Quantum phase transition in a quantum Ising chain at nonzero temperatures

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We study the response of a thermal state of an Ising chain to a nonlocal non-Hermitian perturbation, which coalesces the topological Kramer-like degeneracy in the ferromagnetic phase. The dynamic responses for initial thermal states in different quantum phases are distinct. The final state always approaches its half component with a fixed parity in the ferromagnetic phase but remains almost unchanged in the paramagnetic phase. This indicates that the phase diagram at zero temperature is completely preserved at finite temperatures. Numerical simulations for Loschmidt echoes demonstrate such dynamical behaviors in finite-size systems. In addition, it provides a clear manifestation of the bulk-boundary correspondence at nonzero temperatures. This work presents an alternative approach to understanding the quantum phase transitions of quantum spin systems at nonzero temperatures.

Introduction.—A conventional quantum phase transition (QPT) [1] describes an abrupt change in matter at zero temperature. At nonzero temperatures, the existence of quantum critical behavior depends on the competition between thermal and quantum fluctuations. At higher temperatures, thermal fluctuations conceal the quantum criticality, thus leaving no residuals of quantum phase diagram at absolute zero temperature. On the other hand, variations in a parameter across the critical point induce a symmetry spontaneous breaking of the ground state. The underlying mechanism is the degeneracy of the ground states. These features have been demonstrated in a one-dimensional (1-D) quantum Ising model with a transverse field, which is exactly solvable, so as to be a unique paradigm for understanding conventional QPTs. In the recent works [2, 3], it turns out that the local order parameter and topological index can coexist to characterize the QPT.

In this Letter, we revisit the Ising model to investigate the existence of QPT at nonzero temperatures—a seldom discussed topic. It is motivated from the duality of the Kitaev model, which describes 1-D spinless fermions with superconducting $p$-wave pairing [4]. The Kitaev model is the fermionized version of the familiar 1-D transverse-field Ising model [5], an easily solvable model exhibiting quantum criticality and QPT with spontaneous symmetry breaking [1]. Also, as the gene of a Kitaev model, the Majorana lattice is the Su-Schrieffer-Heeger (SSH) model [6], which has served as a paradigmatic example of a 1-D system supporting topological characteristic [7]. It manifests the key features of topological order because the number of zero-energy levels and edge states are immune to local perturbations [8].

A typical method for detecting QPT is to monitor the response of the ground state under a perturbation through the implementation of Loschmidt echo (LE) and fidelity [9–15]. Most perturbations applied to the Ising model are Hermitian terms, the simplest example of which is the shift of the transverse field. Nevertheless, since the discovery that a class of non-Hermitian Hamiltonians could exhibit entirely real spectra [16–19], the non-Hermitian Hamiltonian is no longer a forbidden regime in quantum mechanics. A certain type of non-Hermitian term may have exclusive effects never before observed in a Hermitian system [20–23]. More importantly, natural quantum systems such as cold atom systems are intrinsically non-Hermitian because of spontaneous decay [24–29]. In this work, we study the response of a thermal state of an Ising chain to a non-Hermitian perturbation, which coalesces the topological Kramer-like degeneracy in the ferromagnetic phase. We use LEs to measure the response and observe that they are distinct for initial thermal states in different quantum phases. The exceptional point (EP) drives a thermal state approaching to its half component in the ferromagnetic phase but remain unchanged in the paramagnetic phase. Numerical simulations for LE demonstrate such dynamical behaviors in finite-size systems. In addition, it presents a clear manifestation of the bulk-boundary correspondence at nonzero temperature. The underlying mechanism is that within the ferromagnetic phase, the robust degeneracy occurs not only in the ground states, but in all energy levels, allowing the identification of the nature of quantum phases from a thermal state. It indicates that the phase diagram at zero temperature is completely preserved at finite temperatures. This property promises the stable ground states, and enables theoretical and experimental investigations of QPT through dynamical control and testing. We present an alternative approach for understanding the QPT of quantum spin systems at nonzero temperatures.

Model and degenerate spectrum.—The model considered is the transverse field Ising chain with open boundary condition, defined by the Hamiltonian

$$H = -J \sum_{j=1}^{N-1} \sigma_j^x \sigma_{j+1}^x + g \sum_{j=1}^{N} \sigma_j^z,$$

(1)

where $\sigma_j^\alpha$ ($\alpha = x, y, z$) are the Pauli operators on site $j$ and parameter $g$ ($g \geq 0$) is the transverse field strength. For simplicity, the following discussion assumes that $J = 1$. We first review some well-known model properties that...
are crucial to our conclusion. The parity \( p = \prod_{j=1}^{N} (-\sigma_j^z) \) is determined to be conservative; that is, \([p, \hat{H}] = 0\) is always true.

The model with periodic boundary condition is exactly soluble and has been well studied [5]. At zero temperature, QPT at \( g = 1 \) separates a ferromagnetic phase of the system (\( g < 1 \)) from a paramagnetic phase (\( g > 1 \)). In general, model properties are not sensitive to the boundary condition in thermodynamic limit. However, herein we consider the model with open boundary condition, which notably possesses an exclusive symmetry in the ferromagnetic phase \( g < 1 \), and it is also the key point of this work. It can be check that in thermodynamic limit, we have a nonlocal operator [30]

\[
D = \frac{1}{2} \sqrt{1 - g^2} \sum_{j=1}^{N} g^{j-1} D_j,
\]

with a position-dependent component

\[
D_j = \prod_{l<j} (-\sigma_l^z) \sigma_j^x - i \prod_{l<N-j+1} (-\sigma_l^z) \sigma_{N-j+1}^y,
\]

satisfying the commutation relations

\[
[D, H] = [D^\dagger, H] = 0,
\]

that can be regarded as a symmetry of the system. In addition, the relations \( [D, D^\dagger] = 1 \) and \( D^2 = (D^\dagger)^2 = 0 \) [30] suggest that \( D \) is a fermion operator. Importantly, such a symmetry is a little special, because it is contingent on the following conditions: \( g < 1 \), a large \( N \) limit, and open boundary. Particularly, operator \( D \) is non-universal and Hamiltonian-dependent because it contains the parameter \( g \) from the Hamiltonian. The first two conditions accord with the symmetry breaking mechanism of QPT [1]. Actually, the commutation relations in Eq. (4) guarantee the existence of eigenstates degeneracy. Specifically, there is a set of degenerate eigenstates \( \{ |\psi^+_n \rangle, |\psi^-_n \rangle \} \) of \( H \) with eigenenergy \( E_n \), in two invariant subspaces, i.e., \( H |\psi^+_n \rangle = E_n |\psi^+_n \rangle \) and \( p |\psi^+_n \rangle = \pm |\psi^-_n \rangle \). Fig. 1 presents the spectrum of the low-lying states, which possess distinct degenerate structures in two phases. Furthermore, we have the relations

\[
D |\psi^+_n \rangle = |\psi^-_n \rangle, D^\dagger |\psi^-_n \rangle = |\psi^+_n \rangle, D^\dagger |\psi^+_n \rangle = D |\psi^-_n \rangle = 0,
\]

in the ferromagnetic phase. We refer to this property as topological Kramers-like degeneracy for two reasons: (i) the two-fold degeneracy lies in the full spectrum, and (ii) it is invariant in the presence of random, position-dependent deviation on the field \( g \), where a new operator \( D \) is redefined accordingly [30]. Because of this property, operator \( D \) plays an important role in the quench dynamics, as demonstrated in the following section.

*Non-Hermitian perturbation and EP dynamics.*—In general, a Hermitian perturbation can lift the degeneracy. However, a non-Hermitian perturbation may take a surprising effect. A fascinating phenomenon is the coalescence of two degenerate states, which supports exclusive dynamics never occurs in a Hermitian system. Such degeneracy-related dynamics differentiates the quantum phases at any temperature, not only in the ground states. To this end, we introduce operator \( D \) into the post-quench Hamiltonian \( \mathcal{H} \) by treating it as a perturbation

\[
\mathcal{H} = H + \kappa D,
\]

with \( \kappa \ll g \). For a system in the ferromagnetic phase, where \( 0 < g < 1 \), any pair of degenerate eigenstates \( (|\psi^+_n \rangle, |\psi^-_n \rangle) \) with energy \( E_n \) spans a diagonal block with the sub-Hamiltonian

\[
\mathcal{H}_n = \left( \begin{array}{cc} E_n & 0 \\ \kappa & -E_n \end{array} \right),
\]

which has a Jordan block structure. This means that in the ferromagnetic phase, the degenerate spectrum becomes an exceptional spectrum with a set of coalescing states \( \{ |\psi^+_n \rangle \} = \{ |\psi^-_n \rangle \} \) when the non-Hermitian term \( \kappa D \) is introduced. The diagonal Jordan block is exact for any values of \( \kappa \). By contrast, for a system in the paramagnetic phase, \( \kappa D \) does not considerably affect the energy levels of \( H \) when \( g \) is much larger than 1 (\( H \approx g \sum_{j=1}^{N} \sigma_j^z \) in this case); this is because the gap between energy levels with different parities is at least in the order of \( g \) (see Fig. 1).

On the basis of this analysis, the dynamics in the ferromagnetic phase is governed by the time evolution op-
where the time evolution operator in the \( n \)-th subspace has the form \( U_n(t) = \exp(-i\mathcal{H}_n t) = \exp(-i\mathcal{E}_n t) [1 - i(\mathcal{H}_n - \mathcal{E}_n) t] \) based on the identity \((\mathcal{H}_n - \mathcal{E}_n)^2 = 0\) for \( g < 1 \). The dynamics of a pure initial state are then clarified, as given in \( U_n(t)(a|\psi_n^+\rangle + b|\psi_n^−\rangle) = \exp(-i\mathcal{E}_n t) [(a - ib\kappa)|\psi_n^+\rangle + b|\psi_n^−\rangle] \). The action of \( U_n(t) \) over a long period projects any pure initial state on the component \(|\psi_n^−\rangle\), which is completely different from that in the paramagnetic phase. These features allow us to observe significantly different dynamical behaviors for an initial thermal state.

**QPT at nonzero temperatures.**—We have observed that the difference between spectra in two regions not only lies in the ground states but also the full spectrum. This results in the exclusive EP dynamics for the initial state involving any excited eigenstates in the ferromagnetic phase, from which two phases at finite temperatures can be identified. Notably, bulk-boundary correspondence can manifest at nonzero temperatures. In the following, we focus on the dynamics of a initial thermal state with density matrix \( \rho(0) = e^{-\beta \mathcal{H}} / \text{Tr} e^{-\beta \mathcal{H}} \) at temperature \( \beta \) for a system (pre-quench Hamiltonian) \( \mathcal{H} \) under a quenched non-Hermitian Hamiltonian \( \mathcal{H}' = H + \kappa \mathcal{H}' \) where \( \mathcal{H}' \) is non-Hermitian, and \( \kappa \) is real.

As mentioned, operator \( D \) is \( g \)-dependent, and a matching \( D \) in the perturbation leads to an exact EP. Nevertheless, operator \( D_j \) (or \( D_j^\dagger \)) still takes the role to switch the parity of an eigenstate and forms a Jordan block approximately for a sufficiently small \( \kappa \). We consider two cases of \( \mathcal{H}' \) where it is (i) a dominant term of operator \( D \) (i.e., \( \mathcal{H}' = D_j \)) and (ii) position dependent (i.e., \( \mathcal{H}' = D_j^\dagger \)). After the quench, the time evolution of the thermal state obeys the equation

\[
i\frac{\partial}{\partial t} \rho(t) = \mathcal{H} \rho(t) - \rho(t) \mathcal{H}^\dagger,
\]

which admits the formal solution

\[
\rho(t) = e^{-i\mathcal{H} t} \rho(0) e^{i\mathcal{H}^\dagger t}.
\]

Unlike the Hermitian case, the time evolution of the density matrix is no longer unitary. Thus, in the following numerical calculation, we normalize \( \rho(t) \) by taking [31, 32]

\[
\rho(t) = e^{-i\mathcal{H} t} \rho(0) e^{i\mathcal{H}^\dagger t} / \text{Tr} \left[ e^{-i\mathcal{H} t} \rho(0) e^{i\mathcal{H}^\dagger t} \right].
\]

To characterize the degree of distinguishability between the initial state \( \rho(0) \) and evolved state \( \rho(t) \), we introduce the LE

\[
L(t) = \left[ \text{Tr} \sqrt{\rho(0) \rho(t) \sqrt{\rho(0)}} \right]^2.
\]

also known as the Uhlmann fidelity [33, 34]. The value of \( L(t) \) after a sufficient period can be estimated intuitively. In general, an initial mixed state \( \rho(0) \) contains equal-amplitude components of two parities. In the ferromagnetic phase, the component with a certain parity of the thermal state \( \rho(t) \) is dominant because of EP dynamics, and in large \( t \) limits, the LE \( L(t) \) approaches 0.5 . In the paramagnetic phase, a non-Hermitian perturbation does not substantially affect the dynamics; this is expressed by \( L(t) \approx L(0) = 1 \). We now numerically demonstrate the decay behavior of \( L(t) \) within a short period.

First, we consider the quench dynamics under the post-quench Hamiltonian \( \mathcal{H} = H + \kappa D_j \). We conduct numerical simulations for \( L(t) \) for the initial state \( \rho(0) \) at different phases in the finite system. The computations are performed using a uniform mesh in the time discretization for the Hamiltonian \( \mathcal{H} \). As mentioned, the spectral degeneracy is dependent on a large \( N \) limit. However, exact zero-mode solutions for an SSH chain demonstrate that even a sufficiently small \( g \) leads to perfect quasi-degeneracy in finite-size systems. Consistent with our prediction, the numerical results of LEs in Fig. 2 are insensitive to temperature and tend towards different values in different phases.

To determine the effect of \( g \), we introduce an average LE in the time interval \([\tau, \tau + T]\), defined as follows:

\[
\bar{L} = \frac{1}{T} \int_{\tau}^{\tau+T} L(t) \, dt,
\]

where \( \tau \gg 1 \). Average LEs as functions of parameter \( g \) for different \( N \) values are plotted in Fig. 3. When \( N \) is larger, the average LE is closer to the ideal values.
that expected in the thermodynamic limit. This indicates that the LEs can be used to identify the quantum phase diagram at nonzero temperatures even in small size systems.

Second, we investigate the bulk-boundary correspondence at nonzero temperatures through quench dynamics. Consider the post-quench Hamiltonian with the form

$$\mathcal{H} = H + \kappa D_j,$$

where $D_j$, defined in Eq. (3), is the component of operator $D$. In this case, the LE is denoted by $L_j(t)$. The long-term behavior of $L_j(t)$ when $j > 1$ is expected to be similar to $L(t)$ of the post-quench Hamiltonian in the first case. We are interested in the dependence of $L_j(t)$ in different phases on position over a short period. The numerical simulation results are plotted in Fig. 4. We can see that, (i) in the case of $g < 1$, $L_j(t)$ tends towards 0.5 for the $j$ near the end and decays more rapidly as $j$ approaches the boundary. By contrast, in the case of $g > 1$, $L_j(t)$ remains at 1.0 for all $j$. And (ii) in the case of $g = 0.1$, the LEs in the middle do not decay but remain near 1.0, which implies the LE behavior in long chains. This is a clear manifestation of the bulk-boundary correspondence at nonzero temperatures.

![FIG. 3. Average LEs as functions of $g$ when $N = 8, 9, \text{and } 10$. The dashed line represents the ideal average LEs expected for large $N$ limits. Here we set $\tau = 500$ and $T = 500$. Other parameters: $\kappa = 0.1$, $J = 1$, and $\beta = 1$. It indicates that as $N$ increases, the plots have the trends to the prediction in thermodynamic limit.](image)

![FIG. 4. Simulation results for LEs under the post-quench Hamiltonian (14) for different $j$ values. (a) and (c) LEs in the ferromagnetic phase when $g = 0.1$ and 0.5. (b) and (d) LEs in the paramagnetic phase when $g = 1.1$ and 1.5. Other parameters: $N = 8$, $J = 1$, $\kappa = 0.1$, and $\beta = 1$. The LE decays rapidly to 0.5 at the end of the chain in the ferromagnetic phase, whereas it remains at one in the paramagnetic phase. In the case (a), where $g$ is small, the LEs in the middle do not decay but remain near 1.0, which implies the LE behavior in long chains. This is a clear manifestation of the bulk-boundary correspondence at nonzero temperatures.](image)
natural state always has a fixed parity in the ferromagnetic phase, while it has half component with each party in the paramagnetic phase. This leads to a sudden drop in the thermal fidelity at the critical point.

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A. The derivation of the operator $D$: uniform case

Starting from the Ising chain Hamiltonian $H$ with $J = 1$ in the Letter, one can perform the Jordan-Wigner transformation [35]

$$\sigma^z_j = \prod_{i<j} \left( 1 - 2c_i^\dagger c_i \right) \left( c_j + c_j^\dagger \right),$$

$$\sigma^x_j = 2c_j c_j^\dagger - 1,$$

(S1)

to replace the Pauli operators by the fermionic operators $c_j$. The Hamiltonian is transformed to the Kitaev model

$$H_{\text{Kitaev}} = -\sum_{j=1}^{N-1} \left( c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right) + \text{H.c.} + g \sum_{j=1}^{N} \left( 2c_j^\dagger c_j - 1 \right).$$

(S2)

To get the solution of the model, we introduce the Majorana fermion operators $a_j = c_j^\dagger + c_j$, $b_j = -i \left( c_j^\dagger - c_j \right)$, which satisfy the commutation relations $\{a_j, a_{j'}\} = 2\delta_{j,j'}$, $\{b_j, b_{j'}\} = 2\delta_{j,j'}$, $\{a_j, b_{j'}\} = 0$. Then the Majorana representation of the original Hamiltonian is

$$H_M = -\frac{i}{2} \sum_{j=1}^{N-1} b_j a_{j+1} - \frac{i}{2} g \sum_{j=1}^{N} a_j b_j + \text{H.c.},$$

(S3)

the core matrix of which is that of a $2N$-site SSH chain in single-particle invariant subspace. Based on the exact diagonalization result of the SSH chain, the Hamiltonian $H_{\text{Kitaev}}$ can be written as the diagonal form

$$H_{\text{Kitaev}} = \sum_{n=1}^{N} \varepsilon_n (d_n^\dagger d_n - \frac{1}{2}).$$

(S4)

Here $d_n$ is a fermionic operator, satisfying $\{d_n, d_{n'}\} = 0$, and $\{d_n, d_{n'}^\dagger\} = \delta_{n,n'}$. On the other hand, we have the relations

$$[d_n, H_{\text{Kitaev}}] = \varepsilon_n d_n, [d_{n'}^\dagger, H_{\text{Kitaev}}] = -\varepsilon_n d_{n'}^\dagger,$$

(S5)

which result in the mapping between the eigenstates of $H_{\text{Kitaev}}$. Direct derivation show that, for an arbitrary eigenstate $|\psi\rangle$ of $H_{\text{Kitaev}}$ with eigenenergy $E$, i.e., $H_{\text{Kitaev}} |\psi\rangle = E |\psi\rangle$, state $d_n |\psi\rangle$ ($d_{n'}^\dagger |\psi\rangle$) is also an eigenstate of $H_{\text{Kitaev}}$ with the eigenenergy $E - \varepsilon_n$ ($E + \varepsilon_n$), i.e.,

$$H_{\text{Kitaev}} (d_n |\psi\rangle) = (E - \varepsilon_n) (d_n |\psi\rangle)$$

(S6)

and

$$H_{\text{Kitaev}} (d_{n'}^\dagger |\psi\rangle) = (E + \varepsilon_n) (d_{n'}^\dagger |\psi\rangle),$$

(S7)

if $d_n |\psi\rangle \neq 0$ ($d_{n'}^\dagger |\psi\rangle \neq 0$).

In large $N$ limit, and within the topologically nontrivial region $|g| < 1$ ($g \neq 0$), the edge modes appear with $\varepsilon_N = 0$ and the edge operator $d_N$ can be expressed as

$$d_N = \frac{1}{2} \sqrt{1 - g^2} \sum_{j=1}^{N} \left[ (g^{j-1} + g^{N-j}) c_j^\dagger + (g^{j-1} - g^{N-j}) c_j \right].$$

(S8)
i.e., $d_N$ is a linear combination of particle and hole operators of spinless fermions $c_j$ on the edge, and we have $[d_N, H_{\text{Kitaev}}] = \varepsilon_N d_N = 0$. Furthermore, applying the inverse Jordan-Wigner transformation, $d_N$ can be expressed as the combination of spin operators,

$$D = \frac{1}{2} \sqrt{1 - g^2} \sum_{j=1}^{N} \prod_{l<j} (-\sigma_l^z) \left( g^{j-1} \sigma_j^x - ig^{N-j} \sigma_j^y \right)$$

$$= \frac{1}{2} \sqrt{1 - g^2} \sum_{j=1}^{N} g^{j-1} D_j,$$

where $D_j = \prod_{l<j} (-\sigma_l^z) \sigma_j^x - i \prod_{l<N-j+1} (-\sigma_l^z) \sigma_{N-j+1}^y$.

In fact, $d_N$ and $D$ are identical, but only in different representations. Thus, from $[d_N, H_{\text{Kitaev}}] = 0$, we have

$$[D, H] = [D^\dagger, H] = 0,$$

which lead to the degeneracy of the eigenstates. Furthermore, from the canonical commutation relations $\{d_N, d_N^\dagger\} = 1$ and $\{d_N, d_N\} = 0$, we have

$$\{D, D^\dagger\} = 1, D^2 = (D^\dagger)^2 = 0.$$

**B. Disordered case**

For the Ising chain with position-dependent random $\{J_j, g_j\}$, i.e., $H = -\sum_{j=1}^{N-1} J_j \sigma_j^x \sigma_{j+1}^x + \sum_{j=1}^{N} g_j \sigma_j^z$, the operator $D$ still exists. In this case, one can perform the above procedure and solve the Schrödinger equation for the corresponding SSH chain with random hopping in single-particle invariant subspace [8]. We have the following solution:

$$D = \frac{1}{2} \sum_{j=1}^{N} \prod_{l<j} (-\sigma_l^z) \left( h_j^+ \sigma_j^x - ih_j^- \sigma_j^y \right),$$

where

$$h_j^+ = h_j^+ \prod_{m=1}^{j-1} \frac{g_m}{J_m},$$

$$h_j^- = h_j^- \frac{g_N}{J_j} \prod_{m=j+1}^{N-1} \frac{g_m}{J_m},$$

and $h_j^+ (h_j^-)$ is determined by the normalization condition $\sum_{j=1}^{N} |h_j^+|^2 = 1$. The solution of $D$ is robust against disordered perturbation and the corresponding energies of the edge modes are still exponentially small in $N$ under the condition of the average value of $J_m$ is stronger than the average value of $g_m$ [8]. Then it can be checked that the commutation relations in Eqs. (S10) and (S11) still hold for the operator $D$ with disordered perturbation in large $N$ limit.