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Conformal mappings versus other power series methods for solving ordinary differential equations: illustration on anharmonic oscillators

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Abstract

The simplicity and the efficiency of a quasi-analytical method for solving nonlinear ordinary differential equations (ODE) is illustrated on the study of anharmonic oscillators (AO) with a potential $V(x) = \beta x^2 + x^{2m}$ ($m > 0$). The method (Bervillier 2008 *Nucl. Phys.* **B801** 296) applies *a priori* to any ODE with two-point boundaries (one being located at infinity), the solution of which has (fixed) singularities in the complex plane of the independent variable x . A conformal mapping of a suitably chosen angular sector of the complex plane of x upon the unit disc centered at the origin makes convergent the transformed Taylor series of the generic solution so that the boundary condition at infinity can be easily imposed. In principle, this constraint, when applied on the logarithmic derivative of the wavefunction, determines the eigenvalues to an arbitrary level of accuracy. In practice, for $\beta \geq 0$ or slightly negative, the accuracy of the results obtained is astonishingly large with regard to the modest computing power used. Various aspects of the method and comparisons with some seemingly similar methods, based also on expressing the solution as a Taylor series, are shortly reviewed, presented and discussed.

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1. Introduction

The accurate determination of the spectrum of the anharmonic oscillator (AO) is an old problem which has attracted much interest (for recent reviews, see [1]). This is certainly due to the asymptotic character of its perturbative expansion [2], but also because it is intrinsically hard to solve accurately for sizeable values of the coupling parameter. The eigenvalues may be numerically determined using shooting or relaxation methods, and extremely accurate results

may be obtained that way (e.g. see [3]). It is also interesting to develop simple and efficient (quasi-) analytical methods which may be implemented using symbolic calculation softwares and modest computation powers¹.

Sophisticated methods have recently been proposed [4, 5]. They are all based on a Taylor series in the independent variable x of the solution of the ordinary differential equation (ODE). Methods of this kind have previously been developed in different contexts [6, 7].

The object of the present paper is to illustrate, by the computation of the spectrum of the AO, the simplicity, the efficiency and the limitations of one of these methods: the mapping method [5].

The paper is organized as follows. In section 2, the AO is introduced together with a change of function (a logarithmic derivative) which transforms the originally linear ODE into a nonlinear ODE. In doing so, the essential singularity at infinity of the wavefunctions is softened but the new functions are no longer analytic in the complex x -plane. The common characteristics of the Taylor-series-based methods are then presented. Section 3 presents a short review of these methods utilized in the past to solve the AO. In section 4 the principle of the mapping method is briefly reminded. Though several configurations of the AO have been explicitly treated, only one is presented here in detail. We also explain how highly accurate estimates of the eigenvalues are obtained for a potential given by (2) with $\lambda = 1$, $\beta = 1$ and $m = 2$. Other cases are discussed elsewhere [8]. A conclusion is presented in section 5. Some numerical results are displayed in the appendix.

2. The ODE of the anharmonic oscillator

2.1. The linear ODE

The usual eigenvalue problem associated with the AO is to find the spectrum E_n which corresponds to the solutions $\psi_n(x)$ of the following linear ODE:

$$\psi''(x) + (E - V(x))\psi(x) = 0, \quad (1)$$

with the condition that the $\psi_n(x)$ vanish at infinity so as to be squared integrable. In (1) a prime denotes a derivative with respect to x and the potential $V(x)$ is

$$V(x) = \beta x^2 + \lambda x^{2m}, \quad (2)$$

with $m = 2, 3, \dots$, β a given real number and λ can be set equal to unity due to Symansik's scaling:

$$E_n^m(\beta, \lambda) = \lambda^{1/(m+1)} E_n^m(\beta \lambda^{-2/(m+1)}, 1).$$

With the potential (2), the general solution of (1) is analytic on the whole complex x -plane with an irregular singular point located at infinity (see, e.g. [9, p 195]).

The two boundary conditions on the corresponding wavefunctions $\psi_n(x)$ are as follows:

- (1a) either $\psi_n(0) = 0$ or $\psi_n'(0) = 0$ (odd or even eigenfunctions) and
 (1b) $\psi_n(x) \rightarrow 0$ as $x \rightarrow \infty$.

For given β and m , the general solution involves three constants: two integration constants—fixed by the parity condition (1a) and by a free normalization—and the yet unknown

¹ The calculations are performed, with the help of Mathematica 5.0.1.0. running on a laptop with a processor Intel Pentium M 2.00 GHz, 1.00 Go RAM.

‘energy’ parameter E . The spectrum of (1) is then determined by imposing the condition (1b). Actually, without this condition and for large x , the general solution of (1), satisfying the condition (1a), has the following asymptotic form:

$$\psi(x) \underset{x \rightarrow +\infty}{\simeq} e^{-\frac{x^{m+1}}{m+1}} + B e^{+\frac{x^{m+1}}{m+1}}, \tag{3}$$

where B is some constant depending on E .

Determining the spectrum of (1) amounts to finding the discrete set of values E_n ($n = 0, 1, \dots, \infty$) for which B vanishes.

2.2. The nonlinear ODE

In order to remove the essential singularity at infinity displayed in (3), it is worth considering the following change of function:

$$\psi(x) = x^\epsilon e^{W(x)}, \tag{4}$$

in which $\epsilon = 0$ or $\epsilon = 1$ according to the parity of the solution of (1) looked for. Then, (1) becomes equivalent to

$$E - V(x) + W'^2 + W'' + \frac{2\epsilon}{x} W' = 0, \tag{5}$$

with the boundary conditions

$$W(0) = 0, \quad W'(0) = -\epsilon, \quad W(x) \underset{x \rightarrow +\infty}{\simeq} -\frac{x^{m+1}}{m+1}. \tag{6}$$

If instead of $W(x)$, one considers the derivative

$$h(x) = W'(x), \tag{7}$$

then (5) takes the form of a Riccati ODE. More important is the fact that

$$h(x) = \psi'(x)/\psi(x) - \epsilon/x, \tag{8}$$

so that any zero of $\psi(x)$ in the complex x -plane becomes a pole for $h(x)$. Hence, the nodes of the excited states ψ_n ($n \geq 2$) of the AO become poles for $h(x)$ located on the positive real x -axis.

Note that, for a given n , a solution $W_n(x)$ of interest is no longer a ‘vanishing separatrix’ between two blowing behaviors when $x \rightarrow \infty$ (see equation (3) for opposite values of B). For large values of x , $W_n(x)$ may not distinguish itself clearly from a ‘wrong’ solution. Fortunately, equation (5) provides a solution which involves a movable singularity of the form

$$W_{\text{Sing}}(x) = \ln |x_0 - x|,$$

where x_0 is a constant which depends on E (the initial conditions being fixed). Determining the ‘physical’ eigenfunctions amounts to pushing this movable singularity up to infinity.

2.3. Generalities on the Taylor-series-based methods

The methods for solving ODEs based on expressing the solution as a Taylor series rely upon the following considerations.

It is convenient to first perform the change of variable $x \rightarrow z = x^2$ and to redefine the wavefunction as

$$\psi(x) = x^\epsilon f(x^2), \tag{9}$$

in which $\epsilon = 0$ or $\epsilon = 1$ according to the parity of the solution of (1) looked for. Then (1) becomes equivalent to

$$4z f''(z) + 2(1 + 2\epsilon) f'(z) + (E - \tilde{V}(z))f(z) = 0, \tag{10}$$

with

$$\tilde{V}(z) = \beta z + z^m,$$

and the boundary conditions

$$f(0) = 1, \tag{11}$$

$$f(\infty) = 0. \tag{12}$$

Express $f(z)$ as a truncated Taylor series about the origin $z = 0$:

$$f_M(z) = \sum_{i=0}^M a_i z^i, \tag{13}$$

in which $a_0 = 1$ in agreement with (11).

For $f_\infty(z)$ to be a solution of (10), the coefficients a_i must satisfy the following recurrence relation:

$$2(k+1)[2k+1+2\epsilon]a_{k+1} + Ea_k - \beta a_{k-1} - a_{k-m} = 0, \tag{14}$$

with the writing convention that $a_i = 0$ if $i < 0$.

Using the recurrence relation (14), one determines iteratively the coefficients $a_i(E)$ so that $f_\infty(z)$ is a solution of (10) for arbitrary E . The coefficients $a_i(E)$ so determined are polynomials in E .

Similar considerations hold for the nonlinear ODE (5) and the expansion

$$W(x) = g(x^2), \tag{15}$$

$$g_M(z) = \sum_{i=0}^M c_i z^i, \tag{16}$$

in which $c_0 = 0$ in agreement with (6). The corresponding recurrence relation is

$$2k(2k-1+2\epsilon)c_k + 4 \sum_{i=0}^{k-2} (i+1)(k-i-1)c_{i+1}c_{k-i-1} = \beta \delta_{k,2} - E \delta_{k,1} + \delta_{k,m+1}, \tag{17}$$

in which $\delta_{i,j}$ is the Kronecker delta symbol. From this relation one can determine iteratively the coefficients c_k as polynomial functions of E .

The expansion of the function $h(x)$ corresponding to the logarithmic derivative-like transform (8) is obtained from (16) and (17) using

$$h_M(x) = 2x g'_M(z),$$

with $z = x^2$.

To determine the set of values E_n which potentially correspond to the wavefunctions $\psi_n(x)$ (satisfying the boundary condition (1b)), one has to find one auxiliary condition on the

coefficients $a_i(E)$ or $c_i(E)$. The various methods described in sections 3 and 4 differ by the choice of the auxiliary condition.

3. The Taylor-series-based methods used to solve the AO

3.1. The power-series method [10]

Because the Taylor series $f_\infty(z)$ has an infinite radius of convergence, one may estimate the set \tilde{E}_n for which $f_\infty(z_0)$ vanishes at a given finite z_0 by simply imposing that the sum of the series (13) vanishes at this point. This zero located on the positive part of the real axis of z exists because there are solutions of (10) having asymptotic forms (3) with opposite values of $B \neq 0$. Then, the limit $z_0 \rightarrow \infty$ should correspond to $B \rightarrow 0$, and \tilde{E}_n should approach the spectrum E_n of the AO (as actually observed in several studies of ‘bounded’ oscillators [11]).

For finite values of M , $f_M(z)$ represents approximately $f_\infty(z)$ only in a finite range of values of z whereas for larger values the sum goes to $\pm\infty$ according to the sign of the last term. The procedure for determining the spectrum of the AO may then be sketched as follows.

- (2a) One fixes M , chooses a sensible value of z_0 and determines the zeros of the polynomial in E associated with the solution of the equation

$$f_M(z_0) = 0 \quad (18)$$

(this is the effective auxiliary condition at z_0).

- (2b) On increasing z_0 one observes a convergence of the zeros toward definite values up to a value $z_0^{(M)}$ where the convergence terminates. At this point, one gets the best values of the spectrum $E_n(z_0^{(M)})$ for the given M .
- (2c) One increases M and repeats the process from step (2a).
- (2d) One observes that $z_0^{(M)}$ is an increasing function of M and that $E_n(z_0^{(M)})$ quickly approaches the spectrum E_n as M increases.

This method has been applied in 1961 by Secret *et al* [10] with $M \sim 1000$. They notably have determined the ground-state energy E_0 with 12 significant figures in the case $m = 2$, $\beta = 0$. A new calculation during the present work, for $m = 2$, $\beta = 1$ and $M = 250$, gives the ground-state energy E_0 with 41 significant figures.

As illustrated by figure 1, the determination of all the real zeros of the condition (18) provides an estimation of the complete spectrum, the number of states being only limited by the order of the polynomial in E corresponding to the value of M chosen. The excited states may be hierarchically determined provided z_0 is chosen larger than the location of the last node. As a consequence the number of significant figures obtained slowly decreases as the quantum number n increases (for a given M).

It may occur (for some values of the potential parameters β and m) that too large values of z_0 or M be required to get a satisfactory accuracy (see the caption of figure 1). In that case Secret *et al* [10] have suggested to reach the value z_0 in more than one step using the Taylor expansion about a non-zero value $z_l < z_0$. This suggestion is already the analytic-continuation method introduced later on by Holubec and Stauffer [12].

3.2. The analytic-continuation method [12]

Let us consider the Taylor expansion of $f(z)$ about an arbitrary point $z_l \neq 0$:

$$f_{M,l}(z) = \sum_{i=0}^M b_i (z - z_l)^i. \quad (19)$$

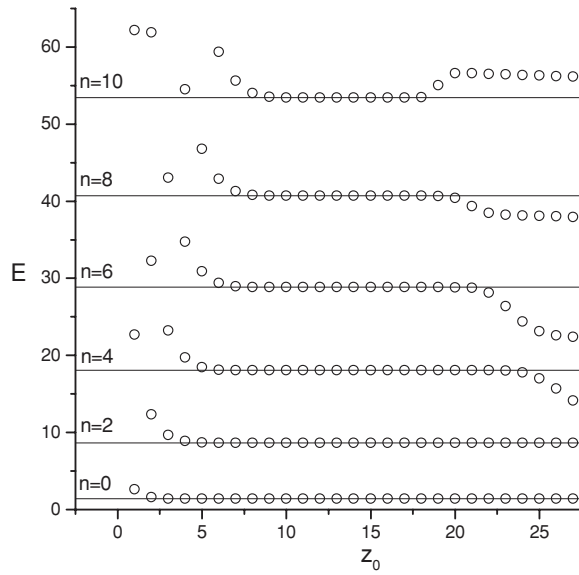


Figure 1. Part of the even spectrum obtained using the power-series method for $\beta = 1$, $m = 2$ and with $M = 100$ terms in the series. The open circles correspond to the real zeros of the polynomial condition (18) for varying z_0 . The horizontal lines indicate the ‘true’ values of the spectrum (E_0, E_2, E_4, \dots) as displayed in the appendix. For sufficiently high values of z_0 , the points reach a first plateau and then deviate from the horizontal lines because the truncated series $f_M(z)$ no longer represents approximately the function $f_\infty(z)$. For the displayed values of n , the succession of the large and stable (relatively to changing M) plateaux allows a clear determination of E_n . However, those plateaux may disappear when n increases (because the value of z_0 at which they would take place may exceed the range where the truncated series represent the function), in such cases, larger values of M should be required to get correct approximations of high eigenvalues E_n . For different values of β and m , this difficulty may occur for much smaller values of M and n so that the power-series method may completely fail.

For $f_{\infty,l}(z)$ to be a solution of (10), the coefficients b_i must satisfy the following recurrence relation:

$$\begin{aligned}
 4 z_l (k + 2)(k + 1)b_{k+2} &= 2(k + 1)[2k + 1 + 2\epsilon]b_{k+1}, \\
 &+ (E - \beta z_l - z_l^m)b_k - (\beta + m z_l^{m-1})b_{k-1}, \\
 &- \sum_{i=0}^{m-2} \frac{m!}{i!(m-i)!} z_l^i b_{k-m+i},
 \end{aligned} \tag{20}$$

which determines them in terms of E and of the two coefficients b_0 and b_1 . Those two quantities may be calculated using the series (13) so as to account for the conditions (1a) at the origin with

$$b_0 = f_\infty(z_l), \quad b_1 = f'_\infty(z_l). \tag{21}$$

Choosing $z_l = z - z_l = h$ to be small, one estimates $f_M(h)$ and $f'_M(h)$ and then $f_M(2h)$ as a function of the unique unknown parameter E . One estimates again b_0 and b_1 at this point in order to reach the point $3h$ and so on until the point $z_0 = N h$.

The following of the procedure is identical to the preceding one (steps (2a)–(2d) above). Despite a relative heaviness, the method is very efficient provided a well-balanced choice of M, N and h is done. For example, with $M = N = 40$, 22 significant figures have been obtained

this way [13], in the case of the ground-state energy of the double-well potential $\beta = -50$ and $m = 2$ for which it is almost degenerated with the first excited state (the splitting occurs at the 21st figure only). In the circumstances, it is more efficient than the mapping method (see [8]).

Note that, contrary to the power-series method, the analytic-continuation method could apply even in configurations where the range of analyticity of ψ about the origin is limited.

3.3. The Hill determinant method [14]

One of the most popular methods used to solve the eigenvalue problem of the AO is the so-called Hill determinant method [14] which is (partly) based on a Taylor expansion of the solution in powers of the independent variable x such as (9, 13).

Actually it is traditionally considered as a variational method because an exponential prefactor is usually introduced in the relation (9) between ψ and the power series (13). In [14], Biswas *et al* use a fixed exponential factor $e^{-x^2/2}$ but subsequent studies considered $e^{-\gamma x^2}$ with γ adjustable [15–17] and even $e^{-\gamma x^2 + \rho x^4}$ with γ and ρ adjustable [18]. Nevertheless, this method may well be sketchily introduced without considering any prefactor.

Let us consider the recurrence relation (14) as an infinite system of linear algebraic equations for the coefficients a_i . For this homogeneous linear system, to have a solution, its (infinite) determinant (namely, the Hill determinant; see, e.g. [9]), if it converges, must vanish. This condition is a transcendental equation for E the infinite number of solutions of which should coincide with the complete spectrum of the AO (provided the condition at infinity is satisfied).

Practically, one deals with finite values of M and the effective auxiliary condition reduces to

$$D_M(E) = 0, \quad (22)$$

where $D_M(E)$ is the Hill determinant truncated at order M .

In fact, the auxiliary condition (22) is not always sufficient to determine the solution looked for. This is due to the analyticity of the general solution of (1): the blowing parts of the solution also correspond to convergent series and may be selected by the iterative procedure so defined. In practice, one should verify that the wavefunction selected by the Hill criterion (22) actually vanishes at infinity.

Using an exponentially decreasing prefactor, one may improve the method. It is a matter of fact that this ‘genuine’ Hill determinant method works in certain circumstances (see for example [17]). But it fails in certain other circumstances. In particular, it is unable [19] to furnish the full spectrum of the quasi-exact configurations [18, 20], see [21] for a review of the reasons of failure.

3.4. A simplistic method

It is interesting to realize that

$$a_{M+1}(E) = (-1)^{M+1} \frac{D_M(E)}{d_{M+1,0}} a_0,$$

where $d_{M+1,0}$ is the $(M+1, 0)$ minor of the matrix of the system of linear equations (14). Hence, the condition (22) is equivalent to the condition that the next coefficient $a_{M+1}(E)$ vanishes (e.g. see [18, 22]). This is the condition imposed in certain studies of nonlinear ODEs (e.g. see [23, 25]), thus assuming implicitly that the Taylor series of the solution looked for has an infinite radius of convergence. Unfortunately, in general, this is not true [24, 26], due to the presence of (fixed) singularities in the complex x -plane [27] in the case of a nonlinear ODE.

The solutions of the nonlinear ODE (5) have such singularities: e.g. for $\beta = 1$ and $m = 2$, one deduces from the exact study [28] that they are all located on the imaginary axis of the complex x -plane. Consequently, the auxiliary condition

$$c_M(E) = 0 \tag{23}$$

is not sufficient to impose the required condition at infinity because the series has a finite radius of convergence. However, condition (23) may, sometimes, give approximate estimates of the true spectrum. In particular, if a large accuracy on E_0 is required to push the movable singularity beyond the (limited) range of convergence of the series, then (23) will give a good estimate of E_0 . In contrast, the procedure simply may not work at all. This phenomenon explains why the simplistic method ‘works’ in some case and does not in another case despite similar radius of convergence for the respective Taylor series [29].

The simplistic method is extremely easy to implement and, when it works, may serve to get a primary estimate of the solution looked for before using more sophisticated methods.

3.5. The Padé method [6]

The Padé method (originally proposed in [6]) relies upon an attempt to represent the solution of (5) looked for by successive rational functions of the form

$$P_{N_1, N_2}(z) = \frac{\sum_{i=0}^{N_1} p_i z^i}{\sum_{i=0}^{N_2} q_i z^i},$$

which involves $N_1 + N_2 + 1$ coefficients and $z = x^2$. The procedure of the method may be described as follows.

The coefficients p_i and q_i may be determined from the Taylor series (16) at order $M = N_1 + N_2$ according to the usual rules of construction of a Padé approximant. This determines the coefficients p_i and q_i as functions of the unknown parameter E . The auxiliary condition is obtained by imposing that the Padé approximant constructed at order M still reproduces the truncated function at next order $M + 1$. Setting $N_1 = s + \omega$ and $N_2 = s$, one gets the following linear system of equations for the coefficients p_i and q_i (using the convention that $c_k = 0$ for $k < 0$):

$$\begin{aligned} p_i &= \sum_{j=0}^s c_{i-j} q_j & \text{for } i = 1, \dots, s + \omega, \\ 0 &= \sum_{j=0}^s c_{i-j} q_j & \text{for } i = s + \omega + 1, \dots, 2s + \omega + 1. \end{aligned}$$

The second line is a homogeneous system of $s + 1$ linear algebraic equations. To have a solution, the determinant of the matrix

$$\hat{T}_{i,j} = c_{s+\omega+1+i-j} \quad (i = 0, \dots, s; \quad j = 0, \dots, s)$$

must vanish:

$$\det(\hat{T}) = 0. \tag{24}$$

That is the auxiliary condition looked for to determine the spectrum provided that one chooses ω in agreement with the boundary condition at infinity. In general, it is sufficient to choose one of the three values $\omega = 1, 0, -1$ according to whether the function to be determined goes to $\pm\infty$, a constant or 0 when $z \rightarrow \infty$. Eventually, considering two successive values of ω gives upper and lower bounds on the eigenvalues [6, 30, 31].

The Padé method is well adapted to reproduce the analytic structure of a meromorphic function in particular if it has poles. If one writes the logarithmic derivative $\psi'(x)/\psi(x)$ under the form of a ratio L/K , then $L(x)$ and $K(x)$ are analytic functions in the complex x -plane (see [32] for an efficient use of this property). Since the transform (8) changes the zeros of $\psi(x)$ into poles for $h(x)$, the Padé method is better adapted to sum the Taylor series of $h(x)$ rather than that of $\psi(x)$ (however, see [33]). Moreover, it is also able to determine the energies of the excited states despite the poles located on the positive real x -axis (the nodes of $\psi_n(x)$ for $n \geq 2$).

The Padé method (named the Riccati–Padé method in [34] and later on the Hankel–Padé method in [35]) has been first introduced in [6] in conjunction with a logarithmic derivative transform like (8) to calculate, notably, the even and odd ground-state energies of the AO with $\beta = 1$ and $m = 2$ and for various values of λ . Typically the accuracy obtained was about eight significant figures. In [30], the excited-state energies have been estimated for the pure quartic and sextic AO (i.e. $\beta = 0$, $m = 2$ and 3), 11 significant figures were obtained on the estimate of E_0 for the quartic AO. The method has then been utilized several times (see, e.g. [31] for a list of references). In [31], the first two eigenvalues of both the quartic AO and the double well down to $\beta = -15$ are estimated with 18–20 significant figures. In addition, Amore and Fernández [36] have shown that the Padé method may also be applied to solve the two-point boundary value problem associated with several nonlinear ODEs.

The Padé method is easy to use. It has appeared robust in several occasions. However, its effectiveness is limited because the (repeated) calculations of determinants of large matrices are extremely time consuming. Sometimes, the Padé approximants introduce ‘spurious’ poles or zeros that can perturb a clear determination of the spectrum E_n . Though it is not as refined as the following methods, the Padé method is extremely useful.

3.6. The contour-integral method

3.6.1. The ground state. Leonard and Mansfield [7, 37] have proposed the recourse to a contour integral in the complex x -plane to perform an analytic continuation of the Taylor series of $W(x)$ (satisfying (5)) toward the large x values so that the asymptotic behavior (6) can be effectively imposed. The method may be described as follows.

Starting with the Taylor series (16), the coefficients of which satisfy the recurrence relation (17), one rewrites this series in terms of large $s = 1/x$:

$$\tilde{g}_M(s) = \sum_{i=0}^M \frac{c_i}{s^{2i}}. \tag{25}$$

According to (6), one is interested in finding the values of E for which this series, for $M \rightarrow \infty$, has a pole of order $m + 1$ at the origin $s = 0$:

$$\tilde{g}_\infty(s) \stackrel{s \rightarrow 0}{\simeq} -\frac{1}{(m+1)s^{m+1}}. \tag{26}$$

To this end, one considers the following integral over a large circle contour C around the origin:

$$F_\infty(\sigma) = \frac{1}{2i\pi\sigma^{m+1}} \int_C \frac{e^{\sigma s}}{s} \tilde{g}_\infty(s) ds.$$

According to the Cauchy formula, the contribution of the pole (26) to this function is $-\frac{1}{(m+1)!(m+1)}$. Assuming that all the other singularities of $\tilde{g}_\infty(s)$ are located to the left of

the imaginary axis in the complex s -plane then their contributions to $F_\infty(\sigma)$ will be made negligible as $\sigma \rightarrow \infty$, so that

$$\lim_{\sigma \rightarrow \infty} F_\infty(\sigma) = -\frac{1}{(m+1)!(m+1)}. \tag{27}$$

The truncated series (25) is then used to estimate $F_\infty(\sigma)$, leading to

$$\begin{aligned} F_M(\sigma) &= \frac{1}{2i\pi\sigma^{m+1}} \sum_{i=0}^M c_i \int_C \frac{e^{\sigma s}}{s} s^{-2i} ds, \\ &= \sum_{i=0}^M \frac{c_i}{\Gamma(2i+1)} \sigma^{2i-m-1}. \end{aligned} \tag{28}$$

Owing to the Euler Gamma function in the denominator, this series converges (the original series had a finite radius of convergence) and may be summed term by term to estimate $F_\infty(\sigma)$ when σ becomes large. Then a procedure similar to that described in points (2a)–(2d) in section 3.1 may be applied with z_0 replaced by σ_0 at which point the condition (27) is tentatively imposed.

If the region of analyticity of $\tilde{g}_\infty(s)$ does not correspond to the assumption that all the singularities are located to the left of the imaginary axis of s , the convergence may be spoiled by steady oscillations. To circumvent such difficulties, Leonard and Mansfield [7, 37] propose to modify (28) by introducing a parameter α_I , so that

$$F_{M,\alpha_I}(\sigma) = \sum_{i=0}^M \frac{c_i}{\Gamma(2i\alpha_I+1)} \sigma^{2i-m-1},$$

what corresponds to having performed some rotation of the complex s -plane (on the left-hand side if $\alpha_I < 1$).

3.6.2. The excited states. Because the excited states $\psi_n(x)$ for $n \geq 2$ have nodes on the positive real part of the x -axis, the corresponding $W_n(x)$ have (fixed) singularities on the positive real part of the s -axis which cannot be moved by α_I . Hence, the method does not apply directly to the determination of the excited states. In order to have access to them, Leonard and Mansfield [7] propose to use $W_0(x)$ (determined by the procedure described just above) as a basis to write (here accounting for the odd ($\epsilon = 1$) and even ($\epsilon = 0$) possibilities)

$$\psi(x) = x^\epsilon e^{W_\epsilon(x)} P(x). \tag{29}$$

The ODE satisfied by $P(x)$ is then

$$P'' + \frac{2\epsilon}{x} P' + 2W'_\epsilon P' + (E - E_\epsilon)P = 0.$$

This differential equation has two types of large x solution:

$$P(x) \stackrel{x \rightarrow \infty}{\simeq} \exp\left[-\frac{E - E_\epsilon}{2(m-1)x^{m-1}}\right], \tag{30}$$

$$P(x) \stackrel{x \rightarrow \infty}{\simeq} \exp\left[2\frac{x^{m+1}}{(m+1)}\right]. \tag{31}$$

Only (30) is compatible with the boundary condition at infinity for $\psi_n(x)$. Taking into account (6), the second behavior (31) reconstructs the blowing part proportional to B in (3).

With the behavior (30), $P_n(1/s)$ has no singularity at $s = 0$ and the contour integral procedure may again be applied to determine the values of $E_n - E_\epsilon$ that make this integral vanish when $\sigma \rightarrow \infty$.

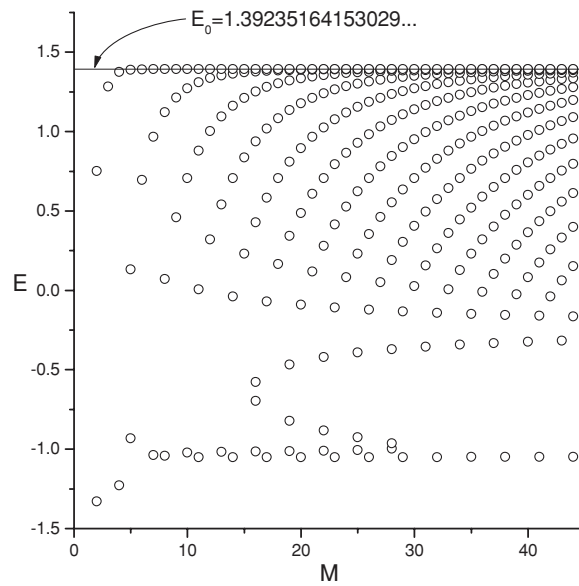


Figure 2. Evolution with the order M of all the real zeros corresponding to the auxiliary condition (34) for the AO with $\beta = 1$, $m = 2$. The mapping transform (32) is used with $R = 5.192695$ and $\alpha = 2$ corresponding to the expected analytic structure of the ground state ψ_0 [28] (see the text). The candidate to the ground-state energy E_0 is well evidenced.

3.6.3. Rescaling. In order to improve the efficiency of their method applied to the AO, Leonard and Mansfield [7, 37] utilize a rescaling which allows them to assign to the third coefficient c_3 the role of the adjustment parameter instead of E whereas c_2 is fixed instead of β . With this trick and $M = 300$, they have been able to estimate E_0 with an accuracy of 65 significant figures (for $\beta = 0$ and $m = 2$). The remaining of the spectrum of the AO up to $n \simeq 40$ is determined with an accuracy of 48 significant figures.

It is to be noted that the rescaling trick is not very convenient when $\beta \neq 0$ since then a supplementary adjustment of c_2 is required [7].

As indicated below, the mapping method appears to be more efficient than the contour-integral method, since, using the same rescaling trick, it yields a much greater accuracy with $M = 250$ only for the configuration $\beta = 0$ and $m = 2$ (see [8]). Also, the contour integral method has recourse to an iterative uncomfortable adjustment procedure for approaching the infinite boundary (similar to that of the power-series method described in section 3.1).

4. The mapping method

4.1. Introduction

The mapping method introduced in [5] leans also on an analytic continuation after a logarithmic-derivative-like transformation but in addition, the infinite boundary is brought close to the origin using the following conformal transformation:

$$z \rightarrow w = \frac{(1 + z/R)^{1/\alpha} - 1}{(1 + z/R)^{1/\alpha} + 1}, \tag{32}$$

in which R and α characterize the position of the vertex and the angle of an angular sector of the complex plane of z as shown in figure 2 of [5].

The conformal transformation (32) maps the interior of the angular sector of the z -plane into the interior of the unit circle centered at the origin of the w -plane so that $z = \infty$ corresponds to $w = 1$ (whereas $z = 0$ corresponds to $w = 0$).

If the interior of the angular sector is a region of analyticity of the original function $g(z)$ then the transformed series

$$\tilde{g}_M(w) = \sum_{i=0}^M u_i(E) w^i, \quad (33)$$

converges in the unit disk $|w| < 1$.

4.2. Example of the AO with $\beta = 1$ and $m = 2$

In this configuration, all the zeros of the ground state $\psi_0(x)$ are located on the imaginary axis of the x -plane [28]. For $g(z)$, they become (fixed) singularities located on the negative part of the real z -axis. Performing simple partial sums of the series in powers of x of $\psi_0(x)$ with $E = 1.392\,351\,641\,530\,29$ (close to the true value E_0 , see the appendix), it is easy to estimate the location of the (fixed) singularity of $g(z)$ the closest to the origin. This provides the radius of convergence $R_0 \simeq 5.192\,695$ for the series of $g(z)$. In addition, the plane cut on the negative real axis, starting from the point $z = -5.192\,695$, forms an angular sector such that $R = R_0$ and $\alpha = \alpha_0 = 2$. Choosing those values in the conformal mapping (32) and accounting for the constraint (6) at infinity (and the definitions (15) and (16)), the auxiliary condition looked for to estimate E_0 can be expressed as

$$\tilde{g}_M^{(2)}(w)_{w=1} = 0, \quad (34)$$

in which $\tilde{g}^{(2)}(w)$ stands for the conformal mapping applied on the function $g''(z)$ which goes to zero as $z \rightarrow \infty$.

The condition (34) is a polynomial equation for E , the solutions of which effectively display a stable real value as M is increased. Figure 2 shows that, even when M is small, this value is easily identified and can be followed without difficulty. Actually this stable value converges quickly to the true value E_0 . For example, with $M = 150$, E_0 is determined with an accuracy of 83 significant figures (see the appendix). Only the choice of the order M limits the accuracy of this estimation which is much more accurate than the previously published values [14, 16, 38].

A convenient variant to the auxiliary condition (34) consists in simply imposing the vanishing of the last term of the series (33):

$$u_M(E) = 0. \quad (35)$$

This simplified condition is justified because, for a generic E , $g(z)$ has movable singularities which limit the convergence of the series $\tilde{g}_M(w)$ except for the value E_0 for which they are sent to infinity. Hence, imposing the condition (35) amounts to force the convergence of the series and this procedure enables the determination of the value of E_0 .

4.3. Practical use of the mapping method

In general one does not know the location of the (fixed) singularity closest to the origin of $g(z)$. One must thus consider R and α as free parameters. Several procedures may be conceived to approximately determine the ‘best’ values of R and α .

Suppose first that R_0 and α_0 define an angular sector in which $g(z)$ is analytic. If $R < R_0$ and $\alpha < \alpha_0$, the mapping method should provide a convergent result as the order M is increased. If it does not, then a decrease of the trial value of R (also of α even) is necessary.

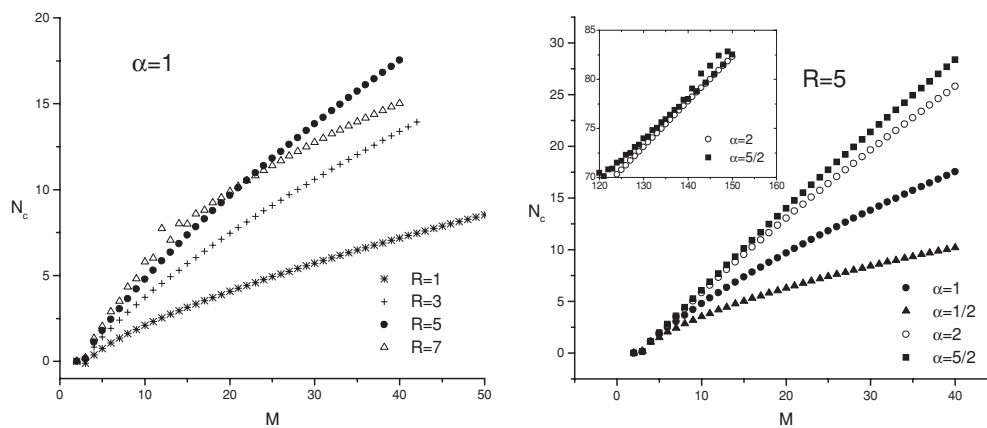


Figure 3. Illustration, on the AO with $\beta = 1$, $m = 2$, of the respective importance of the free parameters R and α , the correct values of which would be $R_0 \simeq 5.192\,695$ and $\alpha = 2$. N_c is an approximate estimate of the number of stabilized figures ($N_c = -\log|1 - E_M^{(0)}/E_{M-1}^{(0)}|$ where $E_{M-1}^{(0)}$ and $E_M^{(0)}$ are two successive estimates of E_0 on varying the order of the Taylor series). On the left, α is fixed to 1 and R is varied. It is clear that the best convergence corresponds to $R = 5$. For smaller values of R , the convergence seems to be monotonically increasing whereas for $R = 7$ (larger than the radius of convergence R_0), a relatively important decrease of the slope shows a greater deterioration of the convergence compared to the other curves. On the right, R is fixed to 5 and α is varied. The best convergence seems to correspond to $\alpha = 5/2$ which is a too large value. Actually, the small rule box shows that at larger values of the order M , this choice, most probably, is no longer the best one.

One proceeds by successive trial and error to find one couple of value $\{R_1, \alpha_1\}$ such that the mapping procedure begins to converge. In the example $\beta = 1$ and $m = 2$, if one sets $R = 1$, $\alpha = 1$ and $M = 50$ one obtains an estimate of E_0 with eight significant figures (1.392 351 63). One may then look at the effective radius of convergence of the original series with the help of the d’Alembert or the Cauchy rule or the plot of the sum of the series as a function of z . This could give a better estimate of R_0 leading to a better convergence toward E_0 . However, a large accuracy on R_0 is not required to get a large accuracy on E_0 .

The determination of the best value of α proceeds also by trial and error and is determined by the criterion of best convergence as shown by figure 3. For small values of M , it may appear that ‘exotic’ effective best values of α may be observed. Figure 3 shows that the value $\alpha = 5/2$ provides, for small M , an apparent better convergence than the true value $\alpha = 2$. But, for larger values of M , one observes that the former case finally yields perturbed convergence whereas with the second case, the convergence remains smooth (see figure 3).

4.4. Excited states

The determination of the excited states proceeds as in section 3.6. The ground state $W_0(x)$ (or the first odd state $W_1(x)$) is used as a basis through (29). Consequently, there is no need to look for new determinations of R and α . The values obtained previously for $W_{0,1}(x)$ work also for the excited states. At a given order M , the corresponding auxiliary condition yields a polynomial equation for E , the real zeros of which form the approximate spectrum of the AO (see figure 4). The values of the spectrum are given in the appendix, and they are much more accurate than (and compatible with) the existing previous estimates [14, 16, 38].

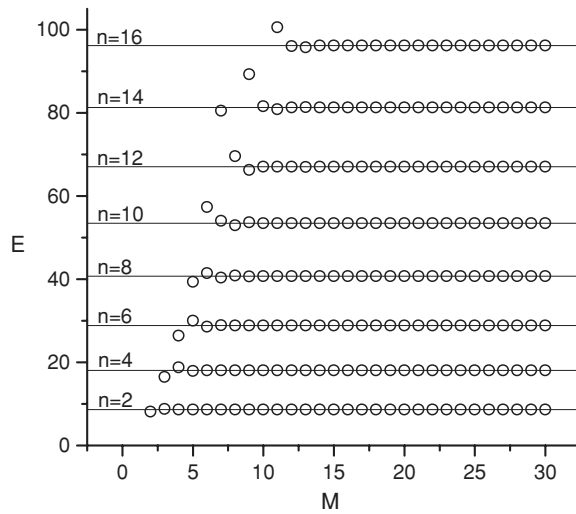


Figure 4. Evolution with M of the distribution of the real zeros (open circles) corresponding to the auxiliary condition of the mapping method applied on the function $P(x)$ defined by (29) in the case $\beta = 1$ and $m = 2$ (even case). The horizontal lines correspond to the ‘exact’ values of the spectrum given in the appendix.

4.5. Other examples treated

Configurations which are more difficult to treat than the previous one have been also considered. For a detailed discussion, the interested reader may look at the previous version of this paper [8]. Let me simply mention that the ground-state energy of the configuration $\beta = 0$ and $m = 2$ has been determined with an accuracy of 114 significant figures in the even case and of 120 significant figures in the odd case! A complication arises when β is more and more negative (double-well configurations). The efficiency of the mapping method decreases as β becomes more and more negative due to the decreasing of the radius of convergence of the series of g .

5. Summary and conclusion

Different potential configurations of the AO have been considered to illustrate the efficiency and the limitations of the mapping method for solving nonlinear ODE [5]. As several other quasi-analytic methods encountered here and there in the literature of the AO, it is based on a generic Taylor series in powers of the independent variable. After a short presentation of those methods, the mapping method has been introduced and its use is illustrated on the basis of the simplicity of the analytic properties of the AO. In particular, the practical determination of the two adjustable parameters R and α , inherent to the method (see equation (32)), corresponds precisely to those analytic properties. Extremely high accurate estimates of the spectrum of the AO have been easily obtained (see the appendix and [8]). The efficiency of the method decreases with the radius of convergence R . In the case of very small R , the analytic continuation method or the Padé method have appeared to be more efficient.

Finally the mapping method [5] is an extremely refined method, easy to use and which provides clear convergence toward the values looked for provided the radius of convergence of the initial Taylor series is not too small. The Padé method [6] is also an easy-to-use method

Table A1. Estimates of even excited-state energies for $\beta = 1$, $m = 2$ as obtained by the mapping method with $M = 115$. The last column displays an approximate value of the number of significant figures obtained in each case.

n	E_n	N_c
2	8.655 049 957 759 309 688 116 539 457 377 308 026 275	40
4	18.057 557 436 303 252 894 771 239 646 525 434 8531	39
6	28.835 338 459 504 248 840 133 635 715 499 838 17	37
8	40.690 386 082 106 444 725 278 931 481 582 464	35
10	53.449 102 139 665 264 600 831 506 459 7595	33
12	66.995 030 001 247 166 061 019 704 904 702	32
14	81.243 505 050 767 152 737 066 521 470 34	31
16	96.129 642 045 234 052 046 811 222 396	29
18	111.601 815 045 172 958 533 701 5116	28
20	127.617 777 795 354 918 333 962 292	27
22	144.142 195 296 398 163 731 983	24
24	161.144 990 694 512 951 868 62	23
26	178.600 192 366 875 761 1938	22
28	196.485 102 910 220 443 66	20
30	214.779 683 549 176 627	18
32	233.466 087 479 3752	16
34	252.528 299 061 4935	16

which is more robust but less refined than the mapping method. The two methods (and also the analytic continuation method [10, 12]) may certainly be advantageously associated in the process of solving a two-point boundary problem of a nonlinear ODE.

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Appendix

In this appendix, we present the estimates of the energy spectrum of the configuration $\beta = 1$, $m = 2$ of the AO as obtained using the mapping method.

With $M = 150$, $R = 5.192\ 694\ 846\ 776\ 623\ 5669$ and $\alpha = 2$, the ground-state energy has been determined with 83 significant figures:

$$E_0 = 1.392\ 351\ 641\ 530\ 291\ 855\ 657\ 507\ 876\ 609\ 934\ 184\ 600\ 066\ 711\ 220\ 834\ 088\ 906\ 349\ 323\ 877\ 567\ 431\ 875\ 646\ 5286.$$

The estimates of the 17 first even excited states, obtained with $M = 115$, are given in table A1.

With $M = 115$, $R = 6.033\ 449\ 839\ 500\ 17$ and $\alpha = 2$ the first odd state has been determined with 70 significant figures:

$$E_1 = 4.648\ 812\ 704\ 212\ 077\ 536\ 377\ 032\ 917\ 260\ 584\ 488\ 898\ 860\ 447\ 882\ 825\ 934\ 823\ 424\ 910\ 341\ 006.$$

Table A2. Estimates of odd excited-state energies for $\beta = 1$, $m = 2$ as obtained by the mapping method with $M = 121$. The last column displays an approximate value of the number of significant figures obtained in each case.

n	E_n	N_c
3	13.156 803 898 049 875 079 209 772 040 382 314 674 650 1484	45
5	23.297 441 451 223 189 084 864 481 992 098 123 828 1208	42
7	34.640 848 321 111 332 542 884 527 618 156 342 033 769	41
9	46.965 009 505 675 527 984 096 443 324 175 114 2524	39
11	60.129 522 959 157 771 315 848 016 059 852 822 16	37
13	74.035 874 359 102 530 180 741 205 487 403 699 15	37
15	88.610 348 800 799 158 873 039 105 371 324 88	34
17	103.795 300 322 272 609 678 111 687 955 7136	34
19	119.544 170 733 050 311 130 026 949 345 64	32
21	135.818 417 325 610 373 340 451 430 114	30
23	152.585 504 205 573 921 566 866 1903	28
25	169.817 528 001 595 348 199 877 321	27
27	187.490 242 692 950 322 544 8058	25
29	205.582 346 604 423 518 718 34	23
31	224.074 947 852 600 306 2853	22
33	242.951 154 951 147 123 53	20
35	262.195 757 468 519 8472	19
37	281.794 972 923 819 312	18
39	322.008 069 744 848	15
41	363.501 894 8643	13

The estimates of the 20 first odd excited states, obtained with $M = 121$, are given in table A2.

All the estimates obtained are in agreement with the existing literature [14, 17, 38] at least up to 10–16 significant figures they quote.

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