Hilbert space inner products for PT-symmetric Su-Schrieffer-Heeger models

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March 3, 2022

Abstract

A Su-Schrieffer-Heeger model with added PT-symmetric boundary term is studied in the framework of pseudo-hermitian quantum mechanics. For two carefully chosen special cases, a complete set of pseudometrics is constructed in closed form. When complemented with a condition of positivity, the pseudometrics determine all the physical inner products of the considered model.

1 Introduction

The Su-Schrieffer-Heeger (SSH) model [1, 2] is one of the benchmark topologically nontrivial models in physics of condensed matter. It provides a convenient description of certain physical systems [3, 4], and serves as one of the simplest examples of topological insulators [5]. The $n$-site SSH model may be expressed as

$$H_{\text{SSH}}^{(n)} = \sum_{i=1}^{N} \left[ t(1 - \Delta \cos \theta) a_{2i}^\dagger a_{2i-1} + t(1 + \Delta \cos \theta) a_{2i}^\dagger a_{2i+1} + h.c. \right]$$

with $a_i^\dagger, a_i$ being the $i$-th site fermionic creation and annihilation operators. It has been suggested [2] to complement this hermitian SSH model with a non-hermitian $\mathcal{PT}$-symmetric (invariant under simultaneous action of parity and time reversal) boundary term

$$H_I = \gamma a_1^\dagger a_1 + \gamma^* a_n^\dagger a_n$$

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with $\gamma = i\alpha, \alpha \in \mathbb{R}$. Despite apparent non-hermicity of the resulting operator $H = H_{SSH} + H_I$, it has been shown that its eigenvalues remain real for $|\alpha|$ sufficiently small. This motivates further examination of this model from the viewpoint of $\mathbb{PT}$-symmetric quantum mechanics.

$\mathbb{PT}$-symmetric quantum mechanics [6, 7, 8] is a theoretical framework for studying representations of quantum observables by non-hermitian operators. It is based on a simple fact, that an observable may be represented by a non-hermitian operator on a given Hilbert space $\mathcal{H}^{(F)} = (\mathcal{V}, \langle \cdot | \cdot \rangle)$, as long as such operator is hermitian in another Hilbert space $\mathcal{H}^{(S)} = (\mathcal{V}, \langle \phi | \psi \rangle_\Theta)$ [9]. The inner products on $\mathcal{V}$ are in one-to-one correspondence with so-called metric operators $\Theta$ through the formula

$$\langle \phi | \psi \rangle_\Theta = \langle \phi | \Theta | \psi \rangle$$

where we require $\Theta$ to be bounded, hermitian and positive in order to generate a genuine inner product [10]. The hermicity condition of $H$ in $\mathcal{H}^{(S)}$ could be expressed in operator form as

$$H^\dagger \Theta = \Theta H$$

which is a direct generalization of the standard condition $H = H^\dagger$. Operators $H$ satisfying eq. 4 for at least one metric operator $\Theta$ are called quasi-hermitian [11]. It is clear that on a given Hilbert space $\mathcal{H}^{(F)}$, all admissible observables are described by quasi-hermitian instead of hermitian operators. Furthermore, recall that for any bounded, positive $\Theta$, there always exists a decomposition $\Theta = \Omega^\dagger \Omega$ with $\Omega$ bounded. Inserting this decomposition into eq. 4 yields

$$h := \Omega H \Omega^{-1} = (\Omega H \Omega^{-1})^\dagger = h^\dagger$$

which shows that being quasi-hermitian is equivalent to being boundedly diagonalizable with real spectrum (instead of unitarily diagonalizable). However, the construction of the similarity transformation $\Omega$ may be in general very difficult for a given $H$. Special attention is usually given to parametric quasi-hermitian models with nontrivial domains of observability. The boundaries of such domains are formed of the so-called exceptional points (EPs) [12, 13], points in parameter space, where the operator ceases to be diagonalizable. The boundary crossings of physical parameters (e.g. time) are studied under the name quantum catastrophes [14], which emphasizes close relationship to classical catastrophe theory [15].

This paper is divided as follows: in section 2, we introduce the general case of the examined $\mathbb{PT}$-symmetric SSH model. In section 3, we link its special case $\cos \theta = 0$ to a discretized Robin square well, and construct a complete set of pseudometrics. In section 4, we repeat this procedure for a dual SSH nearest-neighbor interaction. In section 5, we consider the general case $H = H_{SSH} + H_I$, and address the questions of pseudometric construction and cutoff emergence. Section 6 is devoted to discussion and remarks.

2 The $\mathbb{PT}$-symmetric SSH model

Inspired by [2], we examine a SSH model with open boundary conditions, complemented by the $\mathbb{PT}$-symmetric boundary term as in eq. 2. Throughout this paper, we set with no loss of generality $t = 1, \Delta = 1$, and denote $\lambda = \cos \theta$ in eq. 1. The coupling constant $\gamma$ was taken to be purely imaginary in [2], while we assume a more general case $\gamma = \rho + i\omega \in \mathbb{C}$. In order to apply powerful tools of linear algebra, we work in a matrix representation of the creation and
annihilation operators. The basis of a corresponding two-dimensional Hilbert space is chosen, such that

\[
\begin{align*}
a|0\rangle &= 0, & a^\dagger|0\rangle &= |1\rangle \\
a|1\rangle &= |0\rangle, & a^\dagger|1\rangle &= 0
\end{align*}
\]  

(6)

In such case, the model from eq. 1 becomes a family of \(n \times n\) matrices with \(n = 2N\). We adopt a strategy of printing the matrices explicitly for the \(n = 4\), as long as the extrapolation pattern for higher \(n \in \mathbb{N}\) is clear enough. That means we may write

\[
H^{(4)} = H_{SSH}^{(4)} + H_I^{(4)} = \begin{bmatrix}
\gamma & -1 - \lambda & -1 + \lambda & -1 - \lambda \\
-1 - \lambda & -1 + \lambda & -1 - \lambda & -1 + \lambda \\
-1 + \lambda & -1 - \lambda & -1 + \lambda & -1 - \lambda \\
-1 - \lambda & -1 + \lambda & -1 - \lambda & -1 + \lambda 
\end{bmatrix}
\]  

(7)

In parallel with numerical experiments of [2], we illustrate the effects of general complex coupling in fig. I. Clearly, there is no reason to confine attention to purely imaginary \(\gamma\) in our \(\mathcal{PT}\)-symmetric considerations, as for \(\rho\) reasonably small, there always exists a nonempty interval of \(\omega\) with real spectrum. Size of such interval shrinks with growing \(\rho\), and finally vanishes completely, in the present case for \(\rho \approx 1\).

\[\text{Figure I: } \Re[\sigma(H)] \text{ and } \Im[\sigma(H)] \text{ for the } n = 50 \text{ SSH model as a function of } \theta. \text{ The values of } \gamma \text{ are } 0.5i, 0.5i + 1 \text{ and } 0.5i + 2.\]

\[\text{Figure II: } \text{Exceptional points of eq. 8 for } n = 3, 4, 5 \text{ in the } (\alpha, \beta) \text{ and } (\rho, \omega) \text{ coordinates.}\]
3 The Robin square well

The construction of Θ for infinite-dimensional quasi-hermitian models is in general a highly nontrivial task, which has to be approached perturbatively. An exceptional operator admitting exact metric construction (Laplacian on a real interval with imaginary Robin boundary conditions) was introduced in [16]. This inspired a subsequent paper [17], which applied discretization techniques on this continuous model, resulting in a $\mathbb{PT}$-symmetric family of matrices

$$H_{DR}^{(4)} = \begin{bmatrix} \gamma & -1 & & & \\ -1 & -1 & -1 & & \\ & -1 & -1 & \gamma^* & \\ & & & & \end{bmatrix} \quad \text{with} \quad \gamma = \frac{1}{1 - \alpha - i\beta}$$

which clearly coincides with eq. 7 for $\lambda = 0$. Throughout this paper, we shall use the natural parametrization $\gamma = \rho + i\omega$ instead of eq. 8. The coordinate transformation connecting these parametrizations is

$$\omega = \frac{\beta}{(1 - \alpha)^2 + \beta^2}, \quad \rho = \frac{1 - \alpha}{(1 - \alpha)^2 + \beta^2}$$

The domains of quasi-hermicity in both coordinate systems are shown in fig. II. The non-shrinking behavior of the domains in the limit $n \to \infty$ agrees with the existence of a quasi-hermitian operator in the continuous limit. Now, recall that any $n \times n$ metric may be expressed as $\Theta = \sum_{k=1}^{n} \kappa_{nk} |n\rangle\langle n|$ [18], where $|n\rangle$ are the eigenvectors of $H^\dagger$. Thus, a general metric depends on $n$ arbitrary parameters. Equivalently, we can construct $n$ linearly independent hermitian (but not necessarily positive) matrices $P^{(k)}$ for a given $H$, such that

$$\Theta = \sum_{k=1}^{n} \epsilon_k P^{(k)}$$

with $\epsilon_k$ being constrained by the condition $\Theta > 0$. Such a set of $P^{(k)}$ is called a complete set of pseudometrics. Although the decomposition from eq. 10 may be in general quite arbitrary, our aim is to find the pseudometrics in a form, which admits extrapolation to general $n \in \mathbb{N}$. Already in [17], the authors appreciated the existence of a particular metric $\Theta$ with elements

$$\Theta_{jk} = \begin{cases} 1 & j = k \\ -i\omega(\rho - i\omega)^{j-k-1} & j > k \\ i\omega(\rho + i\omega)^{j-k-1} & j < k \end{cases}$$

which served also as a starting point of our considerations. For sufficiently low dimensions, we can construct pseudometrics explicitly with the help of symbolic manipulation on any computer algebra system. For the present two-site model, after denoting $\xi = \rho - i\omega$, we get
\[ P^{(1)} = \begin{bmatrix} 1 & -i\omega & -i\omega\xi & -i\omega\xi^2 \\ i\omega & 1 & -i\omega & -i\omega \\ i\omega\xi^* & i\omega & 1 & -i\omega \\ i\omega\xi^2 & i\omega\xi^* & i\omega & 1 \end{bmatrix} \]

\[ P^{(2)} = \begin{bmatrix} 1 -i\omega & 1 -i\omega \\ 1 & 1 -i\omega \\ 1 & 1 -i\omega \\ 1 & 1 -i\omega \end{bmatrix} \]

\[ P^{(3)} = \begin{bmatrix} 1 -i\omega \\ 1 & 1 -i\omega \\ 1 & 1 -i\omega \\ 1 & 1 -i\omega \end{bmatrix} \]

\[ P^{(4)} = \begin{bmatrix} 1 -i\omega & 1 -i\omega \\ 1 & 1 -i\omega \\ 1 & 1 -i\omega \\ 1 & 1 -i\omega \end{bmatrix} \]

(12)

Note that \( P^{(1)} \) coincides with eq. 11, while \( P^{(4)} \) realizes a discrete operator of parity, and the condition \( H^\dagger P^{(4)} = P^{(4)} H \) demonstrates the \( \mathcal{PT} \)-symmetry of the present model. The two-site case suggests an extrapolation pattern for higher \( n \in \mathbb{N} \) with the \( k \)-th pseudometric having only \( 2(n-k) + 1 \) nonzero antidiagonals. The nonzero elements of such metrics are given by the following table

\[
\begin{array}{c|c}
-i\omega\xi^{(i-j-k)} & i-j \geq k \\
i\omega\xi^{*(i-j-k)} & j-i \geq k \\
\rho & |i-j| < k, \ i+j-k \text{ even} \\
1 & |i-j| < k, \ i+j-k \text{ odd}
\end{array}
\]

(13)

A rigorous proof of the above proposition by double induction \( n \to n+1 \) and \( k \to k+1 \) would be a straightforward, although lengthy, generalization of proposition 2 in [17] (which is essentially the proof of \( n \to n+1 \) for \( k = 1 \)), and therefore may be omitted. The positivity of the resulting metric as a function of \( \varepsilon_i \) is a generally nontrivial problem, which lies outside of the scope of the present discussion. We can however make use of the fact, that the pseudometric \( P^{(1)} \) is a genuine metric, and treat other \( \varepsilon_i \) using tools of perturbation theory.

4 The dual-SSH model

A large subclass of tridiagonal quasi-hermitian matrices has a close connection to the theory of orthogonal polynomials [19, 20]. Inspired by these models, we define the dual-SSH (or dSSH) model, which, in parallel with the operator-matrix correspondence of eq. 7 has its two-site form

\[ H_{dSSH}^{(4)} = \begin{bmatrix} \gamma & -1-\lambda & -1-\lambda & -1-\lambda \\ -1+\lambda & -1+\lambda & -1-\lambda & -1+\lambda \\ -1+\lambda & -1-\lambda & -1+\lambda & -1+\lambda \\ -1+\lambda & -1-\lambda & -1+\lambda & -1+\lambda \end{bmatrix} \]

(14)

A schematic drawings of the both dSSH and the original SSH interaction are shown for \( N = 4 \) in fig. III, with black circle denoting the boundary term from eq. 2, and solid, respectively dashed lines denoting the \(-1-\lambda\), respectively \(-1+\lambda\) interaction.

In this section, we study the special case of eq. 14 with \( \gamma = 0 \). This matrix family indeed belongs to a class of tridiagonal models admitting elegant treatment using theory of orthogonal polynomials. Recall that any orthogonal polynomial sequence \( p_n(x) \) obeys a three-term recurrence relation.
\[ xp_n(x) = a_{n(n+1)} p_{n+1}(x) + a_{nn} p_n(x) + a_{n(n-1)} p_{n-1}(x) \]  

Figure III: Schemes of the four-site SSH and dSSH models.

with \( a_{n(n+1)} a_{(n+1)n} > 0 \) and \( a_{nn} \in \mathbb{R} \). The coefficients \( a_{ij} \) may be understood as elements of truncated three-diagonal \( n \times n \) matrices with characteristic polynomial \( p_n(x) \). Consequently, the eigenvalues of such matrices (the roots of \( p_n \)) are real and distinct, which is a sufficient condition for matrix quasi-hermicity. Moreover [21], a complete set of pseudometrics for such models has a very feasible form, with \( P^{(k)} \) having only \((2k + 1)\) nonzero diagonals, and may be constructed by solving the recurrences

\[
\sum_{j=0}^{k-1} a_{(k+j)(k)} P^{(k)}_{(k+j)(k+1)} = \sum_{j=0}^{k-1} a_{(k+j)(k+1)} P^{(k)}_{(k)(k+j)}
\]

The matrix elements of eq. 14 obey the condition \( a_{n(n+1)} a_{(n+1)n} > 0 \) for any \( \theta \neq k\pi \). At the exceptional points \( \theta = k\pi \) the operator is not diagonalizable despite the reality of its spectrum, and its quantum-mechanical interpretation is lost. For \( \theta \neq k\pi \), we may construct pseudometrics using eq. 16, or again with the help of computer-based symbolic manipulations. In either case, we arrive at the two-site formulae

\[
P^{(1)} = \begin{bmatrix} + & - \\ - & + \end{bmatrix}, \quad P^{(2)} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \quad P^{(3)} = \begin{bmatrix} + & - \\ - & + \end{bmatrix}, \quad P^{(4)} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}
\]

where we have denoted \( \pm = (1 \pm \lambda) \). These formulae suggest an extrapolation pattern with \( k \)-th pseudometric having \( 2k + 1 \) nonzero diagonals and \( 2(n - k) + 1 \) nonzero antidiagonals. Moreover, the nonzero elements are arranged in a chessboard-like pattern, in accordance with [20]. We may write formula for zero elements as

\[
P^{(k)}_{ij} = 0 \begin{cases} \text{for } |i + j - k| \text{ odd} \\ \text{for } |i - j| \geq k \text{ or } |i + j - n - 1| > n - k \end{cases}
\]

Nonzero elements of \( P^{(k)} \) are given by the following table. In the left column, we have listed for comparison also nonzero pseudometric elements for the classical SSH interaction from eq. 7 with \( \gamma = 0 \). The hermicity of such model is apparent from \( \Theta = I \) being among the admissible metrics.
The inner products

After examining two special cases $\gamma = 0$ and $\lambda = 0$, we are ready to address the model of eq. 7 in full generality. In order to print the resulting matrices explicitly, we define $\pm = (1 \pm \lambda)w$, where $w$ appearing in the $(ij)$-th element of the $k$-th pseudometric denotes the $(ij)$-th element of the $k$-th pseudometric of eq. 12. Explicit construction of metric operators remains feasible for sufficiently low dimensions. For the two-site model, we get the following results (we shall explain shortly why $\mathcal{P}^{(1)}$ is missing from the list)

\[
\mathcal{P}_{\text{SSH}}^{(2)} = \begin{bmatrix}
+ & + & + & 1 \\
+ & - & - & 2 & + \\
+ & - & - & 2 & + \\
1 & + & + & + & +
\end{bmatrix},
\mathcal{P}_{\text{SSH}}^{(3)} = \begin{bmatrix}
+ & 1 \\
- & 1 \\
+ & 1 \\
1 & 1 & 1
\end{bmatrix},
\mathcal{P}_{\text{SSH}}^{(4)} = \begin{bmatrix}
1 \\
1 \\
1 \\
1 & 1
\end{bmatrix}
\]

\[
\mathcal{P}_{\text{dSSH}}^{(2)} = \begin{bmatrix}
- & 2 & - & 1 \\
- & - & - & - & 2 \\
- & - & - & - & 2 \\
1 & + & + & + & +
\end{bmatrix},
\mathcal{P}_{\text{dSSH}}^{(3)} = \begin{bmatrix}
- & 1 \\
- & 1 \\
- & 1 \\
1 & 1 & 1
\end{bmatrix},
\mathcal{P}_{\text{dSSH}}^{(4)} = \begin{bmatrix}
1 \\
1 \\
1 \\
1 & 1
\end{bmatrix}
\]

Extrapolation formulae for general $n \in \mathbb{N}$ are clear from these matrices, again with the $k$-th pseudometric having $2(n - k) + 1$ nonzero antidiagonals. However, as long as we wish to impose the same ansatz for pseudometrics $\mathcal{P}^{(k)}, k < n - 2$, we discover the emergence of a cutoff value, for which the pattern ceases to be valid. This phenomenon can be seen already in the case of hepta-antidiagonal pseudometrics. We illustrate this behavior on the following three-site models

\[
\mathcal{P}_{\text{SSH}}^{(3)} = \begin{bmatrix}
+ & - & + & - & 2 & - & + & 1 \\
+ & - & + & - & - & - & + & + & 2 & - & + & - & -
\end{bmatrix},
\mathcal{P}_{\text{dSSH}}^{(3)} = \begin{bmatrix}
- & 3 & - & 2 & 1 \\
- & 3 & - & 2 & + & 2 & - & + & + & + & + & + & +
\end{bmatrix}
\]

where $+-^2$ stands for $+(-)^2$. If we insert these matrices into the equation $H \mathcal{P}^{(3)} = \mathcal{P}^{(3)} H$, we obtain complex solutions for $\Lambda_i$, which violate the hermicity condition. Thus, in the general case of eq. 7, we are able to build just three pseudometric families $\mathcal{P}^{(n-2)}, \mathcal{P}^{(n-1)}$ and $\mathcal{P}^{(n)}$ before cutoff emergence. Still, the pattern of matrix elements not approaching infinity as $n \to \infty$ is strongly conjectured to be preserved, suggesting that the resulting metrics $\Theta$ remain bounded in appropriate continuous limit. Such a continuous analogue is well-known for $\lambda = 0$ [16], but the examination of the continuous limit for general $\theta \neq 0$ remains open.
6 Discussion

We have successfully constructed a complete set of pseudometrics for the discrete Robin square well, as well as for the hermitian SSH model and its dual counterpart. In the general case of eq. 1, we encountered a cutoff preventing the construction of pseudometrics beyond three particular families. While this may sufficient in many scenarios, we emphasize two reasons for the importance of constructing a complete set of pseudometric. As long as the Hamiltonian is not the only dynamical observable, the presence of additional observables \( \Lambda_i \) imposes additional constraints on the metric, in the form of equations

\[
\Lambda_i^\dagger \Theta = \Theta \Lambda_i
\] (22)

Furthermore, the physical Hilbert spaces \( \mathcal{H}^{(S)} \) generated by different metrics are in general not unitarily equivalent. In particular, for parametric models, some metrics may have larger domains of positivity than others [22, 23]. The choice of a correct physical metric is then dictated by other physical principles of, for example, locality.

Figure IV: Eigenvalues of the \( n = 50 \) SSH, dSSH and the model \(-1 - \lambda \to -1 + \lambda \) for \( \gamma = 0.5i + 0.8 \).

Spectral behavior of the discussed models is briefly outlined for a single parameter value in fig. IV, where we have, for comparison, shown also the operator obtained from eq. 7 by transforming all elements \(-1 - \lambda \) into \(-1 + \lambda \). All three models exhibit nontrivial domains of observability occurring for non-zero \( \gamma \). For non-hermitian operators, it may show rewarding, in addition to studying the spectrum, to examine their \( \epsilon \)-pseudospectrum [24, 25]

\[
\sigma_\epsilon(H) = \{ \lambda \in \mathbb{C} \mid \| (H - \lambda)^{-1} \| \geq \epsilon^{-1} \}
\] (23)

While the pseudospectrum of a general operator may behave quite arbitrarily, pseudospectra of quasi-hermitian operators admit a simple characterization based on the spectral theorem. Using the decomposition \( \Theta = \Omega^\dagger \Omega \), we may write

\[
\frac{1}{\rho(\lambda, \sigma(H))} \leq \| (H - \lambda)^{-1} \| \leq \frac{\| \Omega \| \| \Omega^{-1} \|}{\rho(\lambda, \sigma(H))}
\] (24)

therefore the \( \epsilon \)-pseudospectrum is contained in the \( \kappa \epsilon \)-neighborhood of the spectrum, with \( \kappa = \| \Omega \| \| \Omega^{-1} \| \). Clearly, the pseudospectrum contains information unavailable from the spectrum itself, with the resolvent norm being pronounced near the eigenvalues, which are likely to complexify by a small perturbation of parameters.
Figure V: Pseudospectra of eq. 8 for $n = 8$ and $\alpha = 1, \beta = 1$, respectively $\alpha = 1, \beta = 0.7$.

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