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## LETTER TO THE EDITOR

**Complex HVPT and hyperasymptotics****John P Killingbeck<sup>1,2</sup>, Alain Grosjean<sup>2</sup> and Georges Jolicard<sup>2</sup>**<sup>1</sup> Mathematics Department, University of Hull, Hull HU6 7RX, UK<sup>2</sup> Laboratoire d'Astrophysique de l'Observatoire de Besançon (CNRS, UMR 6091),  
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Online at [stacks.iop.org/JPhysA/39/L547](http://stacks.iop.org/JPhysA/39/L547)**Abstract**

Complex hypervirial perturbation theory (HVPT) is applied to the problem of a harmonic oscillator with a perturbation  $gx^3 \exp(i\varphi)$ , for which the traditional Rayleigh–Schödinger perturbation theory has to be supplemented by hyperasymptotics for obtaining accurate resonance energies in the negative  $\varphi$  region. Complex HVPT gives accurate results for positive  $\varphi$  and for negative  $\varphi$  up to about  $|\varphi| = \frac{\pi}{24}$ . The case of a quartic perturbed oscillator is also treated.

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In their work on the harmonic oscillator with a cubic perturbation  $gx^3 \exp(i\varphi)$  Alvarez and Casares [1] explained the use of hyperasymptotic techniques to correct the perturbation-theoretic complex eigenvalues in the region of negative  $\varphi$ . They pointed out that the use of the traditional (real) perturbation series for the problem would necessarily make  $E(-\varphi)$  be the complex conjugate of  $E(\varphi)$  when a complex perturbation parameter is used. Their complex rotation matrix results indicated, however, that there is an exponentially small extra contribution at negative  $\varphi$  values. They showed how to estimate this contribution by hyperasymptotics. The first point worth noting is that the results of [1] are somewhat better than would be supposed by studying table 2 of [1], since the table takes the [14, 14] Padé approximant estimate at positive  $\varphi$  as the perturbation reference energy at the corresponding negative  $\varphi$  value, whereas it would be more appropriate to take the accurate complex dilatation result at positive  $\varphi$  as the correct ‘sum to infinity’ of the perturbation method. For example, at  $\varphi = -\frac{\pi}{24}$  the use of the correct perturbation reference energy instead of the [14, 14] estimate would correct the quoted perturbation plus hyperasymptotic result at  $g = 0.1$  from  $0.485\,197\,91 + 0.004\,677\,90i$  to  $0.485\,200\,99 + 0.004\,675\,34i$ , which is in close agreement with the quoted complex rotation matrix result,  $0.485\,201\,00 + 0.004\,675\,34i$ . The application of our complex HVPT to the case directly gives the result  $0.485\,200\,996 + 0.004\,675\,342i$ . The complex HVPT has been described previously and applied to several resonance problems [2]; the essential step in the method is the straightforward one of making all of the quantities in the problem complex while using a reference potential of the form  $(WR + iWI)x^2$  in a

renormalized perturbation theory calculation [3]. The method was applied to the Hamiltonian treated in [1]:

$$H = -\frac{1}{2}D^2 + \frac{1}{2}x^2 + gx^3 \exp(i\varphi). \quad (1)$$

The Hamiltonian was written in the partitioned form

$$\left[-\frac{1}{2}D^2 + Wx^2\right] + \lambda\left[\left(\frac{1}{2} - W\right)x^2 + gx^3 \exp(i\varphi)\right]. \quad (2)$$

The usual equations of hypervirial perturbation theory were used [3], except that the real  $W$  of standard theory was replaced throughout by the complex form  $WR + iWI$ , which then means that the other variables (in particular the perturbed energy coefficients) must be allowed to become complex. In the numerical calculations  $\lambda$  is held at the value 1 [3]. The sequence of partial sums of the energy series was treated by a complex variable form of the Wynn algorithm [2] to yield an accurate complex energy. Experience shows that the best choice for  $WR$  is usually the ‘raw’ oscillator coefficient, so  $WR$  was held at the value  $\frac{1}{2}$ . In principle the results can be optimized by varying  $WI$  to give the greatest number of stable digits of output from the Wynn algorithm. For the ground state, the fixed value  $WI = -\frac{1}{2}$  turns out to be reasonably optimal for the range of  $\varphi$  values treated and so the results are reported for the fixed choice  $W = \left(\frac{1}{2}, -\frac{1}{2}\right)$ .

For positive  $\varphi$ , the complex hypervirial method using a perturbation order of 98 (with  $g = 0.1$ ) gives results of very high accuracy; for example at  $\varphi = \frac{\pi}{2}$  it gives the real energy as 0.512 538 145 939 327, while at  $\varphi = 0$  it gives the complex energy as 0.484 315 997 00 + 8.060 211(−6)i. On moving to negative  $\varphi$  values the ‘obvious’ procedure would be to change  $WI$  to  $\frac{1}{2}$ . However, this would give exactly the wrong complex conjugation symmetry between the results for positive and negative  $\varphi$ . Thus the choice  $WI = -\frac{1}{2}$  was retained as  $\varphi$  was moved through zero into the negative region. The surprising result found was that for a reasonable distance into the negative  $\varphi$  region the complex HVPT results were still of considerable accuracy. We used the complex basis matrix approach [4] to check the results; it gives results of up to 16 digit accuracy and agrees (to the number of digits quoted) with the complex dilatation ones quoted in [1, 5]. Table 1 shows the results (truncated for positive  $\varphi$ ), with a sufficiently small interval in  $\varphi$  to reveal the gradual build-up of the exponentially small contribution to the energy which destroys the complex conjugation symmetry between positive and negative  $\varphi$  values. The results of table 1 show that the extra contribution for negative  $\varphi$  is not the usual ‘exponentially small’ type of term which grows very rapidly in some non-analytic manner (like the bound state energy contribution described in section 7 of [3].) The extra contribution  $DR + iDI$  is a smooth function which varies linearly near  $\varphi = 0$ ; the results show that  $DR$  has a maximum in the vicinity of  $|\varphi| = 0.065$ , while  $DI$  has a zero at roughly the same position. The complex energy is a smooth function of  $\varphi$ ; as was emphasized by the authors of [1], the essential feature is the presence of a Stokes line at  $\varphi = 0$ , so that the traditional perturbation series cannot represent the smooth complex energy function on both sides of that line. The complex HVPT can be applied equally well to the excited states, although the accuracy attainable is less than for the ground state. For example, the result obtained for the  $n=1$  resonance at  $\varphi = -0.1$  (with  $g = 0.1$ ) is 1.381 5536 + 0.0390 993i. The results reported here do indicate, however, that the use of the complex variable form of the perturbation theory can provide a direct estimate of the hyperasymptotic corrections worked out in [1] for the Hamiltonian of equation (1). In [5] a method of Borel–Padé summation with complex integration was used to produce complex energies from the Rayleigh–Schrödinger perturbation theory. The complex hypervirial method was checked against the resonance energies given in table 2 of [5] and was found to be able to give 2 or 3 extra decimal digits of accuracy for the complex energy levels quoted in the table for the cubic perturbed oscillator

**Table 1.** The complex HVPT resonance energies for the ground state of the Hamiltonian of equation (1), with  $g = 0.1$ ,  $W = (\frac{1}{2}, -\frac{1}{2})$  and perturbation order 98.  $DR = ER(\varphi) - ER(-\varphi)$  and  $DI = EI(\varphi) + EI(-\varphi)$ .

$\varphi$	$ER$	$EI$	$DR$	$DI$
0.10	0.484 845 0636	-3.604 2792 (-3)	-	-
0.09	0.484 748 8132	-3.257 4455 (-3)	-	-
0.08	0.484 661 6500	-2.090 693 2 (-3)	-	-
0.07	0.484 583 7953	-2.553 0214 (-3)	-	-
0.06	0.484 515 4621	-2.196 0130 (-3)	-	-
0.05	0.484 456 8547	-1.836 2256 (-3)	-	-
0.04	0.484 408 1667	-1.473 9960 (-3)	-	-
0.03	0.484 369 5788	-1.109 6801 (-3)	-	-
0.02	0.484 341 2577	-7.436 5307 (-4)	-	-
0.01	0.484 323 3533	-3.763 0879 (-4)	-	-
0.00	0.484 315 9970	-8.060 2106 (-6)	-	-
-0.01	0.484 319 2988	3.606 6126 (-4)	4.0545 (-6)	-1.564 75 (-5)
-0.02	0.484 333 3451	7.294 0633 (-4)	7.9126 (-6)	-1.424 67 (-5)
-0.03	0.484 358 1957	1.097 7087 (-3)	1.138 31 (-5)	-1.197 14 (-5)
-0.04	0.484 393 8810	1.465 0867 (-3)	1.428 57 (-5)	-8.9093 (-6)
-0.05	0.484 440 3991	1.831 0426 (-3)	1.645 56 (-5)	-5.1830 (-6)
-0.06	0.484 497 7123	2.195 0695 (-3)	1.774 98 (-5)	-9.435 (-7)
-0.07	0.484 565 7441	2.556 6486 (-3)	1.805 12 (-5)	3.6272 (-6)
-0.08	0.484 644 3760	2.915 2553 (-3)	1.727 40 (-5)	8.3231 (-5)
-0.09	0.484 733 4438	3.270 3620 (-3)	1.536 94 (-5)	1.291 65 (-5)
-0.10	0.484 832 7348	3.621 4425 (-3)	1.232 88 (-5)	1.716 33 (-5)

**Table 2.** The complex HVPT resonance energies for the ground state of the Hamiltonian of equation (3), with  $g = 0.02$ ,  $W = (\frac{1}{2}, -\frac{1}{2})$  and perturbation order 98.  $DR = ER(\varphi) - ER(-\varphi)$  and  $DI = EI(\varphi) + EI(-\varphi)$ .

$\varphi$	$ER$	$EI$	$DR$	$DI$
0.14	0.483 940 2106	-2.485 3276 (-3)	-	-
0.12	0.483 883 6453	-2.133 9120 (-3)	-	-
0.10	0.483 835 6137	-1.780 8663 (-3)	-	-
0.08	0.483 796 1882	-1.426 4457 (-3)	-	-
0.06	0.483 765 4307	-1.070 9109 (-3)	-	-
0.04	0.483 743 3922	-7.145 2750 (-4)	-	-
0.02	0.483 730 01121	-3.575 6542 (-4)	-	-
0.00	0.483 725 6176	-2.982 6537 (-7)	-	-
-0.02	0.483 729 9231	3.569 9751 (-4)	1.890 (-7)	-5.6791 (-7)
-0.04	0.483 743 303 00	7.140 4344 (-4)	3.622 (-7)	-4.8406 (-7)
-0.06	0.483 764 9258	1.070 5600 (-3)	5.049 (-7)	-3.5090 (-7)
-0.08	0.483 795 5844	1.426 2676 (-3)	6.038 (-7)	-1.781 (-7)
-0.10	0.483 834 9653	1.780 8877 (-3)	6.484 (-7)	2.140 (-8)
-0.12	0.483 883 0135	2.134 1443 (-3)	6.318 (-7)	2.323 (-7)
-0.14	0.483 939 660	2.485 7647 (-3)	5.507 (-7)	4.371 (-7)

at  $\varphi = 0$ . The main feature of the calculation above is the lack of symmetry between the real parts of the complex energy at  $\varphi$  and  $-\varphi$ . That there will not be perfect complex conjugation symmetry of the FULL complex energy is clear at once, since there is a non-zero  $EI$  at  $\varphi = 0$ , associated with a resonance. Table 2 of [1] gives no perturbation estimate for  $\varphi = 0$

since the simple Rayleigh–Schrödinger perturbation series will give a zero imaginary part for the complex energy at  $\varphi = 0$ . Numerical experiments showed that it is quite easy to apply the complex HVPT to another case for which this perfect complex conjugation is obviously lacking, namely the case of the Hamiltonian:

$$H = -\frac{1}{2}D^2 + \frac{1}{2}x^2 - gx^4 \exp(i\varphi). \quad (3)$$

The behaviour of this Hamiltonian at  $\varphi = 0$  was studied in [6] in connection with the use of dispersion relations in the theory of the perturbed oscillator. We found that the complex HVPT gives accurate complex energies for a wide range values of positive  $g$  at  $\varphi = 0$ ; the results at small  $g$  fit accurately to the non-analytic form  $0.8g^{-\frac{1}{2}} \exp\left(-\frac{1}{3g}\right)$  predicted by the analysis given in [6]. Of more interest, however, is the variation of the complex energy with  $\varphi$  at fixed  $g$ . Table 2 shows the complex HVPT results for the case  $g = 0.02$  and shows that the behaviour of the ground state resonance energy as  $\varphi$  varies is quite similar to that appearing in table 1, provided that the more complicated behaviour in the vicinity of branch points is avoided. In table 2 a sufficient range of  $\varphi$  values is presented to make clear the presence of a minimum in DR as a function of  $\varphi$ , just as was found for the Hamiltonian (1).

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