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LETTER TO THE EDITOR

A complex variable form of the HEG technique**John P Killingbeck¹, Alain Grosjean² and Georges Jolicard²**¹ Mathematics Department, University of Hull, Hull HU6 7RX, UK² Laboratoire d'Astrophysique de l'Observatoire de Besançon (CNRS, UMR 6091),
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Online at stacks.iop.org/JPhysA/38/L695**Abstract**

A previously reported simple method for calculating complex matrix eigenvalues is modified to incorporate the traditional HEG approach for the case of even parity potentials. Two examples of resonance calculations are given. Our matrix and perturbation results agree with each other, but are not in full accord with previously published results for one of the test potentials. New results are given for the resonances of the inverted Gaussian potential.

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Two recent works [1, 2] have explained the 'naive' complex variable form of two traditional computational methods (hypervirial perturbation theory and matrix diagonalization) for the calculation of the resonances of perturbed oscillator systems. In the 'naive' approach, the usual perturbation or matrix method is applied within a basis of harmonic oscillator states referring to an oscillator with the potential term Wx^2 . In every formula in which the parameter W appears, a complex W value $WR + iWI$ is used and all other quantities appearing in the calculation are allowed to take complex values. That this simple approach in the matrix case could be as effective in calculating resonances as the more common full complex rotation approach was suggested long ago [3]; the calculations of resonances in [1, 2] illustrated this for several problems which had previously been treated using more complicated techniques. The problems treated in [1, 2] involved perturbed oscillators with single-term x^3 and x^4 perturbations. This letter treats two smooth perturbations which are represented by infinite series. We combine a complex variable approach with an early forerunner of discrete variable methods, the method of Harris, Engerholm and Gwinn [4]. The complex variable form of the HEG approach is easily obtained by applying the complex matrix technique described in [2], together with a slight modification which is described below.

The original HEG approach [4] used a matrix transformation to diagonalize the matrix of the coordinate x and then back-transformed the resulting diagonal matrix of the potential $V(x)$. Our procedure is slightly different, partly because of the even parity of the Hamiltonians which we are considering. First, we take as a complex basis set the even or odd eigenfunctions

of the Hamiltonian $T + (\text{WR} + i\text{WI})x^2$ and set up the matrices of x^2 and $T = -D^2$. Then we apply the complex similarity transformation method of [2] to diagonalize the x^2 matrix, while at the same time subjecting the T matrix to the same transformation. The diagonal matrix of the potential $V(x^2)$ is then produced by appropriate substitution along the diagonal of the x^2 matrix. The resulting $V(x^2)$ matrix is then added to the transformed T matrix to give the Hamiltonian matrix (with no back-transformation). The resulting matrix is diagonalized to produce the final set of complex energies. Experience with the numerical calculations revealed the value of two modifications of the simple method reported in [2]. Since the HEG approach requires the x^2 matrix to be totally diagonal, it is important to ensure that the sum of the off-diagonal elements in every column is reduced to a very small value. Experience shows that sometimes one or two ‘stubborn’ columns freeze their sum at a non-zero value and so prevent full convergence. In all cases encountered, this problem was resolved by adding two or three cycles of transformation with the parameter SF defined in [2] being set at zero. If in the final diagonalization only the lowest few complex eigenvalues are required then at the second stage it is not obligatory to use the matrix transformation technique. For example, a complex variable form of the Gauss–Seidel iterative approach suffices to extract a few of the low resonances from the final complex $T + V$ matrix, particularly when the sequence of iterates is treated by using the complex variable form of the Wynn algorithm which was found to be effective in the perturbation approach [1].

The first problem treated to test the ‘naive’ complex HEG method was one which has been extensively treated from the point of view of complex resonance energies [5–7] and also via a real variable approach using the concept of spectral concentration [8]. In [5–7], a method was proposed for the accurate calculation of the resonances associated with the Hamiltonian

$$H = -D^2 + x^2 \exp(-v^2 x^2) \quad (1)$$

and a study of the condition numbers of the resonance energies led to the conjecture that for the higher resonances the method of complex rotation might give unreliable results. For the small values of v^2 (0.01 and 0.001) which are used in several of the tables presented in [5], it is possible to apply both the matrix method of [2] and the hypervirial perturbation approach of [1]. It was found that the two methods were in agreement and that they gave results which differed from some of those of [5], even for low-lying resonances (where the criticisms about the limitations of a complex oscillator basis are presumably not applicable). In applying the complex HEG approach, it is, of course, necessary to remember that a diagonal element of the transformed x^2 matrix must be treated as a complex number of the form $X + iY$. Replacing this diagonal element to produce the potential matrix for the (real) potential in equation (1) thus requires replacing $X + iY$ by

$$(X + iY) \exp(-v^2(X + iY)) = \exp(-v^2 X)((XC + YS) + i(YC - XS)), \quad (2)$$

where $C = \cos(v^2 Y)$ and $S = \sin(v^2 Y)$.

In the hypervirial renormalized perturbation theory approach, the complex HVPT method of [1] is applied to the partitioned Hamiltonian

$$\begin{aligned} H &= -D^2 + x^2 \exp(-v^2 x^2) = -D^2 + x^2 + V_2 x^4 + V_3 x^6 + \dots \\ &= -D^2 + W x^2 + \lambda(1 - W)x^2 + \lambda V_2 x^4 + \lambda^2 V_3 x^6 + \dots, \end{aligned} \quad (3)$$

where λ is set equal to 1 in the numerical calculation, as explained in [9].

Tables 1 and 2 show some results for the v^2 values 0.0001 and 0.01, with results from [5] shown for comparison. In both the perturbation and the matrix calculations, the complex parameter $W = \text{WR} + i\text{WI}$ was chosen to make WR equal to the ‘unperturbed’ value $\text{WR} = 1$, while WI was varied over a wide range, both to search for a region of optimum convergence

Table 1. Resonances of even parity for $\nu^2 = 0.01$: (A) present calculation; (B) results of [5].

n	A		B	
	ER	EI	ER	EI
0	0.992 46	0.0	0.9925	0.0
2	4.900 93	0.0	4.9009	0.0
4	8.683 58	0.0	8.6836	0.0
6	12.335 02	0.0	12.3350	0.0
8	15.848 84	0.0	15.8488	0.0
10	19.217 38	0.0	19.2174	0.0
12	22.431 17	0.0	22.4312	0.0
14	25.478 16	0.0	25.4782	0.0
16	28.342 24	0.0	28.3422	0.0
18	31.000 37	0.0	31.0004	0.0
20	33.415 52	6.50 (−7)	33.7512	3.0 (−4)
22	35.509 82	1.355 (−3)	35.5098	1.4 (−3)
24	37.069 32	1.5925 (−1)	37.0693	1.593 (−1)
26	38.375 47	9.346 (−1)	38.7468	1.0004
28	39.789 02	2.033 94	39.8045	2.0367
30	41.234 29	3.319 38	41.2601	3.2488
32	42.687 86	4.757 40	42.6021	4.7565
34	44.138 30	6.328 03	44.1410	6.3314
36	45.578 74	8.017 88	45.6102	8.020 30
38	47.004 58	9.817 26	47.0034	9.8515

and to confirm that a reasonable number of digits are the same over a wide range of WI values. The results quoted are thus very conservative ‘most pessimistic’ values. This approach was considered to be necessary to ensure that the differences between our results and those of [5] are genuine and not an artefact due to a special choice of the complex parameters in our calculations. As an individual example of a result not given in the tables, we may quote our result for the $n = 1$ resonance at $\nu^2 = 0.04$. We calculate this to have a real part of 2.843 057 25, after truncating our result; [5] gives the result 2.824 312. In general, our results vary smoothly with ν^2 and with the state number n , while the ‘anomalous’ results of [5] seem to represent deviations from a smooth behaviour. Where the imaginary part of the energy is given as zero, this indicates that it is typically less than 10^{-12} and so is not stable as WI is varied.

The second problem which we studied was that of the resonances of the inverted Gaussian potential subjected to a power law perturbation:

$$H = -D^2 - 10 \exp(-0.1x^2) - \lambda x^4. \quad (4)$$

Here again, the potential is suitable for treatment by both the perturbation method of [1] and the HEG approach using the matrix eigenvalue method of [2]. The two techniques gave the same results and a selection of the resonance energies is shown in table 3. Several checking calculations were also carried out for the case of a harmonic oscillator perturbed by the term $-\lambda x^4$; in all cases the complex HEG method reported here gave results which agreed to very high precision with those given for this problem in the tables of [1, 2]. In their treatment of spectral concentration, Brown and Eastham [8] commented that for a given ν^2 value in the potential of equation (1), there are only a finite number of points of spectral condensation in the spectrum of the odd parity states of the Hamiltonian. They noted that the presence of these points is related to the values of the complex resonance energies $ER + iEI$ found in [5].

Table 2. Resonances of selected states for $\nu^2 = 0.0001$: (A) present calculation; (B) results of [5].

n	A	B
0	0.999 9250	0.999 925
1	2.999 6250	2.999 677
2	4.999 0248	4.999 025
3	6.998 1246	6.998 125
4	8.996 9242	8.996 924
5	10.995 4235	10.995 877
6	12.993 6226	12.993 623
7	14.991 5213	14.991 344
8	16.989 1196	16.989 119
9	18.986 4174	18.986 242
10	20.983 4148	20.983 418
12	24.976 5078	24.976 502
14	28.968 3982	28.968 399
16	32.959 0855	32.959 086
18	36.948 5693	36.948 571
20	40.936 8493	40.936 844
22	44.923 9248	44.923 925
24	48.909 7957	48.909 797
26	52.894 4613	52.894 462
28	56.877 9213	56.877 922
30	60.860 1753	60.860 175
40	80.753 3396	80.753 321
50	100.616 2884	100.616 298
60	120.448 9676	120.449 097
70	140.251 3227	140.237 430
80	160.002 3299	160.000 434
90	179.764 8408	179.874 965
100	199.475 8931	199.664 121

Table 3. Some resonances for the perturbed inverted Gaussian potential of equation (4) ($WR = 1.0$; $WI = 1.0$).

λ	$n = 0$		$n = 1$	
	ER	EI	ER	EI
0.0	-9.037 639 8798	0.0	-7.191 689 3344	0.0
0.01	-9.046 965 7444	2.206 822 (-7)	-7.246 633 8687	6.769 099 (-5)
0.02	-9.056 982 9644	2.574 034 (-5)	-7.312 539 7507	3.420 164 (-3)
0.03	-9.067 950 2211	2.699 506 (-4)	-7.388 431 6838	2.027 596 (-2)
0.04	-9.079 987 3698	1.158 950 (-3)	-7.463 883 1819	5.474 928 (-2)
0.05	-9.092 923 8655	3.155 366 (-3)	-7.531 286 0559	1.022 625 (-1)
0.06	-9.106 375 5455	6.556 980 (-3)	-7.588 602 2560	1.570 888 (-1)
0.07	-9.119 903 7580	1.143 983 (-2)	-7.636 454 8008	2.152 353 (-1)
0.08	-9.133 131 0187	1.770 689 (-2)	-7.676 207 0180	2.743 216 (-1)

Beyond a certain threshold ER value, the EI values increase rapidly. This rapid departure of the resonance energies from the real axis prevents the appearance of a spectral concentration on the real axis. Table 4 shows for $\nu^2 = 0.02$ how the complex resonances found by our

Table 4. Complex resonances (B) and spectral concentration points (A) (from [8]) for the potential of equation (1) at $\nu^2 = 0.02$ (WR = 1; WI = 1).

n	A		B	
	E	ER	ER	EI
1	2.92	2.923 39		0.0
3	6.61	6.606 93		0.0
5	10.01	10.010 69		0.0
7	13.10	13.097 40		3.0 (−9)
9	15.80	15.801 97		1.20 (−5)
11	–	17.947 23		2.50 (−2)
13	–	19.378 12		5.95 (−1)

calculations (both perturbation and matrix) compare with the spectral concentration points found in [8]. The phenomenon described in [8] is clearly visible.

The specimen results given in this letter show that the complex matrix method of [2] can be effectively combined with the HEG approach to deal with the resonances arising from smooth perturbations of the harmonic oscillator. It should be noted that the numerical results given in the tables have been presented in a compact manner, for ease of display and comparison. Most of the results are severe truncations of results which were calculable to several more decimal digits by the techniques set out in this letter.

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