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Determination of singularities of a function from its perturbation expansion

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Abstract

The method for the determination of the position of the pair of complex conjugate branch points suggested in previous studies is generalized here. The method is modified in order to consider cases where the value of the function at the singularity is not real. A method is proposed for the determination of single isolated singularities located either on the real axis or in the complex plane. These methods are applied to three eigenvalue problems, namely the bounded delta-potential atom, the Mathieu equation and the hydrogen atom in a spherically symmetric cavity. We show that the position of the singularities can be obtained very accurately with minimal number of perturbation coefficients. If we take the characteristic polynomial for variational energy levels as an approximate implicit equation, the method can be used for the investigation of the analytic structure of the energy considered as a function of complex coupling constant. In particular, we show that the first singularity appears at the point of intersection of the ground and the first excited states. The second singularity, when the first and second excited states intersect, can be determined either from the expansion at the first singularity or from the expansion of the second excited state at the origin.

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1. Introduction

This paper is in a sense a continuation of the studies in [1, 2]. In [1], a method for the determination of the position of the pair of complex conjugate branch points from the perturbation series was suggested. This step was very important, because when the singularities lie in the complex plane, the perturbation series exhibits oscillatory behaviour. In such a case, the methods of classical analysis for the determination of the radius of convergence of power

series, namely D'Alembert and Cauchy criteria, cannot be used. The method proposed in [1] was further substantially extended in [2] by expanding the function around the singularity beyond the leading term. This method, when applied to the anharmonic oscillator, yielded the position of the singularity and hence the radius of convergence of the series with much greater accuracy and using much fewer perturbation coefficients than with the original formulation given in [1].

The key idea of the method suggested in [1, 2] is the following. Let us consider an implicitly defined function $E(z)$,

$$G(E(z), z) = 0. \quad (1)$$

Let us then expand the function $E(z)$ as a power series in the powers of variable z , namely

$$E(z) = \sum_{n=0}^{\infty} K_n z^n. \quad (2)$$

The behaviour of this perturbation series as well as its radius of convergence is determined by the nature and the position of the closest singularity z_0 of the expanded function to the origin. For the purposes of this paper it is sufficient, although not necessary [1, 2], to assume that the singularity z_0 is a square-root branch point. As argued in [3], this type of singularities is most likely to appear in eigenvalue problems, see also [4, 5]. If the function $E(z)$ is an eigenvalue of a Hermitian operator, it must have the property $E(z^*) = E^*(z)$. It was suggested in [1, 2] to write this function in the form

$$E(z) = b_1[(z - z_0)(z - z_0^*)]^{1/2} + b_3[(z - z_0)(z - z_0^*)]^{3/2} + \dots \\ + b_0 + b_2(z - z_0)(z - z_0^*) + b_4[(z - z_0)(z - z_0^*)]^2 + \dots \quad (3)$$

In this paper, we first investigate this expansion by studying equation (1) around z_0 for the problem discussed in [1]. We find that for eigenvalue problems, it is not very likely that the value of the function at the singularity is real. Consequently, the assumption made in [1, 2], namely that the value of the coefficients b_i in equation (3) is real, is not likely to hold for physically interesting eigenvalue problems. Moreover, we observe that expanding the function in the variable $[(z - z_0)(z - z_0^*)]^{1/2}$ introduces, in most cases, an artificial singularity at $z = \text{Re}(z_0)$. Therefore, equation (3) is not likely to be the best representation of the behaviour of the eigenvalue in the vicinity of its singular points. In fact, assumption (3) is too strong. It is just sufficient for the function $E(z)$ to be an eigenvalue of a Hermitian operator and to have branch points at z_0 and z_0^* .

In this paper, an alternative expression to replace equation (3) is sought. We first consider the existence of a single singularity, whether lying on the real axis or in the complex plane. We derive equations for the determination of the position of the singularity from the perturbation coefficients. An alternative method for determination of the single singularity lying on the real axis was suggested in [6]. We believe that the method described here is somewhat simpler from both a conceptual and a technical point of view. In the development of our method suggested here, we were inspired by the procedure given in [2] and proceeded along its lines.

After establishing this method, it is then natural to ask for its generalization for the case of the pair of complex conjugate singularities. We derive equations for the determination of the position of the singularities from the perturbation series. In addition, the equations derived here asymptotically approach those given in [1, 2]. Therefore, for large order perturbation theory, they yield the same results. However, for low order they differ. Examples presented in this paper illustrate a better accuracy of our method than in [1, 2] for low orders of the perturbation theory.

Finally, a method is suggested for the determination of the analytic structure of the function for which the exact implicit equation is not known. This is the case for most of physically interesting eigenvalue problems. Using the Ritz variation method, we can consider an approximate implicit equation. This approximate implicit equation is obtained by first truncating the Hamiltonian matrix at a certain size and then by calculating its characteristic polynomial. Expanding the energy $E(z)$ in the series in the coupling constant z , equation (2), we obtain the ‘variational’ perturbation coefficients. These ‘variational’ perturbation coefficients differ from the ‘exact’ ones. In the ‘exact’ perturbation theory, we should sum over an infinite number of the intermediate states. For example in the second order of the perturbation theory, we have

$$K_2 = \sum_{n=1}^{\infty} \frac{W_{n0}^2}{E_0^{(0)} - E_n^{(0)}}, \quad (4)$$

where W_{n0} are matrix elements of the perturbation between unperturbed states and $E_n^{(0)}$ are the unperturbed energies. In the ‘variational’ perturbation theory, we sum implicitly only over intermediate states belonging to the truncated basis set. For example in the second order, we have

$$K_2 = \sum_{n=1}^O \frac{W_{n0}^2}{E_0^{(0)} - E_n^{(0)}}, \quad (5)$$

where O is the order of the truncated Hamiltonian matrix. This summation is, however, only implicit since we do not actually use these formulae to calculate the coefficients K_i . These are calculated by expanding the characteristic polynomial into the series in equation (2) and comparing the same powers of z . Consequently, the position of the branch points of the energy determined from the characteristic polynomial for variational energy levels differs from the exact one. However, as argued in [3] for regular perturbation theory, if the exact implicit equation is replaced by the characteristic polynomial for variational eigenvalues, then the analytic structure of the energy considered as a function of the coupling constant is not qualitatively changed. Truncating the Hamiltonian matrix at a certain size and calculating its characteristic polynomial, should thus yield meaningful results. By increasing the size of the Hamiltonian matrix, we achieve a clear improvement of this approximate implicit equation towards the exact one. Since the examples considered in this paper belong to the class of regular perturbation theories, we use the characteristic polynomial for variational eigenvalues for the determination of the analytic structure of the energy considered as a function of the complex coupling constant. Thus, the method given here can serve to investigate the analytic structure of the eigenvalue problem independently to the ones given in [4, 7, 8]. In addition, this method provides a basis for the exact determination of the singularities in the following sense. We find that by expanding the energy at the first branch point where the ground and first excited states intersect, we determine the next branch point where the first and second excited states intersect. This point is identical with the one determined from the expansion of the second excited state of the energy at the origin. It is likely that the third branch point, where the second and third excited states intersect, can be determined either from the expansion of the energy at the point where the first and second excited states intersect or from the expansion of the third excited state of the energy at the origin. Presumably, analogous relations hold for additional singularities. That means that we can reach the n th branch point either by starting from the ground-state energy at the origin $z = 0$ and then passing through the points of the intersection of the ground and first excited states, the first and second excited states and so on or by expanding the n th state of the energy at the origin. This statement is in one-to-one correspondence with the conclusion drawn in [4] for the case of the anharmonic oscillator

described by the Hamiltonian $H = -d^2/dx^2 + x^2/4 + \lambda x^4/4$. The analytic structure of the eigenvalue E considered as a complex function of the coupling constant λ , $E = E(\lambda)$, was investigated by WKB method in the complex plane and it was found that ‘once one knows the ground-state energy of the anharmonic oscillator, one knows all the energy levels by analytic continuation. Or, in other words, the physical energy levels of the anharmonic oscillator for a given positive real λ are the positive real values of $E(\lambda)$ on each of the infinite number of branches of a Riemann surface. Each energy level corresponds to a sheet of this Riemann surface’ [4, p 1242]. It follows from this that all the singularities of the energy should be possible to determine from the perturbation expansion of all the states of the energy at the point $z = 0$. Then we also have the method of determining the number of the branch points of the energy exactly, other than increasing the size of the Hamiltonian matrix and calculating its characteristic polynomial; namely, to calculate the ‘exact’ perturbation expansion for the corresponding number of the energy levels at the point $z = 0$ using standard formulae. For example, in the second order this standard formula reads as equation (4); for higher orders see any textbook on quantum mechanics. We note, however, that there is no clear and simple way how to expand the energy at the branch point within the ‘exact’ perturbation theory. Therefore the results about analytic structure of the energy can be established only within the ‘variational’ perturbation theory, i.e. using characteristic polynomial for variational energies as an approximate implicit equation.

This paper is organized as follows. In section 2 we summarize the method suggested in [1, 2] and apply it, as in [1], to the bounded delta-potential atom. We show that with the improvement of the method given in [2], the position of the branch point can be determined with greater accuracy and considerably fewer perturbation coefficients than with the original method. We note, however, that the value of the function at the singularity is not real. In section 3, we then suggest a method for the determination of the position of the single isolated singularity from the perturbation series. We apply this method first to the Mathieu equation to demonstrate its validity for the case of the singularity lying on the real axis, and then second to the bounded delta-potential atom to demonstrate its validity when the singularity lies in the complex plane. In section 4, the method suggested in section 3 is modified in order to study the pair of complex conjugate branch points. We apply the method to the bounded delta-potential atom and to the hydrogen atom in a spherically symmetric cavity. The analytic structure of the energy of the hydrogen atom in a spherically symmetric cavity considered as a function of the coupling constant that is equal to the product of the nuclear charge and radius of the cavity is, for the first time, explicitly presented here. In the case of the bounded delta-potential atom we compare the performance of the method suggested in section 4 with the methods given in [1, 2]. In the conclusions, the discussion of the method and perspectives of its further development including possible physical applications are outlined.

2. The method

In this section, we first summarize the method proposed in [1, 2] and then apply it to the bounded delta-potential atom. The performance of the improved method [2] is compared with the original one [1]. We point out the shortcoming of both methods.

2.1. Description of the method

As mentioned in the introduction, let us suppose that in the neighbourhood of the branch point z_0 the energy can be written as

$$\begin{aligned}
 E(z) &= b_1[(z - z_0)(z - z_0^*)]^{1/2} + b_3[(z - z_0)(z - z_0^*)]^{3/2} + \dots \\
 &\quad + b_0 + b_2(z - z_0)(z - z_0^*) + b_4[(z - z_0)(z - z_0^*)]^2 + \dots \\
 &= b_1|z_0|(u^2 - 2u \cos \varphi + 1)^{1/2} + b_3|z_0|^3(u^2 - 2u \cos \varphi + 1)^{3/2} + \dots \\
 &\quad + b_0 + b_2|z_0|^2(u^2 - 2u \cos \varphi + 1) + b_4|z_0|^4(u^2 - 2u \cos \varphi + 1)^2 + \dots, \tag{6}
 \end{aligned}$$

where b_i are supposed to be real constants, $u = z/z_0$ and $\varphi = \arg z_0$.

As shown in [2, 9], this series expansion leads to the following behaviour of the perturbation coefficients K_n ,

$$K_n = A \frac{\cos(n\varphi + \delta)}{|z_0|^n n^{3/2}} [1 + O(1/n)]. \tag{7}$$

The oscillatory character of these coefficients prevents the use of D'Alembert or Cauchy convergence criteria. To determine the radius of convergence, we make use of the fact that, as observed in [2], the function $(u^2 - 2u \cos \varphi + 1)^{\alpha_i}$ is the generating function of the Gegenbauer polynomials $C_n^{(-\alpha_i)}(\cos \varphi)$ [10]:

$$(u^2 - 2u \cos \varphi + 1)^{\alpha_i} = \sum_{n=0}^{\infty} u^n C_n^{(-\alpha_i)}(\cos \varphi), \tag{8}$$

where $\alpha_1 = \frac{1}{2}, \alpha_2 = \frac{3}{2}$ and so on. The Gegenbauer polynomials satisfy the following recurrence relation [10]:

$$(n - 2\alpha_i - 1)C_{n-1}^{(-\alpha_i)} - 2(n - \alpha_i)(\cos \varphi)C_n^{(-\alpha_i)} + (n + 1)C_{n+1}^{(-\alpha_i)} = 0. \tag{9}$$

The terms in equation (3) with integer powers do not influence the large-order behaviour of the K_n coefficients. Consequently, the radius of convergence is not affected by these terms with integer powers. Thus, comparing equations (2), (3) and (8), we get the following expression for the K_n coefficients at large-order, namely

$$K_n = \sum_{i=1}^j x_n^{(i)}, \tag{10}$$

where j is the number of terms with half integer power in equation (3) and

$$x_n^{(i)} = \frac{b_{2i-1}}{|z_0|^{n-2i+1}} C_n^{(-\alpha_i)}(\cos \varphi). \tag{11}$$

Substituting the polynomials $C_n^{(-\alpha_i)}$ from equation (11) into equation (9) yields

$$(n - 2\alpha_i - 1)x_{n-1}^{(i)} - 2(n - \alpha_i) \operatorname{Re}(z_0)x_n^{(i)} + (n + 1)|z_0|^2 x_{n+1}^{(i)} = 0, \tag{12}$$

where we used the fact that $\operatorname{Re}(z_0) = |z_0| \cos \varphi$. In order to implement the method, we have to consider equation (10) for n running from $(n_0 - 1)$ to $(n_0 + 2j)$, equation (12) for i running from 1 to j , and n running from n_0 to $(n_0 + 2j - 1)$. The choice of n_0 and j is arbitrary, but the accuracy of the final results strongly depends on these values. To improve the accuracy, we should increase n_0 as well as j . However, it is of interest to find the lowest values of these parameters that yield meaningful, i.e. accurate enough, final results. This is because, in more complicated perturbation problems, the calculation of the perturbation coefficients poses serious computational problems. For this reason, the motivation of this paper was to minimize the number of such coefficients rather than to obtain the best possible final results.

From a computational point of view, it is interesting to note that this procedure requires the solution of a system of $2j^2 + 2j$ linear equations with $2j^2 + 2j$ unknowns $x_n^{(i)}$, as well as the solution of a system of two nonlinear equations with two unknowns $\operatorname{Re}(z_0)$ and $|z_0|^2$. The solution of the linear system is obtained using a MAPLE procedure while the solution of the nonlinear system requires the application of the two-dimensional Newton–Raphson method. After determining z_0 and $x_n^{(i)}$, we can calculate the coefficients b_{2i-1} from equation (11) for $n = n_0$.

Table 1. The position of branch point of the bounded delta-potential atom calculated by the method described in section 2. n_0 is equal to 5 and j denotes the number of terms taken in equation (10). The number of the needed perturbation coefficients is $n_0 + 2j$ for $j > 1$ and $n_0 + 1$ for $j = 1$. The percentage error is calculated with respect to the exact value $z_0 = 1.895\,282\,288 + i3.719\,436\,139$. This result is obtained with 100 perturbation coefficients and taking eight terms in equation (10), see also [1].

j	$ z_0 $ (error (%))	φ (error (%))
1	4.765 571 544 (14.1)	1.039 111 512 (5.49)
2	4.259 363 383 (2.03)	1.100 688 790 (0.10)
3	4.206 330 302 (0.76)	1.097 088 165 (0.22)
4	4.188 992 766 (0.34)	1.096 816 518 (0.24)
5	4.181 378 948 (0.16)	1.097 128 616 (0.21)

2.2. Bounded delta-potential atom

To illustrate the method described above, let us consider, as in [1], the one-dimensional bounded delta-potential atom

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} - Z\delta(x) \right] \psi(x) = \tilde{E}\psi(x). \quad (13)$$

Here we impose the boundary condition $\psi(\pm L) = 0$, because the particle moves inside impenetrable walls fixed at $x = \pm L$. Since the value of the odd parity solutions at the origin is zero, only the even parity solutions differ from those of the free particle in the box. They are the roots of the equation, see e.g. [11],

$$z = E^{1/2} \cot E^{1/2}, \quad (14)$$

where $z = ZL$ and $E = 2L^2\tilde{E}$. Differentiating equation (14) with respect to E and setting $dz/dE = 0$, we get that the singularities of the energy correspond to the roots

$$2E^{1/2} = \sin 2E^{1/2}. \quad (15)$$

As pointed out in [1], the series (2) is easier to calculate, not from equation (14), but from the differential equation

$$(E + z^2 - z)E' + 2E = 0, \quad (16)$$

which is obtained by differentiating equation (14) with respect to z . Substituting now expansion (2) into equation (16), we obtain the following recurrence relation for the perturbation coefficients: $K_1 = -2$ and

$$K_{n+1} = \frac{1}{K_0(n+1)} \left\{ (n-2)K_n - (n-1)K_{n-1} - \sum_{j=0}^{n-1} (j+1)K_{j+1}K_{n-j} \right\} \quad (17)$$

for $n \geq 1$, where $K_0 = (2i+1)^2\pi^2/4$ and i denotes the state of the energy. We note that equation (28) in [1] contains small typographical errors. We also note that the radius of convergence for the ground state, $i = 0$, is not infinite as assessed in [1], but it is the same as for the first excited state when $i = 1$.

After applying the method described in section 2, very accurate numerical results are obtained for the ground state using only few perturbation coefficients K_n , as can be seen in table 1. We note that greater accuracy can be achieved by using larger number of perturbative coefficients and by increasing the number of terms in the series expansion. Working with 64 digits, taking $n_0 = 40$ and eight terms in equation (10), we obtain $z_0 = 1.895\,282 + i3.719\,436$,

this result improving the one obtained in [1] where 500 coefficients and only one term in equation (10) were considered.

However, assumption (3) is not satisfied, namely, the coefficients b_i are *not real* in this case. To see this observation, we analyse equation (16) at the singular point z_0 . For that purpose, we make the transformation

$$t = [(z - z_0)(z - z_0^*)]^{1/2}. \tag{18}$$

Inverting this equation, we obtain

$$z = \text{Re}(z_0) \pm i\sqrt{(\text{Im}(z_0))^2 - t^2} \tag{19}$$

and substitute it into equation (16)

$$[E + (\text{Re}(z_0) + i\sqrt{(\text{Im}(z_0))^2 - t^2})^2 - (\text{Re}(z_0) + i\sqrt{(\text{Im}(z_0))^2 - t^2})] \times \frac{dE}{dt} \frac{i\sqrt{(\text{Im}(z_0))^2 - t^2}}{t} + 2E = 0. \tag{20}$$

Substituting E by the series

$$E(t) = \sum_{i=0}^{\infty} b_i t^i, \tag{21}$$

expanding equation (20) in the powers of t and comparing terms with the same powers of t , we get $b_0 = z_0 - z_0^2$, $b_1 = 2(-z_0 + z_0^2)^{1/2} / (2i \text{Im}(z_0))^{1/2}$ and so on. Clearly, the coefficients b_i are complex. Furthermore, after calculating the expansion in equation (21) to large order, we observe two series: one for the real part of the b_i coefficients, one for the imaginary part. In addition, each of these two series possesses two subseries, one for odd powers of t and one for even powers. There are thus four series altogether. We note that the signs in all these series do not change, implying that the singularity is on the real axis in the variable t . Using the method explained in detail in section 3.1, we find that the radius of the convergence of all four series is the same and is determined by the square-root branch point at $t^2 = (\text{Im}(z_0))^2$. Therefore, the real axis is outside the radius of convergence of the series in equation (21). The radius of convergence just touches the real axis at the point $z = \text{Re}(z_0)$. If we sum the series in equation (21) at this point, on the border of convergence, the real part approaches the correct value 18.464 069, while the imaginary part slowly converges to zero. This result explains the apparent contradiction that equation (21) has an imaginary part and that the value of the energy for the real values of the coupling constant is real.

However, the singularity at $|t| = \text{Im}(z_0)$ found above is an artificial one, introduced by equation (18). The reason is that the inversion, equation (19), has branch point at $t = \text{Im}(z_0)$. If the square-root factors in the implicit equation do not cancel out then this singularity enters into the function $E(t)$. That the function $E(z)$ does not have at the point $z = \text{Re}(z_0)$ any singularity is easily seen from equation (14). This can also be seen when we use, instead of equation (18), the transformation

$$u = \left(1 - \frac{z}{z_0}\right)^{1/2}. \tag{22}$$

This transformation has the advantage that its inversion is

$$z = z_0(1 - u^2), \tag{23}$$

and therefore no artificial square roots are introduced into equation (1) by such a transformation. Consequently, we can expand the function $E(u)$ in the series

$$E(u) = \sum_{i=0}^{\infty} c_i u^i. \tag{24}$$

Substituting equations (23) and (24) into equation (16), we find the following expressions for the coefficients of the expansion: $c_0 = z_0 - z_0^2$, $c_1 = \pm 2(-z_0)^{1/2}c_0^{1/2}$ and

$$c_k = -\frac{(-z_0)^{k/2}}{(k+1)c_1} \left\{ \sum_{n=1}^{k-2} c_{k-n}c_{n+1}(n+1) + [(k-1)(2z_0-1)+4]c_{k-1} + (k-3)c_{k-3} \right\}, \quad (25)$$

for k larger than 1. Calculating about fifty of these coefficients we determine the position $z = z_2$ of the next singularity that differs from the position $z = \text{Re}(z_0)$ of the singularity determined from series (21). The position z_2 of the next singularity will be determined in section 3.3.

In the other examples treated in this paper, namely the Mathieu equation and the hydrogen atom in a spherically symmetric cavity, the same conclusions can be drawn. The coefficients b_i in equation (3) are not real and the introduction of transformation (18) into equation (1) just creates an artificial singularity at the point $z = \text{Re}(z_0)$. Nevertheless, as can be seen from table 1, the method still provides very accurate estimates of the position z_0 of the first singularity, even if equation (3) is not satisfied. Therefore, in the following sections, we modify and clarify the method for the cases when the coefficients b_i in equation (3) are not real.

Before doing so, it will be helpful to first consider the case when we have just a single isolated singularity.

3. Single isolated singularity

In this section, we propose the method for the determination of one isolated singularity from the perturbation series. We apply the method to Mathieu equation and the bounded delta-potential atom.

3.1. Description of the method

Let us assume that the function $E(z)$ behaves at the neighbourhood of the singularity as

$$E(z) = c_1 \left(1 - \frac{z}{z_0}\right)^{\alpha_1} + c_2 \left(1 - \frac{z}{z_0}\right)^{\alpha_2} + \dots, \quad (26)$$

where α_i are supposed to be rational and non-integer. If they are positive integers, they do not influence the large-order behaviour of series (2).

First, we show how from this assumption the large-order behaviour of K_n coefficients can be deduced or, conversely, how we can determine equation (26) from large order of K_n coefficients. For this purpose, we use the generalized binomial theorem and write

$$\left(1 - \frac{z}{z_0}\right)^\alpha = \sum_{n=0}^{\infty} \frac{\Gamma(\alpha+1)}{\Gamma(n+1)\Gamma(\alpha-n+1)} \frac{(-1)^n}{z_0^n} z^n. \quad (27)$$

Considering only the first term in equation (26), substituting equation (27) into equation (26), and then comparing terms of the same powers of z with equation (2), we get for large n

$$K_n \approx c_1 \frac{\Gamma(\alpha_1+1)}{\Gamma(n+1)\Gamma(\alpha_1-n+1)} \frac{(-1)^n}{z_0^n}. \quad (28)$$

To arrive at the asymptotics of the coefficients K_n we use the asymptotics of the product of gamma functions, namely

$$\Gamma(n+1)\Gamma(\alpha-n+1) = \frac{\pi n^{1+\alpha}(-1)^n}{\sin(\pi(\alpha+1))} [1 + O(1/n)], \quad (29)$$

and insert it into equation (28) to get

$$K_n \approx c_1 \frac{\Gamma(\alpha_1 + 1) \sin(\pi(\alpha_1 + 1))}{\pi} \frac{1}{n^{1+\alpha_1} z_0^n}. \tag{30}$$

The values of z_0 and α_1 can be deduced as follows. Taking the ratio of two successive coefficients K_n , we obtain from equation (28)

$$\frac{K_{n-1}}{K_n} \approx z_0 \frac{n}{n - \alpha_1 - 1}. \tag{31}$$

Taking the limit of this ratio to infinity, we obtain an estimate of z_0 . Inserting this estimate of z_0 back to equation (31), we get an estimate for α_1

$$\alpha_1 \approx n \left(1 - \frac{z_0 K_n}{K_{n-1}} \right) - 1. \tag{32}$$

Let us now describe how equation (26) can be used for very accurate determination of z_0 and the coefficients c_i if the values of the coefficients α_i are known. Taking j terms in equation (26), using equation (27) and comparing again terms with the same powers of z in equations (26) and (2), we obtain

$$K_n = \sum_{i=1}^j x_n^{(i)}, \tag{33}$$

where

$$x_n^{(i)} = c_i \frac{\Gamma(\alpha_i + 1)}{\Gamma(n + 1)\Gamma(\alpha_i - n + 1)} \frac{(-1)^n}{z_0^n}. \tag{34}$$

Considering equation (34) for successive n and taking the ratio of such equations, we express $x_{n-k}^{(i)}$ through $x_n^{(i)}$

$$\frac{x_{n-k}^{(i)}}{x_n^{(i)}} = \frac{n(n-1) \cdots (n-k+1)}{(n-\alpha_i-1)(n-\alpha_i-2) \cdots (n-\alpha_i-k)} z_0^k. \tag{35}$$

Inserting this into equation (33), we get a system of $j + 1$ equations

$$K_{n_0-k} = \sum_{i=1}^j x_{n_0}^{(i)} \frac{n_0(n_0-1) \cdots (n_0-k+1)}{(n_0-\alpha_i-1)(n_0-\alpha_i-2) \cdots (n_0-\alpha_i-k)} z_0^k, \tag{36}$$

for k going from 0 to j . We first solve j linear equations for $x_{n_0}^{(i)}$ using MAPLE procedure and then insert them into the last nonlinear equation for z_0 . This equation is solved by the Newton–Raphson method. The coefficients c_i are then determined from equations (34) for $n = n_0$.

To illustrate the method, we first consider the case when the singularity lies on the real axis. In the following subsection, we consider the case when the singularity is lying in the complex plane.

3.2. Odd parity solution of the Mathieu equation with period π

The Mathieu equation arises in the study of motion of a particle in a periodic potential. This equation reads

$$\left[-\frac{d^2}{dx^2} + 2q \cos(2x) \right] \psi(x) = E\psi(x). \tag{37}$$

Table 2. The position of branch point of odd parity solution of Mathieu equation with period π calculated by the method described in section 3 from 10 perturbation coefficients. The perturbation coefficients were obtained by expanding the characteristic polynomial that was calculated from 20 basis functions. j denotes the number of terms taken in equation (33). The percentage error is calculated with respect to the exact values $z_0 = -48.010414048$, $c_1 = -6.209046297$ and $c_3 = 0.218203105$. The exact value of z_0 was calculated using 130 perturbation coefficients and 10 terms in equation (33). The exact values of the coefficients c_1 and c_3 were obtained by inserting equation (24) into the characteristic polynomial, see the text for details.

j	z_0 (error (%))	c_1 (error (%))	c_3 (error (%))
1	-48.050907031 (0.84×10^{-1})	-6.300919191 (0.14×10^1)	
2	-48.009799452 (0.12×10^{-2})	-6.207103750 (0.31×10^{-1})	0.227335819 (4.18)
3	-48.010158287 (0.53×10^{-3})	-6.208173405 (0.14×10^{-1})	0.222814664 (2.11)
4	-48.010365007 (0.10×10^{-3})	-6.208883238 (0.27×10^{-2})	0.218993430 (0.36)
5	-48.010387567 (0.55×10^{-4})	-6.208965084 (0.12×10^{-2})	0.218512198 (0.14)

We will consider only the odd parity solutions with period π . This means that the unperturbed, i.e. for $q = 0$ in equation (37), wavefunctions and energies are of the form

$$\psi_n^{(0)} = \sqrt{\frac{2}{\pi}} \sin(2nx), \quad E_n^{(0)} = (2n)^2. \quad (38)$$

The matrix elements of the perturbation $W = 2 \cos(2x)$ between these unperturbed states have a very simple form

$$W_{n,m} = \delta_{m,n\pm 1}. \quad (39)$$

As mentioned in the introduction, we will work with an approximate implicit equation for the energy E and coupling constant q . We calculate the characteristic polynomial of this problem considering 20 basis functions in equation (37). Expanding this characteristic polynomial in powers of q we find that all perturbation coefficients with odd powers of q vanish. Calculating series (2) with $z = q^2$ for the lowest state $n = 1$ to the large order, we find that the coefficients alternate sign. That means that the closest singularity lies on the real axis. Thus, we determine the position of the singularity by the method described in the previous subsection, where we take $\alpha_1 = 1/2$, $\alpha_2 = 3/2$, $\alpha_3 = 5/2$ and so on.

The position of the singularity where the ground and first excited states of given symmetry intersect obtained with just ten perturbation coefficients is given in table 2. This value does not differ much from the exact position of the singularity of the lowest eigenvalue of equation (37). Due to the simplicity of the matrix elements of interaction (39), the first 20 perturbation coefficients calculated from the characteristic polynomial of Hamiltonian matrix of order 20 are exact.

The results displayed in table 2 can be verified independently of the numerical method described in this section, in the following way. The square-root branch point is at the point where the ground and the first excited states of the energy intersect. Therefore, the two lowest roots of the characteristic polynomial calculated at the point $z = z_0 = -48.010414048$ (see table 2) should be identical. Calculating these roots, we obtain $E_1 = 11.1904715$ and $E_2 = 11.1904756$, a satisfactory agreement indeed. If we make the transformation $u = (1 - z/z_0)^{1/2}$ and expand the energy and the characteristic polynomial in the powers of u , we obtain equations for the coefficients c_i in equation (24). Since the calculations of these coefficients are not entirely straightforward, let us discuss their calculation in more detail. For the sake of transparency we shall illustrate the calculation on the characteristic polynomial,

obtained from equation (37) considering just four basis functions. Expanding the characteristic polynomial in powers of u yields, in the zeroth order, just the equation for the eigenvalues

$$G(E = c_0, z = z_0) = 0. \tag{40}$$

Considering four basis functions in equation (37) the last equation reads

$$G(c_0, z_0) = c_0^4 - 120c_0^3 + (4368 - 3z_0)c_0^2 + (188z_0 - 52\,480)c_0 + 147\,456 - 2624z_0 + z_0^2 = 0. \tag{41}$$

The two lowest roots of this equation are $c_0 = 11.1897 \pm i0.0725$. In the first order of u , we get in general

$$c_1 \left. \frac{\partial G(E, z)}{\partial E} \right|_{E=c_0, z=z_0} = 0. \tag{42}$$

With the characteristic polynomial (41) we obtain

$$c_1 [4c_0^3 - 360c_0^2 + (8736 - 6z_0)c_0 + 188z_0 - 52\,480] = 0. \tag{43}$$

This, however, is not an equation for c_1 because the intersection of two eigenvalues at the point z_0 simply means that the derivative of the secular polynomial with respect to the energy at this point is zero [3]. This could be well illustrated numerically because from equation (43) we get the lowest root $c_0 = 11.1899$. Using 20 basis functions in equation (37) we get from equation (42) the lowest root $c_0 = 11.1904735$. In the second order, we get using equation (42), a quadratic equation for c_1 without a linear term. For example, from the characteristic polynomial (41) we obtain

$$c_2 [4c_0^3 - 360c_0^2 + (8736 - 6z_0)c_0 + 188z_0 - 52\,480] + z_0 (2624 - 2z_0 - 188c_0 + 3c_0^2) + (4368 - 3z_0 - 360c_0 + 6c_0^2)c_1^2 = 0. \tag{44}$$

Since the first term vanishes we get $c_1 = \pm 6.2099$. Considering 20 basis functions we obtain $c_1 = \pm 6.209\,046\,297$. The two signs correspond to the fact that we can approach the branch point either from the ground state $n = 1$ or from the first excited state $n = 2$. In the next orders of u , we get in the k th order of u , a linear equation for c_{k-1} . The coefficients c_k are in the k th order multiplied by $\partial G(E, z)/\partial E|_{E=c_0, z=z_0}$ that vanishes. For example, in the fourth order of u we get from the characteristic polynomial (41)

$$c_4 [4c_0^3 - 360c_0^2 + (8736 - 6z_0)c_0 + 188z_0 - 52\,480] + 3350.1237 - 15337.9733c_3 = 0 \tag{45}$$

where we inserted the values of z_0, c_0 and c_1 obtained earlier, the coefficient c_1 that with the negative sign, and $c_2 = -1.1745$. From the last equation we obtain $c_3 = 0.2184$, considering 20 basis functions we get $c_3 = 0.218\,203\,105$. The coefficients c_1 and c_3 are in excellent agreement with the coefficients obtained from equation (34), as can be seen from table 2.

3.3. Bounded delta-potential atom continued

Let us now consider a case where the isolated singularity lies in the complex plane, namely the case provided by equation (24) of the eigenvalue of the bounded delta-potential atom at the singular point z_0 . The energy $E(z)$ has complex conjugate branch points with respect to the variable z . However, in the variable u , the pairs of the branch points are not complex conjugates. Therefore, the next singularity of the function $E(z)$ should be obtained by applying the method suggested in this section. Looking at table 3, we see that this is really the case. When transforming the singularity from the variable u to the variable z , we find

Table 3. The position of the second branch point of the bounded delta-potential atom calculated by the method described in section 3 from 50 perturbation coefficients c_i given by equation (25). j denotes the number of terms taken in equation (33). The percentage error is calculated with respect to the exact value $z_2 = 2.180218061 + i6.932966534$. This exact value was obtained from the series (2) for the second excited state of the energy with 100 perturbation coefficients and taking 8 terms in equation (10), see also [1].

j	$ z_2 $ (error (%))	$\arg z_2$ (error (%))
1	7.269 319 869 (0.22×10^{-1})	1.266 652 807 (0.42×10^{-1})
2	7.267 771 248 (0.10×10^{-2})	1.266 075 607 (0.32×10^{-2})
3	7.267 679 138 (0.20×10^{-3})	1.266 121 971 (0.41×10^{-3})

that this second singularity exactly coincides with the singularity obtained from the series in equation (2) for the second excited state $i = 2$.

From this, we can conclude that the closest singularity to the origin is the one where the ground and first excited states intersect. The next singularity is the one where the first and second excited states intersect. This singularity can be reached from the ground state by passing through the first singularity. As mentioned in the introduction it is likely that every additional singularity can be reached either by expanding the energy at the origin for the next excited state in the series in equation (2) or by expanding the energy in the previous singularity in the series in equation (24). We verified this statement also for the third branch point.

4. Pair of complex conjugate singularities

In the previous section, we showed how to obtain the position of the singularity closest to the point where the function is expanded. Since the method holds also when the singularity is in the complex plane, it is natural to ask what happens if the closest singularities to the origin are the pair of complex conjugate branch points.

4.1. Modification of the method

Let us suppose that the function $E(z)$ has two complex conjugate square-root branch points and that in the neighbourhood of these points it behaves like

$$E(z) = c_0 + c_1 \left(1 - \frac{z}{z_0}\right)^{1/2} + c_2 \left(1 - \frac{z}{z_0}\right) + c_3 \left(1 - \frac{z}{z_0}\right)^{3/2} + \dots + c_0^* + c_1^* \left(1 - \frac{z}{z_0^*}\right)^{1/2} + c_2^* \left(1 - \frac{z}{z_0^*}\right) + c_3^* \left(1 - \frac{z}{z_0^*}\right)^{3/2} + \dots \quad (46)$$

Note that this assumption is weaker than equation (3). Comparing equations (2) and (46), we can write in analogy with equations (33) and (34), neglecting the terms with the integer powers that do not contribute at large order,

$$K_n = \sum_{i=1}^j x_n^{(i)}, \quad (47)$$

where j again denotes the number of terms in equation (46) with non-integer powers and

$$x_n^{(i)} = (-1)^n \frac{\Gamma(\alpha_i + 1)}{\Gamma(n+1)\Gamma(\alpha_i - n + 1)} \left(\frac{c_{2i-1}}{z_0^n} + \frac{c_{2i-1}^*}{z_0^{*n}} \right). \quad (48)$$

Here, $\alpha_1 = 1/2$, $\alpha_2 = 3/2$ and so on. Note that the last factor can be written in the form

$$\left(\frac{c_{2i-1}}{z_0^n} + \frac{c_{2i-1}^*}{z_0^{*n}} \right) = \frac{|c_{2i-1}|}{|z_0|^n} 2 \cos(\varphi n - \delta_i), \tag{49}$$

where $\varphi = \arg z_0$ and $\delta_i = \arg c_{2i-1}$.

Let us consider just one term with $i = 1$ in equation (47) and equation (48) together with equation (49) and the asymptotics of the product of Gamma functions, equation (29). We then obtain equation (7) describing the large-order behaviour of the coefficients K_n where $A = -|c_1|/\sqrt{\pi}$ and $\delta = -\delta_1$. From all the derivations given so far in the literature [2, 9], this one is perhaps the most simple.

A procedure to determine the position of the singularity at z_0 follows. Let us consider the ratios of two successive coefficients $x_n^{(i)}$

$$\frac{x_{n-1}^{(i)}}{x_n^{(i)}} = |z_0| \frac{n}{n - \alpha_i - 1} \frac{\cos[(n - 1)\varphi - \delta_i]}{\cos[n\varphi - \delta_i]} = |z_0| \frac{n}{n - \alpha_i - 1} [\cos \varphi + \sin \varphi \tan(n\varphi - \delta_i)] \tag{50}$$

and

$$\frac{x_{n+1}^{(i)}}{x_n^{(i)}} = |z_0|^{-1} \frac{n - \alpha_i}{n + 1} [\cos \varphi - \sin \varphi \tan(n\varphi - \delta_i)]. \tag{51}$$

Adding equation (50) multiplied by $|z_0|^{-1}(n - \alpha_i - 1)/n$ and equation (51) multiplied by $|z_0|(n + 1)/(n - \alpha_i)$, we get

$$x_{n-1}^{(i)}(n - \alpha_i - 1)(n - \alpha_i) - 2|z_0|(\cos \varphi)x_n^{(i)}n(n - \alpha_i) + |z_0|^2x_{n+1}^{(i)}n(n + 1) = 0. \tag{52}$$

Division of equation (52) by n yields almost the same recurrence relations as in equation (12), the only difference being in the factor multiplying $x_{n-1}^{(i)}$. However, since

$$\frac{(n - \alpha_i - 1)(n - \alpha_i)}{n} = (n - 2\alpha_i - 1)[1 + O(1/n)], \tag{53}$$

these recurrence relations are identical for large n . For lower n , they can, however, yield different results. Determining $|z_0|$ and φ from equations (47) and (52) in the same way as in section 2, we can use equation (50) to determine δ_i and then equations (48) and (49) to determine $|c_{2i-1}|$.

4.2. Bounded delta-potential atom revisited

To compare this modified method with the original method described in section 2, let us consider again the series in equation (2) for the ground state of the bounded delta-potential atom under the same circumstances as in section 2. Table 4 illustrates that the modified method yields more accurate position of the singularity both in radius and phase than the method suggested in [1, 2]. Moreover, the coefficients of the expansion c_1 and c_3 agree with those calculated from equation (25). The performance of the method again improves with increasing values of n_0 and j .

4.3. Hydrogen-like atom in a spherically symmetric cavity

As a last example, we discuss the problem not treated so far in the literature in a systematic manner, namely the case of the hydrogen atom in a spherically symmetric cavity. This case is of interest from a practical point of view, namely for understanding the spatial confinement effect on different atomic and molecular particles [12] or for bag model of quarks [13], as well

Table 4. The position of branch point of the bounded delta-potential atom calculated by the method described in section 4. n_0 is equal to 5 and j denotes the number of terms taken in equation (47). The number of the needed perturbation coefficients is $n_0 + 2j$ for $j > 1$ and $n_0 + 1$ for $j = 1$. The percentage error is calculated with respect to the exact values $z_0 = 1.895\,282\,288 + i3.719\,436\,139$, $c_1 = -16.017\,257\,367 - i3.180\,632\,202$ and $c_3 = 7.004\,494\,836 + i7.096\,114\,357$. The exact form of the coefficients c_1 and c_3 was obtained from equation (25).

j	$ z_0 $ (error (%))	φ (error (%))
1	4.934 125 188 (18.1)	0.998 159 396 (9.21)
2	4.073 950 025 (2.40)	1.103 357 857 (0.34)
3	4.162 417 140 (0.28)	1.100 249 138 (0.065)
4	4.172 806 221 (0.040)	1.099 514 977 (0.0012)
5	4.174 562 511 (0.0019)	1.099 366 234 (0.014)
j	Re(c_1) (error (%))	Im(c_1) (error (%))
1	-55.887 592 271 (248)	5.203 740 218 (263)
2	-10.606 537 905 (33.7)	-1.843 181 931 (42.0)
3	-14.955 157 101 (6.63)	-2.889 697 742 (9.14)
4	-15.855 955 099 (1.00)	-3.049 780 180 (4.11)
5	-16.087 927 377 (0.44)	-3.086 357 868 (2.96)
j	Re(c_3) (error (%))	Im(c_3) (error (%))
2	17.113 690 772 (144)	12.894 973 458 (81.7)
3	10.163 828 509 (45.1)	10.042 310 613 (41.5)
4	7.276 958 887 (3.88)	8.378 728 760 (18.0)
5	5.984 680 836 (14.5)	7.609 684 417 (7.23)

as from a theoretical point of view as is the calculation of binding energies in the quantum field theory [14]. There is a long-term confusion on the application of Rayleigh–Schrödinger perturbation theory on this system going back to the paper by Wigner [15]. Since there is a continuing interest in this subject [16], we believe that our results will be useful in the study of this problem.

The Schrödinger equation for the hydrogen-like atom takes the well-known form

$$\left[-\frac{\nabla^2}{2} - \frac{Z}{r} \right] \psi = \tilde{E} \psi. \quad (54)$$

Separating, as usual, the radial and angular degrees of freedom, we get, for the states with zero angular momentum, the radial equation

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} - \frac{Z}{r} \right] R(r) = \tilde{E} R(r). \quad (55)$$

We can eliminate the second term by the transformation $R(r) = r^{-1} \varphi(r)$. We then obtain

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} - \frac{Z}{r} \right] \varphi(r) = \tilde{E} \varphi(r). \quad (56)$$

If the hydrogen atom is in a box of radius L , we impose the boundary condition on the wavefunction

$$\varphi(r = L) = 0. \quad (57)$$

By the scaling $r \rightarrow rL$, we can move the boundary condition to the point $r = 1$. The scaled Schrödinger equation (56) then reads

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} - \frac{z}{r} \right] \varphi(r) = E \varphi(r), \quad (58)$$

Table 5. The position of the first two branch points of hydrogen atom in a spherically symmetric cavity calculated by the method described in section 4. The perturbation coefficients in equation (2) were obtained by expanding the characteristic polynomial that was calculated from 15 basis functions. n_0 is equal to 90 and j denotes the number of terms taken in equation (47). The number of the needed perturbation coefficients is $n_0 + 2j$ for $j > 1$ and $n_0 + 1$ for $j = 1$.

j	$ z_0 $	$\arg z_0$	$\text{Re}(c_1)$	$\text{Im}(c_1)$	$\text{Re}(c_3)$	$\text{Im}(c_3)$
1	6.027 383 739	0.802 387 720	12.453 353	-0.062 027		
2	6.026 577 753	0.802 347 795	12.162 818	-0.149 503	-8.333 556	-2.592 904
3	6.026 592 196	0.802 349 250	12.170 641	-0.144 670	-7.880 537	-2.301 821
4	6.026 591 758	0.802 349 261	12.170 321	-0.144 624	-7.908 949	-2.298 475
5	6.026 591 774	0.802 349 257	12.170 336	-0.144 647	-7.907 113	-2.301 117
j	$ z_2 $	$\arg z_2$	$\text{Re}(c_1)$	$\text{Im}(c_1)$	$\text{Re}(c_3)$	$\text{Im}(c_3)$
1	9.069 691 370	1.018 299 648	24.911 486	6.331 433		
2	9.068 250 195	1.018 160 558	24.373 904	5.551 286	-15.345 756	-22.551 988
3	9.068 282 775	1.018 164 559	24.391 177	5.583 231	-14.340 521	-20.676 352
4	9.068 279 296	1.018 164 500	24.387 926	5.581 901	-14.627 860	-20.796 223
5	9.068 279 651	1.018 164 479	24.388 414	5.581 777	-14.569 595	-20.810 375

where

$$E = \tilde{E}L^2, \quad z = ZL. \tag{59}$$

Since the exact wavefunction satisfies the conditions

$$\varphi(r = 0) = 0, \quad \varphi(r = 1) = 0, \tag{60}$$

we impose the same conditions on the unperturbed wavefunction. We then get the well-known solution of the particle in a box, namely

$$\varphi_n^{(0)}(r) = \sqrt{2} \sin(n\pi r), \quad E_n^{(0)} = \frac{(n\pi)^2}{2}. \tag{61}$$

The matrix elements of the perturbation $W = -1/r$ between the unperturbed states are given by

$$W_{n,m} = -2 \int_0^1 \sin(n\pi r) \frac{1}{r} \sin(m\pi r) dr = -Ci[(n - m)\pi] + Ci[(n + m)\pi] + \ln \frac{n - m}{n + m}. \tag{62}$$

There is no singularity for the case $n = m$. In this case $W_{n,n}$ is given by

$$W_{n,n} = -\ln(2n\pi) + Ci(2n\pi) - \gamma, \tag{63}$$

where $Ci(x)$ is the cosine integral.

As mentioned in the introduction, we consider an approximate implicit equation for the energy $E(z)$ and the coupling constant z . We calculate the characteristic polynomial of the Hamiltonian matrix taking 15 basis functions given by equation (61) and find that the structure of the series in equation (2) is again the same as in the previous cases. Calculating 100 coefficients of the expansion in equation (2), we find $z_0 = 4.188 599 \pm i4.333 064$, see table 5.

Since we are using ‘variational’ perturbation theory, instead of ‘exact’ perturbation theory, this position of the branch point differs from the exact one. In the ‘exact’ perturbation theory we sum over infinite number of the intermediate states. In the ‘variational’ perturbation theory used here we are implicitly summing just over 15 intermediate states.

In contrast to the case of Mathieu equation where, due to equation (39), the perturbation coefficients were exact to the order of the perturbation theory equal to the size of the truncated Hamiltonian, in the case of the hydrogen atom in spherically symmetric cavity, the ‘variational’ perturbation coefficients deviate from the ‘exact’ perturbation coefficients very early and profoundly. To determine the exact position of the branch point, we perform standard perturbation theory and calculate perturbation energies using 300 and 360 intermediate states. Only the digits that agree in both cases are considered as significant. We calculate 20 perturbation coefficients in this way and obtain an estimate $z_0 = 4.212 \pm i4.32$ using $n_0 = 10$ and 5 terms in equation (10). It is seen that this value does not differ significantly from the value obtained from the approximate implicit equation.

The convergence of the method described in this section for the first two singularities of the approximate characteristic polynomial is displayed in table 5. The values of the coefficients c_i were verified by substituting equation (24) for the energy at the singularities into the characteristic polynomial in similar way as in section 3.2. We also encountered the same phenomenon as in the case of bounded delta-potential atom, namely that substituting equation (24) for the energy at the singular points, we obtain the next singularity exactly at the same point as the singularity of the next excited state of the energy expanded at the point $z = 0$, namely equation (2). It can be seen from table 5 that the convergence of the method is better for the ground state than for the second excited state.

Applying the method to the next excited states, we observe again that the convergence slows down. On the basis of this and our experience with other problems, we are tempted to generalize this decrease of convergence when considering higher excited states, see also [1].

5. Conclusions

In this paper, the method for the determination of the singularities of the function from its perturbation expansions was suggested and illustrated on three simple eigenvalue problems.

With regard to the convergence of the method, it is observed that it strongly depends on the nature of the problem. If the singularity, or complex conjugate pair of the singularities, are well isolated from the other singularities, then the method works very well, as can be seen from the tables. This requirement is usually satisfied for the ground and first excited states.

However, problems appear when the other singularities are near to the one closest to the origin. This is usually the case when treating higher excited states [1, 4, 7, 8].

One can see this from equation (7) describing the large-order behaviour of the coefficients K_n . The contribution of the singularity located at the point z_1 to that located at the point z_0 , $|z_0| < |z_1|$, goes roughly like $(|z_0|/|z_1|)^n$. Now, if $|z_1|$ is close to $|z_0|$, we have to go to huge values of n to get the ratio $(|z_0|/|z_1|)^n$ substantially smaller than 1, or in the other words, to suppress the contribution of the singularity at z_1 with respect to that at z_0 .

The presence of another singularity close to the first one has also another consequence. In all considered eigenvalue problems, the radius of convergence of the series in equation (24) is smaller than that of the series in equation (2). This means that equations (33) and (47) hold only asymptotically, i.e. for sufficiently large values of n . If the closest singularity is well isolated from the others, these asymptotic formulae start to apply very early. In the examples given in this paper, they are valid in the fourth or fifth order of the perturbation theory. Taking then more terms in equations (33) and (47) improves the accuracy of the method substantially. However, when two singularities interfere having similar but not equal distance from the origin then equations (33) and (47) hold for very large n only and taking more terms in the expansion does not lead to the improvement in the accuracy. Therefore, future development of the method should be aimed at dealing with the problem of two interfering singularities.

We note that the finite radii of convergence of all three eigenvalue problems discussed in this paper clearly illustrate that the bound states are nonperturbative effects. This means that they cannot be reached by starting from the description of the free particle in a box, taking the binding potential as a perturbation and then letting the boundaries of the box to go to the infinity. This is the main physical result of the paper.

We would like to point out that the method given here is not at all restricted to eigenvalue problems. The method described in this paper can be used, for example, for the determination of the parameters of the phase transitions from high or low temperature expansions (see, e.g., [17]) or for the determination of the singular points of nonlinear differential equations arising in classical physics (see, e.g., [18]). Therefore, we believe that it is of general interest.

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References

- [1] Fernández F M, Arteca G A and Castro E A 1987 *J. Math. Phys.* **28** 323
- [2] Skála L, Čížek J and Zamastil J 1999 *J. Phys. A: Math. Gen. A* **32** L123
- [3] Bender C M and Orszag S A 1978 *Advanced Mathematical Methods for Scientists and Engineers* (New York: McGraw-Hill)
- [4] Bender C M and Wu T T 1969 *Phys. Rev.* **184** 1231
- [5] Simon B 1970 *Ann. Phys. NY* **58** 76
Simon B 1972 *Cargese Lectures in Physics 1970* vol 5, ed D Bessis (New York: Gordon and Breach) p 383
- [6] Arteca G A, Fernández F M and Castro E A 1986 *J. Chem. Phys.* **84** 1624
- [7] Alvarez G and Silverstone H J 1994 *Phys. Rev. A* **50** 4679
- [8] Shanley P E 1986 *Phys. Lett. A* **117** 161
- [9] Usveridze A G 1989 *Bulg. J. Phys.* **16** 137 (in Russian)
See also Zamastil J, Skála L and Čížek J 2000 *Int. J. Theor. Phys.* **39** 2415
- [10] Abramowitz M and Stegun I (ed) 1965 *Handbook of Mathematical Functions* (New York: Dover)
- [11] Atkinson D A and Crater H W 1975 *Am. J. Phys.* **43** 301
- [12] Changa M E, Scherbinin A V and Pupyshv V I 2004 *Int. J. Quantum Chem.* **96** 167
- [13] Horvat D, Podobnik B and Tadic D 1998 *Phys. Rev. D* **58** 034003
- [14] Gat G and Rosenstein B 1993 *Phys. Rev. Lett.* **70** 5
- [15] Wigner E P 1954 *Phys. Rev.* **94** 77
- [16] Hai W, Feng M, Zhu X, Shi L, Gao K and Fang X 2000 *Phys. Rev. A* **61** 052105
- [17] Butera P and Comi M 1996 *Phys. Rev. B* **54** 15828
Butera P and Comi M 2003 *Phys. Rev. B* **67** 054402
- [18] Kivshar Y S and Malomed B A 1989 *Rev. Mod. Phys.* **61** 763