 'two and a half' Riemann sheets joined to each other at exactly four square root branch points. Numerical calculations for arbitrary values of $|g|$ and analytic arguments for sufficiently small values of $|g|$ confirmed that the eigenvalues are real for $\arg g = \frac{\pi}{2}$ and 3π (and purely imaginary for $\arg g = \frac{7\pi}{4}$ and $\frac{17\pi}{4}$).

Our main goal in this paper is to study the structure and summability of the asymptotic expansion for the eigenvalues beyond the real axis. For concreteness, consider the analytic continuation of the unperturbed $n = 0$ eigenvalue across $\arg g = 0$. The first singularity met is the (0, 1)-type Bender–Wu branch point located at $|g| \approx 0.138\,096$, $\arg g = -\frac{\pi}{8}$ (see figure 1 and [14]). That is to say, there is a sector of opening larger than π in which the $n = 0$ eigenvalue is analytic. In a recent paper [16] we showed that the positive real axis, $\arg g = 0$, is a Stokes line of the asymptotic expansion for the eigenvalues, i.e. the asymptotic expansion changes discontinuously from the Borel summable RSPT power series valid in $0 < \arg g < \pi$ to a more complicated expansion valid (for our $n = 0$ example) in $-\frac{\pi}{8} < \arg g < 0$, and reduced the problem of finding the new expansion to the solution of an 'exact matching condition'. In this paper we show that the new asymptotic expansion consists of the RSPT power series plus an infinite sequence of exponentially smaller subseries, where the kth subseries is the kth power of a common exponentially small prefactor times a sum of products of power series and logarithmic terms. Thanks to an observation of Hoe *et al* [17] we are able to give a simple algorithm for the calculation of these subseries (to any desired order) in terms of the elementary calculation of the RSPT coefficients as polynomials in the quantum number n. We find that all the power series coefficients grow only slightly faster than the RSPT coefficients, and our conjecture is that these power series are Borel summable, a conjecture supported by numerical Borel–Padé summations in the sector $-\frac{\pi}{8} < \arg g < 0$ up to third exponentially small order.

The layout of the paper is as follows: in the next section we summarize the main ideas of the matching procedure of [16] with just enough detail to explain the origin of the matching condition and the analytic reason for the discontinuous change of the asymptotic expansion across the real axis; section 3 is devoted to the iterative solution of the matching condition beyond the real axis, and to the analysis of the structure of the successively exponentially smaller contributions; section 4 deals with the asymptotic behaviour of the power series coefficients and the numerical Borel–Padé summation; the paper ends with a summary.

2. Matching condition

Although we refer to [16] for a detailed account, in this section we outline the main ideas of the matching procedure used to obtain the asymptotic expansion that includes exponentially small subseries beyond the standard RSPT power series. The solution of the eigenvalue problem posed in the introduction consists of three steps: (i) scale the independent variable in the Schrödinger equation to obtain an equation with an unperturbed double turning point fixed at the origin and an unperturbed simple turning point fixed at (say) one; (ii) build uniform, Borel summable asymptotic expansions of the wavefunction around these turning points; and (iii) match these expansions in the 'under the barrier' region.

The unperturbed turning points are fixed by the new independent variable

$$z = -h^{1/2}x \tag{3}$$

where

$$h = (2g)^2 \tag{4}$$

and the resulting Schrödinger equation is

$$-h^2\psi''(z) + (z^2 - z^3 - 2hE)\psi(z) = 0. \tag{5}$$

Table 1. Lowest $E^{(2k)}(\nu)$ and $f^{(2k)}(\nu)$ coefficients as polynomials in ν. The RSPT coefficient of g^{2k} for the nth eigenvalue is $E^{(2k)}(n+\frac{1}{2})$.

k	$-E^{(2k)}(\nu)$	$f^{(2k)}(\nu)$
0	$-\nu$	
1	$\frac{7}{16}+\frac{15}{4}\nu^2$	$\frac{77}{128}+\frac{141}{32}\nu^2$
2	$\frac{1155}{64}\nu+\frac{705}{16}\nu^3$	$\frac{13\,937}{2048}\nu+\frac{7717}{512}\nu^3$
3	$\frac{101\,479}{2048}+\frac{209\,055}{256}\nu^2+\frac{115\,755}{128}\nu^4$	$\frac{43\,147\,783}{7864\,320}+\frac{5153\,379}{65\,536}\nu^2+\frac{2663\,129}{32\,768}\nu^4$
4	$\frac{129\,443\,349}{16\,384}\nu+\frac{77\,300\,685}{2048}\nu^3+\frac{23\,968\,161}{1024}\nu^5$	$\frac{1769\,452\,671}{8388\,608}\nu+\frac{240\,109\,947}{262\,144}\nu^3+\frac{282\,482\,109}{524\,288}\nu^5$

(The role of the minus sign in equation (3) is to make the convention of this paper, standard when dealing with the cubic oscillator, conform to the convention of [16] which deals simultaneously with even and odd oscillators.)

The origin-anchored solution which is exponentially decreasing at minus infinity can be written in terms of the parabolic cylinder function $D_{\nu-1/2}(z)$,

$$\psi(z) = [u'(z)]^{-1/2} D_{\nu-1/2}\left[-\left(\frac{2}{h}\right)^{1/2} u(z)\right] \tag{6}$$

which, put into equation (5), gives the following equation for $u(z)$:

$$u(z)^2 u'(z)^2 = z^2 - z^3 - 2h[E - \nu u'(z)^2] + \frac{h^2}{2}\left[\frac{u'''(z)}{u'(z)} - \frac{3}{2}\left(\frac{u''(z)}{u'(z)}\right)^2\right]. \tag{7}$$

Substituting the asymptotic expansions

$$u(z) = \sum_{k=0}^{\infty} u_k(z) h^k \tag{8}$$

$$E = \sum_{k=0}^{\infty} E^{(2k)}(\nu)\frac{h^k}{4^k} \tag{9}$$

into equation (7) and equating powers of h, we obtain a system of differential equations that can be integrated recursively for the $u_k(z)$ in terms of elementary functions. The $E^{(2k)}(\nu)$, which are fixed by the requirement that $u_k(z)$ be regular at the origin, turn out to be precisely the RSPT coefficients expanded as polynomials in $n+\frac{1}{2}$, except that they are now functions of the as yet unspecified parameter ν. For later reference, the first five $E^{(2k)}(\nu)$ are listed in table 1.

The uniform expansion anchored at the unperturbed simple turning point $z = 1$ is built following the same steps, except that the solution with outgoing wave behaviour at infinity is written in terms of the Airy function $\mathrm{Ai}^{(+)}(z) = \mathrm{Bi}(z) + \mathrm{i}\mathrm{Ai}(z)$. Therefore we set

$$\psi(z) = [v'(z)]^{-1/2}\mathrm{Ai}^{(+)}[h^{-2/3}v(z)] \tag{10}$$

into equation (5) and obtain the corresponding equation for $v(z)$:

$$v(z)v'(z)^2 = z^2 - z^3 - h2E + \frac{h^2}{2}\left[\frac{v'''(z)}{v'(z)} - \frac{3}{2}\left(\frac{v''(z)}{v'(z)}\right)^2\right]. \tag{11}$$

Again, substituting the asymptotic expansion for $v(z)$

$$v(z) = \sum_{k=0}^{\infty} v_k(z) h^k \tag{12}$$

and the asymptotic expansion for the energy (9) into equation (11) we obtain a system of equations for the $v_k(z)$ which can be integrated recursively in terms of elementary functions.

The final step is to match the Borel summable asymptotic expansions for the wavefunctions that result from the composition of (6) and (8) (around the origin), and of (10) and (12) (around the outer turning point) in their common region of validity—the 'under the barrier' region.

Comparing the Borel summable asymptotic expansions for the Airy and parabolic cylinder functions [16] in the region $0 < \arg g < \pi$, it turns out that the exponentially increasing term in the asymptotic expansion of (6) must vanish, which leads to the exact matching condition

$$\nu = n + \tfrac{1}{2} \qquad (n = 0, 1, 2, \ldots) \tag{13}$$

and to the ensuing expansion for the energy

$$E \sim E^{(\mathrm{PT})} \equiv \sum_{k=0}^{\infty} E_n^{(2k)} \frac{h^k}{4^k} \tag{14}$$

where we have denoted

$$E_n^{(2k)} \equiv E^{(2k)}(n + \tfrac{1}{2}). \tag{15}$$

This is, of course, the region of Borel summability of the RSPT series mentioned above.

For sufficiently small $\arg g < 0$, however, both the asymptotic expansions of the Airy and parabolic cylinder functions are the sum of a dominant and a subdominant series uniquely defined by Borel summability, and we implement the matching by equating the ratios of the dominant to the subdominant terms in the asymptotic expansions of equations (6) and (10). This matching condition, which is an equation for ν, can be written as

$$f(\nu) = \mathrm{e}^{\mathrm{i}\pi}(\mathrm{e}^{\mathrm{i}2\pi\nu} + 1) \tag{16}$$

where

$$f(\nu) = \frac{(2\pi)^{1/2}}{\Gamma(\nu + \frac{1}{2})}\left(\frac{32}{h}\right)^{\nu} \exp\left[-\frac{8}{15h} - \sum_{k=1}^{\infty} f^{(2k)}(\nu)h^k\right] \tag{17}$$

and the $f^{(2k)}(\nu)$ are polynomials in ν which can be calculated explicitly in principle to any desired order. We list the first four $f^{(2k)}(\nu)$ in the last column of table 1.

As we mentioned in the introduction, the calculation of the polynomials $E^{(2k)}(\nu)$ is trivial and can be carried out to high order with just a few lines of code. Although equally algorithmic, a direct calculation of the $f^{(2k)}(\nu)$ from the matching algorithm is much more time- and memory-consuming, essentially because it involves the composition and expansion of series with a rapidly increasing number of terms. The calculation of the $f^{(2k)}(\nu)$ to high order can be carried out, however, without any difficulty thanks to an observation made by Hoe *et al* [17] in the context of the Stark effect in hydrogenic ions. In fact, the Stark effect Hamiltonian, after separation into parabolic coordinates, is equivalent to a two-dimensional isotropic quartic oscillator, and Hoe *et al* noticed that the ionization rates could be expressed in terms of the energies. A similar relation seems to be true for the cubic anharmonic oscillator: the data in table 1 illustrate that

$$f^{(2k)}(\nu) = -\frac{2}{15}\frac{1}{k4^k}\frac{\partial E^{(2k+2)}(\nu)}{\partial \nu} \tag{18}$$

or in a more condensed form

$$f(\nu) = \frac{(2\pi)^{1/2}2^{5\nu}}{\Gamma(\nu + \frac{1}{2})} \exp\left[\frac{8}{15}\int \frac{\partial E}{\partial \nu}\frac{\mathrm{d}h}{h^2}\right]. \tag{19}$$

We do not have a proof of these equations (probably related to the elliptic character of cubic and quartic polynomials), but we have checked their validity by direct calculation with the matching algorithm up to $k = 10$. Then we used a standard RSPT algorithm to calculate the $E^{(2k)}(\nu)$, and from these and equation (18) the $f^{(2k)}(\nu)$ to a sufficiently high order to perform the numerical Borel–Padé summations of section 4 and check our large-k asymptotic estimates.

3. Iterative solution of the matching condition beyond the real axis

First note that, if the matching functions $f(\nu)$ were identically zero, then the solutions of equation (16) would be precisely those given by equation (13). Since $f(\nu)$ is exponentially small, we put

$$\nu = n + \tfrac{1}{2} + \Delta\nu \qquad (n = 0, 1, 2, \ldots) \tag{20}$$

and rewrite the matching condition in a form suitable for iterative solution. We keep track of the exponentially small order by introducing a parameter λ (that ultimately will be set to one) which appears in two places: multiplying the matching function $f(\nu)$ and as the ordering parameter in the series for $\Delta\nu$. That is to say, we write

$$\Delta\nu = \frac{1}{2\pi \mathrm{i}} \ln\left[1 + \lambda f\left(n + \frac{1}{2} + \Delta\nu\right)\right] \tag{21}$$

where

$$\Delta\nu = \lambda\Delta\nu_1 + \lambda^2\Delta\nu_2 + \lambda^3\Delta\nu_3 + \cdots. \tag{22}$$

Expanding the right-hand side of equation (21) as a Taylor series in λ, we can find immediately the first three terms (which will be enough to infer the general pattern) of the solution for $\Delta\nu$:

$$\Delta\nu_1 = -\frac{\mathrm{i}}{2\pi} f_n \tag{23}$$

$$\Delta\nu_2 = -\frac{1}{4\pi^2} f_n f_n' + \frac{\mathrm{i}}{4\pi} f_n^2 \tag{24}$$

$$\Delta\nu_3 = -\frac{\mathrm{i}}{6\pi} f_n^3 + \frac{3}{8\pi^2} f_n^2 f_n' + \frac{\mathrm{i}}{8\pi^3} f_n (f_n')^2 + \frac{\mathrm{i}}{16\pi^3} f_n^2 f_n'' \tag{25}$$

where again we have denoted by a subindex n the value of the matching function $f(\nu)$ and its derivatives at $\nu = n + \frac{1}{2}$.

The corresponding expansion for the eigenvalues up to third exponentially small order is easily obtained by first putting equation (20) into (9) and expanding to third order in $\Delta\nu$

$$E \sim E^{(\mathrm{PT})} + \frac{\Delta\nu}{1!}\frac{\partial E^{(\mathrm{PT})}}{\partial n} + \frac{\Delta\nu^2}{2!}\frac{\partial^2 E^{(\mathrm{PT})}}{\partial n^2} + \frac{\Delta\nu^3}{3!}\frac{\partial^3 E^{(\mathrm{PT})}}{\partial n^3} + \mathrm{O}(\Delta\nu^4) \tag{26}$$

and subsequently substituting equations (22)–(25) into (26) and collecting powers of λ. We will write the final asymptotic expansion as

$$E \sim E^{(\mathrm{PT})} + \Delta E_1 + \Delta E_2 + \Delta E_3 + \cdots \tag{27}$$

where we have already set $\lambda = 1$ and the subindex labels the exponentially small order.

The first exponentially small subseries is formally purely imaginary

$$\Delta E_1 = -\frac{\mathrm{i}}{2\pi} f_n \frac{\partial E^{(\mathrm{PT})}}{\partial n} \tag{28}$$

$$= -\mathrm{i}C(h)B_1(h) \tag{29}$$

where we have defined the exponentially small prefactor

$$C(h) \equiv \frac{2^{5n+2}}{\pi^{1/2} n!} \mathrm{e}^{-8/(15h)} h^{-(n+1/2)} \tag{30}$$

and $B_1(h)$ is the $p = 1$ instance of

$$B_p(h) = \sum_{k=0}^{\infty} b_{n,p}^{(2k)} h^k \equiv \exp\left[- p \sum_{k=1}^{\infty} f_n^{(2k)} h^k \right] \left(\sum_{k=0}^{\infty} \frac{\partial E_n^{(2k)}}{\partial n} \frac{h^k}{4^k} \right). \tag{31}$$

The last two factors in equation (28) are readily interpreted in the context of the elementary semiclassical derivations of the imaginary part of the resonances: $\frac{\partial E^{(\mathrm{PT})}}{\partial n}$ corresponds to the 'frequency of collisions with the barrier', while f_n represents the 'tunnelling probability'. Although this seems to be the natural factorization from the physical point of view, for our purposes the factorization of equation (29) is more convenient, in which we separate the exponentially small prefactor from the Borel summable power series.

The second exponentially small correction to the eigenvalue (i.e. proportional to the square of $C(h)$) has both formally real and formally imaginary parts, which we denote with superindices:

$$\Delta E_2^{(r)} = -\frac{1}{8\pi^2} \frac{\partial}{\partial n} \left(f_n^2 \frac{\partial E^{(\mathrm{PT})}}{\partial n} \right) \tag{32}$$

$$= C(h)^2 \left\{ \left[\ln\left(\frac{h}{32}\right) + \psi(n+1) \right] B_2(h) - \frac{1}{2} \frac{\partial B_2(h)}{\partial n} \right\} \tag{33}$$

$$\Delta E_2^{(i)} = \frac{1}{4\pi} f_n^2 \frac{\partial E^{(\mathrm{PT})}}{\partial n} \tag{34}$$

$$= \pi C(h)^2 B_2(h). \tag{35}$$

(In these and the following equations ψ stands for the logarithmic derivative of the gamma function.) We point out the first appearance of a logarithmic term, namely in $\Delta E_2^{(r)}$. The structure of $\Delta E_2^{(i)}$, however, is not yet typical. The generic form is reached at the level of the third exponentially small subseries, in which both the formally real and imaginary parts are the cube of the exponentially small prefactor $C(h)$ times a sum of products of power series and logarithmic terms:

$$\Delta E_3^{(r)} = \frac{1}{8\pi^2} \frac{\partial}{\partial n} \left(f_n^3 \frac{\partial E^{(\mathrm{PT})}}{\partial n} \right) \tag{36}$$

$$= -\pi C(h)^3 \left\{ 3 \left[\ln\left(\frac{h}{32}\right) + \psi(n+1) \right] B_3(h) - \frac{\partial B_3(h)}{\partial n} \right\} \tag{37}$$

$$\Delta E_3^{(i)} = \frac{1}{48\pi^3} \frac{\partial^2}{\partial n^2} \left(f_n^3 \frac{\partial E^{(\mathrm{PT})}}{\partial n} \right) - \frac{1}{6\pi} f_n^3 \frac{\partial E^{(\mathrm{PT})}}{\partial n} \tag{38}$$

$$= C(h)^3 \left\{ \left[\frac{3}{2} \left(\ln\left(\frac{h}{32}\right) + \psi(n+1) \right)^2 - \frac{1}{2}\psi'(n+1) - \frac{4\pi}{3} \right] B_3(h) \right.$$
$$\left. - \frac{1}{2} \left[\ln\left(\frac{h}{32}\right) + 2\psi(n+1) \right] \frac{\partial B_3(h)}{\partial n} + \frac{1}{6} \frac{\partial^2 B_3(h)}{\partial n^2} \right\}. \tag{39}$$

This procedure can be applied without any difficulty to calculate explicitly higher exponentially small corrections. In fact, the solution for $\Delta\nu_k$ in equation (22) is a sum of homogeneous terms of degree k in f_n and its derivatives up to order $f_n^{(k-1)}$. Since the logarithmic terms come from these derivatives, the expression for ΔE_k will have $\ln h$ up to the power $k - 1$. The global structure inferred for equation (27) is therefore the same as the multi-instanton expansion conjectured by Zinn-Justin [18–20] for real potentials with degenerate symmetric minima, except that in the Zinn-Justin case both the perturbative and one-instanton contributions are needed to determine the complete multi-instanton expansion. Analytically, in the Zinn-Justin expansion the power series have to be summed first for complex values of the coupling constant and continued back to the real axis, where the imaginary contributions from the Borel sums and logarithms must cancel (these cancellations between the Borel sums of consecutive contributions are equivalent to dispersion relations, as put forward in essence by Damburg and Propin [21]).

The form of the exponentially small factor $C(h)$ in equation (29) has been derived by several authors: for example, Schmid [22] used what can be described as a 'first-order' version of our matching method, but apparently did not realize the role of the RSPT series and did not reach higher-order results; in a series of papers, Jafarizadeh *et al* [23–25] have discussed the derivation of the same expression by instanton methods combined with the heat kernel method; the highest result thus far seems to be by Kleinert and Mustapic [26], who using the JWKB method and a current–density formula were able to derive the expression for $C(h)$ and the first eight terms of the series for $B_1(h)$ in our equation (29), but to our knowledge there was not yet a systematic algorithm to calculate all the exponentially small subseries ΔE_k.

4. Asymptotic behaviour of the coefficients and Borel–Padé summations

Our next goal is to study the asymptotic behaviour of the coefficients of the power series $B_p(h)$ (and their derivatives) which appear in the exponentially small subseries, and to implement a numerical Borel–Padé summation algorithm for the compound asymptotic expansion (27). Substituting equation (29) into the dispersion relation in h

$$E_n^{(2k)} = \frac{4^k}{2\pi \mathrm{i}} \int_0^\infty \Delta E_1 h^{-k-1}\, \mathrm{d}h \tag{40}$$

yields the large-order asymptotic behaviour of the RSPT coefficients

$$E_n^{(2k)} \sim E_n^{[2k]} \equiv -\frac{60^n}{\pi^{3/2} n!} \left(\frac{15}{2}\right)^{k+\frac{1}{2}} \Gamma(n + \tfrac{1}{2} + k) \qquad (k \to \infty) \tag{41}$$

where we have marked with square parentheses in the superindex the functional form of the asymptotic behaviour. It follows immediately that

$$\frac{\partial E_n^{(2k)}}{\partial n} \sim E_n^{[2k]} \left[\psi\left(n + \frac{1}{2} + k\right) + \ln 60 - \psi(n+1)\right] \qquad (k \to \infty) \tag{42}$$

and since $\psi(k) = \Gamma'(k)/\Gamma(k) \sim \ln k$ as $k \to \infty$, the coefficients of the derivative grow only slightly faster than the RSPT coefficients. Furthermore, the lowest-order term of the series in the exponential of equation (31) is not a constant but proportional to h, and the series itself has factorially growing coefficients, from which it follows that the $b_{n,p}^{(2k)}$ also grow only slightly faster than the RSPT coefficients:

$$b_{n,p}^{(2k)} \sim (p+1) E_n^{[2k]} [\psi(n + \tfrac{1}{2} + k) + \ln 60 - \psi(n+1)] \qquad (k \to \infty). \tag{43}$$

Considering the gamma functions in the asymptotic behaviours (41)–(43), we have implemented the Borel–Padé summations of the power series for the nth eigenvalue of the cubic anharmonic oscillator as

$$b(h) \approx \int_0^\infty \mathrm{e}^{-t} t^{n-1/2} P^{[p,q]}(ht)\, \mathrm{d}t \tag{44}$$

where $P^{[p,q]}(t)$ is the $[p,q]$-Padé approximant for

$$\hat{b}(t) = \sum_{k=0}^{p+q} \frac{b_k t^k}{\Gamma(n + \frac{1}{2} + k)}. \tag{45}$$

Furthermore, to avoid problems with the numerical integration we expand the Padé approximant as a polynomial plus partial fractions, i.e. assuming that all the poles are simple

$$P^{[p,q]}(t) = \sum_{k=0}^{p-q} p_k t^k + \frac{R(t)}{S(t)} = \sum_{k=0}^{p-q} p_k t^k + \sum_{k=1}^{q} \frac{R(t_k)}{S'(t_k)(t-t_k)} \tag{46}$$

and the integration in equation (44) can be carried out in terms of complete and incomplete gamma functions evaluated at the q poles t_k of $P^{[p,q]}(t)$:

$$b(h) \approx \sum_{k=0}^{p-q} p_k h^k \Gamma(n + \tfrac{1}{2} + k) + \frac{\Gamma(n+\frac{1}{2})}{h} \sum_{k=1}^{q} \frac{R(t_k)}{S'(t_k)} \mathrm{e}^{-t_k/h} \left(-\frac{t_k}{h}\right)^{n-1/2} \Gamma\left(-n+\frac{1}{2}, -\frac{t_k}{h}\right). \tag{47}$$

We present typical samples of our numerical calculations in tables 2 and 3. The results in table 2 correspond to the $n = 0$ state as the coupling constant g traces an arc of fixed radius $|g| = \frac{1}{10}$ and decreasing argument from $\arg g = \frac{\pi}{2}$ to $\arg g = -\frac{\pi}{8}$. We have used a [14, 14] Padé approximant, which for $\arg g = \frac{\pi}{2}$ (the centre of the summability sector of the RSPT series) gives an error in the last digit shown. The exact energy reported in the last column has been calculated by the complex dilation method [14] and is correct to all the digits shown.

As we have already discussed, for $0 < \arg g < \frac{\pi}{2}$ the Borel–Padé sum of the pure RSPT series reproduces the exact eigenvalue although, since we keep fixed the Padé approximant and hence the number of terms of the RSPT series being summed, the accuracy decreases as $\arg g$ approaches the Stokes line in the real axis.

For $\arg g < 0$ the Borel–Padé sum of the formally real RSPT power series is just the complex conjugate of the sum for $(-\arg g) > 0$, and the Borel–Padé sums of the exponentially small subseries fully account for the difference in the eigenvalue. Again, since we have kept fixed the number of terms being summed, the accuracy increases as $\arg g$ moves away from the Stokes line.

In these numerical results there are two sources of truncation error: truncation in the Borel summation of each series (through the heuristic analytic continuation furnished by the Padé approximants), and truncation (to third exponentially small order) of the full asymptotic expansion (27). The effect of these truncations is illustrated in table 3, which shows the results of a similar calculation with $|g| = \frac{1}{8}$. Accuracy is more rapidly lost as $\arg g$ approaches the Stokes line from $\arg g > 0$, and is not regained at the same rate as in table 2 when $\arg g$ moves away towards $-\frac{\pi}{8}$.

We would finally like to stress that these results are presented as numerical evidence for the Borel summability of the asymptotic expansion (27), since in this problem the Borel–Padé summation is not a practical alternative to the much more efficient numerical methods for the determination of complex eigenvalues, especially to the complex dilation method [14].

5. Summary

There has been much work on the asymptotic solution of the Schrödinger equation with a polynomial potential and the associated Stokes phenomenon. General results for the Stokes constants can be found in [27], and more specific expressions for special cases of the polynomial in [28] and [29]. In particular, the cubic anharmonic oscillator is trivially equivalent to case (iv) in [29], where convergent series expansions for the corresponding Stokes constants can be found. These series, however, converge very slowly when the transition points are not close together (see p 2712) and are not suitable for solving the eigenvalue problem.

In a recent paper [16] we have shown how to solve this problem for anharmonic oscillators by direct matching of Borel-summable asymptotic expansions obtained from suitable comparison equations. This matching shows that the positive real axis is a Stokes line of the asymptotic expansion of the eigenvalues of the cubic anharmonic oscillator (1), where the expansion changes discontinuously from the Borel summable RSPT power series to a more complicated expansion.

In the present paper we have given an explicit method to calculate to any desired order this new asymptotic expansion, which consists of the RSPT power series plus an infinite sequence of exponentially smaller subseries, where the kth subseries is the kth power of a common exponentially small prefactor times a sum of products of power series and logarithmic terms (the same structure as the multi-instanton expansion conjectured by Zinn-Justin for real potentials with degenerate symmetric minima). We have also implemented a numerical Borel–Padé summation algorithm for the power series which appear in this expansion, and checked

Table 2. Borel–Padé sums of the asymptotic expansions for the $n = 0$ state of the cubic anharmonic oscillator as the coupling constant g traces an arc of fixed radius $|g| = \frac{1}{10}$ and decreasing argument that starts at $\arg g = \frac{\pi}{2}$, crosses the Stokes line at $\arg g = 0$, and goes down to $\arg g = -\frac{\pi}{8}$ where the first Bender–Wu branch point is met.

$\arg g$	Series	[14, 14] Borel–Padé sum	E (exact)
$\frac{\pi}{2}$	RSPT	0.512 538 12	0.512 538 15
$\frac{\pi}{6}$	RSPT	0.494 175 31 − 0.013 063 21i	0.494 175 33 − 0.013 063 20i
$\frac{\pi}{8}$	RSPT	0.490 604 86 − 0.011 351 75i	0.490 604 88 − 0.011 351 76i
$\frac{\pi}{12}$	RSPT	0.487 466 36 − 0.008 530 35i	0.487 465 90 − 0.008 530 31i
$\frac{\pi}{24}$	RSPT	0.485 194 35 − 0.004 652 55i	0.485 197 43 − 0.004 649 99i
$\frac{\pi}{100}$	RSPT	0.484 374 36 − 0.001 155 77i	0.484 374 42 − 0.001 161 38i
0			0.484 316 00 − 0.000 008 06i
$-\frac{\pi}{100}$	RSPT	0.484 374 36 + 0.001 155 77i	
	$+\Delta E_1$	0.484 362 52 + 0.001 144 19i	
	$+\Delta E_2$	0.484 362 52 + 0.001 144 19i	
	$+\Delta E_3$	0.484 362 52 + 0.001 144 19i	0.484 362 59 + 0.001 149 79i
$-\frac{\pi}{24}$	RSPT	0.485 194 35 + 0.004 652 55i	
	$+\Delta E_1$	0.485 197 92 + 0.004 677 90i	
	$+\Delta E_2$	0.485 197 91 + 0.004 677 90i	
	$+\Delta E_3$	0.485 197 91 + 0.004 677 90i	0.485 201 00 + 0.004 675 34i
$-\frac{\pi}{12}$	RSPT	0.487 466 36 + 0.008 530 35i	
	$+\Delta E_1$	0.487 461 21 + 0.008 431 54i	
	$+\Delta E_2$	0.487 461 14 + 0.008 431 58i	
	$+\Delta E_3$	0.487 461 14 + 0.008 431 58i	0.487 460 68 + 0.008 431 54i
$-\frac{\pi}{8}$	RSPT	0.490 604 86 + 0.011 351 75i	
	$+\Delta E_1$	0.490 214 32 + 0.012 101 52i	
	$+\Delta E_2$	0.490 209 93 + 0.012 098 29i	
	$+\Delta E_3$	0.490 209 97 + 0.012 098 25i	0.490 209 98 + 0.012 098 27i

Table 3. Borel–Padé sums of the asymptotic expansions for the $n = 0$ state of the cubic anharmonic oscillator as the coupling constant g traces an arc of fixed radius $|g| = \frac{1}{8}$ and decreasing argument that starts at $\arg g = \frac{\pi}{2}$, crosses the Stokes line at $\arg g = 0$, and goes down to $\arg g = -\frac{\pi}{8}$ where the first Bender–Wu branch point is met.

$\arg g$	Series	[14, 14] Borel–Padé sum	E (exact)
$\frac{\pi}{2}$	RSPT	0.518 760 32	0.518 760 34
$\frac{\pi}{6}$	RSPT	0.492 163 45 − 0.021 081 87i	0.492 163 03 − 0.021 081 21i
$\frac{\pi}{8}$	RSPT	0.486 209 34 − 0.019 154 44i	0.486 210 47 − 0.019 154 90i
$\frac{\pi}{12}$	RSPT	0.480 451 82 − 0.015 314 87i	0.480 411 87 − 0.015 338 72i
$\frac{\pi}{24}$	RSPT	0.475 281 84 − 0.009 592 61i	0.475 417 03 − 0.009 279 23i
$\frac{\pi}{100}$	RSPT	0.472 453 66 − 0.002 751 11i	0.472 847 57 − 0.002 993 41i
0			0.472 398 73 − 0.000 702 62i
$-\frac{\pi}{100}$	RSPT	0.472 453 66 + 0.002 751 11i	
	$+\Delta E_1$	0.471 794 19 + 0.001 476 27i	
	$+\Delta E_2$	0.471 791 70 + 0.001 491 73i	
	$+\Delta E_3$	0.471 791 93 + 0.001 491 55i	0.472 185 37 + 0.001 724 47i
$-\frac{\pi}{24}$	RSPT	0.475 281 84 + 0.009 592 61i	
	$+\Delta E_1$	0.473 502 86 + 0.010 386 44i	
	$+\Delta E_2$	0.473 511 26 + 0.010 359 47i	
	$+\Delta E_3$	0.473 511 57 + 0.010 360 10i	0.473 647 71 + 0.010 055 46i
$-\frac{\pi}{12}$	RSPT	0.480 451 82 + 0.015 314 87i	
	$+\Delta E_1$	0.483 664 96 + 0.018 874 65i	
	$+\Delta E_2$	0.483 712 71 + 0.019 035 48i	
	$+\Delta E_3$	0.483 710 37 + 0.019 045 29i	0.483 667 94 + 0.019 067 94i
$-\frac{\pi}{8}$	RSPT	0.486 209 34 + 0.019 154 44i	
	$+\Delta E_1$	0.500 191 68 + 0.005 502 84i	
	$+\Delta E_2$	0.499 305 31 + 0.002 909 58i	
	$+\Delta E_3$	0.498 653 25 + 0.002 795 66i	0.498 690 10 + 0.002 987 32i

numerically up to third exponentially small order the very likely conjecture that the expansion is Borel summable to the eigenvalues. It might be possible to prove rigorously this summability, at least for small values of $|g|$, from the general results of [10] but, to our knowledge, a complete and mathematically rigorous proof of the required resurgence properties of suitably normalized WKB wavefunctions is still not available. We would finally like to mention as another open problem the proof of the relation between the the perturbation series and the matching function given by equation (19) and the analogous equation valid for quartic oscillators.

Acknowledgments

The financial support of the Universidad Complutense under project PR156/97-7100 and the Comisión Interministerial de Ciencia y Tecnología under project PB98-0821 are gratefully acknowledged.

References

[1] Yang C N and Lee T D 1952 *Phys. Rev.* **87** 404
[2] Lee T D and Yang C N 1952 *Phys. Rev.* **87** 410
[3] Fisher M E 1978 *Phys. Rev. Lett.* **40** 1610
[4] Yaris R, Bendler J, Lovett R A, Bender C M and Fedders P A 1978 *Phys. Rev.* A **18** 1816
[5] Balslev E and Combes J C 1971 *Commun. Math. Phys.* **22** 280
[6] Naimark M A 1964 *Linear Differential Operators* Part II (London: Harrap)
[7] Caliceti E, Graffi S and Maioli M 1980 *Commun. Math. Phys.* **75** 51
[8] Siegert A J F 1939 *Phys. Rev.* **56** 750
[9] Delabaere E and Pham F 1998 *Phys. Lett.* A **250** 25
[10] Delabaere E, Dillinger H and Pham F 1997 *J. Math. Phys.* **38** 6126
[11] Delabaere E and Pham F 1999 *Ann. Inst. Henri Poincaré* A **71** 1
[12] Bender C M and Dunne G V 1999 *J. Math. Phys.* **40** 4616
[13] Bender C M and Wu T T 1969 *Phys. Rev.* **184** 1231
[14] Alvarez G 1995 *J. Phys. A: Math. Gen.* **27** 4589
[15] Simon B 1970 *Ann. Phys., NY* **58** 76
[16] Alvarez G and Casares C 2000 *J. Phys. A: Math. Gen.* **33** 2499
[17] Hoe N, D'Etat B, Grumberg J, Caby M, Leboucher E and Couland G 1982 *Phys. Rev.* A **25** 891
[18] Zinn-Justin J 1981 *Nucl. Phys.* B **192** 125
[19] Zinn-Justin J 1983 *Nucl. Phys.* B **218** 333
[20] Zinn-Justin J 1984 *J. Math. Phys.* **25** 549
[21] Damburg R J and Propin R Kh 1983 *J. Phys. B: At. Mol. Phys.* **16** 3741
[22] Schmid A 1986 *Ann. Phys., NY* **170** 333
[23] Jafarizadeh M A and Fakhri H 1997 *Phys. Lett.* A **230** 157
[24] Jafarizadeh M A, Darabi F and Rastegar A 1998 *Phys. Lett.* A **248** 19
[25] Jafarizadeh M A and Jalalzadeh S 2000 *J. Math. Phys.* **41** 701
[26] Kleinert H and Mustapic I 1996 *Int. J. Mod. Phys.* A **24** 4383
[27] Sibuya Y 1975 *Global Theory of a Second Order Linear Ordinary Differential Equation with a Polynomial Coefficient* (Amsterdam: North-Holland)
[28] Dzieciol A 1992 *J. Math. Phys.* **33** 840
[29] Zhu C and Nakamura H 1992 *J. Math. Phys.* **33** 2697