How to Test for Diagonalizability: The Discretized PT-Invariant Square-Well Potential

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Abstract

Given a non-hermitean matrix $M$, the structure of its minimal polynomial encodes whether $M$ is diagonalizable or not. This note will explain 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. It turns out not to be diagonalizable for a critical strength of the interaction, also indicated by the transition of two real into a pair of complex energy eigenvalues. 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.

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 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-hermitean 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.

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,

$$V(x) = \begin{cases} -iZ, & -2L < x < 0, \\ 0, & x = 0, \\ iZ, & 0 < x < 2L, \end{cases} \quad Z \in \mathbb{R},$$

which has proved a useful testbed for the discussion of PT-symmetric systems. Its eigenvalues are given as the zeros of a transcendental equation [4], and, for each value of $Z$, the lowest two real eigenvalues are known to coalesce and then disappear jointly at critical values of the parameter.

Let us introduce a toy-version of this system by discretizing its configuration space. This strategy has been applied successfully to describe tunneling 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 $-2L \leq x \leq 2L$, are replaced by five equidistant points at $0, \pm L, \pm 2L$. The wave function is allowed to take nonzero values only at these points, so it will be a vector with five components at most. However, the hard walls of the square well at $\pm L$ force the wave function to vanish there, leaving us with only three non-zero components, $\psi \rightarrow \psi_k = \psi(kL), k = 0, \pm 1$. The potential energy defined in (1) turns into a diagonal matrix, $V(x) \rightarrow V = \text{diag}(-iZ, 0, iZ)$. The operator for the kinetic energy follows from replacing $\partial^2 \psi(x)/\partial x^2 \rightarrow (\psi_{k+1} - 2\psi_k + \psi_{k-1})/L^2$.

Putting all this together, the Hamiltonian operator of the discrete version of this system reads

$$H_0 \simeq 2E - \mathbf{H}, \quad \text{where} \quad \mathbf{H} = \begin{pmatrix} i\xi & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & -i\xi \end{pmatrix}, \quad \xi = Z/\eta;$$

here $E$ is the $(3 \times 3)$ 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 $\mathbf{H}$, and hence $H_0$, is invariant under the combined action of parity $\mathbf{P}$, represented by a matrix with unit entries equal to one along its minor diagonal and zero elsewhere, and $\mathbf{T}$, 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, $m_M(M) = 0$. This polynomial is unique if the coefficient of its highest power is taken to be one: the minimal polynomial is monic. Since any matrix $M$ of size $N$, say, is annihilated by its own characteristic polynomial, $p_M(M) = 0$, the degree of the minimal polynomial does not exceed $N$. Once $m_M$ has been found, one needs to determine whether it has only single roots, i.e. whether

$$m_M(\lambda) = \prod_{\nu=1}^{m_0(\leq N)} (\lambda - M_\nu), \quad \text{all } M_\nu \text{ distinct}. \quad (3)$$

holds. If it does, the matrix $M$ is diagonalizable - otherwise, it is not diagonalizable since multiple roots of $m_M$ indicate the presence of Jordan blocks larger than one.

The procedure to determine the minimal polynomial of $M$, as 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 size $N$ constitute a vector space of dimension $N^2$. This is seen immediately by setting up a one-to-one correspondence between matrices of size 3 and vectors of length $9 \equiv 3^2$, for example, simply by rearranging the elements $M_{jk}$ of each $M$ systematically according to

$$M \leftrightarrow (M_{11}, M_{12}, M_{13}; M_{21}, M_{22}, M_{23}; M_{31}, M_{32}, M_{33})^T. \quad (4)$$

In view of this correspondence, the theorem by Cayley-Hamilton - every matrix satisfies its own characteristic equation, $p_M(M) = 0$, - turns into a statement about linear dependence of the $(N + 1)$ vectors $E \equiv M^0, M, M^2, \ldots, M^N$. In order to find the minimal polynomial of a matrix $M$ one thus simply calculates $M^n, n = 1 \ldots N$, and then determines successively 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 $M^n$ containing only the smallest powers necessary. 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 $M^n, n = 0 \ldots N$. 

3
Applying these ideas explicitly to the matrix $H$ in \( \text{(2)} \) leads to

\[
\begin{align*}
\mathbf{E} & \leftrightarrow (1, 0, 0; 0, 1; 0, 0, 1), \\
\mathbf{H} & \leftrightarrow (i\xi, 1; 0, 1, 0, 1, -i\xi), \\
\mathbf{H}^2 & \leftrightarrow (1 - \xi^2, -i\xi, 1; -i\xi, 2, i\xi; 1, i\xi, 1 - \xi^2), \\
\mathbf{H}^3 & \leftrightarrow (2 - \xi^2) (i\xi, 1, 0; 1, 0, 1, 0, 1, -i\xi) \equiv (2 - \xi^2)\mathbf{H}.
\end{align*}
\]

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 $\mathbf{H}^3$ in terms of the others, and indeed, the minimal polynomial follows immediately from

\[
(2 - \xi^2)\mathbf{H} - \mathbf{H}^3 = 0 \quad \Rightarrow \quad m_{\mathbf{H}}(\lambda) = \lambda^3 + (\xi^2 - 2)\lambda.
\]

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

If one is not able to factor the resulting minimal polynomial, one needs to check whether the minimal polynomial and its derivative $m'_{\mathbf{H}}(\lambda)$ have a common factor which can be achieved by applying the Euclidean algorithm to this pair (cf. \( \text{[2, 3]} \)). In this present case, this amounts to writing $m_{\mathbf{H}}(\lambda) = (\lambda - \alpha)m'_{\mathbf{H}}(\lambda)/3 + R_1(\lambda)$, 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 the derivative is equal to one - thus, the minimal polynomial is of the form \( \text{[5]} \) and the matrix $\mathbf{H}$ must have three different eigenvalues making it diagonalizable. If $\xi^2 = 2$, the algorithm immediately stops and thus identifies $\lambda^2$ as the highest common factor of $m_{\mathbf{H}}(\lambda)$ and its derivative. Consequently, the minimal polynomial has a three-fold root $\lambda(= 0)$, indicating that $\mathbf{H}$ is not diagonalizable.

### 4 Discussion and Outlook

The properties of $\mathbf{H}$ at the exceptional points defined by $\xi_{\pm} = \pm \sqrt{2}$ deserve a brief discussion. It is not difficult to see that the geometric multiplicity of the eigenvalue $0$ is one at the exceptional points ($\mathbf{H}$ has only one non-zero eigenvector) while its algebraic multiplicity equals three (zero is a triple root of $m_{\mathbf{H}}$). Contrary to previously studied cases, three eigenvalues coalesce for $\xi \rightarrow \xi_{\pm}$. For all values of $\xi$, the vector $(1, -i\xi, -1)$ is an eigenstate of $\mathbf{H}(\xi)$ with eigenvalue $0$, and it does not exhibit any particular behaviour at the critical values $\xi_{\pm}$. Therefore, it seems reasonable to say that the eigenstates associated with the two $\lambda$-dependent eigenvalues 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 living 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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