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. Among them we mention the complex versions of the Barbanis and Hénon-Heiles Hamiltonians. Several methods have been applied to the calculation of their spectra: the diagonalization method, perturbation theory, classical and semiclassical approaches, among others. 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 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. 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). Klaiman and Cederbaum 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\cite{11} 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 $\lambda$). 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\cite{17}. The PT
phase transition is determined by the smallest $|g_c|$.

By means of PGS Fernández and García\cite{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 sym-
metry is not as robust as the PT one and contradict some of the conjectures
put forward by Klaiman and Cederbaum\cite{11} based on PGS. In this paper we
discuss this point in more detail, improve and extend the results and con-
cclusions 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\cite{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

\[ H(\lambda) = H_0 + \lambda H', \]

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 \( H(\lambda)\psi_n(\lambda, r) = E_n(\lambda)\psi_n(\lambda, r) \) and the expression above that \( UH(\lambda)\psi_n(\lambda, r) = H(-\lambda)U\psi_n(\lambda, r) = E_n(\lambda)U\psi_n(\lambda, r) \). We appreciate that \( U\psi_n(\lambda, r) \) is an eigenfunction \( \psi_m(-\lambda, r) \) of \( H(-\lambda) \) with eigenvalue \( E_m(-\lambda) = E_n(\lambda) \). Since this equality holds for all \( \lambda \) 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:

\[ E_n(\lambda) = \sum_{j=0}^{\infty} E_n^{(2j)}(\lambda)^{2j}. \]

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\cite{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\cite{16}. For a detailed discussion of antiunitary operators see the paper by Wigner\cite{21}.

The situation may be quite different when $H_0$ exhibits degenerate eigenfunctions

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

If there are nonzero matrix elements of the form

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

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

$$E_{n,j} = E_{n}^{(0)} + E_{n,j}^{(1)} \lambda + \ldots$$  \hfill (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 \hfill (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\cite{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 $U_i \in G \setminus G'$. 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 $\psi$ is an eigenfunction of $H$ with eigenvalue $E$ and $\hat{A}$ is an antiunitary symmetry of $H$, then

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

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. Klaiman and Cederbaum 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 $P: (x, y, z) \rightarrow (-x, -y, -z)$. 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 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 $\psi_{n,i}(0)$ and $H'$ belong to the irreps $\Gamma_n$ 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 $0 < g < g_c$. 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 $H_0O\psi^{(0)} = OH_0\psi^{(0)} = E^{(0)}O\psi^{(0)}$. 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 $F^S = \{f^S_1, f^S_2, \ldots\}$ for each irrep $S$ [22, 23]. Instead of diagonalizing and $M \times M$ matrix representation $H$ of the Hamiltonian operator in the basis set $F$ we diagonalize $M_S \times M_S$ matrix representations $H^S (M_S < M)$ 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:

\[ \psi^S = \sum_j c_j^S f_j^S. \]  

(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

\[ U f_j^S = \sum_k d_{kj}^S S f_k^S, \]  

(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 \( HA\psi^S = (E^S)^* A\psi^S \) and we conclude that \( E^{S'} = (E^S)^* \) 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

\[ H_0 = p_x^2 + p_y^2 + x^4 + y^4, \]  

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

$$
\begin{align*}
\varphi_{2m,2m} & \quad A_1 \\
\varphi_{2m+1,2m+1} & \quad B_2 \\
\varphi_{2m,2n} & \quad A_1 \\
\varphi_{2m,2n} & \quad B_1 \\
\varphi_{2m+1,2n+1} & \quad B_2 \\
\varphi_{2m+1,2n+1} & \quad A_2 \\
\{\varphi_{2m,2n+1}, \varphi_{2n+1,2m}\} & \quad E
\end{align*}
$$

(10)

where

$$
\varphi_{m,n}^\pm = \frac{1}{\sqrt{2}} (\varphi_{m,n} \pm \varphi_{n,m}), \quad m \neq n.
$$

(11)

According to Equation (11) 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

$$
O = p_x^2 + x^4 - p_y^2 - y^4,
$$

(12)

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

$$
O \varphi_{m,n}^\pm = (\epsilon_m - \epsilon_n) \varphi_{m,n}^\mp.
$$

(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 $A_1(A_2)$. 

10
$B_1(B_2)$. Similar dynamical symmetries for simpler, exactly solvable, two-dimensional models have been discussed elsewhere\cite{25, 26}.

The first eigenvalues of the Hermitian Hamiltonian \cite{9} calculated by means of the Riccati-Padé method\cite{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\cite{22, 23}). The reflection operators in the $C_{4v}$ point group are defined as $\sigma_v : (x, y) \rightarrow (-x, y)$, $\sigma'_v : (x, y) \rightarrow (x, -y)$, $\sigma_d : (x, y) \rightarrow (y, x)$ and $\sigma'_d : (x, y) \rightarrow (-y, -x)$. 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 $C_2 : (x, y) \rightarrow (-x, -y)$ 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 $\sigma_d$ and $\sigma'_d$ instead of the usual $\sigma_v$ and $\sigma'_v$ 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 $\sigma_v$ and $\sigma'_v$. 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 \((x + y, x - y)\) 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 \( E_{nB_1} = (E_{mB_2})^* \) 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 \( \langle \varphi^{A_1} | H' | \varphi^{A_1} \rangle = \langle \varphi^{B_1} | H' | \varphi^{B_1} \rangle = 0 \). 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:

\[
\begin{align*}
A_1 & \rightarrow A_1 \\
A_2 & \rightarrow A_2 \\
B_1 & \rightarrow A_2 \\
B_2 & \rightarrow A_1
\end{align*}
\]
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 and diagonalization of a truncated matrix representation $H$ 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 $H_{HO} = \frac{p_x^2}{2} + \frac{p_y^2}{2} + x^2 + y^2$. It is worth noting that the coefficients of the characteristic polynomial $|H - EI| = 0$, where $I$ is the identity matrix, are real when we use the complete basis set, as discussed by Fernández. 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. Here we diagonalize matrix representations $H^S$ 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 outlined in section 3.

In the case of Hermitian operators there is the well known non-crossing rule 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 antiumitary 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 $C_2 : (x, y) \rightarrow (-x, -y)$. Because of the perturbation the symmetry of the eigenfunctions changes in the following way: $\{A_1, A_2, B_1, B_2\} \rightarrow A, E \rightarrow B$. 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 $|H^B - EI| = 0$ 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 $\sigma: (x, y) \rightarrow (x, -y)$. 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:

\[
\begin{array}{ccc}
A_1 & \rightarrow & A' \\
A_2 & \rightarrow & A'' \\
B_1 & \rightarrow & A' \\
B_2 & \rightarrow & A'' \\
E & \rightarrow & A', A''
\end{array}
\]  

(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,

\[
H_0 = p_x^2 + p_y^2,
\]

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

$$H_0 = p_x^2 + p_y^2 + x^2 + y^2, \quad (17)$$

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 Barbánis 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

$$H_0 = p_x^2 + p_y^2 + p_z^2 + \alpha_x x^4 + \alpha_y y^4 + \alpha_z z^4, \quad (18)$$
where \( \alpha_x, \alpha_y \) and \( \alpha_z \) are real and positive. If the three potential parameters \( \alpha_q \) 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 \( H_0 \varphi_{ijk}(x, y, z) = \phi_i(x)\phi_j(y)\phi_k(z), i, j, k = 0, 1, \ldots, \) 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):

\[ \begin{align*}
\end{align*} \]
\begin{align*}
\{2n, 2n, 2n\} & \quad A_{1g} \\
\{2n + 1, 2n + 1, 2n + 1\} & \quad A_{2u} \\
\{2n + 1, 2n + 1, 2m\}_P & \quad T_{2g} \\
\{2n, 2n, 2m + 1\}_P & \quad T_{1u} \\
\{2n, 2n, 2m\}_P & \quad A_{1g}, E_g \\
\{2n + 1, 2n + 1, 2m + 1\}_P & \quad A_{2u}, E_u \\
\{2n, 2m, 2k\}_P & \quad A_{1g}, A_{2g}, E_g, E_g \\
\{2n + 1, 2m + 1, 2k + 1\}_P & \quad A_{1u}, A_{2u}, E_u, E_u \\
\{2n, 2m, 2k + 1\}_P & \quad T_{1u}, T_{2u} \\
\{2n + 1, 2m + 1, 2k\}_P & \quad T_{1g}, T_{2g}
\end{align*}

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{align*}
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{align*}

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. \cite{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 \ref{table:character_table}, 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 $C'_2 : (x, y, z) \rightarrow (-x, -y, z)$ and $\sigma_h : (x, y, z) \rightarrow (x, y, -z)$. 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: $C_2 : (x, y, z) \rightarrow (-y, -x, -z)$, $\hat{i} : (x, y, z) \rightarrow (-x, -y, -z)$ and $\sigma_h : (x, y, z) \rightarrow (y, x, z)$ as shown in Table 7. Note that $H'$ is invariant under parity inversion $P = \hat{i}$.

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

\[
\begin{align*}
A_{1g} & \rightarrow A_g \\
A_{2g} & \rightarrow B_g \\
E_g & \rightarrow A_g, B_g \\
T_{1g} & \rightarrow A_g, 2B_g \\
T_{2g} & \rightarrow 2A_g, B_g \\
A_{1u} & \rightarrow A_u \\
A_{2u} & \rightarrow B_u \\
E_u & \rightarrow A_u, B_u \\
T_{1u} & \rightarrow A_u, 2B_u \\
T_{2u} & \rightarrow 2A_u, B_u,
\end{align*}
\]

(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 N 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 [3].

Another model with the same symmetry is given by

$$H_0 = p_x^2 + p_y^2 + p_z^2,$$

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
\[
E_{n_1n_2n_3} = \frac{\pi^2}{4}(n_1^2 + n_2^2 + n_3^2)
\]
\[
\psi_{n_1n_2n_3}(x,y,z) = \sin \left( \frac{n_1 \pi (x + 1)}{2} \right) \sin \left( \frac{n_2 \pi (y + 1)}{2} \right) \sin \left( \frac{n_3 \pi (z + 1)}{2} \right),
\]
(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:

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

\[
\begin{align*}
\{2, 2, 2\} & \rightarrow \begin{cases} 
\frac{7\pi^2}{2} - \frac{1024\sqrt{922066}\lambda}{50625\pi^4} + O(\lambda^2) \\
\frac{7\pi^2}{2} - \frac{1024\sqrt{922066}\lambda}{50625\pi^4} + O(\lambda^2) 
\end{cases} \\
\{1, 2, 3\}_p & \rightarrow \begin{cases} 
\frac{7\pi^2}{2} + O(\lambda^2) \\
\frac{7\pi^2}{2} + O(\lambda^2) \\
\frac{7\pi^2}{2} + \frac{1024\sqrt{922066}\lambda}{50625\pi^4} + O(\lambda^2) \\
\frac{7\pi^2}{2} + \frac{1024\sqrt{922066}\lambda}{50625\pi^4} + O(\lambda^2) 
\end{cases} \\
\{2, 2, 3\}_p & \rightarrow \begin{cases} 
\frac{17\pi^2}{4} - \frac{9216\sqrt{7}}{625\pi^4} + O(\lambda^2) \\
\frac{17\pi^2}{4} + O(\lambda^2) \\
\frac{17\pi^2}{4} + \frac{9216\sqrt{7}}{625\pi^4} + O(\lambda^2)
\end{cases} 
\]

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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References

[1] C. M. Bender, G. V. Dunne, P. N. Meisinger, and M. Simsek, Quantum complex Hénon-Heiles potentials, Phys. Lett. A 281 (2001) 311-316.

[2] A. Nanayakkara and C. Abayaratne, Semiclassical quantization of complex Henon-Heiles systems, Phys. Lett. A 303 (2002) 243-248.

[3] A. Nanayakkara, Real eigenspectra in non-Hermitian multidimensional Hamiltonians, Phys. Lett. A 304 (2002) 67-72.

[4] A. Nanayakkara, Comparison of quantal and classical behavior of PT-symmetric systems at avoided crossings, Phys. Lett. A 334 (2005) 144-153.

[5] H. Bíla, M. Tater, and M. Znojil, Comment on: ”Comparison of quantal and classical behavior of PT-symmetric systems at avoided crossings” [Phys. Lett. A 334 (2005) 144], Phys. Lett. A 351 (2006) 452-456.

[6] Q-H Wang, Level crossings in complex two-dimensional potentials, Pramana J. Phys. 73 (2009) 315-322.

[7] F. Cannata, M. V. Ioffe, and D. N. Nishnianidze, Exactly solvable non-separable and nondiagonalizable two-dimensional model with quadratic complex interaction, J. Math. Phys. 51 (2010) 022108.

[8] C. M. Bender and D. J. Weir, PT phase transition in multidimensional quantum systems, J. Phys. A 45 (2012) 425303.

[9] C. R. Handy and D. Vrincenau, Orthogonal polynomial projection quantization: a new Hill determinant method, J. Phys. A 46 (2013) 135202.
[10] W. D. Heiss and A. L. Sannino, Avoided level crossing and exceptional points, J. Phys. A 23 (1990) 1167-1178.

[11] W. D. Heiss, Repulsion of resonance states and exceptional points, Phys. Rev. E 61 (2000) 929-932.

[12] W. D. Heiss and H. L. Harney, The chirality of exceptional points, Eur. Phys. J. D 17 (2001) 149-151.

[13] W. D. Heiss, Exceptional points - their universal occurrence and their physical significance, Czech. J. Phys. 54 (2004) 1091-1099.

[14] R. A. Pullen and A. R. Edmonds, Comparison of classical and quantal spectra for a totally bound potential, J. Phys. A 14 (1981) L477-L484.

[15] R. A. Pullen and A. R. Edmonds, Comparison of classical and quantal spectra for the Hénon-Heiles potential, J. Phys. A 14 (1981) L319-L327.

[16] S. Klaiman and L. S. Cederbaum, Non-Hermitian Hamiltonians with space-time symmetry, Phys. Rev. A 78 (2008) 062113. See also: Erratum: Non-Hermitian Hamiltonians with space-time symmetry [Phys. Rev. A 78, 062113 (2008)], Phys. Rev. A 89 (2014) 039908(E).

[17] F. M. Fernández and J. Garcia, Critical parameters for non-hermitian Hamiltonians, arXiv:1305.5164 [math-ph].

[18] F. M. Fernández and J. Garcia, Non-Hermitian Hamiltonians with unitary and antiunitary symmetries, Ann. Phys. 342 (2014) 195-204.
[19] F. M. Fernández and J. Garcia, PT-symmetry broken by point-group symmetry, J. Math. Phys. 55 (2014) 042107. arXiv:1308.6179v2 [quant-ph].

[20] C. E. Porter, Fluctuations of quantal spectra, in: C. E. Porter (Ed.), Statistical theories of spectra: fluctuations, Vol. Academic Press Inc., New York and London, 1965.

[21] E. Wigner, Normal Form of Antiunitary Operators, J. Math. Phys. 1 (1960) 409-413.

[22] M. Tinkham, Group Theory and Quantum Mechanics, (McGraw-Hill Book Company, New York, 1964).

[23] F. A. Cotton, Chemical Applications of Group Theory, (John Wiley & Sons, New York, 1990).

[24] H. V. McIntosh, On Accidental Degeneracy in Classical and Quantum Mechanics, Am. J. Phys. 27 (1959) 620-625.

[25] F. Leyvraz, A. Frank, R. Lemus, and M. V. Andrés, Accidental degeneracy in a simple quantum system: A new symmetry group for a particle in an impenetrable square-well potential, Am. J. Phys. 65 (1997) 1087-1094.

[26] R. Lemus, A. Frank, M. V. Andrés, and F. Leyvraz, Accidental degeneracy and hidden symmetry: Rectangular wells with commensurate sides, Am. J. Phys. 66 (1998) 629-631.
[27] F. M. Fernández, On the symmetry of the quantum-mechanical particle in a cubic box, arXiv:1310.5136 [quant-ph].

[28] A. O. Hernández-Castillo and R. Lemus, Symmetry group of an impenetrable cubic well potential, J. Phys. A 46 (2013) 465201.

[29] F. M. Fernández, Q. Ma, and R. H. Tipping, Tight upper and lower bounds for energy eigenvalues of the Schrödinger equation, Phys. Rev. A 39 (1989) 1605-1609.

[30] F. M. Fernández, Q. Ma, and R. H. Tipping, Eigenvalues of the Schrödinger equation via the Riccati-Padé method, Phys. Rev. A 40 (1989) 6149-6153.

[31] P. Amore and F. M. Fernández, Variational collocation for systems of coupled anharmonic oscillators, Phys. Scr. 81 (2010) 045011.

[32] P. Amore, F. M. Fernández, and M. Rodriguez, Comment on 'Coupled anharmonic oscillators: the Raileigh-Ritz approach versus the collocation approach', Phys. Scr. 83 (2011) 047003.

[33] F. M. Fernández, On the real matrix representation of PT-symmetric operators, arXiv:1301.7639v3 [quant-ph].

[34] M. Teller, The Crossing of Potential Surfaces, J. Phys. Chem. 41 (1937) 109-116.

[35] K. Razi Naqvi and W. Byers Brown, The non-crossing rule in molecular quantum mechanics, Int. J. Quantum Chem. 6 (1972) 271-279.
Table 1: Character table for $C_{4v}$ point group

| $C_{4v}$ | $E$ | $2C_4$ | $C_2$ | $2\sigma_v$ | $2\sigma_d$ | $x^2 + y^2, z^2$ |
|-----------|-----|--------|-------|-------------|-------------|----------------|
| $A_1$     | 1   | 1      | 1     | 1           | 1           | $z$            |
| $A_2$     | 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

| $C_{2v}$ | $E$ | $C_2$ | $\sigma_d$ | $\sigma'_d$ | $x^2 + y^2$ |
|-----------|-----|-------|-------------|-------------|-------------|
| $A_1$     | 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 $H_0$ \[9\]

| $E_{n_1n_2}$ | $n_1$ | $n_2$ |
|-------------|-------|-------|
| 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

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

30
### Table 5: Character table for $C_s$ point group

| $C_s$ | $E$ | $\sigma$ |
|-------|-----|---------|
| $A'$  | 1   | 1 $x$  |
| $A''$ | 1   | -1 $y$ |

### Table 6: Character table for $O_h$ point group

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

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

| $C_{2h}$ | $E$ | $C_2$ | $i$ | $\sigma_h$ |
|----------|-----|-------|-----|-----------|
| $A_g$    | 1   | 1 1   | 1   | 1         |
| $B_g$    | 1   | -1 1  | -1  | 1         |
| $A_u$    | 1   | 1 -1  | -1  | 1         |
| $B_u$    | 1   | -1 -1 | 1   | 1         |

$x^2 + y^2, z(x + y), xy, z^2$

$x^2 - y^2, z(x - y)$

$x - y$

$x + y, z$
Table 8: First eigenvalues of $H_0$ with $\alpha_x = \alpha_y = \alpha_z = 1$.

| $E_{n_1n_2n_3}$ | $n_1$ | $n_2$ | $n_3$ |
|------------------|-------|-------|-------|
| 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     |