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Asymptotic shooting method for the solution of differential equations

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Abstract. We present a method for the solution of ordinary differential equations over a semi-infinite interval, including the determination of eigenvalues, which is in principle capable of arbitrary accuracy. The solution is expressed in terms of finite polynomials, rendering the integration or determination of zeros of such solutions a straightforward matter. We have applied the method to a number of examples including the determination of the eigenvalues of the screened Coulomb potential and the three-dimensional quartic oscillator.

1. Introduction

Most ordinary differential equations (ODEs) of mathematical physics are of second order with a regular singularity at the origin and an irregular singularity at infinity. In addition, the imposition of boundary conditions on the solution at infinity, such as that the solution remain finite or have a specific form, often requires the determination of an eigenvalue or similar parameter of the ODE. In this paper we present a method which we call the asymptotic shooting method, which enables one to find the solutions to such ODEs, including the determination of eigenvalues or similar parameters to arbitrary accuracy. The solutions are given in terms of finite polynomials over certain intervals, so that the integration or determination of zeros of such solutions is a straightforward matter.

2. General theory

We shall present the theory in terms of second-order ODEs. The generalisation to higher-order ODEs presents no difficulties. We shall assume the situation which usually occurs in ODEs from mathematical physics, i.e. one solution of the ODE is regular at the origin and the other is singular while at infinity both solutions are irregular. However, the method does not depend on these assumptions, which are used primarily to motivate the development.

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Let $u_1(z)$ and $u_2(z)$ be two independent solutions of the ODE obtained about the origin, in our case by the method of Frobenius. We take u_1 to be the regular solution and u_2 to be singular at the origin. Similarly, let $u^+(z)$ and $u^-(z)$ be two independent asymptotic solutions of the ODE, i.e. they form a natural basis at infinity. Then there exist constants (connection coefficients) C_i^+, C_i^-, $i=1,2$, such that

$$\begin{aligned} u_1(z) &= C_1^+ u^+(z) + C_1^- u^-(z) \\ u_2(z) &= C_2^+ u^+(z) + C_2^- u^-(z). \end{aligned} \tag{1}$$

If we now consider the case where the ODE contains a parameter (eigenvalue) E, and we are interested in a solution regular at the origin, we are led to a study of the dependence of the connection coefficients C^+ and C^- on the parameter E in the equation

$$u_1(E, z) = C^+(E)u^+(E, z) + C^-(E)u^-(E, z). \tag{2}$$

In the case of solutions over a finite interval the (ordinary) shooting method can be used to obtain the desired solution, including the determination of the parameter E, in order to satisfy the required boundary conditions. If the interval is infinite, such a method cannot be applied directly. The problem becomes even more difficult if one of the asymptotic solutions is unbounded, as is often the case. The purpose of this paper is to present a method which will allow these connection coefficients to be determined with high accuracy, and in addition to determine the allowed values of the parameter E to similar accuracy. This latter problem reduces to finding E so that one of the connection coefficients in (2) vanishes. For example, if u^+ is an exponentially increasing function at infinity and we require a solution which remains bounded, then we must determine E so that $C^+(E)$ vanishes.

We shall consider a second-order ODE (without a first derivative term) of the form

$$z^2 u'' + Q(z)u = 0 \tag{3}$$

(although ODEs with a first derivative term present no difficulty and can be treated in a similar manner) and assume

$$Q(z) = \sum_{i=0}^{\infty} Q_i z^i. \tag{4}$$

Then it is well known (Birkhoff and Rota 1978, Coddington and Levinson 1955, Ince 1956) that there exists a solution regular at the origin of the form

$$u(z) = z^r \sum_{i=0}^{\infty} a_i z^i \qquad a_0 \neq 0. \tag{5}$$

The exponent r and coefficients a_i can be obtained in the usual way by substituting (4) and (5) into (3). Detailed formulae are given in Holubec and Stauffer (1985).

The series in (5) will have some radius of convergence R. If we truncate the series after n_1 terms, say, then there will be another radius $R_1 < R$ such that the truncated series will approximate the exact solution to within a preset accuracy for $|z| < R_1$. If we choose a value z_0 with $|z_0| < R_1$ we can expand the solution about this point as

$$u(z) = z^r f(z) = z^r \sum_{i=0}^{\infty} b_i (z - z_0)^i \tag{6}$$

where $b_0 = f(z_0)$ and $b_1 = f'(z_0)$ and the remaining coefficients b_i can be found by substituting (6) into (3). Since our ODE clearly satisfies a Lipschitz condition (Birkhoff and Rota 1978, chapter 6), the series in (6) truncated to n_2 terms will then approximate the exact solution to within our tolerance for $|z - z_0| < R_2$ for some R_2. A new z_0 can be chosen within this circle and the solution expanded about it as in (6). Thus we can analytically continue the solution of (3) to any desired non-singular point of the ODE in the complex plane with our polynomial approximations of the required accuracy. This problem was dealt with by Holubec and Stauffer (1985), which paper includes detailed formulae for the coefficients b_i. This solution is the function u_1 referred to above. Note that if (3) contains a parameter E then the coefficients a_i and b_i are functions of such a parameter.

The next problem is to approximate the asymptotic solutions u^+ and u^- in a similar manner. Rewriting (3) as

$$u'' + q(z)u = 0 \tag{7}$$

with $q(z) = z^{-2}Q(z)$ we assume that $q(z)$ has the following asymptotic expansion for large $|z|$:

$$q(z) \asymp z^m \sum_{i=0}^{\infty} q_i z^{-i} \quad \text{as} \quad |z| \to \infty \qquad q_0 \neq 0 \tag{8}$$

with m a positive or negative integer or zero. The various forms of the asymptotic solution of (7) depend on the value of m and are well known (Dieudonné 1971). They are summarised in table 1. The explicit values for the coefficients c_i, s_i and r can be obtained by substituting the appropriate form into (7). (See Holubec 1985, appendix 3 for detailed formulae.) Note that in the first two cases in table 1, s_0 has two possible values yielding the two solutions u^+ and u^-. Likewise in the last two cases r has two possible values. However, when $m = -2$ and the two values of r differ by an integer, the second solution may contain a logarithmic term as in the usual method of Frobenius. Since these solutions may in principle be asymptotic series in z^{-i} they must be truncated and there will be a radius R_∞ such that these truncated solutions will have the desired numerical accuracy for $|z| > R_\infty$.

Having extended our solution u_1 to some point z_1 with $|z_1| > R_\infty$ we may determine the connection coefficients from the equations

$$\begin{aligned} u_1(E, z_1) &= C^+(E)u^+(E, z_1) + C^-(E)u^-(E, z_1) \\ u'(E, z_1) &= C^+(E)u^{+\prime}(E, z_1) + C^-(E)u^{-\prime}(E, z_1). \end{aligned} \tag{9}$$

Table 1. Asymptotic solutions for $u'' + q(z)u = 0$ with $q(z) \asymp z^m \sum_{i=0}^{\infty} q_i z^{-i}$, $q_0 \neq 0$.

m		$u(z)$
$2n$	$(n \geqslant 0)$	$\exp\left(\sum_{j=0}^{n} s_j z^{n-j+1}\right) z^{-r} \sum_{i=0}^{\infty} c_i z^{-i}$
$2n+1$	$(n \geqslant -1)$	$\exp\left(\sum_{j=0}^{2n+2} s_j z^{(n-j+2)/2}\right) z^{-r} \sum_{i=0}^{\infty} c_i z^{-i/2}$
-2		$z^{-r} \sum_{i=0}^{\infty} c_i z^{-i}$
$-n$	$(n \geqslant 3)$	$z^{-r} + z^{-n-r+2} \sum_{i=0}^{\infty} c_i z^{-i}$

Note that the solutions u_1', $u^{+\prime}$ and $u^{-\prime}$ are derivatives with respect to the variable z and can easily be obtained by differentiating the appropriate polynomial solutions.

Obtaining the coefficients C^+ and C^- to the required accuracy from (9) completes the problem in those cases where u^+ and u^- are both admissible solutions. This occurs, for example, in potential scattering problems in quantum mechanics where u^+ and u^- are sinusoidal functions. Obtaining C^+ and C^- in these cases is then equivalent to finding the amplitude and phase of the scattered wavefunction, the quantities of physical interest.

However, if, for example, u^+ is unbounded at infinity, then we must proceed further and determine the values of E such that $C^+(E)$ vanishes. The problem we now consider is that of finding a sequence of values of E that converges to the desired root efficiently and accurately.

Treating this problem as one of finding the zeros of the function $C^+(E)$, we propose to use Newton's method so that an approximate root E is obtained by the following iteration

$$E \leftarrow E - \frac{C^+(E)}{\mathrm{D}_E C^+(E)} \tag{10}$$

where D_E represents differentiation with respect to E.

The local rate of convergence of Newton's method is quadratic and thus gives an efficient method provided we can determine $\mathrm{D}_E C^+(E)$ to high accuracy. This can be done in a straightforward manner as we show below.

Let us differentiate (9) with respect to E to yield

$$\begin{aligned} \mathrm{D}_E u_1 &= C^+(\mathrm{D}_E u^+) + C^-(\mathrm{D}_E u^-) + (\mathrm{D}_E C^+)u^+ + (\mathrm{D}_E C^-)u^- \\ \mathrm{D}_E u_1' &= C^+(\mathrm{D}_E u^{+\prime}) + C^-(\mathrm{D}_E u^{-\prime}) + (\mathrm{D}_E C^+)u^{+\prime} + (\mathrm{D}_E C^-)u^{-\prime}. \end{aligned} \tag{11}$$

Then (9) and (11) represent two sets of two equations in the two pairs of unknowns C^+, C^- and $\mathrm{D}_E C^+$, $\mathrm{D}_E C^-$, since the functions $\mathrm{D}_E u_1$, $\mathrm{D}_E u_1'$, $\mathrm{D}_E u^-$, $\mathrm{D}_E u^{-\prime}$, $\mathrm{D}_E u^+$, $\mathrm{D}_E u^{+\prime}$ can be found by differentiating with respect to E the corresponding series solution for the functions and their derivatives with respect to z. Because the coefficients of the series solutions depend on E their derivatives with respect to E can be found by differentiating the corresponding recurrence relation. Thus, for example, from (6) we get

$$\mathrm{D}_E u_1 = \sum_{i=0}^{\infty} (\mathrm{D}_E b_i)(z - z_0)^{i+r}.$$

Hence (9) and (11) can be solved for C^+ and $\mathrm{D}_E C^+$, say, and then Newton's method (10) employed to find the desired value of E to high accuracy.

We illustrate this method with specific examples in the next section.

3. Examples of the use of the asymptotic shooting method

In this section we present four examples which are based on differential equations that arise in quantum mechanical potential problems.

Given a spherically symmetric potential $V(z)$ the Schrödinger equation containing this potential can be reduced to the radial form (in atomic units)

$$z^2 u'' - [l(l+1) + 2z^2 V(z) - 2Ez^2]u = 0 \tag{12}$$

where l is the angular momentum quantum number which takes non-negative integer values and E is the energy eigenvalue to be determined.

We will now treat the problem of solving (12) for four different potentials.

3.1. The perturbed spherical oscillator potential, $Az^{-2}+2z^2$

As a check on our method, we found the eigenvalues of equation (12) for this potential. Equation (12) becomes

$$z^2u''-[s(s+1)-2Ez^2+4z^4]u=0 \tag{13}$$

where s is the positive root of $s(s+1)=l(l+1)+2A$. Equation (13) has a known solution (Landau and Lifshitz 1965)

$$u=e^{-z^2}z^{s+1}F\left(-\frac{E-2s-3}{4}, s+\frac{3}{2}, 2z^2\right) \tag{14}$$

where F is the confluent hypergeometric function, and in order that $u\to 0$ as $z\to\infty$ we must have $E=4n+2s+3$ where n is a non-negative integer. In this case, the confluent hypergeometric function in (14) becomes the (generalised) Laguerre polynomial of degree n in z^2, i.e. $[n!/(s+\frac{3}{2})_n]L_n^{(s+1/2)}(2z^2)$, where we have used Pochhammer's notation $(x)_n=x(x+1)\ldots(x+n-1)$ and $(x)_0=1$.

A solution regular at the origin has the form (5) with $r=s+1$ and

$$a_i=\frac{-2Ea_{i-2}+4a_{i-4}}{i(i+2s+1)} \qquad a_0=1$$

(we use the convention that $a_i=0$ if $i<0$). Hence $a_i=0$, i odd, and

$$D_Ea_i=\frac{-2a_{i-2}-2ED_Ea_{i-2}+4D_Ea_{i-4}}{i(i+2s+1)} \qquad D_Ea_0=0.$$

Thus both sets of coefficients a_i and D_Ea_i can be found from the above recurrence relations. Now $u(z_0)$, $u'(z_0)$, $D_Eu(z_0)$ and $D_Eu'(z_0)$ can be evaluated from (5) and its derivative with respect to E and then we expand u as in (6). We find that

$$b_{i+2}=[-(i+1)(i+2s+2)b_{i+1}+z_0(-2E+4z_0^2)b_i$$
$$+(-2E+12z_0^2)b_{i-1}+12z_0b_{i-2}+4b_{i-3}]/[z_0(i+1)(i+2)]$$

where $i\geqslant 0$ and

$$D_Eb_{i+2}=[-(i+1)(i+2s+2)D_Eb_{i+1}-2z_0b_i+z_0(-2E+4z_0^2)D_Eb_i$$
$$-2b_{i-1}+(-2E+12z_0)D_Eb_{i-1}$$
$$+12z_0D_Eb_{i-2}+4D_Eb_{i-3}]/[z_0(i+1)(i+2)] \qquad i\geqslant 0$$

$$b_0=f(z_0) \qquad b_1=f'(z_0)$$

$$D_Eb_0=D_Ef(z_0) \qquad D_Eb_1=D_Ef'(z_0)$$

where f is defined in (6). Again the sets of coefficients b_i and D_Eb_i can be found from the above relations and the analytic continuation then proceeds as described above.

For this potential the value of m in (8) is 2. Hence from table 1 the asymptotic solutions are given by

$$u^{\pm} = e^{\pm z^2} \sum_{i=0}^{\infty} A_i^{\pm} z^{r_{\pm}-i} \tag{15}$$

where $r_{\pm} = \mp E/2 - \frac{1}{2}$ and

$$A_i^{\pm} = \pm[(r_{\pm}-i+2)(r_{\pm}-i+1) - s(s+1)]A_{i-2}^{\pm}/(4i)$$

$$D_E A_i^{\pm} = [(r_{\pm}-i+\tfrac{3}{2})A_{i-2}^{\pm} \pm [(r_{\pm}-i+2)(r_{\pm}-i+1) - s(s+1)]D_E A_{i-2}^{\pm}]/(4i) \qquad i \geqslant 2$$

$$A_0^{\pm} = 1 \qquad A_1^{\pm} = 0 \qquad D_E A_0^{\pm} = 0 \qquad D_E A_1^{\pm} = 0.$$

Substituting $A_i^{\pm}$ in (15) gives $u^{\pm}$, and $D_E u^{\pm}$ may be obtained from

$$D_E u^{\pm} = \mp \tfrac{1}{2}(\ln z)u^{\pm} + e^{\pm z^2} \sum_{i=0}^{\infty} D_E A_i^{\pm} z^{r_{\pm}-i} \tag{16}$$

$u'^{\pm}$ and $D_E u'^{\pm}$ are obtained by differentiating (15) and (16). Having these, we solve (9) and (11) for C^+ and $D_E C^+$. Iteration (10) then gives us a new estimate of E and the process is repeated until $|C^+/D_E C^+|$ is less than a preset tolerance.

3.2. The Kratzer's molecular potential, $Ar^{-2} + Br^{-1}$

This is another case which has a known solution (Kratzer 1920, Fues 1926). Equation (12) may be transformed into

$$z^2 u'' - [s(s+1) - \varepsilon z + \tfrac{1}{4}z^2]u = 0 \tag{17}$$

by the substitutions $z = 2\sqrt{-2E}\, r$, $\varepsilon = -B/\sqrt{-2E}$, $s(s+1) = l(l+1) + 2A$, $s > 0$. Equation (17) has the solution (see e.g. Landau and Lifshitz 1965)

$$u = z^{s+1} e^{-z/2} F(-\varepsilon + s + 1, 2s+2, z) \tag{18}$$

and $\varepsilon - s - 1 = n$, say, must be a non-negative integer if u is to be bounded at infinity, in which case the confluent hypergeometric function reduces to the Laguerre polynomial $[n!/(2s+2)_n]L_n^{(2s+1)}(z)$.

The solution regular at the origin is given by (5) with $r = s+1$ and

$$a_{i+1} = \frac{a_{i-1} - 4\varepsilon a_i}{4(i+1)(i+2s+2)} \qquad a_0 = 1. \tag{19}$$

The coefficients b_i for the analytic continuation (6) are given by

$$b_{i+2} = \frac{b_{i-1} - (4\varepsilon - z_0)b_i - 4(i+1)(i+2s+2)b_{i+1}}{4z_0(i+1)(i+2)}. \tag{20}$$

The expressions for $D_\varepsilon a_i$ and $D_\varepsilon b_i$ can be easily obtained from (19) and (20). In this case, the value of m in (8) is zero and the asymptotic expansion (obtained from table 1) is

$$u^{\pm} = e^{\pm z/2} \sum_{i=0}^{\infty} A_i^{\pm} z^{\mp\varepsilon - i} \tag{21}$$

with

$$A_{i+1}^{\pm} = \pm\left[\frac{(i \pm \varepsilon)(i \pm \varepsilon + 1) - s(s+1)}{i+1}\right] A_i^{\pm}. \tag{22}$$

Hence we may find $D_\varepsilon A_i^{\pm}$ and proceed as above to determine the eigenvalue ε.

3.3. The screened Coulomb potential

Here we will find accurate energy eigenvalues of the screened Coulomb potential (as it is known in atomic physics; in nuclear physics it is called the Yukawa potential (Yukawa 1935) and in plasma physics the Debye-Hückel potential (Debye and Hückel 1923))

$$V(z) = -z^{-1}\exp(-az) \tag{23}$$

where a is a given parameter. For convenience we write $E = -s^2/2$. Thus substituting (23) into (12) we get

$$z^2u'' + [2z\exp(-az) - s^2z^2 - l(l+1)]u = 0. \tag{24}$$

Expanding the exponential in a power series we can find a regular Frobenius solution of the form (5) with $r = l+1$ (since u must be zero at the origin) and

$$a_{i+1} = \left(s^2a_{i-1} - \sum_{j=0}^{i}[2(-a)^j/j!]a_{i-j}\right)[(i+1)(i+2l+2)]^{-1} \qquad a_0 = 1. \tag{25}$$

Extending these solutions analytically we have from (6)

$$b_{i+2} = -\left((i+2l+2)(i+1)b_{i+1} + \exp(-az_0)\sum_{j=0}^{i}[2(-a)^j/j!]b_{i-j} - s^2z_0b_i - s^2b_{i-1}\right)$$
$$\times[(i+1)(i+2)z_0]^{-1}. \tag{26}$$

The coefficients D_sa_i and D_sb_i can be easily obtained from (25) and (26).

At this point we must calculate two independent asymptotic solutions to (24) which in this case are simply

$$u^+ = \exp(sz) \qquad \text{and} \qquad u^- = \exp(-sz) \tag{27}$$

neglecting the contribution of the exponential term in the ODE.

For this problem we require u to remain bounded at infinity, which implies that $C^+(s)$ must vanish. Hence we may employ the algorithm (10) to find the values of s which satisfy this condition. Having found s we have then found the energy eigenvalues $E = -s^2/2$.

3.4. The three-dimensional quartic oscillator

In this case the potential is taken as $V(z) = z^4$ so that the differential equation (12) becomes

$$z^2u'' - [l(l+1) + 2z^6 - 2z^2E]u = 0. \tag{28}$$

This has a regular solution at the origin of the form (5) with $r = l+1$, $a_0 = 1$ and

$$a_i = [2a_{i-6} - 2Ea_{i-2}]/[i(2l+i+1)]. \tag{29}$$

Continuing the solution analytically as in (6) we have

$$b_{i+2} = -[b_{i+1}(i+1)(i+2l+2) + b_i(2Ez_0 - 2z_0^5) + b_{i-1}(2E - 10z_0^4) + b_{i-2}(-20z_0^3)$$
$$+ b_{i-3}(-20z_0^2) + b_{i-4}(-10z_0) - 2b_{i-5}]/[z_0(i+1)(i+2)]. \tag{30}$$

Thus we may extend the functions u, u', D_Eu, D_Eu' into the asymptotic region.

By comparing (28) with (7) and (8) we see that the exponent in (8) equals 4 so that using table 1 and substituting into (28) we find the asymptotic solutions to be

$$u^{\pm} = \exp(\pm 2^{1/2} 3^{-1} z^3) \sum_{i=0}^{\infty} A_i^{\pm} z^{-i-1} \tag{31}$$

with $A_0^{\pm} = 1$ and

$$A_{i+1}^{\pm} = \pm[2EA_i^{\pm} + [i(i-1) - l(l+1)]A_{i-2}^{\pm}]/[(i+1)8^{1/2}] \tag{32}$$

and we may proceed to find E as in the other examples.

4. Results

In this section we discuss the details of the calculations for the examples in section 3 and present numerical results. In the first two examples the eigenvalues are known exactly, so we have used these to test the efficiency of the method. For the last two examples we have presented extensive tables of what we believe to be the most accurate determination to date of the eigenvalues for these potentials.

In all of the examples below, we used a constant step size between values of z_0 in the analytic continuation which was equal to the value of z_0 in (5). All calculations were carried out in quadruple precision on VAX and IBM computers. The CPU times quoted all refer to execution on a VAX 8600.

4.1. The perturbed spherical oscillator potential, $Az^{-2} + 2z^2$

We performed these calculations for $A = 0.05$, 0.5 and 10, each for two different eigenvalues E. In each case we were able to obtain the exact eigenvalue correct to 31 significant figures provided that the step size was sufficiently small (~ 0.1) and the number of terms in the Frobenius and analytic continuation series were sufficiently large (~ 30 in both cases). If these conditions were not met, the sequence of eigenvalues converged to an incorrect answer.

When E has the value $4n + 2s + 3$, then our method will produce the exact solution in the asymptotic region (for this particular potential) if $2n$ terms are used in the asymptotic expansion. In practice, we found that, with an initial estimate of E within 1% of its exact value, the procedure would converge (to 31 significant figures) in about 10 iterations on E when z_1 was taken equal to z_0, the point at which the Frobenius series was evaluated. In order to test the validity of the method, we used values of z_1 in the region of 10–20. In this case, it was possible to use as few as 2 or 3 terms in the asymptotic expansion and still obtain an answer correct to 31 significant figures. When $A = 0.05$ and $z_1 = 20$, with 30 terms in all the expansions and a step size of 0.1, each iteration on E took about 2.8 seconds of CPU time.

4.2. The Kratzer's molecular potential, $Ar^{-2} + Br^{-1}$

This potential was investigated for a variety of values of s and ε. In this case we again needed a step size of the order of 0.1 to achieve 31 significant figure accuracy, but only about 20 terms were required in the Frobenius and analytic continuation series.

When $\varepsilon = n + s + 1$ and n terms were retained in the asymptotic expansion, (21) again gave the exact solution, and so any $z_1 \geqslant z_0$ could be used. However, we found

here that the coefficients A_i in (21) increased faster than 10^i, which meant that z_1 needed to be prohibitively large if we were to use fewer than the exact number of terms in the asymptotic expansion. Using more than the exact number of terms also made the results worse, as expected from the nature of the asymptotic expansion.

For $s = 0.7$ and $n = 15$, z_1 had to be 120 in order to obtain an accuracy of 30 significant figures if the asymptotic expansion had 14 instead of the exact 15 terms. In this case, the CPU time required was about 5 seconds per iteration.

4.3. The screened Coulomb potential

We have performed these calculations for $l = 0$ retaining 25 terms in the series (5) and (6) and taking successive points z_0 along the positive real axis in steps of 0.125, with $z_1 = 70$. In order to ensure that the procedure was converging to the correct eigenvalue, we varied z_1, the step size, and the number of terms in (5) and (6) until no change in the energy eigenvalue was obtained in the first 31 figures when these were changed. In this case it was necessary to take such a large value of z_1 in order that the neglect of the exponential term in the asymptotic region not affect the result. We would like to point out that this requirement for large values of z_1 holds generally for short-range, i.e. exponentially decaying, potentials. Thus the present method is more efficient for long-range (inverse-power) potentials than for short-range ones since in the former case we have asymptotic solutions.

For $l = 1$ and $l = 2$ it was necessary to use even larger values of z_1 (~135–200) to obtain the desired accuracy, and the problem became worse as s decreased. This is presumably due in the main to the neglect (in the asymptotic form) of the exponential term in (24) with respect to $s^2 z$, an approximation which requires larger values of z as s decreases.

The results for the lowest energy eigenvalue when $a = 1$ are shown in table 2, where we show the convergence of the iterations and the values for the connection coefficient C^+. Table 3 shows our values for the energy eigenvalues for the 1s, 2s, 3s, 2p, 3p and 3d states for a selection of values of the screening parameter chosen in order to make comparisons with other calculations. We have compared our results with those of Rogers *et al* (1970), who integrated the differential equation numerically, with the results of Lam and Varshni (1979) and Gerry and Laub (1985) who used variational methods, and with those of Vrscay (1986) who used perturbation theory. Our results agree with those of Rogers *et al*, and with those of Lam and Varshni. We disagree in the last two or three digits with Gerry and Laub, but agree with the more precise results of Vrscay except for the last one or two digits in three cases. (Rogers *et al* show a 3s eigenvalue for $a = \frac{1}{7}$, but this is clearly a misprint since $1/a$ is less than their value of 7.171 for the critical screening length.) CPU time for the 3d, $a = 0.08$ case was about

Table 2. Convergence of the iterations for the ground state of the Debye potential with $a = 1$.

E (energy in atomic units)	$C^+(E)$
0.010 3	0.167 088 257 277 544 870 010 842 573 347 95 E − 03
0.010 285 780 500 626 976 991 427 109 796 2276	−0.111 705 141 077 050 244 428 873 361 805 99 E − 06
0.010 285 789 990 013 461 817 346 010 633 6786	−0.498 524 647 747 527 578 845 004 044 E − 13
0.010 285 789 990 017 696 804 774 214 471 4263	−0.992 919 541 680 24 E − 26
0.010 285 789 990 017 696 804 774 215 314 9156	0.120 160 42 E − 33
0.010 285 789 990 017 696 804 774 215 314 9156	

Table 3. Eigenvalues for the Debye potential.

Screening constant	Energy (atomic units)
1s states	
0.10 D − 08	0.499 999 990 000 000 074 999 999 500 000 0
0.002	0.498 002 996 010 958 192 329 750 599 565 0
0.005	0.495 018 687 925 632 530 667 468 329 151 7
0.01	0.490 074 506 746 694 171 809 208 252 333 0
1/70	0.485 865 917 090 562 630 036 073 901 839 0
0.02	0.480 296 105 983 785 084 553 167 568 707 6
0.025	0.475 461 193 929 886 825 872 623 664 866 1
1/30	0.467 482 280 049 066 081 567 670 988 589 6
0.05	0.451 816 428 524 505 543 856 217 075 755 4
1/60	0.436 530 596 749 779 333 824 958 411 769 0
0.10	0.407 058 030 613 403 156 754 507 070 361 1
1/7	0.371 218 339 072 510 415 667 839 618 386 5
0.20	0.326 808 511 369 193 384 882 495 419 281 8
0.25	0.290 919 587 521 274 339 752 038 013 101 1
0.30	0.257 638 586 303 054 148 878 964 069 306 2
1/3	0.236 832 670 269 605 426 282 956 980 344 9
0.40	0.198 376 083 361 850 216 608 413 859 925 9
0.50	0.148 117 021 889 932 616 711 758 220 725 5
0.60	0.106 135 907 505 814 193 000 738 693 811 0
0.70	0.071 833 555 904 512 213 040 262 126 802 38
5/7	0.067 529 595 032 881 321 277 456 778 844 31
0.80	0.044 704 304 497 359 663 200 348 766 240 37
0.90	0.024 314 193 827 502 054 887 384 150 887 19
1.00	0.010 285 789 990 017 696 804 774 215 314 92
1.10	0.002 287 244 234 053 485 463 476 080 685 041
1.15	0.000 455 889 021 355 957 785 682 927 445 887
1.16	0.000 258 622 006 376 600 045 257 206 291 145
1.17	0.000 117 073 729 761 480 412 255 495 394 286
1.18	0.000 030 985 910 874 039 344 565 231 310 402
1.19	0.000 000 103 031 961 498 984 588 555 542 475 15
2s states	
0.10 D − 08	0.124 999 990 000 000 299 999 993 000 000 0
0.002	0.123 011 944 478 134 440 620 850 031 615 3
0.005	0.120 074 143 345 598 522 611 020 393 629 7
0.01	0.115 293 285 167 994 256 222 045 516 170 4
1/70	0.111 307 282 110 805 718 822 370 612 271 4
0.020	0.106 148 320 244 695 503 250 708 341 185 9
0.025	0.101 775 903 096 982 713 088 091 927 353 3
0.03	0.097 531 786 134 660 862 770 039 060 920 2
1/30	0.094 771 911 987 607 611 315 164 185 389 3
0.04	0.089 414 634 185 159 188 415 714 621 025 4
0.05	0.081 771 195 795 253 124 173 489 413 770 4
0.06	0.074 578 534 412 709 709 694 885 171 159 2
1/60	0.070 023 560 580 275 226 569 089 511 905 1
0.07	0.067 815 959 981 462 181 222 810 363 310 6
0.08	0.061 464 656 212 300 385 911 466 251 113 4
0.09	0.055 507 388 553 290 736 394 798 978 073 6
0.01	0.049 928 271 331 918 889 234 996 681 037
1/7	0.029 969 939 257 143 878 404 743 800
0.15	0.027 222 190 725 688 518 250 187 27

Table 3. (continued)

Screening constant	Energy (atomic units)
2s states	
0.20	0.012 107 865 195 440 464 385 85
0.25	0.003 395 906 283 239 307 796 4
0.30	0.000 091 602 443 891 898 904
0.31	0.000 000 037 992 565 724 03
3s states	
0.10 D−08	0.055 555 554 555 555 562 306
0.20 D−02	0.053 582 284 478 315 489 495
0.50 D−02	0.050 720 178 473 178 174 475
0.10 D−01	0.046 198 857 799 033 191 519
1/70	0.042 557 959 016 724 088 371
0.20 D−01	0.038 020 014 393 017 364 13
0.25 D−01	0.034 329 509 911 543 775 44
1/30	0.028 721 590 492 195 219 0
0.50 D−01	0.019 352 554 814 752 34
1/60	0.012 157 785 987 924
0.10 D+00	0.003 208 046 744 69
2p states	
0.20 D−02	0.123 009 960 375 459 483 764 728 914 927 3
0.50 D−02	0.120 061 889 409 835 274 244 767 176 072 6
0.10 D−01	0.115 245 224 090 564 185 894 783 216 335 9
1/70	0.111 210 824 186 077 817 703 880 030 072 8
0.20 D−01	0.105 963 398 179 939 904 755 731 028 037 1
0.25 D−01	0.101 492 463 570 784 334 495 260 636 444 4
0.30 D−01	0.097 131 366 795 691 310 671 783 889 214 14
1/30	0.094 283 812 211 279 496 494 008 933 417 74
0.40 D−01	0.088 729 373 582 879 526 287 939 141 467 60
0.50 D−01	0.080 740 387 037 784 609 712 102 743 610 07
0.60 D−01	0.073 149 619 385 860 625 023 805 418 420 83
1/15	0.068 303 903 388 944 102 080 294 905 665 65
0.70 D−01	0.065 944 176 996 156 573 384 560 516 651 78
0.80 D−01	0.059 112 804 787 031 234 635 692 332 927 76
0.90 D−01	0.052 645 701 331 584 274 463 576 906 198 28
0.10 D+00	0.046 534 390 486 724 608 386 600 840 395 37
1/7	0.024 225 265 220 566 561 482 473 144 684 42
0.15 D+00	0.021 104 888 927 736 242 916 943 382 961 43
0.20 D+00	0.004 101 646 530 784 090 388 446 61
0.21 D+00	0.001 808 760 066 281 795 366 987
0.22 D+00	0.000 028 697 244 985 229 83
3p states	
0.20 D−02	0.053 580 320 031 419 632 788 495 514 717 51
0.50 D−02	0.050 708 224 175 839 214 790 596 302 367 71
0.01 D−01	0.046 153 104 829 162 287 315 273 878 682 40
1/70	0.042 468 034 317 299 059 101 925 455 275 01
0.20 D−01	0.037 852 389 200 223 176 326 568 017 591 23
0.25 D−01	0.034 078 910 428 938 130 548 463 162 217 41
1/30	0.028 308 156 245 525 399 794 062 086 734 19

Table 3. (continued)

Screening constant	Energy (atomic units)
3p states	
0.50 D − 01	0.018 557 751 883 405 996 604 893 993 884 09
1/15	0.010 973 206 620 963 914 224 134 538 27
0.80 D − 01	0.006 329 995 439 268 113 269 338 1
0.10 D + 00	0.001 589 001 525 867 560
3d states	
0.20 D − 02	0.053 576 390 876 136 829 815 017 304 590 99
0.50 D − 02	0.050 684 305 832 852 586 439 627 393 339 32
0.10 D − 01	0.046 061 454 160 659 627 138 130 277 716 71
1/70	0.042 287 618 160 654 326 942 778 643 967 37
0.20 D − 01	0.037 515 127 700 686 930 313 438 432 490 28
0.25 D − 01	0.033 573 122 086 666 003 102 965 090 942 85
1/30	0.027 468 297 378 410 478 968 864 947 978 70
0.50 D − 01	0.016 915 570 569 815 842 886 114 758 243 58
1/15	0.008 476 557 099 266 295 856 418 97
0.80 D − 01	0.003 248 360 428 751 993 572 5

35 seconds per iteration, the larger time being due partly to the greater complexity of the recursion relation (26) and partly to the larger z_1 required.

As a further check on our method and computer program, we also calculated the ground-state energy eigenvalue for this potential with $a = 0$. This corresponds to the potential for the hydrogen atom with a known lowest energy of -0.5. The convergence of our method to this result is shown in table 4.

4.4. The three-dimensional quartic oscillator

In table 5 we present to 10 decimal places the results of applying our method to the three-dimensional quartic oscillator. In this case, the step size required was about $\frac{1}{16}$, 25 terms were kept in the three series expansions, and $z_1 = 10$. These same energy levels were calculated by Bell *et al* (1970). Some of their results differ from ours in the last

Table 4. Convergence for the 1s-eigenvalue of H.

n	$E_{1s}^{(n)}$
0	0.8
1	0.602 116 129 526 180 714 424 611 728 441 021 E0
2	0.521 543 732 140 591 483 130 662 376 439 319 E0
3	0.501 418 490 320 542 520 969 252 083 905 473 E0
4	0.500 006 970 533 708 686 781 484 215 311 404 E0
5	0.500 000 000 169 908 547 629 803 838 297 194 E0
6	0.500 000 000 000 000 000 100 956 388 597 809 E0
7	0.500 000 000 000 000 000 000 000 000 000 000 E0
8	0.500 000 000 000 000 000 000 000 000 000 000 E0

Table 5. Energy levels for the three-dimensional quartic oscillator.

$l=0$	$l=2$	$l=4$	$l=6$	$l=8$
2.393 644 016 5				
7.335 729 995 2	6.830 307 934 3			
13.379 336 552 6	13.004 562 954 6	12.159 017 182 7		
20.220 849 464 1	19.915 973 018 2	19.217 580 482 7	18.152 410 722 0	
27.706 393 442 8	27.445 940 483 4	26.845 204 418 1	25.919 403 470 4	24.688 862 663 7
35.740 315 268 7	35.510 999 923 9	34.980 151 538 3	34.157 245 349 1	33.055 556 655 3
44.256 235 399 1	44.050 163 171 7	43.572 088 795 0	42.828 323 324 3	41.827 976 478 2
53.204 869 790 3	53.016 926 485 5	52.580 305 878 8	51.899 433 998 5	50.980 826 621 5
62.547 902 773 1	62.374 565 038 1	61.971 496 783 5	61.341 930 038 2	60.490 688 095 4
72.254 530 285 7	72.093 256 171 4	71.717 989 783 8	71.131 168 923 1	70.336 467 433 2
82.299 346 209 1	82.148 234 794 4	81.796 443 536 8	81.245 860 488 8	80.499 351 764 0
92.660 970 002 0	92.518 558 295 5	92.186 897 317 0	91.667 481 874 6	90.962 593 725 4
103.321 113 098 4	103.186 248 331 5	102.872 073 186 5	102.379 793 306 7	101.711 257 005 2
114.263 919 606 8	114.135 675 437 4	113.836 855 595 0	113.368 448 044 3	112.731 972 576 8
125.475 486 227 5	125.353 105 776 9	125.067 896 911 8	124.620 680 391 0	124.012 722 282 7
136.943 503 599 5	136.826 359 558 7	136.553 313 592 1	136.125 055 751 9	135.542 652 889 6
148.656 982 474 0	148.544 548 442 3	148.282 448 615 5	147.871 269 288 6	147.311 918 596 4
160.606 040 707 0	160.497 870 141 3	160.245 683 151 3	159.849 982 541 4	159.311 548 346 5
172.781 734 848 2	172.677 445 300 7	172.434 285 350 7	172.052 689 804 4	171.533 334 100 1
185.175 925 076 7	185.075 186 190 5	184.840 287 541 5	184.471 607 952 7	183.969 736 562 5
197.781 165 506 2	197.683 689 732 9	197.456 385 434 8	197.099 584 892 5	196.613 805 365 5
210.590 614 085 8	210.496 149 411 7	210.275 854 604 1	209.930 022 908 1	209.459 111 200 7
223.597 957 848 3	223.506 282 022 8	223.292 480 667 7	222.956 814 024 2	222.499 687 847 3
236.797 350 322 3	236.708 266 230 1	236.500 500 455 3	236.174 285 130 5	235.729 982 418 5
250.183 358 697 1	250.096 690 608 0	249.894 552 064 7	249.577 151 099 1	249.144 812 457 5
$l=1$	$l=3$	$l=5$	$l=7$	$l=9$
4.478 039 219 5				
10.099 944 419 6	9.401 160 155 8			
16.599 520 882 9	16.046 193 351 2	15.081 646 864 4		
23.796 217 400 0	23.331 473 229 7	22.511 045 919 2	21.358 310 363 7	
31.578 082 210 1	31.173 557 744 5	30.454 795 012 4	29.436 169 241 9	28.135 402 860 2
39.869 011 642 4	39.508 457 405 2	38.865 427 716 6	37.949 363 977 9	36 772 408 659 5
48.613 504 047 4	48.286 683 831 4	47.702 456 022 2	46.867 355 674 0	45.790 023 817 3
57.769 020 921 9	57.469 034 094 6	56.931 941 002 2	56.162 458 584 4	55.166 943 708 1
57.769 020 921 9	57.469 034 094 6	56.931 941 002 2	56.162 458 584 4	55.166 943 708 1
67.301 750 275 6	67.023 703 317 7	66.525 351 382 1	65.810 216 413 4	64.883 109 665 0
77.184 061 133 7	76.924 345 267 7	76.458 482 734 3	75.789 177 334 0	74.920 159 742 2
87.392 876 591 7	87.148 746 218 5	86.710 582 534 3	86.080 509 833 1	85.261 481 407 7
97.908 582 079 1	97.677 894 588 5	97.263 671 363 3	96.667 614 293 4	95.892 103 284 3
108.714 263 471 1	108.495 311 185 6	108.102 020 757 5	107.535 778 577 8	106.798 532 312 8
119.795 157 983 3	119.586 555 451 1	119.211 749 925 0	118.671 887 143 0	117.968 582 650 1
131.138 247 623 1	130.938 853 601 5	130.580 511 464 4	130.064 180 006 4	129.391 215 245 5
142.731 951 237 0	142.540 813 211 1	142.197 243 797 8	141.702 054 228 8	141.056 394 674 4
154.565 886 621 7	154.382 200 420 8	154.051 973 974 3	153.575 900 379 4	152.954 964 350 4
166.630 683 607 0	166.453 763 406 7	166.135 658 881 3	165.676 967 359 1	165.078 538 971 7
178.917 834 980 2	178.747 090 617 7	178.440 056 055 4	177.997 250 106 3	177.419 412 253 3
191.419 576 016 8	191.254 495 563 5	190.957 617 552 1	190.529 395 772 9	189.970 477 851 7
204.128 785 979 0	203.968 922 160 6	203.681 401 971 4	203.266 624 858 1	202.725 161 156 6
217.038 906 726 4	216.883 866 206 9	216.605 000 919 0	216.202 664 512 8	215.677 362 736 6
230.143 874 828 4	229.993 309 656 0	229.722 477 058 7	229.331 691 799 8	228.821 404 392 1
243.438 064 450 4	243.291 665 157 7	243.028 311 552 2	242.648 285 147 4	242.151 989 162 8
256.916 238 928 6	256.773 728 914 6	256.517 359 165 6	256.147 382 583 6	255.664 161 642 7

one or two decimal places (see also footnote, table 3, Mathews *et al* 1982, who calculated some of the same values).

We also present in table 6 a more accurate determination of the $n=24$, $l=1$ eigenvalue, using a step size of $\frac{1}{32}$, and compare it with previous work by Bell *et al* (1970), Mathews *et al* (1982) and Killingbeck (1982). Approximate CPU time per iteration for this case was about 3.9 seconds.

Table 6. Comparison of results for the $E(n=24, l=1)$ eigenvalue (quartic oscillator).

E (energy in atomic units)	Source
256.916 220	Bell *et al* (1970) (variational method)
256.916 238	Mathews *et al* (1982) (perturbation theory)
256.916 239	Killingbeck (1982) (the finite-difference method)
256.916 238 928 607 025 721 207 966 4048	present work

Hodgson (1988) has calculated eigenenergies of the equation

$$-\Psi''+x^4\Psi=E_H\Psi \qquad \Psi(0)=c \qquad \Psi'(0)=0 \tag{33}$$

where c is an arbitrary normalisation constant, to 32 significant figures. Putting $l=1$ in (28) and $z=x\times 2^{1/6}$, we obtain (33) with $E_H=2^{2/3}E$. We have run this case with the same step size and number of terms as above, and obtain full agreement with Hodgson's results using $z_1=6$ in the case where Hodgson used the boundary condition $\Psi(8)=0$.

5. Conclusions

In this paper we have presented a method for finding analytic approximations of arbitrary accuracy for ordinary differential equations over a semi-infinite interval. More importantly, the method produces eigenvalues of the ODE, again to arbitrary accuracy. We have tested this method on four different ODEs and have reported eigenvalues for the screened Coulomb potential and quartic oscillator and which are the most accurate to date.

It is of interest to compare our work with that of Hodgson (1988) who used a similar method to find eigenvalues of the harmonic and quartic oscillators. Whereas Hodgson used the secant method to generate successive approximations to the eigenvalue, we use Newton's method which is known to converge more quickly. On the other hand, our method requires the calculation of the derivatives of the polynomial coefficients with respect to the eigenvalues, which approximately doubles the amount of calculation per iteration.

In addition, Hodgson calculates the eigenvalue by requiring $u(z_1)=0$. This requires a sufficiently large z_1 to satisfy this condition to the degree of accuracy required for the eigenvalue. In our method we determine the eigenvalue by matching onto the exact asymptotic form, which requires a z_1 only large enough for this asymptotic form to be within the desired accuracy. Thus we were able to use $z_1=6$ to obtain the same accuracy on the quartic oscillator as Hodgson obtained with $z_1=8$. This is a particularly favourable example for Hodgson's method since from (31) $u\propto\exp(-2^{1/2}3^{-1}z^3)$ and

hence decreases very rapidly. If we determine the eigenvalue for the screened Coulomb potential by solving $u(z_1) = 0$ by Newton's method, we get only about half the significant figures when $a = 0.1$ than we did by matching onto the asymptotic expression at the same value of z_1.

We have the further advantage of having an asymptotic approximation for the solution for $z > z_1$ with a continuous derivative at the matching point. Furthermore, the method we have proposed will work for the case where we wish to match onto the asymptotic solution u^+ rather than u^-, whereas Hodgson's method is not applicable in this case. Such cases arise, for example, in the calculation of resonances in atomic systems, in which case the eigenvalues are complex numbers (cf Holubec 1985). Thus we have developed a method which is applicable to a wide variety of situations and produces highly accurate results for a modest amount of computational effort.

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