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# ON THE REAL MATRIX REPRESENTATION OF PT-SYMMETRIC OPERATORS

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Abstract. We discuss the construction of real matrix representations of PT-symmetric operators. We show the limitation of a general recipe presented some time ago for non-Hermitian Hamiltonians with antiunitary symmetry and propose a way to overcome it. Our results agree with earlier ones for a particular case.

Keywords: non-Hermitian Hamiltonians, antiunitary symmetry, PT-symmetry, real matrix.

## 1. Introduction

At first sight it is suprising that a subset of eigenvalues of a complex-valued non-hermitian operator $\hat{H}$ can be real (see [1] and references therein). In order to provide a simple and general explanation of this fact Bender et al. [2] showed that it is possible to construct a basis set of vectors so that the matrix representation of such an operator is real. As a result the secular determinant is real (the coefficients of the characteristic polynomial are real) and its roots are either real or appear in pairs of complex conjugate numbers. The argument is based on the existence of an antiunitary symmetry $\hat{A}\hat{H}\hat{A}^{-1} = \hat{H}$, where the antiunitary operator $\hat{A}$ satisfies $\hat{A}^k = \hat{1}$ for $k$ odd. Bender et al. [2] showed some illustrative examples of their general result.

The procedure followed by Bender et al. [2] for the construction of the suitable basis set is reminiscent of the one used by Porter [3] in the study of matrix representations of Hermitian operators. However, the ansatz proposed by Porter appears to be somewhat more general.

The purpose of this paper is to analyse the argument given by Bender et al. [2] in more detail. In Section 2 we outline the main features of an antiunitary or antilinear operator and in Section 3 we briefly discuss the concept of antiunitary symmetry. In Section 4 we review the argument given by Bender et al. [2] and show that under certain conditions it does not apply. We illustrate this point by means of the well known harmonic-oscillator basis set and show how to overcome that shortcoming. In Section 5 we discuss the harmonic-oscillator basis set in more detail and in Section 6 we draw conclusions.

## 2. Antiunitary operator

As already mentioned above, a wide class of non-hermitian Hamiltonians with unbroken PT symmetry exhibits real spectra [1]. 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 [4]

$$\begin{aligned} \hat{A}\big(|f\rangle + |g\rangle\big) &= \hat{A}|f\rangle + \hat{A}|g\rangle \\ \hat{A}c|f\rangle &= c^*\hat{A}|f\rangle, \end{aligned} \tag{1}$$

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

$$\langle \hat{A}f | \hat{A}g\rangle = \langle f|g\rangle^*. \tag{2}$$

One can easily derive the pair of equations (1) from (2) so that the latter can be considered to be the actual definition of an antiunitary operator [4].

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 ($\hat{U}^\dagger = \hat{U}^{-1}$); that is to say the inner product $\langle f|g\rangle$ remains invariant under $\hat{U}$:

$$\langle \hat{A}\hat{K}f | \hat{A}\hat{K}g\rangle = \langle \hat{K}f|\hat{K}g\rangle^* = \langle f|g\rangle. \tag{3}$$

In other words, any antilinear operator $\hat{A}$ can be written as a product of a unitary operator and the complex conjugation operation [4]. In exactly in the same way we can easily prove that $\hat{A}^{2j}$ is unitary and $\hat{A}^{2j+1}$ antiunitary.

In their discussion of real matrix representations of non-hermitian Hamiltonians Bender et al. [2] considered Hamiltonians $\hat{H}$ with antiunitary symmetry

$$\hat{A}\hat{H}\hat{A}^{-1} = \hat{H}, \tag{4}$$

where $\hat{A}$ satisfies the additional condition

$$\hat{A}^{2k} = \hat{1}, \quad k \text{ odd}. \tag{5}$$

Since $\hat{B} = \hat{A}^k$ is antiunitary and satisfies $\hat{B}^2 = \hat{1}$ we can restrict our discussion to the case $k = 1$ without loss of generality. Therefore, from now on we substitute the condition

$$\hat{A}^2 = \hat{1} \tag{6}$$

for the apparently more general equation (5). From now on we refer to equation (4) as $A$-symmetry and to the operator $\hat{H}$ as $A$-symmetric for short.

## 3. Antiunitary symmetry

It follows from the antiunitary invariance (4) that $[\hat{H}, \hat{A}] = 0$. Therefore, if $|\psi\rangle$ is an eigenvector of $\hat{H}$ with eigenvalue $E$

$$\hat{H}|\psi\rangle = E|\psi\rangle, \tag{7}$$

we have

$$\begin{aligned}[\hat{H}, \hat{A}]|\psi\rangle &= \hat{H}\hat{A}|\psi\rangle - \hat{A}\hat{H}|\psi\rangle \\ &= \hat{H}\hat{A}|\psi\rangle - E^*\hat{A}|\psi\rangle = 0. \end{aligned} \tag{8}$$

This equation tells us that if $|\psi\rangle$ is an eigenvector of $\hat{H}$ with eigenvalue $E$ then $\hat{A}|\psi\rangle$ is also an eigenvector with eigenvalue $E^*$. That is to say: the eigenvalues are either real or appear as pairs of complex conjugate numbers. In the former case

$$\hat{H}\hat{A}|\psi\rangle = E\hat{A}|\psi\rangle, \tag{9}$$

which contains the condition of unbroken symmetry [1]

$$\hat{A}|\psi\rangle = \lambda|\psi\rangle \tag{10}$$

as a particular case. Note that equation (9) applies to the case in which $\hat{A}|\psi\rangle$ is a linear combination of degenerate eigenvectors of $\hat{H}$ with eigenvalue $E$. An illustrative example of this more general condition for real eigenvalues is given elsewhere [5].

## 4. Real matrix representation

Bender et al. [2] put forward a straightforward procedure for obtaining a basis set in which an $A$-symmetric Hamiltonian has a real matrix representation. They proved that for an $A$-adapted basis set $\{|n_A\rangle\}$

$$\hat{A}|n_A\rangle = |n_A\rangle \tag{11}$$

the matrix elements of the invariant Hamiltonian operator are real

$$\langle m_A|\hat{H}|n_A\rangle = \langle m_A|\hat{H}|n_A\rangle^* \tag{12}$$

These authors proposed to construct $|n_A\rangle$ as (remember that we have restricted present discussion to $k = 1$ without loss of generality)

$$|n_A\rangle = |n\rangle + \hat{A}|n\rangle \tag{13}$$

where $\{|n\rangle\}$ is any orthonormal basis set.

It is not difficult to prove that this recipe does not apply to any basis set. According to equation (6) we can find a basis set $\{|n, \sigma\rangle\}$ that satisfies

$$\hat{A}|n, \sigma\rangle = \sigma|n, \sigma\rangle,\ \sigma = \pm 1 \tag{14}$$

Consequently, all the vectors

$$|n, \sigma\rangle_A = |n, \sigma\rangle + \hat{A}|n, \sigma\rangle = (1 + \sigma)|n, \sigma\rangle \tag{15}$$

with $\sigma = -1$ vanish and the resulting $A$-adapted vector set is not complete. We conclude that the basis set $\{|n\rangle\}$ should be chosen carefully in order to apply the recipe of Bender et al. [2]. In fact, the authors showed a particular example where it certainly applies.

We can construct the basis set $\{|n, \sigma\rangle\}$ from any orthonormal basis set $\{|n\rangle\}$ in the following way

$$|n, \sigma\rangle = N_{n,\sigma}\hat{Q}_\sigma|n\rangle,\ \hat{Q}_\sigma = \frac{1}{2}\big(1 + \sigma\hat{A}\big) \tag{16}$$

where $N_{n,\sigma}$ is a suitable normalization factor. It already satisfies equation (14) because $\hat{A}\hat{Q}_\sigma = \sigma\hat{Q}_\sigma$. In order to overcome the shortcoming in the recipe (13) we define the $A$-adapted basis set $B_A = \{|n_A^+\rangle = |n, 1\rangle, |n_A^-\rangle = i|n, -1\rangle\}$. Note that the vectors $|n_A^\pm\rangle$ satisfy the requirement (11) and that $B_A$ is complete. In principle there is no guarantee of orthogonality, but such a difficulty does not arise in the examples discussed below.

The vectors $|v_n^\pm\rangle = \frac{1}{\sqrt{2}}\big(|n_A^+\rangle \pm |n_A^-\rangle\big)$ also satisfy the requirement (11) and in the particular case of a two-dimensional space they lead to the $A$-adapted basis set chosen by Bender et al. [2] to introduce the issue by means of a simple example.

As a particular case consider the parity-time antiunitary operator $\hat{A} = \hat{P}\hat{T}$, where $\hat{P}$ an $\hat{T}$ are the parity and time-reversal operators, respectively [3]. Let $\{|n\rangle, n = 0, 1, \ldots\}$ be the basis set of eigenvectors of the Harmonic oscillator $\hat{H}_0 = \hat{p}^2 + \hat{x}^2$ that are real and satisfy $\hat{P}|n\rangle = (-1)^n|n\rangle$ so that $\hat{A}|n\rangle = (-1)^n|n\rangle$. It is clear that the recipe (13) does not apply to this simple case. On the other hand, the present recipe yields the $A$-adapted basis set $B_A^{HO} = \{|2n\rangle, i|2n + 1\rangle, n = 0, 1, \ldots\}$ which is obviously complete.

Every vector of the orthonormal basis set $B_A^{HO}$ in the coordinate representation can be expressed as a linear combination of the elements of the nonorthogonal basis set $\{f_n(x) = e^{-x^2/2}(ix)^n, n = 0, 1, \ldots\}$. By means of a slight generalization of the latter, Znojil [6] derived a recurrence relation with real coefficients for a family of complex anharmonic potentials. He also constructed a real matrix representation of a PT-symmetric oscillator in terms of the eigenvectors of $\hat{A} = \hat{P}\hat{T}$ [7]. Note that his vectors $|S_n\rangle$ and $|L_n\rangle$ are our $|n, 1\rangle$ and $|n, -1\rangle$ respectively.

Following Porter [3] we can try the ansatz

$$|n_A\rangle = a_n|n\rangle + \hat{A}a_n|n\rangle = a_n|n\rangle + a_n^*\hat{A}|n\rangle \tag{17}$$

which already satisfies $\hat{A}|n_A\rangle = |n_A\rangle$. This definition of an $A$-adapted basis set is slightly more general than equation (13). When $\hat{A}|n\rangle = (-1)^n|n\rangle$ we simply choose $a_n = \frac{1}{2}(1 + i)$ and obtain the result above for the particular case of the harmonic-oscillator basis set. Note that the resulting expressions (we can also choose $a_n = \frac{1}{2}(1 - i)$) are similar to those in equation (16) in the paper of Bender et al. [2].

## 5. The harmonic-oscillator basis set

Many examples of $PT$-symmetric Hamiltonians are one-dimensional models of the form [1]

$$\hat{H} = \hat{p}^2 + V(x), \tag{18}$$

where

$$V(-x)^* = V(x). \tag{19}$$

We can write $V(x)$ as the sum of its even $V_e(-x) = V_e(x)$ and odd $V_o(-x) = -V_o(x)$ parts

$$V(x) = V_e(x) + V_o(x), \tag{20}$$

where

$$\begin{aligned} V_e(x) &= \frac{1}{2}\left[V(x) + V(-x)\right] = \Re V(x), \\ V_o(x) &= \frac{1}{2}\left[V(x) - V(-x)\right] = i\Im V(x). \end{aligned} \tag{21}$$

For convenience we change the notation of the preceding section and define the $A$-adapted basis set $\{\varphi_n\}$ as

$$\begin{aligned} |\varphi_{2n}\rangle &= |2n\rangle \\ |\varphi_{2n+1}\rangle &= i|2n+1\rangle,\ n = 0, 1, \ldots, \end{aligned} \tag{22}$$

where $\{|n\rangle\}$ is the harmonic-oscillator basis set. Therefore

$$\begin{aligned} \langle\varphi_{2n}|\hat{p}^2|\varphi_{2m}\rangle &= \langle\phi_{2n}|\hat{p}^2|\phi_{2m}\rangle \\ \langle\varphi_{2n}|\hat{p}^2|\varphi_{2m+1}\rangle &= \langle\phi_{2n}|\hat{p}^2|\phi_{2m+1}\rangle = 0 \\ \langle\varphi_{2m+1}|\hat{p}^2|\varphi_{2n}\rangle &= \langle\phi_{2m+1}|\hat{p}^2|\phi_{2n}\rangle = 0 \\ \langle\varphi_{2n+1}|\hat{p}^2|\varphi_{2m+1}\rangle &= \langle\phi_{2n+1}|\hat{p}^2|\phi_{2m+1}\rangle \end{aligned} \tag{23}$$

and

$$\begin{aligned} \langle\varphi_{2n}|V|\varphi_{2m}\rangle &= \langle\phi_{2n}|\Re V|\phi_{2m}\rangle \\ \langle\varphi_{2n+1}|V|\varphi_{2m}\rangle &= \langle\phi_{2n+1}|\Im V|\phi_{2m}\rangle \\ \langle\varphi_{2n}|V|\varphi_{2m+1}\rangle &= -\langle\phi_{2n}|\Im V|\phi_{2m+1}\rangle \\ \langle\varphi_{2n+1}|V|\varphi_{2m+1}\rangle &= \langle\phi_{2n+1}|\Re V|\phi_{2m+1}\rangle \end{aligned} \tag{24}$$

It is clear that all the matrix elements $H_{mn} = \langle\varphi_m|\hat{H}|\varphi_n\rangle$ are real and the basis is complete since

$$\sum_n |\varphi_n\rangle\langle\varphi_n| = \sum_n |n\rangle\langle n| = \hat{1} \tag{25}$$

Besides, the matrix representation of the Hamiltonian operator in the basis set discussed above

$$\hat{H} = \sum_m \sum_n |\varphi_m\rangle\langle\varphi_m|\hat{H}|\varphi_n\rangle\langle\varphi_n| \tag{26}$$

is similar to the one proposed by Znojil [7] some time ago.

The unitary basis transformation (22) is given by the unitary operator

$$\hat{U} = \sum_{n=0}^{\infty}\left(|2n\rangle\langle 2n| + i|2n+1\rangle\langle 2n+1|\right) \tag{27}$$

that satisfies $\hat{U}^\dagger = \hat{U}^* = \hat{T}\hat{U}\hat{T}$ and $\hat{U}^2 = \hat{P}$. If $\mathbf{H}$ and $\mathbf{U}$ are the matrix representations of the operators $\hat{H}$ and $\hat{U}$, respectively, in the basis set $\{|n\rangle\}$ and $\mathbf{I}$ is the identity matrix, then the secular determinant $|\mathbf{H} - E\mathbf{I}| = |\mathbf{U}(\mathbf{H} - E\mathbf{I})\mathbf{U}^\dagger| = |\mathbf{U}\mathbf{H}\mathbf{U}^\dagger - E\mathbf{I}|$ is real because the matrix elements of $\mathbf{U}\mathbf{H}\mathbf{U}^\dagger$ are all real. This result applies even to the approximate finite matrix representations of operators appearing in the diagonalization method [5, 8]. As a consequence, the coefficients of the characteristic polynomial are real and their roots are either real or complex conjugate numbers.

## 6. Conclusions

We have shown that the recipe proposed by Bender et al. [2] for the construction of real matrix representations of $A$-symmetric Hamiltonians may fail under certain conditions, for example, when $\hat{A}|n\rangle = (-1)^n |n\rangle$. In this case one can easily construct an $A$-adapted basis set as $|n_A\rangle = i^n|n\rangle$ that is complete and satisfies the required condition $\hat{A}|n_A\rangle = |n_A\rangle$. One of the most commonly used basis sets, the harmonic-oscillator one, already belongs to this class. There is no unique way of constructing the $A$-adapted basis set; for example, the ansatz proposed by Porter [3] (in the form outlined above in section 4) yields basically the same basis vectors except for the phase factors.

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