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Precise shooting methods for the Schrödinger equation

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Abstract. An analytic continuation procedure using Taylor series is utilised to produce very accurate wavefunctions and eigenvalues for the Schrödinger equation.

1. Introduction

The recent work by Killingbeck (1987) has demonstrated that there is still considerable interest in obtaining accurate solutions to simple one-dimensional problems which can arise in quantum mechanics. The above reference focuses on a standard two-point boundary value problem

$$-D^2\psi + x^2\psi = E\psi \tag{1}$$

with $E = -1$, $\psi(0) = 1$ and $\psi(5) = 0$ which has been studied by several authors (e.g. Holt 1964, Osborne 1969, Roberts and Shipman 1971, Gupta and Agarwal 1985). It is observed that standard shooting methods are unstable, and that beyond $x \sim 3.5$ they do not produce the correct values. Killingbeck has demonstrated that, by viewing the equation from the quantum mechanics viewpoint, new insights can be achieved and more accurate shooting methods can be derived.

In another work Killingbeck (1986) has employed perturbation theory to generate a family of high-order shooting methods in order to obtain eigenvalues for the Schrödinger equation. These procedures lead to results with a higher accuracy than the standard Numerov method can achieve.

In this work we outline an alternative approach which has been proposed by others (Holubec and Stauffer 1985) and which leads to very precise results. The technique is applied to the above problems in order to demonstrate its accuracy, stability and speed. We have found it very easy to implement as well.

2. Analytic continuation

The standard Taylor series approach to the solution of a differential equation (DE) with initial values given at z_0 is to approximate the solution in the neighbourhood of z_0 by a truncated Taylor series. The values of the derivatives at z_0 are determined from successive differentiations of the DE. One then proceeds to construct a new Taylor series about $z_1 = z_0 + h$ using the derivatives of the first series. This process continues to generate an analytic continuation of the solution of the DE along the path $\{z_0, z_1, z_2, \ldots\}$. This technique requires successive differentiation of the DE, and becomes restricted if the DE has singularities anywhere in the complex z plane.

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Holubec and Stauffer (1985) have proposed a way around this problem based on the idea of analytically continuing a Frobenius series rather than a Taylor series. The method is applied to second-order linear DE with a regular singularity and with analytic coefficients which are finite polynomials. In practice the method works for arbitrary order and for more general analytic coefficients.

We start by writing the test problem in the form

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

with $Q(z) = E - z^2$. The solution u is expanded in a Taylor series about the point z_0 as

$$u = \sum_{i=0}^{N_t} c_i (z - z_0)^i. \tag{3}$$

In the general case $Q(z)$ is expanded in a similar fashion

$$Q(z) = \sum_{i=0}^{q} \tilde{Q}_i (z - z_0)^i \tag{4}$$

which for the test problem we are looking at reduces to

$$Q(z) = E - z_0^2 - 2z_0(z - z_0) - (z - z_0)^2. \tag{5}$$

Substituting these expansions for u and Q into the DE, and setting the coefficients of the different powers of $(z - z_0)$ to zero, we arrive at a set of recurrence relations to generate the coefficients c_i:

$$c_{i+2} = -[(E - z_0^2)c_i - 2z_0 c_{i-1} - c_{i-2}]/(i+2)(i+1). \tag{6}$$

The initial values $c_0 = u(z_0)$, $c_1 = u'(z_0)$ are used to start the series.

If we start from the origin, we can use the above results with $z_0 = 0$. In the general case a Frobenius series is used, with the appropriate characteristic exponent. For the test problem under evaluation here, the characteristic exponent is 0, and so the regular Taylor series about $z_0 = 0$ suffices.

3. Results

We have first of all examined the test problem

$$-D^2\psi + x^2\psi = E\psi \tag{1}$$

with $E = -1$, $\psi(0) = 1$ and $\psi(5) = 0$ in order to compare our results with those obtained by Killingbeck (1987). In employing the shooting methods or the above analytic continuation procedure, we start by choosing an initial slope $\psi'(0) = G$, and then compute the solution out to the endpoint. The value of G is varied until the condition $\psi(5) = 0$ is satisfied as well as possible within the precision of the calculations.

In applying the method of analytic continuation we subdivide the interval into N_s subintervals bounded by $z_0, z_1, \ldots, z_{N_s}$. The expansion about z_0 is used first to find the function and its first derivative at z_1, and the process is repeated out to the endpoint. The other variable is the number of terms N_t retained in the polynomial expansion (3).

We have carried out the computations using 32-digit precision, and have found that it is very easy to retain this level of accuracy in the wavefunction. We obtained

the best G value by using the secant method, starting with two G values which generate values of $\psi(5)$ having different signs:

$$G^{i+1} = G^i - \psi^{G^i}(5)\frac{(G^i - G^{i-1})}{\psi^{G^i}(5) - \psi^{G^{i-1}}(5)}. \tag{7}$$

Only three or four iterations are required to obtain the best G. We compare our results with those of Killingbeck (1987) in table 1. These were obtained with $N_s = N_t = 40$.

Table 2 illustrates how the value of G affects the value of $\psi(5)$ for a region close to the best fit. We also show in table 3 that the results are almost insensitive to the value of N_s. Small values of N_s work quite well. Note that far fewer terms are required in our expansion than were used by Killingbeck (1987).

A comparison of the values of $\psi(x)$ for sample x values in table 4 demonstrates that the power series employed by Killingbeck (1987) gives reasonably good results whereas the simple forward-shooting method is quite poor.

We have also used this procedure to compute the eigenvalues for the Schrödinger equation

$$-D^2\psi + V\psi = E\psi \tag{8}$$

Table 1. Values of $\psi'(0) = G$.

Method	G
Power series	−1.128 379
Simple method ($N_0 = 200$)	−1.128 379 (extrapolated)
Numerov ($N_0 = 100$)	−1.128 378
Analytic continuation	−1.128 379 167 097 247 411 498 441 114 3125

Table 2. Variation of $\psi(5)$ with G. Here $G = G_0 + \Delta G$ with $G_0 =$ 1.128 379 167 097 247 411 498 441 114 3125.

ΔG	$\psi(5)$
-2.0×10^{-31}	$5.694\,4\times10^{-26}$
-1.0×10^{-31}	$3.371\,77\times10^{-26}$
0.0	$9.680\,09\times10^{-27}$
1.0×10^{-31}	$-1.425\,79\times10^{-26}$
2.0×10^{-31}	$-3.823\,27\times10^{-26}$
3.0×10^{-31}	$-6.152\,682\times10^{-26}$

Table 3. Values of $\psi(5)$ for $G = -1.1285$. Here $\psi(5) = \psi_0 + \Delta\psi$ with $\psi_0 =$ −28.734 998 121 669 412 565 557 31.

N_s	$\Delta\psi(N_t = 35)$	$\Delta\psi(N_t = 40)$
5	$1.199\,21\times10^{-13}$	$5.700\,46\times10^{-17}$
10	$2.371\,229\times10^{-22}$	$-8.853\,2\times10^{-26}$
15	$-9.175\,1\times10^{-26}$	$-9.273\,2\times10^{-26}$
20	$-9.269\,6\times10^{-26}$	$-9.269\,6\times10^{-26}$
30	$-9.271\,4\times10^{-26}$	$-9.271\,4\times10^{-26}$
40	$-9.242\,9\times10^{-26}$	$-9.242\,9\times10^{-26}$
50	$-9.224\,6\times10^{-26}$	$-9.224\,6\times10^{-26}$

Table 4. Values of $\psi(x)$ for $G = -1.1284$.

x	Simple forward	Power series	Analytic continuation
1	0.259 422	0.259 317	0.259 316 896 872 082 861 227 589 025 777 26
2	0.034 977	0.034 428	0.034 428 262 550 995 016 172 316 972 485 97
3	0.007 011	0.000 327	0.000 326 602 312 256 525 396 865 431 966 08
4	0.166 086	−0.054 989	−0.054 990 517 021 047 522 316 406 867 847 41
4.5	1.388 501	−0.460 808	−0.460 809 864 741 366 069 908 977 205 543 97
5	14.902 7	−4.954 08	−4.954 225 279 932 937 034 405 761 036 392 9

for the special case $V = x^4$, in order to compare with the results of Killingbeck (1986). In this case the recurrence relation (6) must be replaced by

$$c_{i+2} = -[(E - z_0^4)c_i - 4z_0^3 c_{i-1} - 6z_0^2 c_{i-2} - 4z_0 c_{i-3} - c_{i-4}]/(i+2)(i+1). \qquad (9)$$

Table 5 lists our results in comparison with those of Killingbeck (1986) for the different boundary conditions in the ground state. Here we have used $D\psi(0) = 0$ for the even-parity ground state.

Note that the eigenvalue is a function of the boundary condition. In particular, the result obtained with the boundary condition $\psi(5) = 0$ is in agreement with the result over the full semiaxis as computed in the work of Richardson and Blankenbecler (1979). Increasing the x axis boundary to values larger than 5 has no effect on the result given in table 5.

Table 6 lists the eigenvalues for specific even-parity states with $\psi(8) = 0$. In all cases it is very straightforward to obtain very high accuracy in the results. The initial conditions at $x = 0$ are chosen to produce either even or odd wavefunctions. Wavefunctions with even parity are generated by choosing $\psi(0) = c$ and $\psi'(0) = 0$ with c an arbitrary normalisation constant. Two values of E are then found which lie on either side of the eigenvalue being sought, such that they produce values for ψ at the endpoint having opposite signs. The secant method is then employed to generate a new E value, and the process iterated until convergence is obtained.

Table 5. E values for the ground state with $V = x^4$.

Boundary condition	$N = 200$[a]	Analytic continuation
$D\psi(1) = 0$	0.194 546 03	0.195 538 344 346 823 549 850 451 169 344 56
$\psi(1) = 0$	2.508 197 0	2.508 196 963 966 213 487 445 409 411 048 7
$D\psi(3) = 0$	1.060 362 0	1.060 362 037 084 543 847 537 461 886 445 2
$\psi(3) = 0$	1.060 362 1	1.060 362 139 972 967 736 810 136 864 277 6
$\psi(5) = 0$		1.060 362 090 484 182 899 647 046 016 692 7

[a] Perturbation approach of Killingbeck (1986).

Table 6. E values for the 6th, 10th and 16th even-parity states for $V = x^4$ and $\psi(8) = 0$.

Eigenstate	$N = 200$[a]	Analytic continuation
6th	50.256 254	50.256 254 516 682 919 039 744 588 105 263
10th	106.923 31	106.923 307 381 732 525 653 075 102 136 17
16th	208.232 34	208.232 339 005 143 948 502 723 477 141 22

[a] Perturbation with correction term (Killingbeck 1986).

4. Conclusions

The analytic continuation procedure of Holubec and Stauffer (1985) offers a straightforward solution to the problem of obtaining high-accuracy wavefunctions and eigenvalues for Schrödinger's equation. Although the procedure is based on functions $Q(z)$ which are finite polynomials, in practice it works very well in any case where the function (or the potential) can be expanded in a Taylor series, and analytic coefficients obtained. This was demonstrated in their paper by computing the phase shifts for the potential

$$V(r) = -(2+2/r)\exp(-2r). \tag{10}$$

The only real limit to the precision is the precision of the computer employed to carry out the calculations. The disadvantage of this technique lies in the requirement to construct the Taylor series (4) and the corresponding recurrence relations (6) for each specific potential under study. However, if high precision is required in the result, this is not an exorbitant cost.

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