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Structure of avoided crossings for eigenvalues related to equations of Heun's class

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Abstract. We study the phenomenon of avoided crossings of eigenvalue curves for boundary value problems related to differential equations of Heun's class. The eigenvalues are given explicitly in asymptotic form taking into account power-type as well as exponentially small terms. It is exhibited that the phenomenon of avoided crossings of eigenvalue curves show a 'periodical' structure in the sense that at any integer value of the additional controlling parameter an infinite (in the sense of a large parameter) number of avoided crossings take place simultaneously. Some relations to other phenomena of the asymptotics of exponentially small terms are discussed at the end of the article.

1. Introduction

The first publication in which the phenomenon of avoided crossings of eigenvalue curves for a specific equation of Heun's class was exposed was the paper by Komarov and Slavyanov [1]. In this paper two Coulomb centres with different charges Z_1, Z_2 have been studied under the condition of a large centre separation. It has been shown that the structure of avoided crossings of the eigenvalue curves in this model reveals much more specific features than in other models studied. This physical problem has been further studied intensively and the original result has been corrected and numerically approved [2–4]. However, the phenomenon has been explained purely on the basis of the properties of Coulomb fields without sufficiently generalizing to other types of potentials.

In recent years several attempts have been made to make a comprehensive study of Heun's class of special functions—next in complexity to the hypergeometric class. Heun's class originates from Heun's equation—the Fuchsian second-order linear homogeneous equation with four singularities—by the confluence process of its singularities and the specialization of its parameters. These attempts result in a book on Heun's equation [5] in which the phenomenon of avoided crossings of eigenvalue curves has been dealt with from the viewpoint of a more general problem than the one discussed above. These studies, however, were still not comprehensive enough because as in the earlier publications, only Coulomb-type potentials were considered.

In this paper we go beyond Coulomb-type potentials, taking into account oscillator-type potentials as well. This forms the basis for us to show that avoided crossings of eigenvalues is a phenomenon for the majority of the confluent cases of Heun's differential equation. It

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occurs when the exponent of the power-type term of the asymptotic factor in the Thomé-type representation of the eigensolution in an integer. This phenomenon should be regarded along with the other discontinuity effects which are typical to ‘exponential asymptotics’, as, for example, the Stokes’ phenomenon.

The basic conjectures of our studies are the following.

• In one-dimensional models there is no single avoided crossing of only two eigenvalue curves. If there exists one avoided crossing of curves then there is a large number of them (in the sense of the large parameter). They occur at certain values of an additional parameter which controls the phenomenon.

• These values of the controlling parameter constitute a periodic sequence.

The present paper cannot be regarded as the source of new or rigorous methods in asymptotics. We use practical methods as proposed in previous publications [1, 6, 7]. We hope that scientists developing more sophisticated and rigorous approaches like resurgence theory and Borel summation [8, 9] will give more ‘polish’ to our presentation.

The effect of avoided crossings has been largely studied in JWKB approximations for more general models than ours [10–12]. It has been used for qualitative and quantitative explanations of many other observable phenomena appearing in different fields of physics including charge transfer, instantons, propagation of waves in underwater acoustics and tropospheric propagation of radio waves.

Without going into detail we stress that our models can be to some extent useful in these problems. In quantum-mechanical language they comprise (i) two interacting oscillators, (ii) two interacting Coulomb-type potentials and (iii) an interacting Coulomb-type potential and an oscillator-type potential. It should be mentioned that the approximation in which we treat the problem is *not* semi-classical (at least in the conventional sense). This fact implies several changes in the computational scheme. For instance, turning points are *not* the branching points of the action function but its poles; quantization conditions reduce to residue calculations, etc.

In the first section of the article we give the major definitions of the equations of Heun’s class. In the following three sections we study three physical models and the last section is devoted to a general discussion of the phenomenon.

2. Heun’s differential equations

The class of special functions most studied in the literature is the hypergeometric one. There are two reasons for this: first, many physical problems can be formulated in terms of functions belonging to this class; and secondly many specific properties of hypergeometric functions can be obtained in terms of explicit formulae. However, this simplicity results in the fact that these functions are short of free parameters and are too simple to explain a lot of phenomena we encounter in physical sciences. Moreover, all parameters in the equations of this class are related to power-type behaviour of the functions at singularities and as a consequence the JWKB expansions are reduced to Thomé-type solutions at the irregular points. The other consequence is that eigenfunctions of hypergeometric type are exclusively expressed in terms of polynomials, and eigenvalues are easily calculated in terms of the order of these polynomials.

In contrast to the hypergeometric class, the equations of Heun’s class are characterized by additional parameters: first, by the parameter related to the scaling of the equation (further denoted by p), and, secondly, by the ‘accessory’ parameter (further denoted by λ). The accessory parameter is characterized by not being related to the local behaviour of solutions at the singularities and is usually regarded as the eigenvalue (spectral) parameter.

As a consequence, there are solutions for equations of Heun's class being constructed as asymptotic series in the large parameter p. They differ from asymptotic solutions in large values of the independent variable z. The eigensolutions are, in general, no longer polynomials but their asymptotics in p at bounded numbers can be expressed in terms of polynomials of the hypergeometric class.

Heun's class originates from the following differential equation:

$$L_z^{(1,1,1;1)}(a,b,c,d;s;\lambda)y(z) = (z(z-1)(z-s)D^2 + (c(z-1)(z-s) \\ +dz(z-a) + (a+b+1-c-d)z(z-1))D + (abz+\lambda))y(z) = 0. \qquad (1)$$

It is a second-order differential equation with four regular points called Heun equation in its canonical natural form. The upper index of the operator L is the s-rank multisymbol of equation (1) showing that there are four singularities of the equation each characterized by an s-rank equal to unity. The definitions of the notions 's-rank' and 's-rank multisymbol' can be found in [13, 15].

The generalized Riemann scheme (GRS) [14] for equation (1) reads

$$\begin{pmatrix} 1 & 1 & 1 & 1 & \\ 0 & 1 & s & \infty & ;z \\ 0 & 0 & 0 & a & ;\lambda \\ 1-c & 1-d & c+d-a-b & b & \end{pmatrix}. \qquad (2)$$

The two lower rows comprise characteristic exponents at regular singularities of (1), the locations of which are exposed in the second row. In the first row the s-ranks of the singularities are given. The notion 'canonical' we used above means that, first, two of the singularities are positioned at $z = 0$ and $z + 1$ and, secondly, one set of characteristic exponents at the finite singularities is zero. The notion 'natural' means that the point at infinity is a singularity of the equation. The relation between the Heun equation in general form and in canonical natural form is similar to the relation between the hypergeometric equation and the general Riemann equation. More precise definitions are given in [15].

Equation (1) does not reveal a phenomenon of avoided crossings and is therefore not studied here. However, several other equations can be derived from it with the help of confluence processes [13].

First comes the single confluent case of Heun's equation (CHE)

$$L_z^{(1,1,2)}(c,d;a;p;\lambda)y(x) = (z(z-1)D^2 + (-pz(z-1) + c(z-1) + dz)D \\ +(-paz+\lambda))y(z) = 0. \qquad (3)$$

In this equation two regular singularities of the original equation (1) at $z = s$ and $z = \infty$ have coalesced resulting in an irregular singularity at infinity having s-rank 2.

Then come two equations: the biconfluent case of Heun's equation (BHE)

$$L_z^{(;3)}(c;a,p;\lambda)y(z) = (zD^2 + (-z^2 - pz + c)D + (-az+\lambda))y(z) = 0 \qquad (4)$$

originating from a confluence process of the regular point at $z = 1$ and the irregular point at $z = \infty$ in (3) resulting in an irregular point at infinity as s-rank 3 and the double-confluent case of Heun's equation (DHE)

$$L_z^{(2;2)}(a,c,p;\lambda)y(z) = (z^2D^2 + (-z^2 + cz - p)D + (-az+\lambda))y(z) = 0 \qquad (5)$$

originating from a confluence of two regular singularities in (3) at $z = 0$ and $z = 1$ resulting in an irregular singularity at zero of s-rank 2.

Lastly comes the triconfluent case of Heun's equation (THE) which arises when all singularities of Heun's equation coalesce into one irregular singularity at infinity having s-rank 4:

$$L_z^{(;4)}(a,p;\lambda)y(z) = (D^2 + (-z^2 - p)D + (-az+\lambda))y(z) = 0. \qquad (6)$$

Throughout equations (3)–(6) we have used one and the same notation for all parameters representing specific properties of its solutions. The first letters of the alphabet $a, b, c \ldots$ denote the parameters which relate to the power-type behaviour of solutions at the singularities, p denotes the parameter which characterizes the chosen scale of the dependent variable; moreover, it plays the role of a large parameter. λ represents the eigenvalue parameter of the corresponding boundary value problem. We hope that this practice is not a source for confusion.

Equations (3)–(6) are distinguished by their s-rank multisymbols which respectively are $\{1, 1; 2\}$, $\{1; 3\}$, $\{2; 2\}$, $\{; 4\}$. As already mentioned above the s-rank multisymbol is used as the upper index of the corresponding operator. The semi-colon in these symbols separates the s-rank of the singularity at infinity from the finite ones.

Equations (1), (3)–(6) can be arranged into the following confluence diagram:

$$L^{(1,1,1;1)} \to L^{(1,1;2)} \to L^{(1;3)} \to L^{(;4)} \to L^{(2;2)}.$$

Besides the equations which are written above there are several others having so-called ramified singularities at infinity [13, 15]. The ramified singularities are characterized by a half-integer s-rank. It is important that these equations do not possess the parameter a occurring in (3), (5)–(6) which—as we shall see later—is controlling the phenomenon of avoided crossings. As a result, the eigenvalue curves of these equations do not show the effect of avoided crossings. Therefore, they are beyond the scope of this article. Moreover, the eigenvalue curves of the DHE also do not reveal the phenomenon of avoided crossings.

The following lemma clarifies the role of the parameter a:

Lemma 1. For every equation (3)–(4), (6) these exists a solution $y(p, z)$ which has the following asymptotic expansion:

$$y(p, z) = \exp(T_n(z)) z^{-a} \sum_{k=0}^{\infty} g_k z^{-k} \tag{7}$$

valid within a Stokes' sector at infinity and where $T_n(z)$ is a polynomial function.

The proof follows from the explicit substitution of (7) into the corresponding equation.

The canonical forms of equations (3)–(6) means that it is not convenient to treat them asymptotically and to interpret them physically. Therefore, in the following sections we transform the equations to their normal (e.g. Schrödinger-type) form. This form has more in common with conventional treatments of second-order equations since the physical notions of the potential and the energy can be used. In these notions the avoided crossings of the eigenvalue curves for the THE appear as a result of the interaction of eigenstates belonging to two oscillator-type potential wells. In the case of BHE avoided crossings appear as a result of the interaction of states in a Coulomb-type potential well and in an oscillator-type potential well. In the case of CHE the states in two Coulomb-type potential wells interact.

3. Avoided crossings for THE

We shall start with the triconfluent case of Heun's equation which possesses fewer parameters than the other equations. Hence, the phenomenon of avoided crossings is expressed in the simplest way (similar to Airy's equation which is the simplest equation revealing Stokes' phenomenon). The substitution

$$y(z) = G(z)w(z) = \exp(z^3/6 + pz)w(z) \tag{8}$$

transforms equation (6) to its normal (or Schrödinger) form characterized by the lack of the term with the first derivative:

$$M_z^{(;4)}w(z) = (D^2 + (\lambda - (a-1)z - (z^2+p)^2/4))w(z) = 0 \qquad (9)$$

where $M^{(;4)} = G^{-1}L^{(;4)}G$. For large values of p there are two different types of potentials $V(z)$:

$$V(z) = (z^2+p)^2/4 + (a-1)z$$

depending on the sign of p: at positive values of p we have a single potential well at zero while at negative values of p we have two potential wells located in the vicinities of $z = \sqrt{-p}$ and $z = -\sqrt{-p}$. Only the latter case is interesting for our purposes and it is studied below. The substitutions

$$p \mapsto -p, p > 0 \qquad z \mapsto \sqrt{p}z \qquad z \mapsto \sqrt{p}\lambda \qquad a-1 \mapsto b \qquad p^{3/2} \mapsto p \qquad (10)$$

lead us to an equation with a large parameter p and two pairs of close turning points in the vicinities of $z = \pm 1$:

$$\tilde{M}_z^{(;4)}w(z) = (D^2 + (p(\lambda - bz) - p^2(z^2-1)^2/4))w(z) = 0. \qquad (11)$$

Each of these pairs can be regarded as a second-order turning point or as a cluster of turning points as well.

The comprehensive study of asymptotic solutions of equations with two close turning points has been proposed by one of the authors and can be found in [7]. The main technical tool is the transformation of the independent variable in terms of formal asymptotic series changing the equation studied to a Weber equation. In the case of equation (1), it is needed in addition to match the solutions obtained in different potential wells.

On the qualitative level three different possibilities should be distinguished. In the first case eigensolutions are concentrated in the right potential well and eigenvalues—up to exponentially small terms—are determined from the quantization condition for the right well. Exponentially small corrections to the eigenvalues are found from matching conditions with the exponentially small representation of the eigensolutions in the left well. The second case is equivalent to the first with the only difference being that the roles of left and right potential wells are interchanged. The third case which is the most interesting for our study is the case when:

(i) the maximal values of the eigensolutions in the left and right potential wells are of the same order of magnitude (in terms of the large parameter),

(ii) the quantization conditions are fulfilled in both potential wells simultaneously,

(iii) there exist two eigenvalues with exponentially small splitting. For the upper of these eigenvalues the corresponding eigensolution has an additional zero in the sub-barrier region.

This latter case is the most interesting for us.

Later on, we denote quantities related to the right potential well by a superscript '+' and to the left one by '−'.

As a first step, power series in p (as a large parameter) for the eigenvalues λ are calculated with the help of the quantization condition at the right well. This condition was first formulated by Wentzel [16] and afterwards rigorously proved in [17]. Although proved under an additional supposition of a single well this quantization condition enables us to obtain the correct result by neglecting the exponentially small terms in the above-mentioned cases (i) and (iii).

The eigensolutions concentrated in the right potential well (neglected exponentially small terms) are sought in the form

$$w^+(p,z) = (u^+(p,z))^{1/2} \exp\left(-p \int (u^+(p,z))^{-1} dz \right) \tag{12}$$

valid for a complete complex neighbourhood of the point $z = 1$. It reflects the fact that this method of asymptotics for the eigenfunctions does not reveal the Stokes' phenomenon. Moreover, it imposes that successive approximations for the function $u^+(p,z)$ can have only poles (not branching points) at $z = 1$. The cancelling of the branching points originating from the multiplier $(u^+(p,z))^{1/2}$ will be discussed below. The use of the function $u^+(z)$ instead of its reciprocal leads to a simpler presentation of the results to our computations.

The substitution of (12) into (11) results in the following equation for $u^+(z)$:

$$p^2(1-(z^2-1)^2u^2/4) + p(\lambda - bz)u^2 + (u''u - u'^2/2)/2 = 0. \tag{13}$$

The condition for the function $w(z)$ to be single-valued imposes the following quantization condition:

$$-p\,\mathrm{Res}_{z=1}(u^+(p,z))^{-1} = n^+ + \tfrac{1}{2} \tag{14}$$

where, once again, we neglect exponentially small terms. Here, n^+ is an integer ($n^+ = 0, 1, \ldots$) which is equal to the number of zeros of the eigensolution $w^+(p,z)$ at the right well and the term $\frac{1}{2}$ is needed for the sake of cancelling the branching behaviour of the multiplier $(u^+(p,z))^{1/2}$ in (12).

If the eigensolution is exponentially small at the right well the relation between the right-hand side and the left-hand side of (14) still holds in the conventional sense of asymptotics but n^+ is no longer an integer. In the latter case n^+ will be substituted for ν^+ below.

We expand $u^+(p,z)$ and λ^+ in a formal asymptotic series of the form

$$u^+(z,p) = \sum_{k=0}^{\infty} u_k(z) p^{-k} \tag{15}$$

$$\lambda^+(p) = \sum_{k=0}^{\infty} \lambda_k p^{-k}. \tag{16}$$

Successive terms in expansions (15), (16) are obtained recursively by equating terms of the same order of p in equations (13), (14). We explicitly mention that in order to obtain λ_k it is sufficient to know k terms of the Taylor expansion for $u_j(z)$, $j = 0, \ldots, k-1$ in the vicinity of $z = 1$.

The first three terms of expansion (15) are

$$\begin{aligned} u_0 &= \frac{2}{z^2-1} \qquad u^1 = (\lambda_0 - bz)u_0^3/2 \\ u_2 &= \frac{u_0}{2}(\lambda_1 u_0^2 + \tfrac{3}{4}(\lambda_0 - bz)^2 u_0^4 + \tfrac{1}{2}(u_0''u_0 - \tfrac{1}{2}u_0'^2)). \end{aligned} \tag{17}$$

The corresponding terms of the expansion for the eigenvalues λ^+ are

$$\begin{aligned} \lambda^+ = \lambda^+(n^+, b) &= (2n^+ + 1) + b \\ &\quad - \frac{1}{p}\left[\frac{3}{2}((2n^+ + 1)^2 + b(2n^+ + 1)) + \frac{b^2}{4} + \frac{1}{8}\right] + \mathrm{O}(p^{-2}). \end{aligned} \tag{18}$$

There is no need to recompute the function $u^-(p,z)$ and the eigenvalue λ^- at the left well, namely at the point $z = -1$. If we make the substitution

$$z \mapsto -z \qquad b \mapsto -b \tag{19}$$

equation (5) stays unchanged. Thus, there is another set of eigenvalues related to the left potential well which can be obtained with the help of (18), (19):

$$\lambda^- = \lambda^+(n^-, -b) = (2n^- + 1) - b - \frac{1}{p}\left[\frac{3}{2}((2n^- + 1)^2 - b(2n^- + 1)) + \frac{b^2}{4} + \frac{1}{8}\right] + \mathrm{O}(p^{-2}). \qquad (20)$$

Here, the integers n^- correspond to the number of zeros of the eigensolution $w^-(p, z)$ at the left potential well.

If we try to draw the curves of the eigenvalues on the b, λ-plain we would immediately find that there are crossings of these curves (straight lines in the first approximation) at the points with coordinates ($b = n^- - n^+, \lambda = n^+ + n^- + 1$) (the λ coordinate in the first approximation). However, it is well known that there are no degenerate eigenvalues for self-adjoint boundary value problems of second-order differential equations. Hence, the contradiction should be settled by taking into account exponentially small terms.

Compared with (12), we now seek the solution of equation (1) in a more sophisticated form:

$$w(z) = [(\xi^+(p, z))']^{-1/2} D_{\nu^+}(\sqrt{p}\xi^+(p, z)) \qquad (21)$$

where $D_\nu(t)$ are parabolic cylinder functions with

$$\xi^+(p, z) = \sum_{k=0}^{\infty} \xi_k^+ p^{-k} \qquad (22)$$

and

$$\nu^+ = n^+ + \delta^+. \qquad (23)$$

We will see later that this form of the solution includes two exponents in the sub-barrier region.

For our goals we need two terms of the asymptotic expansion in the large parameter p of $\xi^+(p, z)$ or as is more convenient for further computations, of $(\xi^+(p, z))^2$. The following holds:

$$((\xi_0^+)^2)' = 2(z^2 - 1) \qquad (\xi_0^+\xi_1^+)' = 2(z^2 - 1)^{-1}[(\nu_0^+ + 1/2)\xi_0'^2 - \lambda_0^+ + bz] \qquad (24)$$

with the solution

$$(\xi^+)^2 = 2\left(\frac{z^3}{3} - z\right) + \frac{4}{3} + \frac{1}{p}[(2\nu_0^+ + 1)(2\ln(z + 1) + \ln(z + 2)) + 2b\ln(z + 2)] + \mathrm{O}(p^{-2}). \qquad (25)$$

The following asymptotic formula for $D_\nu(t), t = \sqrt{p}\xi^+$ including two exponents is valid at large negative values of t (see [7]):

$$D_{\nu^+}(\sqrt{p}\xi^+) = \cos(\pi\nu^+)\exp(-p(\xi^+)^2/4)(-\sqrt{p}\xi^+)^{\nu^+}[1 + \mathrm{O}(p^{-1})] + \frac{\sqrt{2\pi}}{\Gamma(-\nu^+)}\exp(p(\xi^+)^2/4)(-\sqrt{p}\xi^+)^{-\nu^+-1}[1 + \mathrm{O}(p^{-1})]. \qquad (26)$$

This formula lies beyond Poincaré's definition of an asymptotic expansion but has several reasonable explanations in modern exponential asymptotics (optimal asymptotic approximation for a large but fixed parameter [18], resurgence theory [9], variational best approximation [19] etc).

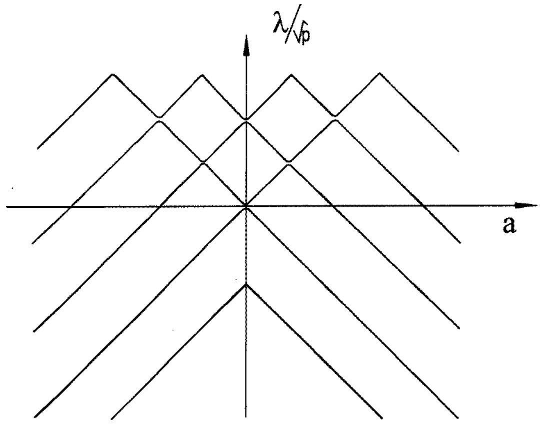

Figure 1.

As a result we obtain for the solution $w^+(p,z)$ of (5) in the sub-barrier region:

$$w^+(p,z) = \cos(\pi\nu^+)\mathrm{e}^{-\frac{p}{6}(z-1)^2(z+2)}\left(\sqrt{\frac{2p}{3}}\right)^{\nu^+}\frac{(z-1)^{\nu^+}}{(z+1)^{\nu^++b+1}}[1+\mathrm{O}(p^{-1})]$$
$$+\frac{\sqrt{2\pi}}{\Gamma(-\nu^+)}\mathrm{e}^{\frac{p}{6}(z-1)^2(z+2)}\left(\sqrt{\frac{2p}{3}}\right)^{-\nu^+-1}\frac{(z+1)^{\nu^++b}}{(z-1)^{\nu^++1}}[1+\mathrm{O}(p^{-1})]. \tag{27}$$

The same solution constructed at the left well and for that sake denoted by $w^-(p,z)$ is

$$w^-(p,z) = \cos(\pi\nu^-)\mathrm{e}^{-\frac{p}{6}(z-1)^2(2-z)}\left(\sqrt{\frac{2p}{3}}\right)^{\nu^-}\frac{(z+1)^{\nu^-}}{(z-1)^{\nu^--b+1}}[1+\mathrm{O}(p^{-1})]$$
$$+\frac{\sqrt{2\pi}}{\Gamma(-\nu^-)}\mathrm{e}^{\frac{p}{6}(z-1)^2(2-z)}\left(\sqrt{\frac{2p}{3}}\right)^{\nu^-}\frac{(z-1)^{\nu^--b}}{(z+1)^{\nu^-+1}}[1+\mathrm{O}(p^{-1})]. \tag{28}$$

Matching the solutions w^+ and w^- we first get the connection formula for ν^+ and ν^-:

$$\nu^+ - \nu^- = -b \tag{29}$$

as a necessary condition. Now the three different behaviours of eigenvalues which have been discussed above may be considered in connection with (29) and the quantization conditions at both wells. Suppose that b is not an integer. Then either $\nu^+ = n^+ + \delta^+$ and the eigenvalues λ are obtained from the quantization condition for the right well (18) or $\nu^- = n^- + \delta^-$ and the eigenvalues λ are obtained from the quantization condition for the left well (20). It is necessary to mention here that the connection formula (29) is compatible with the above-mentioned symmetry property for the eigenvalues λ^+ and λ^-.

The exponentially small corrections δ^+, δ^- are easily found from the condition that the Wronskian of the solutions w^+, w^- should be zero:

$$W(w^+(p,z), w^-(p,z)) = 0. \tag{30}$$

Formally in the case only one of the Γ-functions (27), (28) has a value near its poles.

Another possibility appears when the parameter b is an integer. Then the quantization conditions independently hold at both potential wells. As a result we obtain

$$\nu^+ = n^+ \pm \delta \qquad \nu^- = n^- \pm \delta. \tag{31}$$

The exponentially small value of δ is obtained from equation (30) which turns out to be a quadratic equation at small values of δ. After a simplification it takes the form

$$\delta^2 = \frac{e^{-\frac{4p}{3}} \left(\frac{2p}{3}\right)^{(n^- + n^+ + 1)}}{2\pi(n^-)!(n^+)!}[1 + O(p^{-1})]. \tag{32}$$

Note that this time both Γ-functions in (27), (28) have values near their poles.

The splitting of two eigenvalues $\Delta\lambda$ at the avoided crossing points is given by

$$\Delta\lambda = 4|\delta| = \frac{4e^{-\frac{2p}{3}} \left(\frac{2p}{3}\right)^{(n^- + n^+ + 1)/2}}{[2\pi(n^-)!(n^+)!]^{1/2}}[1 + O(p^{-1})]. \tag{33}$$

Roughly speaking, the values of δ^+, δ^- are of the order of magnitude of δ^2 at the points of avoided crossings but there is still a slight difference of order in the main term of explicit asymptotics.

4. Avoided crossings for BHE

In the case of the biconfluent equation (4) it is convenient to perform the transformation to the Schrödinger from in two steps. First, we transform (4) to the self-adjoint form by means of a substitution similar to (8):

$$y(z) \mapsto w(z) \qquad y(z) = G(z)w(z) = \exp(z^2/4 + pz/2 + (1-c)\ln z/2)w(z) \tag{34}$$

$$M_z^{(1;3)}w(z) = \left(D(zD) + \left[\lambda + \frac{pc}{2} - \left(a - \frac{1+c}{2}\right)z - z(z+p)^2/4 - \frac{(1-c^2}{4z}\right]\right)w(z) = 0 \tag{35}$$

where $M^{(1;3)} = G^{-1}L^{(1;3)}G$. Once again we shall study the case when the large parameter p is negative. For this case we have a typical Coulomb-type behaviour at zero and an oscillator-type well in the vacinity of the point $z = p$. After carrying our the following substitutions:

$$\begin{aligned} &p \mapsto -p,\ p > 0 \qquad z \mapsto pz \qquad \lambda + \frac{pc}{2} \mapsto p\lambda \\ &a - \frac{1+c}{2} \mapsto b \qquad w(z) \mapsto z^{-1/2}w(z) \end{aligned} \tag{36}$$

equation (35) transforms to

$$\tilde{M}_z^{(1;3)}w(z) = \left(D^2 + \left[p\frac{\lambda - bz}{z} - p^2(z-1)^2/4 - \frac{1-(1-c)^2}{4z^2}\right]\right)w(z) = 0. \tag{37}$$

Equation (37) will be studied in the same way as equation (11) but this time we will denote by the sign '+' our constructions in the vicinity of the point $z = 1$ (i.e. related to the oscillator-type potential well) and by the sign '−' the constructions for the Coulomb-type singularity at zero.

By the use of the representation (11) and the quantization condition (12) we obtain as the first terms of an asymptotic power-type expansion for $u^+(p, z)$

$$\begin{aligned} &u_0 = \frac{2}{z-1} \qquad u_1 = (\lambda_0 - bz)\frac{u_0^3}{2z} \\ &u_2 = \frac{u_0}{2}\left[\lambda_1\frac{u_0^2}{z} + \frac{3}{8}(\lambda_0 - bz)^2\frac{u_0^4}{z^2} + (1-(1-c)^2)\frac{u_0^2}{4z^2} + \frac{5}{16}u_0^4\right]. \end{aligned} \tag{38}$$

The corresponding terms of the expansion for the eigenvalues λ^+ are

$$\lambda^+ = \lambda^+(n^+, b) = n^+ + \tfrac{1}{2} + b$$
$$- \frac{1}{p}\left[\frac{3}{2}((n^+ + \tfrac{1}{2})^2 + 2b(n^+ + \tfrac{1}{2})) + \frac{b^2}{2} + \tfrac{1}{4}c(c-2)\right] + \mathrm{O}(p^{-2}). \qquad (39)$$

Here n^+ is a constant indicating the number of zeros of the eigensolutions at the potential well.

Now it is necessary to construct the same terms of the expansions in the vicinity of the Coulomb-type potential well at zero. For this sake in the expressions for $u_k(z)$ we need to change the sign to the opposite for $u_0(z)$. In order to calculate the successive terms of λ^- another quantization condition should be used instead of (14) which takes into account not only zeros of the eigensolutions but also a possible singularity at $z = 0$:

$$-p\,\mathrm{Res}_{z=0}(u^-(p,z))^-1 = n^- + \frac{c}{2}. \qquad (40)$$

Later on, we consider the parameter c being positive [7]. Once again we neglect exponentially small terms. In (40) n^- is an integer ($n^- = 0, 1, \ldots$) which is equal to the number of zeros of the eigensolutions $w^-(p,z)$ at the left Coulomb-type well. Calculations of the residue give the asymptotic expression for λ^-:

$$\lambda^- = n^- + \frac{c}{2} = \frac{1}{p}\left[\frac{3}{4}\left(\left(n^+ + \frac{c}{2}\right)^2 - b\left(n^- + \frac{c}{2}\right)\right) + \frac{c(c-2)}{4}\right] + \mathrm{O}(p^{-2}) \qquad (41)$$

where n^- is an integer indicating the number of zeros of the eigensolutions at the Coulomb-type potential. Unfortunately, there is no simple relation connecting λ^- and λ^+ on the basis of the symmetry properties of the equation.

The study of the solutions at the right well when two exponents are kept is equivalent to the one given in the previous section. So, we only give the formulae corresponding to (24), (25):

$$((\xi_0^+)^2)' = 2(z-1) \qquad (\xi_0^+\xi_1^+)' = \frac{(2\nu^+ + 2b + 1)}{z} \qquad (42)$$

which gives

$$(\xi^+)^2 = z(z-2) + 1 + \frac{1}{p}(2\nu^+ + 2b + 1)\ln z + \mathrm{O}(p^{-2}). \qquad (43)$$

At the Coulomb-type singularity the eigensolution $w^-(p,z)$ is sought in the form

$$w^-(p,z) = (\xi^{-'}(p,z))^{-1/2} M_{\kappa^-,m}(p\xi^-(p,z)) \qquad (44)$$

where $M_{\kappa,m}(t)$ is the bounded solution at zero of the Whittaker equation with $m = (c-1)/2$ and κ^- should be found from matching conditions. The first terms of the asymptotic expansion for ξ^- are

$$\xi^-(p,z) = z(1 - \frac{z}{2}) + \frac{1}{p}\left[\frac{2b - 2\kappa^-}{1-z} - \frac{\kappa^-}{(1-z/2)}\right] + \mathrm{O}(p^{-2}). \qquad (45)$$

In order to match the asymptotic expansions the formula

$$M_{\kappa,m}(p\xi) = \frac{\cos(\pi(m - \kappa + \frac{1}{2}))}{\Gamma(m - \kappa + \frac{1}{2})} \mathrm{e}^{-p\xi/2}(p\xi)^{\kappa}[1 + \mathrm{O}(p^{-1})]$$
$$+ \frac{1}{\Gamma(m + \kappa + \frac{1}{2})} \mathrm{e}^{p\xi/2}(p\xi)^{-\kappa}[1 + \mathrm{O}(p^{-1})] \qquad (46)$$

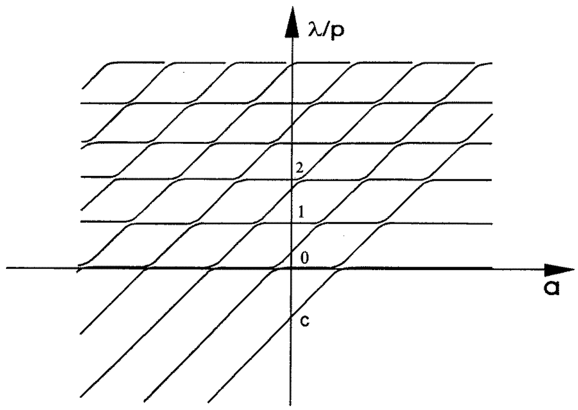

Figure 2.

is needed where both exponents—dominant and recessive— are preserved. Note that in (46) we have chosen a non-standard normalization of the function $M_{\kappa,m}(t)$. After substitutions of (45), (46) in (44) we obtain the asymptotic expression for $w^-(p,z)$ in the sub-barrier region in the form

$$w^-(p,z) = \frac{\cos(\pi(m-\kappa^-+\frac{1}{2}))}{\Gamma(m-\kappa^-+\frac{1}{2})} e^{-p\frac{z}{2}(1-\frac{z}{2})}(1-z)^{b-1/2}\left(\frac{pz}{1-z}\right)^{\kappa^-}[1+O(p^{-1})] + \frac{1}{\Gamma(m+\kappa^-+\frac{1}{2})} e^{p\frac{z}{2}(1-\frac{z}{2})}(1-z)^{-b-1/2}\left(\frac{pz}{1-z}\right)^{-\kappa^-}[1+O(p^{-1})]. \quad (47)$$

The other asymptotic expression for the function $w^+(p,z)$ reads

$$w^+(p,z) = \cos(\pi\nu^+) e^{p\frac{z}{2}(1-\frac{z}{2})-\frac{p}{4}} z^{\nu^++b+1/2}(\sqrt{p}(1-z))^{\nu^+}[1+O(p^{-1})] + \frac{\sqrt{2\pi}}{\Gamma(-\nu^+)} e^{-p\frac{z}{2}(1-\frac{z}{2})+\frac{p}{4}} z^{-(\nu^++b+1/2)}(\sqrt{p}(1-z))^{-\nu^+-1}[1+O(p^{-1})]. \quad (48)$$

As a necessary condition for matching (47) and (48) we have

$$\nu^+ + b + 1/2 = \kappa^-. \quad (49)$$

As in the previous case of the THE the use of the eigenvalue dispersion equation (30) gives rise to two sequences of eigenvalues. One sequence relates to the eigensolutions concentrated at $z = 1$. The other sequence relates to the eigensolutions concentrated at $z = 1$. The asymptotic formulae for these sequences (neglecting exponentially small corrections) have already been obtained by simpler considerations in (39) and (41). Avoided crossings of eigenvalue curves in the $\{\lambda, b\}$-plane occur if $b + (1-c)/2$ is an integer. It is more natural to come back to the original parameters of the BHE and to rewrite this condition as

$$c - a = n^+ - n^-. \quad (50)$$

The splitting of the eigenvalue curves at this point is obtained from (30) as

$$\delta^2 = \frac{e^{-\frac{p}{2}} p^{(2n^-+n^++c+1/2)}}{\sqrt{2\pi}\,\Gamma(c)\Gamma(n^-+c)(n^-)!(n^+)!}[1+O(p^{-1})] \quad (51)$$

with

$$\nu^+ = n^+ \pm \delta \qquad \kappa^- = n^- + \frac{c}{2} \pm \delta. \quad (52)$$

5. Avoided crossings for CHE

As the study of this case has already been published in [5] here we consider it only for the sake of completeness and simply give the initial setting of the problem and the final results for the splittings of the eigenvalue curves at avoided crossings. All technical details of calculations are the same as in the previous sections.

As a starting point for constructing the asymptotics we use the normal form of the CHE in which—for the sake of symmetry—the regular singularities are positioned at $z = \pm 1$ and the parameters c, d in (3) are substituted for m, s according to $c = m+s+1$, $d = m-s+1$:

$$v''(z) + \left(-p^2 + 2p\frac{\lambda - bz}{1-z^2} - \frac{m^2+s^2+2msz-1}{(1-z^2)^2}\right) v(z) = 0. \tag{53}$$

The potential in (53) can be considered as a sum of two one-dimensional Coulomb potentials. Therefore, for $p \mapsto \infty$ the spectrum of the eigenvalues resembles that of two Coulomb spectra.

The eigenvalues related to the eigensolutions concentrated in the left well are presented by the formula

$$\begin{aligned}\lambda^-(p,\chi,b) = {} & (2\chi - b) + \frac{1}{2p}(-2\chi(\chi-b) + \tfrac{1}{2}(m^2+s^2-1)) \\ & + \frac{1}{(2p)^2}(-\chi(\chi-b)^2 + \chi^2(\chi-b) - \tfrac{1}{4}(\chi-b)(1-(m-s)^2) \\ & - \tfrac{1}{4}\chi(1-(m+s)^2)) \\ & + \frac{1}{8p^3}(-3\chi^2(\chi-b)^2 - \chi(\chi-b)^3 - \chi^3(\chi-b) - \chi(\chi-b) \\ & - \tfrac{1}{2}(\chi-b)^2(1-(m-s)^2) - \tfrac{1}{2}\chi^2(1-(m+s)^2) \\ & - \chi(\chi-b)(1-(m^2-s^2)) - \tfrac{1}{16}(1-(m-s)^2)(1-(m+s)^2)) \\ & + \mathrm{O}\left(\frac{1}{p^4}\right)\end{aligned} \tag{54}$$

where

$$\chi = \kappa^-. \tag{55}$$

The asymptotic formula for the eigenvalues $\lambda^+(p,\chi,-b)$ constructed in the right Coulomb-type well is obtained by substitutions

$$\chi \mapsto \kappa^+ \qquad b \mapsto -b \qquad m-s \mapsto m+s \qquad m+s \mapsto m-s$$

in (55). The relation between κ^- and κ^+ that can be regarded as a necessary matching condition reads

$$\kappa^+ = \kappa^- - b. \tag{56}$$

In order to get an equation for the parameter κ^- we calculate the Wronskian of the asymptotic representations of the eigensolutions in the sub-barrier region and put to zero. The corresponding result reads

$$\begin{aligned}& \frac{1}{\pi}\tan\pi\left(\frac{1}{2} + \frac{m+s}{2} - \kappa^+\right)\frac{1}{\pi}\tan\pi\left(\frac{1}{2} + \frac{m-s}{2} - \kappa^-\right) \\ & = \frac{\mathrm{e}^{-4p}(4p)^{2(\kappa^+\kappa^-)}}{\Gamma(\frac{1}{2}+\frac{m+s}{2}+\kappa^+)\Gamma(\frac{1}{2}+\frac{m-s}{2}+\kappa^-)\Gamma(\frac{1}{2}+\kappa^+-\frac{m+s}{2})\Gamma(\frac{1}{2}+\kappa^--\frac{m-s}{2})(1+\mathrm{O}(p^{-1}))}.\end{aligned} \tag{57}$$

The system of two coupled equations (56), (57) can be solved by successive approximations. In general, it leads to two sets of solutions. If we neglect exponentially small terms they are either

$$\kappa^- = n^- + \frac{m-s}{2} = \frac{1}{2} \tag{58}$$

or

$$k^+ = n^+ + \frac{m+s}{2} + \frac{1}{2}. \tag{59}$$

Here n^-, n^+ are integers indicating the eigenvalues of these two sets. The first set is related to the case when the eigenfunctions are concentrated near the left end of the interval $]-1, 1[$. The second set is related to the case when the eigenfunctions are concentrated near the right end.

Avoided crossings of eigenvalue curved in the $\{\lambda, b\}$-plane occur under the condition

$$b = n^- - n^+ - s. \tag{60}$$

The splitting between the eigenvalue curves can be calculated by the formula

$$\Delta\lambda = \frac{2(4p)^{n^+ + n^- + m + 1} \mathrm{e}^{-2p}}{[n^+! n^-! (n^+ + m + s)! (n^- + m - s)!]^{1/2}} (1 + \mathrm{O}(p^{-1})). \tag{61}$$

The asymptotics of the eigensolutions at the points of avoided crossings can be taken as a sum and a difference of the 'local' asymptotic expansions.

6. Discussion

In the following we give some speculations about the origin and possible relations of the phenomenon of avoided crossings to Stokes' phenomenon. We start with confluent cases of hypergeometric equations having unramified singularities at infinity. There are two such equations, namely the confluent hypergeometric equation and the Weber equation for parabolic cylinder functions (note that the famous Airy equation is not among our list since it has a ramified singularity at infinity).

Two formal asymptotic solutions of these equation at the irregular point at infinity are presented in the form

$$y_m(z) = \exp(P_m(z)) z^{-\alpha_m} v_m(z) \qquad m = 1, 2 \tag{62}$$

where $P_m(z)$ are polynomials of the first or second order, respectively, and $v_m(z)$ are formal asymptotic series in powers of z^{-1}. On the radial rays where the imaginary part of P_m becomes zero the Stokes' phenomenon occurs. This means that the two-dimensional vector which represents the actual solution of the equation in terms of the formal asymptotic solutions is multiplied by a matrix. In a proper basis the matrix is triangular. Then it is called the Stokes' matrix. The non-diagonal element of this matrix is called the Stokes' multiplier. This effect has to be considered in the space of two real variables—one large parameter r, the modulus of the independent variable and the other parameter φ, the angle from the above-mentioned ray. On a formal level in this space the Stokes' phenomenon is a discontinuity phenomenon depending on φ. Further structures can be imported to this space for numerical needs. Instead of considering the infinite number of terms of this expansion only a finite number of terms is taken into account. The number of these terms increases when r becomes larger. It leads to an additional non-holomorphic multiplier in the asymptotic expression. This procedure is known as Berry's smoothing of Stokes' phenomenon [20, 21].

All these speculations are valid unless $a = \alpha_1 - \alpha_2$ is an integer. In this latter case the Stokes' matrix becomes diagonal and the Stokes' phenomenon disappears. One of the solutions for this case is the eigensolution. The effect of the disappearing of the Stokes' constant as a function of the parameter a is continuous. It is senseless to investigate the behaviour of the eigenvalues with respect to the parameter a since the eigenvalue is equal to integer a.

Let us discuss Heun's equations now. Formal asymptotic solutions of equations with unramified singularities (which we have studied above) can be represented once again according to lemma 1 in a form similar to (62). The number of free parameters is much larger here. The eigenvalue parameter and the parameter a are different. Besides asymptotics in large values of the argument it is possible to study asymptotics in large values of the parameter p. Therefore, the space of real parameters is four-dimensional and one can study other discontinuity phenomena in this space. We think that the phenomenon of avoided crossings of eigenvalues λ in the space $\{r, a\}$ has many common features with Stokes' phenomenon in the space $\{r, \varphi\}$: both are discontinuity phenomena when different parts of asymptotics (in the sense of exponential asymptotics) change; both are periodic in the second parameter; both appear to be quite general. For this reason further study of the phenomenon of avoided crossings should include estimates of the large terms of the asymptotic expansions in p, appearing in the smoothing function for large but fixed p, resurgence properties in the terms of the transformation to a new space from the space of the parameters $\{p, a\}$.

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