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Avoided crossings of the quartic oscillator

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Abstract. The phenomenon of avoided crossings of energy levels in the spectrum of quantum systems is well known. However, being of an exponentially small order it is hard to calculate. In particular, this is the case when the potential is generating a Schrödinger equation of a type which is beyond the hypergeometric one. Recently, there have been attempts to understand this phenomenon in connection with Heun-type differential equations. The most famous example of this class is the quantum quartic oscillator which is governed by the triconfluent case of Heun's differential equation. In the following we consider situations where the fourth-order potential has two minima and we calculate the avoided crossings of its eigenvalue curves in dependence on the asymmetry and the barrier height between the two wells. The results are compared with those obtained from an asymptotic approach of the problem for large values of the control parameter that governs the barrier height.

1. Introduction

The phenomenon of avoided and hidden crossings of eigenvalue curves is deeply related to quantum molecular physics and has been well known for decades. As far as we know, Komarov and Slavyanov [8] were the first who attempted to get a mathematical understanding of the phenomenon by means of asymptotic methods. Afterwards, Solov'ev and his coworkers clarified the difficult items, developed new methods of calculation and carried on to discuss not only problems of molecular physics but also collision problems in atomic physics. Their main articles are [5, 14, 17].

The common property of all of these works is that the underlying eigenvalue problem requires the treatment of linear difference equations of at most second order which can be handled by well converging infinite continued-fraction methods. However, physical problems that can be treated within these limits are rare.

Recently there have been efforts to establish a theory on the basis of which one can elaborate methods to treat a much larger class of equations than it was possible hitherto. This theory is deeply connected to the investigation of Heun's class of differential equations (being beyond the hypergeometric one) and mainly contains a classification on the basis of their singularities and the investigation of confluence processes of these singularities (see [15, p 291]) as well as a discussion on the central two-point connection problem of all of the confluent cases of Heun's equation (see [10–12]).

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As a first test on how the new methods work, we have solved the boundary-eigenvalue problem of the general (asymmetric) quartic oscillator as the most famous non-trivial example in quantum mechanics (see [9]). We could get the spectrum of the quartic oscillator with an astonishingly low calculatory effort and an accuracy only limited by the representation of numbers on the computer (see [1]).

However, there was still a basic problem in the above-cited papers of Lay and Bay that was noted in other earlier works (see e.g. [13, p 1253]). It seems that we could recently do an important step here as will be explained in the follows section. The problem can be stated as follows. Suppose that we have a linear physical problem that can be separated such that we eventually have to treat one or more linear ordinary second-order differential equations. Ansatzes of solutions of such types of equations by means of series result in difference equations, the order of which does not depend on the order of the underlying differential equations but on the structure of their singularities. As a consequence the order of the difference equations in general exceeds 2. But only in the case where the order is at most 2 is there a clear division between those particular solutions that generate eigensolutions of the differential equation and those which do not. If the order of the difference equation exceeds 2 we have additional particular solutions the roles of which in the eigenvalue problem is unclear. The relevance of the above-cited papers [1,9–12] by Lay and coworkers consists of clarifying this problem. Here, we go a step further in such that the role of these additional particular solutions can be identified and eventually a conjecture can be formulated and substantiated.

On the basis of the works on Heun's differential equations as cited above, Slavyanov and Veshev (see [16]) applied well approved asymptotic methods to give an asymptotic solution of the problem of avoided crossings of eigenvalue curves for these equations. Our success with the quartic oscillator encouraged us to give a solution of this problem which is exact in the sense that no approximation entered in our theory and thus phenomena of exponentially small orders can be calculated.

The paper is divided into two sections: in the following section we give a brief account of the theory of the central two-point connection problem developed by Lay [10] and first published in [11]. Thereafter, we are concerned with the numerical methods applied in order to solve the boundary-eigenvalue problems which were developed mainly by Bay [2] and first published in [1].

2. Theory

2.1. Two-point connection problems

Basically, there are two types of boundary-value problems for linear ordinary differential equations in the complex domain, namely central and lateral connection problems. While the latter ones occur mainly in Hill-type problems, which will not be considered here, the former ones are related to differential equations with polynomial coefficients. In quantum mechanical situations these are non-periodic potentials of the underlying Schrödinger equation. In the following we give a short discussion of the central two-point connection problem as far as it is necessary to understand our solution of the quartic oscillator.

Consider a linear ordinary homogeneous second-order differential equation with polynomial coefficients thus having the form

$$P_2(z)\frac{d^2u(z)}{dz^2} + P_1(z)\frac{du(z)}{dz} + P_0(z)u(z) = 0 \qquad z \in \mathbb{C}.$$
 (1)

We suppose that the polynomial $P_2(z)$ has no zeros in common either with the polynomials

 $P_1(z)$ or $P_0(z)$. Under this condition the zeros of $P_2(z)$ are the singularities of equation (1) (see [15]). Moreover, the point at infinity can also be a singularity of equation (1). This can be investigated by an inversion of (1)

$$\zeta = \frac{1}{z}$$

and a discussion of the point $\zeta = 0$. In contrast to the ordinary points of a differential equation (1) its singularities play a predominant role in the central two-point connection problems. Whether they are elementary, non-elementary, regular or irregular (this is determined by their s-ranks (see [15])) is crucial for the ansatzes of the local solutions. On one side the type and the total number of singularities determines the type of equation (1) and on the other side the sum of the s-ranks over all the singularities of a differential equation (1) determines the class to which it belongs. For the hypergeometric class of equations for instance the sum of the s-ranks over all the singularities is three and for this class the central two-point connection problems are solved. The next higher class is Heun's equation and its confluent and special cases which we are dealing with here.

It is well known (see e.g. [3, p 210]) that every equation (1) can be transformed into its normal form

$$\frac{\mathrm{d}^2 y(z)}{\mathrm{d}z^2} + Q(z)y(z) = 0 \qquad z \in \mathbb{C}.$$
(2)

When the s-rank of the singularity at infinity is at least 2, we have a quantum-mechanical problem and thus a Schrödinger equation. Suppose now that equation (2) has precisely one singularity located at infinity the s-rank of which is 4. This is the triconfluent case of Heun's differential equation (see [15]) which for $-\infty \leq z \leq +\infty$, $z \in \mathbb{R}$ describes the one-dimensional quartic oscillator

$$\frac{d^2 y(z)}{dz^2} + \left(E + \sum_{k=1}^4 D_k z^k\right) y(z) = 0 \qquad z \in \mathbb{C}, \, D_4 \in \mathbb{R}^-.$$
(3)

The central two-point connection problem for the triconfluent case of Heun's equation (3) can be stated as follows. Consider the ordinary point z = 0 and the singularity at $z = \infty$ connected by the positive real axis. As the local solutions in the vicinity of the singularity tell us, there is one fundamental system consisting of one solution that is exponentially decreasing and one that is merely exponentially increasing. These particular solutions are called 'normal'. Suppose now that we either fix the value of the solution of (3) at the origin or its derivative. In such a situation the central two-point connection problem of equation (3) can be specified as follows. Assuming that the parameters D_k , $k = 1 \div 4$ are fixed we look for those values of the eigenvalue parameter, E, for which the solution of (3) decreases exponentially as z tends to infinity along the positive real axis.

2.2. Jaffé expansions

We have shown [9, 1] that the solution of this problem is crucial for solving the quantum quartic oscillator. In the following we give a brief account of it as well as an interpretation. It is appropriate not to start with equation (3) but with the form that contains only the irreducible parameters: these are the energy parameter, the asymmetry parameter and a parameter that indicates the barrier height between the two wells of the quantum potential. (This parameter is used as a large parameter in parameter asymptotic methods (see [16]).)

$$\frac{d^2}{dz^2}\Psi(z) + \left(-\frac{p^2}{4}(z^2-1)^2 + p[E-az]\right)\Psi(z) = 0.$$
(4)

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We consider equation (4) on the positive real axis $[0, +\infty)$. This equation is solved by means of the ansatz

$$\Psi(z) = \exp\left(\frac{p}{2}(z-z^3)\right)(z+1)^{-a-1}w(z).$$
(5)

Ansatz (5) follows the singularity-analytic approach [10] by introducing an additional singularity. In order to obey the boundary conditions it selects the exponentially decreasing particular solution. Rearranging the singularities for the differential equation governing w(z) we apply a Jaffé transformation (see [11])

$$x := \frac{z}{z+1} \tag{6}$$

that maps the real axis onto the compact interval [0, 1]. Now, we can expand the function w(x) about z = x = 0 in terms of a Jaffé expansion (see [6, 18, 9])

$$w(x) = \sum_{n=0}^{\infty} a_n x^n \tag{7}$$

that is uniformly convergent within the unit circle. At x = 1 there is an irregular singularity the s-rank R of which is R = 4. Therefore, expansions (7) in general diverge at x = 1. As a result for the coefficients a_n of (7) we get an irregular fourth-order difference equation of the Poincaré–Perron type that can be solved recursively:

 a_0, a_1 arbitrary

$$f_{0}(0)a_{2} + f_{-1}(0)a_{1} + f_{-2}(0)a_{0} = 0$$

$$f_{1}(1)a_{3} + f_{0}(1)a_{2} + f_{-1}(1)a_{1} + f_{-2}(1)a_{0} = 0$$

$$f_{2}(n)a_{n+2} + f_{1}(n)a_{n+1} + f_{0}(n)a_{n} + f_{-1}(n)a_{n-1} + f_{-2}(n)a_{n-2} = 0 \qquad n \ge 2$$
where we have for $n \ge 2$
(8)

where we have for $n \ge 2$

$$f_{2}(n) = 1 + \frac{\alpha_{2}}{n} + \frac{\beta_{2}}{n}$$

$$f_{1}(n) = -4 + \frac{\alpha_{1}}{n} + \frac{\beta_{1}}{n}$$

$$f_{0}(n) = 6 + \frac{\alpha_{0}}{n} + \frac{\beta_{0}}{n}$$

$$f_{-1}(n) = -4 + \frac{\alpha_{-1}}{n} + \frac{\beta_{-1}}{n}$$

$$f_{-2}(n) = 1 + \frac{\alpha_{-2}}{n} + \frac{\beta_{-2}}{n}.$$

ρ

The explicit dependences of the coefficients α_i , β_i , $i = -2 \div +2$ on *E*, *p* and *a* are given in [12].

2.3. The Birkhoff set

Equation (8) is linear and thus its fundamental system consists of four particular solutions. A fundamental system can be given explicitly in terms of a diverging series being asymptotic for *n* tending to infinity [4]:

$$s_l(n) = \exp\left(\sum_{m=1}^{m=3} \gamma_{lm} n^{\frac{4-m}{4}}\right) n^{r_l} \left[1 + \frac{C_{l1}}{n^{\frac{1}{4}}} + \frac{C_{l2}}{n^{\frac{2}{4}}} + \cdots\right].$$
(9)

Normal solutions for difference equations of the Poincaré–Perron type in the form of (9) are called Birkhoff solutions. The totality of all Birkhoff solutions is called a Birkhoff set (see [19, p 274]). The dependence of the coefficients on the parameters involved may be seen from [10]. We thus can represent the general solution of (8) symbolically by

$$a_n = \sum_{l=1}^4 L_l s_l(n) \text{ as } n \to \infty.$$
⁽¹⁰⁾

What is important here is that under the condition that

$$\sum_{i=-2}^{i=+2} \alpha_i \neq 0$$

holds, we have

$$\gamma_{11} = \frac{4}{3} \sqrt[4]{-\sum_{i=-2}^{i=+2} \alpha_i} = \frac{4}{3} \sqrt[4]{2\sqrt{-D_4}} = \frac{4}{3} \sqrt[4]{p}$$

$$\gamma_{21} = -\gamma_{11}, \gamma_{31} = i\gamma_{11}, \gamma_{41} = -i\gamma_{11}$$
(11)

and

$$\gamma_{12} = -\frac{2\alpha_2 + \alpha_1 - \alpha_{-1} - 2\alpha_{-2}}{\frac{9}{8}\gamma_{11}^2} = -\frac{1}{2}\sqrt{2\sqrt{-D_4}} = -\frac{1}{2}\sqrt{p}$$

$$\gamma_{22} = \gamma_{12}, \gamma_{32} = -\gamma_{12}, \gamma_{42} = -\gamma_{12}.$$
(12)

 γ_{l3} and r_l , $l = 1 \div 4$ may be seen from [12] but are not of significance here.

From (11) we see that γ_{11} takes a positive real value while γ_{12} takes a negative real one. Therefore, as a result, three of the four Birkhoff solutions (9) increase exponentially as *n* tends to infinity while the fourth one (represented by $s_2(n)$ in (9)) decreases exponentially in the same limit.

2.4. The eigenvalue condition

From Weierstrass's convergence criterion (see e.g. [7, p 412]) we see that the Jaffé expansions (7) converge at x = 1 when all the exponentially increasing particular solutions of (8) are vanishing, i.e. if the condition

$$L_1(E) = L_2(E) = L_3(E) = 0$$
(13)

holds with respect to (10). In this case Abel's limiting value theorem (see e.g. [7, pp 179, 419]) tells us that the solution of (4) in the form of (5) decreases exponentially as $z \to \infty$ and thus is a solution of the quantum mechanical problem. However, condition (13) is too restrictive since it consists of three single conditions while we have only one parameter to vary, namely *E*. If we restrict ourselves to the eigenvalue condition

$$L_1(E) = 0 \tag{14}$$

expansions (7) do no more converge at x = 1 and we can no longer apply Abel's theorem. In order to resolve this dilemma we tried to calculate the eigenvalue curves for the quartic oscillator based on (14). The result was surprising: we got them with an extraordinary accuracy [1]. This suggested that (14) was the exact eigenvalue condition and not only an approximate one. In order to prove this we constructed the eigensolutions on the same basis; and here we could see that, although series (7) diverges at x = 1, they represent the eigen-solutions of the quantum mechanical problem. So, it turned out that with Jaffé expansions we have an *asymptotic* representation of the eigensolutions of the underlying differential equation at the neighbouring singularity x = 1 and *not* a *converging* one.

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It is tempting to generalize the discovery discussed above to central two-point connection problems of linear second-order differential equations (1) with polynomial coefficients between an ordinary point or a regular singularity on one side of the relevant interval and an irregular singularity on the other side the s-rank of which is arbitrary but finite. For the sake of simplicity we assume that the differential equation has no other singularities.

What are the main elements and results? We once again can make an appropriately generalized ansatz of the form of (5), a Jaffé transformation (6) and a Jaffé expansion (7). The result for the coefficients of this expansion will also be irregular difference equations of the Poincaré–Perron-type the order of which is the same as the s-rank of the irregular singularity involved into the connection problem. For this equation a Birkhoff set also exists consisting of Birkhoff solutions the number of which is equal to the order of the difference equation. In the following we formulate a conjecture consisting of two parts. The first part is about the number of the maximum solutions in such a sort of difference equations and the second one is about the meaning of the additional particular solutions of this difference equation occurring in addition to the minimum and the maximum one.

Conjecture.

(1) Under the conditions explained above exactly one maximum solution of the difference equation exists.

(2) The (necessary and sufficient) eigenvalue condition for the connection problem exhibited above is the vanishing of the maximum solution of the difference equation.

We would like to finish this section with a remark. Up to now, we have discussed only the *central two-point connection problem* of the triconfluent case of Heun's differential equation. In order to solve the quantum mechanical *boundary-eigenvalue problem* one has to apply the above-exhibited method twice, namely on the positive and the negative real axis, separately and then to match the corresponding Jaffé expansions at x = 0. This is explained in more detail in the following section.

2.5. The quantum mechanical problem

We write the equation of the quartic oscillator with respect to [16] in the form of (4). For positive real values of p we have two potential wells in the vicinities of $z = \pm 1$, where the value of p corresponds to the height of the barrier located at z = 0 between the two wells. The parameter a represents the asymmetry of the wells.

For the numerical calculations we split the quantum mechanical problem into two parts and look separately for quadratic integrable solutions $\Psi^+(p, a, z)$ on the positive real axis and $\Psi^-(p, a, z)$ on the negative real axis. This corresponds to two two-point connection problems; one between 0^+ and the singularity at $+\infty$, the other between the singularity at $-\infty$ and 0^- . The split problem is connected by the requirements that

$$\Psi^+|_{z=0} = \Psi^-|_{z=0} \tag{15}$$

and

$$\left. \frac{\mathrm{d}\Psi^+}{\mathrm{d}z} \right|_{z=0} = \left. \frac{\mathrm{d}\Psi^-}{\mathrm{d}z} \right|_{z=0}.$$
(16)

From symmetry considerations it follows immediately that $\Psi^{-}(p, -a, -z) \equiv \Psi^{+}(p, a, z)$. Following the approach outlined in section 2.2 we get the ansatz (5) for the two-point connection problem of the positive real axis. Inserting (5) into (4) in conjunction with the Jaffé transformation (6) and (7) we get the fourth-order difference equation (8). The coupling conditions (15) and (16) yield

$$a_0^+ = a_0^- \tag{17}$$

and

$$a_1^+ + \left(1 - \frac{p}{2}\right)a_0^+ = a_1^- + \left(\frac{p}{2} - 1\right)a_0^-$$
(18)

respectively. In the symmetrical case (a = 0) of (4) the even eigenfunctions are represented exclusively by $a_0 \neq 0$, $a_1 = 0$ and the odd ones by $a_0 = 0$, $a_1 \neq 0$. This suggests to define two different coupling conditions for odd and even eigenvalues with an additional auxiliary parameter for each case denoted by V (value) and G (gradient). To satisfy the conditions (17), (18) we write

$$even \to a_0^+ = a_0^- = 1 \qquad a_1^+ = G + \left(1 - \frac{p}{2}\right) \qquad a_1^- = G + \left(\frac{p}{2} - 1\right) odd \to a_0^+ = a_0^- = V \qquad a_1^+ = 1 + \left(1 - \frac{p}{2}\right) V \qquad a_1^- = 1 + \left(\frac{p}{2} - 1\right) V$$
(19)

this may also be applied to the asymmetrical case. Now we proceed as follows. We consider G (or V) as additional parameters of the eigenvalue problem and ask for those energy values $E^+(p, a, G)$ for which the ansatz (5) defines a quadratic integrable solution on the positive real axis (right-hand eigenvalues). In a second step we consider the energy values $E^-(p, a, G)$ yielding a quadratic integrable solution on the negative real axis (left-hand eigenvalues). Since the procedure of calculation is the same for both cases, we confine our discussion to the calculation of the $E^+(p, a, G)$.

3. Numerical results

3.1. Eigenvalues

We now consider the behaviour of the coefficients a_n^+ of series (7) for large *n*. Provided that the parameter E^+ is *not* an eigenvalue, this is governed by the maximum Birkhoff solution $s_1(n)$ (9)–(12), i.e. the coefficients increase merely exponentially. An eigenvalue corresponding to a quadratic integrable $\Psi^+(z)$ is indicated by the vanishing of this maximum solution. Since the contribution of the other Birkhoff solutions at sufficiently large *n* is negligibly small, this is monitored by a *change in sign* of the corresponding coefficients $a_n^+(E^+)$.

In a first step, we have calculated the coefficient $a_{200}^+(E)$ with fixed parameters p, a, G (figure 1) and used the zeros as approximations of the right-hand eigenvalues. (It will be shown below that n = 200 is sufficiently large in order to yield a high numerical accuracy for the eigenvalues.)

For the following it is important to understand that by varying the additional parameters G, V introduced above the zeros and thus the spectrum of the connection problem change continuously.

In figure 2 we display in dependence on the parameter G the right-hand eigenvalues (full curves) and left-hand eigenvalues (dotted curves). The spectrum of the quantum mechanical problem is defined by the totality of the points of intersection of the full and dotted curves. In particular, we see that the even eigenvalues, E_0 , E_2 , E_4 , of the symmetrical case of the quartic oscillator (4) are related to the parameter G of the matching procedure. There are no crossings for the odd ones; to get these we have to consider the coupling condition (19) for the parameter V instead of G.



Figure 1. Coefficient $a_{200}^+(E)$ for the parameters p = 15, a = 0, G = 0. The zeros of this curve are the eigenvalues of the central two-point connection problem on the postive real axis.



Figure 2. Zeros of the function $a_{200}^+(E) = 0$ (see figure 1) in dependence on the parameter *G*. These eigenvalue curves $E_k^{\pm}(G)$ are calculated by Newton's iteration of the coefficient a_{200}^+ . Full curve: E_k^- , dotted curve: E_k^+ . The crossings of each pair of full and dotted curves at G = 0 are the even eigenvalues E_0, E_2, E_4 of the quartic oscillator for p = 15 and a = 0.

The *a*-dependence of the spectrum is obtained by tracing these points of intersection as they move by varying *a*. For calculating the spectrum we have used Newton's iteration procedure to find the zeros of a_n^{\pm} ; n = 200 as well as the points of intersection exhibited in figure 2 as functions of *E*, *p*, *a*. In figure 3 we present the spectrum for the parameter p = 15. For higher energy levels, the gap δE of the avoided crossings increases while with increasing asymmetry parameter *a* the gaps decrease (see table 1). This is in a qualitative agreement with the behaviour predicted in [16].

3.2. Eigenfunctions

Figure 4 shows the coefficients a_n^+ over *n* for the eigenvalue E_0 . For n > 100 the maximum solution indicated by $s_1(n)$ in (7) dominates. Therefore, n = 200 was a



Figure 3. Avoided crossings of the eigenvalue spectrum $E_k(a)$ of the quartic oscillator for the parameter p = 15. The curves are numbered by the index k.

Table 1. The gap $\delta E_{k,k+1}$ of the avoided crossings in dependece on integer values of the parameter *a* and the eigenvalues E_k .

Gap δ <i>E</i>	Asymmetry			
	a = 0	a = 1	a = 2	<i>a</i> = 3
$\delta E_{0,1}$	$7.1 imes 10^{-4}$			
$\delta E_{1,2}$	_	6.2×10^{-3}		
$\delta E_{2,3}$	4.8×10^{-2}	_	$3 \times 5 \ 10^{-2}$	
$\delta E_{3,4}$	—	$7.6 imes 10^{-1}$	—	3.3×10^{-1}



Figure 4. Coefficients $a_n^+(E)$ in dependence on *n* at $E \approx E_0$ for the parameters p = 15 and a = 0.

sufficiently large index for the preceding calculations. For n < 100 we see the oscillating and exponentially increasing but dominated particular solutions of (8) indicated by $s_3(n)$ and $s_4(n)$ in (9). The eigenfunctions Ψ_k (full curves) of (4) can be approximated via





Figure 5. Comparison of the eigenfunctions $\Psi_k(z)$ at the avoided crossing points a = 0 (left-hand side) and a = 1 (right-hand side), of the quartic oscillator (full lines) with an appropriate arrangement of the related eigenfunctions of the harmonic oscillator (dotted curves).

(5). By using only the coefficients a_n^+ for $n \leq 100$ where the maximum solution is not yet predominant but the increasing oscillating solutions already have a marked influence on the series. The dotted curves in figure 5 are drawn for comparison reasons. They give approximations to the eigenfunctions of the quartic oscillator in terms of linear combinations of eigenfunctions ψ_k of harmonic oscillators centred around the two wells of the quartic one. In the following we give more details: first, we consider the left column of pictures. They pertain to the asymmetry parameter a = 0. The dotted curves $f_0(z)$ show the ground state $\Psi_0(z) = \psi_0(z+1) + \psi_0(z-1)$. The dotted $f_1(z)$ displays the first level as $\Psi_1(z) = \psi_0(z+1) - \psi_0(z-1)$. Eventually, the third level is approximated by $\Psi_2(z) = \psi_1(z+1) - \psi_1(z-1)$. The pictures on the right-hand side show the corresponding arrangement for the asymmetry parameter a = 1.

As a conclusion, we can state that our method allows us to cope with exponentially small effects in quantum systems. Moreover, the numerical calculations only require recursive computations and Newton's iteration. In a first step, we could confirm the asymptotic results given by [16]. The application of the method to other problems in the realm of quantum mechanics and mathematical physics in general will be an important issue of further investigations.

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