

**Non-Hermitian description of the dynamics of interchain pair tunneling**X. Z. Zhang,<sup>1</sup> L. Jin,<sup>2</sup> and Z. Song<sup>2,\*</sup><sup>1</sup>*College of Physics and Materials Science, Tianjin Normal University, Tianjin 300387, China*<sup>2</sup>*School of Physics, Nankai University, Tianjin 300071, China*

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We study interchain pair tunneling dynamics based on an exact two-particle solution for a two-leg ladder. We show that the Hermitian Hamiltonian shares a common two-particle eigenstate with a corresponding non-Hermitian Hubbard Hamiltonian in which the non-Hermiticity arises from an on-site interaction of imaginary strength. Our results provide that the dynamic processes of two-particle collision and cross-leg tunneling are well described by the effective non-Hermitian Hubbard Hamiltonian based on the eigenstate equivalence. We also find that any common eigenstate is always associated with the emergence of a spectral singularity in the non-Hermitian Hubbard model. This result is valid for both Bose and Fermi systems and provides a clear physical implication of the non-Hermitian Hubbard model.

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A complex parameter in a Hamiltonian, such as imaginary potential, has been investigated under the framework of non-Hermitian quantum mechanics [1–12]. The usefulness of the complex parameter can be explored by establishing a correspondence between a non-Hermitian system and a real physical system in an analytically exact manner. The discovery of a parity-time ( $\mathcal{PT}$ )-symmetric non-Hermitian Hamiltonian having an entirely real quantum-mechanical energy spectrum [13] stimulated the efforts of establishing  $\mathcal{PT}$ -symmetric quantum theory as a complex extension of conventional quantum mechanics [14–20]. This complex extension has profound theoretical and methodological implications in many other subjects, ranging from quantum field theory and mathematical physics [19,21–23] to solid-state [24,25] and atomic physics [26–29].

One way of extracting the physical meaning of a pseudo-Hermitian Hamiltonian with a real spectrum is to seek its Hermitian counterparts [8–10]. There exists another Hermitian Hamiltonian that shares the complete or partial spectrum when the spectrum of a pseudo-Hermitian Hamiltonian is real. The metric-operator theory outlined in Ref. [14] provides a mapping between a pseudo-Hermitian Hamiltonian and an equivalent Hermitian counterpart. However, the obtained equivalent Hermitian Hamiltonian is usually quite complicated [14,30], and it is difficult to determine whether it describes real physics or is just an unrealistic mathematical object. An alternative way to establish the connection between a pseudo-Hermitian Hamiltonian and a physical system is to consider the equivalence of eigenstates [31–33]. A Hermitian scattering center at resonant transmission shares the same wave function with the corresponding non-Hermitian tight-binding lattice consisting of the Hermitian scattering center with two additional  $\mathcal{PT}$ -symmetric on-site complex potentials.

In this paper, we extend this approach to interacting particle systems. In condensed-matter physics, interchain (interlayer) pair tunneling is a popular process and is an important component for the mechanism of superconductivity [34,35].

We consider a two-leg system with interchain pair tunneling. Based on the exact two-particle solution, we show that if the two-particle dynamics mainly refers to a specific invariant subspace, then the corresponding two-particle dynamics can be described by an effective non-Hermitian Hubbard system with an imaginary on-site interaction. For a given initial state, the strength of the imaginary on-site interaction is determined by the relative velocity of the two particles. When we consider the two-particle dynamics associated with the probability gain in one leg of the Hermitian system, a set of corresponding non-Hermitian Hamiltonians is related to the spectral singularities. Therefore, the dynamical correspondence is sensitive to the selection of the initial state. The particle-creation dynamics can be realized by considering the time-reversal process of it, which corresponds to the annihilation of two particles. On the other hand, the two-particle tunneling associated with a decrease of the probability in the other leg can be well described by a non-Hermitian Hubbard model with the definite pair dissipation. In particular, when the relative group velocity matches the strength of pair tunneling, the two-particle probability will exhibit a complete transfer from one leg to the other, which corresponds to pair annihilation in the effective non-Hermitian system. From this point of view, we unveil the connection between the interacting Hermitian and non-Hermitian systems in the context of wave-packet dynamics.

This paper is organized as follows. In Sec. II we introduce the model Hamiltonians and their symmetry. In Sec. III, we present the equivalence between the Hermitian Hamiltonian with interchain pair tunneling and non-Hermitian Hamiltonians with an imaginary on-site interaction. Sections IV and V are devoted to constructing the connection between two types of systems through wave-packet dynamics. Section VI provides the summary and discussion.

**II. MODEL HAMILTONIANS**

We address a physically meaningful non-Hermitian Hamiltonian by associating pair tunneling with an imaginary on-site interaction in a non-Hermitian Hubbard model. As an illustration, we consider two simple models described by a Hermitian and a non-Hermitian Hamiltonian.

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The Hermitian Hamiltonian can be written as follows:

$$H = H_A + H_B + H_{AB} \quad (1)$$

and

$$H_\rho = -\kappa \sum_{j=1}^N (a_{\rho,j}^\dagger a_{\rho,j+1} + \text{H.c.}) \quad (\rho = A, B), \quad (2)$$

$$H_{AB} = -\frac{J}{2} \sum_{j=1}^N (a_{A,j}^\dagger a_{A,j}^\dagger a_{B,j} a_{B,j} + \text{H.c.}). \quad (3)$$

Obviously, it represents a tight-binding system consisting of a two-leg ladder, with each leg  $H_\rho$  ( $\rho = A, B$ ) having dimension  $N$ . The two legs are coupled through a pair tunneling term  $H_{AB}$ , which operates on the motion of multiple particles. The Hamiltonian possesses two symmetries. One is the  $\mathcal{P}$  symmetry: here  $\mathcal{P}$  represents the space-reflection operator (or parity operator), and the effect of the parity operator is  $\mathcal{P} a_{A,j}^\dagger \mathcal{P}^{-1} = a_{B,j}^\dagger$ . The other is the particle-number symmetry, which ensures probability conservation and leads to the following commutation relation:

$$[\hat{N}_\rho, H] \neq 0, \quad \text{but} \quad \left[ \sum_\rho \hat{N}_\rho, H \right] = 0, \quad (4)$$

where  $\hat{N}_\rho = \sum_i a_{\rho,i}^\dagger a_{\rho,i}$  ( $\rho = A, B$ ) are the particle-number operators for the upper and lower legs, respectively. The probability is conserved in the entire system  $H$ , but breaks in subsystems  $H_A$  and  $H_B$ . The interchain pair tunneling admits a peculiar symmetry,

$$[(-1)^{\hat{N}_\rho}, H] = 0, \quad (5)$$

i.e., the conservation of particle-number parity.

Another related system is a non-Hermitian system composed by two independent Hubbard chains, which can be expressed as

$$\mathcal{H} = \mathcal{H}_A + \mathcal{H}_B \quad (6)$$

and

$$\mathcal{H}_\rho = -\kappa \sum_{i=1}^N (a_{\rho,i}^\dagger a_{\rho,i+1} + \text{H.c.}) + \frac{iU_\rho}{2} \sum_i n_{\rho,i} (n_{\rho,i} - 1), \quad (7)$$

where  $\rho = A, B$ . The non-Hermiticity of  $\mathcal{H}_\rho$  arises from the complex on-site interaction  $iU_\rho$ .

We note that  $\mathcal{H}$  has the same symmetries as  $H$  does, i.e.,  $[\mathcal{H}_\rho, \sum_i n_{\rho,i}] = 0$ ,  $[\mathcal{H}, \sum_{\rho,i} n_{\rho,i}] = 0$ , except  $[\mathcal{H}_A, \mathcal{H}_B] = 0$ . This allows us to construct the eigenstates of two models in the same invariant subspaces. For instance, particle-preserving symmetry leads to the two-particle invariant subspace, which can be further decomposed into two invariant subspaces with basis sets  $\{a_{A,i}^\dagger a_{B,j}^\dagger |0\rangle\}$  and  $\{a_{\rho,i}^\dagger a_{\rho,j}^\dagger |0\rangle\}$ , respectively. In the next section, we investigate the connection between the two-particle solutions of these two Hamiltonians. In Fig. 1, we schematically illustrate the systems  $H$  and  $\mathcal{H}$ .

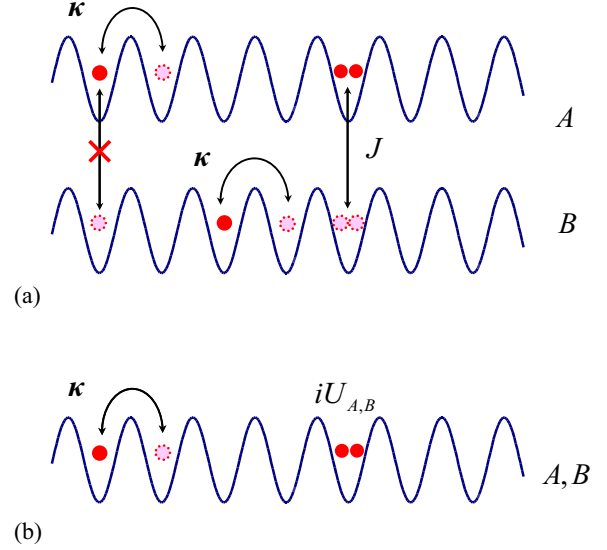


FIG. 1. Schematic illustration of the concerned lattice systems. (a) Two-leg ladder for noninteracting particles. Two particles at the same site can hop simultaneously across two legs with  $J$  being the interchain pair tunneling strength. (b) Two independent Hubbard chains with imaginary on-site interaction  $iU_\rho$  ( $\rho = A, B$ ).

### III. PAIR TUNNELING AND SPECTRAL SINGULARITY

Now we turn to study the two-particle eigenstates of  $H$  and  $\mathcal{H}$ , from which we expect to establish the connection between two models. We focus on the solutions in the invariant subspace spanned by  $\{a_{\rho,i}^\dagger a_{\rho,j}^\dagger |0\rangle\}$ ; i.e., both particles are in either chain A or B. The derivation in Appendix A shows that for each given  $\{K, k\}$  with  $K \in [-\pi, \pi]$ ,  $k \in [0, \pi]$ , there are two degenerate eigenstates of  $H$  with energy

$$\varepsilon_K(k) = -4\kappa \cos(K/2) \cos k. \quad (8)$$

And the associated eigenstates can be written as

$$|\psi_{K,k}^\pm\rangle = \sum_{r \geq 0, \rho=A,B} f_{K,k}^{\rho,\pm}(r) |\phi_r^\rho(K)\rangle, \quad (9)$$

and

$$|\phi_0^\rho(K)\rangle = \frac{1}{2\sqrt{N}} \sum_j e^{iKj} a_{\rho,j}^\dagger a_{\rho,j}^\dagger |\text{vac}\rangle, \quad (10)$$

$$|\phi_r^\rho(K)\rangle = \frac{e^{iKr/2}}{\sqrt{N}} \sum_j e^{iKj} a_{\rho,j}^\dagger a_{\rho,j+r}^\dagger |\text{vac}\rangle \quad (r > 1), \quad (11)$$

where  $|\phi_0^\rho(K)\rangle$  and  $|\phi_r^\rho(K)\rangle$  are translational invariant bases. The corresponding wave functions  $f_{K,k}^{\rho,\pm}(r)$  can be expressed explicitly as

$$\begin{aligned} f_{K,k}^{A,+}(r) &= f_{K,k}^{B,-}(r) \\ &= \begin{cases} e^{-ikr} + \eta_{K,k} e^{ikr}, & r > 0 \\ (1 + \eta_{K,k})/\sqrt{2}, & r = 0, \end{cases} \end{aligned} \quad (12)$$

$$\begin{aligned} f_{K,k}^{B,+}(r) &= f_{K,k}^{A,-}(r) \\ &= \begin{cases} \xi_{K,k} e^{ikr}, & r > 0 \\ (1 + \xi_{K,k})/\sqrt{2}, & r = 0, \end{cases} \end{aligned} \quad (13)$$

where

$$\eta_{K,k} = \frac{\lambda_{K,k}^2 - J^2}{\lambda_{K,k}^2 + J^2}, \quad \xi_{K,k} = -\frac{2i\lambda_{K,k}J}{\lambda_{K,k}^2 + J^2}, \quad (14)$$

$$\lambda_{K,k} = 4\kappa \cos(K/2) \sin k. \quad (15)$$

We note that  $K$  represents the central momentum vector of two particles, while  $k$  represents the relative momentum between the two particles. In this sense, the eigenstates  $|\psi_{K,k}^\pm\rangle$  are associated with the dynamic process in which two particles collide with each other in one leg and then tunnel into the other leg.

Similarly, we can construct the eigenstates of  $\mathcal{H}$  having the same form in Eq. (9) based on the result shown in Appendix B,

$$|\chi_{K,k}^\pm\rangle = \sum_{r \geq 0, \rho=A,B} g_{K,k}^{\rho,\pm}(r) |\phi_r^\rho(K)\rangle, \quad (16)$$

where

$$g_{K,k}^{A,+}(r) = g_{K,k}^{A,-}(r) = \begin{cases} e^{-ikr} + \mu_{K,k} e^{ikr}, & r > 0 \\ (1 + \mu_{K,k})/\sqrt{2}, & r = 0, \end{cases} \quad (17)$$

$$g_{K,k}^{B,+}(r) = -g_{K,k}^{B,-}(r) = \begin{cases} e^{-ikr} + \nu_{K,k} e^{ikr}, & r > 0 \\ (1 + \nu_{K,k})/\sqrt{2}, & r = 0, \end{cases} \quad (18)$$

and the parameters are

$$\mu_{K,k} = \frac{\lambda_{K,k} + U_A}{\lambda_{K,k} - U_A}, \quad \nu_{K,k} = \frac{\lambda_{K,k} + U_B}{\lambda_{K,k} - U_B}. \quad (19)$$

It is easy to check that when the conditions

$$U_A = -J^2/\lambda_{K,k}, \quad U_B = \lambda_{K,k}, \quad (20)$$

are satisfied, we could obtain

$$|\psi_{K,k}^+\rangle = |\chi_{K,k}^+\rangle. \quad (21)$$

Note that the eigenstates  $|\chi_{K,k}^\pm\rangle$  are the functions of  $U_A$  and  $U_B$ . The equivalence condition (21) denotes that  $U_A$  and  $U_B$  are  $\{K,k\}$  dependent. Thus one requires two indices to label the eigenstate as  $|\chi_{K,k}^\pm(U_A, U_B)\rangle$ . For the sake of convenience, we neglect the  $(U_A, U_B)$  of  $|\chi_{K,k}^\pm(U_A, U_B)\rangle$ . If we exchange the values of  $U_A$  and  $U_B$ ,

$$U_A = \lambda_{K,k}, \quad U_B = -J^2/\lambda_{K,k}, \quad (22)$$

we have

$$|\psi_{K,k}^-\rangle = |\chi_{K,k}^+\rangle, \quad (23)$$

which arises from the parity symmetry of both  $H$  and  $\mathcal{H}$ . This indicates that the two Hamiltonians have common eigenstates, revealing the connection between a Hermitian and a non-Hermitian Hamiltonian. This connection has the following features:

(i) We find that  $iU_A$  and  $iU_B$  are  $\{K,k\}$  dependent and for a given  $\{K,k\}$  they are all imaginary but with different signs, representing a complementarity pair gain and loss. Further investigation in the next section shows that this ensures the conservation of particles in the whole system.

(ii) As an independent non-Hermitian Hubbard chain with on-site strength  $iU_\rho$ , the derivation in Appendix C shows that when  $U_\rho = \lambda_{K,k}$  this Hamiltonian has a spectral singularity at point  $\{K,k\}$ .

(iii) Furthermore, we find that in the case of  $J^2 = \lambda_{K,k}^2$  two independent non-Hermitian Hubbard chains have a spectral singularity simultaneously at point  $\{K,k\}$ .

The mechanism of the occurrence of the spectral singularity and the corresponding physical implications are addressed in the next section.

#### IV. TUNNELING DYNAMICS

Considering two local particles in one of two legs which have no overlap with each other, the tunneling term would have zero effect on the dynamics. But when the two particles meet, particle transfer occurs between the two legs. The pair transmission probability depends on many factors as discussed in the following. In this section, we investigate the dynamics of a collision of two wave packets based on the above formalism. We start our investigation from the time evolution of an initial state as

$$|\Phi(0)\rangle = |\Phi_{A,a}\rangle |\Phi_{A,b}\rangle, \quad (24)$$

which represents two separable boson wave packets  $a$  and  $b$ . Here

$$|\Phi_{\rho,\gamma}\rangle = \frac{1}{\sqrt{\Omega}} \sum_j e^{-\alpha^2(j-N_\gamma)^2} e^{ik_\gamma j} a_{\rho,j}^\dagger |\text{vac}\rangle, \quad (25)$$

with  $\gamma = a, b$ , and  $\rho = A, B$  represents a Gaussian wave packet, which has a width  $2\sqrt{\ln 2}/\alpha$ , a central position  $N_\gamma$  in chain  $\rho$ , and a group velocity  $v_\gamma = -2\kappa \sin k_\gamma$ . The condition that  $N_a - N_b \gg 1/\alpha$  ensures that two initial bosons cannot overlap, thus having no pair tunneling. Straightforward derivation shows that

$$\begin{aligned} |\Phi(0)\rangle &= \frac{1}{2} \sum_{\sigma=\pm} (|\Phi_{A,a}\rangle |\Phi_{A,b}\rangle + \sigma |\Phi_{B,a}\rangle |\Phi_{B,b}\rangle) \\ &= \frac{1}{\sqrt{2}\Omega_1} \sum_K e^{-(K-2k_c)^2/4\alpha^2} e^{-iN_c(K-2k_c)} |\psi_K^\pm(r_c, q_c)\rangle, \end{aligned} \quad (26)$$

where

$$|\psi_K^\pm(r_c, q_c)\rangle = \frac{1}{\sqrt{\Omega_2}} \sum_r e^{-\alpha^2(r-r_c)^2/2} e^{iq_c r/2} |\phi_r^\pm(K)\rangle, \quad (27)$$

and  $\Omega_{1,2}$  is the normalized factor. Here we have used the transformations

$$N_c = \frac{1}{2}(N_a + N_b), \quad r_c = N_b - N_a, \quad (28)$$

$$k_c = \frac{1}{2}(k_a + k_b), \quad q_c = k_b - k_a, \quad (29)$$

$$l = j + r, \quad (30)$$

and identities

$$2[(j - N_a)^2 + (l - N_b)^2] = [(j + l) - (N_a + N_b)]^2 + [(l - j) - (N_b - N_a)]^2, \quad (31)$$

$$2(k_a j + k_b l) = (k_a + k_b)(j + l) + (k_b - k_a)(l - j). \quad (32)$$

We note that the component of state  $|\Phi(0)\rangle$  on each invariant subspace represents an incident wave packet along the chains described by  $H_{\text{eq}}^{K,\pm}$  with a width  $2\sqrt{\ln 2}/\alpha$ , a central position  $r_c = N_b - N_a$ , and a group velocity  $v = -4\kappa \cos(K/2) \sin(q_c/2)$ . It is worth pointing out that as  $\alpha \ll 1$ , the initial state is distributed mainly in the invariant subspace  $K = 2k_c$ , where the wave packet moves with the group velocity  $v_r = -4\kappa \cos(k_c) \sin(q_c/2) = v_b - v_a$ . Then the time evolution of state  $|\Phi(t)\rangle$  can be derived by the evolution of the wave packet in two chains  $H_{\text{eq}}^{K,\pm}$ , which eventually can be obtained from the solution in Eq. (A8). Furthermore, according to the solution, the evolved state of  $|\psi_K^\pm(r_c, q_c)\rangle$  can be expressed approximately in the form of  $e^{i\beta(r'_c)} R_{2k_c, q_c/2}^\pm |\psi_K^\pm(r'_c, -q_c)\rangle$ , which represents a reflected wave packet in the equivalent semi-infinite chain  $H_{\text{eq}}^{K,\pm}$ . The expressions of  $R_{2k_c, q_c/2}^\pm$  and  $H_{\text{eq}}^{K,\pm}$  are given in Appendix B. Here  $\beta(r'_c)$ , as a function of the position of the reflected wave packet, is an overall phase and is independent of  $J$ . We assume that the collision occurs at instant  $t_0$ ; the evolved state at time  $t \gg t_0$  has the form of

$$|\Phi(t)\rangle = \sum_{\sigma=\pm} \Omega^{-1} e^{i\beta(|N'_a - N'_b|)} R_{2k_c, q_c/2}^\sigma \times \sum_{j,l} e^{-\alpha^2(l - N'_b)^2} e^{-\alpha^2(j - N'_a)^2} \times e^{ik_b j} e^{ik_a l} (a_{A,j}^\dagger a_{A,l}^\dagger + \sigma a_{B,j}^\dagger a_{B,l}^\dagger) |\text{vac}\rangle, \quad (33)$$

which also represents two separable wave packets at  $N'_a$  and  $N'_b$ , respectively. Comparing Eqs. (26) and (33), it is straightforward to figure out that the two-particle wave packets behave as classical particles, which swap momenta with each other after collision. For simplicity, we denote an incident single-particle wave packet as  $|\lambda, p, A\rangle$ , where  $\lambda = \text{L, R}$  indicates the particle coming from the left or right of the collision zone, and  $p$  is the central momentum. In this context, we give the asymptotic expression for the collision process in the following: at time  $t \ll t_0$ , we have

$$|\text{L}, k_a, A\rangle |\text{R}, k_b, A\rangle = \frac{1}{\sqrt{2}} (|\text{F}^+\rangle + |\text{F}^-\rangle), \quad (34)$$

where

$$|\text{F}^\pm\rangle = \frac{1}{\sqrt{2}} (|\text{L}, k_a, A\rangle |\text{R}, k_b, A\rangle \pm |\text{L}, k_a, B\rangle |\text{R}, k_b, B\rangle), \quad (35)$$

and after collision, at time  $t \gg t_0$ , the wave packets exchange their momenta, which admits

$$|\text{L}, k_a, A\rangle |\text{R}, k_b, A\rangle \pm |\text{L}, k_a, B\rangle |\text{R}, k_b, B\rangle \longmapsto R_{2k_c, q_c/2}^\pm (|\text{L}, k_b, A\rangle |\text{R}, k_a, A\rangle \pm |\text{L}, k_b, B\rangle |\text{R}, k_a, B\rangle). \quad (36)$$

By neglecting the  $J$ -independent overall phase, therefore, we have

$$|\text{L}, k_a, A\rangle |\text{R}, k_b, A\rangle \longmapsto \cos \Delta_{2k_c, q_c/2} |\text{L}, k_b, A\rangle |\text{R}, k_a, A\rangle + i \sin \Delta_{2k_c, q_c/2} |\text{L}, k_b, B\rangle |\text{R}, k_a, B\rangle, \quad (37)$$

where

$$R_{2k_c, q_c/2}^\pm = e^{\pm i \Delta_{2k_c, q_c/2}}, \quad (38)$$

$$\Delta_{2k_c, q_c/2} = 2 \tan^{-1} \left( -\frac{J}{\lambda_{2k_c, q_c/2}} \right), \quad (39)$$

as discussed in Appendix A. Evidently, Eq. (37) shows that after collision, one part of two wave packets in leg  $A$ , which corresponds to the first term in Eq. (37), is reflected as two identical classical particles. Meanwhile another part, which corresponds to the second term in Eq. (37), tunnels into leg  $B$ .

Considering a special case with  $v_r = J$ , i.e., when the pair tunneling amplitude is equal to the relative group velocity, we have  $\Delta_{2k_c, q_c/2} = \pi/2$ , and this leads to

$$|\text{L}, k_a, A\rangle |\text{R}, k_b, A\rangle \longmapsto i |\text{L}, k_b, B\rangle |\text{R}, k_a, B\rangle. \quad (40)$$

Clearly, this represents the process whereby two separable wave packets on leg  $A$  tunnel into leg  $B$  completely.

## V. NON-HERMITIAN DYNAMICS

From the above discussions regarding the dynamics of across-leg tunneling, we see that the two-particle probability transfers from one leg to another. The two-particle probability in one leg is not conserved. Thus, a natural question to ask is whether there exists an effective non-Hermitian Hamiltonian for characterizing such a dynamics. To this end, we first present the connections between Hermitian Hamiltonian  $H$  and  $\mathcal{H}$  in a compact form. There are  $N(N+1)$  eigenstates of  $H$  in the invariant subspace spanned by  $\{a_{\rho,i}^\dagger a_{\rho,j}^\dagger |\text{vac}\rangle\}$ . Each of the eigenstates  $\{|\psi_{K,k}^\pm\rangle\}$  corresponds to a specific eigenstate  $|\chi_{K,k}^+\rangle$  of the non-Hermitian Hubbard chain with the  $(K, k)$ -dependent interaction  $iU_\rho$  as in Eqs. (21) and (23). We note that the eigenstates of  $H$  and  $(K, k)$ -dependent Hamiltonian  $\mathcal{H}$  are related to the index  $(K, k)$ . In the following, we take a single index  $\eta$  to represent  $(K, k)$ . For the system with  $2N$  sites, all possible  $(K, k)$  are denoted as  $\eta = 1, 2, \dots, N(N+1)/2$ . The eigenstates of  $H$  are denoted as  $|\bar{\psi}_l\rangle$  ( $l \in [1, N(N+1)]$ ) with

$$|\bar{\psi}_\eta\rangle \equiv |\psi_{K,k}^+\rangle, \quad |\bar{\psi}_{\eta+N(N+1)/2}\rangle \equiv |\psi_{K,k}^-\rangle. \quad (41)$$

Accordingly, the  $(K, k)$ -dependent Hamiltonian  $\mathcal{H}$  is denoted as  $\bar{\mathcal{H}}_l$  with

$$\bar{\mathcal{H}}_\eta \equiv \mathcal{H}(K, k), \quad \text{for } U_A = -J^2/\lambda_{K,k}, \quad U_B = \lambda_{K,k}, \quad (42)$$

$$\bar{\mathcal{H}}_{\eta+N(N+1)/2} \equiv \mathcal{H}(K, k), \quad \text{for } U_A = \lambda_{K,k}, \quad U_B = -J^2/\lambda_{K,k}. \quad (43)$$

The eigenstate of  $\overline{\mathcal{H}}_l$  is denoted as  $|\overline{\chi}_{l,l'}\rangle$  with

$$|\overline{\chi}_{\eta,\eta'}\rangle \equiv |\chi_{K',k'}^+\rangle, \quad |\overline{\chi}_{\eta,\eta'+N(N+1)/2}\rangle \equiv |\chi_{K',k'}^-\rangle, \quad (44)$$

for  $\mathcal{H}(K,k)$  with  $U_A = -J^2/\lambda_{K,k}$ ,  $U_B = \lambda_{K,k}$ ,

$$|\overline{\chi}_{\eta+N(N+1)/2,\eta'}\rangle \equiv |\chi_{K',k'}^-\rangle,$$

$$|\overline{\chi}_{\eta+N(N+1)/2,\eta'+N(N+1)/2}\rangle \equiv |\chi_{K',k'}^+\rangle,$$

$$\text{for } \mathcal{H}(K,k) \text{ with } U_A = \lambda_{K,k}, \quad U_B = -J^2/\lambda_{K,k}. \quad (45)$$

Note that the eigenstate  $|\overline{\chi}_{l,l'}\rangle$  possesses two subscripts. The first one indicates the  $(K,k)$ -dependent on-site interactions  $U_A$  and  $U_B$ , and the second one denotes the center and relative momenta  $(K',k')$  of the eigenstate for a given  $U_A$  and  $U_B$ . In Fig. 3(a), we illustrate the  $|\overline{\chi}_{l,l'}\rangle$  via ket matrix. The states in the  $l$ th row represent the complete set of eigenstates of  $\overline{\mathcal{H}}_l$ . Based on this notation, the Schrodinger equations become compact:

$$H|\overline{\psi}_l\rangle = E_l|\overline{\psi}_l\rangle, \quad (46)$$

$$\overline{\mathcal{H}}_l|\overline{\chi}_{l,l'}\rangle = \varepsilon_{l,l'}|\overline{\chi}_{l,l'}\rangle. \quad (47)$$

Note that  $\varepsilon_{l,l'}$  is related to the scattering solution of two particles, which possesses the form of  $\varepsilon_{l,l'} = -4\kappa \cos(K'/2) \cos k'$ , where  $(K',k')$  denotes possible center and relative momenta. These eigenstates have simple relations

$$|\overline{\psi}_l\rangle = |\overline{\chi}_{l,l}\rangle, \quad E_l = \varepsilon_{l,l} = -4\kappa \cos(K/2) \cos k, \quad (48)$$

which indicate that the diagonal states  $\{|\overline{\chi}_{l,l}\rangle\}$  of Fig. 3(a) are the complete set of eigenstates of  $H$ . Here,  $|\overline{\psi}_\eta\rangle$  ( $|\overline{\psi}_{\eta+N(N+1)/2}\rangle$ ) represents that the two particles collide with each other in leg A (B) and then tunnel into leg B (A).

When considering the dynamical correspondence in the non-Hermitian Hubbard system, there exist two kinds of dynamical processes corresponding to  $|\overline{\psi}_\eta\rangle$  and  $|\overline{\psi}_{\eta+N(N+1)/2}\rangle$ :

(i)  $|\overline{\chi}_{\eta,\eta}^A\rangle \equiv (|\overline{\chi}_{\eta,\eta}\rangle + |\overline{\chi}_{\eta,\eta+N(N+1)/2}\rangle)/\sqrt{2}$  denotes the two-particle collision process in leg A accompanied by the decrease of the two-particle probability while  $|\overline{\chi}_{\eta,\eta}^B\rangle \equiv (|\overline{\chi}_{\eta,\eta}\rangle - |\overline{\chi}_{\eta,\eta+N(N+1)/2}\rangle)/\sqrt{2}$  represents a process related to the increase of two-particle probability in leg B.

(ii)  $|\overline{\chi}_{\eta+N(N+1)/2,\eta}^B\rangle \equiv (|\overline{\chi}_{\eta+N(N+1)/2,\eta}\rangle - |\overline{\chi}_{\eta+N(N+1)/2,\eta+N(N+1)/2}\rangle)/\sqrt{2}$  represents the two-particle collision process in leg B accompanied by the decrease of the two-particle probability, and  $|\overline{\chi}_{\eta+N(N+1)/2,\eta}^A\rangle \equiv (|\overline{\chi}_{\eta+N(N+1)/2,\eta}\rangle + |\overline{\chi}_{\eta+N(N+1)/2,\eta+N(N+1)/2}\rangle)/\sqrt{2}$  denotes a process associated with the increase of two-particle probability in leg A.

For a collision process along leg  $\rho$  ( $\rho = A, B$ ) in Hermitian systems, there are  $N(N+1)/2$  related non-Hermitian Hamiltonians. Therefore, one cannot obtain a Hubbard chain with a certain value of  $iU_\rho$  to describe the dynamics along one of two legs. However, for an initial state distributed mainly in the vicinity of  $|\overline{\psi}_{l_0}\rangle$ , the correspondence of dynamics can be characterized by the eigenstates around the  $l_0$ th row in which the value of  $l_0$  is determined by the central and relative momenta  $(K_0, k_0)$  of the considered initial state. This corresponds to a block around certain ket  $|\overline{\chi}_{l_0,l_0}\rangle$ , which can be shown in Fig. 3(b). For the sake of simplicity and convenience, we confine the discussions to the case of

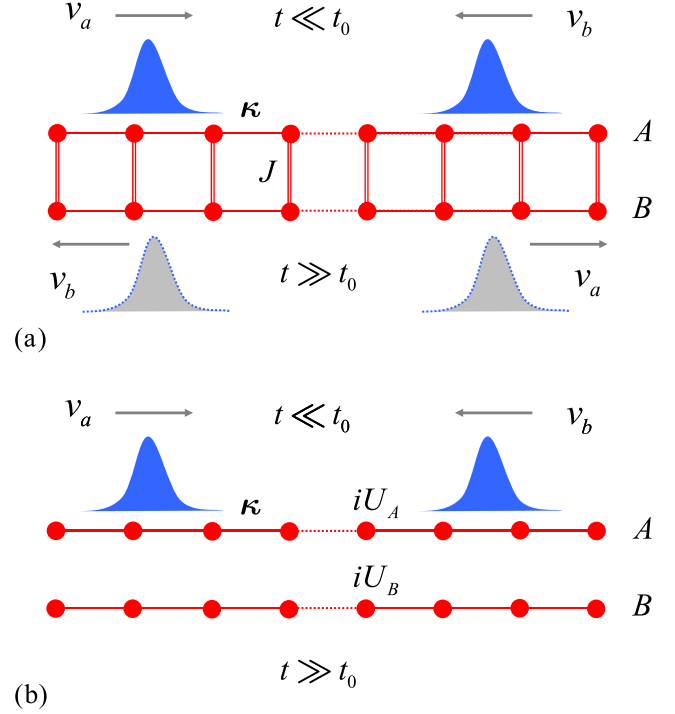


FIG. 2. Schematic illustration of the dynamics of two separable wave packets placed initially at leg A. (a) The two wave packets enter into leg B completely associated with the probability flow from leg A into leg B when  $J = v_r$ . The dynamic process of two such particles in leg A can be described approximately through the non-Hermitian interacting system in (b) with  $U_A = v_r$  ( $v_r < 0$ ), in which the annihilation of the two wave packets occurs through the imaginary on-site interaction.

$l_0 \in [1, (N+1)N/2]$ . The conclusion still holds for the case of  $l_0 \in [(N+1)N/2 + 1, (N+1)N]$ , in which the  $U_A$  and  $U_B$  exchange their values. To seek an effective non-Hermitian Hamiltonian to characterize such a dynamics, we first consider the collision dynamics in leg A, which is accompanied by the decrease of two-particle probability. If the involved wave functions change slowly around  $(|\overline{\chi}_{l_0,l_0}\rangle + |\overline{\chi}_{l_0,l_0+N(N+1)/2}\rangle)/\sqrt{2}$ , then one can use an effective non-Hermitian Hamiltonian  $\mathcal{H}_A(K_0, k_0)$  with a definite  $U_A = -J^2/\lambda_{K_0, k_0}$  as an approximation to describe such a dynamics of leg A in the Hermitian system. To this end, we take the derivative of the function  $\mu_{K,k}$  with respect to  $K$  and  $k$ ,

$$\left(\frac{\partial \mu_{K,k}}{\partial K}\right)_{K_0, k_0} = -\Lambda \sin(K_0/2) \sin k_0, \quad (49)$$

$$\left(\frac{\partial \mu_{K,k}}{\partial k}\right)_{K_0, k_0} = 2\Lambda \cos(K_0/2) \cos k_0, \quad (50)$$

where  $\Lambda = 8\kappa J^2 \lambda_{K_0, k_0} / (\lambda_{K_0, k_0}^2 + J^2)^2$ . The optimal condition can be achieved when  $(\partial \mu_{K,k} / \partial k)_{K_0, k_0} = 0$  and  $(\partial \mu_{K,k} / \partial K)_{K_0, k_0} = 0$ . This can be realized through adjusting the relative group velocity of the initial two wave packets. The condition also indicates that all the rows in such a block are identical approximately as shown in Fig. 3(b). Then the diagonal states of the block can be replaced by that in a row with green shading. On the other hand, for the dynamics

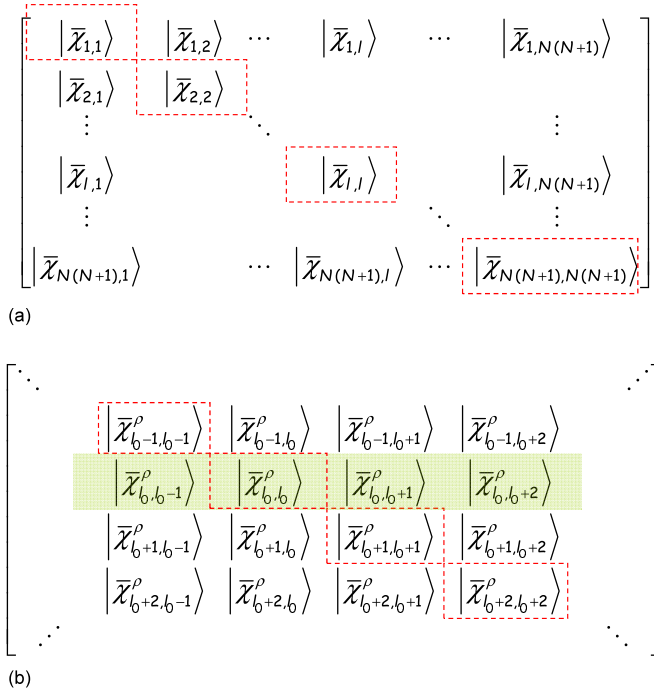


FIG. 3. The ket matrix to illustrate the connection between eigenstates of  $\bar{\mathcal{H}}_l$  and  $H$ . (a) States in the  $l$ th row  $\{|\bar{\chi}_{l,i}\rangle\}$  represent a complete set of eigenstates of  $\bar{\mathcal{H}}_l$ . The diagonal states  $\{|\bar{\chi}_{l,i}\rangle\}$  (dashed box) are the complete set of eigenstates of  $H$ . (b) A block around a certain ket  $|\bar{\chi}_{l_0,l_0}^\rho\rangle$  satisfying Eqs. (49), (50), (52), and (53). All the rows in such a block are identical approximately. Then the diagonal states can be replaced by that in a row (green shaded).

along leg  $B$ , each of the eigenstates in the vicinity of  $|\bar{\chi}_{l_0,l_0}^B\rangle = (|\bar{\chi}_{l_0,l_0}\rangle - |\bar{\chi}_{l_0,l_0+N(N+1)/2}\rangle)/\sqrt{2}$  corresponds to a spectral singularity of the non-Hermitian Hamiltonian  $\mathcal{H}_B(K,k)$ . This leads to the coefficients  $\lambda_{K,k} = U_B$  ( $\nu_{K,k} = \infty$ ). In order to avoid this divergence, we can rewrite the expression of Eq. (18) in the form

$$g_{K,k}^{B,+}(r) = -g_{K,k}^{B,-}(r) = \begin{cases} \varsigma_k e^{-ikr} + \zeta_k e^{ikr}, & r > 0 \\ 2\lambda_{K,k}/\sqrt{2}, & r = 0, \end{cases} \quad (51)$$

where  $\varsigma_k = \lambda_{K,k} - U_B$ , and  $\zeta_k = \lambda_{K,k} + U_B$ . Here we want to point out that the relative magnitude between the amplitudes of right-going wave  $e^{ikr}$  and left-going wave  $e^{-ikr}$  is meaningful, since we focus on the scattering solution in the limit of  $N \rightarrow \infty$ . In this sense, the form of the wave functions  $g_{K,k}^{A,\sigma}(r)$  and  $g_{K,k}^{B,\sigma}(r)$  ( $\sigma = \pm$ ) are not unique. After multiplying by a  $(K - k)$ -dependent constant, the renormalized scattering solutions are still the corresponding eigenstates of  $\mathcal{H}_A$  and  $\mathcal{H}_B$ . In the definition of Eq. (18), the existence of the spectral singularity in the system can be determined by either  $\mu_{K,k} = 0$  ( $\nu_{K,k} = 0$ ) or  $\mu_{K,k} = \infty$  ( $\nu_{K,k} = \infty$ ), which is associated with the pair-annihilation or pair-creation process. This corresponds to the case of  $\zeta_k = 0$  or  $\varsigma_k = 0$  in Eq. (51). To obtain the effective non-Hermitian Hamiltonian, we focus on the variation of  $\varsigma_k$  in the vicinity of  $|\bar{\chi}_{l_0,l_0}^B\rangle$  in the ket matrix.

As we have done in leg  $A$ , we take the partial derivative of the  $\varsigma_k$  with respect to  $K$  and  $k$ , respectively, which yields

$$\left(\frac{\partial \varsigma_k}{\partial K}\right)_{K_0,k_0} = 0, \quad (52)$$

$$\left(\frac{\partial \varsigma_k}{\partial k}\right)_{K_0,k_0} = 0. \quad (53)$$

This indicates that one can replace the diagonal states with row states for any given momenta  $(K_0, k_0)$  in the ket matrix as shown in Fig. 3(b). Thus, an effective Hamiltonian with definite  $U_B = \lambda_{K_0,k_0}$  can be employed to simulate the dynamics of leg  $B$  in the Hermitian system. Here we want to stress that there is no tunneling between non-Hermitian Hamiltonians  $\mathcal{H}_A$  and  $\mathcal{H}_B$ . Thus, we cannot employ an effective non-Hermitian Hamiltonian  $\mathcal{H}$  with definite strengths of the pair dissipation and gain to describe the tunneling dynamics between the two legs. The dynamical correspondence of leg  $B$  can be obtained through another method, which is detailed in the following.

In parallel, we can investigate the dynamics of a two-wave-packet collision by analyzing the time evolution of the initial state  $|\Phi(0)\rangle$  in the effective non-Hermitian system  $\mathcal{H}$  with  $U_A = -J^2/\nu_r$ . Similarly, we can obtain the asymptotic expression for the collision process as

$$|L, k_a, A\rangle |R, k_b, A\rangle \mapsto \cos \Delta_{2k_c, q_c/2} |L, k_b, A\rangle |R, k_a, A\rangle, \quad (54)$$

which has the same form as the wave function in leg  $A$  of Eq. (37). This indicates that the effective non-Hermitian Hamiltonian  $\mathcal{H}$  can describe the wave-packet dynamics in a subsystem (leg  $A$ ) of a Hermitian system  $H$ . Naturally, when the strength of the imaginary on-site interaction  $U_A$  is equal to the relative group velocity  $\nu_r$  ( $\Delta_{2k_c, q_c/2} = \pi/2$ ), the two particles will exhibit a behavior of pair annihilation in leg  $A$  and will never tunnel into leg  $B$ . This process is schematically illustrated in Fig. 2(b). Note that  $\mathcal{H}$  cannot describe the wave-packet dynamics in leg  $B$ , because there is no tunneling between legs  $A$  and  $B$  in  $\mathcal{H}$ . However, the final state  $|L, k_b, B\rangle |R, k_a, B\rangle$  in leg  $B$  as in Eq. (37) can be prepared by using non-Hermitian Hamiltonian  $H_B$  in another way. To this end, we require an initial state to simulate the creation of a pair of particles. Moreover, the modulus of the initial state should tend to be zero, owing to the fact that no one can create a pair of particles out of nothing. Then the initial state driven by the  $\mathcal{H}_B$  will evolve to  $|L, k_b, B\rangle |R, k_a, B\rangle$  accompanied by the increase of two-particle probability. However, the selection of such an initial state is too cumbersome. There are a lot of states with near-zero-modulus value. The different types of the initial states will exhibit distinct dynamical behaviors. In other words, the dynamics of the system is sensitive to the initial state. Therefore, the elaborate selection of the initial state is a crucial step to successfully mimic the dynamics of leg  $B$  in the Hermitian system. Fortunately, we can choose the initial state by considering the time-reversal process of the dynamics of leg  $B$ , which corresponds to the annihilation of two wave packets  $|L, k_b, B\rangle |R, k_a, B\rangle$ . This can be realized through adjusting the on-site interaction  $U_B$  and relative group velocity  $\nu_r$  based on the result obtained in leg  $A$ . In this sense, the final near-zero-modulus state can be selected as an initial state of the particle creation process. And the corresponding driven

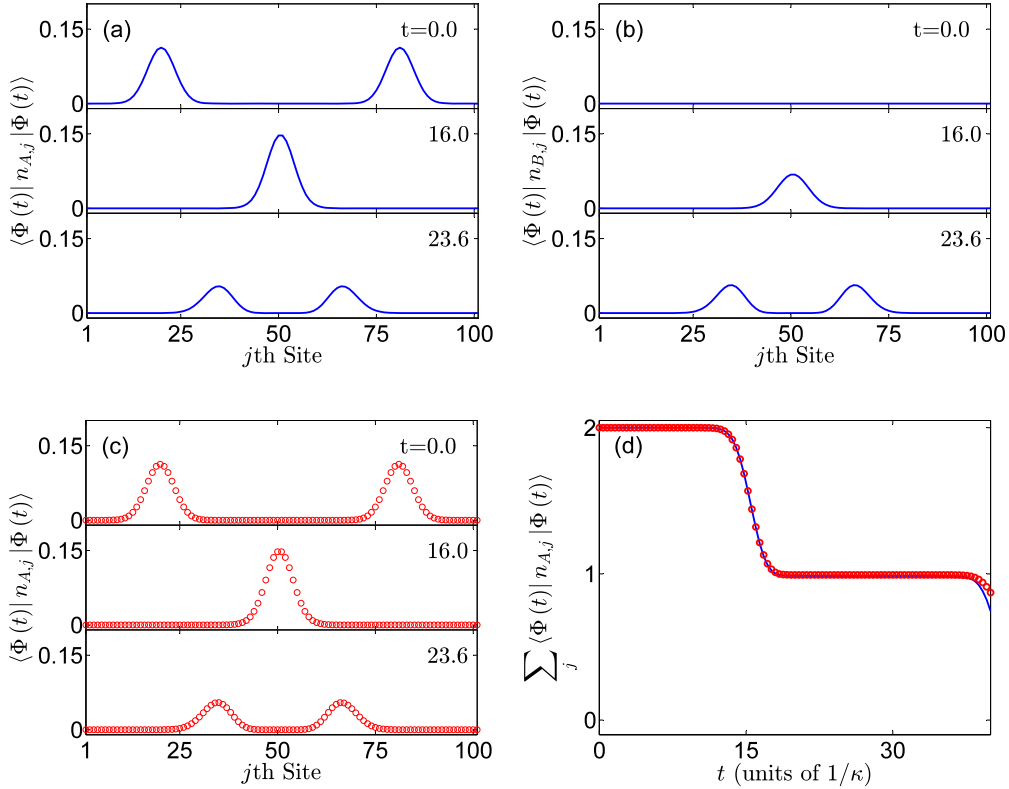


FIG. 4. Probability distribution of the evolved wave function for the initial state being two-particle incident Gaussian wave packets with  $k_a = \pi/2$ ,  $N_a = 20$ ,  $k_b = -\pi/2$ , and  $N_b = 80$  in leg  $A$  of different systems. Probability  $|\langle \Phi(t) | n_{\rho,j} | \Phi(t) \rangle|^2$  ( $\rho = A, B$ ) of the two-leg Hermitian system  $H$  for (a) leg  $A$  and (b) leg  $B$  with a tunneling strength  $J = 4(3 - 2\sqrt{2})$ , respectively. (c) Corresponding probability distribution on leg  $A$  of the non-Hermitian system  $\mathcal{H}$  with imaginary on-site interaction  $U_A = -4(3 - 2\sqrt{2})^2$ . (d) The red circle and blue line represent the total probability  $\sum_j |\langle \Phi(t) | n_{A,j} | \Phi(t) \rangle|^2$  of leg  $A$  as functions of time  $t$  for the Hermitian system  $H$  and the non-Hermitian system  $\mathcal{H}$ , respectively. We plot  $|\langle \Phi(t) | n_j | \Phi(t) \rangle|^2$  at different instants  $t$  in units of  $1/\kappa$ . One can see that when the matching condition  $U_A = -J^2/\nu_r$  is satisfied, the non-Hermitian Hamiltonian can be utilized to describe the dynamics of leg  $A$  of Hermitian Hamiltonian  $H$ , which is in accordance with the theoretical analysis in the text.

Hamiltonian can also be obtained by taking the time-reversal operation on the related non-Hermitian Hubbard Hamiltonian with pair annihilation.

In order to further validate the conclusion obtained above, we compare the local-state dynamics in two such systems by numerical simulation. To do this, we introduce the quantity  $|\langle \Phi(t) | n_j | \Phi(t) \rangle|^2$  to characterize the shape and probability distribution of the two wave packets in Fig. 4. For the Hermitian case as shown in Figs. 4(a) and 4(b), one can see that when the two wave packets enter into the interaction region, the probability of the two wave packets transfers from leg  $A$  to  $B$  due to the pair tunneling  $J$ . The process of the decrease of the two-wave-packet probability in leg  $A$  can also be approximately described through the two-wave-packet dynamics in an effective non-Hermitian Hubbard Hamiltonian  $\mathcal{H}$  with  $U_A = -J^2/\nu_r$ , as is shown in Fig. 4(c).

## VI. SUMMARY

In summary, we have studied the interchain pair tunneling dynamics based on the exact two-particle solution of a two-leg ladder. It is shown that the Hermitian Hamiltonian shares a common two-particle eigenstate with a corresponding non-Hermitian Hubbard model, in which the non-Hermiticity arises

from an imaginary on-site interaction. Such a common state is associated with the spectral singularity of the equivalent non-Hermitian system. The dynamical correspondence is dependent on the selection of the initial state. For the dynamics accompanied with the increase of the two-particle probability, such an initial state can be obtained through a time-reversal process of the annihilation of two wave packets. On the other hand, the reduction of the two-particle probability in the other leg of the Hermitian system can be well characterized by the effective non-Hermitian Hubbard model with the definite strength of pair dissipation, which is also determined by the relative and center momenta of the initial state. In addition, we have also found that the two particles display perfect transfer from one leg to the other when  $\nu_r = J$ , which corresponds to the pair annihilation in the effective non-Hermitian Hubbard system with the strength of the imaginary on-site interaction  $\nu_r = U_\rho$ . This result is valid for both Bose and Fermi systems and provides a clear physical implication of the non-Hermitian Hubbard model.

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### APPENDIX A: SOLUTION OF THE TWO-LEG LADDER

In this section, we derive the solution of the Hamiltonian shown in Eq. (1) in a two-particle invariant subspace. Here, we take the periodic boundary condition that  $a_{\rho,j} = a_{\rho,j+N}$ . Due to the symmetry in Eq. (1), which preserves the parity of particle number in each leg, the  $\mathcal{P}$  symmetry, and the translational symmetry, the basis spanning the subspace can be constructed as

$$|\varphi_0^\pm(K,r)\rangle = \frac{1}{2\sqrt{N}} \sum_j e^{iKj} (a_{A,j}^\dagger a_{A,j}^\dagger \pm a_{B,j}^\dagger a_{B,j}^\dagger) |\text{vac}\rangle, \quad (\text{A1})$$

$$|\varphi_r^\pm(K,r)\rangle = \frac{1}{\sqrt{2N}} e^{iKr/2} \sum_j e^{iKj} (a_{A,j}^\dagger a_{A,j+r}^\dagger \pm a_{B,j}^\dagger a_{B,j+r}^\dagger) |\text{vac}\rangle \quad (r > 1), \quad (\text{A2})$$

where  $K = 2n\pi/N$ ,  $n \in [-N/2, N/2]$ , is the momentum vector, and  $\pm$  denotes two degenerate subspaces originating from the  $\mathcal{P}$  symmetry. A two-particle eigenstate has the form of

$$|\psi_{K,k}^\pm\rangle = \sum_r F_{K,k}^\pm(r) |\varphi_r^\pm(K)\rangle, \quad (\text{A3})$$

with the condition  $F_{K,k}^\pm(-1) = 0$ , where the two degenerate wave functions  $F_{K,k}^\pm(r)$  satisfy the Schrödinger equations

$$Q_r^K F_{K,k}^\pm(r+1) + Q_{r-1}^K F_{K,k}^\pm(r-1) + [\pm J\delta_{r,0} + (-1)^n Q_r^K \delta_{r,N_0} - \varepsilon_K] F_{K,k}^\pm(r) = 0, \quad (\text{A4})$$

with the eigenenergy  $\varepsilon_K$  in the invariant subspace indexed by  $K$ . Here the factors are  $Q_r^K = -2\sqrt{2}\kappa \cos(K/2)$  for  $r = 0$  and  $-2\kappa \cos(K/2)$  for  $r \neq 0$ , respectively. It indicates that the eigenproblem of the two-particle matrix can be reduced to a single particle governed by the equivalent Hamiltonians

$$H_{\text{eq}}^{K,\pm} = \pm J|0\rangle\langle 0| + \sum_{i=1}^{\infty} (Q_i^K |i\rangle\langle i+1| + \text{H.c.}), \quad (\text{A5})$$

which clearly represents a semi-infinite chain with the ending on-site potential  $J$ . We are concerned with only the scattering solution by the zeroth end. The Bethe ansatz solutions have the form

$$F_{K,k}^\pm(r) = e^{-ikr} + R^\pm e^{ikr}. \quad (\text{A6})$$

Substituting  $F_{K,k}^\pm(r)$  into Eq. (A4), we have

$$\varepsilon_K(k) = -4\kappa \cos(K/2) \cos k, \quad k \in [0, \pi], \quad (\text{A7})$$

and

$$R_{K,k}^\pm = \frac{i\lambda_{K,k} \pm J}{i\lambda_{K,k} \mp J} = e^{\pm i\Delta_{K,k}}, \quad (\text{A8})$$

with

$$\lambda_{K,k} = 4\kappa \cos(K/2) \sin k, \quad (\text{A9})$$

$$\Delta_{K,k} = 2 \tan^{-1} \left( -\frac{J}{\lambda_{K,k}} \right). \quad (\text{A10})$$

For convenience in the application of wave-packet dynamics, we rewrite the solutions in the form

$$|\psi_{K,k}^\pm\rangle = \sum_{r,\rho} f_{K,k}^{\rho,\pm}(r) |\phi_r^\rho(K)\rangle, \quad (\text{A11})$$

where  $\rho = A, B$  and

$$|\phi_0^\rho(K)\rangle = \frac{1}{2\sqrt{N}} \sum_j e^{iKj} a_{\rho,j}^\dagger a_{\rho,j}^\dagger |\text{vac}\rangle, \quad (\text{A12})$$

$$|\phi_r^\rho(K)\rangle = \frac{1}{\sqrt{N}} e^{iKr/2} \sum_j e^{iKj} a_{\rho,j}^\dagger a_{\rho,j+r}^\dagger |\text{vac}\rangle \quad (r > 1). \quad (\text{A13})$$

The corresponding wave functions  $f_{K,k}^{\rho,\pm}(r)$  can be expressed as

$$f_{K,k}^{A,+}(r) = f_{K,k}^{B,-}(r) = \begin{cases} e^{-ikr} + \frac{\lambda_{K,k}^2 - J^2}{\lambda_{K,k}^2 + J^2} e^{ikr}, & r > 0 \\ (1 + \frac{\lambda_{K,k}^2 - J^2}{\lambda_{K,k}^2 + J^2}) / \sqrt{2}, & r = 0, \end{cases} \quad (\text{A14})$$

and

$$f_{K,k}^{B,+}(r) = f_{K,k}^{A,-}(r) = \begin{cases} -\frac{2i\lambda_{K,k}J}{\lambda_{K,k}^2 + J^2} e^{ikr}, & r > 0 \\ \frac{-\sqrt{2}i\lambda_{K,k}J}{(\lambda_{K,k}^2 + J^2)}, & r = 0. \end{cases} \quad (\text{A15})$$

### APPENDIX B: SOLUTION OF THE NON-HERMITIAN HUBBARD MODEL

Similarly, considering the Hamiltonian  $\mathcal{H}$ , we find that it admits all the symmetries we used for solving the eigenproblem of  $H$ . Then a two-particle state for  $\mathcal{H}_\rho$  is written as

$$|\kappa_K^\rho\rangle = \sum_r G_{K,k}^\rho(r) |\phi_r^\rho(K)\rangle \quad [G_{K,k}^\rho(-1) = 0], \quad (\text{B1})$$

where wave functions  $G_{K,k}^\rho(r)$  satisfy the Schrödinger equations

$$Q_r^K G_{K,k}^\rho(r+1) + Q_{r-1}^K G_{K,k}^\rho(r-1) + [iU_\rho \delta_{r,0} + (-1)^n Q_r^K \delta_{r,N_0} - \varepsilon_K] G_{K,k}^\rho(r) = 0, \quad (\text{B2})$$

with the eigenenergy  $\varepsilon_K$  in the invariant subspace indexed by  $K$ . We are concerned with only the scattering solution by the zeroth end. In this sense,  $G_{K,k}^\rho$  can be obtained from the two equivalent Hamiltonians in two subspaces:

$$\mathcal{H}_{\text{eq}}^{K,\rho} = iU_\rho |0\rangle\langle 0| + \sum_{i=0}^{\infty} (Q_i^K |i\rangle\langle i+1| + \text{H.c.}). \quad (\text{B3})$$



By the same procedures, we have

$$G_{K,k}^\rho(r) = \begin{cases} e^{-ikj} + \frac{\lambda_{K,k} + U_\rho}{\lambda_{K,k} - U_\rho} e^{ikj}, & r > 0 \\ \left(1 + \frac{\lambda_{K,k} + U_\rho}{\lambda_{K,k} - U_\rho}\right) / \sqrt{2}, & r = 0, \end{cases} \quad (\text{B4})$$

with eigenenergy  $\epsilon_K(k) = -4k \cos(K/2) \cos k$ ,  $k \in [0, \pi]$ . Furthermore, we can rewrite the solution in the form

$$g_{K,k}^\pm(r) = [G_{K,k}^A(r) \pm G_{K,k}^B(r)] / \sqrt{2}. \quad (\text{B5})$$

### APPENDIX C: SPECTRAL SINGULARITY OF THE HUBBARD CHAIN

We note that the wave function  $G_{K,k}^\rho(r)$  only depends on  $\rho$  via  $U_\rho$ . This is because the two chains  $A$  and  $B$  are independent. Then  $G_{K,k}^\rho(r)$  actually represents the two-particle solution of a non-Hermitian Hubbard Hamiltonian on a single chain  $\rho$  with on-site imaginary interaction strength  $iU_\rho$ . We find that  $G_{K,k}^\rho(r) \rightarrow \infty$  as  $U_\rho = \lambda_{K,k}$ , which indicates a spectral singularity at  $\{K, k\}$  [11,36].

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