PHYSICAL REVIEW A **80**, 052107 (2009)

Solutions of $\mathcal{PT}$-symmetric tight-binding chain and its equivalent Hermitian counterpart

L. Jin and Z. Song*

School of Physics, Nankai University, Tianjin 300071, China

(Received 13 April 2009; revised manuscript received 24 September 2009; published 11 November 2009)

We study the non-Hermitian quantum mechanics for the discrete system. This paper gives an exact analytic single-particle solution for an N-site tight-binding chain with two conjugated imaginary potentials $\pm i\gamma$ at two end sites, which Hamiltonian has parity-time symmetry ($\mathcal{PT}$ symmetry). Based on the Bethe ansatz results, it is found that, in single-particle subspace, this model is comprised of two phases: an unbroken symmetry phase with a purely real energy spectrum in the region $\gamma < \gamma_c$ and a spontaneously broken symmetry phase with $N-2$ real and two imaginary eigenvalues in the region $\gamma > \gamma_c$. The behaviors of eigenfunctions and eigenvalues in the vicinity of γ_c are investigated. It is shown that the boundary of two phases possesses the characteristics of exceptional point. We also construct the equivalent Hermitian Hamiltonian of the present model in the framework of metric-operator theory. We find out that the equivalent Hermitian Hamiltonian can be written as another bipartite lattice model with real long-range hoppings.

DOI: 10.1103/PhysRevA.80.052107 PACS number(s): 03.65.−w, 11.30.Er, 71.10.Fd

I. INTRODUCTION

Since the discovery that a non-Hermitian Hamiltonian having simultaneous parity-time ($\mathcal{PT}$) symmetry has an entirely real quantum-mechanical energy spectrum [1], there has been an intense effort to establish a $\mathcal{PT}$-symmetric quantum theory as a complex extension of the conventional quantum mechanics [2–7]. Although there have been no experiments to show clearly and definitively that quantum systems defined by non-Hermitian $\mathcal{PT}$-symmetric Hamiltonians do exist in nature, many models have been proposed to verify theorems and perform numerical and asymptotic analyses (for a recent review, see [8] and references therein). The reality of the spectra is responsible to the $\mathcal{PT}$ symmetry. If all the eigenstates of the Hamiltonian are also eigenstates of $\mathcal{PT}$, then all the eigenvalues are strictly real and the symmetry is said to be unbroken. Otherwise, the symmetry is said to be spontaneously broken. In practice, imaginary potential usually appears in a system to describe physical processes phenomenologically, which have been investigated under the non-Hermitian quantum mechanics framework [9–18]. However it is not clear whether non-Hermitian Hamiltonians describe real physics or are just unrealistic mathematical objects. It is known, for a diagonalizable Hamiltonian, that the presence of $\mathcal{PT}$ symmetry implies the pseudo-Hermiticity of the Hamiltonian [19], i.e., $\mathcal{PT}$ symmetry is a special case of pseudo-Hermiticity. A direct way of extracting the physical meaning of a pseudo-Hermitian Hamiltonian having a real spectrum is to seek for its Hermitian counterparts [16–18]. The metric-operator theory outlined in [2] provides a mapping of such a pseudo-Hermitian Hamiltonian to an equivalent Hermitian Hamiltonian. The construction of the latter is usually quite complicated if the Hilbert space of the systems is infinite dimensional. It is generally more tractable for lattice systems with a finite-dimensional single-particle Hilbert space. Under such circumstances, the study of simple models which are exactly solvable and slight modified version of a practical model, and yet are tractable, is of particular importance to examine the impact of an imaginary potential on the feature of eigenvalues and eigenfunctions of a lattice system.

In this paper, we will focus on the non-Hermitian $\mathcal{PT}$-symmetric quantum theory for a discrete system [20,21], the original form of which is exploited to describe the solid-state system in condensed-matter physics or coupled quantum devices since the advent of quantum information theory [22]. As an illustration, a simple N-site tight-binding chain with the uniform nearest-neighbor (NN) hopping integral is concerned. Such a model is used to describe the Bloch electronic system in condensed-matter physics and now the qubit array relevant to quantum information applications. The corresponding non-Hermitian $\mathcal{PT}$-symmetric version is constructed by adding two conjugated imaginary potentials $\pm i\gamma$ at the end sites. The objective of this paper aims at the exact solutions of such a model so as to confirm the non-Hermitian $\mathcal{PT}$-symmetric quantum theory for the discrete system. Based on the Bethe ansatz results, it is found that, in single-particle subspace, this model exhibits two phases: an unbroken symmetry phase with a purely real energy spectrum when the potentials are in the region $\gamma < \gamma_c$ and a spontaneously broken symmetry phase with $N-2$ real and two imaginary eigenvalues when the potentials are in the region $\gamma > \gamma_c$. Based on the exact solutions, the behaviors of eigenfunctions and eigenvalues in the vicinity of γ_c are investigated. It is shown that the boundary of two phases possesses the characteristics of exceptional point: there are two eigenstates coalescing at γ_c as well as with square-root-type level repulsion in the vicinity of it. We also construct the equivalent Hermitian Hamiltonian of the present model in the framework of metric-operator theory. We find out that the equivalent Hermitian Hamiltonian can be written as another bipartite lattice model with real long-range hoppings.

This paper is organized as follows. In Sec. II, the model is presented. In Sec. III, the Bethe ansatz solutions are given. In Sec. IV, we investigate the characteristics of the critical point γ_c. Section V is devoted to the construction of the equivalent Hermitian Hamiltonian. Section VI is the summary and discussion.

*songtc@nankai.edu.cn

II. $\mathcal{PT}$-SYMMETRIC UNIFORM TIGHT-BINDING CHAIN

We consider a simplest discrete system described by a non-Hermitian Hamiltonian H having the $\mathcal{PT}$ symmetry. It is a tight-binding chain with uniform nearest-neighbor hopping integral and two additional conjugated imaginary on-site potentials on the two end sites, which can be written as follows:

$$H = -J\sum_{l=1}^{N-1}(a_l^\dagger a_{l+1} + \text{H.c.}) + i\gamma a_1^\dagger a_1 - i\gamma a_N^\dagger a_N, \tag{1}$$

where $a_l^\dagger$ is the creation operator of the boson (or fermion) at lth site and the tunneling strength and potential are denoted by J and $\pm i\gamma$. $\mathcal{P}$ and $\mathcal{T}$ represent the space-reflection operator or parity operator and the time-reversal operator, respectively. The effects of $\mathcal{P}$ and $\mathcal{T}$ on a discrete system are

$$\mathcal{T}i\mathcal{T} = -i, \mathcal{P}a_l^\dagger\mathcal{P} = a_{N+1-l}^\dagger. \tag{2}$$

Obviously, the Hamiltonian Eq. (1) has $\mathcal{PT}$ symmetry, i.e., $H^{\mathcal{PT}}=\mathcal{PT}H\mathcal{PT}=H$. According to the $\mathcal{PT}$-symmetric quantum mechanics [7], H can be further classified to be either unbroken $\mathcal{PT}$ symmetry or broken $\mathcal{PT}$ symmetry, which depends on the symmetry of the eigenstates $|\psi_k\rangle$ in different regions of γ. The time-independent Schrödinger equation is

$$H|\psi_k\rangle = \varepsilon_k|\psi_k\rangle, \tag{3}$$

with corresponding eigenvalue ε_k. The system is unbroken $\mathcal{PT}$ symmetry if *all* the eigenfunctions have $\mathcal{PT}$ symmetry

$$\mathcal{PT}|\psi_k\rangle = |\psi_k\rangle \tag{4}$$

and all the corresponding eigenvalues are real simultaneously. This classification depends on the value of the parameter γ. Beyond the unbroken $\mathcal{PT}$ symmetric region, the system is broken $\mathcal{PT}$ symmetry, where Eq. (4) does not hold for *all* the eigenfunctions and the eigenvalues of broken $\mathcal{PT}$ symmetric eigenfunctions are imaginary. One of the aims of this paper is to provide the complete exact eigenfunctions, eigenvalues, and the boundary between unbroken and broken $\mathcal{PT}$ symmetric regions.

Acting the $\mathcal{PT}$ operation on an arbitrary single-particle wave function

$$|\varphi\rangle = \sum_l h_l a_l^\dagger|0\rangle, \tag{5}$$

where $|0\rangle$ denotes the vacuum state, we have

$$\mathcal{PT}|\varphi\rangle = \sum_l (h_l)^* a_{N+1-l}^\dagger|0\rangle = \sum_l (h_{N+1-l})^* a_l^\dagger|0\rangle. \tag{6}$$

Then, in the rest of this paper, we can simply use

$$\mathcal{PT}h_l = (h_{N+1-l})^* \tag{7}$$

to present the $\mathcal{PT}$ operation on the single-particle wave function.

III. BETHE ANSATZ SOLUTIONS

In this paper, we only focus on the single-particle case. We denote the single-particle eigenfunction in the form

$$|\psi_k\rangle = \sum_l f_k^l a_l^\dagger|0\rangle. \tag{8}$$

The Bethe ansatz wave function can be expressed in the form

$$f_k^l = A(k)e^{ikl} + B(k)e^{-ikl}, \tag{9}$$

where the quasimomentum k and amplitudes $A(k)$ and $B(k)$ can be determined from the Eq. (3) and the proper definition of the inner product according to the $\mathcal{PT}$-symmetric quantum theory [7]. The solutions are presented explicitly in the following.

A. Unbroken $\mathcal{PT}$-symmetric region

In the unbroken $\mathcal{PT}$ symmetric region $\gamma < \gamma_c$, where

$$\gamma_c = \begin{cases} J\sqrt{\dfrac{n+1}{n}}, & N = 2n+1 \\ J, & N = 2n, \end{cases} \tag{10}$$

the explicit $\mathcal{CPT}$ normalized wave functions are

$$f_k^l = \frac{e^{ik(l-N_0)} - \eta(k)e^{-ik(l+N_0)}}{|\sqrt{[1+|\eta(k)|^2]\sin(Nk)/\sin k - 2N\eta(k)e^{-ik(N+1)}}|}, \tag{11}$$

where $N_0=(N+1)/2$ is the center of the chain and the coefficient

$$\eta(k) = \frac{\gamma e^{ik} - iJ}{\gamma e^{-ik} - iJ}. \tag{12}$$

The quasimomentum k satisfies the equation

$$\gamma^2 \sin[k(N-1)] + J^2 \sin[k(N+1)] = 0, \tag{13}$$

which has N real solutions. All the corresponding eigenvalues are real

$$\varepsilon_k = -2J\cos k, \tag{14}$$

with the quasimomentum k being more explicit form

$$k = \frac{n_k\pi + \theta_k}{N}, \quad n_k \in [1,N] \tag{15}$$

and

$$\theta_k = \tan^{-1}\left[\frac{(\gamma^2 - J^2)}{(\gamma^2 + J^2)}\tan k\right]. \tag{16}$$

The reality of the spectrum is a consequence of $\mathcal{PT}$ invariance. At $\gamma=0$, we have $\eta(k)=1$ and the eigenfunctions reduce to the form

$$f_l^k(\gamma=0) = (-i)^{n_k} i\sqrt{\frac{2}{N+1}}\sin(kl),$$

$$k = \frac{\pi n_k}{N+1}, \quad n_k \in [1,N], \tag{17}$$

which is the well-known solution of a Hermitian tight-binding chain.

B. Broken $\mathcal{PT}$-symmetric region

In the region $\gamma > \gamma_c$, the $\mathcal{PT}$ symmetry of the Hamiltonian is spontaneously broken; even though $\mathcal{PT}$ commutes with H, the eigenfunctions of H are not *all* simultaneously eigenfunctions of $\mathcal{PT}$. In this region, it can be shown that there are $N-2$ real k for Eq. (13) which corresponds to the eigenfunctions Eq. (11) and real eigenvalues Eq. (14). The rest two eigenfunctions correspond to complex quasimomenta, which are in the form $k=\pi/2 \pm i|\kappa|$, with κ satisfying the equation

$$\gamma^2 \sinh[\kappa(N-1)] = J^2 \sinh[\kappa(N+1)], \quad (\text{odd } N),$$

$$\gamma^2 \cosh[\kappa(N-1)] = J^2 \cosh[\kappa(N+1)], \quad (\text{even } N). \tag{18}$$

The broken $\mathcal{PT}$-symmetric eigenfunctions can be written as

$$f^l_{\pi/2\pm i\kappa} \propto e^{\pm \kappa N_0}\left[(i)^l e^{\mp \kappa l} - (-i)^l \frac{J-\gamma e^{\mp\kappa}}{J+\gamma e^{\pm\kappa}} e^{\pm \kappa l}\right], \tag{19}$$

with the imaginary eigenvalues

$$\varepsilon_k = \pm i2J \sinh \kappa. \tag{20}$$

At this stage, the wave functions Eq. (19) are not normalized since the standard $\mathcal{CPT}$ normalization procedure is invalid for such broken $\mathcal{PT}$-symmetric wave functions.

C. $\mathcal{CPT}$ formalism

In this section, we will elucidate the $\mathcal{CPT}$ formalism based on the solutions of the present model. It can be seen that the solutions have different features compared to that of a Hermitian Hamiltonian. The most intuitive novelties of the eigenfunctions Eq. (11) with real eigenvalues are not standing waves due to $|\eta(k)|$ being not unitary for nonzero γ. According to the $\mathcal{PT}$-symmetric quantum theory [7], the correct inner product is determined by the Hamiltonian itself, so it is necessary for the discrete system Eq. (1) to establish a self-consistent formalism based on the obtained exact solutions.

A straightforward calculation shows that the eigenfunctions Eq. (11) obey the $\mathcal{PT}$ symmetry

$$\mathcal{PT} f^l_k = f^l_k. \tag{21}$$

According to the $\mathcal{PT}$-symmetry quantum theory [7], one can define the coordinate-space representations of the parity operator $\mathcal{P}$ and $\mathcal{C}$ operator for a discrete system as

$$\mathcal{P}(m,l) = \delta_{m,N+1-l}, \tag{22}$$

$$\mathcal{C}(m,l) = \sum_k f^m_k f^l_k, \tag{23}$$

which lead to the $\mathcal{CPT}$ orthogonal and normalization relations

$$\sum_{l,m} f^l_k \mathcal{C}(l,m)\mathcal{P}(m,l)(f^l_{k'})^* = \delta_{kk'}. \tag{24}$$

This guarantees the positive-definite $\mathcal{CPT}$ inner product of two arbitrary states and that the time evolution is unitary. One can verify that the operator $\mathcal{C}$ satisfies

$$\mathcal{C}^2 = 1, \quad [\mathcal{C},\mathcal{PT}] = 0, \quad [\mathcal{C},H] = 0. \tag{25}$$

In the next section, the above formalism will be utilized to establish the canonical basis to construct the equivalent Hermitian Hamiltonian in the unbroken $\mathcal{PT}$-symmetric region. We will see that choosing $\mathcal{CPT}$ normalized eigenstates of H leads the Hermitian equivalence matrix to be more symmetrical.

IV. EXCEPTIONAL POINTS

In this section, we investigate the critical behavior of the system as γ in the vicinity of γ_c. From the obtained solutions of the model, the critical point γ_c has the characteristics of exceptional point [23–26]. We will investigate the feature of eigenvalues and eigenfunctions around the exceptional point in detail.

In unbroken $\mathcal{PT}$-symmetric region, as γ approaches to γ_c, the solutions of Eq. (13) change abruptly. Actually, as the function

$$\mathcal{F}(k) = \gamma^2 \sin[k(N-1)] - J^2 \sin[k(N+1)] \tag{26}$$

is an even (odd) function about $k=\pi/2$ for even (odd) N, two real energy levels, which are closest to zero, disappear when γ passes through the boundary γ_c of the two regions. Meanwhile, two imaginary energy levels appear. Thus, the critical behavior of the eigenstates can be characterized by the two components problem. For $\gamma=\gamma_c-0^+$, we denote the referring eigenfunctions as $f^l_{\pi/2+\delta}$ and $f^l_{\pi/2-\delta}$, with

$$\delta \simeq \begin{cases} \dfrac{1}{\sqrt{-N\alpha}}, & N \text{ is even} \\ \sqrt{\dfrac{3(\alpha-N)}{N^3-\alpha}}, & N \text{ is odd}, \end{cases} \tag{27}$$

$$\alpha = \frac{J^2+\gamma^2}{\gamma^2-J^2}. \tag{28}$$

It follows that such two eigenfunctions approach to a same function and their $\mathcal{PT}$ norms tend to zero when $\mathcal{PT}$ symmetry is broken.

In the broken $\mathcal{PT}$-symmetric region, for $\gamma=\gamma_c+0^+$, such two eigenfunctions are replaced by Eq. (19), while the corresponding eigenvalues turn to imaginary values Eq. (20). Other $N-2$ eigenfunctions in the form of Eq. (11) with real eigenvalues still satisfy the $\mathcal{CPT}$ orthogonal and normalized relations Eq. (24). However, the two eigenfunctions Eq. (19) can no longer be normalized via the above $\mathcal{CPT}$ inner product since they have the following features:

$$\mathcal{PT}[f^l_{\pi/2+i\kappa}] \propto f^l_{\pi/2-i\kappa} \tag{29}$$

and

$$f^l_{\pi/2\pm i\kappa}\mathcal{PT}[f^l_{\pi/2\pm i\kappa}] = 0. \tag{30}$$

On the other hand, the corresponding energy levels experience a switch from real to complex values as well as a coalescence at the exceptional point. In the unbroken symmetric side, from Eq. (27), we have

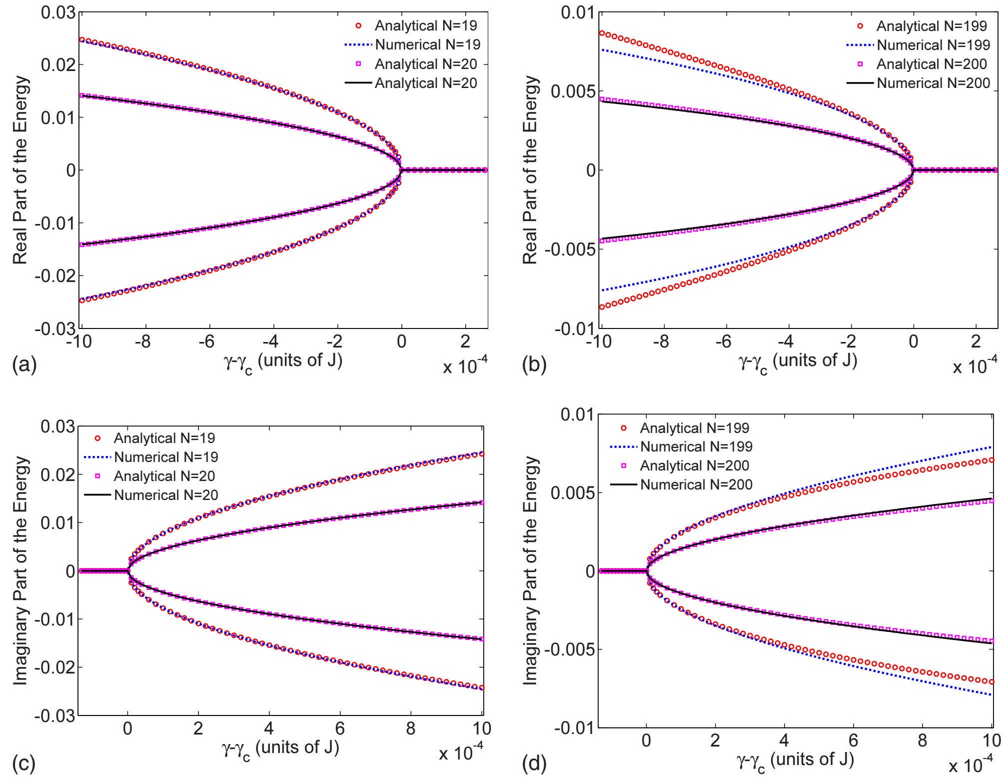

FIG. 1. (Color online) Real and imaginary parts of two repelling levels as functions of $\gamma-\gamma_c$. The plots are obtained from the approximate analytical results Eqs. (31) and (33) and numerical simulations for the systems with $N=19$, 20, 199, and 200. It shows that the analytical eigenvalue expressions are good approximation to the numerically exact results, especially for small N system.

$$\varepsilon_{\pi/2\pm\delta} \simeq \pm 2J \sin \delta \simeq \pm 2J\delta. \tag{31}$$

In the broken symmetric side, from Eq. (18), we have

$$\kappa \simeq \begin{cases} \dfrac{1}{\sqrt{N\alpha}}, & N \text{ is even} \\ \sqrt{\dfrac{3(N-\alpha)}{N^3-\alpha}}, & N \text{ is odd}, \end{cases} \tag{32}$$

which correspond to the eigenvalues

$$\varepsilon_{\pi/2\pm i\kappa} \simeq \pm 2iJ \sinh \kappa \simeq \pm 2iJ\kappa. \tag{33}$$

Alternatively, taking $|\gamma-\gamma_c|$ as the variable, we can see that the two concerned eigenstates satisfy

$$\varepsilon_{\pi/2\pm\delta} \simeq \mathrm{Im}(\varepsilon_{\pi/2\pm i\kappa}) \simeq \begin{cases} \pm 2J\sqrt{\dfrac{|\gamma-\gamma_c|}{N\gamma_c}}, & N \text{ is even} \\ \pm 2J\sqrt{\dfrac{3|\gamma-\gamma_c|}{N\gamma_c}}, & N \text{ is odd} \end{cases} \tag{34}$$

near the critical point, which reveals the symmetry of the critical behavior. In Fig. 1, we plot the real and imaginary parts of two repelling levels as functions of $\gamma-\gamma_c$, which are obtained from the approximate analytical results Eqs. (31) and (33) and numerical simulations for finite systems. The analytical eigenvalue expressions (31) and (33) are good approximations to the numerically exact results. It shows that the exceptional points are always associated with a level repulsion in the vicinity of them. The square-root-type functions for the energy reveal these characteristics. Previous study [24,25] shows that the exceptional point is often related to the emergence of chaotic behavior. However, the quantum chaos is not found in the present model. This may be due to that the coalescence and repulsion of levels in this model only relate to two eigenstates rather than multilevel. Thus, there is no occurrence of quantum chaos.

V. EQUIVALENT HERMITIAN HAMILTONIAN

A natural question to ask is whether such a model Eq. (1) describes real physics or is just an unrealistic mathematical product. While there is as yet no answer to this question, we can gain some insight regarding its equivalent Hermitian counterpart [3,4]. This section aims at seeking the equivalent Hermitian Hamiltonian of the present model in the framework of metric-operator theory [2].

We start with the eigenstates of the Hamiltonian $H^\dagger = H^* = H(-\gamma)$. From Eq. (11), the explicit $\mathcal{CPT}$ normalized wave functions of $H^\dagger$ within the unbroken $\mathcal{PT}$-symmetric region are

$$g_k^l = \frac{e^{ik(l-N_0)} - \zeta(k)e^{-ik(l+N_0)}}{|\sqrt{[1+|\zeta(k)|^2]\sin(Nk)/\sin k - 2N\zeta(k)e^{-ik(N+1)}}|}, \tag{35}$$

where the coefficient is

$$\zeta(k) = \frac{\gamma e^{ik} + iJ}{\gamma e^{-ik} + iJ} \tag{36}$$

and the corresponding eigenvalues are Eq. (14), the same as that of f_k^l. Within the unbroken $\mathcal{PT}$-symmetric region, we have

$$\mathcal{PT}|g_k\rangle = |g_k\rangle \tag{37}$$

and two sets of eigenfunctions $\{g_k^l\}$ and $\{f_k^l\}$ form a biorthonormal system, i.e.,

$$\sum_l (g_k^l)^* f_{k'}^l = \delta_{kk'}. \tag{38}$$

According to the metric-operator theory [2], one can construct a positive-definite operator

$$\eta_+ = \sum_k |g_k\rangle\langle g_k|. \tag{39}$$

From the Appendix, it can be shown that this operator satisfies

$$(\eta_+)^\dagger = \eta_+, \tag{40}$$

$$(\eta_+)^{-1} = (\eta_+)^*, \tag{41}$$

$$\mathcal{PT}\eta_+\mathcal{PT} = \eta_+. \tag{42}$$

In the spatial coordinate space spanned by basis $|m\rangle = a_m^\dagger|0\rangle$, the matrix representation of η_+ has the form

$$\langle m|\eta_+|n\rangle = \sum_k (g_k^m)^* g_k^n. \tag{43}$$

More explicitly, it can be shown that the matrix has the following properties:

$$\langle m|\eta_+|n\rangle = \langle N+1-n|\eta_+|N+1-m\rangle \tag{44}$$

and

$$\langle m|\eta_+|n\rangle = (-1)^{m+n}\langle m|\eta_+|n\rangle^*. \tag{45}$$

In addition, defining the canonical transformation R,

$$R|l\rangle = (-1)^l|l\rangle, \tag{46}$$

we have

$$R\eta_+R^{-1} = (\eta_+)^* = (\eta_+)^{-1}. \tag{47}$$

These features allow characterizing the equivalent physical system of H. In the eigenspace of η_+, we can rewrite η_+ as

$$\eta_+ = \sum_n \epsilon_n|\epsilon_n\rangle\langle\epsilon_n|, \tag{48}$$

where $|\epsilon_n\rangle$ is the eigenvector of operator η_+ with the eigenvalue ϵ_n, i.e.,

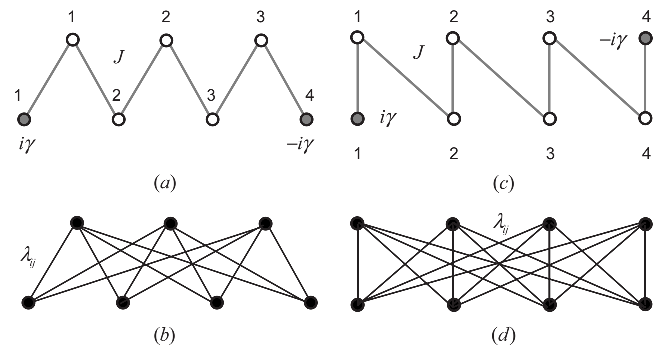

FIG. 2. Schematic illustration of configurations for [(a) and (c)] pseudo-Hermitian system H on seven- and eight-site lattices and [(b) and (d)] their Hermitian counterparts h. Both the original system and its Hermitian counterpart are all bipartite graphs.

$$\eta_+|\epsilon_n\rangle = \epsilon_n|\epsilon_n\rangle. \tag{49}$$

The eigenvalues ϵ_n are all real due to the Hermiticity of η_+ and the complete set $\{|\epsilon_n\rangle\}$ is referred as a canonical metric basis.

Accordingly, the equivalent Hermitian Hamiltonian $\mathcal{H}$ can be obtained by a unitary transformation and can be expressed as

$$\mathcal{H} = \sum_{m,n}\sqrt{\frac{\epsilon_m}{\epsilon_n}}H_{mn}|\epsilon_m\rangle\langle\epsilon_n|, \tag{50}$$

where $H_{mn} = \langle\epsilon_m|H|\epsilon_n\rangle$ is the matrix representation of Hamiltonian H under this canonical metric basis $\{|\epsilon_n\rangle\}$. The Hermitian equivalence matrix $\mathcal{H}$ can be achieved as

$$\mathcal{H}_{mn} = \sqrt{\frac{\epsilon_m}{\epsilon_n}}\sum_{i,j}\langle i|H|j\rangle(\epsilon_m^i)^*\epsilon_n^j, \tag{51}$$

where $\epsilon_m^i = \langle i|\epsilon_m\rangle$ is the component of state $|\epsilon_m\rangle$ in the spatial coordinate basis $|i\rangle$.

Before we explore the features of the equivalent Hermitian Hamiltonian $\mathcal{H}$, it is worthy to point that the ordinal tight-binding chain (1) is a bipartite lattice which can be separated into A and B sublattices with sites N_A and N_B, respectively. We have $N = N_A + N_B$ with $|N_A - N_B| = 1$ (0) for odd (even) N and the two sublattices are connected by hopping terms with strength J [see Figs. 2(a) and 2(c)]. Now we turn to the properties of $\mathcal{H}$. It can be shown, from the Appendix of this paper [27], that under a proper choice of the transformation of $\{|\epsilon_n\rangle\}$, the matrix representation of $\mathcal{H}$ can be in the form of

$$\mathcal{H} = \begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix}, \tag{52}$$

where A^T is the transposed matrix of a $N_A \times N_B$ matrix A and A satisfies

TABLE I. The coupling-constant distributions λ_{ij} for systems with (a) $N=7$ and (b) 8 obtained from numerical simulation for $\gamma=0.00$, 0.50, and 0.99.

γ	$\lambda_{11},\lambda_{34}$	$\lambda_{12},\lambda_{33}$	$\lambda_{13},\lambda_{32}$	$\lambda_{14},\lambda_{31}$	$\lambda_{21},\lambda_{24}$	$\lambda_{22},\lambda_{23}$
0.00	0.6242	1.0068	−0.2997	0.0830	0.2071	−1.2071
0.50	0.5703	0.9731	−0.3089	0.0883	0.2039	−1.2075
0.99	0.3355	0.8949	−0.3280	0.0774	0.1468	−1.2089

γ	$\lambda_{11},\lambda_{44}$	$\lambda_{12},\lambda_{34}$	$\lambda_{13},\lambda_{24}$	λ_{14}	$\lambda_{21},\lambda_{43}$	$\lambda_{22},\lambda_{33}$	λ_{23}	$\lambda_{31},\lambda_{42}$	λ_{32}	λ_{41}
0.00	0.5627	−0.9300	−0.2994	−0.1199	0.1954	1.1615	−1.2411	0.0914	0.3333	0.0277
0.50	0.5153	−0.8918	−0.3057	−0.1304	0.1909	1.1527	−1.2469	0.0972	0.3461	0.0310
0.99	0.1766	−0.9005	−0.3157	−0.1458	0.1005	1.0333	−1.3522	0.0627	0.3505	0.0143

$$A_{ij} = \begin{cases} A_{N_A+1-j,N_B+1-i}, & N \text{ is even} \\ A_{N_A+1-i,N_B+1-j}, & N \text{ is odd.} \end{cases} \quad (53)$$

Then real symmetric matrix $\mathcal{H}$ can be regarded as a single-particle matrix representation of a tight-binding model on a bipartite lattice $N=N_A+N_B$, with $|N_A-N_B|=1$ (0) for odd (even) N. Two sublattices are connected by the long-range hopping terms with strength λ_{ij}. The corresponding tight-binding Hamiltonian can be expressed as

$$\mathcal{H} = \sum_{i=1}^{N_A}\sum_{j=1}^{N_B} \lambda_{ij}(|i\rangle_{AB}\langle j| + \text{H.c.}), \quad (54)$$

where $|l\rangle_A$ and $|l\rangle_B$ denote single-particle states referring to lth site in sublattices N_A and N_B, respectively. Note that both the original model H and its Hermitian counterpart $\mathcal{H}$ are all bipartite. The former contains NN couplings, while the latter contains the long-range couplings. This fact agrees with the observations from other example Hamiltonians that in general, the Hermitian counterpart of a pseudo-Hermitian Hamiltonian obtained by the metric-operator theory is nonlocal operator [2].

In order to exemplify the above analysis, we consider the small systems with $N=7$ and 8. Figure 2 shows the schematics of configurations for (a,c) pseudo-Hermitian system H on seven- and eight-site lattices and (b,d) their Hermitian counterparts $\mathcal{H}$. The corresponding hopping constants λ_{ij} are computed for $\gamma=0.00$, 0.50, and 0.99, which are listed in Table I. It indicates that all the constants vary within a narrow range without changing signs as γ covers the whole unbroken symmetric region and obey the relation of Eq. (53).

VI. CONCLUSION AND DISCUSSION

In conclusion, we have studied the non-Hermitian quantum mechanics for the discrete system. The exact analytic single-particle solution for a tight-binding chain with two end imaginary potentials is obtained, which substantiates the formalism of the $\mathcal{PT}$ quantum theory for discrete system. Based on the Bethe ansatz results, it is found that, in single-particle subspace, this model exhibits two phases: an unbroken symmetry phase with a purely real energy spectrum in the region and a spontaneously broken symmetry phase with a pair of imaginary eigenvalues in the region.

In addition, we have indicated that the boundary of two phases possesses the characteristics of exceptional point. We also construct the equivalent Hermitian Hamiltonian of the present model in the framework of metric-operator theory. We find out that the equivalent Hermitian Hamiltonian can be written as another bipartite lattice model with real long-range hoppings.

It is worthwhile to note that the non-Hermitian Hamiltonian (1) cannot simply be written as the form $\Sigma_k \epsilon_k a_k^\dagger a_k$, where $a_k^\dagger = \Sigma_l f_k^l a_l^\dagger$ is creation operator in k space, since the transition matrix is no longer unitary. However, the equivalent Hermitian Hamiltonian $\mathcal{H}$ can be in such form. It might be interesting to explore the multiparticle sector of the system using the equivalent Hermitian Hamiltonian.

ACKNOWLEDGMENT

We acknowledge the support of the CNSF (Grants No. 10874091 and No. 2006CB921205).

APPENDIX: PROPERTIES OF MATRICES η_+ AND $\mathcal{H}$

According to the definition of the metric operator (39) and the properties of eigenfunctions, Eqs. (37) and (38), we have

$$(\eta_+)^* \eta_+ = \left(\sum_k |g_k\rangle\langle g_k|\right)^* \sum_{k'} |g_{k'}\rangle\langle g_{k'}| = \sum_k |f_k\rangle\langle f_k| \sum_{k'} |g_{k'}\rangle\langle g_{k'}| = 1 \quad (A1)$$

and

$$\mathcal{PT}\eta_+\mathcal{PT} = \mathcal{PT}\sum_k |g_k\rangle\langle g_k|\mathcal{PT} = \sum_k |g_k\rangle\langle g_k| = \eta_+. \quad (A2)$$

On the other hand, Eq. (45) allows the real matrix representation of the metric operator by the transformation on the spatial coordinate basis

$$|l\rangle \to (\sqrt{-1})^{\text{mod}[l,2]}|l\rangle. \quad (A3)$$

For the sake of simplicity, hereafter η_+ denotes a real matrix. Then from Eqs. (41) and (42) indicate

$$\eta_+^T = \eta_+, \quad (A4)$$

$$(\eta_+)^{-1} = R\eta_+ R^{-1}, \tag{A5}$$

$$\mathcal{P}\eta_+\mathcal{P} = \eta_+, \tag{A6}$$

i.e., η_+ is a real unitary and bisymmetric matrix. Then the eigenfunctions $|\epsilon_n\rangle$ of η_+ can always be written as real functions and obey

$$\mathcal{P}|\epsilon_n\rangle = \pm|\epsilon_n\rangle. \tag{A7}$$

These properties are helpful for characterizing the equivalent physical system of H.

Now we focus on the case of even N. A straightforward calculation shows that eigenfunctions $|\epsilon_n\rangle$ and $\mathcal{P}|\epsilon_n\rangle$ have different parities. Then we can reorder the canonical metric basis as

$$|\epsilon_n\rangle = R|\epsilon_{N+1-n}\rangle, \quad n \in [1,N/2], \tag{A8}$$

which satisfy

$$\mathcal{P}|\epsilon_n\rangle = |\epsilon_n\rangle, \quad n \in [1,N/2],$$

$$\mathcal{P}|\epsilon_n\rangle = -|\epsilon_n\rangle, \ n \in [N/2+1,N/2]. \tag{A9}$$

Under such canonical metric basis, we have

$$\begin{aligned}\mathcal{H}_{mn} &= \sqrt{\frac{\epsilon_m}{\epsilon_n}}H_{mn} \\ &= \sqrt{\frac{\epsilon_m}{\epsilon_n}}\langle\epsilon_m|\mathcal{PT}H\mathcal{PT}|\epsilon_n\rangle \\ &= \sqrt{\frac{\epsilon_m}{\epsilon_n}}(-1)^{\vartheta(m)+\vartheta(n)}H_{mn}^* \\ &= (-1)^{\vartheta(m)+\vartheta(n)}\mathcal{H}_{mn}^*,\end{aligned} \tag{A10}$$

where

$$\vartheta(m) = \begin{cases} 0, & m \le N/2 \\ 1, & m > N/2 \end{cases} \tag{A11}$$

is the Heaviside step function. On the other hand, since under the new definition of basis $|l\rangle$ H_{mn} is always imaginary, all the elements $\mathcal{H}_{mn}$ with $\vartheta(m)+\vartheta(n)=0$ or 2 must vanish. Because $|\epsilon_n\rangle$ can always be written as real, one can simply take $|\epsilon_n\rangle \to (\sqrt{-1})^{\vartheta(n)}|\epsilon_n\rangle$ to obtain the final form of the equivalent Hermitian Hamiltonian

$$\mathcal{H} = \begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix}, \tag{A12}$$

where A is real matrix and A^T is its transposed matrix.

[1] C. M. Bender and S. Boettcher, Phys. Rev. Lett. **80**, 5243 (1998).
[2] A. Mostafazadeh and A. Batal, J. Phys. A **37**, 11645 (2004).
[3] A. Mostafazadeh, J. Phys. A **36**, 7081 (2003).
[4] H. F. Jones, J. Phys. A **38**, 1741 (2005).
[5] C. M. Bender, S. Boettcher, and P. N. Meisinger, J. Math. Phys. **40**, 2201 (1999).
[6] P. Dorey, C. Dunning, and R. Tateo, J. Phys. A **34**, L391 (2001); **34**, 5679 (2001).
[7] C. M. Bender, D. C. Brody, and H. F. Jones, Phys. Rev. Lett. **89**, 270401 (2002).
[8] C. M. Bender, Rep. Prog. Phys. **70**, 947 (2007).
[9] S. Klaiman and L. S. Cederbaum, Phys. Rev. A **78**, 062113 (2008).
[10] M. Znojil, Phys. Rev. D **78**, 025026 (2008).
[11] K. G. Makris, R. El-Ganainy, D. N. Christodoulides, and Z. H. Musslimani, Phys. Rev. Lett. **100**, 103904 (2008).
[12] Z. H. Musslimani, K. G. Makris, R. El-Ganainy, and D. N. Christodoulides, Phys. Rev. Lett. **100**, 030402 (2008).
[13] C. M. Bender and P. D. Mannheim, Phys. Rev. Lett. **100**, 110402 (2008).
[14] U. D. Jentschura, A. Surzhykov, and J. Zinn-Justin, Phys. Rev. Lett. **102**, 011601 (2009).
[15] J. T. Shen and S. Fan, Phys. Rev. A **79**, 023837 (2009).
[16] A. Mostafazadeh, J. Phys. A **38**, 6557 (2005).
[17] A. Mostafazadeh, J. Phys. A **39**, 10171 (2006).
[18] A. Mostafazadeh, J. Phys. A **39**, 13495 (2006).
[19] A. Mostafazadeh, J. Math. Phys. **43**, 3944 (2002).
[20] C. Korff and R. Weston, J. Phys. A: Math. Theor. **40**, 8845 (2007).
[21] E. M. Graefe, U. Günther, H. J. Korsch, and A. E. Niederle, J. Phys. A: Math. Theor. **41**, 255206 (2008).
[22] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998).
[23] W. D. Heiss and A. L. Sannino, J. Phys. A **23**, 1167 (1990).
[24] W. D. Heiss, Phys. Rep. **242**, 443 (1994).
[25] W. D. Heiss, J. Phys. A **37**, 2455 (2004).
[26] F. Leyvraz and W. D. Heiss, Phys. Rev. Lett. **95**, 050402 (2005).
[27] In this paper, we only give an exact proof for the even-N system in the Appendix. Numerical results imply that the conclusion also holds for odd-N case.