Physics counterpart of the $\mathcal{PT}$ non-hermitian tight-binding chain

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We explore an alternative way of finding the link between a $\mathcal{PT}$ non-Hermitian Hamiltonian and a Hermitian one. Based on the analysis of the scattering problem for an imaginary potential and its time reversal process, it is shown that any real-energy eigenstate of a $\mathcal{PT}$ tight-binding lattice with on-site imaginary potentials shares the same wave function with a resonant transmission state of the corresponding Hermitian lattice embedded in a chain. It indicates that the $\mathcal{PT}$ eigenstate of a $\mathcal{PT}$ non-Hermitian Hamiltonian has connection to the resonance transmission state of the extended Hermitian Hamiltonian.

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I. INTRODUCTION

Imaginary potential usually appears in a system to describe physical processes phenomenologically due to its simplicity, which has been investigated under the non-Hermitian quantum mechanics framework \[1,10\]. To discuss and explore the usefulness of the imaginary potential, one has to be able to establish a correspondence between a non-Hermitian system and a real physical system in an analytically exact manner. The effort to establish a parity-time ($\mathcal{PT}$) symmetric quantum theory as a complex extension of the conventional quantum mechanics $\{11,17\}$ was stimulated by the discovery that a non-Hermitian Hamiltonian with simultaneous $\mathcal{PT}$ symmetry has an entirely real quantum-mechanical energy spectrum \[18\] and has profound theoretical and methodological implications.

When speaking of physical significance of a non-Hermitian Hamiltonian, it is implicitly assumed that there exists another Hermitian Hamiltonian which shares the complete or partial spectrum with it. Thus one of the ways of extracting the physical meaning of a non-Hermitian Hamiltonian having a real spectrum is to seek for its Hermitian counterparts \[8–10\]. The metric-operator theory outlined in \[11\] provides a mapping of such a pseudo-Hermitian Hamiltonian to an equivalent Hermitian Hamiltonian. However, the obtained equivalent Hermitian Hamiltonian is usually quite complicated \[11,19\] and cannot be judged whether it describes real physics or is just unrealistic mathematical object.

In this paper, we try to find an alternative way to establish the connection between a pseudo-Hermitian Hamiltonian and a physics system. We consider a simple class of discrete systems, which are originally exploited to describe the solid-state system in condensed matter physics. In such systems, the imaginary potential usually appears as source or sink, acting as connection to the outer world. In this sense, the eigenstates of an unbroken $\mathcal{PT}$ non-Hermitian Hamiltonian seem to be the dynamical equilibrium states of an open system. The strategy of this paper is to seek the ways of analytical continuation of the eigenfunctions of a $\mathcal{PT}$ non-Hermitian Hamiltonian into the stationary scattering states of an extended Hermitian system. It indicates that the $\mathcal{PT}$ eigenstate of a $\mathcal{PT}$ non-Hermitian Hamiltonian has connection to the resonance transmission state of the extended Hermitian Hamiltonian.

This paper is organized as follows, in Sec. II, Scattering problem of imaginary potential. In Sec. III, the connection between a resonant transmission state and a $\mathcal{PT}$ symmetry eigenstate is established. In Sec. IV, the illustrative examples are presented to demonstrate the main idea of this paper. Sec. V is the summary and discussion.

II. SCATTERING PROBLEM OF IMAGINARY POTENTIAL

The first problem we address in our search for physically meaningful $\mathcal{PT}$ non-Hermitian Hamiltonian is how to associate the individual imaginary potential with the Hermitian sub-network. Recently the formal theory of scattering for complex potentials in one dimension continuous system has been constructed (for review see Ref. \[20\] and references therein). To establish such a correspondence in a discrete system, we consider a simple model described by a non-Hermitian Hamiltonian $H_\gamma$. It is a tight-binding chain with uniform nearest neighbor hopping integrals and an additional imaginary on-site potential on a site of a semi-infinite chain, which can be written as follows:

\[
H_\gamma = H_{t\gamma} + H_g + H_{\text{sub}},
\]

\[
H_{t\gamma} = -J \sum_{l=-\infty}^{-1} \left( a_{l+1}^\dagger a_l + \text{H.c.} \right) - i\gamma a_0^\dagger a_0,
\]

\[
H_g = -g \left( a_0^\dagger a_1 + a_1^\dagger a_0 \right),
\]

\[
H_{\text{sub}} = \sum_{i,j=1}^{N_x} \kappa_{ij} \left( a_i^\dagger a_j + \text{H.c.} \right),
\]

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where \( a_1^\dagger \) is the creation operator of the boson (or fermion) at the 7th site, the tunneling strengths and imaginary potential are denoted by \( J, g, \) and \( -i\gamma (\gamma > 0) \).

We separate the Hamiltonian into several parts to characterize the configuration of the system. A sketch of such a system is given in Fig. 1(a). Here \( H_{\text{sub}} \) is a semi-infinite uniform chain with one potential \(-i\gamma\) at the edge, \( H_g \) represents the coupling between this chain and an arbitrary sub-network described by a Hermitian Hamiltonian \( H_{\text{sub}} \). In this sense, the conclusion will be obtained is applicable for a large class of systems.

To investigate the role of the imaginary potential in a discrete system, we will be concerned with the scattering problem of such system: an incident plane wave \( e^{ikj} \) or a broad wave packet comes from leftmost and is reflected and transmitted at the imaginary potential. The process can be represented by the wave function \( f_1(j) a_j^\dagger|0\rangle \) with

\[
\hat{f}_1(j \leq 0) = e^{ikj} + r_1 e^{-ikj} ,
\]

where \( r_1 \) represents the reflection amplitude. The explicit form of wave function \( f_1(j > 0) \) within the sub-network depends on the structure of \( H_{\text{sub}} \). General speaking, the solution of \( r_1 \) can not be obtained exactly even the explicit form of \( H_{\text{sub}} \) is given. However, we will see that it does not affect the conclusion below.

In the basis \( \{a_j^\dagger|0\rangle \mid j \in (-\infty, N]\} \), The Schrödinger equation has the explicit form

\[
-Jf_1(j - 1) - Jf_1(j + 1) = Ef_1(j) , \quad (j < 0)
\]
\[
-Jf_1(-1) - gf_1(1) = (E + i\gamma) f_1(0) ,
\]
\[
-gf_1(0) + \sum_{i=1}^{N_j} \kappa_{ij} f_i(1) = Ef_1(1)
\]
\[
\sum_{i=1}^{N_j} \kappa_{ij} f_i(1) = Ef_1(j) , \quad (j \in [2, N])
\]

within all the regions. We will show that, such a scattering process can occur in a Hermitian system.

It has been well known that an imaginary potential, by means of an effective interaction, can serve as a reduced description for the outer world of an open system. Along this line, we consider a similar lattice system to \( H_{\text{sub}} \), described by a Hermitian Hamiltonian \( H_V \). In this network, the imaginary potential is replaced by a real potential \( V \), and a semi-infinite chain is added, which acts as the complementary subspace or outer word if \( H_{\text{sub}} \) is regarded as an open system. The corresponding Hamiltonian has the form

\[
H_V = H_{1V} + H_g + H_{\text{sub}} + H_\nu + H_{1\nu} \quad (4)
\]
\[
H_{1V} = -J \sum_{\nu=-\infty}^{-1} (a_{\nu+1}^\dagger + H.c.) + V a_0^\dagger a_0
\]
\[
H_\nu = -\nu (a_0^\dagger b_1 + b_0^\dagger a_0)
\]
\[
H_{1\nu} = -J \sum_{\nu=1}^{\infty} (b_0^\dagger b_\nu + H.c.)
\]

where \( b_j^\dagger \) is also the creation operator of the boson (or fermion) at the 1th site. \( H_{1V} \) and \( H_\nu \) are two semi-infinite uniform chains with real potential \( V \) at the joint point.

A sketch of such a system is given in Fig. 1(b). Note that the two systems have assigned the same sub-network, \( j \in (-\infty, 0] \), which is referred as the common region. The corresponding scattering wave functions within the two semi-infinite chains are \( f_2(j) a_j^\dagger |0\rangle \) and \( f(j) b_j^\dagger |0\rangle \) with

\[
\hat{f}_2(j \leq 0) = e^{ikj} + r_2 e^{-ikj} \quad (5)
\]
\[
\hat{f}(j > 0) = e^{ikj} .
\]

In the basis \( \{a_j^\dagger |0\rangle \mid j \in (-\infty, N]\}, b_j^\dagger |0\rangle \mid j \in (1, +\infty] \}, \) the Schrödinger equations are

\[
-J f_2(j - 1) - J f_2(j + 1) = E f_2(j) , \quad (j < 0)
\]
\[
-J f_2(-1) - g f_2(1) - \nu \hat{f}(1) = (E - V) f_2(0) ,
\]
\[
-g f_2(0) + \sum_{i=1}^{N_j} \kappa_{ij} f_i(1) = E f_2(1) ,
\]
\[
\sum_{i=1}^{N_j} \kappa_{ij} f_i(1) = E f_2(j) , \quad (j \in [2, N])
\]
and

\[-\nu f_2(0) - J\tilde{f}(2) = E\tilde{f}(1), \tag{7}\]
\[-J\tilde{f}(j-1) - J\tilde{f}(j+1) = E\tilde{f}(j), \quad (j > 1).\]

We can see that the Eqs. (3) and (4) within the common region have the same form except the potentials at the 0th site. For the the same incident plane wave $e^{ikj}$, we have

\[E = -2J\cos k \tag{8}\]

and furthermore, one can find that under the conditions

\[\nu^2 \sin k = \gamma J, \quad \nu^2 \cos k = VJ, \tag{9}\]

the solutions for $r_1$ and $r_2$ are identical. The above equivalent conditions can also be given in the energy-dependent form

\[\nu^2 = \frac{2\gamma J^2}{\Omega}, \quad V = -\frac{\gamma E}{\Omega} \tag{10}\]

where $\Omega = \sqrt{4J^2 - E^2}$. Then the wave functions (2) and (5) within $j \in [-\infty, N]$ are the same. This indicates that for the incident plane wave $e^{ikj}$, the imaginary potential can be regarded as a semi-infinite chain for wave escaping. It is worth to point out that it is a conditional equivalence, which is only for the specific state. This equivalence is the building block for the investigation of this paper.

Now we consider the relevant situations derived from the obtained results. We are interested in the case when the imaginary potential is source like. Actually, applying time-reversal operation on the above scattering processes, i.e., taking complex conjugation for the Eqs. (1) and (4), the corresponding time reversal solutions can be obtained, which are illustrated in Fig. 1(c, d). The Fig. 1(c) shows that the time reversal solution is for the new system $H_\text{r} = H_\text{s} (\gamma \to -\gamma)$. Nevertheless, its counterpart $H_\text{V}$ is invariant under time reversal. The Fig. 1(d) illustrates the corresponding time reversal process of that in Fig. 1(b). Based on the processes in real physical systems illustrated in Fig. 1(b, c), the physics of the imaginary potential becomes clear: $-i\gamma$ acts as a drain lead, while $i\gamma$ acts as a source lead associated with an incoming plane wave. Although this is not a surprising result, we still verify it explicitly in a strict manner and will apply it to a $\mathcal{PT}$ non-Hermitian system.

### III. Resonant Transmission Condition and $\mathcal{PT}$ Symmetry

The above result is essentially about the stationary state for the infinite non-Hermitian system. Intuitively, a source and drain could produce a stationary state in a finite system between them when the gain rate equals to the loss rate, or in an open system with injecting sources and absorbing sinks. The conceptual framework is required to substantiate this idea. In this section, we consider the stationary state of a non-Hermitian system based on the obtained scattering solutions of the imaginary potential.

Although we cannot get the explicit solution about the reflection amplitude $r$, the corresponding time-reversal process illustrated in Fig. 1(c) exhibits the facts: for an incident plane wave with amplitude 1, the reflected amplitude from the absorptive potential $-i\gamma$ is $r$, while for an incident plane wave with amplitude $r^*$, the reflected amplitude from the source potential $i\gamma$ is just 1. The fact $|r| = |r^*|$ indicates that if we combine the building blocks Fig. 1(a) and (c) to construct a finite network with the geometry illustrated in Fig. 4(a), the stationary state may be formed in the manner: a wave coming from the sources and send back its time-reversed version. On the other hand, such a configuration has the $\mathcal{PT}$ symmetry spontaneously, which has been shown to process real-energy eigenstate under certain condition. In the aid of its Hermitian counterpart shown in Fig. 2(b), one can find that in the case of the stationary state being formed, it just corresponds to the resonant transmission. Therefore the existence of the real-energy eigenstate of a $\mathcal{PT}$ symmetric system is connected to the occurrence of resonant transmission in a Hermitian system. It follows that we can find an alternative Hermitian counterpart to a $\mathcal{PT}$ symmetric Hamiltonian in the sense that they share the same eigenfunction within the common region. This should be the way more directly associated with the physics of the $\mathcal{PT}$ symmetric system. In the following sections, we will study the formation of the $\mathcal{PT}$ symmetrical state by dealing with the more tractable models.
Note the region \( \{ a_l^\dagger |0\, l \in (1, N+2N_s) \} \) is regarded as the common region of the two models. In the following, we present the analytical results in the framework of Bethe ansatz for the two models in order to perform a comprehensive study.

### A. \( \mathcal{PT} \) chain \( H_{\gamma \gamma} \)

According to the \( \mathcal{PT} \)-symmetric quantum mechanics \cite{16}, system \( H_{\gamma \gamma} \) can be further classified to be either unbroken \( \mathcal{PT} \) symmetry or broken \( \mathcal{PT} \) symmetry, which depends on the symmetry of the eigenstates \( |\psi^\gamma_k\rangle \) in different regions of \( \gamma \). The time-independent Schrödinger equation is

\[
H_{\gamma \gamma} |\psi^\gamma_k\rangle = \varepsilon^\gamma_k |\psi^\gamma_k\rangle
\]

with corresponding eigenvalue \( \varepsilon^\gamma_k \). The system is unbroken \( \mathcal{PT} \) symmetry if all the eigenfunctions have \( \mathcal{PT} \) symmetry

\[
\mathcal{PT} |\psi^\gamma_k\rangle = |\psi^\gamma_k\rangle
\]

and all the corresponding eigenvalues are real simultaneously. This classification depends on the value of the parameter \( \gamma \). Beyond the unbroken \( \mathcal{PT} \) symmetric region the system is broken \( \mathcal{PT} \) symmetry, where Eq. (16) does not hold for all the eigenfunctions and the eigenvalues of broken \( \mathcal{PT} \) symmetric eigenfunctions are complex.

We denote the single-particle eigenfunction in the form

\[
|\psi^\gamma_k\rangle = \sum_{j=N+1}^{N+N_s} f^\gamma_k (j) a_j^\dagger |0\rangle.
\]

According to Bethe ansatz method, the eigenstates can be in the form of

\[
f^\gamma_k = \begin{cases} 
C_{L} e^{ikj} + D_{L} e^{-ikj}, & \gamma \in [1, N+1] \\
A e^{ikj} + B e^{-ikj}, & \gamma \in [N+1, N+N_s] \\
C_{R} e^{ikj} + D_{R} e^{-ikj}, & \gamma \in [N_s + N + 1, N+2N_s]
\end{cases}
\]

The coefficients \( \{ A, B, C_{L(R)}, D_{L(R)} \} \) and the quasi momentum \( k \) are to be determined by matching conditions

\[
f^\gamma_k (j + 0^+) = f^\gamma_k (j + 0^-),
\]

\[
(j = N_s + 1, N_s + N)
\]

and the corresponding Schrödinger equations of \( j \neq N_s + 1, N_s + N \) in the center of the system,

\[
-J f^\gamma_k (j + 1) - J f^\gamma_k (j - 1) = \varepsilon^\gamma_k f^\gamma_k (j),
\]

the Schrödinger equations of \( j \) for the sites \( j = N_s + 1 \) and \( N_s + N \),

\[
-J f^\gamma_k (N_s + 2) - J f^\gamma_k (N_s + 1) = (\varepsilon^\gamma_k - i\gamma) f^\gamma_k (N_s + 1),
\]

\[
-J f^\gamma_k (N_s + N + 1) - J f^\gamma_k (N_s + N - 1) = (\varepsilon^\gamma_k + i\gamma) f^\gamma_k (N_s + N).
\]
and for the edges of the system \( j = 1 \) and \( N + 2N_s \),
\[
-Jf_k^V (2) = \varepsilon_k^J f_k^V (1) \\
-Jf_k^V (N + 2N_s - 1) = \varepsilon_k^J f_k^V (N + 2N_s).
\]
These lead to the equation of \( k \)
\[
-\gamma^2 \chi_k \left[ e^{ik(N-1)} - e^{-ik(N-1)} \right] = J^2 \left[ e^{ik(N+2N_s-1)} - e^{-ik(N+2N_s+1)} \right],
\]
where
\[
\chi_k = \frac{e^{ik(N+1)} - e^{-ik(N_s+1)}}{e^{ik} - e^{-ik}}.
\]

The solutions of \( k \) can be classified in two categories: physical and unphysical states, which correspond to real and complex \( k \), respectively. The corresponding energy are real or complex and in the form
\[
\varepsilon_k^\gamma = -J \left( e^{ik} + e^{-ik} \right).
\]

A straightforward algebra shows that there are at least \((N-1)\) solutions of real \( k \) for arbitrary \( \gamma/J \). In this paper, we only focus on the physics counterparts of these states rather than the detailed form of the solutions.

### B. Hermitian counterpart \( H_{VV} \)

For the Hamiltonian Eq. (12), it has \( \mathcal{P} \) and \( \mathcal{T} \) symmetry simultaneously, i.e., \( \mathcal{P} H_{VV} \mathcal{P} = \mathcal{T} H_{VV} \mathcal{T} = H_{VV} \). Nevertheless, for a scattering state, a plane wave comes from the leftmost, the \( \mathcal{P} \) and \( \mathcal{T} \) symmetry are broken. We will show that under certain conditions, the wave function within the common region of \( H_{\gamma\gamma} \) and \( H_{VV} \) has \( \mathcal{PT} \) symmetry.

We can set the scattering wave function in the form of
\[
f_k^V = \begin{cases} 
C_L e^{ikj} + D_L e^{-ikj}, & [1, N_s + 1] \\
A_r e^{ikj} + B_r e^{-ikj}, & [N_s + 1, N_s + N] \\
C_R e^{ikj} + D_R e^{-ikj}, & [N_s + N, N + 2N_s]
\end{cases},
\]
and
\[
f_k^V = \begin{cases} 
\varepsilon_k e^{ikj} + r e^{-ikj} & j \in (-\infty, -1] \\
te^{ikj}, & \left[1, +\infty \right)
\end{cases},
\]
where \( f_k^V \) represents the one within the common region, while \( f_k^V \) represents the one in the two leads. The reflection and transmission amplitudes \( r, t \), coefficients \( \{A^s, B^s, C^s_{L(R)}, D^s_{L(R)}\} \) and the quasi momentum \( k \) are to be determined by matching conditions
\[
-f_k^V (j + 0^+) = f_k^V (j + 0^-),
\]
\( (j = N_s + 1, N + N_s) \)
\[
-f_k^V (N_s + 1) = f_k^V (N_s + 1),
\]
\[
f_k^V (N_s + N) = f_k^V (N_s + N)
\]
and the corresponding Schrödinger equations of \( j \) in the center of the system,
\[
-Jf_k^V (j + 1) - Jf_k^V (j - 1) = \varepsilon_k^J f_k^V (j),
\]
\[
-Jf_k^V (j + 1) - Jf_k^V (j - 1) = \varepsilon_k^J f_k^V (j)
\]
Schrödinger equations of \( j \) for the connection sites \( N_s + 1, N_s + N \),
\[
-\nu f_k^V (1) - Jf_k^V (N_s + N + 1) = \varepsilon_k f_k^V (N_s + N),
\]
and for the edges of the system \( j = 1, N + 2N_s \),
\[
-Jf_k^V (2) = \varepsilon_k f_k^V (1)
\]
\[
-Jf_k^V (N + 2N_s - 1) = \varepsilon_k f_k^V (N + 2N_s).
\]

The solution for reflection amplitude \( r \) is given, after a straightforward algebra, by
\[
r = \frac{2i\nu^2 \xi \sin(k) \sin^2[k(N-1)]}{J^2 \sin^2(k) - J^2 \xi^2 \sin^2[k(N-1)]} - 1,
\]
where
\[
\xi = \frac{V}{\mathcal{J}} + \frac{\sin[kN]}{\sin[k(N-1)]} - \frac{\nu^2}{J^2} e^{ik} - \frac{\sin[kN_s]}{\sin[k(N_s + 1)]}.
\]

We are interested in the resonant transmission state, which should be relevant to the \( \mathcal{PT} \) eigenstate of \( H_{\gamma\gamma} \), according to the above time reversal analysis. For \( r = 0 \) we have
\[
2i\nu^2 \xi \sin(k) \sin^2[k(N-1)]
\]
\[
= J^2 \sin^2(k) - J^2 \xi^2 \sin^2[k(N-1)].
\]

The analysis in Sec. II indicates that, under the conditions (9), there should be a resonant transmission state corresponding to the eigenstate of (11). In fact, substituting (9) into (52), one can obtain the
\[
\gamma^2 \sin^2[k(N_s + 1)] \sin[k(1-N)]
\]
\[
= J^2 \sin^2(k) \sin[k(N + 2N_s + 1)],
\]
which is just the reduced form of the Eq. (21) for the real quasi momentum \( k \). It can be shown exactly that there are at least \( N - 1 \) real solutions for the Eq. (33). This exhibits the connection between the two models (11) and (12) predicted by the above mentioned analysis. Accordingly, we have
\[
\frac{C_{L(R)}}{C^s_{L(R)}} = \frac{D_{L(R)}}{D^s_{L(R)}} = \frac{A^s}{A^s} = \frac{B^s}{B^s}
\]

(34)
which shows that both functions within the common region are identical, i.e., the scattering wave function \( \{ r, t, A^s, B^s, C^s_{L(R)}, D^s_{L(R)} \} \) is the analytical continuation of the one \( \{ A, B, C_{L(R)}, D_{L(R)} \} \).

Thus two eigenstates of the Hamiltonian (11) belong to the resonant transmission scattering states of two different systems (with different \( V \) and \( v \)). In this sense, nonorthogonality of the eigenstates of a Pseudo-Hermitian Hamiltonian is obvious. In general the norm of a wave function is conserved in a Hermitian system, while the norm of many components of the wave function is not. These wave components may be associated with a truncated basis set, or a subspace of the full Hilbert space. The common region of \( H_{\gamma \bar{\gamma}} \) and \( H_{VV} \) is a concrete example in the discrete system to demonstrate this fact.

V. CONCLUSION AND DISCUSSION

In conclusion, we have presented an alternative way of finding the link between a \( \mathcal{PT} \) non-Hermitian Hamiltonian and a Hermitian one, based on the analysis of the scattering problem for an imaginary potential. We have found that the on-site absorptive imaginary potential can be equivalent to an attached semi-infinite chain as a drain with respect to a specific wave scattering problem. Applying this result and its extension to the time reversal process on the \( \mathcal{PT} \) non-Hermitian system, the eigenstate problem is connected to that of resonant transmission problem in the corresponding Hermitian system. It is shown that any real-energy eigenstate of a \( \mathcal{PT} \) tight-binding lattice with on-site imaginary potentials shares the same wave function with a resonant transmission state of the corresponding Hermitian lattice embedded in a chain.

It is not surprising that the \( \mathcal{PT} \) eigenstate has connection to the resonance transmission state of the extended system. In general, for an infinite system with parity (\( \mathcal{P} \)) symmetry, it also has the time (\( \mathcal{T} \)) reversal symmetry. An arbitrary scattering state, as an eigenstate of the system, probably breaks the \( \mathcal{P}, \mathcal{T} \) and also \( \mathcal{PT} \) symmetries simultaneously. Interestingly, in the case of the resonance transmission, the corresponding wave function possesses \( \mathcal{PT} \) symmetry. Such wave functions can be the eigenstates of the \( \mathcal{PT} \) non-Hermitian system with the real eigenvalues.

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