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Asymptotic and numeric study of eigenvalues of the double confluent Heun equation

W Lay[†], K Bay and S Yu Slavyanov[‡]

Universität Stuttgart, Institut für Theoretische und Angewandte Physik, Pfaffenwaldring S7/VI,
70550 Stuttgart, Germany

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Abstract. The spectrum of the boundary problems related to the double confluent case of Heun's differential equation is studied numerically and by means of asymptotic methods. The calculation is based on an application of the central two-point connection problem for this equation using Jaffé expansions and Birkhoff sets of irregular difference equations of Poincaré–Perron type. The numerical evaluation based on this approach is compared with results of asymptotic calculations showing several quite interesting features of the eigenvalue curves and of the solution of the equation itself.

1. Introduction

The double confluent Heun equation (DHE) originates from the Heun equation—the Fuchsian equation with four singularities—by means of a confluence process when two regular singularities coalesce pair-wise into an irregular one [8]. From the analytical and the numerical side the solutions of the DHE exhibit very specific features that make them useful in some specific physical problems as for instance in gravitational theory [5]. More precisely, in the case of the DHE there are no convergent Frobenius solutions since there are no regular singularities as is normally the case for other special functions. Moreover, the DHE has a rather specific structure of Stokes lines and Stokes domains [7].

In this paper—after a discussion of the differential equation, its generalized Riemann scheme, some basic forms and simple transformations—we give an asymptotic study resulting in the eigenfunctions and eigenvalues which arise in the central two-point connection problem of the two singularities along the real axis. Thereafter, we propose a numeric procedure for computing the eigenvalues. It is based on an extension of Jaffé expansions introduced by Lay [5] and on an algorithm and programming code developed by Bay *et al* [2]. Moreover, we emphasize polynomial solutions which appear at certain restrictions. Either of the two presented approaches give numerical results that are in good agreement with one another.

2. Forms of equations

The canonical form of the double confluent Heun equation (DHE) reads (see [10])

$$z^2 \frac{d^2 y(z)}{dz^2} + (-z^2 + cz + t) \frac{dy(z)}{dz} + (-az + \lambda)y(z) = 0 \quad z \in \mathbb{C}. \quad (1)$$

[†] E-mail address: lay@itap.physik.uni-stuttgart.de

[‡] On leave from the State University of St Petersburg, Department of Computational Physics.

Here, c , a are local parameters defining the behaviour of the solutions at the irregular singularities located at $z = 0$, $z = \infty$; t is a scaling parameter defining the location of the turning points. The parameter λ is the so-called accessory parameter.

The behaviour of the solutions at the singularities is exposed in the corresponding generalized Riemann scheme [11]

$$\begin{pmatrix} 2 & 2 & \\ 0 & \infty & ; z \\ 0 & a & ; \lambda \\ 2-c & c-a & \\ 0 & 0 & \\ t & 1 & \end{pmatrix}. \quad (2)$$

In the first row of the generalized Riemann scheme the s-ranks [10] of the singularities are exhibited. In the second row the locations of the singularities are exposed and in the further rows the characteristic exponents of the solutions are written. According to the values of these characteristic exponents there exist two pairs of local solutions at the singularities of (1) that behave as

$$\begin{aligned} y_1(a, c; z = 0, z) &= 1(1 + o(1)) & y_2(a, c; z = 0, z) &= z^{2-c} e^{t/z} (1 + o(1)) \\ &\text{as } z \rightarrow +0 & & \\ y_1(a, c; z = \infty, z) &= z^{-a} (1 + o(1)) & y_2(a, c; z = \infty, z) &= z^{a-c} e^z (1 + o(1)) \\ &\text{as } z \rightarrow +\infty. & & \end{aligned} \quad (3)$$

Although equation (1) is not written in a self-adjoint form the corresponding singular boundary-eigenvalue problem defined at $t > 0$, $z \in [0, \infty[$ can be posed by the boundary conditions

$$|y(0)| < \infty \quad e^{-z/2} y(z) \rightarrow_{z \rightarrow \infty} 0 \quad (4)$$

the parameter λ playing the role of the eigenvalue parameter.

From (3) it is clear that the eigensolutions of the boundary problem (1)–(4) are proportional to $y_1(a, c; z = 0, z)$ at zero and are proportional to $y_1(a, c; z = \infty, z)$ at infinity. It also follows the necessary condition for an eigensolution to be a polynomial as

$$a = -n \quad n = 0, 1, \dots \quad (5)$$

Beyond the canonical form other forms of the double confluent equation may be appropriate. First, we carry out a transformation to a more reasonable scaling of the independent variable z when the transition points appear at finite distances:

$$t \mapsto t^2 \quad z \mapsto tz \quad \lambda \mapsto t\lambda \quad (6)$$

$$\implies z^2 \frac{d^2 y(z)}{dz^2} + (cz - t(z^2 - 1)) \frac{dy(z)}{dz} + t(-az + \lambda)y(z) = 0. \quad (7)$$

Taking $t(z^2 - 1)$ as the leading term in equation (7) at large values of t one may see that the transition points are located at $z = 0$, $z = -1$, $z = 1$, $z = \infty$. This is even better seen from the normal form of the DHE

$$z^2 \frac{d^2 w(z)}{dx^2} + \left(t \left[\left(\frac{c}{2} - a \right) z + \left(1 - \frac{c}{2} \right) \frac{1}{z} \right] - t^2 \frac{(z^2 - 1)^2}{4z^2} \right) w + t\tilde{\lambda}w = 0 \quad (8)$$

which follows from (7) by means of the substitution

$$y(z) = \exp \left[\frac{t}{2} \left(z + \frac{1}{z} \right) \right] z^{-\frac{c}{2}} w(z) \quad \tilde{\lambda} := \lambda - \frac{c(c-2)}{4t}. \quad (9)$$

For studying boundary-eigenvalue problems the self-adjoint form of the DHE is used conventionally

$$\frac{d}{dz} \left(z^2 \frac{dv(z)}{dz} \right) + \left(t \left[\left(\frac{c}{2} - a \right) z + \left(1 - \frac{c}{2} \right) \frac{1}{z} \right] - t^2 \frac{(z^2 - 1)^2}{4z^2} \right) v + t\tilde{\lambda}v = 0 \quad (10)$$

where

$$w(z) = zv(z). \quad (11)$$

We introduce new parameters

$$a' := a - 1 \quad c' := \frac{c}{2} - 1. \quad (12)$$

In terms of these parameters equation (8) is rewritten as

$$z^2 \frac{d^2w(z)}{dz^2} - \left(t^2 \frac{(z^2 - 1)^2}{4z^2} + t \left(a'z + c' \frac{1 - z^2}{z} \right) \right) w + t\tilde{\lambda}w = 0. \quad (13)$$

Equation (13) does not change under the simultaneous substitutions

$$z \rightarrow -z \quad a' \rightarrow -a' \quad c' \rightarrow -c'. \quad (14)$$

This means that if we have studied the boundary-eigenvalue problem on the positive real half-axis it is no more necessary to study it on the negative real half-axis since the corresponding eigenvalues $\tilde{\lambda}^-$ are obtained from the eigenvalues of the boundary-eigenvalue problem on the positive half-axis $\tilde{\lambda}^+$ with the help of the following formula:

$$\tilde{\lambda}^-(a', c') = \tilde{\lambda}^+(-a', -c'). \quad (15)$$

The forms (8), (10), (13) of the DHE are appropriate for studying asymptotic expansions.

Another form of the DHE is needed in order to perform the numeric algorithm. First, we make the term $-atz$ vanishing in equation (6) by substituting for the new dependent variable

$$y(z) = (z - 1)^a u(z). \quad (16)$$

The corresponding equation for the function $u(z)$ reads

$$z^2 \frac{d^2u(z)}{dz^2} + \left(-tz^2 + t + cz - \frac{2az^2}{z+1} \right) \frac{du(z)}{dz} + \left(-ta - \frac{acz}{z+1} + \frac{a(a+1)z^2}{(z+1)^2} + \tilde{\lambda} \right) u = 0. \quad (17)$$

Equation (17) has the advantage that the required solution has finite limits at both endpoints of the relevant interval $[0, \infty[$.

The next step is the transformation to a new independent variable ξ

$$\xi := \frac{z - 1}{z + 1} \quad (18)$$

in which the points of the complex z -plane convert into the points of the complex ξ -plane according to

$$z \mapsto \xi \Rightarrow -1 \mapsto \infty \quad 0 \mapsto -1 \quad 1 \mapsto 0 \quad \infty \mapsto 1$$

and the original relevant interval $[0, \infty[$ converts into the interval $[-1, 1]$. This transformation leads to the equation

$$(1 - \xi^2)^2 \frac{d^2u(\xi)}{d\xi^2} + \{-8t\xi - 2(1 - \xi^2)[c + (a + 1)(1 + \xi)]\} \frac{du(\xi)}{d\xi} + \{(1 + \xi)[a(a + 1)(1 + \xi) - 2ac] - 4ta + 4t\tilde{\lambda}\}u(\xi) = 0. \quad (19)$$

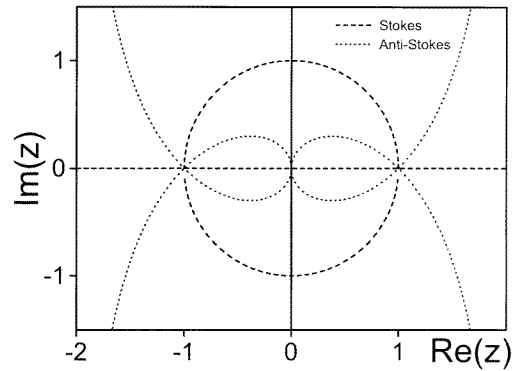


Figure 1. The Stokes set in the complex z -plane.

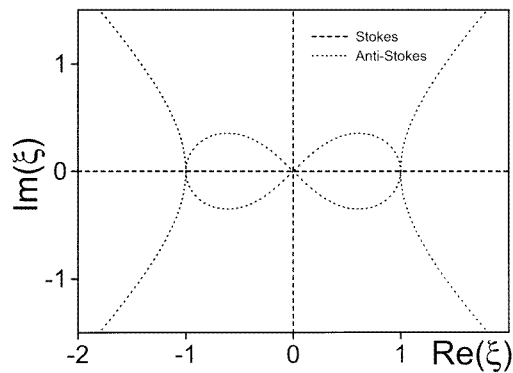


Figure 2. The Stokes set in the complex ξ -plane.

3. Asymptotic study

Here, methods valid in the case of ‘close’ turning points and described in the book [9] are used.

The ‘potential’ related to equations (8), (10), (13) has the shape of two potential wells separated by an irregular singularity at zero.

The Stokes lines defined by

$$\Im \int_{\pm 1}^z \left(\frac{1}{2} - \frac{1}{2z^2} \right) dz = 0 \quad (20)$$

comprise the real axis and the unit circle. The anti-Stokes lines defined by

$$\Re \int_{\pm 1}^z \left(\frac{1}{2} - \frac{1}{2z^2} \right) dz = 0 \quad (21)$$

and represented in polar coordinates r, φ on the z -plane are

$$r(\varphi) = \frac{1 \pm \sin(\varphi)}{\cos(\varphi)}. \quad (22)$$

Stokes as well as anti-Stokes lines on the z - as well as on the ξ -plane are sketched in figures 1 and 2.

We look for asymptotic solutions $w_n(z)$ of the posed boundary problem (13), (4) in the form

$$w_n(z) = \exp \left(-t \int_1^z s_n(z, t) dz \right) \quad (23)$$

where the new semiclassical variable $s(z, t)$ and the eigenvalues $\tilde{\lambda}_n(t)$ are expanded in reciprocal powers of t :

$$s_n(z, t) = \sum_{k=0}^{\infty} s_{nk}(z) t^{-k} \quad (24)$$

$$\tilde{\lambda}_n(t) = \sum_{k=0}^{\infty} \lambda_{nk}(a, c) t^{-k}. \quad (25)$$

It is important to stress that in any approximation when a finite number of terms is taken into account the function on the right-hand side of (23) is single valued. This is a consequence of the quantization condition discussed below.

The quantization condition for the low-lying eigenvalues is given by [3]

$$-t \operatorname{Res}_{|z=1} s_n(t, z) = n \quad (26)$$

where $s_n(t, z)$ is obtained from an asymptotic expansion (24) by recursion processes of

$$z^2 s^2 - \frac{(z^2 - 1)^2}{4z^2} + \frac{1}{t} \left(-\frac{ds(z)}{dz} z^2 - a'z - c' \frac{1 - z^2}{z} + \tilde{\lambda} \right) = 0. \quad (27)$$

The two first terms of the expansion (24) are

$$s_{n0} = \frac{z^2 - 1}{2z^2} \quad s_{n1} = -\frac{c'}{z} + \frac{a' + 1 - \lambda_{n0}}{2(z - 1)} + \frac{a' + 1 + \lambda_{n0}}{2(z + 1)}. \quad (28)$$

The quantization condition (26) gives

$$\lambda_{n0} = 2n + a' + 1. \quad (29)$$

The computation of s_{n2} is rather tiresome and we only give the final result for the correction term to the eigenvalues

$$\lambda_{n1} = \frac{1}{2}n(n + a' + 1) - \frac{1}{4}(a' + 1)(a' + 2) + c'(2 + a' - c'). \quad (30)$$

It is significant and important to realize that the representation (23) is valid all over the complex z -plane without adding another exponential term. The proof follows from the general theory of the Stokes phenomenon as is exhibited in [7]. In this sense the eigenfunctions reveal no Stokes phenomenon. This differs from the behaviour of the eigenfunctions of the other confluent cases of Heun's equations!

The eigenvalues of the boundary-eigenvalue problem on the negative half-axis are obtained by means of the symmetry relation (15). In [12] it has been found that every confluent case belonging to the Heun class, with the exception of the DHE, exhibits the phenomenon of avoided crossings of eigenvalues related to two different potential wells. In the case of DHE we have no phenomenon of avoided crossings but actual crossings of eigenvalue curves which happen approximately at integer values of a' . This does not contradict the theory which forbids degeneration of the eigenfunctions since these eigenfunctions relate to completely disconnected boundary-eigenvalue problems. The numeric study of this phenomenon is given below.

The values of $\tilde{\lambda}$ and a' at which crossings of eigenvalues occur reveal the following very specific feature of the Stokes phenomenon: at these points the eigenfunctions $y_m^-(z)$ and $y_n^+(z)$ related correspondingly to central two-point connection problems on the left and on the right half-axis of the real axis can be taken as asymptotic basis and in this basis the Stokes matrix is trivial (i.e. it is diagonal without mixing matrix elements). As far as the authors know DHE is the only example of such a behaviour.

It is interesting to mention that at

$$a' = -n - 1$$

polynomial eigenfunctions appear for which the formula for the eigenvalues simplifies to

$$\tilde{\lambda}_n = n + \frac{1}{t} \left(-\frac{1}{4}n(n-1) + c'(1-n-c') \right) + \mathcal{O}(t^{-2}). \tag{31}$$

The polynomial solutions cannot arise at crossing points since this would lead to a reduction of the two linearly independent solutions to a unique solution and thus to a degeneration of the fundamental system of the differential equation.

4. Numerical algorithm

The numerical calculation of the eigenvalues and the eigenfunctions within the theory of central two-point connection problems has been extensively exhibited elsewhere (see [1, 2, 4–6, 13]). Therefore, we may restrict ourselves in the following to a brief account.

The relevant solution of (19) may be expanded in a convergent series about $\xi = 0$:

$$u(\xi) = \sum_{k=0}^{k=\infty} g_k \xi^k. \tag{32}$$

The coefficients of (32) obey a fourth-order difference equation of Poincaré–Perron type with an initial condition:

$$\begin{aligned} g_{-1} &= g_{-2} = 0 \\ g_0, g_1 &\text{ arbitrary} \\ 2g_2 + 2(c-a-1)g_1 + (4(t\lambda-ta) + a(a+1) - 2ca)g_0 &= 0 \\ 6g_3 + 4(c-a-1)g_2 + \{-8t - 2(a+1) + 4(t\lambda-ta) + a(a+1) - 2ca\}g_1 \\ &\quad + 2(a(a+1) - ca)g_0 = 0 \\ \left(1 + \frac{\alpha_2}{k} + \frac{\beta_2}{k^2}\right)g_{k+2} + \left(\frac{\alpha_1}{k} + \frac{\beta_1}{k^2}\right)g_{k+1} + \left(-2 + \frac{\alpha_0}{k} + \frac{\beta_0}{k^2}\right)g_k \\ &\quad + \left(\frac{\alpha_{-1}}{k} + \frac{\beta_{-1}}{k^2}\right)g_{k-1} + \left(1 + \frac{\alpha_{-2}}{k} + \frac{\beta_{-2}}{k^2}\right)g_{k-2} = 0 \quad k \geq 2. \end{aligned} \tag{33}$$

The coefficients in (33) are given by

$$\begin{aligned} \alpha_2 &:= 3 & \beta_2 &:= 2 \\ \alpha_1 &:= 2(c-a-1), & \beta_1 &:= 2(c-a-1) \\ \alpha_0 &:= -8t - 2a & \beta_0 &:= 4(t\lambda-ta) + a(a+1) - 2ca \\ \alpha_{-1} &:= -2(c-a-1) & \beta_{-1} &:= -2(a-1)(c-a-1) \\ \alpha_{-2} &:= 2a-3 & \beta_{-2} &:= (a-1)(a-2) \end{aligned}$$

and its Birkhoff set [5, 13] is

$$s_m(k) = \varrho_m^k \exp(\gamma_m k^{\frac{1}{2}}) k^{r_m} \left[1 + \frac{C_{m1}}{k^{\frac{1}{2}}} + \frac{C_{m2}}{k^{\frac{3}{2}}} + \dots \right] \quad m = 1, 2, 3, 4 \tag{34}$$

with

$$\begin{aligned}
 \varrho_m &= 1 & m &= 1, 2 \\
 \varrho_m &= -1 & m &= 3, 4 \\
 \gamma_{m1} &= (-1)^m \sqrt{8t} & m &= 1, 2, 3, 4 \\
 r_1 &= r_2 = -1 + a - \frac{c}{2} \\
 r_3 &= r_4 = -2 - \frac{c}{2}.
 \end{aligned} \tag{35}$$

The general solution of (33) may be put asymptotically in the form

$$g_k \sim \sum_{m=1}^4 L_m s_m(k) \tag{36}$$

with arbitrary coefficients L_i being dependent on all parameters of the differential equation except the index k .

The series (32) have to converge at $\xi = \pm 1$ for λ being an eigenvalue $\tilde{\lambda} = \tilde{\lambda}_n$. Then, it necessarily follows that in this case the asymptotic behaviour of the coefficients g_n must be described by the exponentially decreasing Birkhoff solutions in (34), (36). This leads to the eigenvalue conditions (see [13])

$$L_2(\tilde{\lambda}; t, a', c') = L_4(\tilde{\lambda}; t, a', c') = 0. \tag{37}$$

The consequence of the two eigenvalue conditions in (37) is a set of two eigenvalue parameters $(\tilde{\lambda}; g_1)$ while g_0 in (33) may be normalized to unity without loss of generality. Thus, g_1 in (32) plays the role of a second eigenvalue parameter. As a result of our procedure we have to look for a null-dimensional set $(\tilde{\lambda}_n; g_{1n})$ in a two-parameter space $(\tilde{\lambda}; g_1)$. In the following we exhibit how to convert this problem into an appropriate numerical procedure.

As a first step we solve the difference equation (33) by a *backward recursion* as outlined in [13]. Using the initial conditions

$$g_{N-1}^{(1)} = 1 \quad g_N^{(1)} = g_{N+1}^{(1)} = g_{N+2}^{(1)} = 0$$

for a sufficiently large value N we calculate the coefficients $g_{-1}^{(1)}, g_{-2}^{(1)}$ representing an exponentially *decreasing* particular solution of (33) as $k \rightarrow \infty$ (because of numerical instabilities).

A second linear independent particular solution $g_k^{(2)}$; $k = N, N-1, \dots, 2, 1, 0$ of (33) calculated according to the above-mentioned procedure but which is obtained by starting with a linearly independent initial condition:

$$g_{N-1}^{(2)} = 0 \quad g_N^{(2)} = 1 \quad g_{N+1}^{(2)} = g_{N+2}^{(2)} = 0.$$

The general solution of (33) consisting of the particular ones $g_k^{(1)}$ and $g_k^{(2)}$ is given by

$$g_{-1} = K_1 g_{-1}^{(1)} + K_2 g_{-1}^{(2)} \quad g_{-2} = K_1 g_{-2}^{(1)} + K_2 g_{-2}^{(2)}$$

with two arbitrary and k -independent constants K_1, K_2 .

The eigenvalue conditions (37) are converted into

$$g_{-1} = g_{-2} = 0. \tag{38}$$

The condition (38) is then held by

$$\det A := \begin{pmatrix} g_{-1}^{(1)} & g_{-1}^{(2)} \\ g_{-2}^{(1)} & g_{-2}^{(2)} \end{pmatrix} = 0. \tag{39}$$

Calculating this determinant by a variation of $\tilde{\lambda}$, an eigenvalue is given by its zeros that is indicated by a change of its sign. This zero-condition for the eigenvalue may be detected by a Newton algorithm in the numerical calculations.

5. Results

It is clear that we may consider two relevant intervals of the original equation in z , namely the positive (denoted by $+$) and the negative (denoted by $-$) real half-axis. According to our symmetry considerations we get two sorts of eigenvalue curves in the $\tilde{\lambda} - a'$ -coordinate systems for fixed values of t, c' having the $\tilde{\lambda}$ -coordinate as their symmetry axis.

As can be seen from the difference equation (33) the five-term recurrence relation reduces to a three-term recurrence relation if $c = a + 1$ or $c' = \frac{a'}{2}$, respectively. In this case there is a decoupling between the even and the odd values g_k of (33).

If we interpret the differential equation as a Schrödinger one its potential has the form of a double well the two wells of which are separated by an irregular singularity and thus is the simplest potential that models the suppression of tunnelling fluxes from one well to the neighbouring one. The parameter a in this case is governing the asymmetry between the two wells. If the value of the parameter a exceeds a certain threshold (dependent on the other parameters) there appear eigenvalues lying lower than the minimum of the higher well. It should be mentioned that the corresponding eigenfunctions are generalized polynomials.

In the following we give some examples of our numerical calculations of the nontrivial eigenvalues and eigenfunctions of the double confluent case of Heun's differential equation comparing them with the results of the asymptotics.

Figure 3 shows the behaviour of the determinant (39) in dependence on the eigenvalue parameter $\tilde{\lambda}$. The zeros of this curve give rise to the eigenvalues as indicated. In figures 4–6 we exhibit the six lowest-lying eigenvalue curves $\tilde{\lambda} - a'$ for $c' = 0$ and for $t = 1, t = 3$, and $t = 10$. The ground state is denoted 0 and the excited states are counted according to their

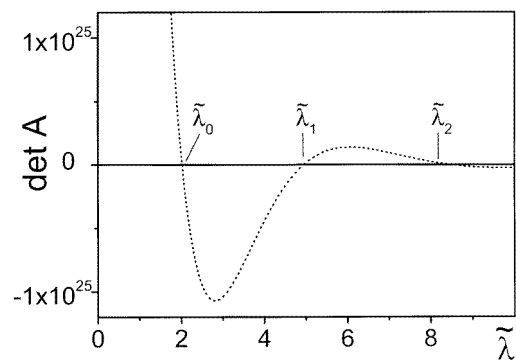


Figure 3. The function $\det A(\tilde{\lambda})$ for $t = 1, a' = 0.5, c' = 0, N = 100$.

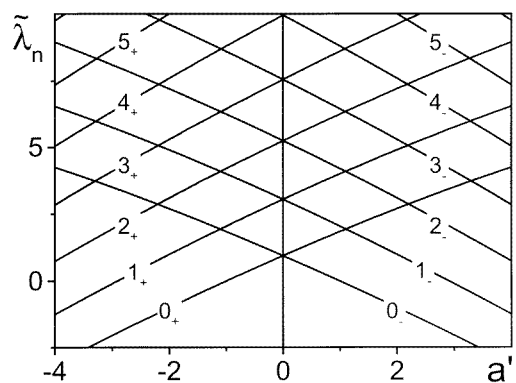


Figure 4. Asymptotic calculation of eigenvalue-curves ($t = 10, c' = 0$).

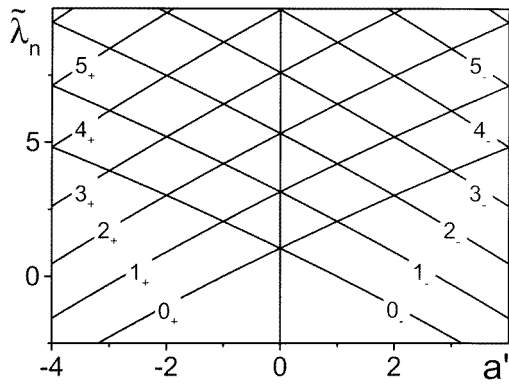


Figure 5. Numeric calculation of eigenvalue-curves ($t = 10, c' = 0$).

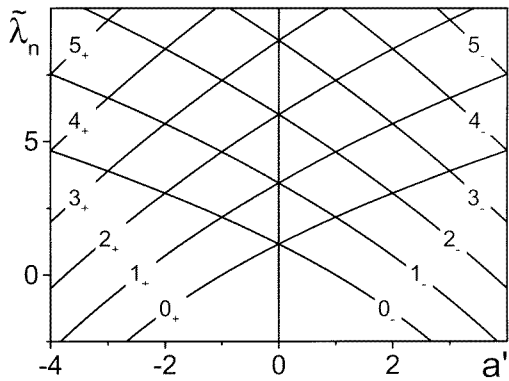


Figure 6. Numeric calculation of eigenvalue-curves ($t = 3, c' = 0$).

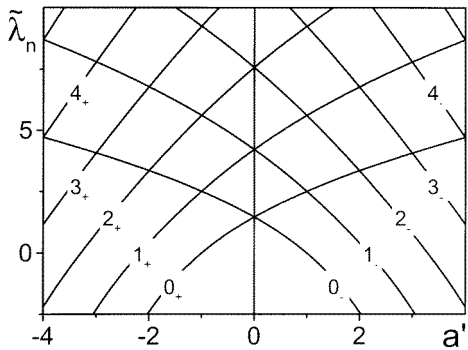


Figure 7. Numeric calculation of eigenvalue-curves ($t = 1, c' = 0$).

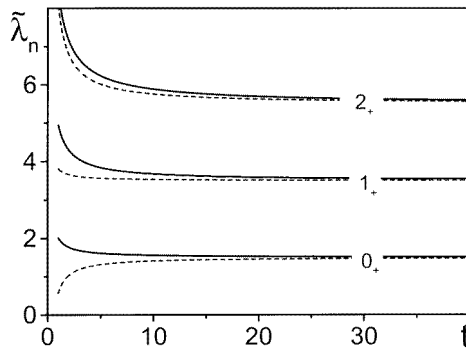


Figure 8. Comparison between asymptotic and numeric calculation in dependence of t for $a' = 0.5, c' = 0$.

number n . The central two-point connection problem on the negative half-axis is denoted by $-$ and on the positive half-axis is denoted by $+$. Figure 7 gives the same curves with the same parameters as figure 6 but as they result from the asymptotic calculation. Thus, it should be compared with figure 6. Figure 8 gives a comparison between the asymptotic calculation for large values of t and the numerical ones in dependence on t for fixed values of $a' = 0.5, c' = 0$ for the three lowest-lying eigenvalues.

6. Conclusion

The double confluent case of Heun's differential equation exhibits several peculiarities: the differential equation has two irregular singularities the s-ranks of both of which is 2. When being placed at the origin and at infinity the differential equation becomes symmetrical with respect to inversion at certain restrictions on the parameters. The generalized Jaffé transformation creates an additional regular singularity at infinity. Such a form is appropriate for solving the central two-point connection problems on the positive as well as on the negative half-axis. The coefficients of the Jaffé expansions obey an irregular fourth-order difference equation of the Poincaré–Perron type. We have shown that the exact eigenvalue-condition for these boundary-eigenvalue problems may be obtained from the Birkhoff set of this difference equation. Moreover, we elaborated a numerical procedure from which we obtained the eigenvalues in dependence on the parameters. It is well understandable but still important to stress that there is no effect of avoided crossing of the eigenvalues in dependence on the asymmetry parameter since—spoken in physical terms—not only the infinite but also the finite singularity is irregular and thus suppresses quantum tunnelling fluxes.

The results of the calculations are compared with an asymptotic investigation of the two-point connection problem. The latter is based on a quantization condition that was developed by SYuS. As is shown graphically even the lowest asymptotic order is in good agreement with the numerical results for values of the large parameter well below 10. In the double confluent case of Heun's differential equation the eigenfunctions reveal no Stokes phenomenon on the entire complex plane of the argument in the sense that at Stokes lines no other asymptotic solution is added to the existing one. As far as we know this has not been discovered before neither for this, nor for any other equation, beyond the hypergeometric class of equations.

Besides the above-mentioned symmetry we discovered another one that occurs with respect to two of the three parameters. As a result the eigenvalue curves of the central two-point connection problems on the positive and on the negative half-axis in dependence on the asymmetry parameter become symmetrical with respect to the energy-parameter axis.

Eventually, we discovered a finite set of generalized polynomial solutions for certain combinations of the parameters. These polynomials are not contained within the set of classical orthogonal polynomials and thus do not seem to be known as yet.

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