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ADDENDUM

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John P Killingbeck¹, Alain Grosjean² and Georges Jolicard²

¹ Mathematics Department, University of Hull, Hull HU6 7RX, UK

² Laboratoire d'Astrophysique de l'Observatoire de Besançon (CNRS, UPRES-A 6091),
41 bis Avenue de l'Observatoire, BP 1615, 25010 Besançon Cedex, France

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Abstract

Complex variable hypervirial perturbation theory is applied to the case of oscillator and Coulomb potentials perturbed by a single term potential of the form Vx^n or Vr^n , respectively. The trial calculations reported show that this approach can produce accurate complex energies for resonant states via a simple and speedy calculation and can also be useful in studies of PT symmetry and tunnelling resonance effects.

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The present note is essentially an addendum to a recent survey of the use of standard hypervirial perturbation theory (HVPT) to calculate bound state energy levels and expectation values for several interesting potentials [1]. After completing that work the authors carried out several trial calculations in which the numerical parameters in the theory were allowed to take complex values. The numerical results were surprisingly good and this note sets out some of them, with the intention of encouraging other workers to apply and extend the simple techniques which are described here. The calculation is a numerical 'direct' one; previous authors using perturbation methods for resonant state calculations [2, 3] have applied various ancillary mathematical techniques to derive the imaginary part of the energy from the coefficients of the traditional energy series, which usually needs to be taken to a very high order or to be expressed in an algebraic form so that the n th order term in the energy series appears as a polynomial in the unperturbed energy. Several authors have used the principle that the complex virial theorem should be obeyed in resonant state calculations [4–6]; here the whole system of complex hypervirial relations is taken to be valid. Comparison with the few very high precision results available (e.g. those of [7]) indicates that the complex HVPT actually produces the complex energies of Siegert states. The results of this note were obtained using ordinary double precision and taking the energy series up to between 50th and 80th orders.

Experience with real variable HVPT suggests that the most favourable case to treat will probably be that of an x^4 perturbation of a harmonic oscillator. For renormalized HVPT the Hamiltonian is written as

$$-\alpha D^2 + Ux^2 + \lambda V_4 x^4 = -\alpha D^2 + Wx^2 + \lambda(V_4 x^4 + V_2 x^2) \quad (1)$$

with the numerical values chosen so that $U = W + V_2$ and with the value of λ always set at 1 in numerical computation, so as to avoid the use of factors λ^n when summing the perturbation series. The novelty here is to let U , W , V_2 and V_4 be complex. The details of the calculation are set out in [1] and in many previous works in the existing literature, except that complex rather than real arithmetic has to be used. Programming languages such as Fortran allow directly for complex arithmetic but it is quite straightforward to write paired real and imaginary part equations to replace each equation appearing in the standard real variable HVPT. Apart from standard multiplication and division, the only new complex variable operation required is that of square root extraction, since the unperturbed energy $E(0)$ of the n th energy level will be equal to $(2n + 1)\beta$, where β is the complex square root of $W\alpha$.

The resulting program is a dual-purpose one. With V_2 and V_4 positive we have the usual renormalized HVPT, giving accurate bound state energy levels [1]. If, however, V_4 is small and negative then the use of real U and W values gives real energies which appear to fall off in accuracy as the modulus of V_4 increases; they are the estimates of the real part of the energy of a resonant state. Making $W = WR + iWI$ a complex number leads to real and complex parts of the energy which both achieve reasonable precision; this precision can be increased by varying W to find an optimum value (taken to be that at which the Wynn epsilon analysis of the partial sums gives the greatest number of converged decimal digits). It turns out that finding the optimum W is hardly any problem when the imaginary part of the energy is greater than about 10^{-10} . As the results of the tables show, it suffices to fix WR at the 'unperturbed' value and to vary WI in steps of roughly 10^{-1} ; even keeping WI fixed gives reasonable results (see table 4) because the optima are extremely broad.

Numerical experiment showed that much more accurate results can be obtained by also using a complex variable form of the Wynn epsilon algorithm subroutine which analyses the partial sums of the energy series. Accuracy is lost if the standard real variable epsilon algorithm is used to treat the real and complex sums separately. The optimum W value as found by studying the epsilon algorithm results is often somewhat different from the W value at which the sequence of complex partial sums appears to be showing the best convergence 'by eye'.

Table 1 shows some typical results for the case of the perturbation $-\lambda x^4$. They compare favourably with most of the previous results arising from methods which are considerably more complicated [2, 6–11, 13]. For the special case $\lambda = 1$ the result $E = (0.74775, 0.60998)$ was quoted in [9]; complex HVPT with the choice $W = (1, 9)$ gives $E = (0.7477478335629, 0.609980500214)$. Table 2 shows some results near the λ values at which the real part of the resonance energy for the first three states has a minimum. These minima were barely visible in the low precision result of [8] but were also detected by workers using other methods [2, 10]. Fernandez and Tipping [2] pointed out that the real variable results of [10] for ER are in error; the complex HVPT method indicates that for the lowest resonance the ER results of [10] are low by roughly one quarter of EI at each λ value. Table 3 shows some results for the case of a $-\lambda x^3$ perturbed oscillator. For this case the results are not as accurate as those for the $-\lambda x^4$ perturbation but are better than most available ones [12–15], except for the very accurate results of [5] and a few of those given in [6]. The use of a complex W value in the HVPT appears to be roughly equivalent to the use of a complex rotated coordinate in the usual matrix or finite difference approaches but leads to a simple and

Table 1. The lowest four resonant state energies for $H = -D^2 + x^2 - \lambda x^4$. The roughly optimized W value has $WR = 1$, $WI = 0.25 + 25\lambda$. A perturbation order of 78 was used. Only the $n = 0$ results of [7] is more accurate than those given here.

n	λ	ER	EI
0	0.02	0.984 427 669 765 3	5.1(-14)
	0.04	0.967 451 235 237 0	5.965 307 36(-7)
	0.06	0.948 329 772 671 7	1.119 115 271(-4)
	0.08	0.925 942 461 073 1	1.544 022 1243(-3)
	0.10	0.900 672 904 092 0	6.693 280 8758(-3)
1	0.02	2.920 282 161 311 84	1.799 685 13(-11)
	0.04	2.827 102 639 47	8.902 964 508(-5)
	0.06	2.706 684 874 05	9.058 977 9587(-3)
	0.08	2.567 498 565 886	6.063 364 402(-2)
	0.10	2.448 334 165 653	1.531 950 6041(-1)
2	0.02	4.786 335 047 926 5	2.842 626 27(-9)
	0.04	4.504 482 756 44	4.670 427 977(-3)
	0.06	4.124 540 696 2	1.414 222 438(-1)
	0.08	3.841 131 497 8	4.320 962 285(-1)
	0.10	3.675 255 765 6	7.440 468 74(-1)
3	0.02	6.573 552 560 950 5	2.632 2967(-7)
	0.04	5.909 093 789 6	8.001 416 68(-2)
	0.06	5.286 435 690	6.382 303 70(-1)
	0.08	5.015 750 038 6	1.269 209 0415(0)
	0.10	4.913 363 916 1	1.808 334 6908(0)

Table 2. The complex energy values around the ER minimum for the lowest three states with $H = -D^2 + x^2 - \lambda x^4$. The fixed choice $WR = 1$, $WI = 4$ sufficed for all results, with a perturbation order of 78. The data show that the minima are very close to the λ values 0.537 75, 0.308 15 and 0.182 65.

λ	ER ($n = 0$)		ER ($n = 1$)		ER ($n = 2$)	
	(0.722 54)	λ	(2.151 26)	λ	(3.5019)	λ
0.5375	731 388	0.3079	028 572	0.1824	07 223	
0.5376	730 658	0.3080	019 690	0.1825	06 749	
0.5377	730 410	0.3081	015 257	0.1826	06 518	
0.5378	730 644	0.3082	015 269	0.1827	06 532	
0.5379	731 360	0.3083	019 720	0.1828	06 789	

speedy calculation. We discovered that in table 1 of [12] the $n = 2$ result for $\lambda = 0.034$ is omitted, so that the quoted energies for the states $n = 2$ and 3 actually refer to the states $n = 3$ and 4.

The complex HVPT has also been tested for the case of the perturbations λr and λr^2 acting on the unperturbed Coulomb Hamiltonian. For this case the renormalized Hamiltonian takes the form

$$-\alpha D^2 - Zr^{-1} + \lambda V_p r^p = -\alpha D^2 - Z_0 r^{-1} + \lambda(V_p r^p + V_{-1} r^{-1}). \tag{2}$$

The basic equations for the calculation were set out in [1]; all that is required is to set out the relevant equations with a real and imaginary part pair of equations to replace each real variable equation in the standard HVPT formalism. The λr^2 perturbation with small positive λ is of interest in the theory of the quadratic Zeeman effect, since for the 1s state the full magnetic perturbation $\lambda(x^2 + y^2)$ can be replaced by $(2/3)\lambda r^2$ to calculate the energy level displacement caused by the magnetic mixing with all higher s type bound state and continuum

Table 3. The lowest four resonant states for $H = -D^2 + 0.25x^2 - \lambda x^3$, for the three λ values used in [6, 12, 14]. The fixed values $WR = 0.25$, $WI = 0.3$ sufficed to obtain greater accuracy than previous results, except for two $n = 0$ results in [6] and the results of [5].

λ	n	ER	EI
0.03	0	0.489 194 714 05	5.537 1 (-8)
	1	1.422 922 457	4.094 1(-5)
	2	2.250 199 8	7.406 4(-3)
	3	2.923 360	1.391 42(-1)
	4	3.618 943	4.688 2(-1)
0.034	0	0.485 679 371 77	2.866 98 (-6)
	1	1.391 574 84	1.341 93(-3)
	2	2.132 136	6.876 23(-2)
	3	2.817 874	3.639 74(-1)
	4	3.586 675	7.772 57(-1)
0.0481	0	0.465 163 672 4	2.262 724(-3)
	1	1.243 100 3	1.132 580(-1)
	2	1.999 877	5.048 11(-1)
	3	2.857 867	1.016 774(0)
	4	3.778 681	1.592 917(0)

Table 4. The lowest resonant state energy for $H = -0.5D^2 - 1/r - \lambda r^p$. For $P = 1$, the choice $Z_0R = 1$, $Z_0I = 0.3 + 5\lambda$ was used. For $P = 2$ both parts of Z_0 were crudely held at the value 1. The perturbation order used was low, 56 for $P = 1$ and 47 for $P = 2$. The results for $P = 1$ are in accord with the highly accurate results of [25].

P	λ	ER	EI
1	0.02	-0.530 663 983 531 828	2.781(-12)
	0.04	-0.563 067 242 935 4	9.607 326 7(-6)
	0.06	-0.598 479 496 219	7.974 050 0(-4)
	0.08	-0.636 534 339 52	5.085 202 5(-3)
	0.10	-0.674 574 135 7	1.346 928 83(-2)
2	0.01	-0.535 047 13	2.223 438(-3)
	0.02	-0.571 711 8	1.691 49(-2)
	0.03	-0.601 622	3.731 7(-2)
	0.04	-0.626 370	5.897 7(-2)
	0.05	-0.647 538	8.062 8(-2)

basis functions [1]. For small positive λ HVPT can thus be used to obtain fairly accurate energy levels for the hydrogen atom in a weak magnetic field. The results for small negative λ values, however, will lead to the complex energy of a resonant state. A search of the literature shows that the case of positive λ has been treated many times. References [16–18] gave a few results for negative λ but the most accurate results for negative λ are those of [25] for r and those of [26] for r^2 . To the smaller number of digits shown our results for the case $-\lambda r$ agree with the highly accurate ones of [25]; our results for $-\lambda r^2$ do not cover the same range as those of [26]. Table 4 shows a selection of complex HVPT results.

Complex HVPT has also been applied to a few PT symmetric potentials. The numerical results in [19] gave the real energy 0.59492 for the lowest eigenvalue of the Hamiltonian $-D^2 + 0.25x^2 + i\lambda x^3$ with $\lambda = 0.125$. Setting $W = 0.75$ in the complex HVPT gives a real energy of 0.594915 222 77. In [20] the Hamiltonian $-D^2 + ix^3 + \lambda x^2$ was treated, with λ as the perturbation parameter, leading (at $\lambda = 10$) to the lowest energy 3.169 096 16. Using complex HVPT with the ix^3 as the perturbation and $W = 5$ gives an energy of 3.169 096 167 272 528.

Complex HVPT also gives very accurate energies for the lowest few energy levels of the Hamiltonian $-D^2 + x^2 + ix^3$. Even for the extreme case $H = -D^2 + ix^3$ the choice $W = 7.0$ gives the energy 1.156 267, agreeing with [21]. As a further extreme test we computed the real ground state energy for the Hamiltonian $-D^2 + x^2 + 0.2ix^3$ using a complex W value, $W = (1, 0.2)$. The resulting energy had the correct real part 1.025 076 291 878 65 and an imaginary part which had been reduced to roughly 2×10^{-16} by the complex epsilon algorithm.

For the case in which U is negative, corresponding to an unperturbed inverted oscillator, complex HVPT based on an origin at $x = 0$ gives complex energies which apparently refer to what are called tunnelling resonances [22, 23], or barrier resonances [3] in the literature. For $H = -D^2 - 0.5x^2 + \lambda x^4$ Sergeev [22] gave the energy $-0.064 750 96 + i0.517 142 56$ at $\lambda = 0.1$. Complex HVPT (with $W = -1$) gives the improved energy value $-0.064 750 956 687 + i0.517 142 561 6210$ and also gives correctly i times this energy for the complex rotated version $H = -D^2 + x^2 - 0.1ix^3$ [3]. Real HVPT, when applied at the potential minimum for a double well potential, gives the average of the lowest even and odd real eigenvalues [1]. To obtain a real energy from the complex HVPT results based on $x = 0$ requires the use of special algebraic approximants which can use the coefficients of the perturbation series to reveal the real energies which are situated on the second Riemann sheet [3, 22].

The selection of results given in this short note is intended to alert journal readers to the potential value of HVPT for the class of problems treated here. There is clearly a further range of problems which should be approached to test the range of applicability of a complex variable modification of standard perturbational techniques. The obvious next problems to look at are those which involve a smooth analytic potential with quickly convergent power series. A survey of the literature for such problems revealed no application of HVPT in complex form, although Germann and Kais [24] did apply a complex variable form of $1/N$ perturbation theory for the potential $r^2 e^{-r}$ and referred to other works which had also done so. It should also be possible to construct a complex variable form of the general moment perturbation theory which was set out in [27]; non-separable problems would then be treatable. It will also be of interest to see how the complex HVPT handles cases which are amenable to treatment by the powerful method of algebraic approximants [28].

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