

# A Gauss elimination method for resonances

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**Abstract** A Gaussian elimination form of inverse iteration within the complex coordinate approach is shown to produce a simple uniform method of finding both real bound state energies and complex resonant state energies for several problems, which have been treated by a variety of methods in the literature. The energy shift method for expectation values is shown to be a useful diagnostic tool.

**Keywords** Complex matrix · Resonant states · Double wells

## 1 Introduction

Several recent works have shown that the resonant state energies for some systems can be calculated by using a straightforward approach in which the equations appearing in a traditional bound state calculation are modified by the simple procedure of making an imbedded parameter become a complex variable. Thus, for example, the coefficient  $\beta$  in a wavefunction factor of type  $\exp(-\beta x^2/2)$  for perturbed oscillator problems or the coefficient  $Z$  in a wavefunction factor of type  $\exp(-Zr)$  for perturbed hydrogen atom problems are usually varied to optimize the calculation of bound state energies; however, they also make it possible to find complex resonant state energies when they are given complex values. This simple complexification approach has been shown to work for hypervirial perturbation theory (HVPT) [1], for matrix diagonalization

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methods [2] and for the Hill-series method [3]. As a remarkable example of this approach, it has been found that for a perturbed hydrogen atom a simple moment method can give either real Zeeman effect energies (with  $Z$  real) or complex Stark effect energies (with  $Z$  complex) [4].

The traditional complex rotation method for locating resonant state energies involves a rotation of all the operators in the Hamiltonian (including the kinetic energy operator) and leads to a complex symmetric matrix eigenvalue problem. There has been some debate in the previous literature about the situations in which the complex rotation method is equivalent to the more simple complex basis approach [5,6], with the authors of [6] claiming that the complex basis approach is the more fundamental one. However, for analytic potentials it is generally agreed that the matrices for the two approaches are related by a similarity transformation and so lead to identical spectra. As explained in Sect. 2, the complex basis approach is more easy to use and in the present work we use it to look at the problem of finding only a selected few of the eigenvalues of a complex symmetric matrix.

In [2], the complex symmetric matrix was transformed by means of a sequence of simple similarity transformations, which is based on first order perturbation theory and which is similar to the complex Jacobi approach. The method is sufficiently general to work even for non-symmetric matrices but has the disadvantages that it sets out to find the full spectrum and that it fills up the matrix as it proceeds. For many test problems, we only require a few low-lying eigenvalues and are dealing with an initial matrix, which has only a small bandwidth. As a method for solving systems of linear equations, the traditional Gaussian elimination method has the special feature that it preserves both the bandwidth and the symmetry of the initial square matrix during the reduction process. The appropriate way to exploit this property while finding only a few eigenvalues is to extract the eigenvalues and eigencolumns by using a complex version of the Gaussian elimination method to perform inverse iteration on the complex symmetric matrix. By finding  $(H - E)^{-N}Y$  for some starting column and a sufficiently large  $N$  we can extract the eigenvalue closest to  $E$ . Because the matrix bandwidth and symmetry is undisturbed during the process the matrix can be stored in a very compact form. Such an approach is more simple than the use of a complex version of other methods such as the Lanczos method, which, although it finally reduces the matrix to tridiagonal form, would require a filter diagonalization approach and the conversion of the basis set by the operator  $(H - E)^{-1}$  to perform the calculations reported here [7]. For small bandwidths, it is obviously easier to deal with the matrix directly, as we do here.

In the present work, we use our method to find the complex energies of resonant states of real potentials as well as the real energies for PT symmetric potentials. Section 2 describes the method and later sections give results for several systems, some of which have been treated in the previous literature. Section 3 produces both bound and resonant state energies for a triple well system which was recently treated by the Hill-series method. Section 4 treats a PT invariant Hamiltonian, which has been much analysed in the literature and for which broken symmetry effects lead to the presence of both real and complex eigenvalues in the spectrum. Section 5 deals with a cubically perturbed oscillator, which has previously been used as an example of hyperasymptotic analysis. Section 6 shows that our approach can handle some unorthodox types

of resonance. Section 7 deals with only bound states but demonstrates that it is not necessary to use basis functions of definite parity to treat a centrosymmetric potential. The numerical results show an initial quasi-convergence of the eigenvalues to the energy given by HVPT. Section 8 gives a brief discussion.

## 2 The method of calculation

All the systems treated in this work can be handled in a matrix approach by using an harmonic oscillator basis set. The advantage of using the complex basis approach is that it can be implemented by using a very simple prescription; we write down the real energy bound state theory and replace the relevant real parameter throughout by a complex one. Thus, if we use a set of basis functions, which are the eigenfunctions of the reference Hamiltonian

$$H(W) = -\alpha D^2 + Wx^2 \quad (1)$$

then we know that the energy of state  $n$  is  $E_n = (2n+1)(W\alpha)^{1/2}$  and that the coordinate operator  $x$  has the matrix element

$$\langle n | x | n+1 \rangle = (\alpha/4W)^{1/4} (n+1)^{1/2} \quad (2)$$

To handle complex eigenvalue problems we simply make  $W$  complex in the formulae given above. This will require the extraction of complex square and fourth roots to evaluate the constants appearing in the formulae. The matrices for higher powers of  $x$  can be constructed by using the complex form of the algebraic formula for the appropriate matrix element or by direct numerical matrix multiplication. To find the exact matrix elements by matrix multiplication we proceed by avoiding the kind of edge effects which would give only approximations similar to those of the DVR or HEG approaches [2]. Thus, for example, to find the  $x^3$  matrix of  $N \times N$  type we would form the  $x$  matrix of  $(N+3) \times (N+3)$  type and then reduce by 1 the dimension at each step of the multiplications. Alternatively, the final matrix can be computed row by row, using a long row which is filled up with the elements of the desired multiple product, which are then loaded into the matrix. We can illustrate the use of the eigenfunctions of Eq. 1 by showing the partitioning of a typical perturbed oscillator Hamiltonian (for a cubic perturbation):

$$H = -\alpha D^2 + Ux^2 + Vx^3 = \left[ -\alpha D^2 + Wx^2 \right] + (U - W)x^2 + Vx^3 \quad (3)$$

The term in square brackets is diagonal with diagonal elements  $E_n$ , while the matrix elements of  $x^2$  and  $x^3$  are found as explained above. For brevity, Eq. 3 shows the real variable case. For a resonance  $W$  becomes complex (e.g.  $W = WR + i WI$ ), while  $V$  can be real or imaginary depending on the problem studied. Most of the oscillator resonant states treated in the literature issue from states which are initially oscillator bound states before the action of some perturbing potential. For such states, the  $WR$  is usually kept equal to the real value of  $W$ , which is associated with the initial bound

state, with WI being varied; when EI is small this choice suffices to give accurate results. The W value involved is, of course, positive. An unphysical negative value would not produce an initial bound state and would give a non-convergent process.

To search for a complex eigenvalue in the neighbourhood of energy E, we use Gaussian elimination to find a sequence of columns  $X(n)$ , which obey the equation

$$X(n + 1) = (H - E)^{-1} X(n) \quad (4)$$

The calculation proceeds as follows. At each stage, we set  $Y = X(n)$  and then solve the linear equation system  $(H - E)X = Y$  for X using Gaussian elimination. We then set  $X(n + 1) = X$ . In all the calculations reported here it sufficed to use Gaussian elimination without pivoting and with a real E, since the complex arithmetic quickly introduced the imaginary part EI of the sought eigenvalue, which is not very large for the lower eigenvalues. The initial column  $X(0)$  is a column with every element given the real value 1. At each iteration, the obtained column  $X(n + 1)$  is scaled to make its first element equal to the real value 1 and then the current eigenvalue estimate is found by evaluating the first row of the complex product  $HX(n + 1)$ . Since complex arithmetic is being used it is possible to seek faster convergence by using the latest complex E in the E position in Eq. 4; however, this loses the advantage of having a fixed form of the reduced matrix  $(H - E)$  throughout the calculation. After N steps of the process we have obtained  $(H - E)^{-N} X(0)$ , which is dominated by the contribution from the eigenvector with its eigenvalue closest to the E value being used. To find several of the low eigenvalues, E is gradually increased to scan the relevant energy range. There are three ways to check the stability of the results. First, the matrix dimension can be gradually increased to check for a stable convergence to a limit, checking that this limit has a negligible dependence on W. Second, as E is varied in small steps  $\Delta E$  through the scanned region, the same eigenvalue should emerge over several successive steps of E if the calculation is initialized at each step. Third, the reference row for the evaluation of E can be varied to see whether the eigenvalue varies. (The essential point is that the basis function associated with the reference row must make a reasonably large contribution to the eigencolumn).

### 3 An interesting triple well system

A recent study of the complexified form of the Hill-series technique [3] included some calculations for a special triple well Hamiltonian

$$H(g) = -D^2 + x^2 - 2g^2x^4 + g^4x^6 \quad (5)$$

which was introduced in [8] and later used to illustrate how the use of complex coordinates in a matrix diagonalization approach can describe tunnelling effects in bound systems [9]. The Riccati-Padé method can also describe these tunnelling effects [10]. By varying the imbedded parameter  $\beta$  in the factor  $\exp(-\beta x^2/2)$  appearing in the Hill-series formalism, it was found possible to produce both real and complex eigenvalues for  $H(g)$  at small g values. From a physical point of view the resonances can

be regarded as referring to the outwards tunnelling of a wavepacket initially sited in the inner well; from a mathematical point of view they are associated with a complex scaled Hamiltonian [8]. The real eigenvalues are just the energies of the traditional bound states, which would be expected for a potential which rises towards infinity at large  $x$  values. The system described by Eq. 5 thus provides an obvious test for the method of the present work (and the prescription described at the start of Sect. 2). The matrix of  $H(g)$  requires the first three powers of the  $x^2$  matrix for its construction. The matrix elements  $H(J,K)$  with  $K=J$  to  $J+3$  are the only ones needing storage, since the matrix is symmetric and we choose a basis with a definite even or odd parity. With this choice, the compact storage scheme uses a linear array  $HC$  for which the  $H(J, K)$  element is stored at the element  $HC(M)$  such that

$$H(J, K) = HC(3J + K - 3) \quad (K = J \text{ to } J + 3) \quad (6)$$

This coding has, of course, to be used in the various matrix operations and a copy of the matrix is used in the elimination process (since this destroys the original matrix). The use of compact storage would make it possible to use very large basis sets for a symmetric matrix with a small bandwidth. Although we only use dimensions up to about 200 in our examples, the approach avoids the large number of arithmetic operations involved in our previous method [2] and so is less subject to the effects of rounding errors when ordinary double precision is used. The full power of the compact matrix operations is obviously not needed for the case of the smooth potentials treated here but is necessary for handling singular perturbations of the oscillator, where it makes basis sizes of up to 20,000 attainable in a simple procedure (work in preparation). Numerical calculations showed that the complex resonance energies  $E = ER + i EI$  with  $ER$  close to 1, as given in Table 3 of [3], were given to double precision by using the complex  $W$  value  $(WR, WI) = (1, 15)$ . The bound state energies of Table 4 of [3] were found by using  $(WR, WI) = (1, 0)$ . For these two cases, an even parity basis set was used. We continued the calculation to give extra resonances which were not studied in previous works. The lowest four resonances found are shown in Table 1 for several  $g$  values. The barrier between the inner and outer well has a height equal to  $(4/27g^2)$ ; the value of  $EI$  increases markedly as  $ER$  passes through that value. A calculation using complex HVPT [1], although less accurate, agreed well with the matrix calculations. This auxiliary perturbation calculation can identify the particular state from which a resonance arises and so indicate the region of  $E$  to scan in the matrix calculation. Table 2 shows some real bound state energies found for several  $g$  values by setting  $(WR, WI) = (1, 0)$ . The states with an energy close to 2 were found by noting that at the outer minimum the potential has a leading term  $4x^2$ . It thus seems likely that they are associated with localized states in the outer well. That this is so was confirmed in two different ways. First, an HVPT calculation with its origin at the centre of the outer well (and using the Taylor expansion of the potential about that point) gave energies, which agree closely with those obtained from the matrix calculation. Second, within the matrix calculation itself the small perturbing term  $0.0005x^2$  was in turn added to and subtracted from the potential; the perturbed eigenvalue was calculated for each case. The results then gave an accurate estimate of the expectation value  $\langle x^2 \rangle = dE/dV_2$  and the result indicated that the wavefunction

**Table 1** The lowest three resonance state energies for the Hamiltonian  $H(g)$  of Eq. 6, obtained using  $W=(1, 15)$  and a matrix dimension of 150

$g$	P	ER	EI
0.20	E	0.9325571582478	7.94775543926(-5)
	O	2.6156743444473	1.21030060549(-2)
	E	3.8713869659323	1.99483314620(-1)
0.24	E	0.8944205532099	2.42463284005(-3)
	O	2.3894780354803	1.11999490115(-1)
	E	3.4581087741326	6.60180783826(-1)
0.28	E	0.8433344239234	1.59158594653(-2)
	O	2.1950967814330	3.02661677759(-1)
	E	3.2043949873518	1.18854425437(0)

The parity P is either even (E) or odd (O)

**Table 2** The lowest four bound state energies for the Hamiltonian  $H(g)$  of Eq. 6, obtained by using  $W=(1, 0)$  and matrix dimension 150

$g$	P	E	$\langle x^2 \rangle$
0.20	E	0.93247629196422	0.596
	O	1.81996584353442	22.315
	E	1.82258016776947	22.423
	O	2.62828330994496	2.438
0.24	E	0.89204244181975	0.768
	O	1.69073242323339	13.508
	E	1.73636556408804	14.348
	O	2.53097937792111	4.093
0.28	E	0.82917630720481	1.121
	O	1.53456526498005	8.495
	E	1.70854344684062	9.587
	O	2.64073480349469	4.817

The parity labels are as in Table 1. The  $\langle x^2 \rangle$  values are found by the energy shift method

is indeed concentrated near the centre of the outer well. This energy shift approach to finding expectation values is widely applicable and here is an efficient alternative to the traditional method of working out  $\langle x^2 \rangle$  by using the matrix of  $x^2$  together with the eigencolumn, particularly since the eigencolumn would have to be normalized in a preliminary step.

#### 4 A system with PT invariance

The Schrödinger equation

$$\left(-D^2 + Aix^3 + Bix\right)\Psi = (ER + iEI)\Psi \quad (7)$$

has been studied by several authors (e.g. [11, 12]). The PT symmetry of the operator in Eq. 7 suggests that the eigenvalues can be real (with  $EI=0$ ). When  $B=0$ , the spectrum is indeed entirely real but for non-zero  $B$  it is possible to have complex eigenvalues, as demonstrated numerically in the moment method calculations of [11]. It is thus a suitable test for the method of this work to see whether it can describe both the real eigenvalues and the complex symmetry breaking eigenvalues for the operator in Eq. 7, by analogy with the way in which it gave both real and complex eigenvalues for the

**Table 3** Low lying eigenvalues for the operator  $-D^2 + Aix^3 + Bix$ , calculated by using a  $W$  value of (1, 15) and a matrix dimension of 150 with an even parity basis

	A	B	ER	EI
Three broken symmetry states with complex energy are shown	1	0	1.15626707198811	
	1	0	4.10922875280966	
	1	0	7.5622738549787	
	1	0	11.3144218201962	
	1	0	15.291553750390	
	1	-3	1.22584757671327	-0.76002247143487
			4.33343983644352	
			7.52519195567867	
	1	-4	1.24865673359469	-1.7617193016512
			3.50876560739555	
			6.37980520633110	
	1	-5	1.34334319874918	-2.9073906160965
			3.43138320167211	
			5.16788868578734	

problem treated in Sect. 3. To set up the matrix, we require the first three powers of the matrix of  $x$ . The  $x^2$  matrix arises because we need to adopt what is essentially a renormalizing approach, in which a term  $-(WR + iWI)x^2$  must be included in the perturbing potential in order to cancel the term, which is implicit in the operator Eq. 2 associated with the basis set. Table 3 shows some typical results for the problem, which are more accurate than those published in previous works. The results for the cases  $A=1$ ,  $B=-3$ ,  $-4$ ,  $-5$  were obtained by gradually increasing  $E$  in the term  $H - E$  of the Gaussian elimination process. If a complex  $W$  is used in an attempt to find a real eigenvalue then the EI value obtained decreases as the iterations proceed, finally oscillating with an amplitude of roughly  $10^{-14}$  at the standard level of double precision which we used. The method of calculating expectation values explained in Sect. 3 can be used for this problem. For example, if we set  $A=-1$  and  $B=0$  (to get a real spectrum) then we can add a very small  $x^2$  perturbing term to the potential to show that for the potential  $Bx^2 - ix^3$  the lowest order correction term for the ground state energy is  $1.9669085B^2$ .

## 5 The cubically perturbed oscillator

Alvarez and Casares [13] described the use of hyperasymptotics to find the complex eigenvalues for the operator

$$H(g, \Phi) = (-1/2) (D^2 + x^2) + gx^3 \exp(i\Phi) \quad (8)$$

Using a complex perturbation parameter in the traditional Rayleigh–Schrödinger perturbation series for the energy would obviously give  $E(g, -\Phi)$  as the complex conjugate of  $E(g, \Phi)$ . However, the authors of [13] pointed out that the presence of a Stokes line at  $\Phi = 0$  means that a hyperasymptotic correction to the perturbative result is needed for negative  $\Phi$  values, so that the complex conjugation symmetry is destroyed. It was later shown that complex HVPT can give these corrected results directly for

**Table 4** Groundstate complex eigenvalues for the cubic perturbed oscillator with the Hamiltonian  $H(g, \Phi)$  given in Eq. 8, for  $g = 0.1$

$\Phi$	ER	EI
-0.10	0.4848327348572	3.621442463000(-3)
-0.08	0.4846443760119	2.91525529968(-3)
-0.06	0.4844977122642	2.19506948166(-3)
-0.04	0.4843938809947	1.46508620844(-3)
-0.02	0.4843333450837	7.29406327924(-4)
0.00	0.4843159970041	-8.06020950000(-6)
0.02	0.4843412576766	-7.43653067984(-4)
0.04	0.4844081666578	-1.47399596288(-3)
0.06	0.4845154620899	-2.19601304015(-3)
0.08	0.4846616500444	-2.90693218571(-3)
0.10	0.4848450636272	-3.60427916939(-3)

An even parity basis with  $W$  set equal to (0.5, 0.5) was used, with a matrix dimension of 150

some distance into the negative  $\Phi$  region [14]. Table 4 shows results obtained by the Gaussian elimination method at  $g = 0.1$ . Although, as explained in the introduction, the complex coordinate method is equivalent to (though more simple than) the complex scaling matrix method used to obtain reference values in [13], our results are more accurate than those given in [13] and cover a finer grid of values of the angle  $\Phi$ .

## 6 Some unorthodox resonances

In [15], some complex energies were calculated for the Hamiltonian

$$H(A, B) = -D^2 + x^M - \lambda x^N \quad (9)$$

The most commonly studied case in the literature is that with  $M = 2$  and  $N = 4$  but in [15] the case  $M = 4$ ,  $N = 6$  was also discussed. Table 5 shows some results for two sets of  $(M, N)$  values, as obtained by the Gaussian elimination method. For negative  $\lambda$  values, of course, bound states exist and the use of a real  $W$  value in the basis set can produce these.

## 7 Symmetry and the double well problem

All the preceding examples studied in this work have involved complex resonances but our final example deals with the ordinary bound states associated with the double well Hamiltonian

$$H(\lambda) = -D^2 - x^2 + \left(\lambda^2/2\right)x^4 \quad (10)$$

When  $\lambda$  is small, this Hamiltonian will have close pairs of states of opposite parity at the bottom of its spectrum. The dominant tradition in matrix approaches is to use the symmetry centre  $x = 0$  as origin and so to build the even or odd parity directly into the basis functions used to set up the matrix of the Hamiltonian. Thus, for example, by using an oscillator basis with  $W = (1, 0)$  in separate even and odd parity calculations



**Table 5** The lowest even and odd parity resonances for the operator  $-D^2 + x^M - \lambda x^N$ , calculated using  $W = (1, 1)$  and matrix dimension 150

M	N	$\lambda$	ER	EI
2	6	0.02	0.9520462653053309	1.402573778245021(-2)
2	6	0.02	2.712788208122200	2.013898488709008(-1)
2	6	0.04	0.9193107387010802	5.273643153667654(-2)
2	6	0.04	2.654858021276504	4.633716332349316(-1)
2	6	0.06	0.9033613239572396	9.127664934058118(-2)
2	6	0.06	2.660081776872349	6.557404144178417(-1)
2	6	0.08	0.8958197460011326	1.254636428092339(-1)
2	6	0.08	2.682850763658098	8.064038265203445(-1)
2	6	0.10	0.8927457964926816	1.555432433598369(-1)
2	6	0.10	2.711585309963890	9.306087123690415(-1)
4	6	0.00	1.060362090484183	0.0
4	6	0.00	3.699156060168530	0.0
4	6	0.04	1.038002353717577	0.0
4	6	0.04	3.699156060168530	0.0
4	6	0.08	1.012731445721011	6.25221492542814(-8)
4	6	0.08	3.581700216602671	1.288075605381661(-6)
4	6	0.12	0.9826725857365955	1.594662368407940(-4)
4	6	0.12	3.431460367418278	2.739336833818093(-3)
4	6	0.16	0.9440969584873676	3.992421290169972(-3)
4	6	0.16	3.22859327560889	5.18915247310509(-2)
4	6	0.20	0.8995394462905228	2.019133790314381(-2)
4	6	0.20	3.036336773026575	1.920564090658734(-1)

The even parity state energy is given first

based on the  $x = 0$  origin, our method gives the low lying pairs of levels. Some authors keep the origin at  $x = 0$  but use a basis which consists of even or odd combinations of oscillator functions centred at the well minima at  $x = 1/\lambda$  and  $x = -1/\lambda$  [16]. While such basis functions show a strong resemblance to the actual eigenfunctions they have the disadvantage of being non-orthogonal, which complicates the matrix eigenvalue problem. We tried a calculation in which only the oscillator functions centred on  $x = 1/\lambda$  were used, to see whether the potential itself would introduce the centrosymmetry into the basis and generate the correct partner peak on the other side of the origin. To perform this calculation with the point  $x = 1/\lambda$  as origin we need to use the correct potential, which has admixtures of both even and odd parity. It is found by performing the Taylor expansion at  $x = 1/\lambda$  of the potential appearing in Eq. 10 and takes the form

$$V = -\left(1/2\lambda^2\right) + 2x^2 + 2\lambda x^3 + \left(\lambda^2/2\right) x^4 \tag{11}$$

This potential naturally suggests the choice  $W = (2, 0)$  for the basis functions, with both even and odd functions being included in the basis. Table 6 shows the results obtained; as the dimension is increased the energies tend correctly to those for the lowest even and odd pair of levels. This effect is explainable in terms of the specially favourable properties of harmonic oscillator basis functions. The virial theorem shows that the value of  $\langle x^2 \rangle$  for an oscillator function is proportional to its energy, i.e. is proportional to  $2n + 1$ . Thus, as more functions are added to the basis set, we reach a stage at which the the basis functions can have an appreciable overlap with the

**Table 6** Energy levels for the double well Hamiltonian using the potential of Eq. 11, with origin at  $x = 1/\lambda$ , for the cases  $\lambda = 0.3$  and  $\lambda = 0.4$ , as a function of the matrix dimension ND

ND	$E(0.3)$	$E(0.4)$
10	-4.1902095978175	-1.8054955213226
20	-4.1902336009106	-1.8068973696846
30	-4.1902339345051	-1.7751402016719
		-1.8207465095929
40	-4.1902342389732	-1.7847047589878
		-1.8267498723262
50	-4.1902508125434	-1.7847050286351
		-1.8267501124629
60	-4.1899127461966	-1.7847050286292
	-4.1905545952753	-1.8267501124656
70	-4.1899128809639	-1.7847050286292
	-4.1905545952753	-1.8267501124656
80	-4.1899128809648	-1.7847050186292
	-4.1905545952761	-1.8267501124656

The E scanning regions used are  $(-4.3, -4.1)$  for  $\lambda = 0.3$  and  $(-1.9, -1.7)$  for  $\lambda = 0.4$ , in steps DE of 0.02

region in the opposite well and so make it possible to describe the partner peak in the wavefunction. This physical argument describes quite well what happens in the numerical calculation. To establish that the correct lowest eigenvalue is indeed associated with the “double peak” symmetric wavefunction we can add small  $x$  and  $x^2$  terms to the potential, as explained previously, to find  $\langle x \rangle$  and  $\langle x^2 \rangle$  and so reveal the presence of the second peak at a distance of about  $2/\lambda$  from our origin at the point  $x = 1/\lambda$ .

An interesting extra effect appeared in the numerical results. For the deeper well (with  $\lambda = 0.3$ ), the results of Table 6 show that the single eigenvalue near  $-4.2$  reaches a semi-converged value of roughly  $-4.190234$  as the matrix dimension increases. This energy is the average of the correct lowest even and odd state energies and is also the energy obtained when a hypervirial perturbation calculation is performed using the potential in Eq. 11. As the matrix dimension is increased further, the original single level eventually begins to descend (to become the lowest level) and is then joined by a level, which moves down from above to form the upper level of the lowest lying doublet. Many years ago Seznec and Zinn-Justin [17] suggested that perturbation theory based on the well centre should give an energy close to the average of the even and odd state energies, and HVPT does this. It would be an interesting calculation (albeit requiring very high precision) to see what trajectory would be followed by the lowest eigenvalue given by a matrix-based perturbation approach which uses exactly the same matrix elements as those of the matrix diagonalization approach based on  $x = 1/\lambda$ . In particular, one could ask whether at a sufficiently high order the perturbation approach would “break through” the region of semi-convergence and descend with the true matrix eigenvalue so as to arrive at the correct even parity ground state energy.

## 8 Conclusion

The results for the specimen systems studied in this work show that by combining Gaussian elimination with inverse iteration using complex basis functions we can

make an accurate study of either real or complex eigenvalues in a desired region of the spectrum while retaining the small bandwidth of the Hamiltonian matrix, which is characteristic of many of the systems, which have been studied by various different methods in the literature. For systems which can have broken PT symmetry the ability to handle both real and complex energies by simple adjusting the reference parameter  $W$  is particularly useful. The relationship between a perturbation approach and the unexpected semi-convergence of the matrix eigenvalues for the double well problem, which were found in Sect. 7 is clearly something which merits further investigation.

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