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Adding a complex shift to HVPT

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Abstract
A complex coordinate shift is incorporated in renormalized hypervirial perturbation theory. Test calculations on harmonic oscillators with cubic perturbations show that the resulting method produces accurate numerical results for the real energies of PT symmetric Hamiltonians with complex potentials and for the complex resonance energies of Hamiltonians with real potentials.

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1. Introduction

The hypervirial relations were first used passively to provide calibratory tests for the accuracy of variational wavefunctions [1, 2] and then in a more active role to find perturbed oscillator energies either by hypervirial perturbation theory (HVPT) [3] or by direct calculation [4]. HVPT is able to calculate expectation values $\langle x^N \rangle$ as well as energies, which gives it an advantage over the Bender–Wu form of perturbation theory [5]. It also works for the perturbed hydrogen atom, for which the unperturbed spectrum has a continuous part [6]. Renormalized perturbation theory [7–10] produces accurate numerical results by making a repartitioning of the perturbed and unperturbed parts of the Hamiltonian. In [10], it was shown that a direct HVPT approach to the repartitioned Hamiltonian gives the better behaved renormalized energy series which had previously been obtained by a transformation of the strongly divergent traditional perturbation series [8]. It was also shown that WKB as well as quantum-mechanical energies can be found by using HVPT [11, 12] and that for some radially perturbed Coulomb potentials even formally non-analytic eigenvalues can be calculated by varying the index I in perturbation terms of the form $\lambda^I r^N$ [13]. A complex variable form of the theory has also been found to give the complex resonant state energies for perturbed oscillator and Coulomb systems [14, 15]. In the 1980s, the renormalized version of HVPT became known as the Caswell–Killingbeck method (CKM), a name that has persisted in the literature [16–18].

The simple CKM form of HVPT not only produced the more recent developments outlined above but also has features which inspired other theoretical methods, as can be seen by considering the standard case of the perturbed oscillator potential $x^2 + \lambda V x^4$. The CKM would rewrite this as $Wx^2 + \lambda(Vx^4 - Ux^2)$, with $U = W - 1$ and with $\lambda = 1$ (to avoid high powers of λ appearing in the perturbation sums). It would also choose W while remembering that the physical results depend only on the full Hamiltonian, so that the results should in principle vary as little as possible with the perturbative partitioning used in the calculation.

These two parts of the CKM were later developed to give the linear delta expansion [17, 19] and the principle of minimal sensitivity (PMS) [20, 21]. Although the method nowadays called variational perturbation theory (VPT) has led to powerful techniques in path integral theory and field theory [22] its origins in the earlier work are visible. The founding work of VPT [23] referred to the work of Caswell [8], while the basic work on the PMS (widely used in VPT) cited the principle as arising within the CKM [21] (with an acknowledgement to the present author).

In recent years there have been several noteworthy advances in the theoretical and numerical aspects of renormalized perturbation theory. It has been shown, for example, how to achieve the perturbed/unperturbed splitting of the Hamiltonian so as to ensure the fastest convergence as the order increases [17, 18] (here the work of [9] is the pioneering one) and how to obtain a strong field perturbation series by an ingenious manipulation of the weak field renormalized series [24]. Since HVPT is often referred to as 'perturbation theory without a wavefunction', one interesting development has been the attempt to estimate the perturbed wavefunction by a careful use of the PMS [25, 26], as well as by using the hypervirial relations and a minimum entropy approach [27].

The present publication extends the CKM version of complex HVPT [13, 14]. We add an extra degree of freedom to the renormalized Hamiltonian by permitting a coordinate shift as well as the usual repartitioning between perturbed and unperturbed terms. Various authors have used the idea of a coordinate shift [e.g. 22, 25, 26] in their work but without exploring its full effectiveness in improving numerical calculations. The present work shows that the use of a complex coordinate shift leads to accurate energies for some systems with PT symmetry and real energies as well as for systems with a real potential and complex resonant state energies. Most of the discussion is concerned with oscillator systems with perturbations of the cubic form Ax^3, with A either pure real or pure imaginary, since for such systems there are many comparison results in the literature.

Section 2 describes the calculation of the shifted potential and section 3 gives some specimen results to illustrate the effectiveness of the process. Section 4 shows how well the method can deal with excited states, which would be difficult to reach by other methods. Section 5 summarizes the experience gained during the calculations and describes some extra numerical work, which arose out of that experience. Section 6 discusses some relevant theoretical background to the work.

2. The basic transformation equations

We adopt throughout a numerical approach, with no use of computer algebra. The advantage of the approach described in this section is that anyone who already has a program which implements complex HVPT for a perturbing potential containing both even and odd powers of x can simply add a short subroutine which produces the modified potential for the existing program to use. We suppose that we are given an initial complex potential of the form

$$U(x) = \sum [UR(J) + \mathrm{i}\, UI(J)]x^J \quad (J = 1 \text{ to } 3). \tag{1}$$

The shift is most simply described by saying that we will replace x by $x + (X + \mathrm{i}Y)$. This fixed-coordinate shift formally leaves the kinetic energy operator invariant but changes the potential from $U(x)$ into a new potential $V(x)$. We expand the powers of the shifted coordinate in the form

$$[x + (X + \mathrm{i}Y)]^M = \sum [A(M, N) + \mathrm{i}B(M, N)]\, x^N \quad (N = 0 \text{ to } M). \tag{2}$$

Considering the action of multiplying this expression by $[x + (X + \mathrm{i}Y)]$ leads us to the recurrence relations

$$A(M + 1, N) = A(M, N - 1) + XA(M, N) - YB(M, N) \tag{3}$$

$$B(M + 1, N) = B(M, N - 1) + XB(M, N) + YA(M, N) \tag{4}$$

with the obvious initial conditions $A(0, 0) = 1$ and $B(0, 0) = 0$. The transformed potential will have contributions to its x^N term coming from each other power x^J in the original potential $U(x)$. The new shifted potential terms thus involve a sum over J involving complex products

$$VR(N) = \sum [UR(J)A(J, N) - UI(J)B(J, N)] \tag{5}$$

$$VI(N) = \sum [UR(J)B(J, N) + UI(J)A(J, N)]. \tag{6}$$

This transformed potential with terms $[VR(N) + \mathrm{i}\, VI(N)]x^N$ is then used as the potential in a complex hypervirial calculation, with the resulting sequence of complex energies being treated by a complex form of the Wynn epsilon algorithm if necessary. The calculation was initially carried out in QBasic interactive mode (before being translated into Fortran), since the choice of the reference oscillator potential $[WR + \mathrm{i}\, WI]x^2$ in the renormalized HVPT has to be based on the knowledge of the modified term $[VR(2) + \mathrm{i}\, VI(2)]x^2$ which emerges after the shift operation has modified the terms in the potential. For most of the calculations reported here $VI(2)$ is zero and so it is not difficult to produce a simple rule that sets a satisfactory real WR which is a fixed multiple of the resulting $VR(2)$ value. The most obvious advantage of using a complex shift for a PT symmetric Hamiltonian is that it increases the magnitude of the x^2 term in the Hamiltonian and thus decreases the effective strength of the perturbation. The shift also introduces a linear term involving x into the perturbation, which requires us to make a further choice about the power of λ to be formally associated with each term. For example, the convention is often used that an x term is prefixed by λ and an x^3 term by λ^2. However, in renormalized perturbation theory there is usually an extra perturbation term involving x^2. We have used the simple convention that the every term in the perturbation is formally associated with the first power of λ in deriving the hypervirial recurrence relations (remembering, of course, that λ is set equal to 1 in numerical calculations). The numerical results show that this choice is adequate. In the literature dealing with perturbed cubic Hamiltonians of the form $-AD^2 + Bx^2 + Cx^3$ (with C real or imaginary) one can find many different numerical values for the coefficients A, B and C. Thus, although we have performed test calculations on the results from a range of published works, we have not undertaken the tedium of presenting a table for every possible case, since readers will find the method of this work so simple that they can apply it themselves to any specific example. We have presented detailed tables for several particular calculations but have simply given selected numerical results in the text to summarize some of the other checking calculations that were performed.

3. Some specimen results

As an initial test during the development of the technique of this work it was decided to take some standard results from the recent literature to give reference values. The results

were somewhat surprising and so were checked by means of an alternative complex matrix method (which gave the same results). In his recent comprehensive review of PT symmetry, Bender [29] gave a table of numerical results for the low-lying real eigenvalues arising from the potentials $\mathrm{i}x^3$ and $-x^4$. The latter potential is a favourite example for workers in spectral theory who like to 'épater la bourgeoisie', since it only acquires its real spectrum by imposing the boundary conditions within two downwards-sloping wedges in the complex plane which meet at the origin. In some remarkable work, using several different methods, Bender and Jones and co-workers [29–31] have shown that the real energies which arise in the complex wedge calculation can be produced by carrying out a traditional real axis calculation using a real potential, which is $4x^4 - 2x$ for the case of the starting potential $-x^4$. It is thus possible to compute the results given in one-half of Bender's table 1 by using several different traditional techniques. We show our results, compared with those of [29] in table 1. The results for the potential $4x^4 - 2x$ were obtainable by using real variable renormalized HVPT with a reference potential of $30x^2$ and were checked by means of a finite difference calculation. The results for the potential $\mathrm{i}x^3$ were obtained by using the complex HVPT with a complex shift (as described in section 1) and were also checked by using a matrix calculation with complex oscillator basis functions.

The discrepancy between our results and those of [29] clearly increases with the state number. Since the results in [29] were obtained by using a Runge–Kutta procedure in the complex plane, it is possible that too large a steplength was being used in the calculations; the safe procedure would be to use a few decreasing steplengths together with Richardson extrapolation. In table 1 most results have been quoted to only the same number of digits as were used in the original table, since that is sufficient to reveal the discrepancy. We note that the authors of [30] perhaps also obtained (unquoted) results of high accuracy but were only trying to match the five or six digit results for the lowest five states, which had appeared in one of the founding papers of PT symmetry theory [32]. At the bottom of table 1 we add some more accurate results for the states $n = 0$ to $n = 4$, obtained by letting the parameter Y in the shift vary in steps of 0.1 between -1 and -2 so as to obtain the greatest number of stable digits in the results. That these more accurate energy values are indeed reliable is indicated by the fact that they fall correctly between the upper and lower bounds produced by highly accurate moment method calculations in [33].

The second recent example which we used as a preliminary test was the set of results for the Hamiltonian

$$H = -(1/2)D^2 + (1/2)x^2 + \mathrm{i}\,ßx^3 \tag{7}$$

given in table 1 of [34]. We used only the fixed complex shift $(0, -1)$ for the test, with no attempt at optimizing the shift. We also used the same shift to treat the real perturbation βx^3, with the surprising result that a complex shift was very efficient for this potential also, whereas intuition might suggest the use of a real shift. Table 2 shows the results, which illustrate how well the complex shift procedure bestows high accuracy on the traditional CKM/HVPT. The slight variation of accuracy in the table is due to the fixed non-optimized value of the shift that is used. For the limited set of β values which we used our resonance results are, of course, more accurate than the complex matrix ones reported in [34], where only low accuracy was needed to make a comparison with the results which were produced by a proposed quantization condition to find the energy levels. In [34], the authors give extra information about the resonance for the perturbation $6^{1/2}x^3$. They state that the use of Borel–Padé summation on the traditional energy perturbation series produces an energy estimate of $0.5541 - 0.035\,16\mathrm{i}$ and that their complex scaling calculation gives $0.554\,053\,519 - 0.351\,401\,778\mathrm{i}$. Our complex shift approach gives

Table 1. HVPT results for the Hamiltonians $-D^2 + U$, with $U = \mathrm{i}x^3$ and $U = 4x^4 - 2x$ (representing $-x^4$).The results of [29] are placed in brackets below the results from the present calculation. The fixed shift $(X, Y) = (0, -1)$ was used for the low precision results. The higher accuracy results for $n = 0$ to 4 were obtained by a rough optimization of the value of Y.

N	$E(\mathrm{i}x^3)$	$E(-x^4)$
0	1.156 267 072	1.477 149 754
	(1.156 267 072)	(1.477 149 753)
1	4.109 228 753	6.003 386 083
	(4.109 228 752)	(6.003 386 082)
2	7.562 273 855	11.802 433 595
	(7.562 273 854)	(11.802 433 593)
3	11.314 421 820	18.458 818 704
	(11.314 421 818)	(18.458 818 694)
4	15.291 553 750	25.791 792 378
	(15.291 553 748)	(25.791 792 423)
5	19.451 529 131	33.694 279 877
	(19.451 529 125)	(33.694 279 298)
6	23.766 740 435	42.093 807 711
	(23.766 740 439)	(42.093 814 569)
7	28.217 524 973	50.937 404 325
	(28.217 524 934)	(50.937 278 826)
8	32.789 082 782	60.184 331 266
	(32.789 082 922)	(60.185 767 651)
9	37.469 825 361	69.802 096 675
	(37.469 824 697)	(69.795 703 031)
0	1.156 267 071 9881	
1	4.109 228 752 8096	
2	7.562 273 854 9788	
3	11.314 421 820 1958	
4	15.291 553 750 3925	

(with $Y = -1$, $W = (0.5, -2.5)$) the real part of the energy as 0.554 053 518 461 01 and the imaginary part as −0.351 401 777 593 69.

The Hamiltonian (7) with a real cubic perturbation βx^3 was also treated in [35] for a range of β values, although only for the states $n = 0$ and $n = 4$. The complex shift method gives highly accurate results for all the cases treated in [35]. As an example we give the results of [35] for the case $\beta = 1$ with the extra digits from the shift method, with shift $(X, Y) = (0, -1)$, added. For the $n = 0$ state we find $E = 0.612\,888\,4333(07\,755) - 0.408\,592\,6669(32\,265)\mathrm{i}$ while for the $n = 4$ state we find $E = 8.136\,859\,247(48\,807) - 5.824\,979\,543(55\,288)\mathrm{i}$. These specimen results show the accuracy of the shift method, although it should be noted that energies with such a large EI value hardly merit the name of resonance state energies, if we think of the reciprocal of EI as being a lifetime for the decay of an initially concentrated wavepacket.

As an example of an individual result from the literature for the perturbation $\mathrm{i}\beta x^3$ we note that [25] quotes the lowest energy for $\beta = 1$ as being 0.797 342 612, as obtained from a matrix calculation. A rough optimization using our method gives $Y = -0.6$ and $W = 6$ and an eigenvalue of 0.797 342 607 508 9055. In a test of the n-loop approximation in VPT a

Table 2. Some specimen results for the ground-state eigenvalue for the Hamiltonian $H = (1/2)\ (-D^2 + x^2)\ + K\beta x^3$, with $K = i$ and $K = 1$. The fixed shift $(X, Y) = (0, -1)$ was used for all calculations. The fixed choice $(WR, WI) = (5/4)(VR(2), VI(2))$ was also used. The complex energy for the case $K = 1$ is given first.

β	ER	EI
1/10	0.484 315 997 004 0.512 538 145 9393	8.060 29 (−6)
1/8	0.472 398 732 48 0.518 760 344 5588	7.026 247 07 (−4)
1/6	0.442 520 045 125 0.530 781 759 3042	1.551 792 5820 (−2)
1/4	0.413 859 273 8354 0.558 372 124 1780	8.902 195 469 26 (−2)
3/8	0.434 523 763 9846 0.602 504 355 6468	1.853 383 603 434 (−1)
1/2	0.472 130 852 566 74 0.645 877 080 9870	2.527 192 945 421 (−1)

numerical reference value of 0.762 851 773 is quoted in [36] for the ground-state energy for $H = -(1/2)D^2 + \mathrm{i}x^3$. HVPT with a complex shift gives the energies 0.762 851 774 227 2636 for the state $n = 0$ and 2.711 079 923 253 886 for the state $n = 1$.

To test the shifted HVPT method for a wider range of perturbation strengths we applied it to the Hamiltonian

$$H = -D^2 + (1/4)x^2 + \mathrm{i}\,ßx^3, \tag{8}$$

which was treated in [37]. The simple choices $(X, Y) = (0, -1)$ and $W = V(2)$ were adequate to give the results shown in table 3, where a comparison with the results of [37] is shown.

4. Excited state calculations

For the study of excited states HVPT has the advantage that a specific state can be selected and studied individually, making it possible to adjust any relevant parameters to improve the accuracy of a particular eigenvalue. Thus for example, we could study the $n = 1000$ perturbed state, which in a standard matrix approach would require a matrix with a dimension of a few thousand. We apply our shifted HVPT method to the cubic Hamiltonian already treated in section 2:

$$H = -D^2 + \mathrm{i}x^3. \tag{9}$$

When a shift of the form $(0, Y)$ is used the most obvious result is a modified x^2 term, which we denote by Vx^2 and which is real for many of our calculations. The key decision to take next is that of the W coefficient in the reference potential Wx^2, so that $(U - W)x^2$ is added to the rest of the potential to give the effective perturbing potential. In interactive computing the operator can select the W value at will, whereas in an automatic program some rule must be incorporated in the program (or a loop scanning a range of choices must be used). Fortunately, a few preliminary calculations quickly give a good idea of the suitable parameter choices (in this case for Y and W). It turns out that the choices become less critical for the higher states,

Table 3. Some energy levels for $-D^2 + (1/4)x^2 + \mathrm{i}\,\beta x^3$. The ground-state result from [37] is shown first, followed by the extra digits given by the shifted HVPT. The fixed shift $(X, Y) = (0, -1)$ is used throughout. The energies for $n = 1$ are also given below the $n = 0$ energies.

β	E
0.015 625	0.502 63(229 852 749)
	1.516 707 457 175 95
0.131 25	0.509 9(8)(759 721 4623)
	1.560 869 385 023 72
0.0625	0.533 93(160 859 384)
	1.689 654 758 742 55
0.125	0.5949(2)(1522 277 104)
	1.971 226 201 092 90
0.25	0.7129(4)(3574 894 383)
	2.450 816 596 177 90
0.50	0.9002(6)(5805 810 384)
	3.156 761 371 513 62
1.00	1.1674(6)(5456 842 266)
	4.128 556 056 50360
2.00	1.5307(8)(7725 501 108)
	5.430 779 723 244 74

Table 4. Some excited state energies obtained by the shifted HVPT method for $H = -D^2 + \mathrm{i}x^3$. The choice $W = VR(2)$ is made for every state and direct convergence is obtained. The shift used is of the form $(X, Y) = (0, -h)$ for every state.

N	h	W	E
25	3	9	122.522 505 832 8462
50	4	12	278.170 980 319 1869
100	6	18	635.272 473 652 1825
150	7	21	1031.345 791 806 419
200	8	24	1455.116 150 440 382
250	9	27	1900.770 320 564 373
300	10	30	2364.687 274 184 924
400	11	33	3337.977 030 787 495
500	12	36	4361.593 699 830 571
1000	16	48	10014.304 805 442 44
2000	20	60	22999.932 295 331 49
3000	24	72	37410.425 463 04816
4000	27	81	52832.044 760 929 74
5000	29	87	65092.023 182 011 52
10 000	38	114	158630.373 430 2000
20 000	50	150	364425.965 460 5554

to such an extent that the perturbation series converges directly without any need for the use of the Wynn epsilon algorithm to treat the partial sums of the series. Table 3 gives results for some high-lying levels for the Hamiltonian in (9), showing the parameters which were used and which led to full double precision convergence for most of the states. It is perhaps useful to add a comment here about the computational procedure. After the action of the shift transformation the new potential V acquires a component $VR(2)x^2$. If the choice $WR = VR(2)$ is made then the resulting perturbation series will have alternate perturbation coefficients equal to zero. This behaviour will arise in general for odd parity perturbations. It is thus important to include a general command in the program which only forms the next partial sum when the current perturbation term is non-zero. The sequence of partial sums then does not have any equal numbers in it, which avoids problems if the sequence of partial sums is acted on by the Wynn epsilon algorithm. In fact, for the results shown, the epsilon algorithm is not needed, since convergence of the partial sums is obtained directly with the choice $W = VR(2)$. We have given results in table 3 for states up to $n = 20\,000$, but an n value of hundreds of thousands is attainable; the results provide an example of a case in which perturbation theory is more effective than the complex matrix approach (and most other methods).

Although we give only a few illustrative results in our tables we have checked many published results. We can, for example, reproduce the full range of complex eigenvalues given in the tables of [38] for a real cubic perturbation and can also treat higher states. Our results indicate that for the particular case $H = -(1/2)D^2 + (1/8)x^2 + 0.5x^3$ some digits have been transposed in table 1 of [38]. The quoted $n = 0$ energy has a real part of 0.466 391 109 8243, which should be 0.466 391 108 9243 according to our calculation.

5. Discussion of the results

In the present short work we have presented some preliminary calculations, which suggest that the use of a complex shift in HVPT can be helpful in improving the accuracy of numerical calculations for some problems involving resonances or PT symmetric Hamiltonians. The reference problems treated were mainly taken from the literature, although the results of section 3 show that the perturbation approach is capable of reaching very high excited states with which other methods would have considerable difficulty. As is usual in the CKM the approach used was largely empirical, with rough rules about how to select optimum parameters being established after a sequence of trial and error calculations (so that interactive computing is a useful first step in gaining experience). To illustrate what happens to the potential during the shift process we quote an example from the reported calculations. For the Hamiltonian $-D^2 + \mathrm{i}x^3$ and the case of the imaginary shift $(X, Y) = (0, -1)$ the transformed potential takes the form $V(x) = -1 - 3\mathrm{i}x + 3x^2 + \mathrm{i}x^3$. Thus the quadratic term has been increased from $0x^2$ to $3x^2$, rendering the problem essentially a weak perturbation problem, while the perturbing potential has acquired an extra imaginary term $-3\mathrm{i}x$. The resulting series converges quickly, even with a reference potential $3x^2$ (i.e. without any extra renormalization being used). This example shows that the HVPT calculation is actually treating a perturbing potential which includes both linear and cubic imaginary terms, of the type treated in the accurate moment calculations of [39]. It thus seems that the method of the present work should be able to deal with the class of problem treated in [39]; we have accordingly made a few test calculations to check this conjecture. We treated the Hamiltonian $-D^2 + \mathrm{i}x^3 + Ax$, using the shift $(X, Y) = (0, -2)$, for the values $A = 1, 2, 3, 4, 5$ and with no further renormalization procedure (i.e. with $W = VR(2)$). The resulting energies were highly accurate; as in the example of section 3 it turned out that the quickest convergence was for excited states. We quote as an example the energies given for the $n = 3$ state in [39], with the extra digits given by our calculation added

at the end: $A = 1$, $E = 12.736\,497\,38(761\,914)$; $A = 2$, $E = 14.244\,0319(3189\,580)$; $A = 3$, $E = 15.836\,8284(4867\,431)$; $A = 4$, $E = 17.513\,684(19\,055\,618)$. Thus for the real energies the method of the present work seems adequate when using only one parameter, the component Y in the complex shift (X, Y). To attack the problem of the broken PT symmetry states which have complex energies [39] would require a more detailed optimization involving both components X and Y. We have made a few rough preliminary attempts in this direction but so far have only managed to obtain a relatively low accuracy (the first 2 or 3 digits of ER and EI for the complex energies of the form $ER + \mathrm{i}EI$). This particular problem thus requires further work to see whether the shift method is sufficiently flexible to handle the broken symmetry states accurately. Since the shift method is such a simple one, we anticipate that our demonstration of its effectiveness will encourage other workers to use and develop it.

The calculations reported here use a complex variable technique to deal with a complex potential, except for the special case of the equivalent potential associated with the PT symmetric potential $-x^4$. In their discussion of the choice between using a complex PT symmetric potential or its Hermitian equivalent Bender *et al* [40] used a Feynman diagram formalism and for the potential $\mathrm{i}\beta x^3$ were only able to obtain a low order perturbative result, since the full Hermitian equivalent for the potential is not explicitly available. Their general conclusion was that a direct attack on the PT symmetric Hamiltonian is preferable to a detour via an Hermitian equivalent. The calculations of the present work represent such a direct attack; they also show that the CKM is still providing an effective tool for extending the range of problems treatable by perturbation theory.

6. Some theoretical background

As is well known, several of the advances in PT symmetry theory were initially due to purely numerical calculations [e.g. 32, 37] and the present work is intended both to give an effective calculational method and to suggest another topic for mathematical investigation. The present author is more experienced in the construction of efficient algorithms and programs than in formal spectral theory but frequently uses the results of that theory to suggest fruitful topics for numerical investigation.

The calculations of this paper were stimulated both by the many previously published numerical results using a range of techniques to treat the cubically perturbed oscillator and by the results and ideas contained in several papers in spectral theory. The first two of these papers [41, 42] discussed the resonances for odd perturbations of the harmonic oscillator. For the special case of a perturbation $(\beta R + \mathrm{i}\,\beta I)x^3$ of the harmonic oscillator the theoretical conclusion was that for non-zero imaginary part βI the perturbed system remains discrete, as was that of the unperturbed oscillator (thus a spectral concentration effect is not involved). This discrete energy is obtainable (by a summation method) from the divergent Rayleigh–Schrödinger perturbation theory and admits an analytic continuation to $\beta I = 0$, where it can be interpreted as a resonance of the perturbed problem. In the other numerical works cited in the present paper only the cases $\beta R = 0$ or $\beta I = 0$ were studied. However, the complex HVPT method of this paper is sufficiently flexible to allow the use of a general complex β. A few trial calculations with fixed βR and gradually decreasing βI showed that the complex energy obtained by the shift method of this paper moves smoothly towards the $\beta I = 0$ results. It is even possible to estimate the first few complex coefficients in a perturbation series in βI for the complex energy $E(\beta R + \mathrm{i}\,\beta I)$ around $\beta I = 0$. Another relevant work [43] leads to the conclusion (for the cases treated in the present work) that the real positive spectrum of a harmonic oscillator remains real and positive for a perturbation $\alpha\,\mathrm{i}\,x^3 + \gamma\,\mathrm{i}x$, provided that α

is non-zero and that the product $\alpha\gamma$ is non-negative. The numerical results of our calculations are in accord with this theoretical conclusion.

The operation of combining a complex coordinate shift with a complex W parameter which is used in the calculations reported here can be regarded as a special case of the general conformal mapping approach which was developed in [44–46] in order to improve the convergence properties of power series. The formal approach of these three papers shows how the choice of the optimal conformal mapping is related to the way in which the mapping displaces the singularities of the underlying function represented by the series (since the radius of convergence is determined by the distance of the nearest singularity from the origin used for the series expansion). The approach of the present paper has, of course, been empirical, using a numerical search for the shift and W values which gave accurate energies.

The present work shows that a generalized form of complex HVPT can reproduce (and improve on) the numerical results for several problems which have been treated by a range of different methods in the literature. When it is recalled that the underlying simple complexification approach has been equally effective in matrix calculations and in moment method calculations [47, 48], it is hardly likely that this impressive range of results can be accidental. The present author believes that the common thread throughout this group of calculations is that they are all in some sense exploiting an equivalence to the complex rotation method, which in many cases has turned out to be effective far beyond the regions in which it is formally justified by the original Balslev–Combes theory. The question of why the shift method works for the family of cubic potentials studied in this paper has been at least partially answered by inspecting the detailed numerical consequences at various stages of the computations. The principal reason for the success of the method in numerical terms is that it converts an initial strong perturbation problem into a weak perturbation problem by increasing the magnitude of the unperturbed harmonic term in the transformed Hamiltonian.

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