Is space-time symmetry a suitable generalization of parity-time symmetry?

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Abstract

We discuss space-time symmetric Hamiltonian operators of the form $H = H_0 + igH'$, where H_0 is Hermitian and g real. H_0 is invariant under the unitary operations of a point group G while H' is invariant under transformation by elements of a subgroup G' of G. If G exhibits irreducible representations of dimension greater than unity, then it is possible that H has complex eigenvalues for sufficiently small nonzero values of g. In the particular case that H is parity-time symmetric then it appears to exhibit real eigenvalues for all $0 < g < g_c$, where g_c is the exceptional point closest to the origin. Point-group symmetry and perturbation theory enable one to predict whether H may exhibit real or complex eigenvalues for $g > 0$. We illustrate the main theoretical results and conclusions of this paper by means of two- and three-dimensional Hamiltonians exhibiting a variety of different point-group symmetries.

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1. Introduction

In the last years there has been great interest in the properties of PT-symmetric multidimensional oscillators[1–9]. Among them we mention the complex versions of the Barbanis[1, 2, 4–6, 8, 9] and Hénon-Heiles[1, 6] Hamiltonians. Several methods have been applied to the calculation of their spectra: the diagonalization method[1–4, 6, 8], perturbation theory[1, 3, 4, 6], classical and semiclassical approaches[1, 2], among others[6, 9]. Typically, those models depend on a potential parameter g so that the Hamiltonian is Hermitian when $g = 0$ and non-Hermitian when $g \neq 0$. Bender and Weir[8] conjectured that the models studied so far may exhibit PT phase transitions so that their spectra are entirely real for sufficiently small but nonzero values of $|g|$. Such phase transitions appear to be a high-energy phenomenon and take place at exceptional points[10–13]. More precisely: as g increases two real eigenvalues approach each other, coalesce at an exceptional point g_c and become a pair of complex conjugate numbers for $g > g_c$. The PT phase transition takes place at the smallest g_c.

Multidimensional oscillators exhibit point-group symmetry (PGS)[14, 15]. Klaiman and Cederbaum[16] were the first to apply PGS to non-Hermitian Hamiltonians of the form $H_0+i\lambda W$ to predict the symmetry of the eigenfunctions associated to the eigenvalues that coalesce at the exceptional points. These authors proposed an interesting approach to study such points in terms of an effective Hermitian operator built from the Hermitian H_0 and non-

Hermitian W parts of the original Hamiltonian operator. They also coined the term space-time symmetry that refers to a class of antiunitary symmetries that contain the PT symmetry as a particular case. The analysis of Klaiman and Cederbaum[16] was restricted to Abelian point groups that exhibit only one-dimensional irreducible representations (irreps).

The main interest in the study of PT-symmetric oscillators has been to enlarge the class of non-Hermitian Hamiltonians that exhibit real spectra, at least for some values of the potential parameter g (or λ). In such cases PT symmetry (or more generally ST symmetry) is broken at the exceptional points g_c already mentioned above which can be efficiently calculated as critical parameters by means of the diagonalization method[17]. The PT phase transition is determined by the smallest $|g_c|$.

By means of PGS Fernández and Garcia[18, 19] found some examples of ST-symmetric multidimensional oscillators that exhibit complex eigenvalues for $g > 0$ so that the phase transition appears to take place at the trivial Hermitian limit $g = 0$. 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[16] based on PGS. In this paper we discuss this point in more detail, improve and extend the results and conclusions of those two papers, and look for more ST-symmetric models with broken ST symmetry for all values of the parameter g that measures the strength of the non-Hermitian part. In Section 2 we argue that perturbation theory is suitable to guess whether ST symmetry is broken at the Hermitian limit $g = 0$ or at an exceptional point $g = g_c > 0$. In Section 3 we outline the main ideas of unitary and antiunitary symmetry in a way that improves

the discussion in the earlier papers[17, 18]. In Section 4 we summarize some well known results about the application of the diagonalization method with symmetry-adapted basis sets. In sections 5 and 6 we illustrate the main ideas of sections 2, 3 and 4 by means of suitably chosen examples in two and three dimensions, respectively. Finally, in Section 7 we summarize the main results and draw conclusions.

2. Perturbation theory

Consider a Hamiltonian operator of the form

$$H(\lambda) = H_0 + \lambda H', \tag{1}$$

where $UH'U^{-1} = -H'$ for some unitary transformation U ($U^{-1} = U^\dagger$). If H_0 is invariant under U ($UH_0U^{-1} = H_0$) then $UH(\lambda)U^{-1} = H(-\lambda)$.

It follows from $H(\lambda)\psi_n(\lambda, \mathbf{r}) = E_n(\lambda)\psi_n(\lambda, \mathbf{r})$ and the expression above that $UH(\lambda)\psi_n(\lambda, \mathbf{r}) = H(-\lambda)U\psi_n(\lambda, \mathbf{r}) = E_n(\lambda)U\psi_n(\lambda, \mathbf{r})$. We appreciate that $U\psi_n(\lambda, \mathbf{r})$ is an eigenfunction $\psi_m(-\lambda, \mathbf{r})$ of $H(-\lambda)$ with eigenvalue $E_m(-\lambda) = E_n(\lambda)$. Since this equality holds for all λ we conclude that $E_n(0) = E_m(0)$. Therefore, if H_0 does not exhibit degenerate eigenfunctions then $m = n$, $E_n(\lambda) = E_n(-\lambda)$, and the perturbation expansion for this eigenvalue will only exhibit even powers of the perturbation parameter:

$$E_n(\lambda) = \sum_{j=0}^{\infty} E_n^{(2j)} \lambda^{2j}. \tag{2}$$

When $\lambda = ig$ is imaginary (g real) this last equation suggests that the eigenvalues of the non-Hermitian operator $H(\lambda)$ may be real for sufficiently small values of $|g|$. Furthermore, if T is the time-reversal operator[20] then $A = TU$

is an antiunitary transformation that leaves the Hamiltonian H invariant $AHA^{-1} = H$ and we say that it is ST symmetric[16]. For a detailed discussion of antiunitary operators see the paper by Wigner[21].

The situation may be quite different when H_0 exhibits degenerate eigenfunctions

$$H_0\psi_{n,i}^{(0)} = E_n^{(0)}\psi_{n,i}^{(0)},\ n = 0, 1, \ldots,\ i = 1, 2, \ldots, \nu_n. \tag{3}$$

If there are nonzero matrix elements of the form

$$H'_{ij} = \left\langle \psi_{n,i}^{(0)} \right| H' \left| \psi_{n,j}^{(0)} \right\rangle \neq 0, 1 \leq i, j \leq \nu_n \tag{4}$$

then some of the perturbation corrections of first order may be nonzero and the corresponding eigenvalues

$$E_{n,j} = E_n^{(0)} + E_{n,j}^{(1)}\lambda + \ldots \tag{5}$$

may be complex, at least for sufficiently small values of $|g|$. In other words: one expects broken ST symmetry for $g > 0$ when H_0 exhibits degenerate eigenfunctions with nonzero matrix elements H'_{ij}. As we will see below, PGS is most helpful for finding such examples.

3. Unitary and antiunitary symmetry

In this paper we consider Hamiltonian operators of the form (1) where $\lambda = ig$, g real. We assume that H_0 is Hermitian and invariant under the operations of the group $G = \{U_1, U_2, \ldots, U_m\}$: $U_i H_0 U_i^{-1} = H_0$ (in this paper we restrict ourselves to point groups[22, 23]). If H' is invariant under the operations of a subgroup $G' = \{W_1, W_2, \ldots, W_k\}$ of G ($W_i H' W_i^{-1} = H'$) then H is invariant under the operations of the point group G'.

Suppose that $U_i H' U_i^{-1} = -H'$, where $U_i \in G \backslash G'$. Then the Hamiltonian exhibits an antiunitary symmetry (space-time symmetry) given by $\hat{A}_i = TU_i$; that is to say, H is invariant under $\hat{A}_i$: $\hat{A}_i H \hat{A}_i^{-1} = H$. Because of this antiunitary symmetry the eigenvalues of H are either real or appear in pairs of complex conjugate numbers. In fact, if ψ is an eigenfunction of H with eigenvalue E and $\hat{A}$ is an antiunitary symmetry of H, then

$$H\hat{A}\psi = \hat{A}\hat{A}^{-1}H\hat{A}\psi = \hat{A}H\psi = E^*\hat{A}\psi. \tag{6}$$

If $\hat{A}\psi = a\psi$ then E is real and we say that the space-time symmetry is unbroken. It may also be possible that $\hat{A}\psi$ is a linear combination of degenerate eigenfunctions of H with eigenvalue E and we arrive at the same conclusion[17]. Klaiman and Cederbaum[16] coined the term space-time symmetry to indicate an antiunitary symmetry $\hat{A} = ST$, where the unitary operator S may be other than the parity operation $P : (x, y, z) \to (-x, -y, -z)$. Obviously, ST symmetry contains PT symmetry as a particular case ($S = P$) and it is understood that in the latter case P belongs to G but not to G'.

Klaiman and Cederbaum[16] argued that in principle one can get an entirely real spectrum for a non-Hermitian Hamiltonian H if H' is chosen such that it transforms as an irrep of the point group or subgroup of H_0. They assumed that the spectrum of H_0 is nondegenerate, thus restricting themselves to Abelian groups with real character tables. This restriction is crucial if H' is to transform as one of the irreps of the point group of H_0 since degenerate states belonging to higher dimensional irreps tend to couple to themselves no matter what irrep one chooses for H'. They also stated that if the non-Abelian point group of H_0 (in the case of a degenerate spectrum) has an Abelian subgroup of order larger than 1, one can still choose H' such that

it transforms under the irreps of the Abelian subgroup and H can still, in principle, have a completely real spectrum. They also pointed out that if one wishes to keep only part of the spectrum of H on the real axis, many more options become available. Fernández and Garcia[19] discussed the non-Hermitian model given by a particle in a square box with the perturbation $H' = xy$. In this case the point group for H_0 is C_{4v} with the Abelian subgroup C_{2v} of order greater than 1. H' transforms as the irrep B_2 of C_{4v} and the irrep A_2 of C_{2v}[22, 23]. However, the spectrum for this model does not appear to be entirely real because some of the eigenvalues are complex for arbitrarily small values of $|g|$.

Because of what we have just discussed, in this paper we are mainly interested in the case that H_0 exhibits degenerate eigenfunctions (3) and G exhibits one or more irreps of dimension greater than one. As argued in Section 2 if there are nonzero matrix elements of the form (4) then some of the perturbation corrections of first order are nonzero and the corresponding eigenvalues (5) are complex for small values of $|g|$. If $\psi_{n,j}^{(0)}$ and H' belong to the irreps Γ_n and $\Gamma_{H'}$, respectively, then the matrix elements H'_{ij} may be nonzero if the decomposition of the reducible representation $\Gamma_n \otimes \Gamma_n \otimes \Gamma_{H'}$ contains the totally symmetric irrep[22, 23]. Since $\psi_{n,i}^{(0)} \psi_{n,j}^{(0)}$ is invariant under P, then H'_{ij} vanishes unless H' is also parity invariant $PH'P = H'$. Therefore, under the latter condition it is likely that an ST-symmetric Hamiltonian may exhibit complex eigenvalues for sufficiently small values of $|g|$. On the other hand, all the PT-symmetric Hamiltonians studied so far exhibit real eigenvalues for $0 \leq g < g_c$. This point has already been discussed in two recent papers[18, 19].

In addition to the unitary and antiunitary symmetries outlined above it is worth considering possible dynamical symmetries. If O is an Hermitian operator that commutes with H_0 and $\psi^{(0)}$ is an eigenfunction of the latter with eigenvalue $E^{(0)}$ then $O\psi^{(0)}$ is also eigenfunction of H_0 with the same eigenvalue as follows from $H_0 O\psi^{(0)} = OH_0\psi^{(0)} = E^{(0)}O\psi^{(0)}$. If, in addition, $\psi^{(0)}$ and $O\psi^{(0)}$ belong to different irreps of the point group G for H_0 then the dimension of some of the eigenspaces of this operator cannot be explained solely by PGS (see [24–28] and the references therein).

4. Diagonalization method

Throughout this paper we calculate the eigenvalues of the non-Hermitian operator H by means of three approaches: the Riccati-Padé method[29, 30], a collocation method[31, 32], and the straightforward diagonalization method[1–4, 6, 8] that consists in obtaining the eigenvalues of a truncated matrix representation of the Hamiltonian operator in a suitable basis set. Commonly, one chooses a complete set of orthonormal functions $F = \{f_1, f_2, \ldots\}$ which we can split into subsets of symmetry-adapted functions $F^S = \{f_1^S, f_2^S, \ldots\}$ for each irrep S[22, 23]. Instead of diagonalizing and $M \times M$ matrix representation $\mathbf{H}$ of the Hamiltonian operator in the basis set F we diagonalize $M_S \times M_S$ matrix representations $\mathbf{H}^S$ ($M_S < M$) of H in each basis set F^S. This strategy not only enables us to reduce the dimension of the matrices to be diagonalized but also facilitates the interpretation of the results[18, 19].

Every eigenfunction of H that belongs to the irrep S can be written as a linear combination of the complete set of functions of the corresponding

symmetry:

$$\psi^S = \sum_j c_j^S f_j^S. \tag{7}$$

Suppose that $\hat{A} = UT$ is an antiunitary symmetry of H such that the space transformation U changes the symmetry of the basis set according to

$$U f_j^S = \sum_k d_{kj}^{S'S} f_k^{S'}, \tag{8}$$

and that $T f_j^S = f_j^S$. Therefore, $\hat{A}\psi^S = \psi^{S'}$ and $H\hat{A}\psi^S = E^{S'}\hat{A}\psi^S$. On the other hand, Equation (6) tells us that $HA\psi^S = \left(E^S\right)^* A\psi^S$ and we conclude that $E^{S'} = \left(E^S\right)^*$ under the conditions just stated. We will see some examples of this result in sections 5 and 6.

5. Two-dimensional models

In this section we consider some two-dimensional examples of the Hamiltonian (1). In order to discuss and illustrate their main ideas Klaiman and Cederbaum[16] chose $H_0 = \frac{1}{2}\left(p_x^2 + p_y^2\right) + \alpha_x x^4 + \alpha_y y^4$. When $\alpha_x \neq \alpha_y$ the point group G for H_0 is C_{2v} (they chose D_{2h}^{2D}) with only one-dimensional irreps and the numerical results suggest that the eigenvalues are real for $0 < g < g_c$, where g_c is the exceptional point closest to the origin. In this section we consider closely related models with different PGS.

The first set of examples that we discuss in what follows is based on the Hermitian part

$$H_0 = p_x^2 + p_y^2 + x^4 + y^4, \tag{9}$$

which is invariant under the operations $\{E, C_4, C_4^2 = C_2, C_4^3, \sigma_v, \sigma_v', \sigma_d, \sigma_d'\}$ of the symmetry point group C_{4v} shown in Table 1. If $\phi_n(q)$ is an eigenfunction

of $p_q^2 + q^4$ with eigenvalue ϵ_n then $\varphi_{m\,n}(x,y) = \phi_m(x)\phi_n(y)$ is eigenfunction of H_0 with eigenvalue $E^{(0)}_{mn} = \epsilon_m + \epsilon_n$. Linear combinations of these eigenfunctions are bases for the irreps of the point group C_{4v} according to the following scheme:

$$\begin{array}{ll} \varphi_{2m\,2m} & A_1 \\ \varphi_{2m+1\,2m+1} & B_2 \\ \varphi^{+}_{2m\,2n} & A_1 \\ \varphi^{-}_{2m\,2n} & B_1 \ , \\ \varphi^{+}_{2m+1\,2n+1} & B_2 \\ \varphi^{-}_{2m+1\,2n+1} & A_2 \\ \{\varphi_{2m\,2n+1}, \varphi_{2n+1\,2m}\} & E \end{array} \tag{10}$$

where

$$\varphi^{\pm}_{m\,n} = \frac{1}{\sqrt{2}} \left(\varphi_{m\,n} \pm \varphi_{n\,m}\right), \ m \neq n. \tag{11}$$

According to Equation (10) we expect one-dimensional eigenspaces of symmetry A_1, A_2, B_1, B_2 and two-dimensional ones of symmetry E. This is the degeneracy predicted by the geometrical symmetry of the Hamiltonian operator.

The Hermitian operator

$$O = p_x^2 + x^4 - p_y^2 - y^4, \tag{12}$$

commutes with H_0 and connects functions of different symmetry as follows from

$$O\varphi^{\pm}_{m\,n} = \left(\epsilon_m - \epsilon_n\right) \varphi^{\mp}_{m\,n}. \tag{13}$$

Since O belongs to the irrep B_1, $B_1 \otimes B_2 = A_2$ and $B_1 \otimes B_1 = A_1$, then some functions of symmetry $A_1(A_2)$ are degenerate with functions of symmetry

$B_1(B_2)$. Similar dynamical symmetries for simpler, exactly solvable, two-dimensional models have been discussed elsewhere[25, 26].

The first eigenvalues of the Hermitian Hamiltonian (9) calculated by means of the Riccati-Padé method[29, 30] shown in Table 3 illustrate the two types of degeneracy (geometrical and dynamical) just discussed.

If we add the perturbation $H' = xy$ then the suitable point group G' results to be C_{2v} that we modify in order to make it compatible with the C_{4v} for H_0. The corresponding modified character table is shown in Table 2 (compare it with the one in the standard textbooks[22, 23]). The reflection operators in the C_{4v} point group are defined as $\sigma_v : (x, y) \to (-x, y)$, $\sigma_v^{'} : (x, y) \to (x, -y)$, $\sigma_d : (x, y) \to (y, x)$ and $\sigma_d' : (x, y) \to (-y, -x)$. Therefore, the antiunitary symmetries $\hat{A}_1 = T\sigma_v$ and $\hat{A}_2 = T\sigma_v'$, which satisfy $\hat{A}_j^2 = 1$, leave H invariant: $\hat{A}_j H \hat{A}_j = H$, $j = 1, 2$. In this example of ST symmetry the rotation operation $C_2 : (x, y) \to (-x, -y)$ plays the role of the parity one and leaves the perturbation invariant $C_2 H' C_2 = H'$.

It is worth noting that we use the symbols σ_d and σ_d' instead of the usual σ_v and σ_v' for the reflection planes in the modified character table C_{2v} in Table 2. The reason is that we have to define the unitary operations of the point group C_{2v} so that $H' = xy$ belongs to the totally symmetric irrep A_1. The point group C_{2v} shown in Table 2 plays the role of the subgroup G' introduced in the general discussion of Section 3. On the other hand, H' belongs to the irrep A_2 of the subgroup C_{2v} that we obtain by choosing the reflection planes σ_v and σ_v'. It is clear that in this example H' belongs to an irrep of an Abelian subgroup of order greater than 1 of the point group for H_0. Therefore, H should have real eigenvalues according to Klaiman and

Cederbaum[16].

$H' = xy$ belongs to the irrep B_2 of the point group C_{4v}. Since $E \otimes E = A_1 \oplus A_2 \oplus B_1 \oplus B_2$ we conclude that two degenerate eigenfunctions of H_0 that are basis for the irrep E will lead to nonzero perturbation corrections of first order and, according to the discussion in Section 2, to complex eigenvalues. More precisely, the perturbation will split a pair of degenerate eigenfunctions E of H_0 into eigenfunctions B_1 and B_2 of H as follows from straightforward inspection of the character tables 1 and 2. Note that (x, y) is basis for the irrep E of C_{4v} and $x+y$ and $x-y$ are bases for B_1 and B_2, respectively, of the modified C_{2v}. Besides, it is clear from $\sigma_v(x+y) = -x+y$ and $\sigma'_v(x+y) = x-y$ that $\hat{A}_j \psi^{B_1}$ belongs to the irrep B_2; therefore $E_n^{B_1} = \left(E_m^{B_2}\right)^*$ as argued in section 4.

On the other hand, the perturbation corrections of first order for the pairs of degenerate states (A_1, B_1) and (A_2, B_2) (coming from dynamical symmetry) vanish as shown, for example, by $\left\langle \varphi^{A_1} \right| H' \left| \varphi^{A_1} \right\rangle = \left\langle \varphi^{B_1} \right| H' \left| \varphi^{B_1} \right\rangle = \left\langle \varphi^{A_1} \right| H' \left| \varphi^{B_1} \right\rangle = 0$. Consequently, the resulting eigenfunctions of H may have real eigenvalues for sufficiently small values of $|g|$.

By means of projection operators[22, 23] we easily prove that the connection between the eigenfunctions of H_0 and those of H is given by the following scheme:

$$\begin{aligned} A_1 &\rightarrow A_1 \\ A_2 &\rightarrow A_2 \\ B_1 &\rightarrow A_2 \\ B_2 &\rightarrow A_1 \end{aligned}$$

$$E \rightarrow B_1, B_2 \tag{14}$$

As pointed out in section 4, in order to obtain the eigenvalues of the models discussed in this paper we resort to two independent methods: a collocation method[31, 32] and diagonalization of a truncated matrix representation $\mathbf{H}$ of the Hamiltonian operator in a suitable basis set. For the two-dimensional anharmonic oscillators discussed in this section we choose the set of eigenfunctions of $H_{HO} = p_x^2 + p_y^2 + x^2 + y^2$. It is worth noting that the coefficients of the characteristic polynomial $|\mathbf{H} - E\mathbf{I}| = 0$, where $\mathbf{I}$ is the identity matrix, are real when we use the complete basis set, as discussed by Fernández[33]. On the other hand, if we resort to symmetry-adapted basis sets F^{B_1} and F^{B_2} as discussed in section 3, then the coefficients of the characteristic polynomials are complex[18, 19]. Here we diagonalize matrix representations $\mathbf{H}^S$ of the Hamiltonian operator using symmetry-adapted basis functions for the irreps $S = A_1, A_2, B_1, B_2$ of the C_{2v} point group of Table 2.

The eigenvalues with eigenfunctions of symmetry A_1 and A_2 are real for sufficiently small values of g. Pairs of them approach each other and coalesce at exceptional points g_c. For $g > g_c$ they become pairs of complex conjugate numbers. On the other hand, the eigenvalues with eigenfunctions of symmetry B_1 and B_2, which emerge from the irrep E of C_{4v}, appear to be complex for all $g > 0$. This result, like the one in reference [19], also appears to contradict the conjecture of Klaiman and Cederbaum[16] outlined in section 3.

In the case of Hermitian operators there is the well known non-crossing rule[34, 35] that states that two eigenvalues with eigenfunctions of the same

symmetry do not cross when they are plotted as functions of a parameter in the Hamiltonian operator. In the case of non-Hermitian operators, on the other hand, there is the coalescence rule that states that only eigenvalues with eigenfunctions of the same symmetry coalesce. This rule is clearly illustrated by the states with symmetry A_1 and A_2 and is an obvious consequence of the fact that we can group the states into different subspaces according to their PGS.

We can easily construct other models based on the same H_0 that exhibit broken ST symmetry for sufficiently small $|g|$. For example, $H' = xy^3$ is a linear combination of functions of symmetry A_2 ($xy(x^2 - y^2)$) and B_2 ($xy(x^2 + y^2)$) of the point group C_{4v} and is also invariant under parity (C_2 in this case). In addition to it, H exhibits the same antiunitary symmetries $\hat{A}_1 = T\sigma_v$ and $\hat{A}_2 = T\sigma_v'$ discussed above. However, in this case H' is invariant under the unitary operations $\{E, C_2\}$ of the point group C_2 with irreps $\{A, B\}$ (see Table 4), where we have obviously chosen $C_2 : (x, y) \to (-x, -y)$. Because of the perturbation the symmetry of the eigenfunctions changes in the following way: $\{A_1, A_2, B_1, B_2\} \to A$, $E \to B$. In this case the perturbation splits pairs of degenerate eigenfunctions of H_0 of symmetry E into eigenfunctions of H that belong to the irrep B and have complex conjugate eigenvalues. The characteristic polynomial $\left|\mathbf{H}^B - E\mathbf{I}\right| = 0$ exhibits real coefficients but complex roots. The eigenvalues with eigenfunctions of symmetry A are real for sufficiently small values of g and pairs of them coalesce at exceptional points as discussed above. On the other hand, the eigenvalues with eigenfunctions of symmetry B are complex for sufficiently small values of $g > 0$. However, some pairs of complex conjugate eigenvalues

exhibit an interesting behaviour. For example, the two complex eigenvalues that stem from $E^{(0)} \approx 12.7$ become real at $g \approx 0.064096$, separate, then approach each other and coalesce at $g \approx 1.08979$ becoming complex again for larger g. This surprising behaviour was not observed in the earlier papers on ST-symmetric Hamiltonians with complex eigenvalues[18, 19].

A slight modification of the perturbation leads to completely different results. For example, $H' = xy^2$ belongs to the irrep E of the point group C_{4v} and H results to be invariant under the unitary transformations $\{E, \sigma\}$ of the point group C_s, where $\sigma : (x, y) \to (x, -y)$. The irreps for C_s are A' and A'' as shown in Table 5. In this case H is PT symmetric, where $P = C_2$, and the perturbation connects the symmetry of the eigenfunctions of H_0 and H in the following way:

$$\begin{aligned} A_1 &\to A' \\ A_2 &\to A'' \\ B_1 &\to A' \\ B_2 &\to A'' \\ E &\to A', A''. \end{aligned} \tag{15}$$

Since the four matrix elements of H' between a pair of E eigenfunctions of H_0 vanish, then the perturbation corrections of first order also vanish and the eigenvalues are expected to be real for $0 \leq g < g_c$. Numerical results confirm our argument based on point-group symmetry and perturbation theory: all the eigenvalues are real for sufficiently small values of g. As g increases pairs of eigenvalues coalesce at exceptional points as expected; however some of them exhibit an interesting behaviour. For example, one of the A' eigenvalues

stemming from $E^{(0)} \approx 27.59$ and one stemming from $E^{(0)} \approx 27.91$ approach each other and coalesce. They become a pair of complex conjugate numbers for some values of g and then separate again as real eigenvalues. One of the resulting branches and the other real eigenvalue stemming from $E^{(0)} \approx 27.59$ coalesce at another exceptional point. On the other hand, the other branch and an eigenvalue stemming from $E^{(0)} \approx 30.33$ coalesce at another exceptional point.

We can also build a non-Hermitian oscillator with unbroken ST symmetry by reducing the geometrical symmetry of H_0. If we choose $H_0 = p_x^2 + p_y^2 + \alpha_x x^4 + \alpha_y y^4$, with $\alpha_x \neq \alpha_y$, the point group for H_0 is C_{2v} with only one-dimensional irreps. Let us consider, for example, the perturbation $H' = xy$ that is invariant under parity (C_2). In this case H is invariant under the antiunitary transformations $\hat{A}_1 = T\sigma_v$ and $\hat{A}_2 = T\sigma_v'$ already introduced above and, therefore, ST symmetric. However, in this case all the perturbation corrections of first order vanish and numerical calculations suggest that the eigenvalues of this Hamiltonian are real for all $0 \leq g < g_c$[16].

We can construct other interesting models by enclosing oscillators in boxes with impenetrable walls and suitable geometries. For example,

$$H_0 = p_x^2 + p_y^2, \tag{16}$$

with the boundary conditions $\psi(\pm 1, y) = 0$ and $\psi(x, \pm 1) = 0$ (square box of length $L = 2$). In this case we can also choose C_{4v} to describe the symmetry of the Hermitian part. When $H' = xy^2$ the eigenvalues are real for all $0 \leq g < g_c$, while $H' = xy$ produces complex eigenvalues of symmetry B_1 and B_2 for sufficiently small $g > 0$. These two models have already been discussed by Fernández and Garcia[19]. On the other hand, $H' = xy^3$

leads to complex conjugate eigenvalues of symmetry B for small $g > 0$ but some pairs of them separate into real ones, then approach each other and coalesce again at exceptional points. Since the symmetry of the Hermitian and non-Hermitian parts is identical to the examples discussed above the behaviour of the eigenvalues for the box models and the anharmonic oscillators is quite similar. The main difference is that in the case of the box models the exceptional points appear at much larger values of g.

The two dimensional isotropic harmonic oscillator

$$H_0 = p_x^2 + p_y^2 + x^2 + y^2, \tag{17}$$

is invariant under the two-dimensional rotation group (we can choose the $C_{\infty v}$ point group[22, 23]). In this case we draw the same conclusions as before. When $H' = xy^2$ we have the non-Hermitian version of the Barbanis Hamiltonian that has been widely studied[1, 2, 4–6, 8, 9]. Numerical calculations based on the diagonalization method, perturbation theory and other approaches suggest that its eigenvalues are real for all $0 \leq g < g_c$, where g_c is the exceptional point closest to the origin. If, on the other hand, $H' = xy$ then some of the eigenvalues of the resulting exactly-solvable model are complex for all g[18].

The models discussed in this section clearly show that ST symmetry does not guarantee a real spectrum unless $S = P$. Note that of all the perturbations studied above only $H' = xy^2$ satisfies this condition.

6. Three-dimensional models

We first consider the Hermitian Hamiltonian oscillator

$$H_0 = p_x^2 + p_y^2 + p_z^2 + \alpha_x x^4 + \alpha_y y^4 + \alpha_z z^4, \tag{18}$$

where α_x, α_y and α_z are real and positive. If the three potential parameters α_q are different then this operator is invariant under the unitary transformations of the point group C_i. Since its eigenfunctions belong to the one-dimensional irreps A_g and B_g, one expects the eigenvalues of any space-time symmetric Hamiltonian H built from it to have real eigenvalues for some interval of parameter values $0 \leq g < g_c$. If, for example, $\alpha_x = \alpha_y \neq \alpha_z$ then H_0 is invariant under the operations of the point group C_{4v} and we expect results similar to those discussed in Section 5; that is to say: for some non-Hermitian perturbations the eigenvalues may be complex for sufficiently small $g > 0$.

Therefore, the most interesting case seems to be $\alpha_x = \alpha_y = \alpha_z = \alpha$ and without loss of generality in what follows we choose $\alpha = 1$. In such a case H_0 is invariant under the unitary transformations of the point group O_h shown in Table 6. The degeneracy of the energy levels of a quantum-mechanical model with this PGS has been recently discussed[27, 28].

If $\{i, j, k\}_P$ denotes all distinct permutations of the subscripts in the eigenfunctions of H_0 $\varphi_{i\,j\,k}(x, y, z) = \phi_i(x)\phi_j(y)\phi_k(z)$, $i, j, k = 0, 1, \ldots$, then their symmetry and dimension of the eigenspaces are given by (see reference [27] for a discussion of another quantum-mechanical problem with the same PGS):

$$
\begin{array}{ll}
\{2n, 2n, 2n\} & A_{1g} \\
\{2n+1, 2n+1, 2n+1\} & A_{2u} \\
\{2n+1, 2n+1, 2m\}_P & T_{2g} \\
\{2n, 2n, 2m+1\}_P & T_{1u} \\
\{2n, 2n, 2m\}_P & A_{1g}, E_g \\
\{2n+1, 2n+1, 2m+1\}_P & A_{2u}, E_u \\
\{2n, 2m, 2k\}_P & A_{1g}, A_{2g}, E_g, E_g \\
\{2n+1, 2m+1, 2k+1\}_P & A_{1u}, A_{2u}, E_u, E_u \\
\{2n, 2m, 2k+1\}_P & T_{1u}, T_{2u} \\
\{2n+1, 2m+1, 2k\}_P & T_{1g}, T_{2g}
\end{array} \quad . \tag{19}
$$

The dynamical symmetries that are responsible for the degeneracy of eigenfunctions belonging to different irreps (which cannot be explained by PGS) are given by the Hermitian operators

$$
\begin{aligned}
O_1 &= 2p_x^2 + 2x^4 - p_y^2 - y^4 - p_z^2 - z^4 \\
O_2 &= 2p_y^2 + 2y^4 - p_x^2 - x^4 - p_z^2 - z^4,
\end{aligned} \tag{20}
$$

which belong to the irrep E_g. In order to obtain them we simply apply the projection operator P^{E_g} to the two pairs of functions (x^2, y^2) and (x^4, y^4) as discussed elsewhere[27].

If we take into account that $T_{1g} \otimes T_{1g} = T_{2g} \otimes T_{2g} = T_{1u} \otimes T_{1u} = T_{2u} \otimes T_{2u} = A_{1g} \oplus E_g \oplus T_{1g} \oplus T_{2g}$, then we realize that a perturbation H' belonging to the irrep T_{2g} will split those degenerate energy levels and produce complex eigenvalues for sufficiently small $g > 0$. According to the character table in Table 6, any linear combination of the functions xy, xz and yz will suffice. If, for example, we choose $H' = z(x + y)$, then the Hamiltonian H is

invariant under the antiunitary transformations $\hat{A}_1 = C_2' T$ and $\hat{A}_2 = \sigma_h T$, where $C_2' : (x, y, z) \to (-x, -y, z)$ and $\sigma_h : (x, y, z) \to (x, y, -z)$. The resulting space-time invariant Hamiltonian H is also invariant under the unitary transformations of the point group C_{2h} if we choose them in the following way: $C_2 : (x, y, z) \to (-y, -x, -z)$, $\hat{\imath} : (x, y, z) \to (-x, -y, -z)$ and $\sigma_h : (x, y, z) \to (y, x, z)$ as shown in Table 7. Note that H' is invariant under parity inversion $P = \hat{\imath}$.

The connection between the eigenfunctions of H_0 and H is given by

$$\begin{aligned}
A_{1g} &\to A_g \\
A_{2g} &\to B_g \\
E_g &\to A_g, B_g \\
T_{1g} &\to A_g, 2B_g \\
T_{2g} &\to 2A_g, B_g \\
A_{1u} &\to A_u \\
A_{2u} &\to B_u \\
E_u &\to A_u, B_u \\
T_{1u} &\to A_u, 2B_u \\
T_{2u} &\to 2A_u, B_u,
\end{aligned} \tag{21}$$

and those corresponding to the three-dimensional irreps will produce complex eigenvalues for $g > 0$ as argued above. Equations (19) and (21) together summarize the splitting of the energy levels of an O_h Hermitian Hamiltonian by a C_{2h} non-Hermitian perturbation.

Table 8 shows the lowest eigenvalues of H_0 calculated by means of the

Riccati-Padé method[29, 30] and the quantum numbers of their corresponding states. The eigenvalue stemming from $E^{(0)} \approx 3.18$ of symmetry A_g is real for all g. The next one starting at $E^{(0)} \approx 5.92$ splits into one real A_u and two complex B_u. The next one at $E^{(0)} \approx 8.66$ gives rise to one real eigenvalue B_g and two complex ones A_g. The next one at $E^{(0)} \approx 9.58$ leads to three real eigenvalues: two A_g and one B_g. The two real eigenvalues B_g approach each other and coalesce at an exceptional point $g_c \approx 1.0713$ where they become a pair of complex conjugate numbers. The next eigenvalue at $E^{(0)} \approx 11.40$ is real and B_u. The sixth-dimensional eigenspace for $E^{(0)} \approx 12.32$ consists of three functions T_{1u} and three T_{2u}. The former split into two complex eigenvalues A_u and one real B_u. The latter split into two complex B_u and one real A_u. The two real eigenvalues B_u just mentioned approach each other and coalesce at an exceptional point $g_c \approx 1.3064$. The eigenfunctions of symmetry T_{1u} with eigenvalue $E^{(0)} \approx 13.77$ are most interesting. They split into two complex B_u and one real A_u; however the two complex B_u eigenvalues become real at $g \approx 0.018578$, separate and then approach each other to coalesce at an exceptional point $g_c \approx 0.83161$. We have already encountered this behaviour in one of the two-dimensional examples discussed in section 5.

Another model with the same symmetry is given by

$$H_0 = p_x^2 + p_y^2 + p_z^2, \tag{22}$$

with the boundary conditions $\psi(\pm 1, y, z) = \psi(x, \pm 1, z) = \psi(x, y, \pm 1) = 0$. The point group for this system is also O_h and was discussed in detail by Fernández[27] and Hernández-Castillo and Lemus[28]. The dimensionless

eigenvalues and eigenfunctions are

$$\begin{aligned} E_{n_1n_2n_3} &= \frac{\pi^2}{4}(n_1^2+n_2^2+n_3^2) \\ \psi_{n_1n_2n_3}(x,y,z) &= \sin\left[\frac{n_1\pi(x+1)}{2}\right]\sin\left[\frac{n_2\pi(y+1)}{2}\right]\sin\left[\frac{n_3\pi(z+1)}{2}\right], \end{aligned} \tag{23}$$

where $n_1, n_2, n_3 = 1, 2, \ldots$. The symmetry of the eigenfunctions is similar to the scheme in equation (19) by substituting $(2n_1 - 1, 2n_2 - 1, 2n_3 - 1)$ for $(2m, 2n, 2k)$ and $(2n_1, 2n_2, 2n_3)$ for $(2m + 1, 2n + 1, 2k + 1)$ [27].

Obviously, the same parity-invariant non-Hermitian perturbations discussed above lead to complex eigenvalues for $g \neq 0$. However, in this case we can easily calculate the perturbation corrections of first order analytically and show which eigenvalues are complex when $g \neq 0$. For example, for $H' = z(x + y)$ we easily obtain the following perturbation expansions for the eigenvalues:

$$\begin{aligned} \{1,1,1\} &\rightarrow \frac{3\pi^2}{4} + O(\lambda^2) \\ \{1,1,2\}_p &\rightarrow \begin{cases} \frac{3\pi^2}{2} - \frac{1024\sqrt{2}\lambda}{81\pi^4} + O(\lambda^2) \\ \frac{3\pi^2}{2} + O(\lambda^2) \\ \frac{3\pi^2}{2} + \frac{1024\sqrt{2}\lambda}{81\pi^4} + O(\lambda^2) \end{cases} \\ \{1,2,2\}_p &\rightarrow \begin{cases} \frac{9\pi^2}{4} - \frac{1024\sqrt{2}\lambda}{81\pi^4} + O(\lambda^2) \\ \frac{9\pi^2}{4} + O(\lambda^2) \\ \frac{9\pi^2}{4} + \frac{1024\sqrt{2}\lambda}{81\pi^4} + O(\lambda^2) \end{cases} \\ \{1,1,3\}_p &\rightarrow \begin{cases} \frac{11\pi^2}{4} + O(\lambda^2) \\ \frac{11\pi^2}{4} + O(\lambda^2) \\ \frac{11\pi^2}{4} + O(\lambda^2) \end{cases} \end{aligned}$$

$$
\begin{aligned}
\{2,2,2\} &\rightarrow 3\pi^2 + O(\lambda^2) \\
\{1,2,3\}_p &\rightarrow \begin{cases}
\frac{7\pi^2}{2} - \frac{1024\sqrt{922066}\lambda}{50625\pi^4} + O(\lambda^2) \\
\frac{7\pi^2}{2} - \frac{1024\sqrt{922066}\lambda}{50625\pi^4} + O(\lambda^2) \\
\frac{7\pi^2}{2} + O(\lambda^2) \\
\frac{7\pi^2}{2} + O(\lambda^2) \\
\frac{7\pi^2}{2} + \frac{1024\sqrt{922066}\lambda}{50625\pi^4} + O(\lambda^2) \\
\frac{7\pi^2}{2} + \frac{1024\sqrt{922066}\lambda}{50625\pi^4} + O(\lambda^2)
\end{cases} \\
\{2,2,3\}_p &\rightarrow \begin{cases}
\frac{17\pi^2}{4} - \frac{9216\sqrt{2}}{625\pi^4} + O(\lambda^2) \\
\frac{17\pi^2}{4} + O(\lambda^2) \\
\frac{17\pi^2}{4} + \frac{9216\sqrt{2}}{625\pi^4} + O(\lambda^2)
\end{cases} ,
\end{aligned}
\tag{24}
$$

for the first eigenvalues. Those states with nonzero perturbation correction of first order are expected to be complex for sufficiently small $|g|$. The splitting of the energy levels of H_0 by the perturbation H' is also summarized by equations (19) and (21) with the substitutions already mentioned above. For example, the three eigenfunctions of order zero generated by the label permutations $\{1,1,2\}_P$ are basis for the irrep T_{1u} when $g = 0$ and split into two B_u with complex conjugate eigenvalues and one A_u with real eigenvalue.

7. Conclusions

Throughout this paper we have discussed non-Hermitian Hamiltonian operators of the form (1) where the Hermitian and non-Hermitian parts exhibit several different PGS. In each case we have clearly indicated how the energy levels of H_0 behave when the perturbation is turned on. The nature of the resulting eigenvalues of H depend on the symmetry of both H_0 and H'. PGS and perturbation theory enable us to predict whether there is a chance

that the eigenvalues of H are real for some values of the strength parameter g. If the perturbation correction of first order is nonzero for at least one state then we expect complex eigenvalues for sufficiently small $|g|$. Complex eigenvalues may become real for some values of g but it is unlikely that such intervals overlap to produce an island of real eigenvalues for all the states of the model. It is worth noting that space-time symmetry only tells us that the eigenvalues of the non-Hermitian Hamiltonian are either real or appear in pairs of complex conjugate numbers. On the other hand, the analysis based on perturbation theory provides a much clearer indication of whether there is any chance that the eigenvalues are real for sufficiently small nonzero values of g.

One of the main conclusions of this paper is that ST symmetry is not a satisfactory generalization of PT symmetry, except when the full point group of symmetry for H_0 is Abelian. An ST-symmetric Hamiltonian may exhibit complex eigenvalues for sufficiently small $|g|$ when the unitary operation S is different from the parity inversion P. On the other hand, PT symmetry has led to real eigenvalues for all $0 < g < g_c$ in all the cases studied so far.

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Table 1: Character table for C_{4v} point group

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$		
A_1	1	1	1	1	1	z	x^2+y^2, z^2
A_2	1	1	1	-1	-1	R_z	
B_1	1	-1	1	1	-1		x^2-y^2
B_2	1	-1	1	-1	1		xy
E	2	0	-2	0	0	$(x,y)(R_x,R_y)$	(xz,yz)

Table 2: Character table for the modified C_{2v} point group

C_{2v}	E	C_2	σ_d	σ_d'		
A_1	1	1	1	1		x^2+y^2, xy
A_2	1	1	-1	-1		x^2-y^2
B_1	1	-1	1	-1	$x+y$	
B_2	1	-1	-1	1	$x-y$	

Table 3: First eigenvalues of H_0 (9)

$E_{n_1 n_2}$	n_1	n_2
2.1207241809683657991	0	0
4.8600351202855770683	0	1
4.8600351202855770683	1	0
7.5993460596027883375	1	1
8.5160600284709212917	0	2
8.5160600284709212917	2	0
11.255370967788132561	1	2
11.255370967788132561	2	1
12.70510760186234492	0	3
12.70510760186234492	3	0
14.911395875973476784	2	2
15.444418541179556189	1	3
15.444418541179556189	3	1
17.322188109334408837	0	4
17.322188109334408837	4	0
19.100443449364900413	2	3
19.100443449364900413	3	2

Table 4: Character table for C_2 point group

C_2	E	C_2		
A	1	1		x^2, y^2, xy
B	1	-1	x, y	

Table 5: Character table for C_s point group

C_s	E	σ		
A'	1	1	x	x^2, y^2
A''	1	-1	y	xy

Table 6: Character table for O_h point group

O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_2(=C_4^2)$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$		
A1g	1	1	1	1	1	1	1	1	1	1		$x^2+y^2+z^2$
A2g	1	1	-1	-1	1	1	-1	1	1	-1		
Eg	2	-1	0	0	2	2	0	-1	2	0		$(2z^2-x^2-y^2, x^2-y^2)$
T1g	3	0	-1	1	-1	3	1	0	-1	-1	(R_x, R_y, R_z)	
T2g	3	0	1	-1	-1	3	-1	0	-1	1	(xz, yz, xy)	
A1u	1	1	1	1	1	-1	-1	-1	-1	-1		
A2u	1	1	-1	-1	1	-1	1	-1	-1	1		
Eu	2	-1	0	0	2	-2	0	1	-2	0		
T1u	3	0	-1	1	-1	-3	-1	0	1	1	(x, y, z)	
T2u	3	0	1	-1	-1	-3	1	0	1	-1		

Table 7: Character table for C_{2h} point group

C_{2h}	E	C_2	i	σ_h		
A_g	1	1	1	1		$x^2+y^2, z(x+y), xy, z^2$
B_g	1	-1	1	-1		$x^2-y^2, z(x-y)$
A_u	1	1	-1	-1	$x-y$	
B_u	1	-1	-1	1	$x+y, z$	

Table 8: First eigenvalues of H_0 (18) with $\alpha_x = \alpha_y = \alpha_z = 1$.

$E_{n_1 n_2 n_3}$	n_1	n_2	n_3
3.1810862714525486987	0	0	0
5.9203972107697599679	0	0	1
5.9203972107697599679	0	1	0
5.9203972107697599679	1	0	0
8.6597081500869712372	0	1	1
8.6597081500869712372	1	0	1
8.6597081500869712372	1	1	0
9.5764221189551041913	0	0	2
9.5764221189551041913	0	2	0
9.5764221189551041914	2	0	0
11.399019089404182506	1	1	1
12.31573305827231546	1	0	2
12.31573305827231546	1	2	0
12.31573305827231546	2	0	1
12.31573305827231546	2	1	0
12.31573305827231546	0	1	2
12.31573305827231546	0	2	1
13.76546969234652782	0	0	3
13.76546969234652782	0	3	0