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## LETTER TO THE EDITOR

**A simple method for complex eigenvalues****John P Killingbeck<sup>1</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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**Abstract**

A simple iterative method is described for finding the eigenvalues of a general square complex matrix. Several numerical examples involving complex symmetric matrices are treated. In particular, it is found that a naive matrix calculation without complex rotation produces resonant state energies in accord with those given by the recently introduced naive complex hypervirial perturbation theory.

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A recent review of a matrix approach to wave operator theory [1] described the recursive distorted wave approximation (RDWA) and the single cycle method (SCM) for the solution of the nonlinear matrix equations for the Bloch wave operator. The present letter sets out for the first time a method which arose from the numerical calculations in that review and which has since been tested by several numerical experiments. The method is probably the most simple one yet devised to find the eigenvalues of a complex square matrix; it is even more simple than the complex extensions of the Jacobi method which have been proposed [2, 3] and it involves only the traditional first-order formula of Rayleigh–Schrödinger perturbation theory.

The basic idea of the method is to use an iterative process which applies a sequence of spectrum-preserving similarity transformations to the complex matrix  $H$ , with the aim of ultimately transforming it to diagonal form. If the transforming matrix is written as  $I + X$ , where  $I$  is the unit matrix and  $X$  has only off-diagonal elements, then the transformation involved at a given step is

$$H \longrightarrow (I + X)^{-1} H (I + X). \quad (1)$$

A little algebra shows that the inverse  $(I + X)^{-1}$  appearing in equation (1) can be written in the form  $(I - X)(I - X^2)^{-1}$ . In an early real variable approach to the iterative use of

similarity transformations [4], the  $X$  used was a full off-diagonal matrix; thus a full matrix inversion was needed at each step of the iterative process described in [4]. To produce a speedy iterative calculation, it is better to follow the tradition in wave operator theory [1] by choosing an  $X$  which obeys the equation  $X^2 = 0$  at each step of the iteration.  $(I + X)^{-1}$  then becomes  $(I - X)$  and only matrix multiplication is required in equation (1). It can quickly be verified that if  $X$  is a single off-diagonal element or even a column of off-diagonal elements then the condition  $X^2 = 0$  is satisfied. Numerical experience has shown [5] that the first choice leads to better convergence properties; each 'single element' transformation modifies the environment for the next one, giving a cooperative effect which leads to quicker convergence. The valuable further discovery reported here is that this cooperative effect is even further enhanced if the 'single element' transformations scan the *whole* off-diagonal region of the matrix (rather than just a small rectangular part of it, as is the tradition in wave operator theory [1]).

To find the appropriate choice for  $X$  at each step of the iterative process, we can use a simple Dirac notation, which is easier to follow than the classical dyadic notation. The product appearing in equation (1) becomes  $(I - X)H(I + X)$  if  $X^2 = 0$ . We take  $X$  to consist of the single non-zero number  $A$  at the position  $(J, K)$ . The required triple product then becomes

$$[I - A|J\rangle\langle K|] \sum_{M,N} H(M, N)|M\rangle\langle N|[I + A|J\rangle\langle K|]. \quad (2)$$

In the  $H(I + X)$  product only the  $N = J$  terms survive in the  $HX$  term and so the total product takes the form:

$$\sum_{M,N} H(M, N)|M\rangle\langle N| + A \sum_M H(M, J)|M\rangle\langle K| \quad (3)$$

which shows that  $A$  times column  $J$  has been added to column  $K$ . In completing the triple product in (2), we note that the term  $-A|J\rangle\langle K|$  only allows terms with  $M = K$  to survive. In words the whole transformation can be described very simply: first add  $A$  times column  $J$  to column  $K$ ; then subtract  $A$  times row  $K$  from row  $J$ . The crucial question is: what happens to the element  $H(J, K)$ ? Tracing this element through the triple product gives

$$H(J, K) \longrightarrow H(J, K) + A[H(J, J) - H(K, K)] - A^2H(K, J). \quad (4)$$

We wish to choose  $A$  so as to render  $H(J, K)$  zero (recalling that we only use elements with  $J \neq K$ ). Numerical experiments have shown that finding  $A$  by treating (4) as a full quadratic equation is less effective than an approach which neglects the second-order term and simply uses the linear approximation:

$$A(J, K) = H(J, K)/[H(K, K) - H(J, J)]. \quad (5)$$

Here the indices  $(J, K)$  have been added to indicate that the  $A$  value is associated with the particular element  $(J, K)$ . In applying the transformations the matrix is scanned sequentially column by column, performing the single element transformations (as described above) down each column, omitting elements  $(J, K)$  for which  $H(J, J) = H(K, K)$  and omitting columns for which the sum of the moduli of the off-diagonal elements is less than a number  $TOL$  (usually  $10^{-12}$ ). To keep the transformation 'small' the  $A(J, K)$  value actually used in the  $(J, K)$  single element transformation is obtained by dividing the number from (5) by  $[1 + SF|A(J, K)|]$ , so as to limit its modulus to be less than  $1/SF$ . The number  $SF$  is set at the initial value  $SFU$  (usually 4 or 5) and is gradually reduced according to the formula:

$$SF = SFU(NACT/ND) \quad (6)$$

where  $NACT$  is the number of active columns (i.e. those which still require to be scanned) and  $ND$  is the dimension of the  $H$  matrix. On each scan every column is checked to see

whether it should be active or not, since ‘revivals’ could in principle be caused by the transformations associated with other columns.

In the formalism described above all the quantities (except  $SF$ ) can be complex and so complex matrices can be treated. At any stage, the diagonal element in an inactive column gives a valid eigenvalue for the matrix. If the final transformation matrix (essentially the right eigenvectors) is required then the  $(I + X)$  parts only of each transformation are applied to a matrix which is initially the unit matrix.

Given the current interest in the complex energies of resonant states and the study of Hamiltonians with  $PT$  symmetry, the simple iterative method for complex matrices described here should be of wide interest and applicability. As an illustrative example, we use the method to settle a problem which has arisen in connection with the recently developed complex variable form of hypervirial perturbation theory ( $HVPT$ ) [6]. This theory simply allows the quantities appearing in traditional renormalized perturbation theory [7] to be complex. For a perturbed oscillator problem, for example, the Hamiltonian would be written as

$$-D^2 + Ux^2 + V_J \lambda x^J = -D^2 + Wx^2 + \lambda[V_J x^J + V_2 x^2]. \quad (7)$$

When the number  $W$  is allowed to be complex it unexpectedly turns out that the complex energies of resonant states for a potential such as, for example,  $x^2 - \lambda x^4$  can be found without introducing the notion of a complex rotation. An interesting problem then arises. In principle the use of a matrix diagonalization of the Hamiltonian, using the basis of oscillator states for the Hamiltonian  $-D^2 + Wx^2$ , should give the same eigenvalues as those which arise from a perturbation approach. However, it is well known that the use of complex rotations is regarded as standard (indeed obligatory) in matrix approaches to resonances. Will a naive complex matrix diagonalization without complex rotation work? The results in the specimen tables of this letter show that it *does* work, simply by making the  $W$  involved in the basis functions be a complex number. That the problem involved is a serious one can be confirmed by noting that for the case of a two-term perturbation of the type  $-V_4 x^4 + V_6 x^6$  preliminary numerical experiments indicate that the perturbation calculation and its associated ‘naive’ matrix calculation do *not* give the same results (it seems that complex rotation really is necessary for the matrix approach to that problem).

The description of the method given above was set out with sufficient care to make it possible for readers to implement it themselves. As a further technical note, we should point out that the complex matrix for the perturbed oscillator Hamiltonians studied was set up by first forming the matrix of  $x$  and then using a complex variable form of nested matrix multiplication to set up the matrix of  $H$ , in a complex number version of the technique described in [8]. Simply replacing a real  $W$  by a complex  $W$  in the standard oscillator formulae involves using a complex continuation of the usual oscillator basis functions. Tables 1 and 2 show matrix results for two problems treated by complex  $HVPT$  in [6]; the results of the two methods agree, except that the matrix approach gives higher accuracy. Table 3 shows some results for a Hamiltonian treated by Alvarez [9], who used complex rotation and searched for an optimum rotation angle. Our results (without complex rotation) agree with his to very high accuracy for the states  $n = 0$  and  $n = 1$  which he treats; accordingly we have given the results for the states  $n = 2$  and  $n = 3$ , which as far as we know have not yet appeared in the literature.

To pick out the resonant states from the matrix spectrum was not difficult for the states treated here; in any doubtful cases, a checking complex  $HVPT$  calculation can be used to confirm that a correct choice has been made.

The applications to resonances studied here are linked (as explained) to those already treated by complex  $HVPT$  [6]. However, since the methods described here and in [6] would

**Table 1.** Resonant state energies for  $H = -D^2 + x^2 - \lambda x^4$ , with the fixed choice  $W = (1, 2)$  for the matrix basis functions. The matrix dimension was gradually increased until convergence for the displayed levels was obtained. The results for the state  $n = 0$  and  $n = 2$  and for  $\lambda = 0.1, 0.2, 0.3$  and  $0.5$  are in accord with those of [15] to the number of digits given in [15].

$\lambda$	$n$	ER	EI
0.1	0	0.900 672 904 092	6.693 280 875 800(-3)
0.2	0	0.794 881 259 6417	8.941 229 506 645(-2)
0.3	0	0.747 533 332 9690	1.901 134 544 866(-1)
0.4	0	0.728 822 270 4051	2.773 516 666 528(-1)
0.5	0	0.722 917 966 8990	3.515 109 888 375(-1)
0.1	1	2.448 334 165 652	1.531 950 604 130(-1)
0.2	1	2.192 903 734 545	6.773 211 281 790(-1)
0.3	1	2.151 412 178 191	1.079 136 316 235(0)
0.4	1	2.165 164 179 279	1.390 463 920 203(0)
0.5	1	2.197 935 183 795	1.645 327 655 904(0)
0.1	2	3.675 255 765 593	7.440 468 742 584(-1)
0.2	2	3.505 179 575 285	1.938 705 455 017(0)
0.3	2	3.591 106 336 645	2.714 658 140 087(0)
0.4	2	3.713 289 298 839	3.296 090 846 404(0)
0.5	2	3.839 404 069 514	3.767 920 202 795(0)

**Table 2.** 'Naive' matrix method results for  $H = -D^2 + 1/4x^2 + \lambda x^3$ , using a basis set with the fixed  $W$  value  $W = (0.25, 0.5)$ . The three  $\lambda$  values are those used by most authors in the literature.

$\lambda$	$n$	ER	EI
0.03	0	0.489 194 714 0504	5.537 124 63(-8)
0.03	1	1.422 922 457 231	4.094 162 126 37(-5)
0.03	2	2.250 199 666 020	7.406 379 930 83(-3)
0.03	3	2.923 360 554 324	1.391 418 351 906(-1)
0.03	4	3.618 941 811 044	4.688 236 258 239(-1)
0.034	0	0.485 679 371 7724	2.866 977 8691(-6)
0.034	1	1.391 574 841 037	1.341 934 012 201(-3)
0.034	2	2.132 135 564 371	6.876 261 021 015(-2)
0.034	3	2.817 874 150 732	3.639 736 670 720(-1)
0.034	4	3.586 674 703 099	7.772 568 840 751(-1)
0.0481	0	0.465 163 672 4277	2.262 723 422 041(-3)
0.0481	1	1.243 100 286 256	1.132 579 639 217(-1)
0.0481	2	1.999 877 445 681	5.0481 115 268 94(-1)
0.0481	3	2.857 867 095 237	1.016 773 861 502(0)
0.0481	4	3.778 681 569 810	1.592 917 151 364(0)

permit *all* the quantities in the problem to be complex, further combined *HVPT* and matrix work is currently being carried out on calculations with or without complex rotations and for several smooth potential described by convergent power series.

As a further test of the simple technique described in this letter, we applied it to the Hamiltonian  $-D^2 + x^4 + iAx$  treated in [10] and found that it correctly shows the appearance of complex conjugate pairs of eigenvalues at critical values of  $A$ , as reported in [10]. The technique also gave a real third excited state energy of 11.314 421 820 19 for the Hamiltonian  $-D^2 - ix^3$ , while the authors of [11] gave the upper and lower bounds 11.314 421 824 and 11.314 421 818. However, it should be noted that the powerful moment techniques developed

**Table 3.** Matrix results for  $H = -1/2D^2 + 1/8x^2 + gx^3$ .  $W$  is held at the value  $W = (0.125, 0.250)$ . The results for the state  $n = 0$  and  $n = 1$  agree with the complex rotation results of [9]. The table shows results for  $n = 2$  and 3, which are not given in [9].

$g$	$n$	ER	EI
0.02	2	1.010 506 816 722	1.271 087 733 661(-1)
0.02	3	1.396 858 157 408	3.375 633 104 266(-1)
0.04	2	1.112 037 640 9941	5.733 799 142 762(-1)
0.04	3	1.661 736 956 999	9.377 546 543 952(-1)
0.06	2	1.129 954 055 8043	8.033 721 113 272(-1)
0.06	3	1.942 482 924 355	1.253 157 108 677(0)
0.08	2	1.456 781 313 592	9.617 819 348 05(-1)
0.08	3	2.181 002 287 79	1.475 821 828 40(0)

in the works [11–14] can produce sequences of upper and lower bounds to desired eigenvalues (real or complex); the present calculation cannot do so but relies instead on the traditional notion that increasing the matrix dimension will ultimately produce a ‘converged’ eigenvalue. For a complex eigenvalue, this notion might not always be reliable, although for the simple one-term perturbations treated here it did operate successfully. The applications of this letter only involved perturbed oscillators, whereas the moment methods can also be applied to potentials involving Coulomb terms in order to yield upper and lower bounds. The complex *HVPT* [6] certainly applies to perturbed Coulomb problems. To apply the matrix approach to them requires either the use of an orthonormal Sturmian or other basis or the use of a non-orthonormal basis together with a straightforward extension of the method of this letter to handle the generalized eigenvalue problem.

As a technique for eigenvalue calculations, the method of this letter should have about the same range of applicability as the complex Jacobi method [2, 3], which essentially uses the arctan of the  $A(J, K)$  of equation (5) in its transformations. The success of the oscillator resonance calculations presented here presumably indicates the existence (for this class of problem) of a continuous family of similarity transformations which connects the usual complex rotated Hamiltonian to the more simple one used here (which simply uses a complex continuation of standard oscillator functions as a basis set). Successful calculations for several other resonance problems have been performed and tend to support this conjecture. A further literature search revealed a previous debate about whether resonances can be calculated by matrix methods without complex rotation [16, 17], although the problems and methods under discussion were more complicated than those presented here.

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