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LETTER TO THE EDITOR

A simple numerical method for singular potentials

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Abstract

A one-parameter family of coordinate transformations is shown to lead to a simple finite difference method which gives highly accurate energies and expectation values for the Schrödinger equation in which the potential consists of a smooth term plus a perturbing term which is singular at the origin. The method is effective down to very small values of the perturbation parameter and supplements the previously reported perturbation approach which is valuable for large λ values.

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In this short letter we present a simple and accurate method for the calculation of the energy levels of a potential which has a strong singularity at the origin $r = 0$. The Schrödinger equation for the spiked oscillator

$$-\mathrm{D}^2\psi + (r^2 + \lambda r^{-M})\psi = E\psi \tag{1}$$

has frequently been treated as a test case in the literature [1–18], and so we give some specimen results for this problem as well as for some others. For a smooth perturbation such as a λr^4 the computational problems arise for large λ values; in contrast, for the singular perturbing potential in (1) it is the small λ region which causes the most difficulty, since the greatest re-shaping of the wavefunction appears in a very small band of r values near to the origin. For large λ values (typically greater than 1) perturbation theory actually becomes easier, since it can be carried out about the minimum of the potential, which is at some distance from the origin. This makes it easy to obtain highly accurate results for the singular potentials by applying the hypervirial perturbation method which was recently applied to a Penning trap calculation [19]. For large λ values this method has provided checking results for our finite difference calculations. The shooting method presented here was developed by the authors during a visit to Besançon in 1992 by one of the authors (JPK). Since then it has been tested for a wide range of singular potentials, both in already published works and in works for which the present authors have acted as referees. This long study has shown that the method presented here still remains original and is more simple and accurate than previously published methods. The only method which is capable of comparable accuracy is the step-by-step analytic continuation method [16],

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which we have tested and which requires a much more complicated computer program; even so, we easily obtain the first 12 decimal digits of the results in [16]. The first point to note is that for the class of problems described by equation (1) the use of the finite difference method based on a fixed steplength h will be inefficient because the difficult region near $r = 0$ will require h to be very small. Both computation and theory [3, 4] have shown that fixed-h methods must use very large numbers of steps to make the calculated energies $E(h)$ fall into the region where Richardson extrapolation becomes meaningful; the error as a function of h contains non-analytic components which spoil its usual smooth $(h^2, h^4, \ldots)$ behaviour [4]. It is intuitively clear that we need a variable steplength, with small h values near $r = 0$. Since this is true for the whole class of problems represented by equation (1), it seems that an analytic change of variable approach should be appropriate; such an approach will obviously lead to a much more simple program than that for methods which continuously monitor the local behaviour in order to adjust the local steplength. Even more importantly, we wish to retain the powerful Richardson extrapolation procedure to obtain highly accurate energies from a few runs with varying numbers of steps. After testing several possible transformation functions we found that the most effective change of variable in (1) is that described by the following simple formula relating the original r coordinate to the transformed coordinate y;

$$1 + Kr = \exp(Ky). \tag{2}$$

In (2) K is an adjustable parameter which is chosen empirically. The explicit formula for y clearly involves a natural log, but the form (2) renders the mathematical analysis very clear and simple. First, (2) directly yields the relationship $\mathrm{d}r = (1 + Kr)\,\mathrm{d}y$ between infinitesimals. This shows that the use of a fixed steplength in y gives a linearly increasing steplength in r, which seems suitable for the class of potentials being studied. After introducing the change of variable into (1) a little algebra gives the transformed equation

$$-\mathrm{D}^2\psi + K\mathrm{D}\psi = (E - V)\exp(2Ky)\psi = (E - V)(1 + Kr)^2\psi. \tag{3}$$

Introducing the lowest-order finite difference representations of the first- and second-order derivatives in (3) then leads to a three-term recurrence relation (with W for 'wavefunction')

$$(1 - Kh/2)W_{N+1} + (1 + Kh/2)W_{N-1} = [2 + h(V_N - E)(1 + Kr_N)^2]W_N. \tag{4}$$

In (4) we have assumed a fixed steplength h in the y variable and so have given the various quantities an index N (with $y = Nh$). We have presented (4) in a form which shows that at $K = 0$ it becomes the well known traditional second-order finite difference equation which can be used for smooth non-singular potentials. In using (4) in a shooting process we have to work out the r value at each step in order to evaluate the potential V. However, from (2) we see that the quantity $(1 + Kr)$ propagates from step to step simply by being multiplied by the fixed number $\exp(Kh)$, so that only the extraction of r requires any extra arithmetic. To perform the shooting we can set $W_0 = 0$, $W_1 = 1$ and vary the trial E in order to search for the result $W_N = 0$ at the desired boundary $r = L$. The appropriate boundary value of y is, of course, found by using the explicit formula for y which follows from (2). In using (4) we can apply the full range of numerical and programming techniques developed previously [20]: we can use scaling to avoid any overflow or underflow problems as the shooting proceeds; we can apply Newton's method to find the eigenvalues for a given number of steps; and we can find expectation values directly without the need for quadratures involving the wavefunction. The key points involved are that the partial derivatives of W_N with respect to E and to the parameter μ (if a potential μU is added to V) obey (4) except for the addition of a single term. For the E derivative this term is equal to $-h^2(1 + Kr_N)^2W_N$ while for the μ derivative it is $h^2(1 + Kr_N)^2U_NW_N$.

Table 1. Results for the potential $r^2 + \lambda r^{-M}$, with $\lambda = 10^{-4}$ and varying M, using five runs plus Richardson extrapolation to find the lowest state of zero angular momentum. For $M = 2$ the accurate analytical result is $E = 3.000\,199\,980\,004$.

M	NS_0	K	E	$\langle r^2 \rangle$
1/2	128	64	3.000 102 276 429	1.500 012 7846
1	128	64	3.000 112 837 138	1.500 028 2095
3/2	128	2 048	3.000 138 270 120	1.500 051 8517
2	512	32 768	3.000 199 979 996	1.500 099 9900
5/2	512	1048 576	3.000 407 898 621	1.500 254 8081
3	128	16 384	3.001 754 252 826	1.501 259 5519
7/2	128	2 048	3.007 864 636 336	1.505 833 4352
4	128	2 048	3.022 274 508 729	1.516 637 7034
5	128	2 048	3.076 852 540 268	1.557 705 9597
6	128	2 048	3.155 573 206 759	1.617 322 8352
7	128	2 048	3.246 263 982 512	1.686 540 6632
8	128	2 048	3.341 068 915 312	1.759 480 1280

Thus by simultaneously propagating the W, $\mathrm{d}W/\mathrm{d}E$, and $\mathrm{d}W/\mathrm{d}\mu$ values (a procedure which involves very little extra computational effort) we can obtain the energy near to any starting E and also find any desired $\langle U(r) \rangle$. The results obtained are striking; using a sufficiently large value of the K parameter and regularly increasing the number of steps NS leads to a regular sequence of $E(NS)$ values which can be used in the usual Richardson extrapolation process to give accurate eigenvalues. Previously reported finite difference results for the class of potentials treated here have usually been of much lower accuracy and have typically used NS values of hundreds of thousands. Table 1 shows a few typical results for potentials of the spiked oscillator type. The table shows E and $\langle r^2 \rangle$ for a sequence of M values. It also shows the typical K value required to give the energy to the displayed accuracy, as well as the step number NS_0 used in a sequence of NS values starting with NS_0 and with ratio 3/2 between successive NS values, standard Richardson extrapolation being used to obtain the final E and $\langle r^2 \rangle$ values. The parameters have to be chosen to ensure that the K value gives a sufficiently small h near $r = 0$, while NS_0 is large enough to keep an h value which is not too large at the upper limit of integration. A wide band of K values around the quoted one will give virtually the same results; indeed, this stability property is obviously necessary if the method is to be widely applicable. The 'difficult' cases are grouped around $M = 5/2$, as was also found in most of the cited references. Our energy values for very small λ obey with high accuracy the law deduced theoretically by Harrell [2], that the energy should vary as λ^A for $\lambda \to 0$, with $A = 1/(M - 2)$ for the case of the singular term λr^{-M} with $M \geqslant 4$. We also checked the computed expectation values by checking that the virial relation $2E = 4\langle r^2 \rangle + \lambda(2 - M)\langle r^{-M} \rangle$ associated with (1) accurately describes the calculated values of the three related quantities. A little algebra shows that the equations quoted above lead to the simple result $3E = 4\langle r^2 \rangle + E_0$ in the limit $\lambda \to 0$, for states with the unperturbed energy E_0; this equation was also used to check the results at very small values of λ.

The method works for cases in which the r^2 term in (1) is replaced by other smooth potentials; for the Lennard-Jones potential of the form $A(r^{-12} - r^{-6})$ we found the two lowest states at $A = 625$ to have the energies $-97.539\,755\,6097$ and $-27.438\,632\,8991$, respectively. The methods described in [21] and [22] only give (differing) results of three or four decimal digits precision. Table 2 shows some results for the slightly unusual example of a singular perturbation of the smooth potential x^4 rather than the usual x^2. We carried out further tests by starting from a postulated wavefunction formed by multiplying a power of r by a term

Table 2. Energies of several states for Hamiltonian $-\mathrm{D}^2 + r^4 + 10^{-4}r^{-M}$, $(M = 4, 6)$. In all cases the upper boundary was at $r = 8$, with $NS_0 = 256$ and $K = 64$. Six runs plus Richardson extrapolation were used.

State number	$E(M = 4)$	$E(M = 6)$
0	3.840 169 8552	4.088 971 7170
1	11.738 134 3778	12.308 538 1420
2	21.383 629 7513	22.269 569 2184
3	32.294 947 7355	33.491 512 3506
4	44.227 966 8383	45.730 963 2455
5	57.030 929 8945	58.836 610 6302
6	70.598 524 9704	72.703 478 9782
7	84.852 563 7887	87.253 651 5892
8	99.732 260 2559	102.426 569 38

$\exp(-Br^2 - Cr^{-2})$ and then formally differentiating twice to give a Schrödinger with an exact eigenvalue and a potential with both r^{-4} and r^{-6} terms, as in [10, 11]. Our method gave energies correct to about 14 decimal digits for these exact test problems. Without giving many tedious tables of results we can summarize the results of our research by noting that the method described here has been applied to the singular potential problems in all of the cited references and in all cases but [16] gives much more accurate results than those reported in the works concerned. The exception [16] is, as noted above, the work which uses the more complicated stepwise analytic continuation approach. We note that many of the results obtained by other techniques and cited in the literature, both for the case of equation (1) with large λ values and for the Lennard-Jones potential with a large A value, can easily be surpassed in accuracy by using the simple hypervirial perturbation method mentioned earlier; the details of that method are given in [19]. For the more difficult case of small λ values, however, the method presented in this paper is believed to be by far the most accurate simple method available and so should be of value to the many workers who deal with singular potential problems.

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