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Non-Hermitian oscillators with T_d symmetry

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HIGHLIGHTS

- PT-symmetric oscillators exhibit real eigenvalues.
- Not all space–time symmetries lead to real eigenvalues.
- Some Hamiltonians are invariant under unitary transformations.
- Point-group symmetry greatly simplifies the calculation of eigenvalues and eigenfunctions.
- Group theory and perturbation theory enable one to predict the occurrence of real eigenvalues.

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ABSTRACT

We analyse some PT-symmetric oscillators with T_d symmetry that depend on a potential parameter g. We calculate the eigenvalues and eigenfunctions for each irreducible representation and for a range of values of g. Pairs of eigenvalues coalesce at exceptional points g_c; their magnitude roughly decreasing with the magnitude of the eigenvalues. It is difficult to estimate whether there is a phase transition at a nonzero value of g as conjectured in earlier papers. Group theory and perturbation theory enable one to predict whether a given space–time symmetry leads to real eigenvalues for sufficiently small nonzero values of g.

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1. Introduction

In the last years there has been great interest in non-Hermitian multidimensional oscillators with antiunitary symmetry $A = UK$, where U is a unitary operator and K is the complex conjugation operation. These Hamiltonians are of the form $H = H_0 + igH'$, where H_0 is Hermitian, $UH_0U^\dagger = H_0$ and $UH'U^\dagger = -H'$ [1–10]. The interest in these oscillators stems from the fact that they appear to exhibit real eigenvalues for sufficiently small values of $|g|$. As g increases from $g = 0$ two eigenvalues E_m and E_n approach each other, coalesce at an exceptional point g_c [11–14] and become a pair of complex conjugate numbers for $g > g_c$. At the exceptional point the corresponding eigenvectors ψ_m and ψ_n are no longer linearly independent [11–14]. It is commonly said that the system exhibits a PT-phase transition at $g = g_{PT} > 0$, where g_{PT} is the exceptional point closest to the origin [9]. The eigenvalues E_m of H are real for all $0 \leq g < g_{PT}$, where the antiunitary symmetry remains unbroken. Based on the multidimensional non-Hermitian oscillators studied so far, Bender and Weir [9] conjectured that the PT phase transition is a high-energy phenomenon.

Point-group symmetry (PGS) [15,16] proved useful for the study of a class of multidimensional anharmonic oscillators [17,18]. Klaiman and Cederbaum [6] applied PGS to non-Hermitian Hamiltonians chosen so that the point group G for H is a subgroup of the point group G_0 for H_0. They restricted their study to Abelian groups, which exhibit only one-dimensional irreducible representations (irreps), and Hermitian operators H_0 with no degenerate states. All such examples exhibit real eigenvalues for sufficiently small values of $|g|$. One of their goals was to predict the symmetry of the eigenfunctions associated to the eigenvalues that coalesce at the exceptional points and coined the term space–time (ST) symmetry that refers to a class of antiunitary symmetries that contain the PT symmetry as a particular case. Strictly speaking we refer to PT symmetry when $U = P$, $P : (\mathbf{x}, \mathbf{p}) \rightarrow (-\mathbf{x}, -\mathbf{p})$, where $\mathbf{x}$ and $\mathbf{p}$ are the collections of coordinate and momenta operators, respectively.

The main interest in the studies of PT-symmetric multidimensional oscillators just mentioned has been to enlarge the class of non-Hermitian Hamiltonians that exhibit real spectra, at least for some values of the potential parameter g. On the other hand, by means of PGS Fernández and Garcia [19,20] found some examples of ST-symmetric multidimensional models that exhibit complex eigenvalues for $g > 0$ so that the phase transition takes place at the trivial Hermitian limit $g_{PT} = 0$. Their results suggest that the more general ST symmetry is not as robust as the PT one and contradict some of the conjectures put forward by Klaiman and Cederbaum [6] based on PGS. By means of PGS and perturbation theory we have considerably improved the results, arguments and conclusions of those earlier papers and also found a greater class of ST-symmetric multidimensional models with broken ST symmetry for all values of $g \neq 0$ [21]. Those results show in a more clear way that the conjecture of Klaiman and Cederbaum does not apply to the general case where the Hermitian Hamiltonian H_0 may exhibit degenerate states.

The purpose of this paper is the study of some tri-dimensional non-Hermitian oscillators by means of PGS. In Section 2 we discuss the diagonalization of the matrix representation of the Hamiltonian operator in symmetry-adapted basis sets. By means of PGS and perturbation theory we develop a straightforward strategy that appears to be suitable for determining whether the Hamiltonian will have real eigenvalues for sufficiently small nonzero values of the parameter g. In Section 3 we choose a non-Hermitian oscillator discussed earlier by Bender and Weir [9] as an illustrative example and exploit the fact that it exhibits T_d symmetry. In Section 4 we discuss a non-Hermitian oscillator where H_0 and H' exhibit symmetry O_h and T_d, respectively. Finally, in Section 5 we draw conclusions.

2. Diagonalization

Several approaches have been applied to the calculation of the spectra of the ST-symmetric multidimensional oscillators: the diagonalization method [1–4,7,9], perturbation theory [1,3,4,7], classical and semiclassical approaches [1,2], among others [7,10]. The diagonalization method consists of expanding the eigenfunctions ψ of H as linear combinations of a suitable basis set $B = \{f_1, f_2, \ldots\}$

$$\psi = \sum_j c_j f_j \tag{1}$$

and then diagonalizing an $N \times N$ matrix representation of the Hamiltonian $\mathbf{H}$ with elements $\langle f_i | H | f_j \rangle$, where $\langle f | g \rangle$ stands for the c-product [22]. Such matrices are complex and symmetric $\langle f_i | H | f_j \rangle = \langle f_j | H | f_i \rangle$ but obviously not Hermitian.

In this paper we take into account that the non-Hermitian multidimensional oscillators exhibit PGS and choose basis sets adapted to the irreps of the point group G of H. In this way we can split the matrix representation $\mathbf{H}$ into representations $\mathbf{H}^S$ for each symmetry S. The eigenfunctions of H are bases for the irreps of G and can be written as linear combinations

$$\psi^S = \sum_j c_j^S f_j^S \tag{2}$$

of the elements of the symmetry-adapted basis sets $B^S = \{f_1^S, f_2^S, \ldots\}$. The matrix elements of $\mathbf{H}^S$ are given by $\left\langle f_i^S \right| H \left| f_j^S \right\rangle$ and the separate treatment of each symmetry is justified by the fact that $\left\langle f_i^S \right| H \left| f_j^{S'} \right\rangle = 0$ if $S \neq S'$ [15,16]. That is to say: functions of different symmetry do not mix.

The construction of symmetry-adapted basis sets is straightforward and is described in most textbooks on group theory [15,16]. One applies a projection operator P^S to a basis function f_j and obtains a symmetry-adapted function u_j^S. If the irrep S is one-dimensional it is only necessary to normalize the resulting function u_j^S; otherwise it may be necessary to combine two or more functions u_j^S to obtain a set of orthonormal functions [15,16].

In what follows we apply this approach to two non-Hermitian three-dimensional oscillators of the form

$$H = H_0 + igH' \tag{3}$$

where H_0 is Hermitian and g is real. In particular, we consider the case that both H_0 and H exhibit eigenspaces of dimension greater than one.

In the examples discussed in this paper the symmetry of H_0 is given by the point group $G_0 = \{U_1, U_2, \ldots, U_m\}$: $U_i H_0 U_i^{-1} = H_0$. If H' is invariant under the operations of a subgroup $G = \{W_1, W_2, \ldots, W_k\}$ of G_0 ($W_i H' W_i^{-1} = H'$) then H is invariant under the operations of the point group G. Suppose that there exists a unitary operator $U_a \in G_0 \backslash G$ with the following properties: (i) it forms a class by itself (that is to say: $U_i U_a U_i^{-1} = U_a, i = 1, 2, \ldots, m$) so that $U_a^{-1} = U_a$, (ii) it changes the sign of $H' U_a H' U_a^{-1} = -H'$. Under these conditions H exhibits the antiunitary symmetry given by $A = U_a K$, $AHA^{-1} = H$, where K is the complex conjugation operation introduced earlier.

If $\psi_m^{(0)}$ is an eigenfunction of H_0 with eigenvalue $E_m^{(0)}$ then $U_a \psi_m^{(0)} = \sigma_m \psi_m^{(0)}$, where $\sigma_m = \pm 1$, as follows from $[H, U_a] = 0$ and $U_a^2 = 1$. Therefore,

$$\left\langle \psi_m^{(0)} \right| H' \left| \psi_n^{(0)} \right\rangle = 0, \tag{4}$$

if $\sigma_m \sigma_n = 1$.

It was shown in our earlier papers that complex eigenvalues appear for sufficiently small values of $|g|$ when H_0 exhibits degenerate eigenfunctions and at least one of the perturbation corrections of first order produced by H' is nonzero [19–21]. The degenerate eigenfunctions of H_0

$$H_0 \psi_{m,k}^{(0)} = E_m^{(0)} \psi_{m,k}^{(0)}, \quad k = 1, 2, \ldots, \nu_m, \tag{5}$$

exhibit the same behaviour with respect to U_a: $U_a \psi_{m,k}^{(0)} = \sigma_m \psi_{m,k}^{(0)}$, so that

$$\left\langle \psi_{m,k}^{(0)} \right| H' \left| \psi_{n,l}^{(0)} \right\rangle = 0 \quad k, l = 1, 2, \ldots, \nu_m, \tag{6}$$

and all the perturbation corrections of first order vanish (see Ref. [21] for more details).

The main conclusion drawn from the discussion above is that the space–time symmetry given by A may not be broken when the space transformation given by $U_a \in G_0$ forms a class by itself. This conjecture is confirmed by all the examples discussed in our earlier paper [21] where we concluded

Table 1
Character table for T_d point group.

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$		
A_1	1	1	1	1	1		$x^2+y^2+z^2$
A_2	1	1	1	−1	−1		
E	2	−1	2	0	0		$(2z^2-x^2-y^2, x^2-y^2)$
T_1	3	0	−1	1	−1	(R_x, R_y, R_z)	
T_2	3	0	−1	−1	1	(x, y, z)	(xz, yz, xy)

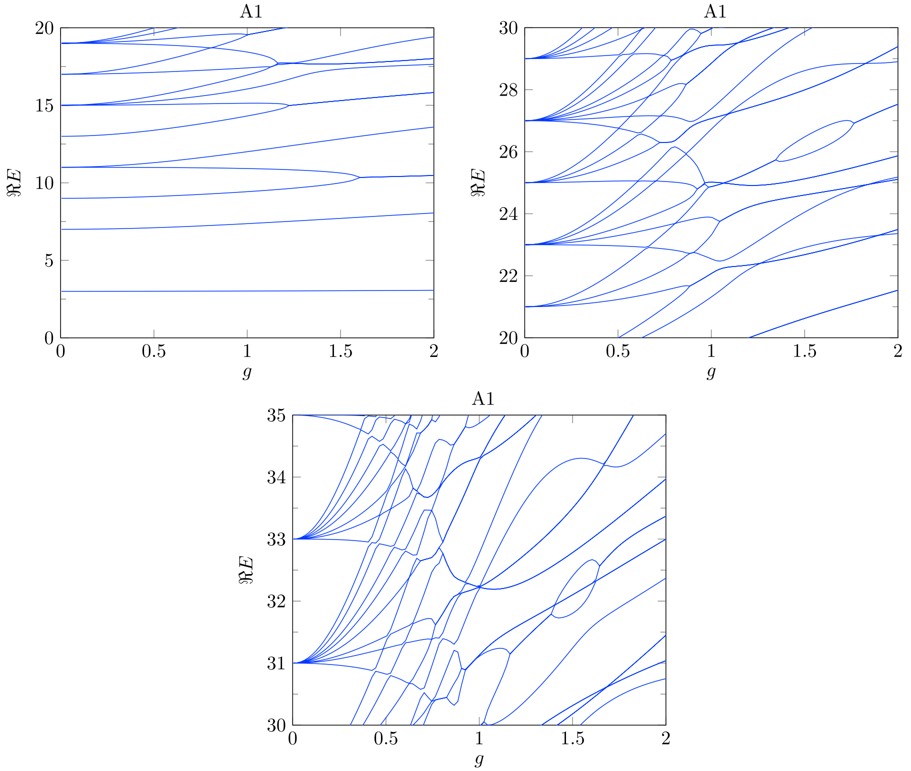

Fig. 1. Real parts of the eigenvalues of symmetry A_1 of the Hamiltonian operator $H = p_x^2 + p_y^2 + p_z^2 + x^2 + y^2 + z^2 + igxyz$.

that the inversion operation $\hat{\imath} : (x, y, z) \to (-x, -y, -z)$ is suitable choice for U_a. Note that in all the point groups $\hat{\imath}$ forms a class by itself [15,16].

In closing this section we outline some features of PGS used throughout this paper. To begin with we mention that a projection operator P^S on the irrep S is given by

$$P^S = \frac{l_S}{h} \sum_{j=1}^{h} \chi_j^S W_j, \tag{7}$$

where l_S is the dimension of the irrep, h the order (total number of elements or operations) of the group and χ_j^S is the character (trace of the matrix representation) of W_j in a basis for the irrep. Tables 1 and 2 show examples of the items enumerated above. For example, the first row exhibits the group name and lists group operations grouped in classes; their symbols having the following meaning:

- E: identity operation
- C_n: rotation by an angle of $2\pi/n$

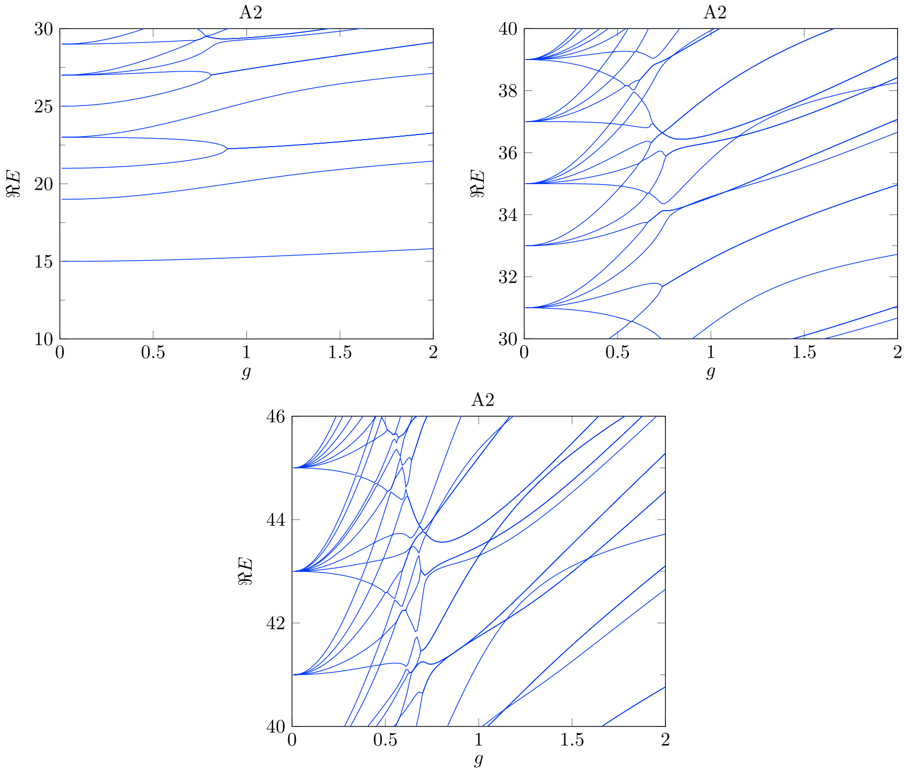

Fig. 2. Real parts of the eigenvalues of symmetry A_2 the Hamiltonian operator $H = p_x^2 + p_y^2 + p_z^2 + x^2 + y^2 + z^2 + igxyz$.

Table 2
Character table for O_h point group.

O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_2(=C_4^2)$	$\hat{\imath}$	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1		$x^2+y^2+z^2$
A_{2g}	1	1	−1	−1	1	1	−1	1	1	−1		
E_g	2	−1	0	0	2	2	0	−1	2	0		$(2z^2-x^2-y^2, x^2-y^2)$
T_{1g}	3	0	−1	1	−1	3	1	0	−1	−1	(R_x, R_y, R_z)	
T_{2g}	3	0	1	−1	−1	3	−1	0	−1	1	(xz, yz, xy)	
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1		
A_{2u}	1	1	−1	−1	1	−1	1	−1	−1	1		
E_u	2	−1	0	0	2	−2	0	1	−2	0		
T_{1u}	3	0	−1	1	−1	−3	−1	0	1	1	(x, y, z)	
T_{2u}	3	0	1	−1	−1	−3	1	0	1	−1		

- $\hat{\imath}$: inversion operation (already discussed above)
- S_n: rotation C_n followed by a reflexion with respect to a plane perpendicular to the rotation axis
- σ_d, σ_h reflexion planes

The first column exhibits the irreps; those labelled A or B are one-dimensional ($l_S = 1$), the ones labelled E are two-dimensional ($l_S = 2$) and those labelled T are three-dimensional ($l_S = 3$). The integers are the characters χ_j^S that appear in Eq. (7). The remaining columns show the bases for the different irreps.

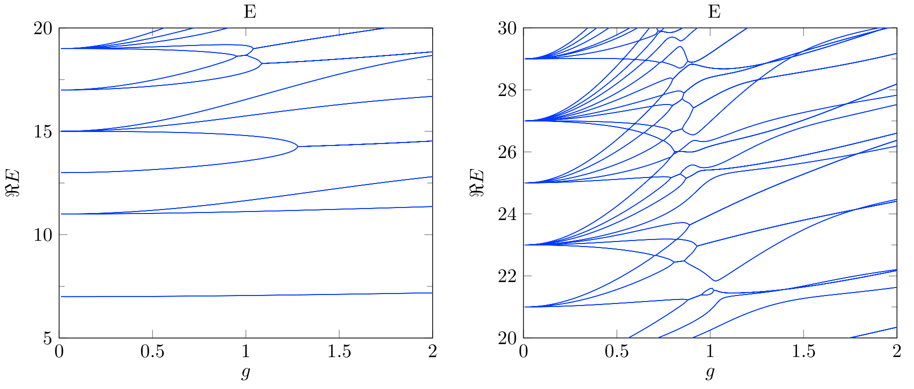

Fig. 3. Real parts of the eigenvalues of symmetry E the Hamiltonian operator $H = p_x^2 + p_y^2 + p_z^2 + x^2 + y^2 + z^2 + igxyz$.

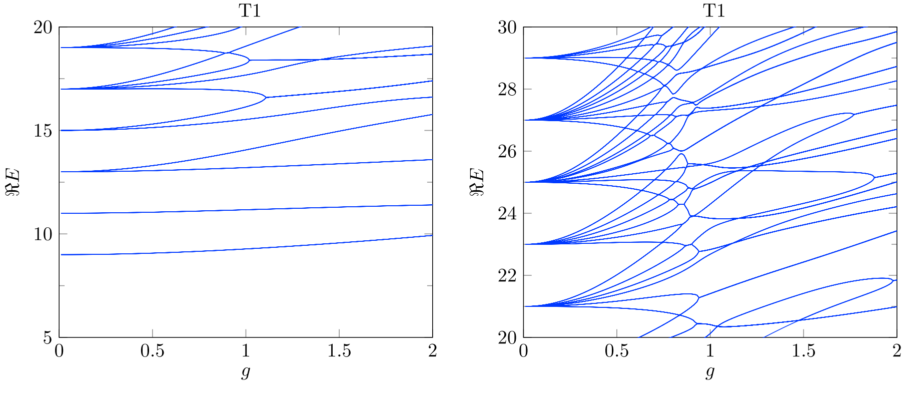

Fig. 4. Real parts of the eigenvalues of symmetry T_1 the Hamiltonian operator $H = p_x^2 + p_y^2 + p_z^2 + x^2 + y^2 + z^2 + igxyz$.

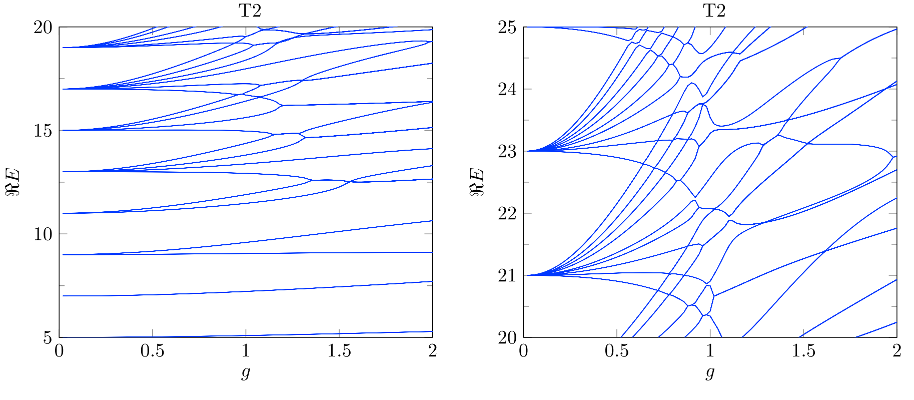

Fig. 5. Real parts of the eigenvalues of symmetry T_2 the Hamiltonian operator $H = p_x^2 + p_y^2 + p_z^2 + x^2 + y^2 + z^2 + igxyz$.

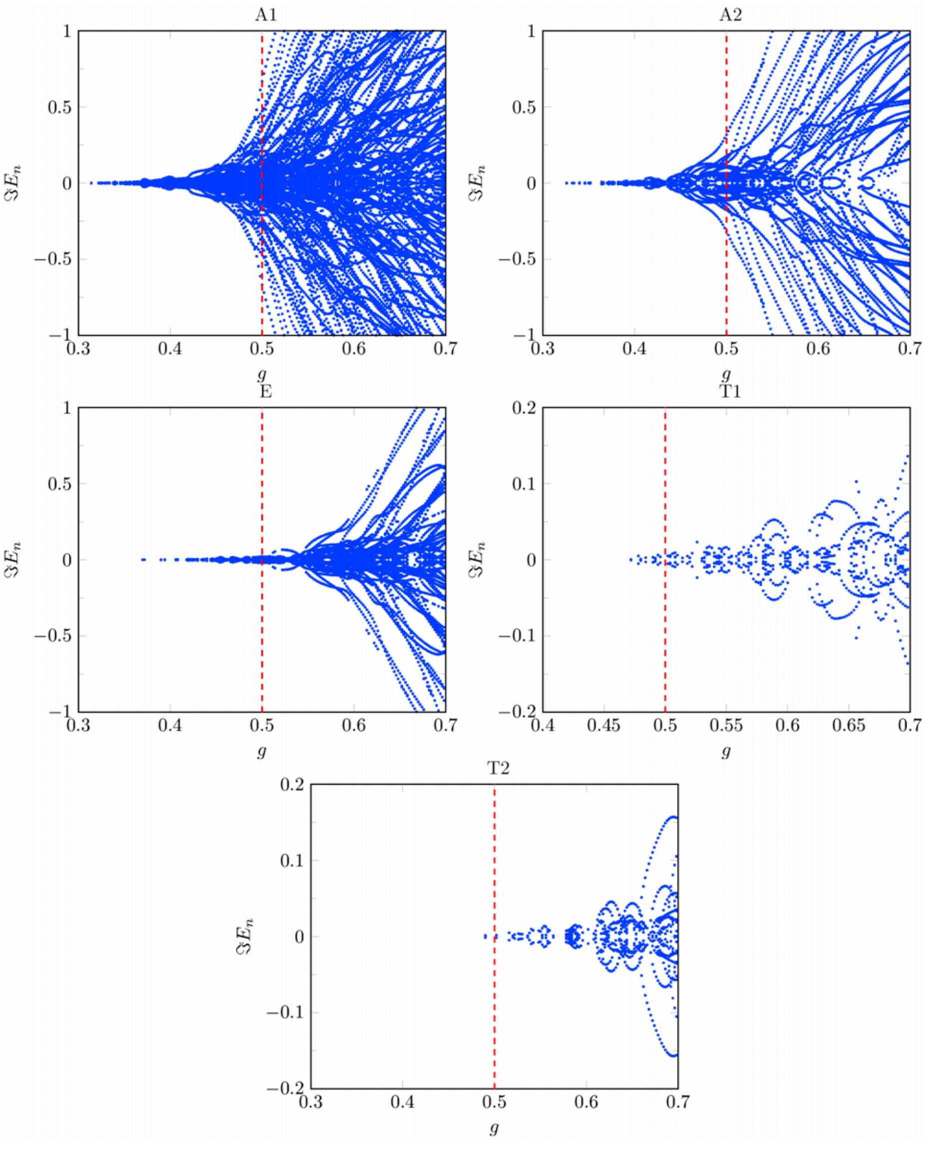

Fig. 6. Imaginary parts of the eigenvalues of the Hamiltonian Operator $H = p_x^2 + p_y^2 + p_z^2 + x^2 + y^2 + z^2 + igxyz$.

3. Example 1

As a first example we choose the non-Hermitian oscillator

$$H = p_x^2 + p_y^2 + p_z^2 + x^2 + y^2 + z^2 + igxyz \tag{8}$$

studied by Bender and Weir [9]. When $g = 0$ the resulting isotropic harmonic oscillator H_0 may be described by the 3D rotation group (the group of all rotations about the origin of the three-dimensional Euclidean space R^3 under the operation of composition). Its eigenfunctions in Cartesian coordinates are

$$\varphi_{m,n,k}(x,y,z) = \phi_m(x)\phi_n(y)\phi_k(z), \quad m,n,k = 0,1,\ldots, \tag{9}$$

where $\phi_j(q)$ is an eigenfunction of $H_{HO} = p_q^2 + q^2$, and the corresponding eigenvalues

$$E_{mnk}^{(0)} = 2\nu + 3, \quad \nu = m+n+k, \tag{10}$$

are $(\nu+1)(\nu+2)/2$-fold degenerate. When $g \neq 0$ the symmetry of the model is determined by $H' = xyz$ and the suitable point group is T_d. The corresponding character table is shown in Table 1. It is not difficult to verify that the 24 symmetry operations in this point group leave the potential-energy function (and, therefore, the whole Hamiltonian operator) invariant.

In this case the obvious choice is $U_a = \hat{\imath} \in G_0$ that satisfies all the conditions outlined in Section 2. Note that $U_a V(x,y,z) U_a = V(-x,-y,-z)$ and $KV(x,y,z)K = V(x,y,z)^*$ so that $AV(x,y,z)A = V(-x,-y,-z)^* = V(x,y,z)$ and the Hamiltonian operator is invariant with respect to the antiunitary transformation $A = U_a K$.

The application of the projection procedure outlined in Section 2 to the eigenfunctions of H_0 yields the following symmetry-adapted basis set for $G = T_d$

$$A_1 : \begin{cases} \varphi_{2m,2m,2m} \\ \dfrac{1}{\sqrt{3}}\left(\varphi_{2m,2m,2n} + \varphi_{2m,2n,2m} + \varphi_{2n,2m,2m}\right) \\ \dfrac{1}{\sqrt{6}}\left(\varphi_{2m,2n,2k} + \varphi_{2k,2m,2n} + \varphi_{2n,2k,2m} + \varphi_{2k,2n,2m} + \varphi_{2m,2k,2n} + \varphi_{2n,2m,2k}\right) \\ \varphi_{2m+1,2m+1,2m+1} \\ \dfrac{1}{\sqrt{3}}\left(\varphi_{2m+1,2m+1,2n+1} + \varphi_{2m+1,2n+1,2m+1} + \varphi_{2n+1,2m+1,2m+1}\right) \\ \dfrac{1}{\sqrt{6}}\left(\varphi_{2m+1,2n+1,2k+1} + \varphi_{2k+1,2m+1,2n+1} + \varphi_{2n+1,2k+1,2m+1} + \varphi_{2k+1,2n+1,2m+1} \right. \\ \quad \left. + \varphi_{2m+1,2k+1,2n+1} + \varphi_{2n+1,2m+1,2k+1}\right) \end{cases} \tag{11}$$

$$A_2 : \begin{cases} \dfrac{1}{\sqrt{6}}\left(\varphi_{2m,2n,2k} + \varphi_{2k,2m,2n} + \varphi_{2n,2k,2m} - \varphi_{2k,2n,2m} - \varphi_{2m,2k,2n} - \varphi_{2n,2m,2k}\right) \\ \dfrac{1}{\sqrt{6}}\left(\varphi_{2m+1,2n+1,2k+1} + \varphi_{2k+1,2m+1,2n+1} + \varphi_{2n+1,2k+1,2m+1} - \varphi_{2k+1,2n+1,2m+1} \right. \\ \quad \left. - \varphi_{2m+1,2k+1,2n+1} - \varphi_{2n+1,2m+1,2k+1}\right) \end{cases}$$

$$E : \begin{cases} \left\{ \dfrac{1}{\sqrt{6}}\left(2\varphi_{2n,2m,2m} - \varphi_{2m,2n,2m} - \varphi_{2m,2m,2n}\right), \dfrac{1}{\sqrt{2}}\left(\varphi_{2m,2n,2m} - \varphi_{2m,2m,2n}\right) \right\} \\ \left\{ \dfrac{1}{\sqrt{6}}\left(2\varphi_{2m,2n,2k} - \varphi_{2k,2m,2n} - \varphi_{2n,2k,2m}\right), \dfrac{1}{\sqrt{2}}\left(\varphi_{2k,2m,2n} - \varphi_{2n,2k,2m}\right) \right\} \\ \left\{ \dfrac{1}{\sqrt{6}}\left(2\varphi_{2n,2m,2k} - \varphi_{2k,2n,2m} - \varphi_{2m,2k,2n}\right), \dfrac{1}{\sqrt{2}}\left(\varphi_{2k,2n,2m} - \varphi_{2m,2k,2n}\right) \right\} \\ \left\{ \begin{matrix} \dfrac{1}{\sqrt{6}}\left(2\varphi_{2n+1,2m+1,2m+1} - \varphi_{2m+1,2n+1,2m+1} - \varphi_{2m+1,2m+1,2n+1}\right), \\ \dfrac{1}{\sqrt{2}}\left(\varphi_{2m+1,2n+1,2m+1} - \varphi_{2m+1,2m+1,2n+1}\right) \end{matrix} \right\} \\ \left\{ \begin{matrix} \dfrac{1}{\sqrt{6}}\left(2\varphi_{2m+1,2n+1,2k+1} - \varphi_{2k+1,2m+1,2n+1} - \varphi_{2n+1,2k+1,2m+1}\right), \\ \dfrac{1}{\sqrt{2}}\left(\varphi_{2k+1,2m+1,2n+1} - \varphi_{2n+1,2k+1,2m+1}\right) \end{matrix} \right\} \\ \left\{ \begin{matrix} \dfrac{1}{\sqrt{6}}\left(2\varphi_{2n+1,2m+1,2k+1} - \varphi_{2k+1,2n+1,2m+1} - \varphi_{2m+1,2k+1,2n+1}\right), \\ \dfrac{1}{\sqrt{2}}\left(\varphi_{2k+1,2n+1,2m+1} - \varphi_{2m+1,2k+1,2n+1}\right) \end{matrix} \right\} \end{cases} \tag{12}$$

$$T_1 : \left\{ \begin{array}{c} \left\{ \begin{array}{c} \frac{1}{\sqrt{2}}\left(\varphi_{2m+1,2n,2k+1} - \varphi_{2k+1,2n,2m+1}\right), \frac{1}{\sqrt{2}}\left(\varphi_{2k+1,2m+1,2n} - \varphi_{2m+1,2k+1,2n}\right), \\ \frac{1}{\sqrt{2}}\left(\varphi_{2n,2k+1,2m+1} - \varphi_{2n,2m+1,2k+1}\right) \end{array} \right\} \\ \left\{ \begin{array}{c} \frac{1}{\sqrt{2}}\left(\varphi_{2m,2n+1,2k} - \varphi_{2k,2n+1,2m}\right), \frac{1}{\sqrt{2}}\left(\varphi_{2k,2m,2n+1} - \varphi_{2m,2k,2n+1}\right), \\ \frac{1}{\sqrt{2}}\left(\varphi_{2n+1,2k,2m} - \varphi_{2n+1,2m,2k}\right) \end{array} \right\} \end{array} \right. \tag{13}$$

$$T_2 : \left\{ \begin{array}{c} \left\{\varphi_{2m+1,2n,2n}, \varphi_{2n,2m+1,2n}, \varphi_{2n,2n,2m+1}\right\} \\ \left\{\varphi_{2m,2n+1,2n+1}, \varphi_{2n+1,2m,2n+1}, \varphi_{2n+1,2n+1,2m}\right\} \\ \left\{ \begin{array}{c} \frac{1}{\sqrt{2}}\left(\varphi_{2m+1,2n,2k+1} + \varphi_{2k+1,2n,2m+1}\right), \frac{1}{\sqrt{2}}\left(\varphi_{2k+1,2m+1,2n} + \varphi_{2m+1,2k+1,2n}\right), \\ \frac{1}{\sqrt{2}}\left(\varphi_{2n,2k+1,2m+1} + \varphi_{2n,2m+1,2k+1}\right) \end{array} \right\} \\ \left\{ \begin{array}{c} \frac{1}{\sqrt{2}}\left(\varphi_{2m,2n+1,2k} + \varphi_{2k,2n+1,2m}\right), \frac{1}{\sqrt{2}}\left(\varphi_{2k,2m,2n+1} + \varphi_{2m,2k,2n+1}\right), \\ \frac{1}{\sqrt{2}}\left(\varphi_{2n+1,2k,2m} + \varphi_{2n+1,2m,2k}\right) \end{array} \right\} \end{array} \right. \tag{14}$$

By means of projection operators one can also prove that the perturbation $H' = xyz$ splits the degenerate states of the three-dimensional harmonic oscillator H_0 in the following way:

$$\begin{array}{ll} \{2n, 2n, 2n\} & \to A_1 \\ \{2n+1, 2m, 2m\}_P & \to T_2 \\ \{2n+1, 2n+1, 2m\}_P & \to T_2 \\ \{2n, 2m, 2m\}_P & \to A_1, E \\ \{2n+1, 2n+1, 2n+1\} & \to A_1 \\ \{2n, 2m, 2k+1\}_P & \to T_1, T_2 \\ \{2n, 2m+1, 2k+1\}_P & \to T_1, T_2 \\ \{2n, 2m, 2k\}_P & \to A_1, A_2, E, E \\ \{2n+1, 2m+1, 2m+1\}_P & \to A_1, E \\ \{2n+1, 2m+1, 2k+1\}_P & \to A_1, A_2, E, E, \end{array} \tag{15}$$

where $\{i, j, k\}_P$ denotes all the distinct permutations of the labels i, j and k.

Bender and Weir [9] diagonalized truncated matrix representations $\mathbf{H}$ of the Hamiltonian operator of dimension $20^3 \times 20^3, 25^3 \times 25^3$ and $30^3 \times 30^3$ in order to estimate the accuracy of their results. They resorted to well known efficient diagonalization routines for sparse matrices. Here, we diagonalize matrix representations $\mathbf{H}^S$ for $S = A_1, A_2, E, T_1, T_2$. This splitting reduces the dimension of the matrices required for a given accuracy and also enables a clearer interpretation and discussion of the results. In this paper we carried out all the calculations with matrices of dimension 5000×5000 for each irrep. Comparison of such results for $g = 1$ with those coming from a calculation with matrices of dimension $10\,000 \times 10\,000$ did not show any relevant difference for present purposes and discussion.

Figs. 1–5 show $\Re E(g)$ for the five irreps. For clarity we split every case into two or three energy intervals where we can appreciate the occurrence of crossings, coalescence of eigenvalues at exceptional points and even what appear to be avoided crossings. Because of the scale used and the separation into irreps our figures reveal a rich pattern of intertwined energy curves that one cannot easily discern when plotting all the symmetries together [9].

Bender and Weir [9] estimated a phase transition near to $g \approx 0.25$ for their Hamiltonian $H^{BW} = H_0^{present}/2 + igxyz$. The relation between present exceptional points and those of Bender and Weir

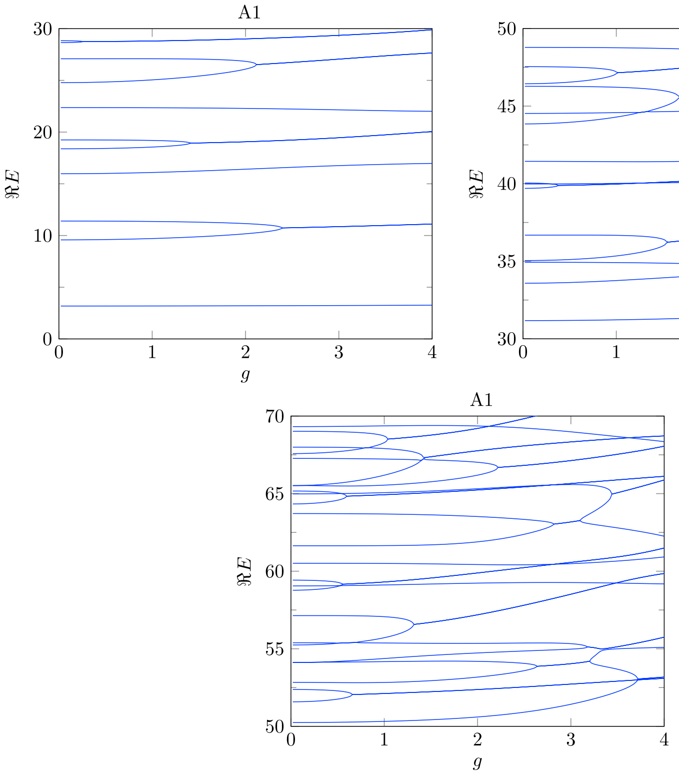

Fig. 7. Real parts of the eigenvalues of symmetry A_1 of the Hamiltonian operator $H = p_x^2 + p_y^2 + p_z^2 + x^4 + y^4 + z^4 + igxyz$.

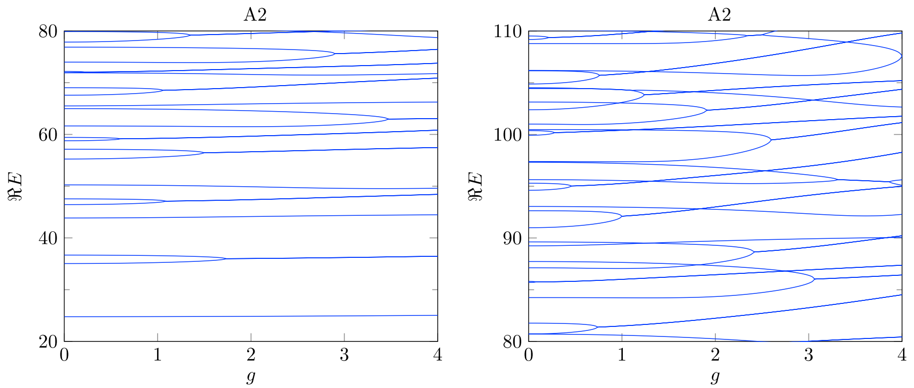

Fig. 8. Real parts of the eigenvalues of symmetry A_2 of the Hamiltonian operator $H = p_x^2 + p_y^2 + p_z^2 + x^4 + y^4 + z^4 + igxyz$.

is therefore $g_c^{present} = 2g_c^{BW}$. Fig. 6 shows the imaginary parts of the eigenvalues for each irrep. We appreciate that complex eigenvalues appear for values of the parameter that are considerably smaller than $g = 0.5$; therefore, we cannot be sure that there is a phase transition for this Hamiltonian. As the energy increases more exceptional points seem to emerge closer to the origin.

All the figures in this paper have been produced by means of the Tikz package [23].

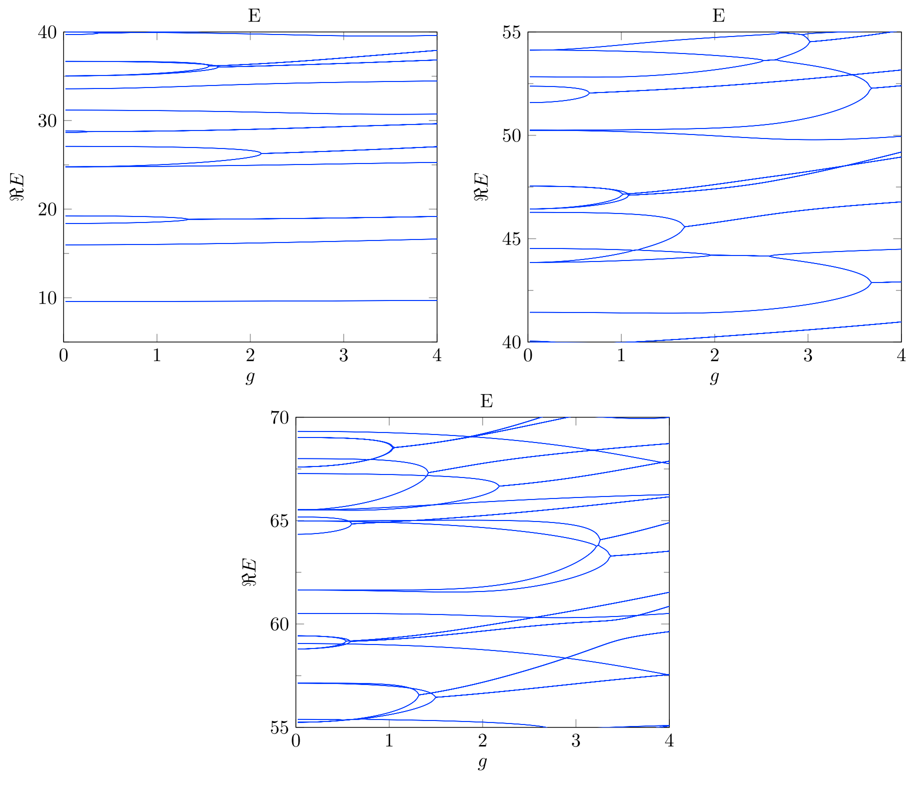

Fig. 9. Real parts of the eigenvalues of symmetry E of the Hamiltonian operator $H = p_x^2 + p_y^2 + p_z^2 + x^4 + y^4 + z^4 + igxyz$.

4. Example 2

The non-Hermitian anharmonic oscillator

$$H = p_x^2 + p_y^2 + p_z^2 + x^4 + y^4 + z^4 + igxyz, \tag{16}$$

is interesting because H_0 is invariant under the unitary operations of the point group O_h and H is invariant under those of T_d.

If $\{i, j, k\}_P$ denotes all distinct permutations of the subscripts in the eigenfunctions $\chi_{ijk}(x, y, z) = \rho_i(x)\rho_j(y)\rho_k(z)$, $i, j, k = 0, 1, \ldots,$ of H_0, then their symmetry is given by (see Ref. [24,25] for a discussion of an exactly solvable quantum-mechanical problem with the same PGS):

$$\begin{array}{ll}
\{2n, 2n, 2n\} & A_{1g} \\
\{2n+1, 2n+1, 2n+1\} & A_{2u} \\
\{2n+1, 2n+1, 2m\}_P & T_{2g} \\
\{2n, 2n, 2m+1\}_P & T_{1u} \\
\{2n, 2n, 2m\}_P & A_{1g}, E_g \\
\{2n+1, 2n+1, 2m+1\}_P & A_{2u}, E_u \\
\{2n, 2m, 2k\}_P & A_{1g}, A_{2g}, E_g, E_g \\
\{2n+1, 2m+1, 2k+1\}_P & A_{1u}, A_{2u}, E_u, E_u \\
\{2n, 2m, 2k+1\}_P & T_{1u}, T_{2u} \\
\{2n+1, 2m+1, 2k\}_P & T_{1g}, T_{2g}.
\end{array} \tag{17}$$

The character table for the point group O_h is shown in Table 2. The dynamical symmetries that are responsible for the degeneracy of eigenfunctions belonging to different irreps (which cannot be

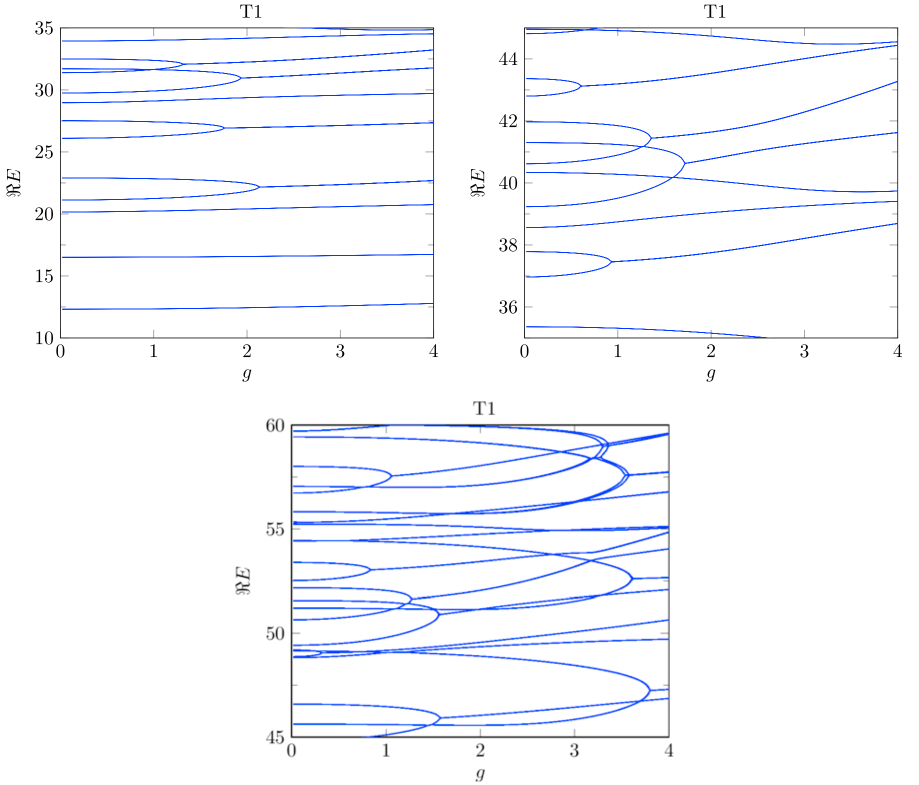

Fig. 10. Real parts of the eigenvalues of symmetry T_1 of the Hamiltonian operator $H = p_x^2 + p_y^2 + p_z^2 + x^4 + y^4 + z^4 + igxyz$.

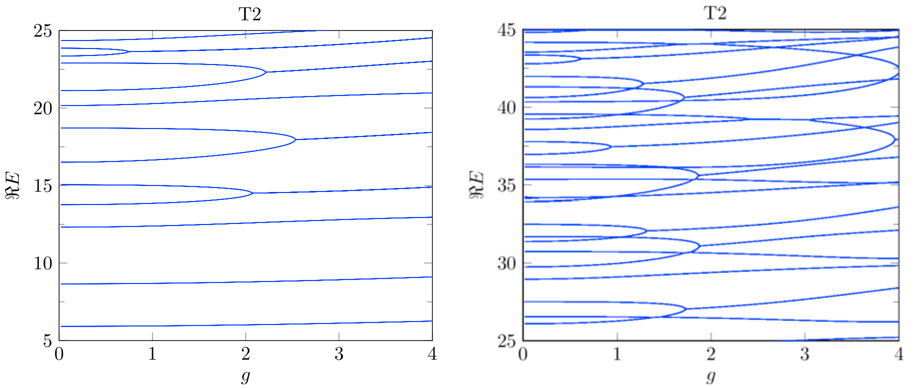

Fig. 11. Real parts of the eigenvalues of symmetry T_2 of the Hamiltonian operator $H = p_x^2 + p_y^2 + p_z^2 + x^4 + y^4 + z^4 + igxyz$.

explained by PGS) are given by the Hermitian operators

$$O_1 = 2p_x^2 + 2x^4 - p_y^2 - y^4 - p_z^2 - z^4$$
$$O_2 = 2p_y^2 + 2y^4 - p_x^2 - x^4 - p_z^2 - z^4. \quad (18)$$

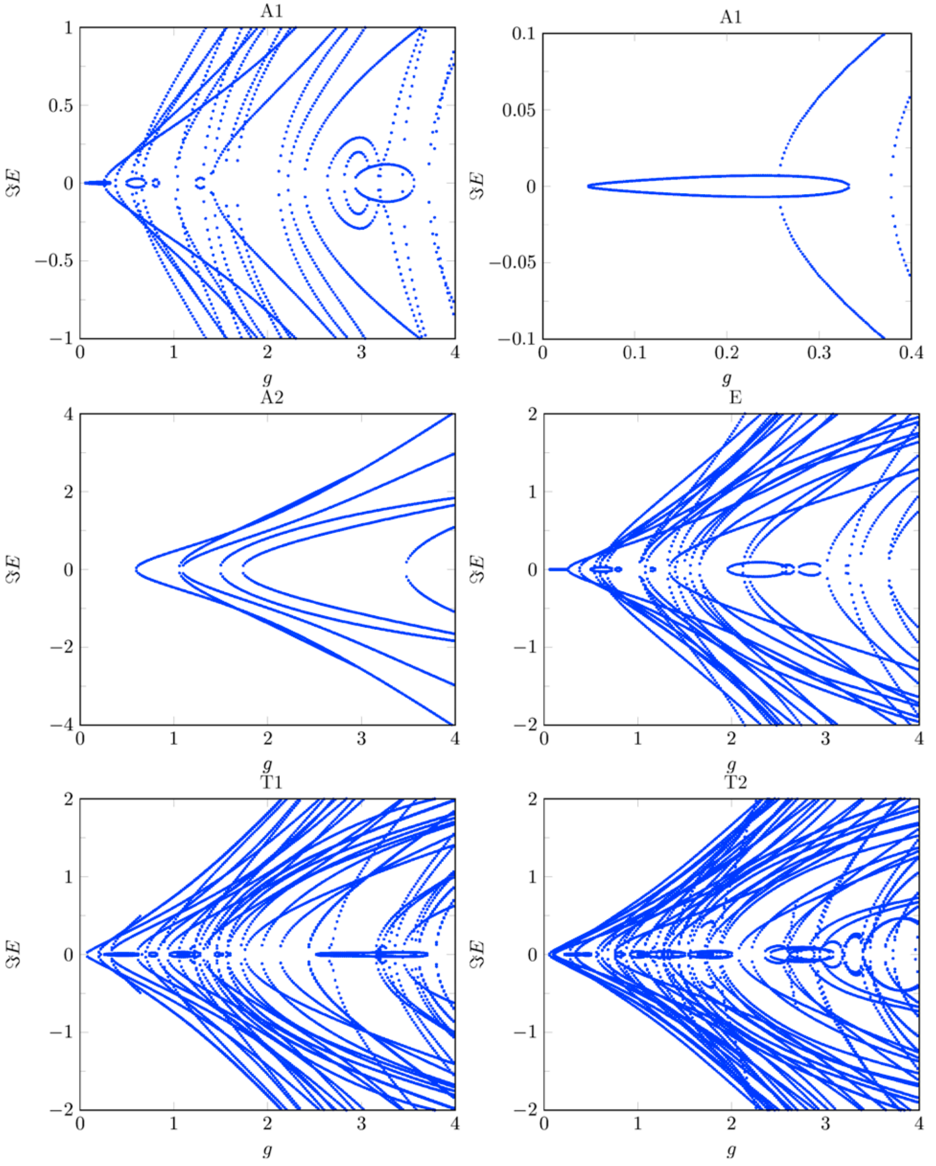

Fig. 12. Imaginary parts of the eigenvalues of the Hamiltonian operator $H = p_x^2 + p_y^2 + p_z^2 + x^4 + y^4 + z^4 + igxyz$.

They belong to the irrep E_g and commute with H_0. We easily obtain them by straightforward application of the projection operator P^{E_g} to the two pairs of functions (x^2, y^2) and (x^4, y^4) as discussed elsewhere [24].

By means of projection operators we can prove that the eigenfunctions of H_0 transform into those of H according to the following symmetry scheme:

$$\begin{aligned} A_{1g}, A_{2u} &\to A_1 \\ A_{2g}, A_{1u} &\to A_2 \\ E_g, E_u &\to E \end{aligned}$$

$$T_{1g},\ T_{2u}\ \rightarrow T_1$$
$$T_{2g},\ T_{1u}\ \rightarrow T_2. \tag{19}$$

Clearly, $A = \hat{\imath}K$ leaves H invariant. Since $\hat{\imath}$ forms a class by itself as shown by the character Table 2 then this antiunitary symmetry is expected to be unbroken for sufficiently small values of g according to the discussion in Section 2. This conclusion is confirmed by Figs. 7–12 where we see that there are real eigenvalues for sufficiently small values of g for the five irreps. However, the values of g_c approach the origin as the eigenvalues increase in such a way that it is difficult to estimate whether there is a high-energy phase transition. It is also worth noting that the pattern of $\Im E$ vs g is not the same for all the irreps. The most striking difference occurs between the irreps A_1 and A_2.

5. Conclusions

In this paper we have studied a few examples of non-Hermitian Hamiltonian operators of the form (3) with a space–time symmetry given by an antiunitary operator $A = U_aK$. The space transformation U_a satisfies $U_aH_0U_a^{-1} = H_0$ and $U_aH'U_a^{-1} = -H'$. Under such conditions our conjecture is that one expects real eigenvalues for sufficiently small values of $|g|$ when U_a forms a class by itself in the point group G_0 that describes the symmetry of H_0. This conclusion is suggested by the fact that the perturbation corrections of first order for all the energy levels vanish. All the known examples with real spectrum already satisfy this condition [1–10]. On the other hand, the recently found space–time symmetric Hamiltonians with complex eigenvalues for $|g| > 0$ [19–21] clearly violate it. Although present proof based on PGS and perturbation theory is not as conclusive as one may desire, at least the examples studied so far support it.

In addition to what was said above, there remains the question whether there is a phase transition in those cases where the eigenvalues are real for $0 < g < g_c$. As E increases the critical values of g approach the origin and it is quite difficult to estimate if there is a nonzero limit.

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