Geometric phase and phase diagram for non-Hermitian quantum XY model

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We study the geometric phase for the ground state of a generalized one-dimensional non-Hermitian quantum XY model, which has transverse-field-dependent intrinsic rotation-time reversal symmetry. Based on the exact solution, this model is shown to have full real spectrum in multiple regions for the finite size system. The result indicates that the phase diagram or exceptional boundary, which separates the unbroken and broken symmetry regions corresponds to the divergence of the Berry curvature. The scaling behaviors of the groundstate energy and Berry curvature are obtained in an analytical manner for a concrete system.

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I. INTRODUCTION

Since the existence of an entirely real quantum mechanical energy spectrum of a non-Hermitian Hamiltonian was proposed in the seminal work of Bender and Boettcher [1], much effort has been devoted to establish a complex extension of the conventional quantum mechanics [1–8]. It has been shown [9] that if a Hamiltonian has a symmetry given by an anti-linear operator $K$, then either the eigenvalues of the Hamiltonian are real or they come in complex conjugate pairs. The eigenvector with real eigenvalue has the symmetry of $K$, while the one with complex eigenvalue breaks the symmetry. As system parameter varying, such a sudden change in the eigenstate can be referred as quantum phase transition in complex quantum mechanics, while the critical point is called exceptional point. The characteristic of the critical behavior is the level repulsion, which leads to the divergence of the first derivative of the eigenvalue with respect to the system parameter. Although we borrow the concept of QPT from the conventional Hermitian system, they differ from each other in many aspects. For instance, the exceptional point can occur in finite non-Hermitian system, while the QPT is the phenomenon for a Hermitian system in the thermodynamic limit. This allows the observation of the critical phenomenon in experiment, since it has been demonstrated that the small size discrete non-Hermitian system could be realized in optics [10–14].

In this paper, we are interested at the critical behavior of the eigenfunction in the vicinity of the boundary. In the realm of traditional quantum mechanics, geometric phase has been introduced to analyze the quantum phase transitions of the XY model [15–17], and much effort has been devoted to various Hermitian many-body systems [18–26]. We study the geometric phase for the ground state of a generalized one-dimensional non-Hermitian quantum XY model, which has transverse-field-dependent intrinsic rotation-time reversal symmetry. Based on the exact solution, this model is shown to have full real spectrum in multiple regions for finite size system. The result indicates that the phase diagram or exceptional boundary, which separates the unbroken and broken symmetry regions corresponds to the divergence of the Berry curvature.

This paper is organized as follows. In Section II we present the model Hamiltonian and the solutions. In Section III we investigate the phase diagram and analyze the symmetry of the ground state base on the properties of the solutions. In Section IV we give the connection between the phase transition and Berry curvature. Finally, we give a summary and discussion in Section V.

II. MODEL AND SOLUTION

Firstly, we consider a generalized non-Hermitian one-dimensional spin-1/2 XY model in a transverse magnetic field $\lambda$ on $N$-site lattice. The Hamiltonian has the form

$$
\mathcal{H} = J \sum_{j=1}^{N} \left[ \mathcal{G} \sigma_j^x \sigma_{j+1}^x - G^* \sigma_j^z \sigma_{j+1}^z \right] + \left( \sigma_j^x \sigma_{j+1}^z + H.c. \right) + 4\lambda \sigma_j^z,
$$

(1)

where $\mathcal{G} = \mathcal{G}(\xi)$ and $\Lambda(\xi)$ are arbitrary functions of an $n$-dimensional parameter vector $\xi = \{\xi_i\} \in [1, n]$, one component of which is the field strength $\lambda$, i.e. $\xi_1 = \lambda$. Here $\sigma_j^\alpha (\alpha = \pm, z)$ are the Pauli operators on site $j$, and satisfy the periodic boundary condition $\sigma_j^\alpha \equiv \sigma_{j+N}^\alpha$. For the sake of simplicity, we only concern the case of even $N$. We note that the non-Hermiticity of the Hamiltonian arises from the coupling constants in terms of $\sigma_j^+ \sigma_{j+1}^-$ and $\sigma_j^- \sigma_{j+1}^+$. In the case of $|\Lambda| \neq 1$, it represents double spin-flip of unequal-amplitude. In the case of $\mathcal{G} = i\gamma$ (real $\gamma$) and $|\Lambda| = 1$, the Hamiltonian (1) reduces to

$$
\mathcal{H}_0 = J \sum_{j=1}^{N} \left( \frac{1 + i\gamma}{2} \sigma_j^x \sigma_{j+1}^x + \frac{1 - i\gamma}{2} \sigma_j^y \sigma_{j+1}^y + \lambda \sigma_j^z \right),
$$

(2)
which has been investigated in the previous work [27]. Here we take the absolute value of the Λ in order to ensure the non-Hermiticity of the Hamiltonian. Once we replace |Λ| by −1 in the Hamiltonian (1), it switches to a Hermitian operator. Likewise, in this work we define a spin rotation operator

$$\mathcal{R} = \exp \left[ -i \phi \sum_{j=1}^{N} \sigma_j^z / 2 \right],$$

which has the function of rotating each spin by angle φ/2 about the z-axis. It turns out that, by taking \( \phi = \arg (\mathcal{G}) \), we have \([\mathcal{R}, \mathcal{H}] \neq 0\) and \([\mathcal{T}, \mathcal{H}] \neq 0\), but

\[ [\mathcal{R} \mathcal{T}, \mathcal{H}] = 0, \]

where the antilinear time reversal operator \( \mathcal{T} \) has the function \( \mathcal{T} \mathcal{T} = -i \), i.e., the Hamiltonian \( \mathcal{H} \) is rotation-time reversal invariant. In contrast to the Hamiltonian \( \mathcal{H}_0 \), the rotation is transverse-field-dependent (\( \lambda \)-dependent) through the function \( \mathcal{G} \), i.e., \( \phi = \phi (\{\xi_i\}) \). It is crucial for the aim of this paper, revealing the connection between the phase diagram and the Berry curvature for a non-Hermitian system, that \( \phi \) and \( \Lambda \) are \( \{\xi_i\} \)-dependent functions. Otherwise, the Berry curvature vanishes, by no means providing any information of the QPT.

Now we consider the solution of the non-Hermitian Hamiltonian of Eq. (1). We start by taking the Jordan-Wigner transformation

$$\sigma_j^+ = -2 \prod_{l<j} \left( 1 - 2c_l^+ c_l \right) c_j,$$

$$\sigma_j^- = -2 \prod_{l<j} \left( 1 - 2c_l^+ c_l \right) c_j^\dagger,$$

$$\sigma_j^z = 1 - 2c_j^+ c_j,$$

to replace the Pauli operators by the fermionic operators \( c_j \). Likewise, the parity of the number of fermions

$$\Pi = \prod_{l=1}^{N} (\sigma_l^z) = (-1)^{N_\eta}$$

is a conservative quantity, i.e., \([\mathcal{H}, \Pi] = 0\), where \( N_\eta = \sum_{j=1}^{N} c_j^\dagger c_j \). Then the Hamiltonian (1) can be rewritten as

$$\mathcal{H} = \sum_{\eta=\pm} P_\eta \mathcal{H}_\eta P_\eta,$$

where

$$P_\eta = \frac{1}{2} (1 + \eta \Pi)$$

is the projector on the subspaces with even \( (\eta = +) \) and odd \( (\eta = -) \) \( N_\eta \). The Hamiltonian in each invariant subspaces has the form

$$\mathcal{H}_\eta = J \sum_{j=1}^{N-1} \left[ c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j - |\Lambda| \mathcal{G}^* c_j^\dagger c_{j+1} + \mathcal{G} c_{j+1} c_j \right]$$

$$-\eta \left[ c_N^\dagger c_1 + c_1^\dagger c_N - |\Lambda| \mathcal{G}^* c_N^\dagger c_1 + \mathcal{G} c_1 c_N \right]$$

$$-2J\lambda \sum_{j=1}^{N} c_j^\dagger c_j + NJ\lambda.$$

Taking the Fourier transformation

$$c_j = \frac{1}{\sqrt{N}} \sum_{k=\pm} e^{ik \pm j} c_k,$$

for the Hamiltonians \( \mathcal{H}_\pm \), we have

$$\mathcal{H}_\eta = -J \sum_{k= \pm} \left[ 2 (\lambda - \cos k_\eta) c_{k_\eta}^\dagger c_{k_\eta} + \left( k_\eta \right)^{1/2} \sin k_\eta \left( e^{i\beta} e^{-k_\eta} c_{k_\eta} + e^{-i\beta} e^{k_\eta} c_{k_\eta}^\dagger \right) - \lambda \right],$$

where the momenta \( k_\pm = 2 (m + 1 / 2) \pi / N, \ k_\pm = 2m\pi / N, \ m = 0, 1, 2, ..., N - 1 \), and

$$\beta = -\frac{1}{2} \ln |\Lambda| + i \left( \phi - \frac{\pi}{2} \right).$$

Employing the Bogoliubov transformation

$$A_{k_\eta} = e^{\beta / 2} \cos \left( \frac{\theta}{2} \right) c_{k_\eta} - ie^{-\beta / 2} \sin \left( \frac{\theta}{2} \right) c_{-k_\eta}^\dagger,$$

$$\overline{A}_{k_\eta} = e^{-\beta / 2} \cos \left( \frac{\theta}{2} \right) c_{k_\eta}^\dagger + ie^{\beta / 2} \sin \left( \frac{\theta}{2} \right) c_{-k_\eta},$$

FIG. 1. (Color online) Schematic of the phase diagram for the Hamiltonian (1) under the condition of Eq. (20), which boundary surface is a hyperboloid of two sheets in 3-dimensional space \( \{\omega, \gamma, \lambda\} \). The red circle denotes the force line of the field \( \Omega \).
where
\[ \tan \theta = \frac{i |G| |\Lambda|^{1/2} \sin k_{n} \sin k_{y}}{(\lambda - \cos k_{y})} , \]

one can recast Hamiltonian \( \mathcal{H}_{n} \) to the diagonal form
\[ \mathcal{H}_{n} = \sum_{k_{n}} \varepsilon_{k_{n}} \left( \mathcal{A}_{k_{n}} \mathcal{A}_{k_{n}}^{\dagger} - \frac{1}{2} \right) , \]

with spectrum being
\[ \varepsilon_{k_{n}} = 2J \sqrt{(\lambda - \cos k_{n})^{2} - \left( |G| \sqrt{|\Lambda|} \sin k_{y} \right)^{2}} . \]

It can be seen that the diagonal form of Hamiltonian \( \mathcal{H}_{n} \) in Eq. (10) is still non-Hermitian due to the fact that \( \mathcal{A}_{k_{n}} \neq \mathcal{A}_{k_{n}}^{\dagger} \). Note that, instead of \( (\mathcal{A}_{k_{n}}, \mathcal{A}_{k_{n}}^{\dagger}) \), we take the Bogoliubov modes \( (A_{k_{n}}, \mathcal{A}_{k_{n}}) \), which satisfy the canonical commutation relations
\[ \{A_{k_{n}}, \mathcal{A}_{k_{n}}^{\dagger}\} = \delta_{k_{n}, k_{n}^{\prime}} , \]
\[ \{A_{k_{n}}, A_{k_{n}^{\prime}}\} = \{\mathcal{A}_{k_{n}}, \mathcal{A}_{k_{n}^{\prime}}\} = 0 . \]

The eigenstates of \( \mathcal{H}_{n} \) and \( \mathcal{H}_{n}^{\dagger} \) can be constructed by mode \( (A_{k_{n}}, \mathcal{A}_{k_{n}}) \), and the complete biorthogonal bases are established.

In the following analysis, we will focus on the ground state of the Hamiltonian. It turns out that the ground state lies in the subspace with \( \eta = + \) in the thermodynamic limit. In addition, the reality of the ground state lies in the subspace with \( \eta = 0 \) and \( \eta = \pi \).

Here it represents the region in which the non-Hermitian Hamiltonian has full real spectrum or not, rather than the quantum phase transition \( 29 \) in the ground state of a Hermitian system. From Eq. (17), it turns out that the Hamiltonian \( \mathcal{H} \) lie in the broken symmetry region when at last one single-particle level becomes the square root of a negative number, an imaginary number.

Precisely, it is clear that when any one of the momentum \( k_{y} \) satisfies
\[ |\lambda - \cos k_{y}| < |G| \sin k_{y} |\Lambda|^{1/2} , \]

the imaginary energy level appears in single-particle spectrum. For finite \( N \) system, there are totally \( 2(N - 1) \) equations in the form of \( |\lambda - \cos k_{n}| = \sqrt{|\Lambda|} |G| \sin k_{y} \) for all possible value of \( k_{y} \) with \( k_{y} \neq 0, \pi \).

Note that the broken region does not include the surface \( \mathcal{G} = 0 \), which is determined by the following set of parametric equations \( 30 \)
\[ \frac{\partial \varepsilon (\xi, k_{n})}{\partial k_{n}} = \varepsilon (\xi, k_{n}) = 0 . \]

Straightforward algebra gives the analytical expression
\[ \lambda_{c}^{2} - \left[ |G| \sqrt{|\Lambda|} (\xi_{c}) \right]^{2} = 1 , \]

which is the common boundary for both \( H_{+} \) and \( H_{-} \). Note that the broken region does not include the surface \( |G| \sqrt{|\Lambda|} (\xi_{c}) = 0 \). In order to illustrate this point, we consider an examples with 3-dimensional parameter vectors \( \{\omega, \gamma, \lambda\} \), and taking
\[ \mathcal{G} \sqrt{|\Lambda|} = \sqrt{\omega^{2} + \gamma^{2} e^{i\lambda}} . \]

The boundary of this examples reads
\[ \lambda^{2} - \omega^{2} - \gamma^{2} = 1 , \]

which is a hyperboloid of two sheets in 3-dimensional space \( \{\omega, \gamma, \lambda\} \) as shown in Fig. 1.

According to the non-Hermitian quantum theory, the occurrence of the exceptional point always accomplishes the \( RT \) symmetry breaking of an eigenstate. Taking the combination of the Jordan-Wigner and Fourier transformations on the rotational operator in Eq. (3), we have
\[ \mathcal{R} = \prod_{k_{+}} \left[ 1 + e^{i\phi} n_{k_{+}} - n_{k_{+}} \right] , \]
where \( n_{k_+} = c_{k_+}^\dagger c_{k_+} \) is the particle number in \( k_+ \) space. Applying the \( \mathcal{RT} \) operator on the fermion operators and its vacuum state \( |\text{Vac}\rangle \), we have
\[
\mathcal{RT} c_{k_+}^\dagger (\mathcal{RT})^{-1} = e^{i\phi} c_{-k_+}^\dagger,
\]
and
\[
\mathcal{RT} |\text{Vac}\rangle = |\text{Vac}\rangle,
\]
which are available in the both regions. However, the coefficients \( \cos (\theta/2) \) and \( \sin (\theta/2) \) experience a transition as following when the corresponding single-particle level changes from real to imaginary: We have \( \{\cos (\theta/2)\}^* = \cos (\theta/2) \) and \( \{\sin (\theta/2)\}^* = -\sin (\theta/2) \) for real levels and \( \{\cos (\theta/2)\}^2 = \sin (\theta/2) \) for the imaginary levels, respectively. This leads to the conclusion that the ground state is not \( \mathcal{RT} \) symmetric in the broken region, i.e., \( \mathcal{RT} |G\rangle \neq |G\rangle \). It shows that the symmetry of the ground state can be an indicator of the phase transition as observed in the quantum phase transition of the Hermitian system. In the following section, we will investigate the connection between the geometric phase and the phase diagram in this non-Hermitian spin model, which has been well established for its Hermitian version [15–17].

IV. GEOMETRIC PHASE

The Berry curvature for the ground state is an anti-symmetric second-rank tensor derived from the Berry connection via
\[
\Omega_{ij} = \frac{\partial}{\partial \xi_i} A_j - \frac{\partial}{\partial \xi_j} A_i,
\]
where
\[
A_j = i \langle G | \frac{\partial}{\partial \xi_j} | G \rangle_b
\]
is known as the Berry connection, an \( n \)-dimensional parameter vector \( A = \{A_i\} \) in the parameter space. Here \( \langle \cdots | \cdots \rangle_b \) represents the biorthogonal inner product. Within the unbroken region, we have
\[
A_i = -\frac{i}{2} \frac{\partial}{\partial \xi_i} \sum_{0 < k_+ < \pi} \frac{(1 - \cos \theta)}{2}.
\]
The Berry curvature can be written as
\[
\Omega_{ij} = \frac{i}{2} \sum_{0 < k_+ < \pi} \left( \frac{\partial \beta}{\partial \xi_j} \frac{\partial \cos \theta}{\partial \xi_i} - \frac{\partial \beta}{\partial \xi_i} \frac{\partial \cos \theta}{\partial \xi_j} \right).
\]
Turning back to the 3-dimensional example system defined in Eq. (26), a straightforward algebra shows that
\[
\mathbf{A} = \mathbf{A}_\lambda \hat{k}
\]
where
\[
\mathbf{A}_\lambda = \sum_{0 < k_+ < \pi} \left[ \frac{1}{2} - \frac{J (\lambda - \cos k_+)}{\epsilon_{k_+}^3} \right].
\]
According to the symmetry of the phase diagram, it is convenient to express the Berry curvature in cylindrical coordinate system as the form of \( \Omega = \Omega_\rho \hat{\rho} + \Omega_\varphi \hat{\varphi} + \Omega_\lambda \hat{k} \). Here \( \hat{\rho}, \hat{\varphi} \) and \( \hat{k} \) denote the unit vectors in cylindrical coordinate system and \( \lambda \) is the axis of symmetry, \( \rho = \sqrt{\omega^2 + \gamma^2} \) is the distance from \( \lambda \) axis. The components are explicitly obtained as
\[
\Omega_\varphi = 4J^2 \rho \sum_{0 < k_+ < \pi} \frac{(\lambda - \cos k_+) \sin^2 k_+}{\epsilon_{k_+}^3},
\]
\[
\Omega_\lambda = \Omega_\rho = 0,
\]
which shows that \( \Omega_\varphi \) is the sum of a series of \( \epsilon_{k_+}^{-3} \). It leads to the following features of the curvature: i) The reality of \( \Omega_\varphi \), depending on the single-particle spectrum of
\( \epsilon_{k_+} \) is the same as that of the groundstate energy \( E_g \). ii) \( \Omega_\varphi \) is divergent at every boundary point, the surface of \( \lambda^2 - \rho^2 = 1 \). iii) Within the exact symmetric region, the direction of the field \( \overrightarrow{\Omega} \) is tangent to a circle on a radius \( \rho \) from \( \lambda \) axis. In Fig. 2 the contours of the field magnitude \( \sqrt{\lambda^2 - \rho^2} \) obtained from Eq. (37) are plotted schematically. These features indicate the connection between the geometric phase and the phase boundary in a pseudo-Hermitian system.

To further understand the relation between geometric phase and quantum criticality, one can investigate the scaling behavior of the geometric phases by direct analytical calculation. We start with the investigation of the scaling behavior of the groundstate energy and Berry curvature \( \Omega_\varphi \). For the special case in Eq. (20), we have

\[
\Omega_\varphi = -4J^2 \sum_{0<k_+<\pi} \frac{\lambda - \cos k_+}{\epsilon_{k_+}},
\]

\[
\frac{\partial E_g}{\partial \rho} = 4J^2 \sum_{0<k_+<\pi} \frac{\rho \sin^2 k_+}{\epsilon_{k_+}}.
\]

In order to investigate the groundstate energy and Berry curvature quantitatively and relate their behavior to the criticality, we consider the two types of approaching paths, parameters tending to the critical point along the two lines: I) \( |\lambda| \to |\lambda_c| = \sqrt{\rho^2 + 1} \) for fixed \( \rho \), and II) \( |\rho| \to |\rho_c| = \sqrt{\lambda^2 - 1} \) for fixed \( \lambda \), respectively. In the thermodynamic limit, we have

\[
\frac{\partial E_g}{\partial \lambda} \to -\frac{\sqrt{2}J (\lambda^2 - 1)^{1/2}}{\lambda_c^{1/2}} (\lambda - \lambda_c)^{-1/2} \quad (I),
\]

\[
\frac{\partial E_g}{\partial \rho} \to \frac{\sqrt{2}J \rho_c^{3/2}}{(\rho_c^2 + 1)^{1/2}} (\rho - \rho_c)^{-1/2} \quad (II),
\]

in the vicinity of the boundary surface.

Now we turn to the investigation of the scaling behavior for the geometric quantity, the groundstate Berry curvature \( \Omega_\varphi \). For the special case in Eq. (20), we have

\[
\Omega_\varphi = -4J^2 \sum_{0<k_+<\pi} \frac{(\lambda - \cos k_+) \sin^2 k_+}{\epsilon_{k_+}^3}.
\]

Similarly, in the vicinity of the boundary surface we have

\[
\Omega_\varphi \to \frac{\sqrt{2} (\lambda_c^2 - 1)}{8 \lambda_c^{3/2}} (\lambda - \lambda_c)^{-3/2} \quad (I),
\]

\[
\Omega_\varphi \to \frac{2 \rho_c^{1/2}}{8} (\rho - \rho_c)^{-3/2} \quad (II).
\]

It indicates that two different approach paths share the same scaling exponent. Before ending this paper, we want to stress that there is an interesting relation between the two quantities \( \Omega_\varphi \) and \( E_g \), emerging in Eq. (43). It reveals the physical meaning of the geometrical quantity \( \Omega_\varphi \) in this concrete example. Further work should be done in considering such a relation in the generic system. Similar work has been done in Hermitian systems, relating the geometric phase to the energy gap [31].

V. SUMMARY

In summary, we have studied the connection between the geometric phase and the phase diagram for the pseudo-Hermitian system. We focused on the ground state of a generalized one-dimensional non-Hermitian quantum XY model, which has transverse-field-dependent intrinsic rotation-time reversal symmetry. Based on the exact solution, this model is shown to have full real spectrum in multiple regions for finite size system. The result indicates that the phase diagram, which separates the unbroken and broken symmetry regions corresponds to the divergence of the Berry curvature. The scaling behavior of the groundstate energy and Berry curvature are also revealed by the analytical analysis for a concrete system. The result for such a non-Hermitian quantum spin model may have profound theoretical and methodological implications.

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