

Solving the anharmonic oscillator: tuning the boundary condition

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2007 J. Phys. A: Math. Theor. 40 10291

(<http://iopscience.iop.org/1751-8121/40/33/020>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.144

The article was downloaded on 03/06/2010 at 06:10

Please note that [terms and conditions apply](#).

Solving the anharmonic oscillator: tuning the boundary condition

David Leonard and Paul Mansfield

Centre for Particle Theory, Durham University, Durham DH1 3LE, UK

E-mail: david.leonard@durham.ac.uk and p.r.w.mansfield@durham.ac.uk

Received 11 April 2007, in final form 3 July 2007

Published 1 August 2007

Online at stacks.iop.org/JPhysA/40/10291

Abstract

We outline a remarkably efficient method for generating solutions to quantum anharmonic oscillators with an x^{2M} potential. We solve the Schrödinger equation in terms of a free parameter which is then tuned to give the correct boundary condition by generating a power series expansion of the wavefunction in x and applying a modified Borel resummation technique to obtain the large x behaviour. The process allows us to calculate energy eigenvalues to an arbitrary level of accuracy. High degrees of precision are achieved even with modest computing power. Our technique extends to all levels of excitation and produces the correct solution to the double well oscillators even though they are dominated by non-perturbative effects.

PACS number: 02.60.–x

1. Introduction

Harmonic oscillators are a corner-stone of many branches of physics. Consequently, a large variety of methods have been used to study the eigenvalue properties of *anharmonic* oscillators (see [1, 2] and references therein for a general review). High levels of accuracy have always been difficult to achieve due to slow convergence or often non-convergence of asymptotic perturbative expansions. For example, the Bender–Wu [3] expansion of the quartic anharmonic oscillator ground state energy eigenvalue in positive powers of the coupling is known to be divergent for all non-zero values of the coupling. Methods of resumming asymptotic series [4] have been applied to generate approximate eigenvalues [5, 6]. In addition, some types of anharmonic oscillators are dominated by non-perturbative effects such as instantons [7]. More innovative approaches have been required to produce a greater level of accuracy and account for these non-perturbative effects [8–11]. In addition to the numerical approaches, some progress has been made in determining the analytic structure of certain anharmonic oscillators [12, 13]. In particular, [13] outlines a type of anharmonic oscillator which is quasi exactly solvable with certain parts of the spectrum known exactly.

These problems extend into the quantum field theory. For example, the renormalization group implies that the energy eigenvalues in the Yang–Mills theory cannot be solved perturbatively. Strongly coupled theories in particular are hard to deal with by using traditional techniques. Anharmonic oscillators are therefore of great interest because of their applicability in many branches of physics and because their mathematical properties often mirror those of other physical systems.

We will outline a method of constructing solutions to the Schrödinger equation for an anharmonic oscillator of the form

$$-\frac{d^2\Psi}{dx^2} + \rho x^2\Psi + gx^{2M}\Psi = E\Psi, \quad (1)$$

$$\lim_{|x|\rightarrow\infty} \Psi = 0, \quad (2)$$

where x is real and units are defined to absorb Planck's constant and mass such that $\hbar = 2m = 1$. We do this initially by constructing a solution to the differential equation (1) in terms of one free parameter for a given ρ and g . We then vary this parameter until we observe the correct large x behaviour determined by the boundary condition (2) using a contour integral method of resummation. We find the energy eigenvalues with an arbitrary level of accuracy. The process is easily automated to produce very high levels of precision even with modest computing power.

In section 2, we will outline the basic method for the ground state of the quartic oscillator, $M = 2$. In section 3, we will extend the method to produce excited wavefunctions and energy eigenvalues. Finally, in section 4, we will show how this method can be extended to general anharmonic oscillators with an x^{2M} potential as in (1).

2. Tuning for large x

In this section, we will find the ground state wavefunction and energy eigenvalues corresponding to the quartic anharmonic oscillator obtained from (1) by setting $M = 2$. Since the ground state has no nodes, we will construct the wavefunction in the form $\Psi = \exp(W)$. We will make an even-powered x expansion $W = \sum_{n=1}^{\infty} a_n x^{2n}$ since both the potential term and boundary condition are even. The coefficients a_n are then determined in terms of the parameters ρ , g and E via (1). Having chosen two of these parameters, the third must be determined by ensuring the correct boundary condition (2), which implies that $W \sim -\sqrt{g}x^3/3$ for large positive real x . Since our expansion for W in positive powers of x is only valid for small x , we shall resum by analytically continuing x into the complex $s \equiv 1/x$ -plane and using Cauchy's theorem to examine the large x behaviour. We define

$$L(\lambda) = \frac{1}{2\pi i} \frac{1}{\lambda^3} \int_C ds \frac{e^{\lambda s}}{s} W(s), \quad (3)$$

where C is a large circular contour about the origin in the complex s -plane. The large x asymptotic behaviour implied by the differential equation requires $W(s)$ to have a third-order pole at the origin. This contributes a term $-\sqrt{g}/18$ to $L(\lambda)$ by Cauchy's theorem. When the boundary condition is satisfied, we find that any remaining singularities of $W(s)$ lie to the left of the imaginary axis. The contribution from these is exponentially suppressed in $L(\lambda)$ so that in the large λ limit only the singular contribution at the origin remains, $\lim_{\lambda\rightarrow\infty} L(\lambda) = -\sqrt{g}/18$. In reality, (3) is not calculated exactly but by truncating W at some order x^{2N} . Thus,

$$L_N(\lambda) \equiv \frac{1}{2\pi i} \frac{1}{\lambda^3} \int_C ds \frac{e^{\lambda s}}{s} \sum_{n=1}^N \frac{a_n}{s^{2n}} = \sum_{n=1}^N a_n \frac{\lambda^{2n-3}}{\Gamma(2n+1)} \approx L(\lambda), \quad (4)$$

where in the evaluation of the contour integral we used the identity $\int_C ds s^{-n} \exp(\lambda s) = 2\pi i \lambda^{n-1} / \Gamma(n)$ for $n < 0$ [14].

We proceed by finding our x expansion in W and look for the correct behaviour in $L_N(\lambda)$. We will consider solutions with a fixed coupling $g = 1$ and look at the relationship between E and ρ . We do this without loss of generality since our parameters are related by scaling properties of the Hamiltonian, as first noted by Symanzik and discussed in [15]. To help us we will scale $x \rightarrow cx$ ($c \in \mathbb{R}$) in the differential equation (1) in such a way that we are free to place a restriction on our expansion for W . We can choose $k \equiv a_1/a_2$ at least up to a sign, say $k = \pm 4$. Now substituting W into our scaled differential equation and comparing coefficients of x^{2n} :

$$Ec^2 = -2a_1, \quad (5)$$

$$\rho c^4 = 4a_1^2 + 12a_2, \quad (6)$$

$$c^6 = 16a_1a_2 + 30a_3. \quad (7)$$

We eliminate c to find expressions for E and ρ in terms of a_2 and a_3 :

$$E = \frac{-2ka_2}{(16ka_2^2 + 30a_3)^{\frac{1}{3}}}, \quad (8)$$

$$\rho = \frac{4k^2a_2^2 + 12a_2}{(16ka_2^2 + 30a_3)^{\frac{2}{3}}}, \quad (9)$$

whilst for $n \geq 3$ we have

$$a_{n+1} = - \left(\sum_{m=1}^n 4m(n-m+1)a_m a_{n-m+1} \right) / (2(n+1)(2n+1)), \quad (10)$$

giving a_{n+1} in terms of a_2 and a_3 .

Our goal is now to determine a_3 for a given a_2 in such a way that the boundary condition is satisfied. We do this by tuning a_3 until the correct large λ behaviour is observed in $L_N(\lambda)$. To illustrate the process, we shall choose positive k , $k = 4$ and $a_2 = -3/16$. With this sign choice and a_2 we get a zero ρ term. We choose a fairly modest N initially, guess a value of a_3 and then plot $L_N(\lambda)$ and $L_{N-1}(\lambda)$. L_N and L_{N-1} only provide a good approximation to $L(\lambda)$ for values of λ up to the point where they appreciably diverge from each other. Therefore, we restrict our consideration of λ to within this range.

With a_3 too small we encounter a curve rapidly decreasing such as in figure 1(a). With a_3 too large we encounter a curve rapidly increasing as in figure 1(c). An optimal value of a_3 will give a curve flattening as we increase λ as in figure 1(b). We tune a_3 until we achieve this. As a_3 gets closer to its correct value, the exponential behaviour in figures 1(a) and (c) becomes less pronounced within our range of acceptable λ and flatness becomes a less well-defined concept. This determines our level of accuracy for determining a_3 . To improve our accuracy we must increase N in order to consider larger λ . As we consider these larger λ , we again encounter the exponentially increasing/decreasing behaviour which enables us to further tune a_3 to a greater accuracy.

We completed this procedure in this zero ρ case and determined a_3 to six significant figures with $N = 20$. With $N = 100$ we tune a_3 to 30 significant figures, and with $N = 300$ we get

$$a_3 = 0.019\ 360\ 437\ 202\ 459\ 504\ 192\ 019\ 975\ 317\ 212\ 335\ 964\ 255\ 895\ 815\ 493\ 975\ 700\ 276\ 151\ 52, \quad (11)$$

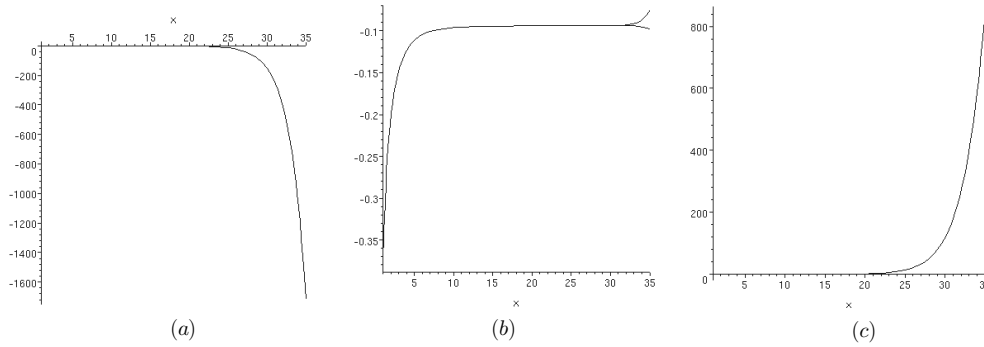


Figure 1. $L_N(\lambda)$ with $N = 19, 20$ for $a_2 = -3/16$: (a) $a_3 = 0.015$ —too small; (b) $a_3 = 0.019\ 3604$ —optimal; (c) $a_3 = 0.025$ —too big.

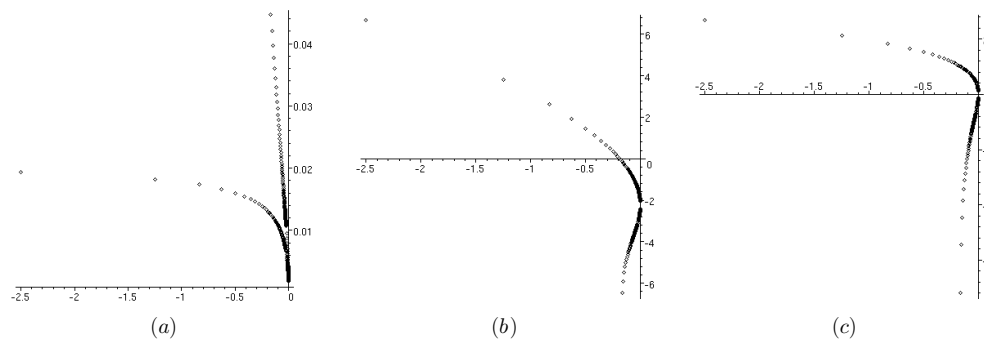


Figure 2. (a) a_3 as a function of a_2 ; (b) ρ as a function of a_2 ; (c) E as a function of a_2 .

to 65 significant figures and we find $L(\lambda) \approx -0.093\ 4774$ which is remarkably close to the predicted value of $-0.093\ 4723$. This calculated figure of a_3 is accurate to the stated number of digits, i.e. 65 significant figures and in agreement with the existing literature [8–11] at least up to 10–16 significant figures they quote. With a_3 determined, we calculate the ground state energy via (8):

$$E_0 = 1.060\ 362\ 090\ 484\ 182\ 899\ 647\ 046\ 016\ 692\ 663\ 545\ 515\ 208\ 728\ 528\ 977\ 933\ 216\ 245\ 2417, \tag{12}$$

again quoted accurately up to 65 significant figures.

Calculating large number of terms is easy, even with modest computing power, given the linear nature of the calculations. The tuning process is easily automated.

We repeat this for various a_2 and plot the results in figures 2 and 3. The two branches correspond to differing sign choices of k . With $k = +4$, we found solutions corresponding to positive energy. The solutions have a positive ρ term for $a_2 < -3/16$ and a negative term for $-3/16 < a_2 \leq 0$. With $k = -4$ and $0 > a_2 > -3/16$, we found negative energy eigenvalues corresponding to $\rho < 0$.

We also verify that non-zero ρ terms correspond to the literature by, for example, calculating the $\rho = -1, g = 1$ energy eigenvalue. In doing so we must tune a_2 with $k = +4$ to obtain the correct ρ term. We found that $a_2 = 0.004\ 048\ 768\ 355\ 681\ 543\ 705$

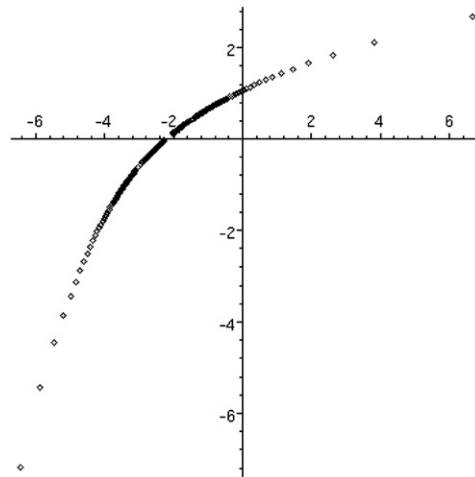


Figure 3. E as a function of ρ .

approximated $\rho = -1$ with an error in the order of 10^{-16} . This value of a_2 is within $\pm 5^{-21}$ of the correct a_2 required to evaluate ρ exactly. The energy eigenvalue produced from this approximate value of a_2 gave us the same eigenvalue as stated in the previous literature to within 16 significant figures available for comparison. This is an example of an eigenvalue where instanton effects would normally dominate and perturbative techniques in \hbar or g would fail.

We now explain why this method of tuning is so sensitive. With $M = 2$, the differential equation (1) without the boundary condition (2) in general has an asymptotic large positive x solution of the form

$$\Psi_l = \exp\left(-\frac{\sqrt{g}}{3}x^3\right) + A \exp\left(\frac{\sqrt{g}}{3}x^3\right). \quad (13)$$

For $A < 0$, Ψ_l has zeros along the real x -axis however for $A > 0$, Ψ_l has zeros in the complex x -plane of the real axis. Our boundary condition (2) requires us to take $A = 0$ in which case Ψ_l has no zeros. We note that for $A \neq 0$, $\log \Psi_l$ will have a pole (possibly part of a cut). Such a pole contribution in the right-half x -plane would spoil our resummation of the large x behaviour. We have numerically determined the location of zeros in our wavefunctions for varying a_3 and shown that they numerically approximate the location of the zeros in our asymptotic large x solution for varying A . Thus, varying a_3 corresponds to varying A in (13). The presence of these poles is responsible for the rapidly increasing/decreasing behaviour for values of a_3 on either side of the correct one due to the exponential factor in (3). It is this behaviour that allows us to select the correct value of a_3 to any specified level of accuracy.

3. Excited states

We now construct the excited states and energy eigenvalues of the quartic anharmonic oscillator. First, we write the q th excited state as $\Psi_q = P_q \Psi_0$, where the energy is $E = E_q + E_0$ and Ψ_0 is the ground state obtained in the previous section. For q odd P_q is odd and for q even P_q is even. We therefore expand $P = \sum_{n=0}^{\infty} c_n x^n$ and sum only over even or odd values of n as appropriate. We set either c_0 or c_1 to unity as a choice of normalization. The remaining

c_n and E_q are then solved for using a recurrence relation in terms of either c_2 or c_3 . This is easily obtained from our new differential equation which comes from substituting Ψ_q into (1) to obtain

$$\frac{d^2 P}{dx^2} + 2 \frac{dW}{dx} \frac{dP_q}{dx} + E_q P_q = 0. \quad (14)$$

This differential equation has two types of large x solution. Either

$$P \sim \exp\left(-\frac{E_q}{2\sqrt{g}x}\right) \quad \text{or} \quad P \sim \exp(2\sqrt{g}x^3). \quad (15)$$

For the correct boundary condition (2), we must choose the first type of solution. We therefore construct

$$T_N(\lambda) \equiv \frac{1}{2\pi i} \int_C ds \frac{e^{\lambda s}}{s} \sum_{n=0}^N \frac{c_n}{s^{2n\alpha}} = \sum_{n=0}^N c_n \frac{\lambda^{2n\alpha}}{\Gamma(2n\alpha + 1)} \quad (16)$$

and look for a flat curve as we tune c_2 or c_3 . We have introduced an additional parameter α by substituting $s \rightarrow s^\alpha$ in $P(s)$ since we find that $P(s)$ has a more limited region of analyticity than $W(s)$ when the boundary condition is satisfied. Here, we only assume that $P(s)$ is analytic in some wedge-shaped region radiating from the origin and containing the real axis. Singularities outside of this region of analyticity are observed in $T_N(\lambda)$ in the form of oscillations. They can however be rotated in the complex s -plane so that they lie to the left of the imaginary axis by reducing the parameter $\alpha < 1$. Having done this the singularities become exponentially suppressed.

We illustrate the process in the zero ρ case for the odd eigenfunctions. There will be multiple values of $\tau \equiv -c_3$ that correspond to different levels of odd excitation. Let us label these τ_n in such a way that $\tau_{n+1} > \tau_n$. With $\tau < \tau_1$ we obtain a rapidly increasing curve however with $\tau_1 < \tau < \tau_2$ we get a rapidly decreasing curve (figure 4). We follow our tuning procedure in the same manner as for the ground state however this time we do not encounter a flat curve but oscillations. These result from a pole or cut outside of our region of analyticity. We could however take a smaller α to recover a flat curve and proceed with our tuning procedure. For $\tau = \tau_1$, we found $\alpha = 0.6$ sufficient to achieve this.

We can produce the full spectrum of eigenvalues by continuing to vary τ . We find that as τ passes through a value τ_n we switch from the rapidly growing to rapidly decreasing behaviour. With $\tau_3 > \tau > \tau_2$, for example, we switch back to the rapidly increasing curve. This alternating behaviour continues with higher excitations as illustrated in figure 4. Exactly the same procedure works for even excitations but we vary c_2 instead of c_3 . Having found an eigenstate through this method, we cannot immediately tell which energy level it corresponds to. To do this, we could plot the prefactor using a similar contour integral method of resummation. We then count the number of nodes. We did this for some of the lower excitations. We calculated excited states up to $q = 39$ with $g = 1$ and again found an exact agreement to the quoted level of accuracy in the previous literature [8–11]. We give some of these eigenvalues in the appendix.

Whilst we cannot attribute the rapidly increasing/decreasing behaviour of $T_N(\lambda)$ to zeros in P_q , we believe that a similar effect is encountered this time due to the large x behaviour. There were two types of the large x behaviour (15) that we were able to derive from the differential equation (14). We chose the first in order to satisfy our boundary condition (2). When c_2 or c_3 do not correspond to an energy eigenstate, we believe that we are obtaining the second type of solution. We note that such large x behaviour would give an additional pole contribution to $T(\lambda)$. Again our resummation is conveniently spoiled. We have numerically verified this result by plotting P for large real values of x for a range of c_3 by exploiting Cauchy's theorem.

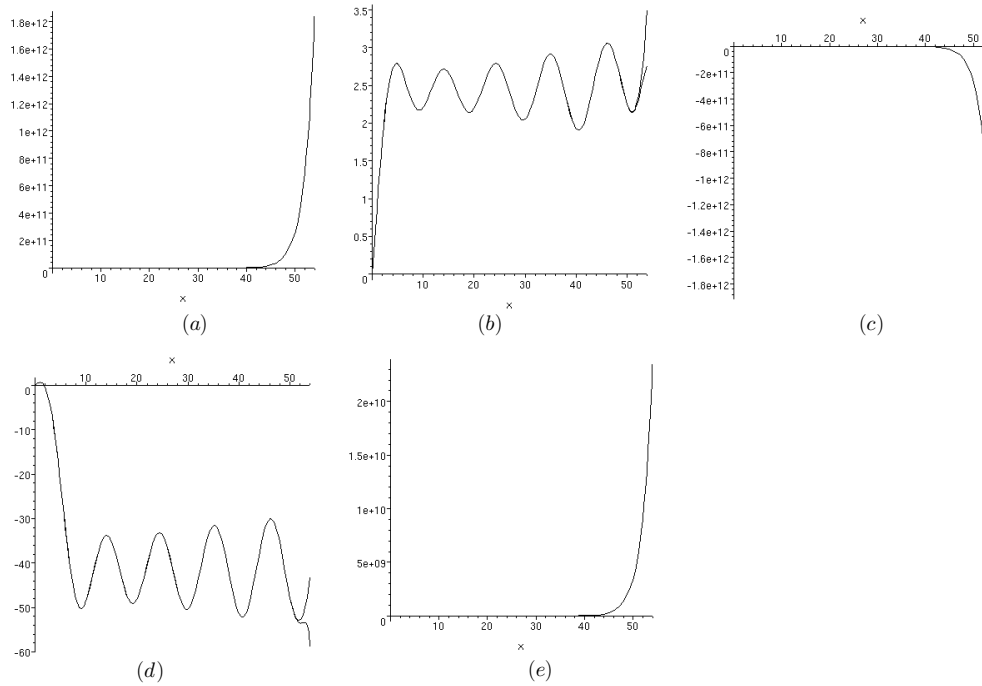


Figure 4. $T(\lambda)$ with an odd prefactor: (a) $\tau = 0.1$; (b) $\tau \approx \tau_1 \approx 0.14584$; (c) $\tau = 0.2$; (d) $\tau \approx \tau_2 \approx 1.99546$; (e) $\tau = 2$.

4. Other potentials

In this section, we consider other values of M in ((1)). The large positive x behaviour is now $W \sim -\sqrt{g}x^{M+1}/(M+1)$. We should therefore redefine our $L_N(\lambda)$ for a general x^{2M} potential

$$L_N^M(\lambda) \equiv \frac{1}{2\pi i} \frac{1}{\lambda^{(M+1)\alpha}} \int_C ds \frac{e^{\lambda s}}{s} \sum_{n=1}^N \frac{a_n}{s^{2n\alpha}} = \sum_{n=1}^N a_n \frac{\lambda^{(2n-M-1)\alpha}}{\Gamma(2n\alpha + 1)}, \tag{17}$$

where again we introduce the parameter α since for $M > 2$ we find that $W(s)$ is analytic within a more limited region. Our prescription of reducing $\alpha < 1$ will therefore be required to rotate these singularities to the left of the imaginary axis where they become exponentially suppressed.

Our a_n are again determined via the differential equation in the same manner as before. We apply the rescaling $x \rightarrow cx$ so that we can fix $a_1/a_2 = \pm 4$ as before. We pick a value of a_2 and use (10) to solve for all of the coefficients in terms of a_{n+1} . This relation now holds for $n \geq 2$ but not $n = M$. In its place we have

$$c^6 g = 2(M+1)(2M+1)a_{M+1} + \sum_{n=1}^M 4n(M-n+1)a_n a_{n-M+1} \tag{18}$$

which is then substituted into (5) and (6) to give E and ρ .

Our procedure is now the same as for the $M = 2$ case. We do find however that for increasing M the region of analyticity becomes smaller and therefore an increasingly small α is required. We performed this procedure with M ranging from 2 to 50 for $g = 1$ and found results matching those in [9] for $M = 2, 3, 4$. Having determined the ground state, we have

applied the technique outlined in section 3 to obtain some excited energy eigenvalues. Again, these are in complete agreement with [9].

5. Summary

We have developed a method for calculating the relationship between the physical parameters of a general x^{2M} anharmonic oscillator. The equations we solve are linear and the process of refining our estimate is easily automated. We can calculate the physical quantities and wavefunctions for all levels of excitation to an arbitrary level of accuracy with an error that can be reduced by increasing the number of terms in our expansion. Using modest computing power, we have demonstrated that high degrees of accuracy can be obtained very quickly. Our technique overcomes some of the deficiencies of traditional perturbative techniques which rely on coupling constant expansions and so do not immediately reveal the effects of instantons, for example. Finally, we note that the analytic continuation of quantum–mechanical systems into complex configuration space has recently been studied in \mathcal{PT} -symmetric quantum mechanics (see [16] and references therein). We believe that understanding the properties of Hermitian theories in the complex plane is still of great interest.

Finally, we note that in the case of the quasi exactly solvable solutions studied in [13] the expansion of both W and P in powers of x becomes truncated. In this type of solution, it is more obvious that the correct boundary condition is satisfied by the large x behaviour. This is trivially reflected in our resummation technique. We have numerically verified that the results of [13] are correctly reproduced for some specific choices of an x^6 polynomial potential.

Appendix

Below we give some of the excited energy eigenvalues for the $\rho = 0$ quartic ($M = 2$) anharmonic oscillator. The results represent accurate eigenvalues rounded to 48 significant figures.

q	$E_0 + E_1$
1	3.799 673 029 801 394 168 783 094 188 512 568 957 766 065 467 33
2	7.455 697 937 986 738 392 156 591 347 185 767 488 137 819 536 750
3	11.644 745 511 378 162 020 850 373 281 370 936 436 550 872 1620
4	16.261 826 018 850 225 937 894 954 430 384 613 534 244 586 5045
5	21.238 372 918 235 940 024 149 711 113 588 636 376 704 832 0597
20	122.604 639 000 999 455 020 762 971 417 615 181 874 976 633 223
38	284.068 590 581 400 743 150 496 281 208 125 064 777 084 713 267
39	293.948 458 266 006 085 433 669 997 483 521 626 303 445 899 275

References

- [1] Hioe F T, Macmillen D and Montroll E W 1978 Quantum theory of anharmonic oscillators: energy levels of a single and a pair of coupled oscillators with quartic coupling *Phys. Rep.* **43** 305
- [2] Müller-Kirsten H J *Introduction to Quantum Mechanics* (Singapore: World Scientific) ISBN 981-256-691-0
- [3] Bender C M and Wu T T 1969 Anharmonic oscillator *Phys. Rev.* **184** 1231
- [4] Hardy G H 1949 *Divergent Series* (Oxford: Oxford University Press)
- [5] Graffi S, Grecchi V and Simon B 1970 Borel summability: application to the anharmonic oscillator *Phys. Lett. B* **32** 631
- [6] Loeffel J J, Martin A, Simon B and Wightman A S 1969 Pade approximants and the anharmonic oscillator *Phys. Lett. B* **30** 656

- [7] Coleman S R 1979 The uses of instantons *Subnucl. Ser.* **15** 805 (also printed in Coleman S R 1985 *Aspects of Symmetry* (Cambridge: Cambridge University Press) ISBN 0-521-31827-0)
- [8] Balsa R, Plo M, Esteve J G and Pacheco A F 1983 Simple procedure to compute accurate energy levels of a double well anharmonic oscillator *Phys. Rev. D* **28** 1945
- [9] Fernandez F M, Meson A M and Castro E A 1985 A simple iterative solution of the Schrödinger equation in matrix representation form *J. Phys. A: Math. Gen.* **18** 1389
- [10] de Saavedra F A and Buenda E 1990 Perturbative-variational calculations in two-well anharmonic oscillators *Phys. Rev. A* **42** 5073
- [11] Yuste S Bravo and Martín Sánchez A 1993 Energy levels of the quartic double well using a phase-integral method *Phys. Rev. A* **48** 3478
- [12] Singh V, Biswas S N and Datta K 1978 The anharmonic oscillator and the analytic theory of continued fractions *Phys. Rev. D* **18** 1901
- [13] Shifman M A 1989 New findings in quantum mechanics (partial algebraization of the spectral problem) *Int. J. Mod. Phys. A* **4** 2897
- [14] Magnus W, Oberhettinger F and Sony R P 1966 *Formulae and Theorems for the Special Functions of Mathematical Physics* 3rd edn (Berlin: Springer)
- [15] Simon B and Dicke A 1970 Coupling constant analyticity for the anharmonic oscillator *Ann. Phys.* **58** 76
- [16] Bender C M 2005 Introduction to PT-symmetric quantum theory *Contemp. Phys.* **46** 277 (Preprint [quant-ph/0501052](https://arxiv.org/abs/quant-ph/0501052))