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A Hill-series method for resonances

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Abstract

A simple algorithm is given to treat perturbed oscillator bound states and resonances. The method is applied to a bound state problem for which the energy is a non-analytic function of a perturbation parameter and also to two resonance problems, one of which has a spectrum with an unusual dual nature.

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1. Introduction

In a recent work [1] which commented on the fashionable AIM approach [2–4] to the calculation of energy levels it was pointed out that a Hill-series approach can treat polynomial potentials much more simply than AIM and can calculate some expectation values along with the energy eigenvalues. It was also shown that the Hill-series approach can easily deal with resonances by making use of the complexification approach which has recently been found to be effective in both perturbation and matrix calculations [5–7]. The initial work [1] dealt with problems involving a perturbed Coulomb potential; the present work treats the other standard case, that of the perturbed oscillator potential. However, rather than just giving illustrative high accuracy versions of numerical results previously obtained by using AIM for some standard problems, we have used the Hill-series approach as a research tool to investigate some unusual perturbed oscillator problems, thereby illustrating that the technique has a flexibility which would require much more complication if it were attempted using AIM. Section 2 describes the technique, with some references to earlier accounts of it. Section 3 treats an interesting problem in which the energy eigenvalue is a non-analytic function of a perturbing parameter; the problem is an oscillator counterpart of a similar problem involving a perturbed Coulomb potential [8–10]. In section 3 only bound states are treated, but section 4 applies the complexification approach to deal with the much-treated case of a harmonic oscillator with a perturbation of the form $-\lambda x^4$, showing that the complex resonance energies can be obtained with an accuracy matching the best ones previously obtained. Section 5 then modifies the standard problem of section 4 by adding an extra term of x^6 type to the

perturbing potential. This converts the potential into one which was treated by Benassi *et al* in 1979 [11] to show the existence of an unusual and unexpected type of resonance. For this unusual case the Hill-series approach shows a remarkable behaviour; depending on the choice of the variable complex parameter which is used, it can give either bound or resonant state results for one and the same potential. Checking calculations using both perturbation theory and an accurate finite difference method [12] confirm this unusual phenomenon, by virtue of which we propose the descriptive (if humorous) name of schizophrenic potentials for the class of potentials concerned. Section 6 in essence explains why the method of this work is called the Hill-series method, since it shows that a simple way to establish the validity of the method is to regard the Hill determinant approach within the context of a power series method which can handle Dirichlet boundary conditions at a finite value of r . Section 7 gives a conclusion, together with some extra numerical results which suggest that one of the conclusions drawn in [11] is incorrect.

2. The basic equations of the method

To treat the case of a harmonic oscillator subject to a few-term perturbing potential of even parity, we start from the Schrödinger radial equation

$$\alpha[-D^2 + L(L+1)r^{-2}]\Psi + \sum_1 V(J)r^{2J}\Psi = E\Psi \quad (1)$$

and take the wavefunction in the form

$$\Psi = \exp\left(\frac{-Wr^2}{2}\right) \sum_0 A(K)r^{2K+L+1}. \quad (2)$$

The wavefunction starts off with an r^{L+1} term so as to fit correctly to the angular momentum L which appears in (1). (We should note that in [1] the $L+1$ part was accidentally omitted from the index of the wavefunction given in equation (2) of that paper, although it appears correctly throughout the calculations). Equation (1) has been presented in a style appropriate for radial problems, but to deal with even and odd states in one dimension it suffices to set $L = -1$ and $L = 0$, respectively. When the postulated wavefunction (2) is used in the Schrödinger equation (1) a little algebra leads to the recurrence relation

$$\alpha(2N+2)(2N+2L+3)A(N+1) = F(N, V, E), \quad (3)$$

with

$$F(N, V, E) = [(4N+2L+3)\alpha W - E]A(N) + \sum_1 V(J)A(N-J) - \alpha W^2 A(N-1). \quad (4)$$

The method of use of this recurrence relation is exactly analogous to that explained in [1]. In our examples we only go up to the term $V(3)$ in the potential appearing in (1) and so can number the $A(N)$ from 1 (for $N-3$) to 5 (for $N+1$), with the replacement $A(J-1) = KA(J)$ at each step, with K being a numerical scaling factor chosen to avoid computational overflow or underflow. The choice $K = \frac{1}{|A(5)|}$ is usually adequate. Differentiating $F(N, V, E)$ with respect to E gives a partner recurrence relation for the energy derivatives of the wavefunction coefficients, which we label $AE(J)$

$$\alpha(2N+2)(2N+2L+3)AE(N+1) = F(N, V, AE) - A(N) \quad (5)$$

Similarly, differentiation with respect to $V(J)$, for $J = 1, 2, 3$ leads to another partner recurrence relation for the $V(J)$ derivatives of the wavefunction coefficients, which we label $AV(J)$;

$$\alpha(2N+2)(2N+2L+3)AV(N+1) = F(N, V, AV) + A(N-J) \quad (6)$$

Since all three recurrence relations involve the same coefficients their simultaneous propagation is computationally inexpensive. As already explained in [1], and also in [13, 14], the ‘infinite space’ eigenvalues of (1) can be found without adding up the terms appearing in the sum (2). By varying E to ensure that $A(N) = 0$ for a sufficiently high N value we are in effect using a Hill determinant approach. The valuable new feature introduced by the complexification approach is that by making W (and thus E and the sets of coefficients) complex the Hill-series technique can handle resonances as well as bound states. By applying the same scaling factor K at each step to the A , AE and AV coefficients we lock their ratios throughout the propagation and so at a high N value can apply the equations (in the form of assignment statements)

$$E := E - \frac{A(5)}{AE(5)} : \quad \langle x^{2J} \rangle := \frac{-AV(5)}{AE(5)} \quad (7)$$

The simultaneous propagation of the three recurrence relations is started with the choice $A(4) = 1$ and $N = 0$; all other coefficients are set equal to zero. The maximum N value used, ND , is gradually increased until the energy value obtained converges as a function of ND . In the following sections we apply the equations described here to give numerical results for a bound state problem and for two resonant state problems. The method is a dual purpose one in that it can deal at will with either type of state. The use of the third recurrence relation for the $AV(J)$ is optional and is not required if only the energy eigenvalues are being calculated.

3. A problem involving non-analytic eigenvalues

An interesting test of the Hill-series method is provided by a model problem due to Herbst and Simon [15]. The normalizable wavefunction

$$\Psi = \exp - \left(\frac{x^2}{2} + \frac{\beta x^4}{4} \right) \quad (8)$$

can quickly be found to obey the Schrödinger equation

$$-D^2\Psi + [(1 - 3\beta)x^2 + 2\beta x^4 + \beta^2 x^6]\Psi = \Psi \quad (9)$$

thus giving an exact ground state energy of 1 for any real positive value of β . However, a negative value of β will not give a normalizable wavefunction, although the double well nature of the potential implies that a well-defined ground state energy should still exist. A simple perturbation calculation based on the unperturbed potential x^2 will give a finite perturbation series consisting of the single term 1, whatever the sign of the real perturbing parameter β . This is quickly confirmed by a simple application of hypervirial perturbation theory. However, the use of renormalized perturbation theory, based on an unperturbed potential $3x^2$, with the rest of the potential regarded as the perturbation, gives results as surprising as those for a similar Coulomb problem [10] and actually succeeds in using perturbation theory to obtain a reasonable value for a non-analytic energy which is supposedly inaccessible to perturbation theory. (Here we should perhaps note that renormalized perturbation theory with an optimized parameter long predates its recent modern retitling as variational perturbation theory). To apply the Hill-series method of the present work to the problem we simply increase the number of terms ND used in the propagation until the calculated eigenvalue settles down to a limiting value. Trial and error showed that the choice $W = 3$ is adequate to obtain double precision energies for an ND value ranging up to 300. Table 1 shows the numerical results, with the less accurate renormalized hypervirial perturbation theory results incorporated in the displayed numbers. The particular choice $\beta = -g^2$ has been used, since the parameter g appears in some of the other examples treated later in the present work. As a further check on

Table 1. The lowest energy level for the Hamiltonian of equation (9), with $L = -1$ (even parity) and with W fixed at the real value 3. The parameter β is set equal to $-g^2$, with g being a positive number. The digits in brackets are those given by the renormalized hypervirial perturbation theory. The extra digits are those given by the Hill-series method.

g	$E(g)$
0.20	(1.000 003 2464)30 177
0.22	(1.000 028 193)570 523
0.24	(1.000 145 48)9201 872
0.26	(1.000 520 20)0715 391
0.28	(1.001 4259)33 439 162
0.30	(1.003 2105)26 205 645

Table 2. Lowest resonant state complex energies for the potential $x^2 - 2g^2x^4$, with $L = -1$ (even parity). A complex W value (1, 1) and an ND value of 350 suffices to give all the results.

g	ER	EI
0.14	0.968 164 247 842 0597	4.297 124 101(-7)
0.16	0.957 085 006 539 8872	1.960 687 029 36(-5)
0.18	0.943 282 187 993 8105	2.569 986 483 606(-4)
0.20	0.925 942 461 073 143	1.544 022 124 3205(-3)
0.22	0.904 825 085 519 8596	5.539 501 705 8573(-3)
0.24	0.880 930 111 973 8638	1.397 847 527 9423(-2)
0.26	0.856 133 537 632 9515	2.767 004 146 1778(-2)
0.28	0.832 259 899 857 6937	4.630 061 197 1066(-2)
0.30	0.810 527 122 179 3937	6.890 850 364 6838(-2)
0.32	0.791 513 679 653 6186	9.439 080 110 482 25(-2)
0.34	0.775 349 598 086 2343	1.217 757 312 654 71(-1)
0.36	0.761 912 598 584 7811	1.503 046 474 073 10(-1)

the results obtained we treated a few selected cases by using the high accuracy finite difference method of [13] and found agreement to double precision.

4. A resonant state example

For the much treated case of equation (1) with $L = -1$, $V(1) = 1$ and $V(2) = 1$, the choice of a real W is appropriate. Thus, for example, the choice $W = 3$, with $\alpha = 1$, gives the lowest energy $E = 1.392 351 641 530 29$ and correspondingly accurate values for excited state energies, as well as for the energies associated with higher values of the angular momentum L . More interesting than this standard problem is that of the resonant states which arise when $V(2)$ is negative but not too great in magnitude (simply because the term ‘resonance’ is not physically appropriate if the imaginary part of the eigenvalue becomes very large). For this $-\lambda x^4$ type of perturbation we must use a complex value of W in the equations and so must write the associated computer program to allow all the quantities appearing to take complex values. A quick preliminary trial calculation with varying W establishes the appropriate (and not too critical) value of W which will suffice to give speedy convergence of the complex eigenvalues as ND is increased. Table 2 sets out some typical results, which are of comparable accuracy to those of the highly accurate Hankel determinant method [16].

5. An interesting schizophrenic potential

In 1979, Benassi *et al* [11] gave numerical results for a potential which corresponds to that of equation (1) of this work, with the special choice $L = -1$, $\alpha = 1$, $V(1) = 1$, $V(2) = -2g^2$, $V(3) = g^4$. This is the potential treated in section 3 but with a very small extra term $g^4 x^6$. Looking at the problem intuitively, we can take two different but apparently reasonable points of view. First, we can suppose that as we add a term $K g^4 x^6$ to the potential, with K gradually increasing from 0 to 1, then the imaginary part of the resonant state eigenvalue should change slowly with K . The Hill-series method with complex W can follow the eigenvalue trajectory and bears out this conjecture; at $K = 1$ it arrives at (or near) the complex eigenvalues given in [1]. However, an equally compelling point of view is to note that as soon as K becomes nonzero the potential can be seen to rise to infinity in both directions, producing a deep outer well in the potential. On physical grounds we thus expect to have only real bound state energies, with many low-lying oscillator-type states being concentrated in the outer well regions of the potential which are far from the origin. Remarkably, we can obtain these energies by using a real W value in the Hill-series approach. The intention of the work [11] was to show that the presence of the outer well leads to the existence of complex eigenvalues without the need for the ever-descending potential which is clearly present for the case $K = 0$ and which is associated with the presence of a continuous spectrum. To make the two apparently contradictory intuitive arguments outlined above consistent requires a complicated analysis of directions in the complex g plane, as given in [11] and the references therein. The gist of the argument is that the resonances are actually associated with a complex scaled Hamiltonian and so make sense in that context. We note that in the history of the Hill determinant method for bound states it was found that two different spectra could be obtained as the W parameter is varied for some perturbed oscillator problems. Znojil [17] eventually resolved this problem by showing that the two spectra refer to two different Hamiltonians which are related by a simple transformation. It seems that in the present case a similar effect is taking place, albeit involving complex transformations. However, our principal intention here is to report the numerical results, since they give a remarkable illustration of the flexibility of the technique which we describe in the present work. Table 3 gives the complex energies for the potential treated in [11], comparing the results of [11] with those obtained using the series-Hill method with a complex W value. Since the latter method gives double precision results, we have used suitably truncated values in making the comparison. Table 4 shows the real eigenvalues which are obtained when real values of W are used. These energies are confirmed by the finite difference method of [12]. For the case $K = 0.5$, for which the x^6 term is $0.5g^4 x^6$, the outer wells are deep enough to contain several energy levels. A hypervirial perturbation calculation carried out at the potential minimum shows that at $g = 0.20$ the lowest state has the energy -51.3619569455867 , with an energy level spacing of around 7.5 between the low-lying oscillator-type levels. The Hill-series method with $L = -1$ and $W = (10, 0)$ can locate this level with high accuracy, as well as all the other levels. Furthermore, the $\langle x^2 \rangle$ value associated with the energy shows correctly that the low states are indeed localized in the outer well. Once again, this calculation shows the great flexibility of the Hill-series method.

6. The use of a finite r value

In [1] and in the present work the principal attention was on the high ND (i.e. Hill determinant) use of the equations. For completeness we should now comment on the modification needed in order to use homogeneous Dirichlet boundary conditions at finite r . To find the energy

Table 3. The lowest even parity complex eigenvalue for the potential $x^2 - 2g^2x^4 + g^4x^6$ as obtained by the Hill-series method with $W = (1, 5)$. An ND value of 350 suffices to give all the results. The bracketed groups of digits show first the result of [11], when applicable, and then the result from the Hill-series method. Our double precision results have been truncated for convenient presentation when they are compared with those of [11].

g	ER	EI
0.14	0.969 129 320 027 18	3.3798(-10)
0.16	0.958 969 970 461 692	1.061 900 17(-7)
0.18	0.946 916 040 677 459	5.180 776 6717(-6)
0.20	0.932 5557(77)(15 825)	7.9(081)(477554)(-5)
0.22	0.915 253(681)(54 748)	5.70(44)(253066)(-4)
0.24	0.894 420(390)(55 321)	2.424(6)(632840)(-3)
0.26	0.870 1153(74)(11 574)	7.10(39)(405834)(-3)
0.28	0.843 3344(92)(23 923)	1.591(6)(585947)(-2)
0.30	0.815 607(847)(95 815)	2.940(0)(0216 892)(-2)

Table 4. The real eigenvalue closest to 1 for the potential used in table 3. The values $W = (3, 0)$ and $ND = 300$ suffice to obtain the results. The L value is -1 . We find that $E \rightarrow (ER - EI)$ as $g \rightarrow 0$.

g	E
0.14	0.969 129 319 6892
0.16	0.958 969 864 2718
0.18	0.946 910 860 1364
0.20	0.932 476 291 9642
0.22	0.914 685 971 0514
0.24	0.892 042 441 8197
0.26	0.863 389 091 5599
0.28	0.829 176 307 2048
0.30	0.791 672 513 9913

levels subject to the condition $\Psi(R) = 0$ it seems to be necessary to revert to the direction summation of the terms appearing in the wavefunction of equation (2), but an approach which is more simple is possible. We set $r = R$ and note that the quantity

$$S(N) = \left[\sum_0^N A(J)R^{2J+L+1} \right] \frac{1}{R^{2N+L+1}} = \sum_0^N \frac{A(N-J)}{R^{2J}} \quad (10)$$

obeys the recurrence relation

$$S(N+1) = S(N)R^{-2} + A(N+1); \quad S(0) = A(0) \quad (11)$$

When comparing the values of the wavefunction $\Psi(R)$ for two slightly different E values at the same N it is quite permissible to drop all common factors and take the $S(N)$ value for the two E values as the representative numbers to consider. Differentiating with respect to E gives the partner recurrence relation

$$SE(N+1) = SE(N)R^{-2} + AE(N+1); \quad SE(0) = 0, \quad (12)$$

with analogous equations for SV if required. With this modification, we can set the boundary at any finite distance R and can also see that in the limit of infinite R we arrive at exactly the test $A(N) = 0$ which is used to find the energy levels in the Hill-series approach used in [1]

Table 5. Values of $F(g) = \text{EI}(g)g^2 \exp(-g^{-2}/2)$, from table 3.

g	This work	[11]
0.14	0.784 66	
0.16	0.825 35	
0.18	0.845 31	
0.20	0.853 07	0.848 82
0.22	0.846 11	0.846 39
0.24	0.822 22	0.822 21
0.26	0.782 87	0.782 86
0.28	0.734 31	0.734 32
0.30	0.684 45	0.684 44

and in the present work. One application of the method described in this section is to locate the nodes of the wavefunction by first finding the infinite space eigenvalue and then locating the R values at which the spectrum contains that same energy. This can be done by making use of the virial theorem together with a Newton's method rootfinder of the type appearing in equation (7) for the energy. The appropriate computer program is under development, and it is hoped to describe the method in a future work.

7. Conclusion and discussion

The examples given in the present work again illustrate the point, made in a previous work [1], that a simple Hill-series approach is adequate to obtain much information about the Schrödinger equation with a polynomial potential and is less complicated for that purpose than the currently fashionable AIM. The complexification process for extending bound state techniques to handle resonant states also seems to be comparatively easy and accurate for the Hill-series approach. The special systems which have been studied in sections 2 and 4 of the present work display interesting features which would merit wider mathematical and computational studies. In particular, it would be of interest to see how a concentrated wave packet in the region of the origin can propagate into the outer well (which for small K values has a dense set of many low-lying levels) in much the same way as if the potential descended monotonically (which case was treated in [18]). On physical grounds we surmise that the difference between the results of tables 3 and 4 is really that between a dynamic and a static process, with the complex W results referring to the behaviour of an initially concentrated oscillator function (in a non-stationary state) which can tunnel into the outer well with a lifetime which is proportional to the reciprocal of EI. With regard to this tunnelling effect the authors of [11] conjectured that EI (in our table 3) should behave as a WKB barrier transmission coefficient, so that $F(g) = \text{EI}(g)g^2 \exp(-g^{-2}/2)$ will tend to a constant as g tends to zero. The results given in [11] do suggest that $F(g)$ reaches an asymptotic value at around $g = 0.20$, which is the lower limit of their displayed results. Our Hill-series results for g less than 0.20 have been checked by using both complex hypervirial [5] and complex matrix [6] methods. The three methods agree; they all indicate that $F(g)$ actually has a maximum very close to 0.20 and shows a high symmetry about that maximum. Accordingly, while revising the manuscript we added table 5 in order to show this effect.

References

- [1] Killingbeck J P 2007 *J. Phys. A: Math. Theor.* **40** 2819
- [2] Cifti H, Hall R L and Saad N 2003 *J. Phys. A: Math. Gen.* **36** 11807

- [3] Barakat T 2005 *Phys. Lett. A* **344** 411
- [4] Cifti H, Hall R L and Saad N 2005 *Phys. Lett. A* **340** 388
- [5] Killingbeck J P, Grosjean A and Jolicard G 2004 *J. Phys. A: Math. Gen.* **37** 7971
- [6] Killingbeck J P, Grosjean A and Jolicard G 2005 *J. Phys. A: Math. Gen.* **38** L695
- [7] Killingbeck J P, Grosjean A and Jolicard G 2006 *J. Phys. A: Math. Gen.* **39** L547
- [8] Killingbeck J P 1980 *J. Phys. A: Math. Gen.* **13** L393
- [9] Pandey R K and Varma V S 1989 *J. Phys. A: Math. Gen.* **22** 459
- [10] Killingbeck J P, Grosjean A and Jolicard G 2001 *J. Phys. A: Math. Gen.* **34** 8309
- [11] Benassi L, Graffi S and Grecchi V 1979 *Phys. Lett. B* **82** 229
- [12] Killingbeck J P, Gordon N A and Witwit M R M 1995 *Phys. Lett. A* **206** 279
- [13] Killingbeck J 1985 *J. Phys. A: Math. Gen.* **18** 245
- [14] Killingbeck J 1985 *J. Phys. A: Math. Gen.* **18** L1025
- [15] Herbst I W and Simon B 1978 *Phys. Lett. B* **78** 304
- [16] Fernandez F M 1995 *J. Phys. A: Math. Gen.* **28** 4043
- [17] Znojil M 1986 *Phys. Lett. A* **116** 207
- [18] Gomez F J and Sesma J 2002 *Phys. Lett. A* **301** 184