Non-Hermitian Hamiltonians with space-time symmetry

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(Received 5 August 2008; published 29 December 2008)

The spectrum of non-Hermitian Hamiltonians is studied using the point-group symmetries of the Hermitian and non-Hermitian parts of the Hamiltonian. We show that, in principle, the symmetry properties of the Hamiltonian are responsible for the appearance of real eigenvalues in the spectrum of the non-Hermitian Hamiltonian. In practice, however, one must take into account the "strength" of the non-Hermitian part of the Hamiltonian. An effective energy-dependent Hermitian Hamiltonian is constructed that has the same real spectrum as the non-Hermitian Hamiltonian. Several properties, including the self-orthogonality of the states at branch points of the spectrum, are proven using this effective representation. An interesting possibility of complex eigenvalues returning to the real axis is exemplified along with several examples of non-Hermitian Hamiltonians with real eigenvalues.

DOI: 10.1103/PhysRevA.78.062113 PACS number(s): 03.65.−w

I. INTRODUCTION

Non-Hermitian Hamiltonians have been widely used in many fields in order to describe the dynamics of a reduced system. These effective Hamiltonians gain from the encapsulation of many degrees of freedom into a non-Hermitian operator, thus making the remaining degrees of freedom tractable both computationally and conceptually. The exact method by which the effective non-Hermitian Hamiltonian is constructed varies according to the application at hand, but in general this can be done either rigorously (usually by some projection into a subspace) or phenomenologically.

Since the introduction of parity and time-reversal symmetric Hamiltonians, briefly referred to as $\mathcal{PT}$-symmetric Hamiltonians, by Bender and Boettcher [1], a new class of non-Hermitian Hamiltonians have been drawing a great deal of attention. For a recent review, see [2] and references therein. As later classified by Mostafazadeh [3], $\mathcal{PT}$-symmetric Hamiltonians are a special case of pseudo-Hermitian Hamiltonians, which are Hamiltonians that have an antilinear symmetry [4]. Consider the antilinear operator: $\mathcal{ST}$, where $\mathcal{S}$ is a linear operator and $\mathcal{T}$ is the antilinear operator of time reversal, i.e., the complex conjugation operator in time-independent systems. If the Hamiltonian H commutes with the antilinear operator $\mathcal{ST}$, then

$$H(\mathcal{ST}|\Psi\rangle) = \mathcal{ST}(H|\Psi\rangle) = E^*(\mathcal{ST}|\Psi\rangle). \tag{1}$$

Therefore, if $|\Psi\rangle$ is an eigenstate of H with the eigenvalue E, then $\mathcal{ST}|\Psi\rangle$ is also an eigenstate with the eigenvalue E^*. We can therefore conclude that the eigenvalues of a Hamiltonian that has an antilinear symmetry, i.e., is pseudo-Hermitian, can be either real or come in complex-conjugate pairs. Several examples of such Hamiltonians with an antilinear symmetry where $\mathcal{S}$ is not the parity operator $\mathcal{P}$ have been given in the literature, e.g., [5,6]. Only if an eigenstate of H is also an eigenstate of $\mathcal{ST}$ is the corresponding eigenvalue real. If all the eigenstates of H are also eigenstates of $\mathcal{ST}$, then all the eigenvalues are strictly real and the symmetry is said to be *exact*. Otherwise, the symmetry is said to be *spontaneously broken*. This is part of the appeal of $\mathcal{PT}$-symmetric Hamiltonians as they can have, under certain conditions, completely real spectra and thus can serve, under the appropriate inner products, as Hamiltonians for unitary quantum systems.

As mentioned above, a $\mathcal{PT}$-symmetric Hamiltonian can possess a completely real spectrum. In most cases, the transition between exact and broken $\mathcal{PT}$ symmetry is governed by some parameter serving as a measure of the non-Hermiticity. At the transition point, two (or more) of the real eigenvalues of the Hamiltonian coalesce [6,7]. However, this is no ordinary degeneracy as the corresponding eigenfunctions coalesce as well forming a *self-orthogonal* state [8]. Such points in the spectrum are often referred to as *exceptional points* [9] and have been studied in connection with several physical systems [10–14]. Beyond this point, the eigenvalues separate into a pair of complex-conjugate solutions and the eigenvalues cease to be simultaneous eigenfunctions of both the Hamiltonian and the $\mathcal{PT}$ operator.

In the past several years, there have been many suggestions of pseudo-Hermitian Hamiltonians, specifically $\mathcal{PT}$-symmetric Hamiltonians; see, for example, [15–21]. These have exemplified in a multitude of one- and multidimensional Hamiltonians the transition from a strictly real spectrum to a spectrum comprised of real and complex-conjugate pairs of eigenvalues. Constructing a one-dimensional $\mathcal{PT}$-symmetric Hamiltonian is a straightforward matter of adding an ungerade perturbation of the form $i\lambda W(x)$, where $W(-x)=-W(x)$ is a real ungerade potential and λ is a real parameter, to a gerade real Hamiltonian, H_0. The resulting Hamiltonian, $H=H_0+i\lambda W$, clearly commutes with the $\mathcal{PT}$ operator, i.e., $[H,\mathcal{PT}]=0$. The real parameter λ then serves as the non-Hermiticity parameter inducing the transition from exact to broken $\mathcal{PT}$ symmetry. In much the same way, a multidimensional $\mathcal{PT}$-symmetric Hamiltonian can be constructed in which the parity operator is now the multidimensional inverse operator.

Although the possibility of finding new fundamental forces that give rise to non-Hermitian Hamiltonians that have

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real spectra is of great interest, to our knowledge there has yet to be any progress in that direction. Still, one can construct an *effective* $\mathcal{PT}$-symmetric Hamiltonian, which can then be studied. Recently, several such effective "Hamiltonians" have been proposed using optical waveguides with complex refractive indices [22–24]. However, as emphasized by the quotation marks, these examples have more to do with $\mathcal{PT}$-symmetric operators in classical optics than with physical Hamiltonians. Until new forces are found, the best one can hope for is to find a physical system that under certain conditions, e.g., a limited energy range, can be described by an effective $\mathcal{ST}$-symmetric non-Hermitian Hamiltonian.

In this work, we aim to give a simple physically oriented method of constructing $\mathcal{ST}$-symmetric Hamiltonians using point-group symmetries. Such considerations can not only facilitate finding effective Hamiltonians with the appropriate symmetry, but, as will be shown below, also provide a deep understanding of the mechanism by which the symmetry is broken.

II. REAL EIGENVALUES OF NON-HERMITIAN HAMILTONIANS

Consider the following non-Hermitian Hamiltonian:

$$H = H_0 + i\lambda W, \tag{2}$$

where H_0 is a real Hermitian Hamiltonian composed as usual of a kinetic and potential energy term, λ is a real parameter, and W is any real local potential. The corresponding Schrödinger equation reads

$$H\Psi = E\Psi. \tag{3}$$

If we limit ourselves to solutions of Eq. (3) that have real eigenvalues and separate between the real part and the imaginary part of the equation, we can rewrite the Schrödinger equation in matrix form,

$$\begin{pmatrix} H_0 & -\lambda W \\ \lambda W & H_0 \end{pmatrix}\begin{pmatrix} \phi \\ \chi \end{pmatrix} = E\begin{pmatrix} \phi \\ \chi \end{pmatrix}, \tag{4}$$

where ϕ and χ are real functions corresponding to the real and imaginary parts of Ψ, respectively, i.e., $\Psi=\phi+i\chi$. The above matrix equation has a very special property. Using the formal solution $\chi=\lambda(E-H_0)^{-1}W\phi$, we can write an equation strictly for ϕ,

$$[H_0 - \lambda^2 W(E-H_0)^{-1}W]\phi = E\phi. \tag{5}$$

Pursuing the same course of action for χ reveals that both χ and ϕ are solution of the same reduced equation. Thus we can write

$$[H_0 - \lambda^2 W(E-H_0)^{-1}W]\varphi = E\varphi, \tag{6}$$

where φ is either ϕ or χ. As it turns out, the real and imaginary parts of the wave function Ψ are degenerate solutions of Eq. (6) with the energy E. As we shall show below, this reduced equation is very helpful in understanding the mechanism leading to symmetry breaking and complex eigenvalues.

Equations of the form

$$[H_{AA} + V_{AB}(E-H_{BB})^{-1}V_{BA}]\psi = E\psi \tag{7}$$

are very common in physics. They often stem from the use of a projection into a smaller space of a matrix eigenvalue equation. In fact, whenever a continuum channel is projected out, the resulting equation is non-Hermitian. The most important difference between such equations and Eq. (6) is the minus sign before the energy-dependent term on the left-hand side. It is this minus sign that brings forth the special spectral properties of real eigenvalues of non-Hermitian Hamiltonians causing them to coalesce and move into the complex energy plane.

Recently, the reality of the spectrum of $\mathcal{PT}$-symmetric Hamiltonians has been proven by showing that all odd-order corrections of the Rayleigh-Schrödinger perturbation expansion in the parameter $i\lambda$ vanish [26]. This is of course a sufficient condition, since all even-order terms are real by definition, so long as the perturbation series converges, i.e., the radius of convergence is not zero. We can now, using Eq. (6), expand this idea and show that it is also a necessary condition under the same limitation of a nonzero radius of convergence. Clearly, the real energy in Eq. (6) is dependent solely on even powers of λ. The even power correction of the Rayleigh-Schrödinger expansion of Eqs. (6) and (3) can be shown to be the same [25], therefore all odd power perturbation corrections must vanish.

As pointed out earlier, in order to find real eigenvalues of the Hamiltonian in Eq. (2), we need two solutions of Eq. (6) to be degenerate. The noncrossing rule ensures that this can only be a direct consequence of symmetry. The role of symmetry was further emphasized by the vanishing odd-order perturbation corrections. As we shall see in the next section, this enforces strict demands on the potential W.

Before delving into the symmetry consideration, let us examine more carefully the solutions of Eq. (6). We can rewrite Eq. (6) as an eigenvalue equation where the Hamiltonian is dependent on the parameter E,

$$[H_0 - \lambda^2 W(E-H_0)^{-1}W]\varphi_n(E) = z_n(E)\varphi_n(E), \tag{8}$$

where $z_n(E)$ denotes the nth eigenvalue, which is now dependent on the parameter E. This type of analysis is often used when dealing with such equations; see, for example, [27]. The solutions we seek correspond to the points where the curves $y=z_n(E)$ cross the line $y=E$, i.e., the solution of the transcendental equation $z(E)=E$. In fact, we expect two such curves to cross each other exactly on the line $y=E$, one belonging to the real part of the wave function, $\varphi=\phi$ while the other will belong to the imaginary part of the wave function, $\varphi=\chi$. Figure 1 displays an example of the curves $z_n(E)$ for different values of λ. Evidently, whenever the equation $z(E)=E$ is satisfied, two curves cross the line $y=E$. Another important feature that is observable in Fig. 1 is the horizontal and vertical asymptotes of the curves $z_n(E)$ at the eigenvalues of H_0 as clearly seen from Eq. (8). The importance of these asymptotes will be made clear below.

Even if the spectrum of the Hamiltonian given in Eq. (2) has a real eigenvalue for a given λ, chances are that if we increase λ, the solution will eventually coalesce with another real eigenvalue and form a complex-conjugate pair of eigen-

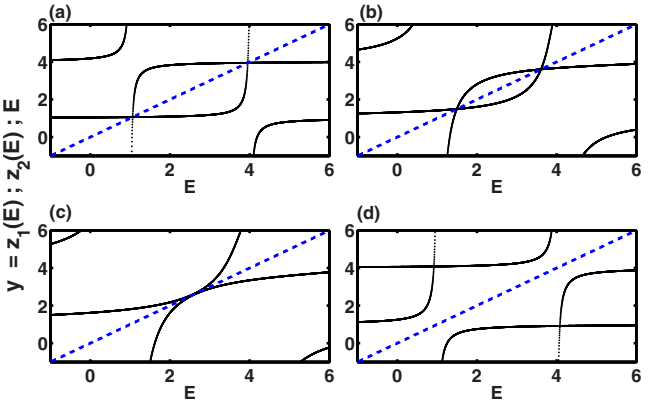

FIG. 1. (Color online) The first two solutions of Eq. (8), $z_1(E)$ and $z_2(E)$, as a function of E (black) measured in atomic units for different values of λ: (a) $\lambda=0.5$, (b) $\lambda=1.5$, (c) $\lambda=1.83\approx\lambda_c$. Also plotted is the line $z=E$ (dashed-blue). The points of intersection between the curves $z_1(E)$ and $z_2(E)$ and the line $z=E$ are the real eigenvalues of the non-Hermitian Hamiltonian in Eq. (2). Here H_0 is the Hamiltonian for a particle in an infinite square well, i.e., $x \in [-L/2, L/2]$, where $L=\sqrt{\pi}/2$. The non-Hermitian potential is taken as $W=\Theta(x)-1$, where Θ is the Heaviside function. The plot (d) displays the resulting curves when the non-Hermitian potential is taken to be a constant potential, i.e., $W=1$, and $\lambda=0.5$. Note that for such a choice of W there are no intersection points.

values. In the reduced equation introduced here, Eq. (7), we expect such a phenomenon to appear as the disappearance of two solutions. As discussed above, the two real solutions correspond to crossing points between the curve $z(E)$ and the line $y=E$. Therefore, at the critical value λ_c at which the solutions coalesce, the curve $z(E)$ becomes tangent to the line $y=E$ [where we have removed the index n from $z(E)$ for brevity]. One can now show using the derivative of $z(E)$ that at this critical point the wave function Ψ corresponding to the real eigenvalue, see Eq. (3), becomes self-orthogonal. Concentrating on one of the crossing curves, for example the one that belongs to a solution for the real part of the wave function, the derivative of $z(E)$ with respect to the energy is given by the Hellmann-Feynman theorem,

$$\frac{dz}{dE} = \frac{\langle\phi|\lambda^2 W(E-H_0)^{-2}W|\phi\rangle}{\langle\phi|\phi\rangle}. \tag{9}$$

From Eq. (4) we have that $|\chi\rangle=\lambda(E-H_0)^{-1}W|\phi\rangle$ and $\langle\chi| =\langle\phi|\lambda W(E-H_0)^{-1}$. Therefore,

$$\frac{dz}{dE} = \frac{\langle\phi|\lambda W(E-H_0)^{-1}\lambda(E-H_0)^{-1}W|\phi\rangle}{\langle\phi|\phi\rangle} = \frac{\langle\chi|\chi\rangle}{\langle\phi|\phi\rangle}. \tag{10}$$

At the critical value of λ where the two solutions merge, the curve $y=z_n(E)$ becomes tangent with the line $y=E$. Therefore, the following condition is fulfilled:

$$\left.\frac{dz}{dE}\right|_{\lambda=\lambda_c} = 1, \tag{11}$$

resulting in

$$\langle\chi|\chi\rangle = \langle\phi|\phi\rangle. \tag{12}$$

Thus the square of the norms of the real and imaginary part of the wave function Ψ becomes the same at the critical point where the two solutions coalesce. The state Ψ can be normalized by using the bi-orthonormal set of H, which for our case where $H^\dagger=H^*$ reads

$$N = \langle\Psi^*|\Psi\rangle = \langle\phi|\phi\rangle - \langle\chi|\chi\rangle, \tag{13}$$

where we have already used the fact that ϕ and χ are real orthogonal solutions of Eq. (6), i.e., $\langle\phi|\chi\rangle=0$. Evidently, at the critical point λ_c the norm of the state Ψ is zero, making the state Ψ self-orthogonal.

Note that the preceding analysis is rather general, imposing only the form of Eq. (2) on the Hamiltonian and the existence of a real eigenvalue. From this alone we have shown that if this real eigenvalue should disappear as λ is increased, then the corresponding eigenstate Ψ would become self-orthogonal. In order to proceed further, we need to look at the symmetries that need to be imposed on the potential W in order for a real solution of Eq. (3) to exist.

Before concluding this section, we return to discuss the differences between the regularly encountered reduced equation, i.e., of the form given in Eq. (7), and our reduced equation, Eq. (6). As already pointed out, the sign difference before the energy-dependant term is very important. This difference in sign causes all the curves $z_n(E)$ to increase monotonously between vertical asymptotes, as can be seen from Eq. (9). Increasing λ changes the slope of these curves and can eventually cause two solutions, i.e., crossing points with the line $y=E$, to coalesce and even disappear. This process is portrayed in Figs. 1(b) and 1(c). At the critical value λ_c, the *two* twofold degenerate solutions of Eq. (6) become a single degenerate pair of eigenvalues. Therefore, given the right conditions, the operator $\tilde{W}(E_c)=-\lambda^2 W(E_c-H_0)^{-1}W$ can make two former nondegenerate eigenvalues of H_0 degenerate at the energy E_c. We call such a special operator a *degenerating operator*. Note that it is hardly a trivial matter to make two solutions of a Hermitian operator degenerate by adding a Hermitian perturbation as done in Eq. (6). The second difference between Eqs. (6) and (7) is the appearance of a different Hamiltonian in the energy-dependent term. The eigenvalues of the Hamiltonian H_{AA} in Eq. (7) will serve as the horizontal asymptotes, i.e., $E\rightarrow\pm\infty$ of the curves $z_n(E)$. In the same manner, the eigenvalues of H_{BB} determine the vertical asymptotes of the curves $z_n(E)$. If a curve $z_n(E)$ has the same horizontal and vertical asymptotes, then it cannot cross the line $y=E$ and therefore there will be no solution to Eq. (7). Such a situation is portrayed in Fig. 1(d). At first glance it seems that Eq. (6) suffers from exactly this problem and could not support any solutions. However, much is dependent on the choice of W, as will be explained in the following section.

III. SPACE-TIME SYMMETRY

After analyzing the general properties of real eigenvalues of non-Hermitian Hamiltonians in the previous section, we are now prepared to classify these non-Hermitian Hamilto-

nians using the symmetry properties of H_0 and W. Let H_0 belong to the Nth-order Abelian point group G, which contains N spatial symmetry operators $\{\mathcal{S}_i\}_{i=1}^N$ (including the identity operator $\mathcal{S}_1=E$) and N irreducible representations (irreps) $\{\Gamma_i\}_{i=1}^N$. We denote the totally symmetric irrep as Γ_1 and assume the spectrum of H_0 has no accidental degeneracies.

Once the symmetry of H_0 is determined, we need to consider the symmetry of W. As shown in the previous section, a real eigenvalue of the Hamiltonian, $H=H_0+i\lambda W$, corresponds to a degenerate solution of the Hermitian energy dependent "Hamiltonian,"

$$\tilde{H}(E)\varphi=[H_0-\lambda^2 W(E-H_0)^{-1}W]\varphi=E\varphi. \tag{14}$$

Such degeneracy must be the result of a symmetry in the energy-dependent term $\tilde{W}(E)=-\lambda^2 W(E-H_0)^{-1}W$. We choose the eigenstates of H_0 as a basis for the representation of $\tilde{H}(E)$, where we order the states according to the irreps to which they belong. In such a representation, in order for the spectrum of $\tilde{H}(E)$ to be degenerate $\tilde{W}(E)$ has to be of block-diagonal form. Clearly, if W transforms as one of the irreps of the group G, then the symmetry of $\tilde{H}(E)$ is the same as that of H_0 since $W\times W\supset\Gamma_1$. However, this is insufficient to ensure the existence of degenerate solutions to Eq. (14). Suppose W transforms as the irrep Γ_p, where $p\in[1,2,\ldots,N]$. Γ_p determines which of the eigenstates of H_0 are coupled through $\tilde{W}(E)$. Consequentially, this determines the relations between the horizontal and vertical asymptotes of the curves $z_n(E)$ introduced in the previous section. As noted there, we must abstain from making the curves $z_n(E)$ have the same horizontal and vertical asymptotes. This can be achieved by preventing the coupling of eigenstates of H_0 to themselves via $\tilde{W}(E)$. It is, therefore, not sufficient that W transforms as one of the irreps of G and we must add the condition that W does not transform as the totally symmetric irrep, i.e., $W\not\supset\Gamma_1$. This shows that one way in which real eigenvalues can appear in the spectrum of H is to choose W such that it transforms as one of the irreps of the point group G excluding the totally symmetric one. Such a choice of W ensures the existence of one or more antiunitary space-time symmetries of the form $\mathcal{S}_i\mathcal{T}$ of the Hamiltonian H. This will be exemplified in detail in the following section. Of course the appearance of real eigenvalues of H is still likely to be constrained by a critical value of λ. If we choose W such that it does not transform as one of the irreps of G, one needs to search for a subgroup of G under which W will transform as one of the subgroup's irreps. If such a subgroup can be found, then the preceding analysis can be done in the same manner considering the subgroup rather than the point group G.

The above analysis shows that in principle one can get an entirely real spectrum for a non-Hermitian Hamiltonian H if W is chosen such that it transforms as an irrep of the point group (or subgroup) of H_0. We assumed all along that the spectrum of H_0 is nondegenerate, thus restricting ourselves to Abelian groups with real character tables. This restriction is crucial if W 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 we choose for W. 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, we can still choose W such that it transform under the irreps of the Abelian subgroup and H can still, in principle, have a completely real spectrum. Note, however, that if one wishes to keep only part of the spectrum of H on the real axis, many more options become available.

TABLE I. Character table for the point group C_i.

C_i	E	$\mathcal{P}$
A_g	1	1
A_u	1	−1

IV. EXAMPLES

A. $\mathcal{PT}$-symmetric Hamiltonians

The majority of research on the real spectrum of non-Hermitian Hamiltonians has been directed to Hamiltonians exhibiting parity-time symmetry. We shall, therefore, start this section by implementing the above analysis on a $\mathcal{PT}$-symmetric Hamiltonian. The parity operator $\mathcal{P}$ stands for the inversion operator, i.e., $\mathcal{P}\vec{r}\mathcal{P}^{-1}=-\vec{r}$.

The time-reversal operator $\mathcal{T}$ is simply the complex conjugation operator in the case of a time-independent Hamiltonian, i.e., $\mathcal{T}i\mathcal{T}^{-1}=-i$. Clearly, if we wish a Hamiltonian of the form $H=H_0+i\lambda W$ to be $\mathcal{PT}$-symmetric, where H_0 and W have been previously defined, we must demand that $\mathcal{P}H_0\mathcal{P}^{-1}=H_0$ and $\mathcal{P}W\mathcal{P}^{-1}=-W$. In one dimension, these conditions imply that H_0 belongs to the point group C_i whose character table is given in Table I. The condition on W means that it transforms as the irrep A_u. For this point group this is the only possible choice for W that will allow the non-Hermitian Hamiltonian H to have real eigenvalues. If we use the eigenstates of H_0 to represent Eq. (14) and order the eigenstates such that we first take all states belonging to A_g, i.e., the even states, and then all the states belonging to A_u, i.e., the odd states, the reduced equation will read

$$\left[\begin{pmatrix}\mathbf{E}^0_{A_g} & \mathbf{0}\\ \mathbf{0} & E^0_{A_u}\end{pmatrix}-\lambda^2\begin{pmatrix}\mathbf{0} & \mathbf{W}\\ \mathbf{W} & \mathbf{0}\end{pmatrix}\begin{pmatrix}(E\mathbf{I}-\mathbf{E}^0_{A_g})^{-1} & \mathbf{0}\\ \mathbf{0} & (E\mathbf{I}-\mathbf{E}^0_{A_u})^{-1}\end{pmatrix}\times\begin{pmatrix}\mathbf{0} & \mathbf{W}\\ \mathbf{W} & \mathbf{0}\end{pmatrix}\right]\begin{pmatrix}\vec{C}_{A_g}\\ \vec{C}_{A_u}\end{pmatrix}=E\begin{pmatrix}\vec{C}_{A_g}\\ \vec{C}_{A_u}\end{pmatrix}, \tag{15}$$

where $\mathbf{E}^0_{A_{g(u)}}$ is a diagonal matrix comprised of the eigenvalues of H_0 corresponding to the even (odd) eigenstates of H_0, $\mathbf{0}$ is a matrix of zeros, $\mathbf{I}$ is the identity matrix, $\mathbf{W}$ is the potential coupling between the different states, and $\vec{C}_{A_{g(u)}}$ is a vector of expansion coefficients belonging to the even (odd) basis functions, respectively. Expanding the left-hand side, Eq. (15) decouples into two equations,

$$[\mathbf{E}^0_{A_g} - \lambda^2 \mathbf{W}(E\mathbf{I} - \mathbf{E}^0_{A_u})^{-1}\mathbf{W}]\vec{C}_{A_g} = E\vec{C}_{A_g}, \tag{16}$$

$$[\mathbf{E}^0_{A_u} - \lambda^2 \mathbf{W}(E\mathbf{I} - \mathbf{E}^0_{A_g})^{-1}\mathbf{W}]\vec{C}_{A_u} = E\vec{C}_{A_u}. \tag{17}$$

As described earlier, the systematic degeneracy required from the solutions of Eq. (15) in order to obtain real eigenvalues depends on the decoupling of the matrix equation. In the case of one-dimensional $\mathcal{PT}$-symmetric Hamiltonians, this is clearly achieved. Note that although originally the odd states were coupled to the even states by the potential W, after the decoupling each symmetry is coupled only within itself. Because there are only two irreps under which we can classify the eigenstates, Eq. (15) is the only way in which Eq. (6) can decouple. Still the knowledge of the original coupling also reveals which of the real eigenvalues of the non-Hermitian Hamiltonian H can eventually coalesce before turning into a complex-conjugate pair. Note that when λ is nonzero it is the real and imaginary parts of the eigenstates $\psi(\lambda)$ of H that have the symmetry A_g and A_u, respectively, or vice versa. The eigenstates $\psi(\lambda)$ of the non-Hermitian Hamiltonian H do not retain the symmetry of A_g or A_u themselves. Still the knowledge of the symmetry of the corresponding eigenstate of H_0, i.e., the symmetry of $\psi(\lambda \to 0)$, is sufficient to determine which of the states may eventually merge. Here, the *gerade* eigenstates of H_0 are coupled to the *ungerade* eigenstates of H_0 through the *ungerade* potential W, therefore originally *gerade* solutions of H_0 can only coalesce with solutions that were originally *ungerade* solutions of H_0 as λ is increased. Even though in the case of the point group C_i there is only one possible answer, for point groups with more than two irreps one can control which of the states eventually coalesce.

In more than one dimension it is rather difficult to construct a Hamiltonian, H_0, belonging to the point group C_i. Still several examples have been given of multidimensional $\mathcal{PT}$-symmetric Hamiltonians. These have been achieved by taking Hamiltonians that possess the point group C_i as a subgroup and taking W to transform as the irrep A_u of the subgroup. One such example was given by Bender *et al.* [6], where $H_0 = -\partial_x^2 - \partial_y^2 + x^2 + y^2$ and $W = x$. In this case, H_0 belongs to the point group $C_{\infty v}$ and possesses the dynamical symmetry of SU(2). The non-Hermitian perturbation, however, transforms as the irrep A_u of the subgroup C_i contained in $C_{\infty v}$ (in the two-dimensional case). Therefore, the entire analysis shown above can be repeated by considering the subgroup C_i and labeling the eigenstates of H_0 only by the irreps A_g and A_u.

B. Multiple space-time symmetries

We move now to consider the two-dimensional Hamiltonian

$$H_0 = -\frac{1}{2}(\partial_x^2 + \partial_y^2) + \alpha_x x^4 + \alpha_y y^4. \tag{18}$$

Figure 2 displays the potential term of H_0.

This Hamiltonian belongs to the two-dimensional analogue of the point group D_{2h}, which is isomorphic to C_{2v}. We will denote this point group by D^{2D}_{2h}. The character table for this point group is given in Table II.

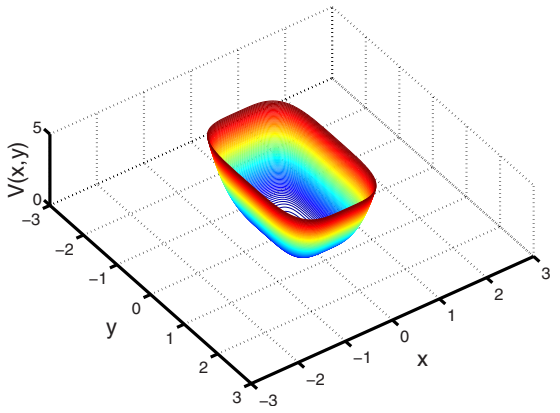

FIG. 2. (Color online) The potential energy function in Eq. (18): $V(x) = \alpha_x x^4 + \alpha_y y^4$, where $\alpha_x = 1$ and $\alpha_y = \sqrt{2}$. Note that the potential belongs to the two-dimensional analogue of the point group D_{2h}; see Table II. All variables depicted are measured in atomic units.

The separability of H_0 allows one to write the eigenstates of H_0 as

$$|n_x, n_y\rangle = |n_x\rangle \otimes |n_y\rangle, \tag{19}$$

where $|n\rangle$ stands for the nth eigenstate of the one-dimensional quartic oscillator and $n_{x(y)} = 0, 1, \ldots$. The eigenstates can be classified into four groups according to the different irreps of the point group. If both quantum numbers n_x and n_y are even (odd), then the eigenstate $|n_x, n_y\rangle$ will transform as A_g (B_g). If, however, n_x is even (odd) and n_y is odd (even), then the eigenstate $|n_x, n_y\rangle$ will transform as A_u (B_u). By appropriately choosing W, one can decide which of the eigenstates will couple to each other.

Suppose one chooses W to transform as the irrep B_g. As an example we choose $W = xy$. The Hamiltonian $H = H_0 + i\lambda W$ is not $\mathcal{PT}$-symmetric but rather $\mathcal{P}_x\mathcal{T}$- and $\mathcal{P}_y\mathcal{T}$-symmetric. Thus unlike the $\mathcal{PT}$-symmetric examples, the Hamiltonian possesses *more than one* antiunitary space-time symmetry. The first seven eigenvalues are depicted in Fig. 3 as a function of λ (see the figure caption for the parameters chosen).

In order to understand which of the eigenstates of H_0 couple to each other via the perturbing potential W, we construct the triple product table with respect to the irrep under which W transforms. Table III contains such a multiplication

TABLE II. Character table for the two-dimensional analog of the point group D_{2h}. As usual, E denotes the identity operator, $\mathcal{P}$ is the two-dimensional inversion operator, $\mathcal{P}_x$ reflects with respect to the y axis, and $\mathcal{P}_y$ reflects with respect to the x axis.

D^{2D}_{2h}	E	$\mathcal{P}$	$\mathcal{P}_x$	$\mathcal{P}_y$
A_g	1	1	1	1
B_g	1	1	−1	−1
A_u	1	−1	1	−1
B_u	1	−1	−1	1

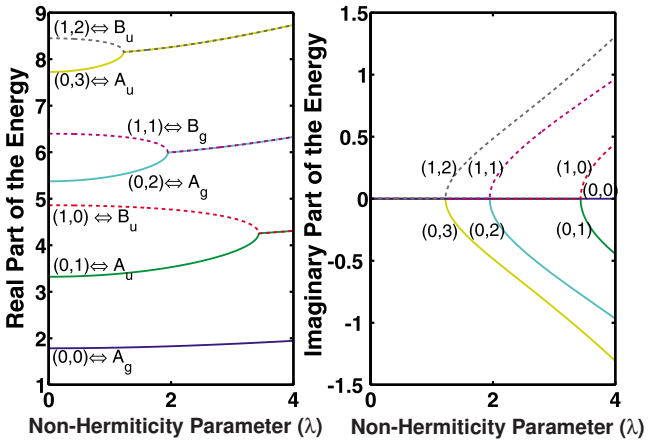

FIG. 3. (Color online) The first seven eigenvalues of the Hamiltonian $H=H_0+i\lambda W$, where H_0 is given in Eq. (18) ($\alpha_x=1$, $\alpha_y=\sqrt{2}$) and $W=xy$. The eigenvalues and λ are given in atomic units.

table for the case in which W transforms as B_g. Only when the multiplication of the irreps includes the totally symmetric irrep, i.e., A_g, are the eigenstates coupled. All other couplings vanish due to symmetry. Therefore, for the W chosen above, eigenstates that transform as A_g (A_u) couple to eigenstates that transform as B_g (B_u). This is clearly portrayed in Fig. 3.

Although Fig. 3 displays only seven of the eigenvalues, our numerical solution of the non-Hermitian Hamiltonian H showed that it is possible to find a range of values of λ for which all the eigenvalues calculated were real.

The fact that H_0 belongs to a point group that has more than two irreps allows one to design which of the eigenvalues of H will eventually coalesce and become complex. The choice made above and depicted in Fig. 3 is but one of several choices allowed for the point group D_{2h}^{2D}. Suppose we choose now W such that it transforms as the irrep A_u, e.g., $W=x^2y$. The corresponding triple product table, see Table IV, now shows that the eigenstates that transform as A_g (B_g) couple to those that transform as A_u (B_u).

The first six eigenvalues of H as a function of λ for this choice of W are displayed in Fig. 4. This second example shows that one can control which of the eigenstates will eventually coalesce by appropriately selecting the potential W. Note that the Hamiltonian H now possesses two different space-time symmetries, i.e., $[H,\mathcal{PT}]=0$ and $[H,\mathcal{P}_y\mathcal{T}]=0$.

So far we have explored two possible ways of choosing W that resulted in different couplings schemes between the eigenstates of H_0 and different space-time symmetries. If we continue to limit ourselves and only choose W such that it

TABLE III. Triple product table for the group D_{2h}^{2D} with respect to the irrep B_g.

$\times B_g \times$	A_g	B_g	A_u	B_u
A_g	B_g	A_g	B_u	A_u
B_g	A_g	B_g	A_u	B_u
A_u	B_u	A_u	B_g	A_g
B_u	A_u	B_u	A_g	B_g

TABLE IV. Triple product table for the group D_{2h}^{2D} with respect to the irrep A_u.

$\times A_u \times$	A_g	B_g	A_u	B_u
A_g	A_u	B_u	A_g	B_g
B_g	B_u	A_u	B_g	A_g
A_u	A_g	B_g	A_u	B_u
B_u	B_g	A_g	B_u	A_u

transforms as one of the irreps of the point group of H_0, we are left with only one unexplored choice for which W transforms as B_u, e.g., $W=xy^2$. For such a choice, the Hamiltonian H will now be $\mathcal{PT}$- and $\mathcal{P}_x\mathcal{T}$-symmetric.

The point group D_{2h}^{2D} has three isomorphic subgroups: C_i, $C_{\mathcal{P}_x}$, and $C_{\mathcal{P}_y}$. Each of these subgroups contains two symmetry operators: the identity and either $\mathcal{P}$, $\mathcal{P}_x$, or $\mathcal{P}_y$, respectively. The character tables are equivalent to that given in Table I with the respective interchange of the second symmetry operator for the groups $C_{\mathcal{P}_x}$ and $C_{\mathcal{P}_y}$, and where the subscript u (g) given to the irreps corresponds to symmetric (antisymmetric) with respect to the appropriate axis reflection. If the potential W does not transform as one of the irreps of D_{2h}^{2D} but transforms as the nontotally symmetric irrep of one of the subgroups of D_{2h}^{2D}, the non-Hermitian Hamiltonian H might still have real eigenvalues. Note that in such a case one analyzes the coupling between the eigenstates of H_0 by using the irreps of the subgroup rather than those of D_{2h}^{2D}. Unlike with the irreps of D_{2h}^{2D}, the subgroups can support only one space-time symmetry. Therefore, one can construct W by combining potentials that transform as different irreps of D_{2h}^{2D}. For example, consider the potential $W=W_{B_g}+W_{A_u}=xy+x^2y$. This potential does not transform as one of the irreps of D_{2h}^{2D} but rather as the irrep A_u of the subgroup $C_{\mathcal{P}_y}$. Note that the Hamiltonian H with each of the potentials W_{B_g} (W_{A_u}) possessed two space-time symmetries, i.e., H was $\mathcal{P}_x\mathcal{T}$ and $\mathcal{P}_y\mathcal{T}$ ($\mathcal{PT}$ and $\mathcal{P}_y\mathcal{T}$) -symmetric. With the combined potential, however, the Hamiltonian possesses only one space-time symmetry, i.e., $\mathcal{P}_y\mathcal{T}$. The coupling be-

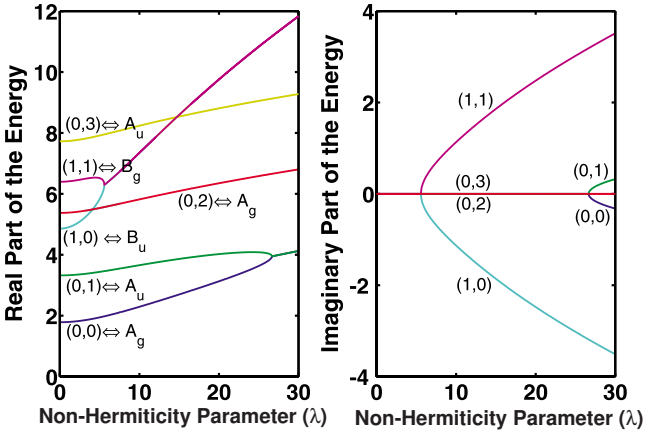

FIG. 4. (Color online) The first six eigenvalues of the Hamiltonian $H=H_0+i\lambda W$, where H_0 is given in Eq. (18) ($\alpha_x=1$, $\alpha_y=\sqrt{2}$) and $W=x^2y$. The eigenvalues and λ are given in atomic units.

tween the eigenstates can be identified by noticing that under the subgroup the irreps A_g (A_u) and B_u (B_g) of D_{2h}^{2D} become the irrep A_g (A_u) of $C_{\mathcal{P}_y}$. Therefore, eigenstates of H_0 for which the quantum number n_y is even will couple to those for which the quantum number n_y is odd.

In the above examples, we have stuck to two-dimensional examples for simplicity and brevity, but the analysis is easily extended to three-dimensional potentials where more interesting space symmetries are available. The important thing to note is that by classifying the point group of H_0 and the irrep under which W transforms, one can know whether real eigenvalues are possible at all, what are the space-time symmetries of the Hamiltonian H, and which of the eigenstates can eventually coalesce. One could also find many other potentials, W, for which the Hamiltonian H will have real eigenvalues by using the irreps of the point group of H_0 and thus control which of the eigenstates coalesce.

V. BACK TO REALITY

In the previous sections we have seen that non-Hermitian Hamiltonians of the form $H=H_0+i\lambda W$ with a correct choice of W can have real eigenvalues for some range of λ. At certain critical points, the real eigenvalues tend to coalesce and form complex-conjugate pairs. It appears as if every pair of real eigenvalues can only remain on the real energy axis up to a certain non-Hermiticity of the Hamiltonian, which is measured by λ. Occasionally, however, one can find real eigenvalues for any value of λ; see, for example, [6].

Suppose that at a certain value of $\lambda=\lambda_c$, two real eigenvalues of the Hamiltonian H coalesced. If we increase λ further, then these previously real solutions form a pair of complex-conjugate eigenvalues that move away from the real axis as λ is increased. Clearly, if we reduce λ, the eigenvalues will return to the real axis but one might still wonder whether the eigenvalues can return to the real axis by further increasing λ, i.e., the non-Hermiticity. To the best of our knowledge, we are unaware of any such examples in the literature. In the following, we shall show that the above scenario is not only possible but actually turns out to be very common.

Consider the Hamiltonian H_0 presented in the previous section, see Eq. (18), along with the potential $W=x^2y+y^2x$. With this choice of W, the Hamiltonian is $\mathcal{PT}$-symmetric and the relevant subgroup is C_i. The potential W transforms as the irrep A_u of this subgroup. Figure 5 shows the first eight eigenvalues of the Hamiltonian $H=H_0+i\lambda W$ as a function of λ.

We first analyze the behavior of the third and fourth eigenvalues. These two states belong to different irreps and are thus coupled by W. At first they approach each other as usual and coalesce at the critical value of $\lambda_b\approx 3.13$. After a short excursion into the complex plane, see the right-hand side frame in Fig. 5, they return to the real axis and coalesce once again at the point $\lambda_c\approx 3.47$. The self-orthogonal state at λ_c now separates into two real eigenvalues as λ is increased and the two eigenvalues start moving on the real axis in different directions. A further increase in the non-Hermiticity causes these two real solutions to move toward each other yet again

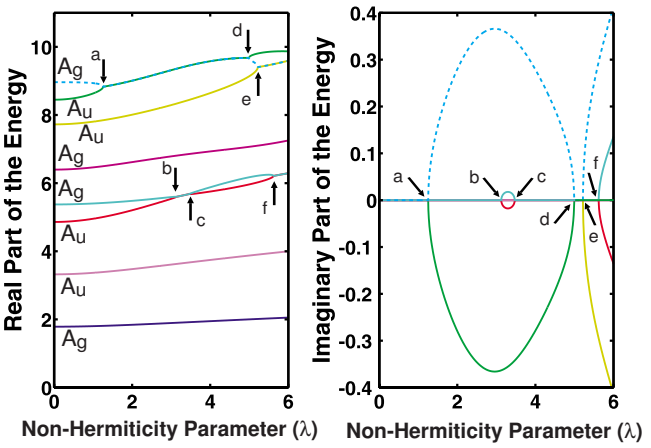

FIG. 5. (Color online) The first eight eigenvalues of the Hamiltonian $H=H_0+i\lambda W$, where H_0 is given in Eq. (18) ($\alpha_x=1$, $\alpha_y=\sqrt{2}$), and $W=x^2y+y^2x$. The eigenvalues and λ are given in atomic units.

and re-coalesce at the point $\lambda_f\approx 5.6$. Note that for the range of λ portrayed in Fig. 5, the third and fourth eigenvalues pass through three exceptional points where the eigenstates coalesce into a self-orthogonal state. Even more interesting is the behavior of the six, seventh, and eighth eigenvalues. The seventh and eighth eigenvalues are coupled via W and increasing λ moves them toward one another until λ reaches $\lambda_a\approx 1.33$, where the two eigenvalues coalesce. Increasing λ further causes the two eigenvalues to separate into a pair of complex-conjugate solutions and moves them away from the real axis. At some value of λ the two complex solutions start moving back toward the real axis, and when $\lambda=\lambda_d\approx 4.93$ they coalesce once again on the real axis. The two real solutions that now form once λ is further increased move to opposite directions on the real axis. One of them now moves toward the sixth eigenvalue and will coalesce with it at the point $\lambda_e\approx 5.3$.

The above example shows that even after the real eigenvalues of the Hamiltonian H became complex-conjugate pairs, they might still return to the real axis for some other value of λ. This could be a mechanism by which a spontaneously broken symmetry returns to an exact symmetry. We have yet to find an example for which this occurs for the entire spectrum. That is an example where a pair of real eigenvalues became complex and returned to the real axis so that the entire spectrum was real once again. For a part of the spectrum, however, this is easily accomplished. For example, the eigenvalues of H portrayed in Fig. 5 are *all* real while $\lambda<1.33$ and are once again *all* real when $4.93<\lambda<5.3$.

VI. CONCLUSIONS

The energy spectra of non-Hermitian Hamiltonians present a very rich foundation where new spectral properties can be observed. At first, the study of non-Hermitian Hamiltonians may seem rather academic or a purely mathematical study, but first impressions can be deceiving. Whenever there is more than one degree of freedom, a non-Hermitian representation of the Hamiltonian is but a projection away. There-

fore, understanding the spectral properties of non-Hermitian Hamiltonians can facilitate the analysis of a quantum system and lead to new understandings and predictions of observed quantities. Such insight into the quantum system is rarely possible when all degrees of freedom are taken into account, i.e., directly from the original Hamiltonian.

Here we have presented a method of characterizing a non-Hermitian Hamiltonian using the point-group symmetries of the Hermitian and non-Hermitian parts of the Hamiltonian. This characterization provides a method of analyzing the spectrum of the non-Hermitian Hamiltonian, thus predicting the possible appearance of real eigenvalues. If the non-Hermitian Hamiltonian indeed originated from a Hermitian counterpart, through a projection, a real eigenvalue indicates the existence of a bound state in the continuum. An example of such a situation was observed in [28], where bound states in the continuum were found in a system composed of two coupled electronic surfaces.

The applicability of the symmetry analysis presented here can be applied to many fields. In the study of complex potential energy surfaces (CPES), for example, one can study the point-group symmetry of the real and imaginary parts of the CPES and determine whether the molecule ionizes. Such a study, however, is beyond the scope of this paper. Another field in which understanding the properties of non-Hermitian Hamiltonians will be invaluable is waveguide optics. In optics, complex potentials are frequent and all the properties presented above can be easily demonstrated by constructing the appropriate waveguide structures [26].

Finally, we emphasize that the several examples of non-Hermitian Hamiltonians presented here are but a few of the myriad possible non-Hermitian Hamiltonians one can construct by first choosing the point-group symmetry of H_0 and then choosing W such that it transforms as one of the nontotally symmetric irreps. Many more possibilities become available if one further chooses W such that it contains more than a single non-Hermiticity parameter. For example, one could modify the potential studied in Sec. V so that it reads $W=\lambda_1 x^2 y+\lambda_2 y^2 x$. One can now study the spectrum as a function of two non-Hermiticity parameters: λ_1 and λ_2.

ACKNOWLEDGMENTS

We thank Professor Nimrod Moiseyev and Dr. Ido Gilary for helpful discussions. S.K. acknowledges the support of the Israel Ministry of Science, Culture and Sports. L.S.C. acknowledges the financial support of the DFG.

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