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Resonances for coupled oscillators

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Abstract

A recently developed complexification approach is shown to lead to a dual purpose method which can find bound state or resonance energies for a two-dimensional perturbed oscillator. Several anisotropic resonance effects are treated by the method.

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In a series of recent works it has been shown that resonant state complex energies can be obtained for several traditional model systems by a very simple approach [1–3]. All that is required is to start from a standard perturbation or matrix method which is able to calculate the real bound state energies of a system and then to switch over to a complex variable form of the theory. In a recent work, we have shown that this approach also works for a power series-Hill determinant approach to a perturbed Coulomb system [4]. The systems treated in the cited works were either directly one-dimensional systems or were radial ones in three dimensions. In the present work, we describe an application of the complexification approach to a method which was applied to the bound states of a two-dimensional perturbed oscillator problem [5]. Once again this simple approach works well and reveals some interesting anisotropic effects which can be given an intuitively reasonable physical interpretation and which do not seem to have been discussed in the previous literature. The Hamiltonian which is treated here and in the work [5], published previously in this journal, is the coupled oscillator one

$$H = -\nabla^2 + V(2)(x^2 + y^2) + V(4)(x^4 + y^4) + V(22)x^2y^2. \quad (1)$$

The coupled oscillator basis set used in the calculation is the set of eigenfunctions for the scaled Hamiltonian

$$H(0) = -\nabla^2 + W(x^2 + y^2), \quad (2)$$

with the extra feature that W is allowed to become complex for resonant state calculations. This is achieved by simply using a complex W instead of a real W in the standard equations of the theory. For example the matrix element of x^2 between the states $|n\rangle$ and $|n+2\rangle$ is

$$\langle n|x^2|n+2\rangle = [(n+1)(n+2)]^{\frac{1}{2}} W^{-\frac{1}{2}}. \quad (3)$$

If W is a complex number then the complex numbers $W^{\frac{1}{2}}$ and $W^{-\frac{1}{2}}$ are evaluated just once at the start of the calculation. The large matrix is never explicitly constructed, since, as in [5], an iterative (essentially Gauss–Seidel) method is used to calculate a desired eigenvalue, with the matrix elements required at any stage being found by means of formulae which are stored in a subroutine of the computer program. By exploiting the even or odd $x \leftrightarrow y$ interchange symmetry of many of the eigenstates it is possible to speed up the iterative process by filling in roughly one half of the eigencolumn coefficients when the other half have been calculated. The high symmetry of the Hamiltonian (1) means that only a restricted set of basis functions is needed for a given state, since the chosen reference product function will only be coupled to other functions which obey the appropriate selection rules. The full point group symmetry of the Hamiltonian is C_{4v} [8], but we only exploit the x and y parity and the $x \leftrightarrow y$ interchange symmetry in our calculations.

The iterative process has been described in [5] but we give a brief sketch of it here. The matrix eigenvalue problem can be written in a form which shows the state indices on the product basis of oscillator functions:

$$\sum_{LM} H(JK, LM)X(LM) + H(JK, JK)X(JK) = EX(JK). \quad (4)$$

Here the summation omits the case $LM = JK$. $H(JK, LM)$ is the matrix element $\langle JK|H|LM\rangle$ and so is a sum of terms representing the various operators in the Hamiltonian. The wavefunction is taken in the form $\sum_{JK} X(JK)|JK\rangle$. When the sum in (4) is worked out, the element $X(JK)$ is then found by dividing the sum by $E - H(JK, JK)$. The chosen range of basis state indices is repeatedly scanned, with one chosen element $X(AB)$ being held at the value 1 (or any suitable fixed numerical value which helps to avoid overflow or underflow). After one or more full scans which adjust the other $X(JK)$, the choice $JK = AB$ is made. Equation (3) is then used to find the current E estimate by working out the full left-hand side and dividing by $X(AB)$. This revised E is then used in the next scan over the $X(JK)$. To avoid divergence it is often necessary to incorporate relaxation parameters into the calculation, so that the actual new value of $X(JK)$ or E is taken as a weighted average of the old value and the new value produced by the calculation based on using equation (4) in the iterations. By using sufficiently small relaxation parameters it is possible to treat the lowest fifteen or so states if the perturbing potential is not too strong.

Numerical experiment showed that the application of the Wynn algorithm to the sequence of E values generated by the iterative process gives a sequence of estimates which converges much more quickly than the raw E sequence and so can give a rapid result to 12 or so digits when using standard double precision throughout the computation. This holds for both the bound state and the resonance calculations; the complex form of the Wynn algorithm has already been applied in the perturbation approach to resonances [1]. By the simple process of making W in equation (2) complex and so making the values of E and of the $X(JK)$ complex (with $X(AB)$ still held at a real fixed value) we found that the iterative process leads to the complex energies of resonant states. Since there does not seem to be a wide range of previous results available, we took care to check the validity of the calculation by applying it to many cases which reduce to either equivalent one-dimensional or radial resonance problems, for which the complex hypervirial perturbation method can give accurate comparison results for any new test problems which are devised. The calculation described in this work is a dual purpose one, since with W real we can also apply it to the bound states of (1), which have already been treated [5–7]. In all cases, both bound states and resonances, we found very close agreement with previous results acknowledged to be of high accuracy. This gives us confidence that the simple complexified iterative method used here will be able to handle

Table 1. Energies and $\langle x^2y^2 \rangle$ values for the degenerate bound states arising from the $(0, 2, o)$ and $(1, 1, e)$ oscillator states, for several potentials with spherical symmetry. The W value $(2, 0)$ was used, with a product basis of dimension 50×50 . The $\langle x^2y^2 \rangle$ values for the two states have the fixed ratio 3 throughout.

$V(2), V(4)$	E	$\langle x^2y^2 \rangle$ (1, 1, e)	$\langle x^2y^2 \rangle$ (0, 2, o)
1, 0	6	2.25	0.75
0, 1	8.928 082 1998	0.558 005 13	0.186 001 71
1, 1	10.390 627 2955	0.474 136 41	0.158 045 47
-1, 1	7.328 144 3881	0.667 765 17	0.222 588 39

anisotropic resonances with a non-zero value of $V(22)$. First, however, we give one set of interesting results which emerged from our real energy test calculations for radial problems. It was observed that for a radial potential the two states $(1, 1, e)$ and $(0, 2, o)$ (using e and o for even and odd $x \leftrightarrow y$ interchange parity) are degenerate in energy to double precision. This result can be understood for the case of the unperturbed oscillator potential r^2 , since the two states transform into one another on a rotation of $\frac{\pi}{4}$; they can be symbolically represented by the functions xy and $(\frac{1}{2})(x^2 - y^2)$. The results show that this rotational energy degeneracy persists for any radial perturbation of this oscillator potential. We were also able to find the variation of the expectation value $\langle x^2y^2 \rangle$ for the two states as the radial potential varies. We calculated this expectation value by finding the energy shifts when a small perturbation λx^2y^2 is added to or subtracted from the otherwise radial potential. For the case of the oscillator potential r^2 we can find the values of $\langle x^2y^2 \rangle$ analytically; they have the exact ratio of 3. The numerical energy shift approach easily gave $\langle x^2y^2 \rangle$ accurate to eight decimal digits, and it was found that the ratio of the $\langle x^2y^2 \rangle$ values remained at the exact value 3 for any radial perturbation of the oscillator potential. Table 1 shows a few typical results. Since the distortion of the radial wavefunction varies markedly from state to state in table 1, it is clear that the constancy of the ratio is due to unchanging angular factors throughout, so that it would more easily be discernible by treating the system using polar coordinates (r, θ) . That the result was found using the (x, y) coordinates indicates the accuracy of the energy differencing method for expectation values (and, of course, of the eigenvalues themselves). For the special case in which we set $V(22) = 2V(4)$ in the Hamiltonian (1), we are dealing with a spherically symmetric potential with the fourth-order term $V(4)r^4$. In two dimensions an isotropic potential $V(r)$ would lead to the Schrödinger equation

$$(-D^2 - r^{-1}D)\Psi - m^2r^{-2}\Psi + V(r)\Psi = E\Psi, \quad (5)$$

for a state with a magnetic quantum number m . To treat this equation by using perturbation or other techniques which have been formulated for a three-dimensional problem with arbitrary angular momentum L , we must convert equation (5) into an equivalent three-dimensional equation. This is done by setting $\Psi = r^{\frac{1}{2}}\phi$. A little algebra then shows that the function ϕ obeys the Schrödinger equation

$$(-D^2 - 2r^{-1}D)\phi + (m^2 - \frac{1}{4})r^{-2}\phi + V(r)\phi = E\phi. \quad (6)$$

This is now a three-dimensional equation containing an effective angular momentum $L = m - \frac{1}{2}$, so that $L(L+1) = m^2 - \frac{1}{4}$. It is this effective L which must be used when applying hypervirial perturbation theory to the Hamiltonian (1) with a radial potential. The eigenstates can thus be classified in terms of their effective angular momentum, which in two dimensions equals $-\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$, etc. A comparison calculation using complex hypervirial perturbation theory gives the angular momentum value and the level of excitation ($n = 0, 1, 2$,

Table 2. Results for the potential $r^2 - 0.1r^4$, showing the complex matrix results. The complex hypervirial perturbation method gives the angular momentum L and the level of excitation n , with somewhat less accurate energies.

State	(L, n)	ER	EI
$(0, 0, e)$	$(-\frac{1}{2}, 0)$	1.713 490 082 291 66	4.543 667 070 259 02 (-2)
$(0, 1)$	$(\frac{1}{2}, 0)$	3.136 365 859 387 4	3.468 244 235 576 37 (-1)
$(1, 1, e)$	$(\frac{3}{2}, 0)$	4.463 978 575 502 85	9.691 550 938 030 89 (-1)
$(0, 2, e)$	$(-\frac{1}{2}, 1)$	4.265 124 214 438 76	1.247 960 230 195 4
$(0, 2, o)$	$(\frac{3}{2}, 0)$	4.463 978 575 502 85	9.691 550 938 030 89 (-1)
$(1, 3, e)$	$(\frac{3}{2}, 0)$	4.463 978 575 502 85	9.691 550 938 030 89 (-1)
$(1, 3, o)$	$(\frac{7}{2}, 0)$	7.045 728 124 508	2.908 145 179 297 4
$(2, 2, e)$	$(-\frac{1}{2}, 1)$	4.265 124 214 438 76	1.247 960 230 195 4
$(1, 2)$	$(\frac{1}{2}, 1)$	5.600 354 031 555 6	2.396 843 437 824
$(3, 3, e)$	$(\frac{3}{2}, 1)$	7.028 042 422 622 0	3.641 224 487 237 07
$(2, 4, e)$	$(-\frac{1}{2}, 2)$	6.973 134 137 355 7	3.878 659 456 302 1
$(2, 4, o)$	$(\frac{3}{2}, 1)$	7.028 042 422 622 0	6.641 224 487 237 07
$(3, 4)$	$(\frac{1}{2}, 2)$	8.441 780 557 286	5.410 421 329 81

etc) of each state which is described by oscillator labels. Table 2 shows some typical results. The complex matrix method gives about four more digits of accuracy than the hypervirial method. The bound state checking calculations are, of course, equally accurate and illustrate the dual purpose nature of the method. By considering the nature of the potential along a straight line from the origin it is possible to build up an intuitive picture of the way in which resonances can be produced or inhibited by the highly symmetric potential appearing in the Hamiltonian (1). For example, if the potential has a positive $V(4)$, then at large distances the potential will be rising steeply and bound states will be expected whatever the sign of $V(2)$, provided that $V(22)$ is zero. If, however, $V(22)$ is made increasingly negative, then for $|V(22)| > 2V_4$ the potential at or around the lines $y = \pm|x|$ will descend rapidly at large distances, thus creating a diagonal escape route for a particle which is originally bound near to the origin. This suggests that the initially bound states will become resonances as $V(22)$ passes through $-2V_4$. The numerical results are in agreement with this intuitive argument, and table 3 shows some illustrative results. The complex W , with $W = WR + iWI$, was found empirically by varying it to give a large number of stable digits in the converged result as the basis size is increased. However, a wide range of W values around the 'optimum' W is found to be equally effective. The use of a complex W in the bound state region leads to an EI value which is negligibly small (typically of modulus less than 10^{-16}), showing that the state is bound. Another case which was treated in detail is that in which $V(2)$ is positive, $V(22)$ is zero and $V(4)$ is small but negative. The resonant state energies for this separable case are simply sums of appropriate one-dimensional resonance energies, and the method of this work gives results in agreement with those of works which have dealt with the one-dimensional problem [1, 2]. By studying the form of the wavefunction for the simple unperturbed oscillator it can be seen that the state labelled $(0, 0, e)$ is (and remains) spherically symmetric while the

Table 3. Complex energies of the $(0, 0, e)$ resonance arising from the $(0, 0, e)$ state with $V(2) = V(4) = 1$ and decreasing $V(22)$. The state changes from bound state to resonance at $V(22) = -2$. Between $V(22) = -2$ and -2.15 the value of EI is too small to be found accurately.

$V(22)$	W	ER	EI
-1.9	(4, 4)	2.575 377 205 954 7	0.0
-2.0	(4, 4)	2.561 626 575 640 03	0.0
-2.15	(4, 4)	2.547 386 907 867 41	5.847 (-12)
-2.20	(4, 4)	2.532 577 658 937 5	2.756 148 (-9)
-2.30	(6, 6)	2.517 077 914 546	1.620 736 (-6)
-2.40	(6, 6)	2.500 680 139 949	4.403 975 88 (-5)
-2.50	(8, 8)	2.483 103 763 760	3.336 917 055 (-4)
-2.60	(8, 8)	2.464 181 203 172 5	1.308 895 243 6 (-3)
-2.70	(8, 8)	2.444 020 105 637 7	3.490 589 739 1 (-3)
-2.80	(8, 8)	2.422 976 522 281 1	7.280 796 160 2 (-3)
-2.90	(8, 8)	2.401 517 162 084 2	1.286 772 155 75 (-2)
-3.00	(8, 8)	2.380 091 738 718 0	2.024 145 310 98 (-2)

Table 4. An isotropic resonance inhibiting effect for the resonances arising from $(0, 0, e)$ and $(1, 1, e)$, with $V(2) = 1$ and $V(4) = -0.1$. The energies have been severely truncated from their original double precision accuracy in order to simplify the table. A comma separates ER and EI in each energy value. A W value gradually increasing from (1, 1) to (4, 4) down the table suffices to give highly accurate results.

$V(22)$	$(0, 0, e)$	$(1, 1, e)$
0.0	1.801 3458, 1.338 6562 (-2)	4.898 8833, 3.063 9102 (-1)
0.5	1.957 1134, 3.026 8898 (-3)	6.259 8911, 1.157 5157 (-2)
1.0	2.066 8438, 1.244 6558 (-3)	7.007 0356, 1.326 0544 (-3)
1.5	2.156 6871, 6.163 8671 (-4)	7.564 7900, 2.220 1615 (-4)
2.0	2.234 4886, 3.382 2639 (-4)	8.025 3613, 4.687 7662 (-5)

state labelled $(1, 1, e)$ has (and retains) a factor of xy . The probability density associated with $(1, 1, e)$ thus has a factor of form x^2y^2 , which means that it has a maximum along the diagonal directions. The complex energy for the $(1, 1, e)$ state has a greater imaginary part than that for the $(0, 0, e)$ state, since for the separable case it is associated with the $n = 1$ perturbed state in one dimension. As the value of $V(22)$ is increased from zero through positive values (with $V(4)$ negative), it appears that the increasing x^2y^2 term in the potential should act so as to block the escape route along the diagonal while leaving unaffected escape routes near the axes. Such a process would have a stronger effect for the $(1, 1, e)$ state than for the $(0, 0, e)$ one. The numerical results confirm this intuitive argument; indeed, as $V(22)$ increases the imaginary part of the $(0, 0, e)$ resonance actually becomes greater than that of the $(1, 1, e)$ resonance. Some results are shown in table 4, and a similar behaviour was found to be shown by the resonances arising from the states $(0, 2, o)$ and $(1, 3, o)$. These results illustrate the interesting anisotropic effects which can arise in the study of resonances in two dimensions and which are not present in the much more studied one-dimensional case. The method described here represents the fourth successful example of the conversion of a traditional bound state technique into a resonant state one by the simple process of using complex numbers to replace the usual real ones in the algorithm. The resulting modified algorithms then become dual purpose ones which can be used to treat either bound states or resonant states at will. The potential treated in this work is an even parity one which can be given both bound and resonant

states by varying the potential parameters. By contrast, the Henon-Heiles potential contains an odd-parity term and so should only have resonances, although the invariable practice in the literature is to produce real ‘bound state’ energies for it. The dual purpose algorithm described in the present work is appropriate for such a problem and is currently being modified to treat the Henon-Heiles potential. The results of this paper show that it is possible to obtain resonant state energies by using a complex oscillator basis set but also without using the traditional formal complex scaling of all the kinetic and potential energy terms in the Hamiltonian [9]. The simple complexification process used here is easy to apply within various formalisms [1–4], although the results obtained do suggest that it is probably formally equivalent to the more complicated complex scaling approach. In the complex scaling approach a rotation angle θ is varied, while in the present approach the value of W is varied.

References

- [1] Killingbeck J P, Grosjean A and Jolicard G 2004 *J. Phys. A: Math. Gen.* **37** 7971
- [2] Killingbeck J P, Grosjean A and Jolicard G 2004 *J. Phys. A: Math. Gen.* **37** L567
- [3] Killingbeck J P, Grosjean A and Jolicard G 2005 *J. Phys. A: Math. Gen.* **38** L695
- [4] Killingbeck J P 2007 *J. Phys. A: Math. Theor.* **40** 2819
- [5] Arias de Saavedra F and Buendia E 1991 *J. Phys. A: Math. Gen.* **24** L1209
- [6] Fernandez F M 1995 *J. Phys. A: Math. Gen.* **28** 4043
- [7] Taseli H and Eid R 1996 *J. Phys. A: Math. Gen.* **29** 6967
- [8] Vrscaj E R and Handy C R 1989 *J. Phys. A: Math. Gen.* **22** 823
- [9] Alvarez G 1988 *Phys. Rev. A* **37** 4079