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A physical interpretation for the non-Hermitian Hamiltonian

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Abstract

We explore a way of finding the link between a non-Hermitian Hamiltonian and a Hermitian one. Based on the analysis of Bethe ansatz solutions for a class of non-Hermitian Hamiltonians and the scattering problems for the corresponding Hermitian Hamiltonians, it is shown that a scattering state of an arbitrary Hermitian lattice embedded in a chain as the scattering center shares the same wavefunction with the corresponding non-Hermitian tight binding lattice, which consists of the Hermitian lattice with two additional on-site complex potentials, no matter whether the non-Hermitian is broken $\mathcal{PT}$ symmetry or even non-$\mathcal{PT}$ symmetry. Exactly solvable models are presented to demonstrate the main points of this paper.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

In general, a non-Hermitian Hamiltonian is said to be physical when it has an entirely real energy spectrum. Much effort has been devoted to establish a parity-time ($\mathcal{PT}$) symmetric quantum theory as a complex extension of the conventional quantum mechanics [1–9] since the seminal discovery by Bender [1]. It is found that non-Hermitian Hamiltonian with simultaneous $\mathcal{PT}$ symmetry can have an entirely real quantum mechanical energy spectrum and has profound theoretical and methodological implications. Research works and findings relevant to the spectra of the $\mathcal{PT}$-symmetric non-Hermitian systems are presented, such as exceptional points [10–13], spectral singularities for complex scattering potentials [14–16], complex crystal and other specific models [17] have been investigated. At the same time, the $\mathcal{PT}$ symmetry is also of great relevance to the technological applications based on the fact that the imaginary potential could be realized by a complex index in optics [18–24]. In fact, such $\mathcal{PT}$ optical potentials can be realized through a judicious inclusion of index guiding and gain/loss regions, and the most interesting aspects associated with the $\mathcal{PT}$-symmetric system are observed during the dynamic evolution process [25].

Thus one of the ways of extracting the physical meaning of a pseudo-Hermitian Hamiltonian with a real spectrum is to seek for its Hermitian counterparts [26–28]. The metric-operator theory outlined in [7] provides a mapping of such a pseudo-Hermitian Hamiltonian to an equivalent Hermitian Hamiltonian. Thus, most of the studies are focused on the quasi-Hermitian system, or unbroken $\mathcal{PT}$-symmetric region. However, the obtained equivalent Hermitian Hamiltonian is usually quite complicated [7, 29], involving long-range or non-local interactions, which is hardly realized in practice.

To anticipate these problems, alternative proposals for the connection between a pseudo-Hermitian Hamiltonian and a real physics system have been suggested in the context of scattering problems [30, 31]. Central to that analysis was the recognition that the $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian may be used to depict the resonant scattering for an infinite system. It is shown that any real-energy eigenstate of a certain $\mathcal{PT}$-symmetric non-Hermitian tight-binding lattice shares the same wavefunction with a resonant transmission state of the corresponding Hermitian lattice. In such a framework, further questions to ask are whether the requirements of the entireness of the real eigenvalues and the $\mathcal{PT}$ symmetry of the non-Hermitian system are really necessary.

In this paper, we propose a physical interpretation for a general non-Hermitian Hamiltonian based on the configurations involving an arbitrary network coupled with the input and output waveguides. Relevant to our previous discussion is the interpretation of the imaginary potentials. Based on this, we make a tentative connection between a non-Hermitian system and the corresponding large Hermitian system. It is shown that for any scattering state of such a Hermitian system, the wavefunction within the center lattice always corresponds to the equal energy eigenfunction of the non-Hermitian Hamiltonian, no matter whether it is $\mathcal{PT}$-symmetric or not. Our formalism is generic and is not limited to the pseudo-Hermitian system.

This paper is organized as follows. Section 2 is the heart of this paper which presents a formulism to reduce a scattering process of a Hermitian system to the eigenproblem of the non-Hermitian system. Section 3 consists of two exactly solvable examples to illustrate our main idea. Section 4 is the summary and discussion.

2. Non-Hermitian reduction of a Hermitian system

A typical scattering tight-binding network is constructed by a scattering-center network and two semi-infinite chains as the input and output leads. The well-established Green function technique [32–34] can be employed to obtain the reflection and transmission coefficients for a given incoming plane wave. The corresponding wavefunction within the scattering center should be obtained via the Bethe ansatz method, which has been widely applied to the systems with real as well as complex potentials [35–38]. In the following, we will show that this can be done by solving a finite non-Hermitian Hamiltonian when dealing with the real potential scattering problem. In our previous work [30], a $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian has been connected to a physical system in such a manner that any real-energy eigenstate of a $\mathcal{PT}$-symmetric non-Hermitian tight-binding lattice with on-site imaginary potentials shares the same wavefunction with a resonant transmission state of the corresponding Hermitian lattice embedded in a chain. The main aim of this paper is to answer the question whether such a statement still holds for the broken $\mathcal{PT}$-symmetric non-Hermitian or non-$\mathcal{PT}$-symmetric non-Hermitian lattice. In the following, we will show that a scattering state of the Hermitian system always has connection to the eigenstate of its non-Hermitian reduction. For certain incident plane wave, the scattering problem of the whole infinite Hermitian system can be reduced to the eigenproblem of a finite non-Hermitian system.

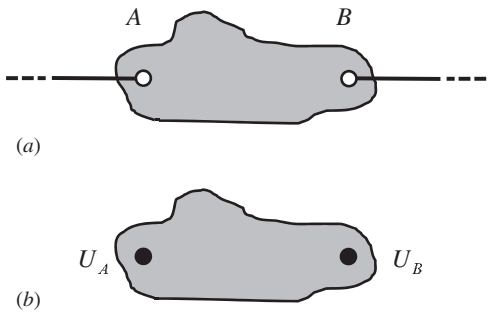

Figure 1. Schematic illustration of the configuration of the concerned network. It consists of an arbitrary graph of a Hermitian tight-binding network (shadow) connecting to two semi-infinite chains L and R as the waveguides. The wavefunction within the scattering center for a scattering state of the whole system is identical to an equal-energy eigenfunction of the non-Hermitian Hamiltonian which is constructed by the center Hermitian network with imaginary potentials added at the joint sites A and B.

The Hamiltonian of a typical scattering tight-binding network has the form

$$H = H_A + H_B + H_c, \tag{1}$$

where

$$H_A = -J\sum_{i=-1}^{-\infty} b_{i-1}^{\dagger} b_i - g_A b_{-1}^{\dagger} a_A + \text{h.c.}, \tag{2}$$

$$H_B = -J\sum_{i=1}^{+\infty} b_i^{\dagger} b_{i+1} - g_B b_1^{\dagger} a_B + \text{h.c.}, \tag{3}$$

represent the left (H_A) and right (H_B) waveguides and

$$H_c = -\sum_{i,j=1,i\leqslant j}^{N} \left(\kappa_{ij} a_j^{\dagger} a_i + \text{h.c.}\right) \tag{4}$$

describes an arbitrary N-site network as a scattering center. Sites A and B are arbitrary sites within the center network as the joints connecting the waveguides H_A and H_B, respectively. Here a_i and b_i are boson (or fermion) operators for the scattering center and waveguides, respectively. Parameter $-\kappa_{ij}$ $(i \neq j)$ represents the hopping between sites i and j of the scattering center, while $-\kappa_{ii} - \kappa_{ii}^*$ indicates the real potential on the ith site. In the following, we denote $V_A = -\kappa_{AA} - \kappa_{AA}^*$, $V_B = -\kappa_{BB} - \kappa_{BB}^*$ as the potentials on the joint sites for the sake of simplicity. Also, J is the hopping integral between the nearest-neighbor sites of the waveguide, while g_A (g_B) is the hopping integral across the left (right) waveguide to the scattering center. $\sum_{i,j=1,i\leqslant j}^{N}$ stands for a summation of i and j both from 1 to N with constraint $i \leqslant j$. Figure 1(a) represents a schematic scattering configuration to illustrate the concerned network.

For an incident plane wave with momentum k incoming from the left waveguide A with energy $E = -2J\cos(k)$, the scattering wavefunction $|\psi_k\rangle$ can be obtained by the Bethe ansatz method. The wavefunction has the form

$$|\psi_k\rangle = \sum_l f_l b_l^{\dagger}|\text{vac}\rangle + \sum_l h_l a_l^{\dagger}|\text{vac}\rangle, \tag{5}$$

where

$$f_l = \begin{cases} e^{ik(l+1)} + r\,e^{-ik(l+1)}, & l \in (-\infty, -1] \\ t\,e^{ik(l-1)}, & l \in [1, \infty), \end{cases} \tag{6}$$

$$h_l = h_l, \qquad l \in [1, N]. \tag{7}$$

Here, r and t are the reflection and transmission coefficients of the incident wave, respectively. Substituting the wavefunction (5) into the Schrödinger equation

$$H|\psi_k\rangle = E|\psi_k\rangle, \tag{8}$$

the explicit form of the Schrödinger equations for the waveguides H_A and H_B are

$$\begin{aligned} &-Jf_{j-1} - Jf_{j+1} = Ef_j, \\ &(j \in (-\infty, -2] \cup [2, +\infty)) \\ &-Jf_{-2} - g_A h_A = Ef_{-1}, \\ &-Jf_2 - g_B h_B = Ef_1. \end{aligned} \tag{9}$$

The first equation of (9) admits $E = -2J\cos(k)$. The Bethe ansatz wavefunction (6) admits

$$\begin{aligned} g_A h_A &= J(e^{ik} + r\,e^{-ik}), \\ g_B h_B &= J\,e^{-ik} t, \end{aligned}$$

or equivalently

$$h_A = \frac{J}{g_A}(e^{ik} + r\,e^{-ik}), \tag{10}$$

$$h_B = \frac{J}{g_B} t\,e^{-ik}. \tag{11}$$

Vanishing h_A (h_B) is beyond our interest. From (10) and (11), one can establish the connections between the wavefunctions of two joints (A, B) and the ends of the waveguides as the form

$$f_{-1} = \frac{g_A}{J}\frac{1+r}{e^{ik} + r\,e^{-ik}} h_A, \tag{12}$$

$$f_1 = \frac{g_B}{J} e^{ik} h_B. \tag{13}$$

Here, the expressions $f_{-1} = 1 + r$ and $f_1 = t$ have been employed, which is obtained by taking $l = \pm 1$ in (6).

Similarly, the explicit form of the Schrödinger equations for H_c can be written as

$$\begin{aligned} &-\sum_{i=1, i\leqslant j}^{N} \kappa_{ij} h_i - \sum_{i=1, i\geqslant j}^{N} \kappa_{ji}^* h_i = E h_j, \qquad (j \neq A, B), \\ &-\sum_{i=1, i<A}^{N} \kappa_{iA} h_i - \sum_{i=1, i>A}^{N} \kappa_{Ai}^* h_i - g_A^* f_{-1} = (E - V_A) h_A, \\ &-\sum_{i=1, i<B}^{N} \kappa_{iB} h_i - \sum_{i=1, i>B}^{N} \kappa_{Bi}^* h_i - g_B^* f_1 = (E - V_B) h_B. \end{aligned} \tag{14}$$

Our aim is to obtain a reduced equation for the wavefunction within the center network. To this end, substituting the expressions of f_{-1} and f_1 from (12) and (13) into the above equation (14), we get the following Schrödinger equations for the center network:

$$\begin{aligned}
&-\sum_{i=1,i\leqslant j}^{N}\kappa_{ij}h_i-\sum_{i=1,i\geqslant j}^{N}\kappa_{ji}^{*}h_i=Eh_j,\ (j\neq A,B),\\
&-\sum_{i=1,i<A}^{N}\kappa_{iA}h_i-\sum_{i=1,i>A}^{N}\kappa_{Ai}^{*}h_i=(E-U_A)h_A,\\
&-\sum_{i=1,i<B}^{N}\kappa_{iB}h_i-\sum_{i=1,i>B}^{N}\kappa_{Bi}^{*}h_i=(E-U_B)h_B,
\end{aligned}\tag{15}$$

with

$$U_A=V_A-\frac{|g_A|^2}{J}\frac{1+r}{\mathrm{e}^{\mathrm{i}k}+r\,\mathrm{e}^{-\mathrm{i}k}},\tag{16}$$

$$U_B=V_B-\frac{|g_B|^2}{J}\mathrm{e}^{\mathrm{i}k}.\tag{17}$$

This is equivalent to the effective non-Hermitian Hamiltonian

$$\mathcal{H}=H_c+(U_A-V_A)a_A^{\dagger}a_A+(U_B-V_B)a_B^{\dagger}a_B,\tag{18}$$

which indicates that U_A (U_B) acts as the on-site potential on the site A (B) for the effective non-Hermitian reduction Hamiltonian.

We now investigate the feature of the effective potentials U_A and U_B. Without losing generality, we take $r=|r|\,\mathrm{e}^{\mathrm{i}\delta}$ with $|r|<1$ (case of $r=1$ leads vanishing h_A (h_B), which is beyond our interest), where δ is the phase of the reflection coefficient. Submitting $r=|r|\,\mathrm{e}^{\mathrm{i}\delta}$ into (16) and (17), we have

$$\mathrm{Im}(U_A)=\frac{|g_A|^2}{J}\frac{(1-|r|^2)\sin k}{1+2|r|\cos(\delta-2k)+|r|^2},\tag{19}$$

$$\mathrm{Im}(U_B)=-\frac{|g_B|^2\sin k}{J}.\tag{20}$$

Based on the inequality $1+2|r|\cos(\delta-2k)+|r|^2\geqslant 1-2|r|+|r|^2>0$, we obtain

$$\mathrm{Im}(U_A)\mathrm{Im}(U_B)=-\frac{(|g_Ag_B|\sin k)^2(1-|r|^2)}{J^2[1+2|r|\cos(\delta-2k)+|r|^2]}<0,\tag{21}$$

which means that the imaginary parts of the additional potentials have opposite signs, one providing gain and the other loss. This is in accordance with the conservation law of the current. It is important to stress that the magnitude of the two imaginary potentials may not be equal, which deviates from the general understanding of an imaginary potential.

The existence of the scattering solution of the Hermitian system H ensures that there must exist at least one real solution of $\mathcal{H}$ with the eigenvalue equals the incident energy E. It possesses the identical wavefunction as that of the scattering state within the region of the scattering center. Then a scattering problem is reduced to the eigenproblem of a non-Hermitian Hamiltonian. This conclusion is an extension of our previous result [30]. In this work, our formalism is generic. The central network is not limited to the linear geometry and the scattering is not restricted to be resonant transmission. Thus, the scattering interpretation for the non-Hermitian Hamiltonian is not limited to the pseudo-Hermitian system. This rigorous conclusion has important implications in both theoretical and methodological aspects.

Likewise, we consider the inverse scattering process, i.e. taking the time-reversal operation on the above-mentioned scattering process. The corresponding Bethe ansatz wavefunction has the form

$$\begin{cases} \mathrm{e}^{-\mathrm{i}k(l+1)} + r^* \,\mathrm{e}^{\mathrm{i}k(l+1)}, & l \in (-\infty, -1] \\ t^* \,\mathrm{e}^{-\mathrm{i}k(l-1)}, & l \in [1, \infty) \\ h_l^*, & l \in [1, N] \end{cases} \tag{22}$$

with energy $E = -2J\cos k$. The above conclusion still holds. The straightforward algebra shows that the corresponding non-Hermitian reduction is $\mathcal{H}^*$. In the framework of non-Hermitian quantum mechanics, $\mathcal{H}^\dagger$ takes an important role to construct a complete biorthogonal basis set, which has no physical correspondence. In the context of our approach, $\mathcal{H}^*$ has the same physics as $\mathcal{H}$, in describing the scattering problem of the same Hermitian system.

3. Illustrative examples

In this section, we investigate simple exactly solvable systems to illustrate the main idea of this paper. We will discuss two examples which correspond to a $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian and a non-$\mathcal{PT}$-symmetric non-Hermitian Hamiltonian, respectively. In the following, based on the formalism presented in this paper, we will demonstrate that the scattering problem of the Hermitian Hamiltonian H_{ss} is equivalent to the eigenproblem of the $\mathcal{PT}$-symmetric non-Hermitian Hamiltonians $\mathcal{H}_{\mathrm{ss}}^{[n]}$ and $\mathcal{H}_{\mathrm{ss}}^{[\varepsilon]}$. The second example shows the same relation between the Hermitian Hamiltonians H_{as} and the non-$\mathcal{PT}$-symmetric non-Hermitian Hamiltonian $\mathcal{H}_{\mathrm{as}}^{[\vartheta]}$. The advantage of these examples is that the non-Hermitian Hamiltonians$\mathcal{H}_{\mathrm{ss}}^{[n]}$, $\mathcal{H}_{\mathrm{ss}}^{[\varepsilon]}$ and $\mathcal{H}_{\mathrm{as}}^{[\vartheta]}$ are exactly solvable (detailed solutions are shown in the appendices B and C).

3.1. Exactly solvable $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian

To exemplify the previously mentioned analysis of relating the stationary states of a $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian to a scattering problem for a Hermitian one, we take the center network to be a simple network: a uniform ring system as shown in figure 2. We start with the scattering problem for a class of symmetric systems; the Hamiltonian can be written as

$$\begin{aligned} H_{\mathrm{ss}} = {} & -J\sum_{i=1}^{2N} a_i^\dagger a_{i+1} + \mathrm{h.c.} - \frac{\varepsilon}{2}\frac{g^2}{J^2}\left(a_1^\dagger a_1 + a_{N+1}^\dagger a_{N+1}\right) \\ & - J\sum_{i=-1}^{-\infty} b_{i-1}^\dagger b_i - J\sum_{i=1}^{+\infty} b_i^\dagger b_{i+1} + \mathrm{h.c.} - g\left(b_{-1}^\dagger a_1 + b_1^\dagger a_{N+1} + \mathrm{h.c.}\right), \end{aligned} \tag{23}$$

where we denote the connection sites as $a_A = a_1$ and $a_B = a_{N+1}$, and the periodic boundary condition denotes $a_1 = a_{2N+1}$. We note the on-site potentials $V_A = V_B = -\varepsilon g^2/(2J^2)$.

The corresponding non-Hermitian reduction Hamiltonian depends on the energy E of the incident plane wave as well as the parameters ε and g. To be concise, as an illustrative example, we would like to present the exactly solvable model, which is helpful to demonstrate our main idea. Therefore, we will focus on the following configurations:

(i) $g \neq \sqrt{2}J$, $E = \varepsilon = \varepsilon_n = -2J\cos(n\pi/N)$, where $n \in [1, N-1]$. Here, we restrict the energy of the incident plane wave since it will lead to the pure imaginary potential for the corresponding non-Hermitian reduction Hamiltonian, thus ensures the existence of the exact solution. According to the analysis in section 2, the straightforward algebra

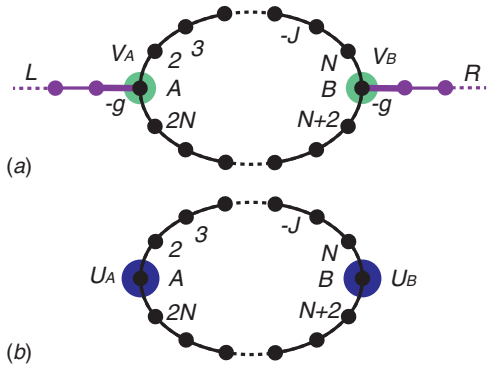

Figure 2. Schematic illustration of the concrete configuration for a scattering system. A ring as a scattering center connects to two semi-infinite chains L and R as waveguides with coupling $-g$. The on-site potentials at the connections are V_A and V_B. The wavefunction within the scattering center for a scattering state of the whole system is identical to an equal-energy eigenfunction of the non-Hermitian Hamiltonian which is constructed by the center Hermitian ring with imaginary potentials U_A and U_B added at the joint sites A and B.

(see appendix A.2.1) shows that the problem of solving the Schrödinger equation of the Hermitian Hamiltonian $H_{\rm ss}$ is reduced to the eigenproblem of the following $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian:

$$\mathcal{H}_{\rm ss}^{[n]} = -J\sum_{i=1}^{2N} a_i^\dagger a_{i+1} + \text{h.c.} + \mathrm{i}\gamma_n a_1^\dagger a_1 - \mathrm{i}\gamma_n a_{N+1}^\dagger a_{N+1}, \tag{24}$$

with the imaginary potential

$$\gamma_n = \frac{g^2}{J}\sin\left(\frac{n\pi}{N}\right). \tag{25}$$

Obviously, this Hamiltonian depicts a $2N$-site ring with two imaginary potentials at two symmetrical sites 1 and $N+1$, which is a $\mathcal{PT}$-invariant non-Hermitian Hamiltonian. Note that the magnitude of the imaginary potential is discrete in order to obtain the exact solutions. In appendix B, it is shown that such lattices can be synthesized from the potential-free lattice by the intertwining operator technique generally employed in supersymmetric quantum mechanics. The eigenspectrum $\{\varepsilon_j\}$ of $\mathcal{H}_{\rm ss}^{[n]}$ consists of

$$\begin{aligned}&\varepsilon_j = -2J\cos(j\pi/N), \\ &(j \in [1, N-1], 2\text{−fold degeneracy}),\end{aligned} \tag{26}$$

and two additional levels

$$\varepsilon_\pm = \pm\sqrt{4J^2 - \gamma_n^2}. \tag{27}$$

The eigenstates with eigenvalue ε_j can be decomposed into two sets: bonding and antibonding, with respect to the spatial reflection symmetry about the axis along the waveguides. For the scattering problem, only the bonding states are involved. It shows that there always exists a solution in $\{\varepsilon_j\}$ to match the energy ε_n of the incident wave.

From (25)–(27), one can see that a pair of imaginary eigenvalues appears, i.e. the $\mathcal{PT}$ symmetry is broken when $g > \sqrt{2}J$. In general, a non-Hermitian Hamiltonian with a broken $\mathcal{PT}$ symmetry is unacceptable because its complex energy eigenvalues make a hash of the physical interpretation. On the other hand, the $\mathcal{PT}$-symmetry breaking was

observed in optics realm experimentally [39]. In theoretical aspects, $\mathcal{PT}$ symmetry in a non-Hermitian spin chain system was discussed [40]. From the point of view of this paper, we note that even $\mathcal{H}_{\rm ss}^{[n]}$ possesses a broken $\mathcal{PT}$ symmetry, the spectrum $\{\varepsilon_j\}$ still contains the state with the energy $\varepsilon_j = \varepsilon_n$. It is worth mentioning that the broken $\mathcal{PT}$ symmetry does not contradict the interpretation of the non-Hermitian Hamiltonian (24). $\mathcal{H}_{\rm ss}^{[n]}$ equivalently depicts the Hermitian-scattering Hamiltonian for the incident energy ε_n. This indicates that even the $\mathcal{PT}$ symmetry is broken, the non-Hermitian Hamiltonian still has physical significance.

(ii) $g = \sqrt{2}J$, $E = \varepsilon \in [-2J, 2J]$. Here, we do not restrict the energy of the incident plane wave but the magnitude of g. The straightforward algebra shows that the problem of solving the Schrödinger equation is reduced to the eigenproblem of the following non-Hermitian Hamiltonian:

$$\mathcal{H}_{\rm ss}^{[\varepsilon]} = -J\sum_{i=1}^{2N} a_i^\dagger a_{i+1} + \text{h.c.} + \mathrm{i}\gamma_\varepsilon a_1^\dagger a_1 - \mathrm{i}\gamma_\varepsilon a_{N+1}^\dagger a_{N+1}, \tag{28}$$

with the imaginary potential

$$\gamma_\varepsilon = \sqrt{4J^2 - \varepsilon^2}. \tag{29}$$

Similar as in appendix A.2.1, we obtain that the solution of the Hamiltonian $\mathcal{H}_{\rm ss}^{[\varepsilon]}$ has the same form of (26), (27) with γ_n replaced by γ_ε. Here, we would like to see the relation between the Hamiltonians $\mathcal{H}_{\rm ss}^{[n]}$ and $\mathcal{H}_{\rm ss}^{[\varepsilon]}$: both of them come from the same model with different coupling constants (with $g \neq \sqrt{2}J$ and $g = \sqrt{2}J$) and different incident plane waves (with discrete and continuous spectra). However, they have the same structure but different values of the imaginary potentials. In appendix B, we provide the universal solution that contains $\mathcal{H}_{\rm ss}^{[n]}$ and $\mathcal{H}_{\rm ss}^{[\varepsilon]}$.

Obviously, Hamiltonian $\mathcal{H}_{\rm ss}^{[\varepsilon]}$ is always exact $\mathcal{PT}$-symmetric. All the eigenvalues are real. Among them we can find that $\varepsilon_\pm = \pm\sqrt{4J^2 - \gamma_\varepsilon^2} = \pm\varepsilon$, and ε_+ is equal to the energy of incident plane wave ε and thus verifies the above-mentioned conclusion that there always exists a solution of the correspondence non-Hermitian Hamiltonian to match the incident wave energy. Furthermore, the solution of it has the following peculiar feature: in the case of $\varepsilon = \varepsilon_n$, i.e. the incident wave has the wave vector $n\pi/N$ ($n \in [1, N-1]$), the exceptional points appear in $\mathcal{H}_{\rm ss}^{[\varepsilon]}$. It is shown in appendix B.3 that the corresponding eigenfunctions of ε_- (ε_+) and ε_n (ε_{N-n}) coalesce.

According to non-Hermitian quantum mechanics, in general, $\mathcal{H}_{\rm ss}^{[\varepsilon]}$ has the Hermitian counterpart $H_{\rm ss}^{[\varepsilon]}$ which possesses the same spectrum. When the potential γ_ε approaches γ_{ε_n}, the similarity transform that connects $\mathcal{H}_{\rm ss}^{[\varepsilon]}$ and $H_{\rm ss}^{[\varepsilon]}$ becomes singular. The Hamiltonian $\mathcal{H}_{\rm ss}^{[\varepsilon]}$ becomes a Jordan-block operator, which is non-diagonalizable and has fewer energy eigenstates ($N-1$) than eigenvalues ($N+1$), (i.e. the lack of completeness of the energy eigenstates). Such a Hamiltonian has no Hermitian counterpart [41]. According to our analysis, one can see that even at the exceptional points [10–13] the coalescence eigenstates still have physical significance.

3.2. Exactly solvable non-$\mathcal{PT}$-symmetric non-Hermitian Hamiltonian

Now we turn to exemplify the previously mentioned analysis of relating the stationary states of a non-$\mathcal{PT}$-symmetric non-Hermitian Hamiltonian to a scattering problem for a Hermitian lattice. We still take the center network as a simple network: a uniform ring system with

uniform coupling but none on-site real potentials. The corresponding Hamiltonian can be written as

$$H_{\rm as} = -J\sum_{i=1}^{2N} a_i^\dagger a_{i+1} + \text{h.c.} - J\sum_{i=-1}^{-\infty} b_{i-1}^\dagger b_i - J\sum_{i=1}^{+\infty} b_i^\dagger b_{i+1} + \text{h.c.}$$
$$- Jb_{-1}^\dagger a_1 - Jb_1^\dagger a_{N+1} + \text{h.c.}, \tag{30}$$

where we denote the connection sites as $a_A = a_1$ and $a_B = a_{N+1}$. In this model the on-site potentials $V_A = V_B = 0$. We consider the incident plane wave with the wave vector ϑ and energy $E = -2J\cos\vartheta$, where $\vartheta \in (\pi, -\pi)$ without any restriction. The straightforward algebra (see appendix A.2.2) shows that the problem of solving the Schrödinger equation is reduced to the eigenproblem of the following non-Hermitian Hamiltonian:

$$\mathcal{H}_{\rm as}^{[\vartheta]} = -J\sum_{i=1}^{2N} a_i^\dagger a_{i+1} + \text{h.c.} + U_A a_1^\dagger a_1 + U_B a_{N+1}^\dagger a_{N+1}, \tag{31}$$

where the complex potentials are

$$U_A = -J\frac{e^{i\vartheta N}\cos[(N-1)\vartheta] + i\sin\vartheta}{e^{i\vartheta N}\sin[(N-1)\vartheta] - \sin\vartheta} 2\sin\vartheta, \tag{32}$$

$$U_B = -J\,e^{i\vartheta}. \tag{33}$$

We can see that, in general, the Hamiltonian $\mathcal{H}_{\rm as}^{[\vartheta]}$ is not $\mathcal{PT}$-symmetric, except in some special cases. It is hard to get the analytical solution of such a Hamiltonian in general cases. Fortunately, what we need to do is to prove that the incident energy $E = -2J\cos\vartheta$ is always one of the eigenvalues of the Hamiltonian $\mathcal{H}_{\rm as}^{[\vartheta]}$. In fact, in single-particle basis the matrix representation $\mathcal{M}^{[\vartheta]}$ of the Hamiltonian (31) satisfies

$$|\mathcal{M}^{[\vartheta]} + 2J\cos\vartheta| = 0, \tag{34}$$

according to the derivation given in appendix C. Now, we know that the incident energy $E = -2J\cos\vartheta$ is a solution of the non-$\mathcal{PT}$-symmetric non-Hermitian Hamiltonian $\mathcal{H}_{\rm as}^{[\vartheta]}$ and the corresponding eigenfunction is the wavefunction within the scattering center. In this sense, one can conclude that a non-$\mathcal{PT}$-symmetric non-Hermitian Hamiltonian still has physical significance when we refer to its real eigenvalue.

4. Conclusion

In summary, we have studied the connection between a non-Hermitian system and the corresponding large Hermitian system. We propose a physical interpretation for a general non-Hermitian Hamiltonian based on the configurations involving an arbitrary network coupled with the input and output waveguides. We employed the Bethe ansatz approach to the scattering problem to show that for any scattering state of a Hermitian system, the wavefunction within the scattering center lattice always corresponds to the equal energy eigenfunction of the non-Hermitian Hamiltonian. It is important to stress that such a physical interpretation for the non-Hermitian Hamiltonian is not limited to the pseudo-Hermitian system. As an application, we examine concrete networks consisting of a ring lattice as the scattering center. Exact solutions for such types of configurations are obtained to demonstrate the results. Such results are expected to be necessary and insightful for the physical significance of the non-Hermitian Hamiltonian, as well as the descriptions of quantum mechanics. It would be interesting if the present formalism could be extended to quantum composite systems [47, 48].

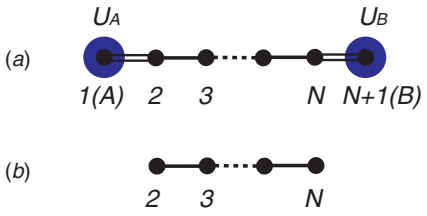

Figure A1. Schematic illustration of the reduction for a ring system by linear transformation. (*a*) Represents the Hamiltonian $\mathcal{H}_\alpha$ and (*b*) represents the Hamiltonian $\mathcal{H}_\beta$.

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Appendix A. The non-Hermitian reduction Hamiltonian

In this appendix, we will derive the central formulae in obtaining the non-Hermitian reduction Hamiltonian of the Hermitian scattering systems we introduced in section 3.

A.1. Linear transformation

First of all, we introduce the linear transformation. The ring Hamiltonian with two potentials at symmetric sites of the form (24) or (28) can be decomposed into two independent sub-Hamiltonians as in figure A1:

$$\mathcal{H} = \mathcal{H}_\alpha + \mathcal{H}_\beta, \tag{A.1}$$

$$\mathcal{H}_\alpha = -J\sum_{i=2}^{N-1}\alpha_i^\dagger\alpha_{i+1} - \sqrt{2}J\left(\alpha_1^\dagger\alpha_2 + \alpha_N^\dagger\alpha_{N+1}\right) + \text{h.c.} + U_A\alpha_1^\dagger\alpha_1 + U_B\alpha_{N+1}^\dagger\alpha_{N+1}, \tag{A.2}$$

$$\mathcal{H}_\beta = -J\sum_{i=2}^{N-1}\left(\beta_i^\dagger\beta_{i+1} + \text{h.c.}\right), \tag{A.3}$$

with $[\mathcal{H}_\alpha, \mathcal{H}_\beta] = 0$ by using the following linear transformation:

$$\begin{aligned} &\alpha_1 = a_1, \alpha_{N+1} = a_{N+1}, \\ &\alpha_j = \tfrac{1}{\sqrt{2}}(a_j + a_{2N+2-j}),\ j \in [2, N], \\ &\beta_j = \tfrac{1}{\sqrt{2}}(a_j - a_{2N+2-j}),\ j \in [2, N]. \end{aligned} \tag{A.4}$$

The anti-symmetric sub-Hamiltonian $\mathcal{H}_\beta$ is a uniform $(N-1)$-dimensional chain, whose spectrum and eigenfunction are well known. We will focus on the solution of the symmetric sub-Hamiltonian $\mathcal{H}_\alpha$.

A.2. $\mathcal{PT}$-symmetric non-Hermitian reduction Hamiltonian

A.2.1. Exactly solvable $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian. The scattering center is a ring system; from the symmetry of the ring system, we perform the linear transformation similarly as we do in appendix A.1 for the Hamiltonian $\mathcal{H}$. After linear transformation, H_{ss} can be separated into symmetric and anti-symmetric sub-Hamiltonians. For the scattering problem

of $H_{\rm ss}$ only related to its symmetric sub-Hamiltonian $H_{\rm ss}^{\alpha}$, we can calculate the scattering of $H_{\rm ss}^{\alpha}$ to get the scattering result of $H_{\rm ss}$:

$$H_{\rm ss}^{\alpha} = -J\sum_{i=2}^{N-1}\alpha_i^{\dagger}\alpha_{i+1} - \sqrt{2}J\left(\alpha_1^{\dagger}\alpha_2 + \alpha_N^{\dagger}\alpha_{N+1}\right) + \text{h.c.} - \frac{\varepsilon g^2}{2J^2}\left(\alpha_1^{\dagger}\alpha_1 + \alpha_{N+1}^{\dagger}\alpha_{N+1}\right)$$
$$-J\sum_{i=-1}^{-\infty} b_{i-1}^{\dagger}b_i - J\sum_{i=1}^{+\infty} b_i^{\dagger}b_{i+1} + \text{h.c.} - g\left(b_{-1}^{\dagger}a_1 + b_1^{\dagger}a_{N+1} + \text{h.c.}\right), \tag{A.5}$$

where α_i has a similar definition as in (A.4). We can obtain the transmission and reflection coefficients by calculating $H_{\rm ss}^{\alpha}$. The Schrödinger equations for site h_1 and h_{N+1} of $H_{\rm ss}^{\alpha}$ are

$$\begin{aligned} -gf_{-1} - \sqrt{2}Jh_2 &= \left(E + \frac{\varepsilon g^2}{2J^2}\right)h_1, \\ -\sqrt{2}Jh_N - gf_1 &= \left(E + \frac{\varepsilon g^2}{2J^2}\right)h_{N+1}. \end{aligned} \tag{A.6}$$

Schrödinger equations for the rest site give $E = \varepsilon = -2J\cos(k)$. Using the ansatz of f_j in (6), we get the continuity equation of the form

$$\begin{aligned} h_1 &= \frac{1}{\sqrt{2}}(u_k\,\mathrm{e}^{\mathrm{i}k} + v_k\,\mathrm{e}^{-\mathrm{i}k}) = \frac{J}{g}(\mathrm{e}^{\mathrm{i}k} + r\,\mathrm{e}^{-\mathrm{i}k}), \\ h_j &= (u_k\,\mathrm{e}^{\mathrm{i}kj} + v_k\,\mathrm{e}^{-\mathrm{i}kj}), \qquad j \in [2, N], \\ h_{N+1} &= \frac{1}{\sqrt{2}}(u_k\,\mathrm{e}^{\mathrm{i}k(N+1)} + v_k\,\mathrm{e}^{-\mathrm{i}k(N+1)}) = \frac{J}{g}t\,\mathrm{e}^{-\mathrm{i}k} \end{aligned} \tag{A.7}$$

and also $f_{-1} = 1 + r$ together with $f_1 = t$, where r and t are the reflection and transmission coefficients, respectively, and u_k and v_k are the undetermined coefficients of the ansatz wavefunction. In this example, we confine the momentum of the incident wave $k = n\pi/N$, $n \in [1, N-1]$. The energy of the wave is $E = \varepsilon = -2J\cos(n\pi/N)$, $n \in [1, N-1]$; then by substituting the ansatz (A.7) into (A.6), the Schrödinger and the continuity equations reduce to

$$-\frac{g}{J}(1+r) - \sqrt{2}(u_k\,\mathrm{e}^{2\mathrm{i}k} + v_k\,\mathrm{e}^{-2\mathrm{i}k}) = \left(E + \frac{\varepsilon g^2}{2J^2}\right)\frac{J}{g}(\mathrm{e}^{\mathrm{i}k} + r\,\mathrm{e}^{-\mathrm{i}k}), \tag{A.8}$$

$$-(-1)^n\sqrt{2}(u_k + v_k) - \frac{g}{J}t = \left(E + \frac{\varepsilon g^2}{2J^2}\right)\frac{J}{g}t\,\mathrm{e}^{-\mathrm{i}k}, \tag{A.9}$$

$$\frac{1}{\sqrt{2}}\left(u_k\mathrm{e}^{\mathrm{i}k} + v_k\mathrm{e}^{-\mathrm{i}k}\right) = \frac{J}{g}\left(\mathrm{e}^{\mathrm{i}k} + r\mathrm{e}^{-\mathrm{i}k}\right) = \frac{J}{g}(-1)^n t\mathrm{e}^{-\mathrm{i}k}. \tag{A.10}$$

From (A.9) and (A.10), we obtain

$$u_k = \frac{(-1)^n\sqrt{2}}{4}\,\mathrm{e}^{-2\mathrm{i}k}\left(\frac{g^2}{J^2} + 2\right)\frac{J}{g}t, \tag{A.11}$$

$$v_k = -\frac{(-1)^n\sqrt{2}}{4}\left(\frac{g^2}{J^2} - 2\right)\frac{J}{g}t. \tag{A.12}$$

From (A.11), (A.12) and (A.8), we obtain

$$[\mathrm{e}^{2\mathrm{i}k} - (-1)^n t](\mathrm{e}^{2\mathrm{i}k} - 1) = 0. \tag{A.13}$$

We obtain the reflection coefficient r from (A.10) and (A.13):

$$r = (-1)^n t - \mathrm{e}^{2\mathrm{i}k} = 0. \tag{A.14}$$

Actually, site 1 denotes A and site $N+1$ denotes B ($a_1 = a_A, a_{N+1} = a_B$). In this example, we have $V_A = V_B = -\varepsilon g^2/(2J^2) = (g^2/J)\cos k$; substituting $r = 0$ into (16) and (17) gives U_A and U_B as

$$U_A = \frac{g^2}{J}\cos k - \frac{g^2}{J}\mathrm{e}^{-\mathrm{i}k} = \mathrm{i}\frac{g^2}{J}\sin k, \tag{A.15}$$

$$U_B = \frac{g^2}{J}\cos k - \frac{g^2}{J}\mathrm{e}^{\mathrm{i}k} = -\mathrm{i}\frac{g^2}{J}\sin k, \tag{A.16}$$

where $k = n\pi/N$, $n \in [1, N-1]$. The reduced non-Hermitian Hamiltonian $\mathcal{H}_{\mathrm{ss}}^{[n]}$ is then the same as (24).

A.2.2. Exactly solvable non-$\mathcal{PT}$-symmetric non-Hermitian Hamiltonian. Using the linear transformation as introduced in appendix A.1, we note that the scattering problem for Hamiltonian H_{as} is equivalent to its symmetric sub-Hamiltonian H_{as}^{α}:

$$\begin{aligned} H_{\mathrm{as}}^{\alpha} = &-J\sum_{i=2}^{N-1}\alpha_i^{\dagger}\alpha_{i+1} - \sqrt{2}J\alpha_1^{\dagger}\alpha_2 - \sqrt{2}J\alpha_N^{\dagger}\alpha_{N+1} + \mathrm{h.c.} \\ &- J\sum_{i=-1}^{-\infty} b_{i-1}^{\dagger}b_i - J\sum_{i=1}^{+\infty} b_i^{\dagger}b_{i+1} + \mathrm{h.c.} - Jb_{-1}^{\dagger}\alpha_1 - Jb_1^{\dagger}\alpha_{N+1} + \mathrm{h.c.}, \end{aligned} \tag{A.17}$$

where α_i has a similar definition as in (A.4); the Schrödinger equation of H_{as}^{α} for sites h_1, h_2, h_N, h_{N+1} is then

$$\begin{aligned} &-Jf_{-1} - \sqrt{2}Jh_2 = Eh_1, \\ &-\sqrt{2}Jh_1 - Jh_3 = Eh_2, \\ &-Jh_{N-1} - \sqrt{2}Jh_{N+1} = Eh_N, \\ &-\sqrt{2}Jh_N - Jf_1 = Eh_{N+1}. \end{aligned} \tag{A.18}$$

The Schrödinger equation of H_{as}^{α} for the other site reduced to $E = -2J\cos k$, where E is energy and k is the momentum of the incident wave. The wavefunction ansatz f_j of H_{as}^{α} is in the form of (6) and h_j is

$$\begin{aligned} &h_1 = \tfrac{1}{\sqrt{2}}(\mu_k\mathrm{e}^{\mathrm{i}k} + \nu_k\mathrm{e}^{-\mathrm{i}k}), \\ &h_j = \mu_k\mathrm{e}^{\mathrm{i}kj} + \nu_k\mathrm{e}^{-\mathrm{i}kj}, \qquad (j \in [2, N]), \\ &h_{N+1} = \tfrac{1}{\sqrt{2}}(\mu_k\mathrm{e}^{\mathrm{i}k(N+1)} + \nu_k\mathrm{e}^{-\mathrm{i}k(N+1)}), \end{aligned} \tag{A.19}$$

where r and t are the reflection and transmission coefficients, and μ_k and ν_k are the undetermined coefficients of the ansatz wavefunction. Together with the continuity condition, the wavefunction must obey

$$\begin{aligned} &h_1 = \mathrm{e}^{\mathrm{i}k} + r\mathrm{e}^{-\mathrm{i}k} = \tfrac{1}{\sqrt{2}}(\mu_k\mathrm{e}^{\mathrm{i}k} + \nu_k\mathrm{e}^{-\mathrm{i}k}), \\ &h_2 = \mu_k\mathrm{e}^{2\mathrm{i}k} + \nu_k\mathrm{e}^{-2\mathrm{i}k} = \tfrac{1}{\sqrt{2}}(\mathrm{e}^{2\mathrm{i}k} + r\mathrm{e}^{-2\mathrm{i}k}), \\ &h_N = \mu_k\mathrm{e}^{\mathrm{i}kN} + \nu_k\mathrm{e}^{-\mathrm{i}kN} = \tfrac{1}{\sqrt{2}}t\mathrm{e}^{-2\mathrm{i}k}, \\ &h_{N+1} = t\mathrm{e}^{-\mathrm{i}k} = \tfrac{1}{\sqrt{2}}(\mu_k\mathrm{e}^{\mathrm{i}k(N+1)} + \nu_k\mathrm{e}^{-\mathrm{i}k(N+1)}). \end{aligned} \tag{A.20}$$

Using the Gaussian elimination method, eliminating μ_k, ν_k and t, we obtain

$$r = \mathrm{e}^{2\mathrm{i}k}\frac{-2\sin[k(N-2)] + \sin(kN)}{-4\mathrm{e}^{-\mathrm{i}k(N-1)}\sin k + \mathrm{e}^{-2\mathrm{i}k}\sin(kN)}. \tag{A.21}$$

Actually, site 1 denotes A and site $N+1$ denotes B ($a_1 = a_A, a_{N+1} = a_B$). We note that in this example $V_A = V_B = 0$; substituting (A.21) into (16) and (17), we obtain (32) and (33). The reduced non-Hermitian Hamiltonian $\mathcal{H}_{\mathrm{as}}^{[\vartheta]}$ is then the same as (31).

Appendix B. Construction of $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian by the intertwining operator technique

In this appendix, we will derive the central formulae for studying the eigenproblem of the $\mathcal{PT}$-symmetric non-Hermitian ring system. Typically, the solution can be obtained via the Bethe ansatz method as shown in [34]. In this appendix, we will use the intertwining operator technique to get the solutions in order to reveal their characteristic features.

B.1. The intertwining operator technique

The intertwining operator technique is generally employed in supersymmetric quantum mechanics, which provides the universal approach for creating new exactly solvable models. Recently, it is applied to discrete systems in order to construct the model which supports the desirable spectrum [42–46].

The critical idea of the intertwining operator technique is as follows. Consider an $N \times N$ Hamiltonian H_1 which has the form $H_1 = \mathcal{Q}_1\mathcal{R}_1 + \mu_1$, where $\mathcal{Q}_1$ and $\mathcal{R}_1$ represent $N \times (N+1)$ and $(N+1) \times N$ matrices, respectively. One can construct an $(N+1) \times (N+1)$ new Hamiltonian H_2 ($H_2 = \mathcal{R}_1\mathcal{Q}_1 + \mu_1$) by interchanging the operators $\mathcal{R}_1$ and $\mathcal{Q}_1$. The spectrum of H_1 is the same as that of H_2 except for the energy level μ_1. Iterating this method results in a series of Hamiltonians H_3, H_4, H_5, ..., whose energy spectra differ from that of H_1 owing to the addition of the discrete energy levels $\{\mu_1, \mu_2\}$, $\{\mu_1, \mu_2, \mu_3\}$, $\{\mu_1, \mu_2, \mu_3, \mu_4\}$, ...

Our aim is to construct a $\mathcal{PT}$-invariant non-Hermitian Hamiltonian H_3 by adding two energy levels $E = -\mu$ and $E = \mu$ ($0 \leqslant \mu \leqslant 2$; the obtained conclusion will be extended beyond this region later) into the energy spectrum of a uniform chain system. We will show the processes of this construction explicitly. We start with the following $(N-1) \times (N-1)$ uniform chain Hamiltonian:

$$H_1 = -\sum_{n=1}^{N-2}(|n\rangle\langle n+1| + \text{h.c.}), \tag{B.1}$$

which depicts an $(N-1)$-site uniform chain. The spectrum of H_1 can be expressed as

$$\varepsilon_n = -2\cos\left(\frac{n\pi}{N}\right), \qquad n \in [1, N-1]. \tag{B.2}$$

On the other hand, H_1 can be written in the form

$$H_1 = \mathcal{Q}\mathcal{R} - \mu, \tag{B.3}$$

where

$$\mathcal{Q} = \sum_{n=1}^{N-1}(q_n|n\rangle\langle n| + \bar{q}_n|n\rangle\langle n+1|), \tag{B.4}$$

$$\mathcal{R} = \sum_{n=1}^{N-1}(r_n|n\rangle\langle n| + \bar{r}_n|n+1\rangle\langle n|) \tag{B.5}$$

and

$$\begin{aligned} &\mu = 2\cos\kappa, (\kappa > 0),\\ &r_n = q_n = -\mathrm{e}^{-\mathrm{i}\kappa/2},\\ &\bar{r}_n = \bar{q}_n = \mathrm{e}^{\mathrm{i}\kappa/2}. \end{aligned} \tag{B.6}$$

Then the Hamiltonian H_2 can be constructed in the form

$$\begin{aligned} H_2 &= \mathcal{R}\mathcal{Q} - \mu \\ &= -\sum_{n=1}^{N-1}(|n\rangle\langle n+1| + \text{h.c.}) - \mathrm{e}^{\mathrm{i}\kappa}|1\rangle\langle 1| - \mathrm{e}^{-\mathrm{i}\kappa}|N\rangle\langle N|, \end{aligned} \tag{B.7}$$

which possesses an extra eigenvalue $-2\cos\kappa$ based on the spectrum ε_n.

Next step, we repeat the above procedure based on a new Hamiltonian H_2', which is obtained from H_2 under parity operation P, i.e.

$$\begin{aligned} H_2' &= P^{-1}H_2P \\ &= -\sum_{n=1}^{N-1}(|n\rangle\langle n+1| + \text{h.c.}) - \mathrm{e}^{-\mathrm{i}\kappa}|1\rangle\langle 1| - \mathrm{e}^{\mathrm{i}\kappa}|N\rangle\langle N|, \end{aligned} \tag{B.8}$$

where

$$P_{ij} = \delta_{i,N+1-j} \tag{B.9}$$

is the matrix representation of the mirror reflection. Note that H_2' and H_2 have identical spectra. Accordingly, H_2' can be written in the form

$$H_2' = \mathcal{Q}'\mathcal{R}' + \mu, \tag{B.10}$$

where

$$\mathcal{Q}' = \sum_{n=1}^{N}(q_n'|n\rangle\langle n| + \bar{q}_n'|n\rangle\langle n+1|), \tag{B.11}$$

$$\mathcal{R}' = \sum_{n=1}^{N}(r_n'|n\rangle\langle n| + \bar{r}_n'|n+1\rangle\langle n|) \tag{B.12}$$

and

$$\begin{aligned} r_n' &= q_n' = \mathrm{i}\mathrm{e}^{-\mathrm{i}\kappa/2}, \\ \bar{r}_n' &= \bar{q}_n' = \mathrm{i}\mathrm{e}^{\mathrm{i}\kappa/2}, \\ r_1' &= q_1' = \mathrm{i}\sqrt{2}\mathrm{e}^{-\mathrm{i}\kappa/2}, \\ \bar{r}_N' &= \bar{q}_N' = \mathrm{i}\sqrt{2}\mathrm{e}^{\mathrm{i}\kappa/2}. \end{aligned} \tag{B.13}$$

Finally, the target Hamiltonian H_3 can be constructed in the form

$$\begin{aligned} H_3 &= \mathcal{R}'\mathcal{Q}' + \mu \\ &= -\sum_{2}^{N-1}|n\rangle\langle n+1| - \sqrt{2}|1\rangle\langle 2| - \sqrt{2}|N\rangle\langle N+1| + \text{h.c.} \\ &\quad + 2\mathrm{i}\sin\kappa\,(|1\rangle\langle 1| - |N+1\rangle\langle N+1|). \end{aligned} \tag{B.14}$$

We note that H_3 is the symmetric sub-Hamiltonian of $\mathcal{H}^{[n]}$ ($\mathcal{H}^{[\varepsilon]}$); together with the anti-symmetric sub-Hamiltonian ($(N-1)$-dimension uniform chain), we obtain $\mathcal{H}^{[n]}$ ($\mathcal{H}^{[\varepsilon]}$). The energy spectra ((26) and (27)) of $\mathcal{H}^{[n]}$ and $\mathcal{H}^{[\varepsilon]}$ can be obtained by adding the unit J.

B.2. Eigenfunctions of H_3

Now we turn to derive the eigenfunctions of H_3. The eigenfunctions of the Hamiltonians H_1, H_2 and H_3 are denoted by ϕ_n, φ_n and ψ_n, respectively. The eigenfunctions of a uniform chain can be readily written as

$$\phi_n(j) = \sqrt{\frac{2}{N}}\sin\left(\frac{n\pi j}{N}\right), \qquad (n \in [1, N-1]). \tag{B.15}$$

According to the intertwining operator technique of supersymmetry theory, we have

$$\varphi_n(j) = \mathcal{R}\phi_n, \qquad n \in [1, N-1], \tag{B.16}$$

$$\varphi_N(j) = \mathrm{e}^{-\mathrm{i}\kappa j}, \qquad j \in [1, N] \tag{B.17}$$

and

$$\psi_n(j) = \mathcal{R}' P \varphi_n, \qquad n \in [1, N], \tag{B.18}$$

$$\psi_{N+1}(j) = (-1)^j \mathrm{e}^{-\mathrm{i}\kappa j} \begin{pmatrix} \frac{1}{\sqrt{2}}, j = 1, N+1 \\ 1, j \in [2, N] \end{pmatrix}. \tag{B.19}$$

Note that the eigenfunctions are not normalized.

In the above, we restricted μ in the region $[0, 2]$ for the purpose of obtaining H_3 as an unbroken $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian with imaginary potentials at the edges in the form of (B.14). However, the obtained result can be extended beyond the region. Actually, one can simply replace κ by $-\mathrm{i}\omega$ in all the expressions. Then, one can obtain a $\mathcal{PT}$-symmetric Hermitian Hamiltonian with two added bound states with energy $\pm\mu$, where $\mu = 2\cosh\omega > 2$. On the other hand, if κ is replaced by a complex number $\kappa = \pi/2 - \mathrm{i}\omega$, one can obtain a $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian in the broken phase. In this case, the two added eigenstates have pure imaginary eigenvalues $\mu = \pm 2\mathrm{i}\sinh\omega$.

B.3. Coalescence of eigenstates

Now, we investigate the eigenfunctions in the case of $\kappa = k$ ($k = n\pi/N, n \in [1, N-1]$). In this situation, all the coalescence eigenfunctions in (B.18) can be written explicitly as

$$\begin{cases} \psi_n(1) = -\mathrm{i}\sqrt{2}(-1)^n \sin k \\ \psi_n(j) = -2\mathrm{i}\mathrm{e}^{-(N+1-j)\mathrm{i}k} \sin k \\ \psi_n(N+1) = -\mathrm{i}\sqrt{2}\sin k, \end{cases} \tag{B.20}$$

$$\begin{cases} \psi_{N-n}(1) = -\mathrm{i}\sqrt{2}(-1)^{N+n} \sin k \\ \psi_{N-n}(j) = (-1)^{N+n+j} 2\mathrm{i}\mathrm{e}^{-\mathrm{i}(j-1)k} \sin k \\ \psi_{N-n}(N+1) = -\mathrm{i}\sqrt{2}\sin k, \end{cases} \tag{B.21}$$

$$\begin{cases} \psi_N(1) = \mathrm{i}\sqrt{2}(-1)^n \mathrm{e}^{-\mathrm{i}k/2} \\ \psi_N(j) = 2\mathrm{i}\mathrm{e}^{-(N+1-j)\mathrm{i}k}\mathrm{e}^{-\mathrm{i}k/2} \\ \psi_N(N+1) = \mathrm{i}\sqrt{2}\mathrm{e}^{-\mathrm{i}k/2}, \end{cases} \tag{B.22}$$

$$\begin{cases} \psi_{N+1}(1) = -\mathrm{e}^{-\mathrm{i}k}/\sqrt{2} \\ \psi_{N+1}(j) = (-1)^j \mathrm{e}^{-\mathrm{i}kj} \\ \psi_{N+1}(N+1) = -(-1)^{N+n}\mathrm{e}^{-\mathrm{i}k}/\sqrt{2}. \end{cases} \tag{B.23}$$

For odd N, we have $\psi_n \propto \psi_N$ and $\psi_{N-n} \propto \psi_{N+1}$, which means the coalescence of eigenstates. Also the norms of the above four eigenstates vanish. For even N, we have the same conclusion except when $n = N/2$. In this case, ψ_N is ψ_{N-n}, and we have $\psi_n \propto \psi_N = \psi_{N-n} \propto \psi_{N+1}$, which means the coalescence of the three eigenstates. Also, the norms of the above three eigenstates vanish.

Appendix C. Zero determinant

In this appendix we will prove (34). Applying the linear transformation introduced in appendix A, the $2N$-dimensional matrix $\mathcal{M}^{[\vartheta]}$ can be written in a diagonal block form, i.e.

$$\mathcal{M}^{[\vartheta]} + 2\cos\vartheta = \begin{bmatrix} \mathcal{D} & 0 \\ 0 & \mathcal{A} \end{bmatrix}, \tag{C.1}$$

where $\mathcal{D}$ is $(N+1)$ dimensional, while $\mathcal{A}$ is $(N-1)$ dimensional. Here, we take $J = 1$ for simplicity. Then, we have

$$\left|\mathcal{M}^{[\vartheta]} + 2\cos\vartheta\right| = |\mathcal{D}|\,|\mathcal{A}|\,. \tag{C.2}$$

Consider the $(N+1)$-dimensional matrix $\mathcal{D}$, where determinant $D = |\mathcal{D}|$ has the form

$$D = \begin{vmatrix} U_A - E & -\sqrt{2} & & & & & & & \\ -\sqrt{2} & -E & -1 & & & & & & \\ & -1 & -E & -1 & & & & & \\ & & -1 & \ddots & \ddots & & & & \\ & & & \ddots & \ddots & -1 & & & \\ & & & & -1 & -E & -1 & & \\ & & & & & -1 & -E & -\sqrt{2} & \\ & & & & & & -\sqrt{2} & U_B - E \end{vmatrix}. \tag{C.3}$$

Using cofactor expansion along the first and last rows, we obtain

$$D = [E^2 + U_A U_B - E(U_A + U_B) - 4]D_{N-1} - 2(U_A + U_B)D_{N-2}, \tag{C.4}$$

where D_j is the $j \times j$ determinant

$$D_j = \begin{vmatrix} -E & -1 & & & & \\ -1 & -E & -1 & & & \\ & -1 & \ddots & \ddots & & \\ & & \ddots & \ddots & -1 & \\ & & & -1 & -E & -1 \\ & & & & -1 & -E \end{vmatrix}. \tag{C.5}$$

Such kinds of determinants follow the recursion formula

$$D_j = -ED_{j-1} - D_{j-2}, \tag{C.6}$$

which leads to

$$D_j = \frac{1 - \mathrm{e}^{2(j+1)\mathrm{i}\vartheta}}{1 - \mathrm{e}^{2\mathrm{i}\vartheta}}\,\mathrm{e}^{-j\mathrm{i}\vartheta}, \qquad (j < N). \tag{C.7}$$

Substituting (32), (33), (C.7) and $E = -2\cos\vartheta$ into (C.4), we obtain $D = 0$. Thus, (34) is proved.

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