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Finite-temperature scaling of magnetic susceptibility and the geometric phase in the XY spin chain

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Abstract

We study the magnetic susceptibility of the 1D quantum XY model, and show that when the temperature approaches zero, the magnetic susceptibility exhibits finite-temperature scaling behavior. The scaling behavior of the magnetic susceptibility in the 1D quantum XY model, due to the quantum-classical mapping, can easily be experimentally tested. Furthermore, the universality in the critical properties of the magnetic susceptibility in the quantum XY model is verified. Our study also reveals the close relation between the magnetic susceptibility and the geometric phase in some spin systems, where the quantum phase transitions are driven by an external magnetic field.

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

1. Introduction

Quantum phase transitions (QPTs), which occur at absolute zero and are driven by zero-point quantum fluctuations, are one of the most fascinating aspects of many-body systems. QPTs and related quantum critical phenomena have been a topic of tremendous interest in condensed matter physics and have been extensively studied in the past decade [1]. In recent work, quantum criticality has been characterized by using the methods and notions borrowed from quantum information science, such as the concurrence [2], the entanglement entropy [3], geometric phase (GP) [4], Loschmidt echo [5], and quantum fidelity [6], in the place of traditional criteria, such as specific heat or magnetic susceptibility (MS). Most of these studies focus on the zero-temperature properties of the critical systems. In recent years, the finite-temperature properties of QPTs [7, 8], such as thermal entanglement [9], have begun to attract more attention. This is because, firstly, all experiments are confined to finite temperature. Thus, to experimentally verify the theoretical results, knowing only the zero-temperature properties of the quantum system is not sufficient. Secondly, though genuine QPTs occur only at absolute zero, quantum criticality has profound influence on system properties up to a surprisingly high temperature [7]. Interesting phenomena at finite temperature related to QPTs

have been experimentally observed in various systems, such as the heavy fermion system and the BEC [10].

On the other hand, it has been shown that a QPT in d space dimensions is related to a classical transition in $d+z$ space dimensions [1, 11], where z is the dynamical critical exponent. Under this quantum-classical mapping, the temperature T of the quantum system maps onto an imaginary time direction: $\tau = -it/\hbar \in (0, 1/k_B T)$, where τ and t are imaginary and real time [11]. Accordingly accessing the QPT by reducing the temperature amounts to increasing the size of imaginary time dimension toward infinity, and leads to a divergence of the spatial correlation length ξ . This one-to-one mapping motivates us to study the finite-temperature properties of QPTs through its higher dimensional classical counterpart. Studies of these QPTs and the quantum-classical mapping rely heavily on the exactly solvable models. One of the most common examples is the one-dimensional quantum transverse Ising model (1D TIM) [12], which exhibits a second-order QPT at the critical point $\lambda_c = 1$, and its classical counterpart—the two-dimensional classical Ising model [13], which exhibits a second-order thermal phase transitions at the Curie point.

Historically, scaling has played a central role in the study of classical criticality. It is well known that the 2D classical Ising model obeys finite-size scaling behavior [14]. A straightforward idea is to study $T \neq 0$ scaling laws of the 1D TIM. In [9] and [15], the authors use the Gruneisen parameter and concurrence to characterize finite-temperature properties induced by QPT at zero temperature. In this paper, instead we will use a classical macroscopic thermodynamic observable—the MS—to study the finite-temperature properties of the generalized 1D TIM—the quantum XY chain. The MS has the advantage of being easily experimentally accessible and has been used as a witness of macroscopic quantum entanglement [16]¹. We will show how the finite-temperature scaling is manifested when the temperature approaches zero, in analogy with finite-size scaling in the imaginary time direction of the 2D classical Ising model. We will also verify the universality in the properties of the MS in the quantum XY chain. Finally, we will elucidate the close relation between the MS and another well-studied observable—the GP [4, 17–19].

2. Magnetic susceptibility of the quantum XY chain at finite temperature

The Hamiltonian of the quantum XY chain can be written as [12]

$$H(\gamma, \lambda) = J \sum_{i=1}^N \left[\frac{1+\gamma}{2} \sigma_i^x \sigma_{i+1}^x + \frac{1-\gamma}{2} \sigma_i^y \sigma_{i+1}^y + \lambda \sigma_i^z \right], \quad (1)$$

where N is the number of spins in the chain; J is the coupling strength (for simplicity we choose $J = 1$ hereafter); λ is an external magnetic field, and γ describes the anisotropy of the system; σ_i^α , $\alpha = x, y, z$, are the Pauli matrices on the i th site of the chain. After a standard procedure [12], this Hamiltonian can be diagonalized as $H(\gamma, \lambda) = \sum_k 2\Lambda_k (\eta_k^\dagger \eta_k - 1/2)$, where η_k is the Fermionic annihilation operator of the k th mode quasiparticle; $\Lambda_k = \sqrt{(\lambda - \cos k)^2 + \gamma^2 \sin^2 k}$ are one-half of the excitation energy for modes $k = 2\pi(i - 0.5)/N$, $i = 1, 2, \dots, N/2$. The partition function of the system can be obtained as $Z = \prod_k (e^{-\beta\Lambda_k} + e^{\beta\Lambda_k}) = \prod_k 2 \cosh(\beta\Lambda_k)$, where $\beta = 1/k_B T$ is the inverse temperature and k_B is the Boltzmann constant. Accordingly, the free energy per spin of the

¹ The use of thermodynamic observables to witness quantum entanglement is studied in [16]. For the XY chain, the separable bound of the MS is given by the sum of three susceptibilities along three orthogonal axes $\chi_x + \chi_y + \chi_z \geq N(2k_B T)^{-1}$. We know that when $0 \leq \gamma \leq 1$ and at $T = 0$, $\chi_x \approx (1 - \lambda)^{-7/4}$, $\chi_y = 0$ and $\chi_z \approx (\gamma\pi)^{-1} \ln|1 - \lambda|$. Hence, except for $\lambda = 1$, the MS cannot be explained without entanglement at $T = 0$. The above result agrees with the analysis using the specific heat as an entanglement witness [16].

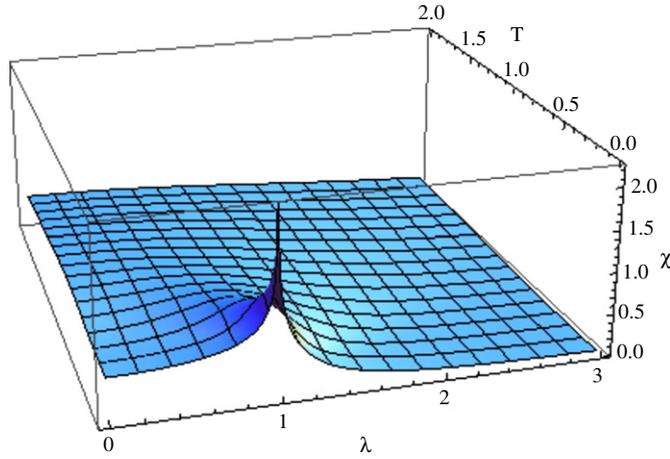


Figure 1. MS χ_z of the 1D TIM as a function of the external magnetic field λ and temperature T . It can be seen that the MS at zero temperature show logarithmic divergence at the QCP $\lambda_c = 1$. At nonzero temperature the MS is analytical. This agrees with the known result that the 1D TIM does not exhibit thermal phase transition at nonzero temperature.

system can be calculated as $F = -k_B T \ln Z/N = -k_B T \sum_k \ln [2 \cosh(\beta \Lambda_k)]/N$. In the thermodynamic limit, $N \rightarrow \infty$, we use an integral to replace the sum and obtain the exact expression of the free energy per spin at temperature T [12]:

$$F = -k_B T \ln 2 - k_B T \times \frac{1}{\pi} \int_0^\pi dk \ln[\cosh(\beta \Lambda_k)]. \tag{2}$$

The magnetization per spin along the direction of the external magnetic field λ at temperature T can be obtained,

$$M_z(T) = -\frac{\partial F}{\partial \lambda} = \frac{1}{\pi} \int_0^\pi \tanh(\beta \Lambda_k) \frac{\lambda - \cos k}{\Lambda_k} dk, \tag{3}$$

and then the MS along the z -direction $\chi_z = -\partial^2 F/\partial \lambda^2$ as a function of the temperature T and the magnetic field λ of the system can also be obtained:

$$\chi_z(\lambda, T) = \frac{1}{\pi} \int_0^\pi \left[\frac{\beta}{\cosh^2(\beta \Lambda_k)} \frac{(\lambda - \cos k)^2}{\Lambda_k^2} + \tanh(\beta \Lambda_k) \frac{\gamma^2 \sin^2 k}{\Lambda_k^3} \right] dk. \tag{4}$$

We plot the MS χ_z of the 1D TIM ($\gamma = 1$) as a function of the external magnetic field λ and the temperature T in figure 1. Clearly, it can be seen that the logarithmic divergence of the MS at zero temperature indicates the second-order QPT at the QCP $\lambda_c = 1$. We would like to point out that at zero temperature, the magnetization is reduced to $M_z(T = 0) = \int_0^\pi (\lambda - \cos k)/(\pi \Lambda_k) dk$.

For the convenience of later study, we introduce another observable—the GP, which is a fundamental concept in quantum mechanics [20]. To obtain a geometric phase, we rotate the Hamiltonian (1) around the the z -axis at an angle ϕ . The effective Hamiltonian after the rotation is

$$H_\phi = U_\phi H U_\phi^\dagger, \quad U_\phi = \prod_{j=1}^N e^{i\phi \sigma_j^z/2}. \tag{5}$$

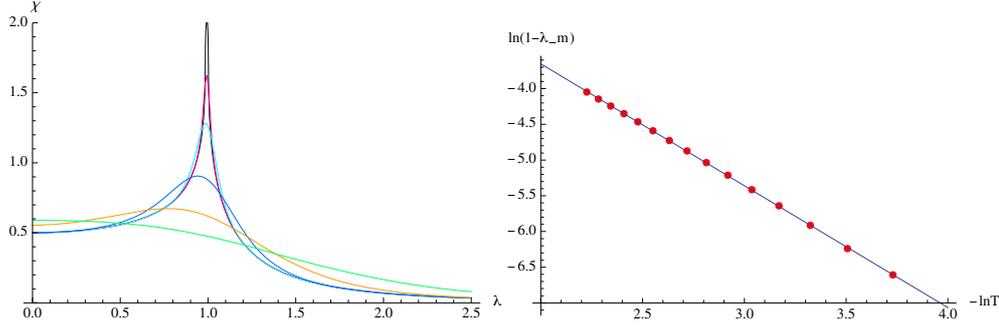


Figure 2. (Left) The MS for the 1D TIM ($\gamma = 1$) as a function of the controlling parameter λ . The curve corresponds to different temperatures $k_B T = 0$ J, 0.02 J, 0.06 J, 0.21 J, 0.5 J, and 1.01 J. With the decrease of the temperature, the maximum gets pronounced, and (right) the pseudopoint λ_m changes and tends as $T^{1.706}$ toward the QCP $\lambda_c = 1$.

The periodicity of the Hamiltonian in ϕ is π . After we rotate the Hamiltonian back to its initial form ($\phi = \pi$), the GP of the ground state accumulated by varying the angle ϕ from 0 to π is given by

$$\beta_g = -i \frac{2}{N} \int_0^\pi ((GS|U_\phi^\dagger) \frac{\partial}{\partial \phi} (U_\phi|GS)) d\phi, \tag{6}$$

which is an extra phase in addition to the usual dynamic phase. From references [4, 17–19] we know that the ground-state GP studied there can be expressed as

$$\beta_g = \pi + \int_0^\pi \frac{\lambda - \cos k}{\Delta_k} dk = \pi + \pi M_z(T = 0). \tag{7}$$

Hence, the derivative $\partial\beta_g/\partial\lambda$ of the ground-state GP over the external field is π times of the zero-temperature MS $\chi_z = \partial M_z(T = 0)/\partial\lambda$. We can understand this relation in the following way: the ground-state GP studied in [4, 17–19] is a function of the derivative of the ground-state energy with respect to the external magnetic field [17–19], and at zero temperature, the free energy is equal to the ground-state energy. Thus, at zero temperature, the GP is a function of the magnetization.

As is well known, at zero temperature, the MS of the 1D TIM shows logarithmic singularity at the QCP and exhibits finite-size scaling behavior in the proximity of the QPT point $\lambda_c = 1$. Thus, it is not surprising that the GP exhibits singularity and finite-size scaling behavior near the QCP [17]. Instead of studying the finite-size scaling of the GP (MS at zero temperature), in this paper, we will study finite-temperature scaling of the quantum XY chain. We will see that when the temperature approaches zero, in analogy with the imaginary time direction approaching the infinity in the finite-size scaling, the MS obeys $T \neq 0$ scaling behavior in the proximity of the QPT.

3. Scaling of the magnetic susceptibility of the quantum XY chain

In order to further understand the relation between the 1D TIM and the 2D classical Ising model, we investigate the finite-temperature scaling behavior of the MS by the finite-size scaling ansatz [21]. For simplicity, we first look at the 1D TIM ($\gamma = 1$), and we will discuss the properties of the family of $\gamma \neq 1$ later. The MSs as a function of the external magnetic field λ at different temperatures T (including zero temperature) are presented in figure 2. At

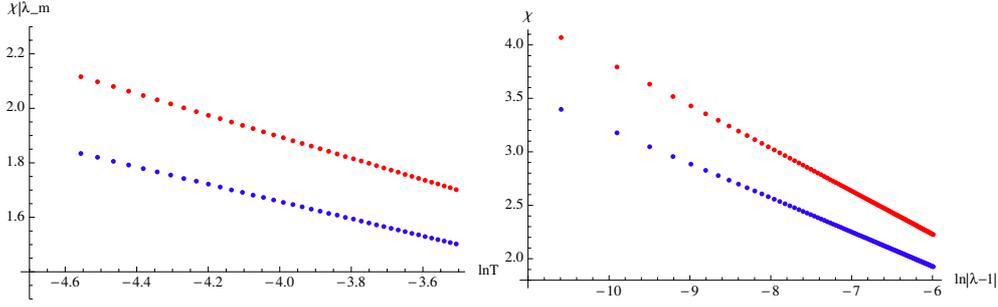


Figure 3. (Left) The maximum value of the MS at the pseudocritical point λ_m of the 1D quantum XY chain as a function of temperature T . The slope of the line is 0.317 (0.394) for $\gamma = 1$ (below) ($\gamma = 0.8$ (above)). (Right) The MS at zero temperature diverges logarithmically in the proximity of the QCP $\lambda_c = 1$. The slope of the line is 0.320 (0.401) for $\gamma = 1$ (below) ($\gamma = 0.8$ (above)). The ratio of the two slopes (below and above) for a fixed parameter γ is equal to the critical exponent ν . Here $\nu \approx 1.009$ ($\nu \approx 1.017$) for $\gamma = 1$ ($\gamma = 0.8$) is obtained. The numerical results agree with the scaling ansatz and the universality of the XY model.

zero temperature the MS shows a singularity at $\lambda_c = 1$, but at nonzero temperature, there is no real divergence of χ_z . Nevertheless, there are clear anomalies at low temperature, and the height of which increases with the decrease of the temperature. This can be regarded as the precursors of the QPT. What is more, the position λ_m of the maximum susceptibility (pseudocritical point) [21] changes and tends as $T^{1.704}$ toward the QCP and clearly approaches λ_c when $T \rightarrow 0$ (see figure 2(b)). Meanwhile, the maximum value $\chi_z|_{\lambda_m}$ of the MS diverges logarithmically with the decrease of the temperature:

$$\chi_z|_{\lambda_m} \approx \kappa_1 \ln T + \text{const.} \tag{8}$$

Our numerical results (see figure 3(a)) give $\kappa_1 = 0.320$. On the other hand, when $T = 0$, from [22] we know that the MS in the proximity of the QCP exhibits logarithmic singularity

$$\chi_z \approx \kappa_2 \ln |\lambda - \lambda_c| + \text{const.} \tag{9}$$

Our numerals in figure 3(b) give the result $\kappa_2 \approx 0.317$, while the exact result [22] gives $\kappa_2 = 1/\pi \approx 0.3183$. We would like to point out that the coefficient κ_2 here is the same as that in [17], where the author gives $\kappa_2 \approx 0.3123$ and our numerical result is closer to the exact result $\kappa_2 = 1/\pi$. According to the scaling ansatz in the logarithmic singularities, the ratio $|\kappa_2/\kappa_1|$ gives the critical exponent ν that governs the divergence of the correlation length $\xi \sim |\lambda - \lambda_c|^{-\nu}$. In our case, $\nu \approx 1.009 \sim 1$ is obtained in the numerical calculation for the 1D TIM, which agrees well with the known results about the 1D TIM [12]. Furthermore, by proper scaling and taking into account the distance of the maximum χ_z from the QCP, it is possible to make all the data for the value of $F = 1 - \exp[\chi_z(\lambda) - \chi_z|_{\lambda_m}]$ as a function of $(\lambda - \lambda_m)/T$ for different temperatures T to collapse onto a single curve (see figure 4). This figure contains the data for temperatures ranging from $k_B T = e^{-3}J, e^{-4}J, e^{-5}J, e^{-5.5}J$. These results demonstrate that the MS obeys the scaling behavior as the temperature decreases to zero, in analogy with the lattice size approaching the infinity in the finite-size scaling cases.

In the following, we will study the universality of the critical behavior of the MS. It is well known that the anisotropic XY chain ($\gamma \ni (0, 1]$) belongs to the 1D TIM universality, while the isotropic XY chain ($\gamma = 0$) belongs to the XX universality. For the 1D TIM universality, $\nu = 1$, while for the XX universality, $\nu = 1/2$. We will show that the finite-temperature scaling

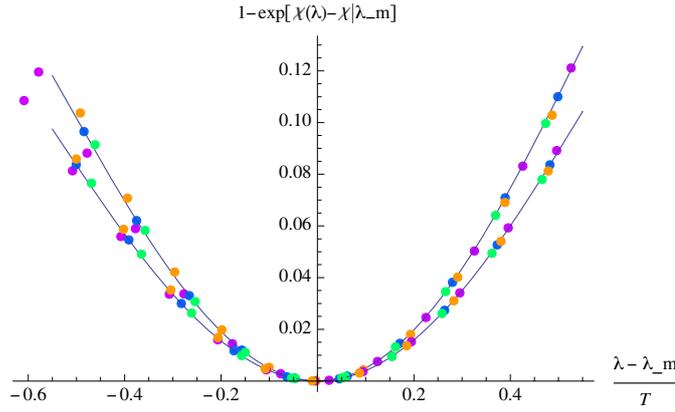


Figure 4. The value of $F = 1 - \exp[\chi_z(\lambda) - \chi_z[\lambda_m]]$ as a function of $(\lambda - \lambda_m)/T$ for different temperatures $k_B T = e^{-3} J, e^{-4} J, e^{-5} J,$ and $e^{-5.5} J$. For fixed γ (here we choose $\gamma = 1$ and $\gamma = 0.8$), all data collapse on a single curve, which agrees with the finite-size scaling behavior. The critical exponent $\nu = 1$ can be obtained from this figure.

behavior of χ_z also manifests the universality principle—the critical properties depend only on the dimensionality of the system and the broken symmetry in the ordered phase. To verify the universality principle of the XY model, we consider the case for $\gamma \neq 1$. The asymptotic behavior is also described by equations (8) and (9). From figure 3 we see that for $\gamma = 0.8$ numerical simulation gives $\kappa_1 \approx 0.394$ and $\kappa_2 \approx 0.401$, while the exact result [22] should be $\kappa_2 = (\gamma\pi)^{-1} \approx 0.398$. As a result, the critical exponent for $\gamma = 0.8$ is $\nu = |\kappa_2/\kappa_1| \approx 1.017$, very close to the exact value $\nu = 1$. Moreover, we also verify that by proper scaling, all data for different temperatures T but a specific γ will collapse onto the same curve. The data for $\gamma = 0.8$ are shown in figure 4.

What is more, through a similar analysis to that in [17], we can directly extract the finite-temperature scaling behavior of the XX ($\gamma = 0$) universality class. It can be found that, at zero temperature $T = 0$, for the XX universality, the magnetization can be written in the following compact form:

$$M_z = \begin{cases} 1 - \frac{2}{\pi} \arccos \lambda & (0 \leq \lambda \leq 1) \\ 1 & (\lambda > 1). \end{cases} \quad (10)$$

Accordingly, the critical exponent $\nu = 1/2$ and $z = 2$ can be extracted from the MS $\chi_z = \sqrt{2}(1 - \lambda)^{-\frac{1}{2}}, (\lambda \rightarrow 1^-)$ [17], which is different from the TIM universality ($\nu = 1$ and $z = 1$). When we change the anisotropy γ from 1 to 0, we find the range of the validity of the quantum scaling ansatz in λ (equation (9)) shrinks gradually. The leading term of the MS changes from $\frac{1}{\pi\gamma} \ln(1 - \lambda)$ to $\sqrt{2}(1 - \lambda)^{-\frac{1}{2}}$. Hence, when $0 < \gamma \leq 1$, the scaling belongs to XY universality, while when $\gamma = 0$, the scaling belongs to XX universality. Finally, we would also like to point out that our numerical result shows that the scaling behavior of equation (8) can persist up to a temperature $k_B T \approx 0.5 J$. This result agrees well with that of [7]. In addition, the crossover line in the region $0 < \lambda < 1$ given by the MS χ_z is roughly $T_c \sim |\lambda - \lambda_c|^{\nu z}$, which agrees well with the result obtained in the analysis elsewhere [9]. Hence, the boundary of the quantum critical scaling region can be confirmed by the behavior of the MS χ_z .

4. Magnetic susceptibility and the geometric phase

As we have mentioned before, the derivative of the ground-state GP discussed in [4, 17–19] is equal to π times of the MS, and the finite-size scaling of the GP [17] actually represents the finite-size scaling of the MS. Based on these studies, we would like to further study the relation between the thermal-state GP and the MS at a finite temperature. Similar to the definition of the ground-state GP in [4, 17–19], we define the thermal-state GP in the following way: four eigenstates of the modes $(k, -k)$ of H_ϕ (see [4, 17–19]) can be expressed as $|00\rangle_k = \cos(\theta_k/2)|0\rangle_k|0\rangle_{-k} + i e^{i2\phi} \sin(\theta_k/2)|1\rangle_k|1\rangle_{-k}$, $|11\rangle_k = i e^{-i2\phi} \sin(\theta_k/2)|0\rangle_k|0\rangle_{-k} + \cos(\theta_k/2)|1\rangle_k|1\rangle_{-k}$, $|01\rangle_k = |0\rangle_k|1\rangle_{-k}$, and $|10\rangle_k = |1\rangle_k|0\rangle_{-k}$ with the angle θ_k defined by $\theta_k = \arctan[-\sin k/(\cos k - \lambda)]$. The GP of the thermal state at temperature T accumulated by varying the angle ϕ from 0 to π is described by

$$\beta_T = \frac{-2i}{N} \sum_{k=1}^{N/2} \sum_n \int e^{-\beta E_n} \langle n|_k \frac{\partial}{\partial \phi} |n\rangle_k d\phi, \quad (11)$$

where $|n\rangle_k = |00\rangle_k, |01\rangle_k, |10\rangle_k, \text{ and } |11\rangle_k$. After a straightforward calculation, we obtain the same relation between the magnetization and the GP as that of zero temperature $\beta_T = \pi + \int_0^\pi (\lambda - \cos k)/\Lambda_k \tanh(\beta \Lambda_k) dk = \pi[1 + M_z(T)]$ (3). Thus, we prove that at both zero temperature and nonzero temperature, the GP of the quantum XY chain is a linear function of the magnetization, and the derivative of the GP is proportional to the MS. The discussions of the finite-temperature scaling of the MS in this paper can be alternatively regarded as the finite-temperature scaling of the GP in the proximity of the QPT point. Finally, the close relation between the GP and the MS is not confined to the 1D quantum XY chain. In [23] the ground-state GP of the Dicke model and its relation to quantum criticality are studied. We would like to point out that, similar to the discussions about the 1D XY chain, the ground-state GP of the Dicke model is a linear function of the ground-state magnetization $\beta_g = \pi(1 + \langle S_x \rangle/N)$, where $\langle S_x \rangle/N$ is the magnetization M_x per spin in the Dicke model. Hence, the derivative of ground-state GP of the Dicke model is also equal to π times of the MS. Besides the above two examples, it can be proved that for any QPTs driven by an external magnetic field, such as the Lipkin–Meshkov–Glick model [18] and the 1D XXZ model², the relation between the GP and the magnetization still holds true. The proof is given as follows. For those QPTs driven by an external magnetic field, we apply a π -rotation along the z -axis for every spin $U_\phi = \prod_{j=1}^N e^{i\phi\sigma_j^z/2}$ to obtain the GP. The GP of the ground state can be expressed as (6)

$$\begin{aligned} \beta_g &= -i \frac{2}{N} \int_0^\pi \langle GS|U_\phi^\dagger \left(i \sum_j \frac{\sigma_j^z}{2} \right) (U_\phi|GS) \rangle d\phi \\ &= \frac{2\pi}{N} \sum_j \langle GS| \frac{\sigma_j^z}{2} |GS \rangle = \pi M_z(T = 0), \end{aligned} \quad (12)$$

where $|GS\rangle$ is the ground state of the Hamiltonian (1) before the rotation, and $U_\phi|GS\rangle$ is the instantaneous ground state after the rotation for an angle ϕ . We know that $\frac{2}{N} \sum_j \langle GS| \frac{\sigma_j^z}{2} |GS \rangle$ is the definition of the GP of the ground state. Thus, we prove that the GP obtained by applying a rotation around the z -axis to each spin, is proportional to the magnetization along the z -axis (similarly, if we rotate along the x -axis, the GP will be proportional to the magnetization along

² The Hamiltonian of the XXZ model is $H = \sum_{i=1}^N [\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z + \lambda \sigma_i^z]$. Here both the anisotropy Δ and the external magnetic field λ can induce QPTs [24]. However, only the QPTs induced by λ can be characterized by the GP induced by a rotation $U_\phi = \prod_{j=1}^N e^{-i\phi\sigma_j^z/2}$. Because $\frac{\partial F}{\partial \Delta}$ is not proportional to the magnetization in the z -direction M_z , and hence is not proportional to $\langle \sigma^z \rangle$.

the x -axis). We would also like to point out that the GP in equation (12) differs from that in equation (7) by a constant π . This is because the ground state of $U_\phi H U_\phi^\dagger$ has an uncertainty of the global phase. When we choose a proper global phase, we can eliminate the difference between equation (7) and equation (12). In addition, we can generalize the above discussions to eigenstates other than the ground state. We find the same proportional factor between the GP and the magnetization for all eigenstates. Thus, the relation between the GP and the magnetization can be straightforwardly generalized to a thermal state at finite temperature. The above XY model is a good example.

In summary, we study the finite-temperature scaling of the MS of the quantum XY chain. All key features of the quantum criticality, such as scaling, critical exponent, the universality, etc are presented in the MS of the XY spin chain. Although the nature of the QPT and the $T \neq 0$ scaling is purely quantum mechanical, the classical macroscopic thermodynamic observable MS, which can be easily accessed experimentally, can be used to witness and characterize the quantum features of the system [16] (see footnote 1). Our studies shed light on the mechanism of bringing quantum criticality up to a finite temperature, and open the possibility of observing the footprint of quantum criticality experimentally. We would also like to point out that the results obtained in this paper do not depend on the model and thermodynamic observables used here, and can be generalized to other QPT models with the only change of MS to a ‘controlling parameter-dependent susceptibility’. For example, in a QPT driven by the pressure instead of the external magnetic field, the observable $\chi_p = -\partial^2 F / \partial p^2$ is expected to exhibit the finite-temperature scaling behavior, and the critical exponent can be extracted through a similar analysis. Finally, our study establishes the connection between the MS and the GP at both zero temperature and nonzero temperature in a family of spin systems, where the QPTs are driven by an external magnetic field.

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