How to test for diagonalizability: the discretized PT-invariant square-well potential *)

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Given a non-Hermitian matrix M, the structure of its *minimal* polynomial encodes whether M is diagonalizable or not. This note explains how to determine the minimal polynomial of a matrix without going through its *characteristic* polynomial. The approach is applied to a quantum mechanical particle moving in a square well under the influence of a piece-wise constant PT-symmetric potential. Upon discretizing the configuration space, the system is described by a matrix of dimension three which turns out not to be diagonalizable for a critical strength of the interaction. The systems develops a *three-fold* degenerate eigenvalue, and *two* of the three eigenfunctions disappear at this exceptional point, giving a difference between the *algebraic* and *geometric* multiplicity of the eigenvalue equal to two.

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1 Introduction

Genuinely PT-invariant operators may or may not possess a complete set of eigenstates. In other words, PT-invariance of a matrix M is compatible with the presence of (non-trivial) Jordan blocks while hermiticity is not. When considering a family of PT-invariant operators depending on a parameter, their spectra often change qualitatively if one passes through an *exceptional* point [1] where diagonalizability breaks down. It is thus important to be able to either check whether a given matrix is diagonalizable or to locate exceptional points when presented with a continuous family of matrices.

The purpose of this note is to describe a method which allows one to identify exceptional points of finite-dimensional non-Hermitian matrices by means of an algorithm. It is different from the method outlined in [2, 3] as it directly aims at the *minimal* polynomial containing the relevant information about (non-) diagonalizability. While being more transparent in the first place, it also requires no knowledge of the *characteristic* polynomial of the given matrix.

The presentation to follow is problem-based: the algorithm will be developed while studying a specific example, the discretized PT-invariant square well. This physical system is introduced in Section 2, and it is subjected to the test for diagonalizability in the subsequent section. The results will be discussed in Section 4 and some open questions will be addressed.

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2 The discretized PT-symmetric square well

Consider a quantum particle in a one-dimensional box of length $4L$ subjected to a piece-wise constant PT-symmetric potential,

$$V(x) = \begin{cases} -\mathrm{i}Z, & -2L < x < 0, \\ 0, & x = 0, \\ \mathrm{i}Z, & 0 < x < 2L, \end{cases} \qquad Z \in \mathbb{R}\,, \tag{1}$$

which has proved a useful testing ground for the discussion of PT-symmetric systems [4]. Its eigenvalues are given as the zeros of a transcendental equation, and for increasing values of Z, the lowest two real eigenvalues are known to approach each other, finally disappearing jointly at critical values of Z.

Let us introduce a toy-version of this system by discretizing its configuration space. This strategy has been applied successfully to describe tunnelling phenomena in a driven double-well potential in terms of a three-state model [5]. Effectively, this technique corresponds to turning Feynman's "derivation" of Schrödinger's equation from a discrete lattice [6] upside down. Explicitly, the continuous set of points of configuration space with labels $-2L \le x \le 2L$, is replaced by *five* equidistant points at $0, \pm L$, and $\pm 2L$. The wave function is allowed to take nonzero values only at these points, so it will be a vector with at most five components. However, the hard walls of the square well at $x = \pm L$ force the wave function to vanish there, leaving us with only three non-zero components, $\psi(x) \to \psi_k = \psi(kL), k = 0, \pm 1$. The potential energy defined in (1) turns into a diagonal matrix, $V(x) \to \mathsf{V} = \mathrm{diag}(-\mathrm{i}Z, 0, \mathrm{i}Z)$. The operator for the kinetic energy follows from the substitution $\partial^2\psi(x)/\partial x^2 \to (\psi_{k+1} - 2\psi_k + \psi_{k-1})/L^2$. Putting all this together, the Hamiltonian operator of the discrete version of this system reads

$$\mathsf{H}_0 \simeq 2\mathsf{E} - \mathsf{H}\,, \quad \text{where} \quad \mathsf{H} = \begin{pmatrix} \mathrm{i}\xi & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & -\mathrm{i}\xi \end{pmatrix}, \quad \xi = \frac{Z}{\eta}\,; \tag{2}$$

here E is the (3×3) identity matrix, and an overall factor $\eta = \hbar^2/2mL^2$ has been dropped. The matrix H_0 inherits PT-invariance from the square well: the matrix H, and hence H_0, is invariant under the combined action of parity P, represented by a matrix with unit entries equal to one along its minor diagonal and zero elsewhere, and T, effecting complex conjugation. In the next section, the diagonalizability of H, the nontrivial part of the Hamiltonian H_0, will be studied.

3 Diagonalizability of the PT-symmetric square well

The *minimal* polynomial m_{M} of a matrix M is defined (see [7], for example) as the polynomial of least degree in M which annihilates M, that is, $m_{\mathsf{M}}(\mathsf{M}) = 0$. This polynomial is unique if the coefficient of its highest power is taken to be one: the minimal polynomial is *monic.* Since any square matrix M of size N, say, is annihilated by its own *characteristic* polynomial, $p_{\mathsf{M}}(\mathsf{M}) = 0$, the degree of the minimal polynomial cannot exceed N. Once the minimal polynomial has been found, one needs to determine whether it has only *single* roots, i.e., whether

$$m_{\mathsf{M}}(\lambda) = \prod_{\nu=1}^{\nu_0(\leq N)} (\lambda - M_\nu)\,, \quad \text{all } M_\nu \text{ distinct}\,, \tag{3}$$

holds. If it does, the matrix M *is* diagonalizable, otherwise it is *not* diagonalizable: multiple roots of m_{M} indicate the presence of Jordan blocks larger than one.

The procedure to determine the minimal polynomial of M, outlined in [3], invokes the characteristic polynomial of M and repeated applications of the Euclidean algorithm generalized to polynomials. The method presented below, taken from [8], aims at directly constructing the minimal polynomial. The fundamental observation is that matrices of dimension N constitute a vector space of dimension N^2. This is seen immediately by setting up a one-to-one correspondence between matrices of dimension three and vectors of length $9 \equiv 3^2$, for example, by rearranging the elements M_{jk} of each M systematically according to

$$\mathsf{M} \Leftrightarrow (\mathsf{M}_{11}, \mathsf{M}_{12}, \mathsf{M}_{13}; \mathsf{M}_{21}, \mathsf{M}_{22}, \mathsf{M}_{23}; \mathsf{M}_{31}, \mathsf{M}_{32}, \mathsf{M}_{33})^{\mathrm{T}}. \tag{4}$$

In view of this correspondence, the Cayley–Hamilton theorem - every matrix satisfies its own characteristic equation, $p_{\mathsf{M}}(\mathsf{M}) = 0$, turns into a statement about linear *dependence* of the $(N+1)$ *vectors* $\mathsf{E} \equiv \mathsf{M}^0, \mathsf{M}, \mathsf{M}^2, \ldots, \mathsf{M}^N$. In order to find the minimal polynomial of a matrix M, one thus calculates $\mathsf{M}^n, n = 1, \ldots N$, and then determines whether the vectors E and M are linearly independent; if not, one adds M^2 and asks the same question; etc. Proceeding in this way, one is obviously able to identify linear dependence among the vectors M^n with the smallest possible number n. This, however, comes down to the definition of the minimal polynomial of M. Gram–Schmidt orthonormalization effectively provides a systematic test for linear dependence among the first k elements of $\mathsf{M}^n, n = 0, \ldots N$.

Applying these ideas explicitly to the matrix H in (2) leads to

$$\mathsf{E} \Leftrightarrow (1,0,0;0,1;0;0,0,1)\,, \tag{5}$$

$$\mathsf{H} \Leftrightarrow (\mathrm{i}\xi, 1, 0; 1, 0, 1; 0, 1, -\mathrm{i}\xi)\,, \tag{6}$$

$$\mathsf{H}^2 \Leftrightarrow (1-\xi^2, -\mathrm{i}\xi, 1; -\mathrm{i}\xi, 2, \mathrm{i}\xi; 1, \mathrm{i}\xi, 1-\xi^2)\,, \tag{7}$$

$$\mathsf{H}^3 \Leftrightarrow (2-\xi^2)\,(\mathrm{i}\xi, 1, 0; 1, 0, 1; 0, 1, -\mathrm{i}\xi) \equiv (2-\xi^2)\mathsf{H}\,. \tag{8}$$

It is easy to see that neither the first two nor the first three vectors in this sequence are linearly dependent. Consequently, there must be a relation expressing H^3 in terms of the others, giving rise to the desired minimal polynomial,

$$(2-\xi^2)\mathsf{H} - \mathsf{H}^3 = 0 \quad \Rightarrow \quad m_{\mathsf{H}}(\lambda) = \lambda^3 + (\xi^2 - 2)\lambda\,. \tag{9}$$

In addition, the characteristic polynomial of H must coincide with m_{H} since there is only one monic polynomial of third degree annihilating H.

If one is not able to factor the resulting minimal polynomial, one needs to check whether the minimal polynomial and its derivative $m'_{\mathsf{H}}(\lambda)$ have a common factor. This can be achieved by applying the Euclidean algorithm to this pair of polynomials (cf. [2, 3]). In this present case, it amounts to writing $m_{\mathsf{H}}(\lambda) = (\lambda - \alpha)m'_{\mathsf{H}}(\lambda)/3 + R_1(\lambda)$, implying that $\alpha = 0$ and $R_1(\lambda) = (2/3)(\xi^2 - 2)(\lambda + 1/2)$. Two different cases arise: if $\xi \neq 2$, one finds that the only common factor of the minimal polynomial and its derivative is equal to one - thus, the minimal polynomial is of the form (3) and the matrix H must have three different eigenvalues making it diagonalizable. If $\xi^2 = 2$, the algorithm immediately stops and thus identifies λ^2 as the highest common factor of $m_{\mathsf{H}}(\lambda)$ and its derivative. Consequently, the minimal polynomial has a three-fold root $\lambda\,(= 0)$, indicating that H is not diagonalizable.

4 Discussion and outlook

The properties of H at the exceptional points $\xi_\pm = \pm\sqrt{2}$ deserve a brief discussion. It is not difficult to see that the *geometric* multiplicity of the eigenvalue 0 is one at the exceptional points (H has only one non-zero eigenvector) while its *algebraic* multiplicity equals three (zero is a triple root of m_{H}). Contrary to previously studied cases, *three* eigenvalues coalesce for $\xi \to \xi_\pm$.

For all values of ξ, the vector $(1, -\mathrm{i}\xi, -1)$ is an eigenstate of $\mathsf{H}(\xi)$ with eigenvalue 0, and it is well-behaved near and at the critical values $\xi_\pm$. Therefore, it seems reasonable to say that it is the eigenstates associated with the two λ-dependent eigenvalues which disappear at the exceptional point. It is not obvious from a physical point of view why this scenario is preferred over the familiar situation of just one disappearing eigenstate.

The natural question to ask now is whether one can expect algorithmic tests for diagonalizability to exist for a quantum system existing in a Hilbert space accommodating a countable infinity of states. As one needs to potentially perform an infinite number of steps, the idea of a useful algorithm gets somewhat blurred. Nevertheless, it is likely that one can search for systematic properties of finite-dimensional approximations which, hopefully, behave smoothly in the limit of infinite dimension.

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