ORIGINAL PAPER

Numerical computation of the coefficients in exponential fitting

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Abstract

We show that a direct numerical computation of the coefficients of any method based on the exponential fitting is possible. This makes unnecessary the knowledge of long sets of analytical expressions for the coefficients, as usually presented in the literature. Consequently, the task of any potential user for writing his/her own code becomes much simpler. The approach is illustrated on the case of the Numerov method for the Schrödinger equation, on a version for which the analytic expressions of coefficients are not known.

Keywords Numerov method · Schrödinger equation · Regularization · Coffey-Evans potential

1 Introduction

Exponential fitting (ef for short) is a mathematical procedure for generating numerical methods for various operations (solution of differential or integral equations, numerical differentiation, quadrature, least-square approximation, interpolation, etc.) on functions with a pronounced oscillatory or hyperbolic variation. The typical condition for generating the coefficients of such methods is that the method must be exact for a set of functions including exponential functions.

The literature is very vast, see, e.g., [1–17] and references therein, but in the large majority of papers the efforts were directed on the analytic determination of the coefficients. However, the resulting expressions are often so long and cumbersome that their use becomes a difficult task for any potential reader who wants to apply such

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methods. Attempts of reducing the number of the expressions do also exist, e.g., in [18], but for a potential user the problem continues to remain quite complicated.

As a matter of fact, the need for analytic expressions was important especially in the early stages of the field when properties of the new ef versions, for example the stability properties of solvers of differential equations, were better seen on analytic expressions. At present, however, the main interest consists in applications such that by now only the numerical determination of the coefficients is sufficient.

In this paper, we consider the problem from this perspective. The need of analytic expressions, which in many papers fill pages and pages of formulas, becomes redundant. Only the generating system of equations has to be mentioned, and everything after that is done numerically by using a dedicated subroutine.

We illustrate this on the case of the Numerov method for the Schrödinger equation.

2 Numerov method

This is to solve the Schrödinger equation

$$y'' = (V(x) - E)y, \quad x \in [a, b], \tag{1}$$

where $V(x)$, called the potential, is a given function, and E, the energy, is a constant. Two problems are usually considered: (i) initial value problem, with initial values $y(a)$ and $y'(a)$, with unique solution for any E, and (ii) eigenvalue problem where conditions at the two ends are given, $\alpha_1 y(a) + \beta_1 y'(a) = 0$ and $\alpha_2 y(b) + \beta_2 y'(b) = 0$. Here the weights have to satisfy the conditions $|\alpha_i| + |\beta_i| \neq 0$, $i = 1, 2$. The eigenvalues and their eigenfunctions have to be computed in this case.

Let us introduce an equidistant partition of $[a, b]$ with the step h: $x_i = a + ih$, $i = 0, 1, 2, ..., i_{max}$; Of course, $x_{i_{max}} = b$. The Numerov method links the numerical values of y at three consecutive points,

$$y_{i+1} + a_1 y_i + y_{i-1} = h^2 [b_0(f_{i+1} y_{i+1} + f_{i-1} y_{i-1}) + b_1 f_i y_i] \tag{2}$$

where $f_i = V(x_i) - E$. It allows computing y_{i+1} in terms of y_{i-1} and y_i (forwards propagation) or y_{i-1} in terms of y_i and y_{i+1} (backwards propagation).

In the frame of the exponential fitting, four different versions of this method (schemes), denoted S_m, $m = 0, 1, 2, 3$, are available, see [1, 19]. In each, the coefficients a_1, b_0, and b_1 are known in analytic form but there is one restriction. While in principle each scheme depends on three parameters, Z_1, Z_2, Z_3, of the form $S(Z_1, Z_2, Z_3)$, in the existing publications, the maximal number of parameters that can be different is only two: one is 0 and the other, Z, allowed to be not vanishing. Specifically, the existing schemes are: $S_0 = S(0, 0, 0)$ (classical), $S_1 = S(0, 0, Z)$, $S_2 = S(0, Z, Z)$, and $S_3 = S(Z, Z, Z)$.

A scheme where all three parameters Z_1, Z_2 and Z_3 are different can be also derived in analytic form but an accurate numerical procedure to compute its coefficients is available.

The theory behind this procedure is presented in [20]. In that paper, the following system of linear algebraic equations is examined:

$$\sum_{n=1}^{N} F_n(Z_k)v_n = B(Z_k)\,, \ k = 1, 2, \cdots, N\,, \tag{3}$$

written compactly as $\mathbf{Fv} = \mathbf{B}$, where $\mathbf{F}_{kn} = F_n(Z_k)$ and $\mathbf{B}_k = B(Z_k)$. We see that a set of $N + 1$ functions, $F_n(Z)$, $n = 1, 2, \cdots, N$ and $B(Z)$, and of N arguments Z_k, $k = 1, 2, \cdots, N$, are involved. Each column n of matrix $\mathbf{F}$ contains one and the the same function F_n and each row k has one and the same argument Z_k. The latter holds true also for the column vector $\mathbf{B}$.

The numerical problem with this system is that any standard numerical method to solve it meets difficulties when some arguments are close together. For example, the first two equations coincide if $Z_1 = Z_2$ and then the determinant of the system vanishes. To solve this type of difficulty, authors of [20] develop a regularization procedure for the system. The numerical solution of the resulting regularized system is free of difficulties such that its results are uniformly accurate irrespective of how close or separated are the arguments. A code is also available. This is Fortran subroutine REGSOLV (double precision arithmetics) in the CD attached to book [1].

The approach developed in [20] and the associate REGSOLV are rather general, and many existing investigations on ef methods lead to the need of solving systems of this form. For the Numerov method, the system for computing the three coefficients consists of three equations:

$$-a_1 + 2Z_k\eta_{-1}(Z_k)b_0 + Z_kb_1 = 2\eta_{-1}(Z_k)\,, \ k = 1, 2, 3. \tag{4}$$

see [20]. For the set $\eta_{-1}(Z),\ \eta_0(Z),\ \eta_1(Z), \cdots$ see the Appendix.

To build up this system, we associate to the Numerov algorithm (2) the functional

$$\mathcal{L}[h, a_1, b_0, b_1]y(x) = y(x + h) + a_1y(x) + y(x - h) - h^2[b_0(y''(x + h)$$
$$+y''(x - h)) + b_1y''(x)], \tag{5}$$

and ask that this is identically vanishing if $y(x)$ is any of the six functions

$$e^{\pm\mu_1 x},\ e^{\pm\mu_2 x},\ e^{\pm\mu_3 x}, \tag{6}$$

where μ_k may be either real or purely imaginary. We get

$$\mathcal{L}[h, a_1, b_0, b_1]e^{\pm\mu_k x} = e^{\pm\mu_k x}\{e^{\mu_k h} + a_1 + e^{-\mu_k h} - \mu_k^2 h^2[b_0(e^{\mu_k h} + e^{-\mu_k h}) + b_1]\} = 0 \tag{7}$$

for each k. By expressing the expression in the curly brackets in terms of η_{-1},

$$e^{\mu_k h} + a_1 + e^{-\mu_k h} - \mu_k^2 h^2[b_0(e^{\mu_k h} + e^{-\mu_k h}) + b_1]$$
$$= 2\eta_{-1}(Z_k) + a_1 - Z_k(2\eta_{-1}(Z_k)b_0 + b_1),\ Z_k = \mu_k^2 h^2,$$

system (4) results. We have preferred to write the system in terms of η functions because, on one hand, REGSOLV works for real arguments and functions and therefore, if $\mu_k h$ were used as arguments, a system in complex arithmetics would result and, on the other hand, this subroutine asks for the expressions of the derivatives of the involved F_n and B, and these are very short if written in terms of the η functions, see again the Appendix.

By solving this system with REGSOLV, the computed coefficients are highly accurate. Their errors are quite often within the round-off limits. Thus, for example, if we put here $Z_1 = Z_2 = Z_3 = 0$, we reobtain the numerical values of the coefficients of the classical S_0. In the following, the scheme $S(Z_1, Z_2, Z_3)$ with the coefficients computed numerically will be denoted S_3^*.

The expressions of the leading term of local truncation error, denoted lte, are known for versions $S_m, m = 0, 1, 2, 3$. As for the new S_3^*, we follow the general theory, see, e.g., [1, 19].

The point is that the functions in (6) are six linear independent solutions of the sixth order differential equation $Dy(x) = 0$, where

$$Dy = y^{(6)} - (\mu_1^2 + \mu_2^2 + \mu_3^2)y^{(4)} + (\mu_1^2\mu_2^2 + \mu_1^2\mu_3^2 + \mu_2^2\mu_3^2)y'' - \mu_1^2\mu_2^2\mu_3^2 y. \quad (8)$$

This means that, if the coefficients are those resulting from solving the generating system (4), then functional $\mathcal{L}$ of (5) can be written as a product of the form

$$\mathcal{L}[h, a_1, b_0, b_1]y(x) = ADy(x), \quad (9)$$

where the factor A must be determined. To do this, we consider the lowest power function for which $\mathcal{L}$ is nonvanishing. This is $y(x) = 1$ in our case. Equation (5) gives $\mathcal{L}[h, a_1, b_0, b_1]1 = 2 + a_1$ and, since $D1 = -\mu_1^2\mu_2^2\mu_3^2$, we obtain

$$A = -\frac{2 + a_1}{\mu_1^2\mu_2^2\mu_3^2} = -h^6\frac{2 + a_1}{Z_1 Z_2 Z_3}, \quad (10)$$

such that finally the lte of S_3^* at x_i is

$$lte = -h^6\frac{2 + a_1}{Z_1 Z_2 Z_3}Dy(x_i). \quad (11)$$

The numerical computation of the middle factor may meet difficulties for small $|Z_k|$ because this factor is of the form $0/0$ if $Z_k = 0$. A direct procedure for determining approximate but reliable values is as follows. To each Z_k, we associate

$$Z_k' = \begin{cases} Z_k & \text{if } |Z_k| > 0.1 \\ -0.1 & \text{if } -0.1 \le Z_k < 0 \\ 0.1 & \text{if } 0 \le Z_k \le 0.1 \end{cases}. \quad (12)$$

and solve (4) for this set. If a_1', b_1', and b_2' are the resulting coefficients then the expression $(2 + a_1')/Z_1' Z_2' Z_3'$ produces values which are exact in at least three figures for any Z_1, Z_2, Z_3.

To conclude, the new S_3^* remains of the same order (four) as any other scheme of this method but a gain in accuracy is expected from the last factor in the lte provided Z_k parameters are advantageously selected.

Remark An extension of REGSOLV is also presented in book [1]. This is subroutine REGSOLV2 which solves a system consisting of two blocks:

$$\sum_{n=1}^{N} F_n^1(Z_k)v_n = B^1(Z_k)\,, \ k = 1, 2, \cdots, \bar{k},$$

$$\sum_{n=1}^{N} F_n^2(Z_k)v_n = B^2(Z_k)\,, \ k = \bar{k}+1, \bar{k}+2, \cdots, N\,, \tag{13}$$

where functions F_n^i, B^i, $i = 1, 2$ and their derivatives have to be furnished by the user. This opens the possibility of solving a substantially larger class of problems related to the ef approach. In particular, for the Numerov method, we may address the problem of generating the most general set of coefficients consistent with the set (6). Specifically, the functional to be addressed is now

$$\mathcal{L}[h, a_1, a_2, b_0, b_1, b_2]y(x) = y(x+h) + a_1 y(x) + a_2 y(x-h) - h^2[b_0 y''(x+h)$$
$$+b_1 y''(x) + b_2 y''(x-h)], \tag{14}$$

instead of (5). On asking that this is identically vanishing for the pair $e^{\pm\mu x}$, we get

$$\mathcal{L}[h, a_1, a_2, b_0, b_1, b_2]e^{\pm\mu x} = e^{\pm\mu x} E^{\pm z} = 0, \ z = \mu h,$$

where

$$E^{\pm z} = e^{\pm z} + a_1 + a_2 e^{\mp z} - z^2(b_0 e^{\pm z} + b_1 + b_2 e^{\mp z}).$$

The set of two equations $E^{\pm z} = 0$ is now expressed in terms of the eta functions of argument $Z = z^2$. The following equivalent pair results:

$$G^+(Z) \equiv (E^z + E^{-z})/2 = \eta_{-1}(Z) + a_1 + a_2\eta_{-1}(Z) - Z(b_0\eta_{-1}(Z) + b_1 + b_2\eta_{-1}(Z)) = 0,$$

$$G^-(Z) \equiv (E^z - E^{-z})/(2z) = \eta_0(Z) - a_2\eta_0(Z) - Z(b_0\eta_0(Z) - b_2\eta_0(Z)) = 0.$$

All together, the five coefficients consistent with the set of six functions (6) satisfy the system of six linear equations $G^{\pm}(Z_k) = 0$, $k = 1, 2, 3$, but, to determine them numerically, one of these equations must be disregarded. For example, if we choose disregarding $G^-(Z_3) = 0$, the following system of five equations and of form (13) remains to be solved:

$$-a_1 - \eta_{-1}(Z_k)a_2 + Z_k\eta_{-1}(Z_k)b_0 + Z_k b_1 + Z_k\eta_{-1}(Z_k)b_2 = \eta_{-1}(Z_k), \ k = 1, 2, 3$$

$$\eta_0(Z_k)a_2 + Z_k\eta_0(Z_k)b_0 - Z_k\eta_0(Z_k)b_2 = \eta_0(Z_k), \ k = 1, 2. \tag{15}$$

As expected, if $a_2 = 1$ and $b_0 = b_2$, as tacitly assumed in (4), system (15) reduces to (4). By solving (15) with REGSOLV2, the values furnished by REGSOLV for (4) and the additional relations $a_2 = 1$ and $b_0 = b_2$ are reproduced with an absolute error which is typically within the round-off limits. As an extra check, we can examine if the disregarded equation $G^-(Z_3) = 0$ is also satisfied for the computed coefficients, to find out that this is indeed confirmed within the same accuracy.

3 A numerical illustration

We take the case of the eigenvalue problem for the Schrödinger equation (1) with the Coffey-Evans potential

$$V(x) = -2\beta \cos(2x) + \beta^2 \sin^2(2x) \tag{16}$$

with $\beta = 25$, see Fig. 1. The domain is $[a = 0, b = \pi/2]$ and the boundary conditions are $y(0) = y(\pi/2) = 0$. As a matter of fact, in the literature related to this problem, e.g., [22, 23], the domain is $[-\pi/2, \pi/2]$, and various values for parameter β are considered. However, the domain and the value of β used by us are sufficient for this illustration.

We compare three schemes: S_0, S_3, and the new S_3^*. The domain is divided in two sectors, $[0, \pi/4]$ and $[\pi/4, \pi/2]$, and the eigenvalues are located by shooting. A set of test values $E \in [50, 400]$ is considered and for each E the equation is propagated forwards with the starting values $y_0 = 0$, $y_1 = h$ up to $\pi/4 + h$ and backwards, with $y_{i_{max}} = 0$, $y_{i_{max}-1} = h$ for start, up to $\pi/4$. The values obtained at $\pi/4$ and $\pi/4 + h$ from the two directions, denoted $y_1^f(E)$, $y_2^f(E)$ and $y_1^b(E)$, $y_2^b(E)$, respectively, are used to form the mismatch function

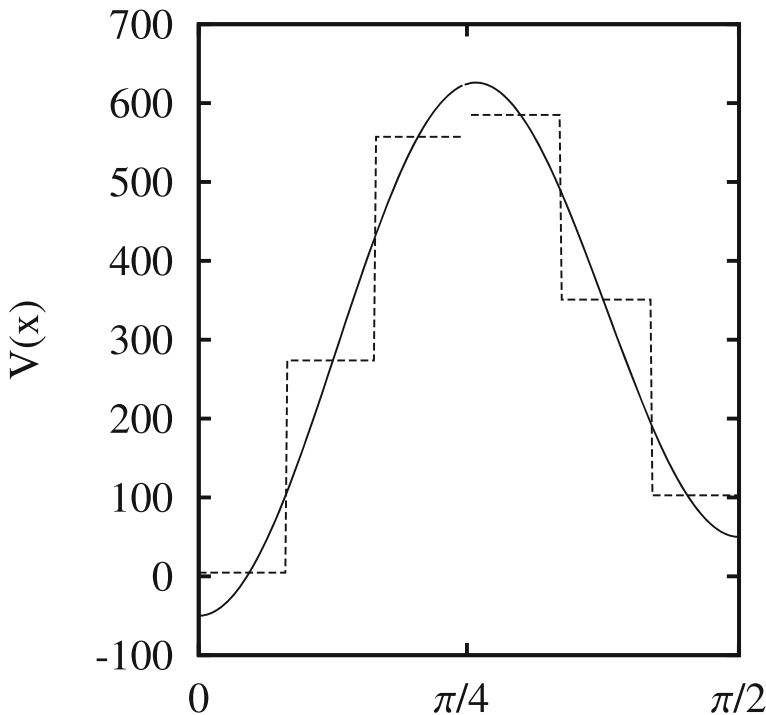$$\Delta(E) = y_1^f(E)y_2^b(E) - y_1^b(E)y_2^f(E). \tag{17}$$

Fig. 1 Coffey-Evans potential function (16) with $\beta = 25$ on interval $[0, \pi/2]$ and the three piecewise average values of it on each sector

The eigenvalues are located as the zeros of this $\Delta(E)$.

Computation of the coefficients:

- S_0: This is the classical scheme. Its coefficients are $a_1 = -2$, $b_0 = 1/12$, and $b_1 = 5/6$.
- S_3: Let $\bar{V}^f$ and $\bar{V}^b$ be the average values of $V(x)$ over the two sectors. Arguments $Z^f = (\bar{V}^f - E)h^2 / Z^b = (\bar{V}^b - E)h^2$ are used in the forwards/backwards propagations with this S_3. The coefficients are computed by the known analytic expressions, see [1, 2, 19].
- S_3^*: Each of the two sectors is divided into three equal subsectors, and let $\bar{V}_k^f$ / $\bar{V}_k^b$, ($k = 1, 2, 3$), be the corresponding average values (horizontal segments in Fig. 1). The three arguments Z_1, Z_2, Z_3 are now $Z_k^f = (\bar{V}_k^f - E)h^2$ / $Z_k^b = (\bar{V}_k^b - E)h^2$ ($k = 1, 2, 3$), and the coefficients are computed by REGSOLV.

Notice that the computational effort is the same for S_3 and S_3^*: for each E they need only two computations of the coefficients, one for each direction.

In Table 1, we give the absolute errors in eigenvalues from the three schemes and different values of h. The reference eigenvalues, denoted E_{exact}, were computed by S_3^* at $h = \pi/1024$.

Table 1 Absolute errors $\Delta E = E_{exact} - E_{comput}$ in 10^{-6} units from the three compared Numerov versions for the first four eigenvalues of the Coffey-Evans potential on $[0, \pi/2]$

E_{exact}	h	S_0	S_3	New S_3^*
			ΔE	
97.9345617	$\pi/32$	36572	555229	5509
	$\pi/64$	2248	32, 423	258
	$\pi/128$	139	1937	14
	$\pi/256$	8	118	0
	$\pi/512$	0	7	0
191.5876333	$\pi/32$	31797	310471	7539
	$\pi/64$	1956	19, 804	411
	$\pi/128$	121	1244	24
	$\pi/256$	7	77	1
	$\pi/512$	0	4	0
280.6142453	$\pi/32$	271059	331072	−7231
	$\pi/64$	16500	18341	−563
	$\pi/128$	1024	1082	−36
	$\pi/256$	63	65	−2
	$\pi/512$	3	4	0
364.5556442	$\pi/32$	228089	184067	2259
	$\pi/64$	13903	11143	54
	$\pi/128$	863	691	2
	$\pi/256$	53	43	0
	$\pi/512$	3	2	0

We see that, as expected, all schemes are of the same order, four. Indeed the errors typically decrease by a factor of around 16 when h is halved. What is also significant is that S_3 does not improve the accuracy if compared with the classical S_0. For contrast, the new S_3^* produces systematically better results than the other two schemes. The accuracy gain with S_3^* is of between one and two decimal figures if compared with the best placed from S_0 and S_3.

Our results suggest that, more general, the use of ef-based versions with one and the same value for the parameters (that is, with $Z_1 = Z_2 = Z_3$) does not automatically lead to an improvement in accuracy for potentials with a pronounced variation. This holds true only for potentials that are reasonably well approximated by a step function, as is the case of the Woods-Saxon potential which is frequently used in the literature. Otherwise, using three different Z_k represents a good idea.

These remarks do not restrict to the Numerov method. For any other method based on exponential fitting, the choice of sets with different values for the parameters, instead of a single one, will add more flexibility and therefore more chances for accuracy gain. The total number of parameters may vary from one method to another. Anyway, in any such situation, the use of the numerical solvers REGSOLV or REGSOLV2 for the coefficients will continue to play a central role.

Also worth adding is that the way how the values of the parameters should be advantageously selected remains open at this stage, especially for second-order differential equations of general form $y'' = f(x, y)$.

4 Conclusions

We have considered the Numerov method to introduce the new scheme S_3^* which is more flexible than the existing ones and includes them as particular cases. The important feature is that now the coefficients are computed numerically, not by analytical expressions, as before, and the numerical values obtained in this way are practically as accurate as those from analytic expressions. Fortran 95 subroutine REGSOLV was used for this purpose. Subroutine REGSOLV2 can be also used according to the case. The major advantage is that now the knowledge of the analytic expressions of the coefficients and their series expansions, which usually consists in sets of lengthy formulas, is no more needed. Only the generating system, as are (4) or (15) for the Numerov method, has to be formulated and communicated to the potential readers.

Appendix

Eta functions $\eta_{-1}(Z)$, $\eta_0(Z)$, $\eta_1(Z)$, ... are defined as follows [1, 19, 21]:

The first two are

$$\eta_{-1}(Z) = \begin{cases} \cos(|Z|^{1/2}) & \text{if } Z \leq 0 \\ \cosh(Z^{1/2}) & \text{if } Z > 0 \end{cases}, \quad \eta_0(Z) = \begin{cases} \frac{\sin(|Z|^{1/2})}{|Z|^{1/2}} & \text{if } Z < 0 \\ 1 & \text{if } Z = 0 \\ \frac{\sinh(Z^{1/2})}{Z^{1/2}} & \text{if } Z > 0 \end{cases} . \quad (18)$$

In some papers, function $\eta_{-1}(Z)$ is denoted $\xi(Z)$.

Functions $\eta_m(Z)$ with $m > 0$ are generated by recurrence

$$\eta_m(Z) = \frac{\eta_{m-2}(Z) - (2m - 1)\eta_{m-1}(Z)}{Z}, \quad m = 1, 2, 3, \dots \quad (19)$$

if $Z \neq 0$, and by following values at $Z = 0$:

$$\eta_m(0) = \frac{1}{(2m + 1)!!}, \quad m = 1, 2, 3, \dots \quad (20)$$

Some useful properties are:

Series expansion:

$$\eta_m(Z) = 2^m \sum_{q=0}^{\infty} \frac{(q + m)!}{q!(2q + 2m + 1)!} Z^q, \quad m = 0, 1, 2, \dots \quad (21)$$

Asymptotic behavior at large $|Z|$:

$$\eta_m(Z) \approx \begin{cases} \frac{\eta_{-1}(Z)}{Z^{(m+1)/2}} & \text{for odd } m \\ \frac{\eta_0(Z)}{Z^{m/2}} & \text{for even } m. \end{cases} \quad (22)$$

Differentiation properties:

$$\eta'_m(Z) = \frac{1}{2}\eta_{m+1}(Z), \quad m = -1, 0, 1, 2, \dots \quad (23)$$

The latter is important in subroutine REGSOLV for solving (3) because there the expressions of the derivatives of functions $F_n(Z)$, $n = 1, 2, \cdots, N$ and $B(Z)$ are also requested.

The expressions needed in system (4) for these functions and their derivatives are:

$$F_1(Z) = -1 \text{ and } F_1^{(m)}(Z) = 0 \text{ for } m \geq 1,$$

$$F_2(Z) = 2Z\eta_{-1}(Z), \quad F_2^{(1)}(Z) = 2\eta_{-1}(Z) + Z\eta_0(Z) \text{ and}$$
$$F_2^{(m)}(Z) = 2^{1-m}[\eta_{m-3}(Z) + 3\eta_{m-2}(Z)] \text{ for } m \geq 2,$$

$$F_3(Z) = Z, \quad F_3^{(1)}(Z) = 1 \text{ and } F_3^{(m)}(Z) = 0 \text{ for } m \geq 2,$$

$$B(Z) = 2\eta_{-1}(Z) \text{ and } B^{(m)}(Z) = 2^{1-m}\eta_{m-1}(Z) \text{ for } m \geq 1.$$

Codes for the computation of the eta functions are available: subroutines GEBASE and GEBASEV (fortran 95, double precision arithmetic) in the compact disk attached to book [1]; see also formConv (mathematica) in [24].

For solving (4), we have used derivatives up to $m_{max} = 30$ with eta functions computed by GEBASEV.

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