PT-symmetry broken by point-group symmetry

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We discuss a PT-symmetric Hamiltonian with complex eigenvalues. It is based on the dimensionless Schrödinger equation for a particle in a square box with the PT-symmetric potential $V(x,y) = iaxy$. Perturbation theory clearly shows that some of the eigenvalues are complex for sufficiently small values of $|a|$. Point-group symmetry proves useful to guess if some of the eigenvalues may already be complex for all values of the coupling constant. We confirm those conclusions by means of an accurate numerical calculation based on the diagonalization method. On the other hand, the Schrödinger equation with the potential $V(x,y) = iaxy^2$ exhibits real eigenvalues for sufficiently small values of $|a|$. Point group symmetry suggests that PT-symmetry may be broken in the former case and unbroken in the latter one.

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I. INTRODUCTION

It was shown some time ago that some complex non-Hermitian Hamiltonians may exhibit real eigenvalues\[1, 2\]. The conjecture that such intriguing feature may be due to unbroken PT-symmetry\[3\] gave rise to a very active field of research\[4\] (and references therein). The first studied PT-symmetric models were mainly one-dimensional anharmonic oscillators\[3–6\] and lately the focus shifted towards multidimensional problems\[7–14\]. Among the most widely studied multidimensional PT-symmetric models we mention the complex versions of the Barbanis\[7, 8, 10–14\] and Hénon-Heiles\[7, 12\] Hamiltonians. Several methods have been applied to the calculation of their spectra: the diagonalization method\[7–10, 12, 13\], perturbation theory\[7, 9, 10, 12\], classical and semiclassical approaches\[7, 8\], among others\[12, 14\]. 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\[13\] conjectured that some of those models may exhibit phase transitions so that their spectra are real for sufficiently small values of $|g|$. Such phase transitions appear to be a high-energy phenomenon.

Multidimensional oscillators exhibit point-group symmetry (PGS)\[15, 16\]. As far as we know such a property has not been taken into consideration in those earlier studies of the PT-symmetric models, except for the occasional parity in one of the variables. It is more than likely that PGS may be relevant to the study of the spectra of multidimensional PT-symmetric Hamiltonians. This paper is expected to be a useful contribution in that direction.

The research on non-Hermitian Hamiltonians has been mainly focused on finding models with real spectrum. It is our purpose to show an example of PT-symmetric Hamiltonian with complex eigenvalues; a Hamiltonian with the
phase transition at the Hermitian limit $g = 0$. We will also show that PGS provides a simple and clear explanation of why the eigenvalues of such model are complex and not real as the other problems discussed so far.

In section II we consider the dimensionless Schrödinger equation for a particle in a square box with the potential $iaxy$ that is obviously PT-symmetric. In section III we show that perturbation theory predicts that some of the eigenvalues are complex for sufficiently small values of $|a|$. In section IV we analyze the eigenfunctions of the unperturbed and perturbed Hamiltonians from the point of view of PGS and show why some eigenvalues are expected to be complex. In section V we obtain the eigenvalues and eigenfunctions accurately by means of the diagonalization method and confirm the conclusions of the preceding sections. In section VI we consider the particle in a square box with the potential $iaxy^2$ that resembles part of the potential of the PT-symmetric version of the Barbanis Hamiltonian. In this case PGS shows that PT symmetry may not be broken for sufficiently small values of $|a|$. This conclusion is confirmed by the diagonalization method. Finally, in section VII we summarize the main results of the paper, draw conclusions and put forward a somewhat general recipe for the appearance of complex eigenvalues in a given multidimensional non-Hermitian Hamiltonian.

II. BOX MODEL WITH $C_{2v}$ POINT-GROUP SYMMETRY

We first consider the Schrödinger equation $H \psi = E \psi$ with the dimensionless Hamiltonian operator

$$ H = p_x^2 + p_y^2 + gxy, \quad (1) $$

and the boundary conditions

$$ \psi(\pm 1, y) = 0, \quad \psi(x, \pm 1) = 0. \quad (2) $$

This Hamiltonian is Hermitian when $g$ is real and PT-symmetric when $g$ is imaginary. In fact, when $g = ia$, a real, the Hamiltonian is invariant under two antiunitary transformations[17]

$$ A_x H A_x = H, \quad A_y H A_y = H \quad (3) $$
generated by $A_x = P_x T$ and $A_y = P_y T$, where $T$ is the time-reversal operator[18] and $P_x$ and $P_y$ are the parity transformations

$$ P_x : (x, y, px, py) \rightarrow (-x, y, -px, py), $$

$$ P_y : (x, y, px, py) \rightarrow (x, -y, px, -py). \quad (4) $$

It follows from equation (3) that

$$ H A_x \psi = A_x H \psi = A_x E \psi = E^* A_x \psi. \quad (5) $$

That is to say, if $\psi$ is eigenfunction of $H$ with eigenvalue $E$ then $A_x \psi$ is eigenfunction with eigenvalue $E^*$. Obviously, the same conclusion applies to $A_y \psi$. When PT symmetry is unbroken

$$ A_x \psi = \lambda \psi, \quad |\lambda| = 1, \quad (6) $$
the corresponding eigenvalue is real\cite{4}. In a recent paper we have shown that the eigenvalue may be real even when this condition is manifestly violated\cite{21}. Later on we will discuss this point in more detail. All the Hamiltonians studied previously exhibit unbroken PT symmetry for sufficiently small values of $|g|$\cite{7–14}. In what follows we show that the model depicted above behaves in a quite different way.

### III. PERTURBATION THEORY

When $g = 0$ the eigenvalues and eigenfunctions of the simple model described in the preceding section are those of the particle in a square box

$$E_{mn}^{(0)} = \frac{(m^2 + n^2) \pi^2}{4}, \quad m, n = 1, 2, \ldots,$$

$$\psi_{mn}^{(0)}(x, y) = \varphi_{mn}(x, y) = \sin \left( \frac{m\pi(x + 1)}{2} \right) \sin \left( \frac{n\pi(y + 1)}{2} \right),$$

and we appreciate that the eigenfunctions with $m \neq n$ are two-fold degenerate. There are accidental degeneracies that occur when $m_1^2 + n_1^2 = m_2^2 + n_2^2$ but they are not relevant for the present discussion. For example, the three eigenfunctions $\psi_{7,1}^{(0)}$, $\psi_{1,7}^{(0)}$ and $\psi_{5,5}^{(0)}$ share the same eigenvalue but only the first two ones are consequence of the symmetry of the problem.

By means of perturbation theory it is quite easy to prove that some of the eigenvalues are complex for sufficiently small values of $|a|$. The perturbation correction of first order $E_{mn}^{(1)}$ vanishes when $n = m + 2j$, $j = 0, 1, \ldots$ but it is nonzero if $n = m + 2j + 1$:

$$E_{mn}^{(1)+} = \frac{256m^2(2j + m + 1)^2}{\pi^4 (2j + 1)^4 (2j + 2m + 1)^4},$$

$$E_{mn}^{(1)-} = -\frac{256m^2(2j + m + 1)^2}{\pi^4 (2j + 1)^4 (2j + 2m + 1)^4}.\quad (8)$$

It is clear that for sufficiently small values of $|a|$ these levels behave approximately as linear functions of $g = ia$. In other words, the phase transition takes place at the Hermitian limit $a = 0$. This result is different from that for the PT-symmetric oscillators studied so far that exhibit a vanishing perturbation correction of first order\cite{7, 12}.

### IV. POINT-GROUP SYMMETRY

We can understand the occurrence of complex eigenvalues more clearly from the point of view of PGS. Since the model is two-dimensional its behaviour with respect to the coordinate $z$ is irrelevant and, consequently, the choice of the point group is not unique. For the description of the unperturbed model $g = 0$ we choose the point group $C_{4v}$ with symmetry operations

$$E : (x, y) \to (x, y),$$

$$C_4 : (x, y) \to (y, -x),$$

$$C_4^3 : (x, y) \to (-y, x).$$
\[ C_2 : (x, y) \rightarrow (-x, -y), \]
\[ \sigma_{v1} : (x, y) \rightarrow (y, x), \]
\[ \sigma_{v2} : (x, y) \rightarrow (-y, -x), \]
\[ \sigma_{d1} : (x, y) \rightarrow (x, -y), \]
\[ \sigma_{d2} : (x, y) \rightarrow (-x, y), \]

where \( C_n^k \) is a rotation by an angle \( 2\pi k/n \) around an axis perpendicular to the center of the square box \((C_2^2 = C_2)\) and \( \sigma_v \) and \( \sigma_d \) are vertical reflection planes\[19, 20\]. For simplicity we omit the transformation of the momenta when it is similar to that of the coordinates. The eigenfunctions form bases for the irreducible representations \( \{ A_1, A_2, B_1, B_2, E \} \) as indicated below

\[
A_1 : \{ \varphi_{2m-12n-1} \}, \{ \varphi_{2m-12n-1}^+ \},
A_2 : \{ \varphi_{2m-2n}^- \},
B_1 : \{ \varphi_{2m-2n}^+ \}, \{ \varphi_{2m-2n}^- \},
B_2 : \{ \varphi_{2m-12n-1}^- \},
E : \{ \varphi_{2m-12n-1}^+, \varphi_{2m-12n-1}^- \},
\]
\[
\varphi_{m,n}^\pm = \frac{1}{\sqrt{2}} (\varphi_{mn} \pm \varphi_{nm})
\]
\[ m, n = 1, 2, \ldots. \]

(10)

As expected some pairs of two-fold degenerate eigenfunctions form bases for the irreducible representation \( E \). In addition to it, pairs of eigenfunctions with symmetry \( A_1 \) and \( B_2 \) \( (\varphi_{2m-12n-1}^+, \varphi_{2m-12n-1}^-) \) as well as \( A_2 \) and \( B_1 \) \( (\varphi_{2m-2n}^-, \varphi_{2m-2n}^+) \) are also degenerate.

When \( g \neq 0 \) a suitable point group is \( C_{2v} \), with symmetry operations \( \{ E, C_2, \sigma_{v1}, \sigma_{v2} \} \) and irreducible representations \( \{ A_1, A_2, B_1, B_2 \} \). The eigenfunctions are linear combinations of the form

\[
\psi_{A1} = \sum_{m, n} (a_{mn}^{A1} \varphi_{2m-12n-1} + b_{mn}^{A1} \varphi_{2m-2n} + c_{mn} \varphi_{2m-12n-1}^+ + d_{mn} \varphi_{2m-2n}^+ )
\]
\[
\psi_{A2} = \sum_{m, n} (a_{mn}^{A2} \varphi_{2m-12n-1}^- + b_{mn}^{A2} \varphi_{2m-2n}^-)
\]
\[
\psi_{B1} = \sum_{m, n} (a_{mn}^{B1} \varphi_{2m-12n-1}^+ + b_{mn}^{B1} \varphi_{2m-2n}^+)\]
\[
\psi_{B2} = \sum_{m, n} (a_{mn}^{B2} \varphi_{2m-12n-1}^- + b_{mn}^{B2} \varphi_{2m-2n}^-) \]

(11)

It is clear that the perturbation removes the degeneracy in such a way that the two-fold degenerate unperturbed eigenfunctions \( E \) become the perturbed eigenfunctions of symmetry \( B_1 \) and \( B_2 \). As a result, every eigenvalue \( E_{B_1} \) is the complex conjugate of an eigenvalue \( E_{B_2} \) \( (E_{B_2} = E_{B_1}^*) \). As shown in the preceding section, the degeneracy of these levels is removed at first order of perturbation theory and it is not difficult to verify that the pair of integrals \( \langle \varphi_{2m-2n}^\pm | xy | \varphi_{2m-2n}^\pm \rangle \) give us exactly the perturbation corrections in equation (8). On the other hand, the degenerate unperturbed eigenfunctions of symmetry \( A_1, A_2, B_1 \) and \( B_2 \) become the perturbed eigenfunctions of symmetry \( A_1 \) and \( A_2 \). In this case the perturbation correction of first order vanishes and the degeneracy is removed at least at second order. If, as in the case of the models studied earlier by other authors, all the perturbation corrections of odd order vanish\[8, 12\], then we may expect real eigenvalues for sufficiently small values of \(|a|\).
PGS gives us a clear description of the occurrence of complex eigenvalues. If we take into account equation (5) and that
\[ A_x \varphi_{2m-1,2n} = -\varphi_{2m-1,2n} \]
then we realize that
\[ A_x \psi = \lambda \psi \]
We appreciate that PT symmetry is broken for all \( |g| \neq 0 \) and that \( E_{B_2} = E_{B_1}^* \) as mentioned above. However, in principle it may be possible that both
eigenvalues were real and degenerate as in the case of the rigid rotor studied in an earlier paper\[21\]. In the present case we know that they are complex as shown in section III. If we apply the same reasoning to the eigenfunctions of symmetry \( A_1 \) and \( A_2 \) we realize that PT-symmetry may not be broken for them because \( A_x \psi^{A_1} = \lambda^{A_1} \psi^{A_1} \) and \( A_x \psi^{A_2} = \lambda^{A_2} \psi^{A_2} \) (where \( |\lambda| = 1 \)) that follows from the fact that the symmetry-adapted basis functions are invariant or merely change sign under this antiunitary operation (and also under \( A_y \)).

V. DIAGONALIZATION METHOD

We can obtain sufficiently accurate eigenvalues and eigenfunctions of the box model by means of the diagonalization method. Diagonalization of the Hamiltonian matrix \( H \) in the basis set \( \{ \varphi_{mn} \} \) gives us the lowest eigenvalues of the Hamiltonian operator as well as the coefficients of the expansion of the eigenfunctions in the basis set
\[ \psi = \sum_m \sum_n a_{mn} \varphi_{mn}. \] (12)
Alternatively, we can diagonalize Hamiltonian matrices \( H^S \) for each of the irreducible representations \( S = A_1, A_2, B_1, B_2 \) of the point group \( C_{2v} \) and thus obtain the corresponding sets of eigenfunctions separately. In this case the dimension of the resulting secular equations is noticeably smaller.

It is well known that the coefficients of the characteristic polynomial generated by the full matrix \( H \) are real\[22\]. The coefficients of the characteristic polynomials generated by \( H^{A_1} \) and \( H^{A_2} \) are polynomial functions of \( g^2 \) and therefore real. On the other hand, the coefficients of the characteristic polynomials generated by the matrices \( H^{B_1} \) and \( H^{B_2} \) are polynomial functions of \( g \) and therefore complex.

Figure 1 shows the real and imaginary parts of the first eigenvalues of the Hamiltonian for a wide range of values of \( a \). The eigenvalues for symmetry \( A_1 \) and \( A_2 \) are real for sufficiently small values of \( a \). Some pairs of them coalesce at critical values \( a_c \) of the coupling constant and emerge as pairs of complex numbers for \( a > a_c \). This occurrence of exceptional points is similar to that already found for other two-dimensional models\[7–14\]. On the other hand, the eigenvalues for symmetry \( B_1 \) and \( B_2 \) are complex for all values of \( a \). This kind of eigenvalues does not appear in those non-Hermitian Hamiltonians studied earlier. We say that the PT-symmetric Hamiltonian exhibits a PT phase transition at the trivial Hermitian limit.

VI. BOX MODEL WITH C₂ POINT-GROUP SYMMETRY

In order to illustrate the difference between present PT-symmetric model and those studied earlier, in this section we choose the particle in a square box with the interaction potential
\[ V(x, y) = g x y^2 \] (13)
that resembles the one in the Barbanis Hamiltonian\[2, 8, 10–14\]. In this case we may choose the point group \( C_2 \) with symmetry operations \( \{ E, C_2 \} \), where \( C_2 : (x, y) \rightarrow (x, -y) \). The bases for the irreducible representations \( \{ A, B \} \) are
\{\varphi_{m,2n}\}$ and \{\varphi_{m,2n}\}, respectively. The antiunitary operator \(A = P_x T\), where \(P_x : (x, y, p_x, p_y) \rightarrow (-x, y, -p_x, p_y)\), leaves the Hamiltonian invariant when \(g = ia\), a real. It follows from \(A \varphi_{m, n} = (-1)^{m+1} \varphi_{m, n}\) and equation (3) that it is possible that \(A \psi^A = \lambda A \psi^A\) and \(A \psi^B = \lambda B \psi^B\); that is to say symmetry may be unbroken and the eigenvalues may be real for sufficiently small values of \(|a|\). This observation is consistent with the fact that the perturbation correction of first order vanishes for all the states which suggests that the perturbation expansion exhibits only even powers of \(g\) as in the case of the Barbanis Hamiltonian \(7, 12\).

The main features of the spectrum of this model resemble those described in earlier problems. For those that are bases for some irreducible representations \((B_1\) and \(B_2\) in the present case). We may formulate the main ideas in a somewhat more general way. In general, the eigenfunctions are of the form

\[\psi^S = \sum_j C_j^S \varphi_j^S\]  

(14)

where \(S\) is an irreducible representation of the point group for the model. If \(A \varphi_j^S = \lambda_j^S \varphi_j^S\), were \(A\) is an antiunitary operation that leaves the Hamiltonian invariant, then it is possible that \(A \psi^S = \lambda S \psi^S\) (unbroken PT symmetry) and the corresponding eigenvalues are real. All the models studied before exhibit this property \(7-14\). The eigenfunctions of symmetry \(A_1\) and \(A_2\) of present \(C_{2v}\) model also behave in this way. The situation is quite different in the case of the eigenfunctions of symmetry \(B_1\) and \(B_2\) that we may generalize it in the following way: when \(A \varphi_j^{S'} = \lambda_k^{S'} \varphi_k^{S'}\) where \(S' \neq S\) then PT symmetry is broken \(A \psi^S = \lambda_{SS'} \psi^{S'}\) and \(E_S = E_{S'}\). However, this relationship is not a rigorous proof that the eigenvalues are complex. In a recent paper we have shown that the eigenvalues of a PT symmetric rigid rotor are real even when PT-symmetry is broken as just indicated \(21\). In the case of present \(C_{2v}\) model the eigenvalues are in fact complex and for this reason we have decided to coin the term **PT-symmetry broken by PGS**.
In closing, we want to put forward an additional argument. Let $H_R$ and $H_I$ be the real and imaginary parts of the non-Hermitian Hamiltonian $H$, and assume that $H_R$ is invariant under the inversion operator $\hat{i}: (x, p) \to (-x, -p)$. Then the product $\varphi_i \varphi_j$ of degenerate eigenfunctions of $H_R$ is invariant under $\hat{i}$ as shown by the character tables of the symmetry point groups [19, 20]. Under such conditions, if $iH_I i = -H_I$ then $\langle \varphi_i | H_I | \varphi_j \rangle = 0$ and the perturbation correction of first order vanishes. The non-Hermitian Hamiltonian $H$ is invariant under the antiunitary operator $A = IT$ and it is possible that the spectrum be real. If, on the other hand, $iH_I i = H_I$ then some of the perturbation corrections of first order for the degenerate states may not vanish and the corresponding eigenvalues are expected to be complex.

In section IV $C_2$ plays the role of $\hat{i}$ and we appreciate that both $H_R = p_x^2 + p_y^2$ and $H_I = ax y$ are invariant under $C_2$. For this reason there are complex eigenvalues even though the non-Hermitian Hamiltonian is invariant under $A_x$ and $A_y$ (it is not invariant under $A$). On the other hand, the inversion operation changes the sign of the potential in equation [13] and the perturbation corrections of first order for all the states vanish. In this case the non-Hermitian Hamiltonian is invariant under $A$ and exhibits real spectrum for sufficiently small values of $a$.

It seems that the argument about unbroken PT symmetry [4] applies to the antiunitary operator $A$ and not to other antiunitary operators like $A_x$ and $A_y$.

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FIG. 1: First eigenvalues of the model (1)

FIG. 2: First eigenvalues of the model (13)