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Finite difference order doubling in two dimensions

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Abstract

An order doubling process previously used to obtain eighth-order eigenvalues from the fourth-order Numerov method is applied to the perturbed oscillator in two dimensions. A simple method of obtaining high order finite difference operators is reported and an odd parity boundary condition is found to be effective in facilitating the smooth operation of the order doubling process.

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1. Introduction

There are two traditional ways of using finite difference methods to find the eigenvalues of the Schrödinger equation in one dimension. The shooting method finds the energy levels one at a time but has the advantage of permitting the calculation of expectation values without any storage of the wavefunction [1]. The matrix approach involves a matrix diagonalization but yields many energy levels along with their associated wavefunctions [2]. The fourth-order Numerov method gives a wavefunction and an energy value both with an error of order h^4 , where h is the constant steplength used in the finite difference calculation. In a previous work [3] we pointed out that a result of higher accuracy can be obtained by applying the ideas of the matrix approach to a wavefunction which has been found by a shooting approach. We simply apply Rayleigh's principle, which says that an energy with h^8 error can be obtained from an approximate eigencolumn with h^4 error by evaluating the Rayleigh quotient for a symmetric matrix. The technical problem is that of producing a finite difference Hamiltonian with an eighth-order kinetic energy operator in order to find the expectation value and so extract the more accurate energy value from the Numerov wavefunction. This approach was found to work in one dimension [1] and the present work reports some results which were obtained by trying a similar order doubling approach in two dimensions. Section 2 describes the construction of high order finite difference versions of the kinetic energy operator, with a few illustrative examples. Section 3 explains the use of a relaxation process for finding the wavefunction of a low-lying state in a square region, with emphasis on the use of special odd parity boundary conditions at the external boundaries. The tables give numerical results which

demonstrate the effectiveness of the order doubling process and also the results obtained by applying it to some perturbed oscillator systems. An appendix describes in more detail how to construct the high order kinetic energy operators.

2. The D^2 operator

The problem treated was that of the perturbed oscillator with the Hamiltonian

$$H = -\nabla^2 + V(2)(x^2 + y^2) + V(4)(x^4 + y^4) + V(22)x^2y^2 \quad (1)$$

for which comparison results are available in the literature. The finite difference approach simply uses the explicit form of the potential function and so does not need complicated matrix elements; we were thus able to carry out a few calibratory calculations for potentials with different coefficients for x^2 and y^2 and with extra terms such as $x^2y^4 + x^4y^2$, for which there are a few previous reported results. The potential energy operator is straightforward but the finite difference kinetic energy operator has to be constructed for gradually increasing orders of accuracy in the calculation.

A perusal of the literature showed that several methods have been proposed for obtaining high order D^2 operators, e.g. [4–7]. However there is an extremely simple approach for producing them which suggests itself quite naturally to anyone used to applying finite difference methods together with Richardson extrapolation. All that is required is to apply vector Richardson extrapolation to the initial family of h^2 type finite difference operators representing D^2 for the steplengths $h, 2h, 3h$, etc. Readers who are not fully familiar with simple Richardson extrapolation will find the explanation of the weighting factors used below set out in the appendix. The first three members of the initial set of D^2 operators are

$$T1 = (-2, 1, 0, 0), \quad T2 = (-2, 0, 1, 0)/4, \quad T3 = (-2, 0, 0, 1)/9 \quad (2)$$

(with a division by h^2 understood and omitted and with only the right-hand half of the stencil used because of the exact left–right symmetry). The first stage of Richardson extrapolation forms a $(4, -1)/3$ combination of $T1$ and $T2$ and a $(9, -4)/5$ combination of $T2$ and $T3$ in the standard manner, giving two fourth-order expressions

$$T12 = (-5/2, 4/3, -1/12, 0), \quad T23 = (-13/18, 0, 9/20, -4/45). \quad (3)$$

The more accurate expression $T12$ is selected as the fourth-order finite difference approximation to the differential operator D^2 . A $(9, -1)/8$ combination of $T12$ and $T23$ is now made to continue the Richardson extrapolation, giving the sixth-order approximation for D^2

$$T123 = (-49/18, 3/2, -3/20, 1/90). \quad (4)$$

It is clear that by setting up an initial row with more members (thus involving longer rows with more initial zeros) we can continue the Richardson extrapolation to obtain finite difference approximations of increasingly high order. The calculation can be programmed to yield the results in the form of exact fractions (as in the example above). Table 1 shows some high order finite difference approximations for D^2 which we obtained by using the exact fraction form of Richardson extrapolation. This simplifies the tabulation of the coefficients, although in numerical calculations it sufficed to use a subroutine which produces a double precision decimal form of them for any required order.

Table 1. Some high order finite difference operators for D^2 . An entry such as (-20572) denotes the fraction $-205/72$. Only the right-hand half of the stencil is given, in the order $C(0), C(1), C(2), \dots$ downwards. The results up to order 6 are derived in the text as an example. The results for orders 12 and 14 agree with those of [15], but our fractions are reduced to their lowest terms.

Order 8		Order16	
-205	72	-1077 749	352 800
8	5	16	9
-1	5	-14	45
8	315	112	1485
-1	560	-7	396
Order 10		112	32 175
-5269	1800	-2	3861
5	3	16	315 315
-5	21	-1	411 840
5	126	Order 18	
-5	1008	-977 8141	317 5200
1	3150	9	5
Order 12		-18	55
-5369	1800	14	165
12	7	-63	2860
-15	56	18	3575
10	189	-2	2145
-1	112	9	70 070
2	1925	-9	777 920
-1	16 632	1	196 9110
Order 14		Order 20	
-266 681	88 200	-196 8329	635 040
7	4	20	11
-7	24	-15	44
7	108	40	429
-7	528	-15	572
7	3300	24	3575
-7	308 88	-5	3432
1	840 84	30	119 119
		-5	155 584
		10	374 1309
		-1	923 7800

3. The relaxation process

We shall suppose that the finite difference operator for D_x^2 at the lattice point (J, K) , for a lattice with uniform spacing h and for a wavefunction W is

$$\sum_M C(M)W(J + M, K)/h^2, \tag{5}$$

where the summation goes from $M = -I$ to $M = I$ for the finite difference operator of order $2I$ and the $C(M)$ are the numbers appearing in the stencils (such as those shown in equations (2)–(4) above). On adding the x and y contributions and multiplying by -1 to get the two-dimensional kinetic energy operator we obtain the finite difference operator equation

at each lattice point (J, K)

$$\begin{aligned}
 & - \sum_M C(M)W(J + M, K)/h^2 - \sum_N C(N)W(J, K + N)/h^2 \\
 & + V(J, K)W(J, K) = EW(J, K).
 \end{aligned}
 \tag{6}$$

This equation is our finite difference simulation of the Schrödinger equation, with $V(J, K)$ being the potential at the lattice point (J, K) .

If a full matrix diagonalization approach to the problem were attempted then the resulting matrix would be very large and would have a large bandwidth, with each basis state needing two labels to identify it. Since our primary aim is to explore the effectiveness of the simple order doubling procedure in two dimensions we have adopted a more simple approach to the eigenvalue problem, by using a relaxation technique. This approach suffices to find five of the low-lying levels for the Hamiltonian (1) and is easily able to incorporate the special boundary conditions which we discuss later. In the relaxation (Gauss–Seidel) calculation one lattice value $W(A, B)$ is held at the fixed value 1 and the lattice is scanned over the indices J and K , excluding (A, B) . Because of the even or odd $x \leftrightarrow y$ interchange symmetry of several states it is often possible to scan only half of the lattice points, with the remainder of the $W(J, K)$ values being written in by using the required symmetry or antisymmetry of the required state. For the mixed parity state $(0, 1)$, however, the full lattice has to be scanned, since that state lacks an $x \leftrightarrow y$ interchange symmetry. At each point the $W(J, K)$ terms are isolated on the right-hand side of equation (6). Thus we have the quantity $[E - V(J, K) + 2C(0)/h^2]W(J, K)$ on the right of the equation and the sum on the left excludes the $M = 0$ and $N = 0$ cases. The sum is evaluated and then a revised value $WR(J, K)$ of $W(J, K)$ is found. The present $W(J, K)$ value is then replaced by the new value $W(J, K) + RX(WR(J, K) - W(J, K))$, where RX is a wavefunction relaxation parameter. After the lattice has been scanned to modify the wavefunction values the choice $J = A, K = B$ is made (having been excluded from the lattice scan). The equation (6) is then used directly; the full left-hand side is evaluated and becomes the revised energy estimate ER . The current estimate E is then replaced by the value $E + RE(ER - E)$, where RE is an energy relaxation parameter. As explained above it is often possible to scan only about half of the lattice points by exploiting the interchange symmetry or antisymmetry of the required wavefunction.

If, to use a shorthand notation, we denote the sum on the left of equation (6) by $HW(J, K)$, then the order doubling process simply involves calculating the sequence of energy expectation values (Rayleigh quotients) of the form

$$\sum W(J, K)[HW(J, K)] / \sum W(J, K)W(J, K)
 \tag{7}$$

for a sequence of kinetic energy operators of increasing order. Thus, if the relaxation process has produced a stable wavefunction throughout space and a converged energy E , then the expectation value sequence extracts more and more digits of the accurate energy ‘hidden’ within the wavefunction. The sums in (7) are taken over all lattice points and the $HW(J, K)$ term at each point includes external point contributions, as explained in the following discussion.

The most complicated part of the relaxation process in evaluating $HW(J, K)$ is that which has to allow for boundary conditions at the x - and y -axes and along the outer boundaries. To incorporate the even or odd parity of the wavefunction about the x - or y -axis we take care to represent the nominal value of a $W(J, K)$ at a point beyond the axis by plus or minus the $W(J, K)$ value at the mirror point which is within the axes. This device is necessary whenever a high order finite difference formula for an inner point requires the wavefunction value at an

Table 2. The sequence of expectation values as a function of the finite difference order for the $(0, 0)$ and $(1, 1)$ states of even $x \leftrightarrow y$ interchange parity, for the potential x^2y^2 and with an initial relaxation order of 14. Only the last few varying digits are shown. The fixed values $NS = 60$ and $L = 12$ were used, with $(A, B) = (1, 1)$.

Order	(1.108 223 157) (0, 0)	(5.0112792) (1, 1)
14	4654	796 494
16	5690	812 514
18	5864	814 872
20	5899	815 279
22	5907	815 360
24	5909	815 377
26	5910	815 382
28	5910	815 384

outer point. For the outer boundaries the crude procedure of setting the wavefunction to zero at all external points as well as on the boundary will introduce errors when a high order finite difference method is used. We found that the best way to proceed is to regard the zeros at the outer walls as being nodes in a wavefunction which is formally regarded as extending smoothly through the boundary. We do this by simply imposing an antisymmetry condition across the outer boundaries between the wavefunction values at internal and external lattice points. This procedure in one dimension was found to lead to a well-behaved Richardson extrapolation process for the energy [3] and numerical experiments showed that it has a similar beneficial effect in two dimensions, as was discovered by a preliminary ‘empty box’ calculation for a system with a zero potential inside a square region. The order doubling procedure converges to give the correct analytic energy to 14 or so digits when the boundary antisymmetry is imposed, while the accuracy falls to only 2 or 3 digits if the wavefunction is crudely set to zero at all external points.

In the relaxation process it is not too difficult to apply the various boundary conditions. Every time a $W(J, K)$ value is called for it is tested to see whether it is beyond a boundary; if it is then it is replaced by plus or minus the value at the mirror image point for the appropriate boundary. Table 2 shows what happens when an initial order of 14 is used in the kinetic energy operator of equation (1), for the interesting case of the potential x^2y^2 , which Simon [8] showed to have bound states, despite the existence of apparent escape routes for a particle along the coordinate axes. Only the first quadrant is used in the relaxation (because of the high symmetry); a square of side $L = 12$ was used, with a 60×60 grid of lattice points. The finite difference step length was thus 0.2 in both x and y directions. The final wavefunction from the 14th-order relaxation was used in a sequence of expectation value calculations up to order 28, with the appropriate kinetic energy operator being generated in a subroutine which applied the vector Richardson extrapolation described earlier. The end result of the relaxation process is quickly predicted by applying the standard Wynn algorithm to the most recent ten E values. This target value then indicates how well the sequence of raw E values and the associated wavefunction have converged towards their final steady state. When this convergence is achieved then the sequence of expectation values of increasing order can be calculated. This way of increasing the effective finite difference order is, of course, much quicker than actually carrying out the relaxation process at each of the higher orders up to 28. Test calculations showed that the energy from the expectation value process at each order agrees very closely with the energy obtained by a full relaxation process at that order. In the calculations reported here we have used ordinary double precision and have quoted the energy values to 14 significant decimal digits.

Table 3. The groundstate (0, 0) energy for $V = \mu(x^2 + y^2) + \lambda x^2 y^2$, obtained with initial relaxation order of 20 and with $NS = 60$. The value of L is decreased as λ increases. $(A, B) = (1, 1)$.

λ	L0, L1	$\mu = 0$	$\mu = 1$
0.5	12, 12	0.879 597 303 087 77	2.024 138 321 4157
1	10, 10	1.108 223 157 5910	2.195 918 085 2001
2	9, 9	1.396 273 684 2299	2.339 566 210 1592
3	8, 8	1.598 334 372 8404	2.458 376 906 2368
4	8, 8	1.759 194 606 1756	2.561 626 575 6400
5	8, 8	1.895 034 943 0308	2.653 909 779 5320
10	8, 8	2.387 594 415 0108	3.019 177 714 7720
100	6, 6	5.143 916 233 4257	5.460 970 397 9234
1000	5, 4	11.082 231 575 908	11.232 439 267 210
10 000	2, 2	23.875 944 150 109	23.945 989 627 820

Table 4. The energies of five low-lying states for the Hamiltonian (1), using an initial relaxation order of 20, with $NS = 60$ and $L = 12$. The potential is denoted by the symbol $[V(2), V(4), V(22)]$. The states (0, 2) and (1, 3) have odd $x \leftrightarrow y$ interchange parity, with $(A, B) = (1, 2)$.

State	[1, 0, 1]	[0, 1, 1]
(0, 0)	2.195 918 080 8520	2.240 910 020 1942
(0, 1)	4.526 743 874 3910	5.151 680 290 3930
(1, 1)	7.444 551 361 5700	8.325 296 529 8155
(0, 2)	6.557 803 326 6723	8.733 164 092 4749
(1, 3)	12.332 331 271 118	16.320 612 931 726
	[0, 0, 1]	[1, 1, 1]
(0, 0)	1.108 223 157 5910	2.872 765 333 0837
(0, 1)	2.378 637 829 3449	6.266 795 083 9935
(1, 1)	5.011 279 281 5384	9.885 096 861 6280
(0, 2)	3.056 081 154 6566	10.226 404 296 576
(1, 3)	8.074 373 925 3878	18.555 036 296 491

The results of table 2 show that the order doubling procedure adds several decimal digits of accuracy for the case of a starting order of 14 and the accuracy obtained is high. The energy obtained is correct to 14 decimal digits and this is so for a wide range of test cases which we have drawn from those tables in the works [9–11] which refer to the Hamiltonian (1). Roughly one half of the cases treated in [10] and [11] actually involve separable potentials with $V(22) = 0$ or radial potentials with $V(22) = 2V(4)$. For these cases hypervirial perturbation theory gives accurate energy levels and thus provides an extra set of test problems to check the accuracy of the technique of this work, when the angular momentum is given the appropriate values $\frac{-1}{2}, \frac{1}{2}, \frac{3}{2}$, etc. For most of the calculations we used a starting order of 20 for the relaxation process, with an escalating order up to 40, so that the expectation value sequence typically adds 4 decimal digits of accuracy. The L value can be adjusted if physical considerations make it clear in which (x, y) region the wavefunction is concentrated. For example table 3 shows results for the groundstate of the potentials $x^2 y^2$ and $x^2 + y^2 + \lambda x^2 y^2$. We found some comparison energies for the second of these potentials in table 3 of [12], although the present calculation is able to give a greater number of accurate decimal digits for large λ values. As λ increases the L value can be reduced, since the wavefunction contracts. Table 4 shows selected energy levels for several potential functions. The energies are quoted to 14 significant digits, using the full relaxation plus expectation value procedure. However, it was found to be very easy to obtain a speedy energy accurate to ten significant digits after a few hundred iterations.

Although the E sequence is far from convergence the sequence of Wynn algorithm extrapolants based on the last ten E values converges quickly to give an energy of high accuracy.

Expectation values for symmetric potentials can be calculated in two ways. Since the lattice of wavefunction values is available a direct numerical quadrature can be performed in principle. However, the expectation value of an even symmetric function $F(x, y)$ can be found by adding a small term $kF(x, y)$ to the potential and recomputing the energy to give the small energy shift $k\langle F(x, y) \rangle$. The use of this energy shift technique confirmed the $\langle x^2 \rangle$, $\langle x^4 \rangle$ and $\langle x^2 y^2 \rangle$ values for the Hamiltonian (1) which were given in table 3 of [11] but were able to add several extra digits of accuracy to the results of [11].

4. Conclusion

The specimen results here show that the simple order doubling procedure previously tested in one dimension is also effective in two dimensions and makes it possible to extract several more digits of accuracy from a finite difference wavefunction of a nominally lower order. The increased eigenvalue accuracy then permits the calculation of accurate expectation values by using an energy differencing approach. Speedy energy estimates of ten or so decimal digits can be found by applying the Wynn epsilon algorithm to the sequence of energy estimates of the relaxation process well before that sequence and the associated wavefunction have converged. While revising this work for publication we made a further literature search and found that appendix A in [13] lists our odd parity outer boundary condition as one of the ways of extending a wavefunction ‘off the grid’ although, of course [13] does not involve an order doubling concept. It is perhaps of interest to note that the approach used in the present work (keeping the grid size fixed and increasing the order) is the analogue of the p version of finite element theory, while the usual procedure of using decreasing step lengths and fixed order is the analogue of the h version of finite element theory [14].

Appendix. The Richardson extrapolation weight table for the D^2 operator

The expression $T(H) = [W(X + H) + W(X - H) - 2W(X)]/H^2$ approximates $D^2W(X)$ with an error which is a sum of terms in even powers of H (with operator coefficients). If we set down the results for $H = h, 2h, 3h, 4h$ we get the first column of an extrapolation table. The second column then gives the weighted combination of neighbouring elements needed to remove the h^2 errors. The third column then gives the weighted combinations of neighbouring second column elements needed to remove the h^4 errors, and so on. It is easy to see how the coefficients in each column are made up from those in the previous column. Several equivalent algorithms can be used to construct the table automatically in a program subroutine. It is important to note that this is a table of weighting factors and is thus generally applicable to many quantities which can be subjected to Richardson extrapolation. The result of applying the factors to the $T(nh)$ operators is shown in table 1 and in equations (2) and (4) of the text.

$T(1)$			
	[4, -1]/3		
$T(2)$		[9, -1]/8	
	[9, -4]/5		[16, -1]/15
$T(3)$		[16, -4]/12	
	[16, -9]/7		
$T(4)$			

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