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Critical parameters for non-hermitian Hamiltonians

Francisco M Fernández*, Javier Garcia

INIFTA (UNLP, CCT La Plata-CONICET), División Química Teórica, Blvd. 113 S/N, Sucursal 4, Casilla de Correo 16, 1900 La Plata, Argentina

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ABSTRACT

We calculate accurate critical parameters for a class of non-hermitian Hamiltonians by means of the diagonalization method. We study three one-dimensional models and two perturbed rigid rotors with PT symmetry. One of the latter models illustrates the necessity of a more general condition for the appearance of real eigenvalues that we also discuss here. © 2014 Elsevier Inc. All rights reserved.

1. Introduction

There has recently been interest in PT-symmetric Hamiltonians that exhibit real eigenvalues for a range of values of a potential parameter. Some of them are anharmonic oscillators [1–9] as well as models with Dirichlet [10–12] periodic and anti-periodic boundary conditions [13,14].

Among the methods used for the study of such models we mention the WKB approximation [3,4], the eigenvalue moment method [5,7], the multiscale reference function analysis [6], the diagonalization method (DM) [8] and the orthogonal polynomial projection quantization (OPPQ) (an improved Hill-determinant method) [9].

For some particular values of the potential parameter the spectrum of those PT-symmetric Hamiltonians exhibits critical points where two real eigenvalues coalesce and emerge as complex conjugate eigenvalues. Such critical points are also known as exceptional points [15–18].

The purpose of this paper is the analysis of the critical points for a variety of simple models. The calculation is based on a well known simple and quite efficient application of the DM [15]. In Section 2 we propose a somewhat more general condition for the existence of real eigenvalues (unbroken symmetry) [19,20] that is suitable for models with degenerate states. In Section 3 we present three one-dimensional examples already discussed earlier by other authors. In Section 4 we outline the procedure for the calculation of critical points based on the DM. In Section 5 we apply perturbation theory to one of the models and discuss the convergence of the perturbation series for the eigenvalues by comparison with the accurate results produced by the DM. In Section 6 we discuss a PT-symmetric perturbed planar rigid rotor that was studied earlier as an example with E2 algebra [14]. In Section 7 we discuss a non-hermitian perturbed three-dimensional rigid rotor that was not treated before as far as we know. This most interesting model illustrates the generalized condition for real eigenvalues mentioned above. Finally, in Section 8 we summarize the main results and draw conclusions.

2. PT Symmetry

It is well known that a wide class of non-hermitian Hamiltonians with unbroken PT symmetry exhibit real spectra [19,20]. In general, they are invariant under an antilinear or antiunitary transformation of the form $\hat{A}^{-1}\hat{H}\hat{A} = \hat{H}$. The antiunitary operator \hat{A} satisfies [21]

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^{*} Corresponding author. *E-mail address:* fernande@quimica.unlp.edu.ar (F.M Fernández).

$$\widehat{A}(|f\rangle + |g\rangle) = \widehat{A}|f\rangle + \widehat{A}|g\rangle,$$

$$\widehat{A}c|f\rangle = c^*\widehat{A}|f\rangle$$
(1)

for any pair of vectors $|f\rangle$ and $|g\rangle$ and arbitrary complex number *c*, where the asterisk denotes complex conjugation. This definition is equivalent to

$$\left\langle \widehat{A}f\middle|\widehat{A}g\right\rangle = \left\langle f|g\right\rangle^*.$$
(2)

It follows from the antiunitary invariance mentioned above that $[\hat{H}, \hat{A}] = 0$. Therefore, if $|\psi\rangle$ is an eigenvector of \hat{H} with eigenvalue E

$$\widehat{H}|\psi\rangle = E|\psi\rangle,\tag{3}$$

we have

$$[\widehat{H},\widehat{A}]|\psi\rangle = \widehat{H}\widehat{A}|\psi\rangle - \widehat{A}\widehat{H}|\psi\rangle = \widehat{H}\widehat{A}|\psi\rangle - E^*\widehat{A}|\psi\rangle = 0.$$
(4)

This equation merely tell us that if $|\psi\rangle$ is eigenvector of \hat{H} with eigenvalue *E* then $\hat{A}|\psi\rangle$ is eigenvector with eigenvalue *E*^{*}. Consequently, *E* is real if

$$\widehat{H}\widehat{A}|\psi\rangle = E\widehat{A}|\psi\rangle,\tag{5}$$

that contains the condition of unbroken symmetry required by Bender et al. [19,20]

$$A|\psi\rangle = \lambda|\psi\rangle,\tag{6}$$

as a particular case. Note that Eq. (5) applies to the case in which $\widehat{A}|\psi\rangle$ is a linear combination of degenerate eigenvectors of \widehat{H} with eigenvalue *E*.

If \hat{K} is an antilinear operator such that $\hat{K}^2 = \hat{1}$ (for example, the complex conjugation operator) then it follows from (2) that $\hat{A}\hat{K} = \hat{U}$ is unitary ($\hat{U}^{\dagger} = \hat{U}^{-1}$). In other words, any antilinear operator \hat{A} can be written as a product of a unitary operator and the complex conjugation operation [21]. In most of the non-hermitian models studied $\hat{U}^{-1} = \hat{U}$ that results in $\hat{A}^2 = \hat{1}$ (as in the case of the parity operator $\hat{U} = \hat{P}$ that gives rise to PT symmetry) [19,20].

3. Some simple one-dimensional examples

In this section we consider three examples of the Schrödinger equation

$$\widehat{H}\psi = E\psi, \widehat{H} = \widehat{p}^2 + \widehat{V}(\mathbf{x}),$$
(7)

with eigenvalues $E_0 < E_1 < \cdots$. The first one [3,5,6]

$$\widehat{H} = \widehat{p}^2 + i\widehat{x}^3 + ia\widehat{x} \tag{8}$$

exhibits an infinite set of critical values $0 > a_0 > a_1 > \cdots > a_n > \cdots$ of *a* so that $E_{2n} = E_{2n+1}$ at $a = a_n$. Both eigenvalues are real when $a > a_n$ and become complex conjugate numbers when $a < a_n$. The eigenfunctions ψ_{2n} and ψ_{2n+1} are linearly dependent at the exceptional point $a = a_n$ [15–18].

The second example is [1,4,7]

$$\hat{H} = \hat{p}^2 + \hat{x}^4 + ia\hat{x}.$$
(9)

If \widehat{P} denotes the parity operator we have $\widehat{P}\widehat{H}(a)\widehat{P} = \widehat{H}(-a)$ so that E(-a) = E(a). Because of this property of the eigenvalues the crossings $E_{2n} = E_{2n+1}$ take place at $\pm a_n$, where $0 < a_0 < a_1 < \cdots < a_n < \cdots$. In this case the pair of coalescing eigenvalues become complex conjugate numbers when $|a| > a_n$.

The third example is given by

$$\hat{H} = \hat{p}^2 + ia\hat{x},\tag{10}$$

with the boundary conditions $\psi(\pm 1) = 0$. In this case we also find that the crossings take place at $\pm a_n$, $a_n > 0$ as in the preceding one. Because of physical reasons Rubinstein et al. [10] considered only the half line a > 0.

4. Diagonalization method

In order to solve the Schrödinger equation (7) we resort to a matrix representation of the Hamiltonian operator $H_{ij} = \langle i|\hat{H}|j\rangle$ in an appropriate orthonormal basis set $\{|j\rangle, j = 0, 1, ...\}$. We obtain the eigenvalues from the roots of the

142

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