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Detecting broken PT-symmetry

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Abstract
A fundamental problem in the theory of PT-invariant quantum systems is to determine whether a given system 'respects' this symmetry or not. If not, the system usually develops non-real eigenvalues. It is shown in this contribution how to algorithmically detect the existence of complex eigenvalues for a given PT-symmetric matrix. The procedure uses classical results from stability theory which qualitatively locate the zeros of real polynomials in the complex plane. The interest and value of the present approach lies in the fact that it avoids diagonalization of the Hamiltonian at hand.

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1. Motivation

When dealing with a non-Hermitian operator such as

$$\mathsf{H} = p^2 + \mathrm{i}x^3, \tag{1}$$

one needs to address two questions which do not arise for a Hermitian operator:

Q1. Is the operator H diagonalizable?
Q2. Does the operator H have real eigenvalues only?

For a randomly picked non-Hermitian operator the answers to both questions are unlikely to be positive: it will have neither a complete set of eigenfunctions nor a real spectrum. However, operators with PT-symmetry [1],

$$[\mathsf{H}, \mathsf{PT}] = 0, \tag{2}$$

invariant under simultaneous application of parity P and time-reversal T, behave somewhat 'better'. PT-invariant operators tend to be diagonalizable but for the rare occurrence of exceptional points, and each of their eigenvalues must be either real or have a complex-conjugate counterpart. Positive answers to Q1 and Q2 are necessary in order to attempt a

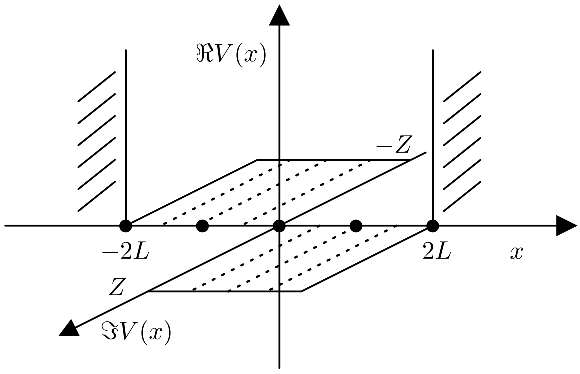

Figure 1. Discretized PT-symmetric well: the wavefunction takes non-zero values at three points $x = 0, \pm L$ only (cf text).

consistent quantum mechanical interpretation of the operator H since it can be similar to a Hermitian operator only then [2].

To answer these questions for a given PT-invariant Hamiltonian is by no means straightforward. It is known, for example, that the operator H in equation (1) does have only real eigenvalues [3, 4] while the (likely) completeness of its eigenfunctions has, apparently, not yet been established rigorously. Perturbative results allow one to confirm that the spectrum of an initially Hermitian operator such as the Hamiltonian of a particle in an oscillator-type potential remains real if a sufficiently weak PT-symmetric term is added [5]. As long as no degeneracies develop, this approach also makes plausible the existence of a complete set of eigenfunctions; they are, however, not necessarily pairwise orthogonal with respect to the standard scalar product in Hilbert space. Technically, the difficulties are due to the fact that the cubic term in equation (1) is unbounded on the real axis, and the unperturbed operator does not provide a bound for it. When restricted to a finite interval, a perturbation such as igx^3, $g \in \mathbb{R}$, *is* bounded, and one can reach general conclusions when perturbing the Hermitian boundary value problem with a non-Hermitian PT-symmetric term. Upon treating the PT-symmetrically perturbed square-well potential [6] in a Krein space setting, one can show [7] that its eigenvalues remain real if the perturbation does not move the (non-degenerate) real eigenvalues far enough along the real axis to create a degeneracy, which is necessary for complex eigenvalues to emerge. A similar result also follows by a non-perturbative approach when a 'slightly' non-self-adjoint term is added to a self-adjoint operator, as is described in [8].

More is known for PT-symmetric systems with a *finite*-dimensional state space which are described by complex symmetric matrices M. Let us consider an example which exhibits the essential features: the *discretized* PT-symmetric square well [9]. This model, sketched in figure 1, is obtained upon discretizing the configuration space of a particle moving freely between walls at $x = \pm 2L$, subjected to a piecewise constant potential $\pm iZ$, $Z \in \mathbb{R}$. Defining a wavefunction which takes values at the points $x = 0, \pm L, \pm 2L$, and satisfies 'hard' boundary conditions at $x = \pm 2L$, an effective Hamiltonian is obtained,

$$\mathsf{H} = \begin{pmatrix} i\xi & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & -i\xi \end{pmatrix}, \qquad \xi = 2mL^2 Z/\hbar^2. \tag{3}$$

This matrix is invariant under the action of parity P, a matrix with ones along the minor diagonal and zeros elsewhere, followed by complex conjugation, overall equivalent to equation (2). The eigenvalues of H are given by the roots of its characteristic polynomial,

$$p_{\mathsf{H}}(\lambda) = \lambda(\lambda^2 - (2 - \xi^2)), \tag{4}$$

reading explicitly,

$$E_0 = 0 \qquad \text{and} \qquad E_\pm = \pm\sqrt{2 - \xi^2} \in \begin{cases} \mathbb{R} & \text{if} \quad |\xi| < \sqrt{2}, \\ \mathrm{i}\mathbb{R} & \text{if} \quad |\xi| > \sqrt{2}. \end{cases} \tag{5}$$

The possibility of analytically determining the eigenvalues of H provides immediate and exhaustive answers to both Q1 and Q2, summarized briefly now. The zero eigenvalue (with its associated eigenstate) persists for all values of ξ, while the remaining two change their character with varying strength of the parameter Z. Three regions can be identified: depending on the magnitude of ξ, there is either a pair of complex conjugate or a pair of real eigenvalues. However, the matrix H is not diagonalizable for $\xi = \pm\sqrt{2}$: only a single eigenvector is associated with $E_\pm = 0$, while the *algebraic* multiplicity of this eigenvalue is 2 [9].

For matrices M of larger dimensions no analytic expressions for the eigenvalues exist. To overcome this shortcoming, an algorithm has been proposed which is capable of detecting whether a PT-invariant matrix is diagonalizable or not [10]. The relevant information is coded in the *minimal* polynomial of the matrix which one can construct without knowing the eigenvalues of M, just like its *characteristic* polynomial. This approach answers Q1 systematically, circumventing the need to numerically calculate the eigenvalues of M. This is important from a conceptual point of view.

In the present contribution, a second, independent algorithm will be presented which answers Q2 for any PT-symmetric matrix. Both the number of its real eigenvalues and the number of pairs of complex eigenvalues are obtained by manipulating the coefficients of the characteristic polynomial of M. This information will be called the *qualitative spectrum* of M.

The interest of the method proposed is due to the fact that it is possible to extract nothing but the desired information about the eigenvalues, namely their location relative to the real axis in the complex plane. Problems of this type arise when the stability of dynamical systems is addressed where it is crucial to determine whether the eigenvalues of a given matrix have negative real parts.

In section 2, the notion of inertia is introduced for Hermitian matrices, followed by Jacobi's criterion of stability for such matrices. Then, the breaking (or not) of PT-symmetry is described in terms of a modified inertia. Next, a theorem by Jacobi and Borhard is presented which locates the zeros of real polynomials in the complex plane. Section 3 combines all this to formulate an algorithm which, given a PT-invariant (or quasi-Hermitian) matrix, outputs the number of its real and complex eigenvalues. Finally, the algorithm is illustrated by applying it to the discretized PT-symmetric square-well potential introduced above, outputting correctly its qualitative spectrum.

2. Stability and inertia of matrices

Consider a dynamical system which is described exactly or, after some approximation, by the equation

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathsf{M} \cdot \mathbf{x}, \tag{6}$$

where M is a fixed Hermitian (or real symmetric) matrix of dimensions $(N \times N)$, and the vector $\mathbf{x}(t)$ gives the state of the system at time t. In many applications, one needs to know

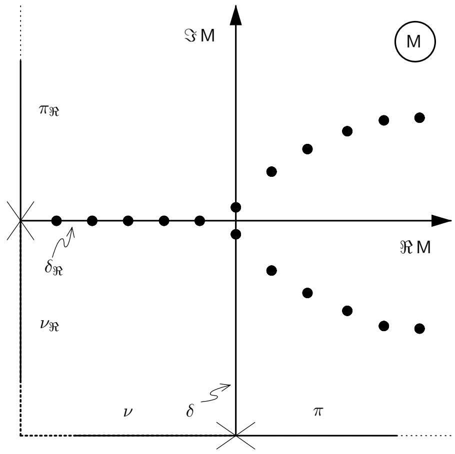

Figure 2. Imaginary and real inertia of a (17×17) matrix M with broken PT-symmetry, having five real eigenvalues and six pairs of complex-conjugate eigenvalues: $\mathtt{In}\,\mathsf{M} = \{5, 2, 10\}$ and $\mathtt{In}_{\Re}\,\mathsf{M} = \{6, 5, 6\}$, see equations (8) and (16), respectively.

whether the solutions of equation (6) are *stable*: this is the case if all eigenvalues M_n of M have negative real parts,

$$\mathfrak{Re}\,\mathsf{M}_n < 0. \tag{7}$$

Indeed, no solution of equation (6) will grow without bounds if (7) holds, making it possible to qualitatively predict the system's long-term behaviour. Let us characterize a matrix M by a triple of non-negative integers, its *inertia* [11] with respect to the imaginary axis,

$$\mathtt{In}\,\mathsf{M} = \{\nu, \delta, \pi\}, \tag{8}$$

where ν and π are the number of its eigenvalues with negative and positive real parts, respectively, while δ counts the eigenvalues on the imaginary axis (cf figure 2 for an illustration). All eigenvalues are counted according to their multiplicities. A stable matrix M has an inertia of the form

$$\mathtt{In}\,\mathsf{M} = \{N, 0, 0\}, \tag{9}$$

while a matrix is called *marginally stable* if all its eigenvalues have non-positive real parts, allowing for the presence of purely imaginary eigenvalues,

$$\mathtt{In}\,\mathsf{M} = \{N - m, m, 0\}, \qquad 0 < m \leqslant N. \tag{10}$$

Whenever $\pi > 0$, the matrix M is called *unstable* since there is at least one solution of (6) which will grow without bound.

2.1. Inertia of Hermitian matrices: Jacobi's method

Jacobi devised an ingenious method [12] to determine the inertia of a given (non-singular) *Hermitian* matrix L of size $(N \times N)$. First, calculate the determinants d_n of its N leading principal submatrices $\mathsf{L}_1, \mathsf{L}_2, \ldots, \mathsf{L}_N \equiv \mathsf{L}$, all of which must be different from zero,

$$d_n \equiv \det \mathsf{L}_n, \qquad n = 1, \ldots, N; \tag{11}$$

second, write down a '+' followed by the sequence of signs σ_n of the N determinants d_n,

$$+, \sigma_1, \sigma_2, \ldots, \sigma_N, \qquad \sigma_n = \frac{d_n}{|d_n|} = \pm 1. \tag{12}$$

These $(N + 1)$ signs encode the inertia of the matrix L: the number of sign *changes* in this sequence equals the number π of eigenvalues with positive real part, while the number of *constancies* in signs equals the number ν of its negative eigenvalues:

$$\left.\begin{array}{l}\text{Number of constancies in (12)} \equiv \pi \\ \text{Number of alterations in (12)} \equiv \nu\end{array}\right\} \quad \Rightarrow \quad \mathtt{In}\,\mathsf{L} = (\nu, 0, \pi). \tag{13}$$

The matrix L cannot have a zero eigenvalue, that is, $\delta \equiv 0$, since all leading subdeterminants including d_N have been assumed to be non-zero.

The following section will show that it is possible to detect the location of the eigenvalues of a PT-symmetric (hence non-Hermitian) matrix relative to the *real* axis by similar methods.

2.2. *Stability and inertia of* PT-*invariant matrices*

A non-Hermitian matrix H with PT-symmetry satisfies (2), which implies that its characteristic polynomial

$$p_{\mathsf{H}}(\lambda) = \sum_{n=0}^{N} h_n \lambda^n \tag{14}$$

has real coefficients h_n only,

$$p^*_{\mathsf{H}}(\lambda) = p_{\mathsf{H}}(\lambda^*). \tag{15}$$

As a consequence, the zeros of this polynomial are either real or they come in complex-conjugate pairs. To distinguish between broken and unbroken PT-symmetry, it is useful to introduce the inertia of a matrix H with respect to the *real* axis,

$$\mathtt{In}_{\Re}\,\mathsf{H} = \{\nu_{\Re}, \delta_{\Re}, \pi_{\Re}\}, \tag{16}$$

where the triple $\{\nu_{\Re}, \delta_{\Re}, \pi_{\Re}\}$ of integers denotes the number of eigenvalues of H with negative, vanishing and positive imaginary part (cf figure 2). The inertia of a matrix with real eigenvalues only, corresponding to *unbroken* PT-symmetry, reads

$$\mathtt{In}_{\Re}\,\mathsf{H} = \{0, N, 0\}, \tag{17}$$

while *broken* PT-symmetry is signalled by an inertia of the form

$$\mathtt{In}_{\Re}\,\mathsf{H} = \{m, N - 2m, m\}, \qquad m > 0, \tag{18}$$

corresponding to m pairs of complex eigenvalues and $(N - 2m)$ real ones. Thus, for any PT-invariant matrix the numbers $\nu_{\Re}$ and $\pi_{\Re}$ coincide, the symmetry being broken or not. Let us now turn to the question how to determine the real inertia of a matrix with PT-symmetry.

2.3. *Zeros of real polynomials*

Given a real polynomial $p(\lambda)$ of degree N, one can proceed as follows to obtain the number of its real zeros. To begin, one determines the first $(2N - 2)$ Newton sums associated with the polynomial $p(\lambda)$ defined by

$$s_0 = N, \qquad s_n = \lambda_1^n + \cdots + \lambda_N^n, \qquad n = 1, 2, \ldots, 2N - 2. \tag{19}$$

This is possible *without* knowing the zeros $\lambda_1, \ldots, \lambda_N$, since one can [11] either define the numbers s_n recursively in terms of the coefficients h_n of the polynomial or generate them by means of the identity

$$\frac{\mathrm{d}p(\lambda)}{\mathrm{d}\lambda} = (s_0\lambda^{-1} + s_1\lambda^{-2} + \cdots)p(\lambda). \tag{20}$$

Once the Newton sums have been calculated, one introduces the real symmetric (and Hermitian) matrix

$$\mathfrak{H}_p = \begin{pmatrix} s_0 & s_1 & s_2 & \cdots & s_{N-1} \\ s_1 & s_2 & & \cdots & s_N \\ s_2 & & & & s_{N+1} \\ \vdots & & & & \vdots \\ s_{N-1} & s_N & & \cdots & s_{2N-2} \end{pmatrix}, \tag{21}$$

which, having constant entries along its minor diagonals, is of Hankel type. One can thus apply the method presented in section 2.1 to determine its imaginary inertia[1]. This is useful since Borhard [14] and Jacobi [15] have shown[2] that the inertia of $\mathfrak{H}_p$, in fact, encodes the structure of the zeros of the polynomial $p(\lambda)$:

$$\mathtt{In}\,\mathfrak{H}_p = \{\nu, 0, \pi\} \quad \Rightarrow \quad p(\lambda) \text{ has } \begin{cases} \pi - \nu \text{ different real zeros,} \\ \nu \text{ different pairs of complex-conjugate zeros.} \end{cases} \tag{22}$$

Let us imagine that the real polynomial $p(\lambda)$ is the characteristic polynomial $p_{\mathsf{H}}(\lambda)$ associated with a PT-invariant matrix H. Then, the result (22) says that H has ν pairs of different complex eigenvalues and $(\pi - \nu)$ different real eigenvalues if the Hankel matrix $\mathfrak{H}_{\mathsf{H}}$ associated with $p_{\mathsf{H}}(\lambda)$ has $\nu(\pi)$ eigenvalues with negative (positive) real part. Expressed in terms of inertias, this result reads

$$\mathtt{In}\,\mathfrak{H}_{\mathsf{H}} = \{\nu, 0, \pi\} \quad \Longrightarrow \quad \mathtt{In}_{\Re}\mathsf{H} = \{\nu, \pi - \nu, \nu\}. \tag{23}$$

The next section will collect the results obtained so far and present them as an algorithm to determine the number of complex pairs and real eigenvalues of a PT-invariant matrix.

3. Algorithm for detecting complex eigenvalues

Given a matrix H of dimensions $(N \times N)$ which is invariant under the combined action of parity P and time-reversal T, equation (2), here is an algorithm that determines its qualitative spectrum.

(1) Calculate the characteristic polynomial $p_{\mathsf{H}}(\lambda)$ of the matrix H.
(2) Determine the first $(2N - 2)$ Newton sums s_n associated with the polynomial $p_{\mathsf{H}}(\lambda)$.
(3) Write down the Hankel matrix $\mathfrak{H}_{\mathsf{H}}$ (21), defined in terms of the sums s_n.
(4) Obtain the number of constancies π and alterations ν in the sequence of signs (12) giving the inertia of $\mathfrak{H}_{\mathsf{H}}$ as $\mathtt{In}\,\mathfrak{H}_{\mathsf{H}} = \{\nu, 0, \pi\}$.
(5) Then, the inertia of the PT-invariant matrix H follows from the inertia $\mathtt{In}\,\mathfrak{H}_{\mathsf{H}}$ using (23) with $N \equiv \pi + \nu$,

$$\mathtt{In}_{\Re}\,\mathsf{H} = \{\nu, N - 2\nu, \nu\}. \tag{24}$$

Consequently, PT-symmetry is broken if $\nu > 0$, and H will have ν pairs of complex-conjugate eigenvalues while the remaining $(N - 2\nu)$ ones are real. Thus, the main result of this paper has been established.

[1] To evaluate the leading principal minors of $\mathfrak{H}_p$ means, in modern terminology [13], to determine the first N terms of the *Hankel transform* of the sequence $s_0, s_1, s_2, \ldots$.
[2] The content of [14] and [15] is described in [11].

3.1. Example: the discretized PT-*symmetric square well*

Let us work through the algorithm to detect the qualitative spectrum of the PT-symmetric discretized square-well potential described by the matrix H in (3)—this time *without* solving for its eigenvalues. The derivative of its characteristic polynomial (4) reads

$$\frac{\mathrm{d}p_{\mathsf{H}}(\lambda)}{\mathrm{d}\lambda} = 3\lambda^2 - (2-\xi^2). \tag{25}$$

Compare the expansion

$$\frac{p'_{\mathsf{H}}(\lambda)}{p_{\mathsf{H}}(\lambda)} = 3\lambda^{-1} + 2(2-\xi^2)\lambda^{-3} + 2(2-\xi^2)^2\lambda^{-5} + \mathcal{O}(\lambda^{-7}) \tag{26}$$

with (20), to read off the first five Newton sums. The Hankel matrix associated with H is given by

$$\mathfrak{H}_{\mathsf{H}} = 2\begin{pmatrix} 3/2 & 0 & (2-\xi^2) \\ 0 & (2-\xi^2) & 0 \\ (2-\xi^2) & 0 & (2-\xi^2)^2 \end{pmatrix}, \tag{27}$$

and its leading principal minors have determinants

$$d_1 = 3, \qquad d_2 = 6(2-\xi^2), \qquad d_3 = 4(2-\xi^2)^3. \tag{28}$$

Depending on the value of the parameter ξ, two different sequences of signs arise; for $\xi^2 < 2$, one has all d_n positive, resulting in *three* constancies and *no* alteration:

$$+ + + + \quad \Rightarrow \quad \mathtt{In}\,\mathfrak{H}_{\mathsf{H}} = \{0, 0, 3\}, \tag{29}$$

while d_2 and d_3 turn negative for $\xi^2 > 2$, implying that

$$+ + - - \quad \Rightarrow \quad \mathtt{In}\,\mathfrak{H}_{\mathsf{H}} = \{1, 0, 2\}. \tag{30}$$

Using relation (24), the inertia of H with respect to the real axis is finally given by

$$\mathtt{In}_{\Re}\,\mathsf{H} = \begin{cases} \{0, 3, 0\} & \text{if} \quad |\xi| < \sqrt{2}, \\ \{1, 1, 1\} & \text{if} \quad |\xi| > \sqrt{2}. \end{cases} \tag{31}$$

Thus, the spectrum of H is *real* for $\xi^2 < 2$, while a pair of *complex* eigenvalues exist whenever $\xi^2 > 2$. This agrees with the exact result given in (5).

For $\xi = \pm\sqrt{2}$, the method cannot be applied since the matrix $\mathfrak{H}_{\mathsf{H}}$ in (27) develops leading principal minors with vanishing determinant. This is consistent with the fact that for these values of ξ the properties of the matrix H undergo qualitative changes such as the 'disappearance' of an eigenstate. However, this does not put the current approach in jeopardy since these exceptional points can be identified *beforehand* by running the algorithm presented in [10], which checks whether a given PT-invariant matrix is diagonalizable. In the present example, the points $\xi = \pm\sqrt{2}$ would be flagged, as shown explicitly in [9].

In fact, modifications of the current approach have been developed by Gundelfinger and Frobenius (cf [11]) which are able to cope with the presence of at most *three* consecutive *vanishing* determinants d_n. The general relation between the vanishing principal subdeterminants d_n of the Hankel matrix $\mathfrak{H}_{\mathsf{H}}$ and the zeros of the polynomial $p_{\mathsf{H}}(\lambda)$ is not obvious. In view of the example discussed above, it seems reasonable to conjecture that there is a close link between the non-diagonalizability of the matrix H and the existence of vanishing leading submatrices d_n of $\mathfrak{H}_{\mathsf{H}}$.

4. Discussion and outlook

An algorithm has been presented which is capable of determining whether the eigenvalues of a PT-invariant matrix H (or possibly a family of such matrices depending smoothly on parameters) are complex or not. It complements an earlier algorithm [10] which detects whether a PT-invariant matrix does have a complete set of eigenstates. Thus, the fundamental questions Q1 and Q2 about PT-invariant system as spelled out in the introduction can be answered in a systematic way if the system is described by a matrix of *finite* but arbitrarily large dimension.

From a numerical point of view, the current algorithm does not appear to be particularly efficient. First, one needs to calculate the characteristic polynomial of the $(N \times N)$ matrix H and, second, all principal minors of $\mathfrak{H}_p$ in equation (21) must be determined, that is, N determinants of matrices with dimensions $1, 2, \ldots, N$. It is likely, however, that these calculations can be simplified due to the structure of $\mathfrak{H}_p$: for example, one can invert *Hankel* matrices using 'superfast' algorithms [16] requiring only $\mathcal{O}(N \log^2 N)$ steps. Furthermore, one is only interested in the *signs* of the principal minors of $\mathfrak{H}_p$ which, under some circumstances, are accessible using particularly efficient methods [17]. The method proposed here has the advantage of being *exact*, contrary to any numerical implementation generating approximations of the eigenvalues of the matrix H. Furthermore, as the example in section 3.1 has shown, it is possible to carry along free parameters allowing for the subsequent investigation of continuous ranges of values.

Although desirable, it is not yet obvious how to generalize the algorithm presented here to operators such as $\mathsf{H} = p^2 + \mathrm{i}x^3$ acting in an *infinite-dimensional* space. This observation also applies to the algorithm for diagonalizability mentioned earlier. Finally, it seems worth while to point out that more efficient algorithms to determine the qualitative spectrum of a PT-invariant matrix are likely to exist—Sturmian sequences based on the Euclidean algorithm for polynomials [18] being the most promising candidates.

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