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Quantum Phase Transition and Finite-Size Scaling of the One-Dimensional Ising Model

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We study the quantum phase transition in the one-dimensional Ising model at zero temperature. As the strength g of the transverse field is changed, the system undergoes a quantum phase transition from an ordered to a disordered phase, characterized by spontaneous magnetization in the z-direction. We apply the standard technique of finite-size scaling in statistical mechanics to detect the nature of the quantum phase transition in the system.

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I. INTRODUCTION

Finite-size scaling is a standard technique which has been widely used to study phase transitions in classical statistical physics [1,2]. If the correlation length diverges at the critical point, the linear dimension L of a sample becomes the relevant scale near the critical point, and one can write the free energy and other thermodynamic quantities in simple forms of scaling functions.

At zero temperature, even without thermal fluctuations, quantum fluctuations instead may cause a quantum phase transition, which is accompanied by a drastic change of the ground state. In this work, we apply the standard finite-size scaling to the quantum phase transition for the one-dimensional (1D) quantum Ising model under a transverse magnetic field. A continuous phase transition occurs at zero temperature in the 1D quantum Ising model when the transverse magnetic field strength g, playing the role of the temperature in classical Ising system, is varied across the critical value g_c. For $g < g_c$, a nonvanishing spontaneous magnetization has been shown to exist in the z-direction while the long-range order is destroyed above g_c. This quantum phase transition belongs to the universality class of the two-dimensional (2D) classical Ising model, which has been analytically solved by Onsager [3]. Since the partition function of the 2D classical Ising model in the thermodynamic limit can be rewritten as that of the 1D quantum Ising chain at zero temperature [4,5], both systems naturally belong to the same universality class.

In this paper, we first compute the ground state of the Hamiltonian of the quantum Ising chain for various L and g through a numerical diagonalization based on the modified Lanczos method [6]. From the obtained ground states, we calculate physical quantities, such as the spontaneous magnetization m, the magnetic susceptibility χ in the $z-$direction, and the transverse susceptibility χ_x, where $g\chi_x$ is analogous to the specific heat in the 2D classical Ising model. We apply the standard method of finite-size scaling, in a more general context than in Refs. 7–9, and confirm that the critical exponents agree with those of the 2D classical Ising model. Furthermore, we define the functional of the magnetization in analogy with the free-energy functional in standard statistical physics to explore the nature of the phase transition of the 1D quantum Ising model. We emphasize that the method presented in this work is applicable to various other quantum systems beyond the simple 1D quantum Ising model [8,9].

II. MODEL AND RESULTS

The Hamiltonian of the quantum Ising chain is given by

$$H = -g \sum_{i=1}^{L} \sigma_i^x - \sum_{i=1}^{L} \sigma_i^z \sigma_{i+1}^z, \tag{1}$$

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where σ_i^α is the Pauli matrix in the α-direction($\alpha = x, y, z$) defined at the ith site. Since $[\sigma^x, \sigma^z] \neq 0$, there exist quantum fluctuations controlled by the parameter g. When $g = 0$ at an infinitesimally small external magnetic field in the z-direction ($B \to \pm 0$), the ground state is completely ordered. In contrast, at $g = \infty$, the spin operator σ_i^x commutes with H, and each spin points in the x-direction, leading to a vanishing spontaneous magnetization m in the z-direction. Consequently, the system is expected to exhibit a phase transition at g_c, separating the ordered phase with $m \neq 0$ and the disordered one with $m = 0$. Indeed, the quantum phase transition has been found to occur at $g_c = 1$ [10].

With the Jordan-Wigner transformation [5,10,11], the quantum Ising Hamiltonian in the momentum space [12] leads to

$$H = \sum_k \epsilon_k \left(\gamma_k^\dagger \gamma_k - \frac{1}{2} \right), \tag{2}$$

where $\gamma_k^\dagger(\gamma_k)$ is the fermion creation (annihilation) operator. For states of even fermions, $\epsilon_k = 2\sqrt{1 + g^2 - 2g\cos k}$ at any g and k while for odd-fermion states [11],

$$\epsilon_k = \begin{cases} 2\sqrt{1 + g^2 - 2g\cos k} & \text{for } k \neq 0, \\ 2(g-1) & \text{for } k = 0. \end{cases} \tag{3}$$

From Eqs. (2) and (3), the ground state for $g > g_c(= 1)$ is found to be the vacuum state with $\gamma_k^\dagger \gamma_k = 0$ for all k with energy $E_G = -(1/2)\sum_k \epsilon_k$. Below g_c, the ground state for the even-fermion state is the vacuum state while it is the one-fermion state for odd fermions ($\gamma_k^\dagger \gamma_k = 1$ for $k = 0$ and $\gamma_k^\dagger \gamma_k = 0$ for $k \neq 0$). Since the energy of the one-fermion state is slightly higher than that of the vacuum state in finite systems, the ground-state energy below g_c is the vacuum state. However, the energy difference between the vacuum state and the one-fermion state approaches zero as the system size is increased [11], yielding a degenerate ground state in the thermodynamic limit below g_c.

Although the ground-state energy is easily found by using the Jordan-Wigner transformation, it is difficult to obtain analytic expressions for the magnetization and the correlation functions within the fermion representation. In contrast, if one can diagonalize the Hamiltonian in Eq. (1) numerically, the physical properties are easily investigated from the numerically obtained eigenstates. We take $|n\rangle \in \{|\uparrow\uparrow\cdots\uparrow\rangle, |\downarrow\uparrow\cdots\uparrow\rangle, \cdots, |\downarrow\downarrow\cdots\downarrow\rangle\}$, *i.e.*, the eigenstates of σ^z, as basis kets, and we diagonalize the Hamiltonian matrix through the use of the modified Lanczos method [6]. It is to be noted that the diagonalization is possible only for systems of small sizes because the dimensionality (2^L) of the Hilbert space grows exponentially as L is increased.

The procedure of the modified Lanczos method is as follows:

1. $|\phi_0\rangle$ is chosen randomly in the 2^L-dimensional ket space.
2. $|\phi_1\rangle$ is constructed to be orthogonal to $|\phi_0\rangle$ as
$$|\phi_1\rangle = H|\phi_0\rangle - \left(\langle\phi_0|H|\phi_0\rangle\right)|\phi_0\rangle. \tag{4}$$
3. The 2×2 matrix $H_{ij} = \langle\phi_i|H|\phi_j\rangle$ with $(i, j = 0, 1)$ is built and then diagonalized.
4. The eigenvector with the lowest eigenvalues is chosen as a new $|\phi_0\rangle$. Go to the step 2 and iterate.

We repeat this procedure until the ground state is obtained within a given numerical accuracy.

Due to the spin reversal symmetry in the z-direction, $\langle\sum_i \sigma_i^z\rangle = 0$ at any g. To avoid this, previous works [11, 13] have defined the spontaneous magnetization m in the z-direction as

$$m \equiv \frac{1}{L} \left| \left\langle \Psi_0^+ \left| \sum_i \sigma_i^z \right| \Psi_{k=0}^- \right\rangle \right|, \tag{5}$$

where $|\Psi_0^+\rangle$ denotes the vacuum state and $|\Psi_{k=0}^-\rangle$ the one-fermion state (at $k = 0$). However, the above definition in Eq. (5) is not directly applicable within the scheme of the modified Lanczos method used in the present work because we find only one ground state. For the ground state written in the form

$$|\Phi\rangle = \sum_n a_n |n\rangle, \tag{6}$$

we define the spontaneous magnetization as

$$m = \sum_n |a_n|^2 |m_n|, \tag{7}$$

where $m_n = (1/L)\langle n|\sum_i \sigma_i^z|n\rangle$. Since the states with $m_n \approx 1$ and $m_n \approx -1$ are mixed in the ground states below g_c, the definition in Eq. (7) captures well the meaning of the spontaneous magnetization.

We plot m versus g for various system sizes L in Fig. 1(a): As g is increased, it is clearly seen that the system undergoes a quantum phase transition near $g = 1$ from the ferromagnetic ordered phase at $g \lesssim 1$ to the paramagnetic disordered phase at $g \gtrsim 1$. As L is increased, the magnetization m changes more sharply near $g = 1$, indicating a singular behavior in the thermodynamic limit at $g_c \approx 1$. The finite-size scaling form of the spontaneous magnetization reads

$$m = L^{-\beta/\nu} \bar{m} \left((g - g_c) L^{1/\nu} \right), \tag{8}$$

where β and ν are critical exponents describing the singular behaviors of the magnetization and the correlation length as $m \sim (g_c - g)^\beta$ $(g \leq g_c)$ and $\xi \sim |g - g_c|^\nu$, respectively. Since the quantum phase transition at zero temperature is controlled by g, we use g in Eq. (8), although the usual scaling forms in classical statistical physics have temperature T instead of g. As expected from Eq. (8), $mL^{\beta/\nu}$ for different sizes cross at g_c with $\beta/\nu = 1/8$ and $g_c = 1$ [see Fig. 1(b)]. Furthermore,

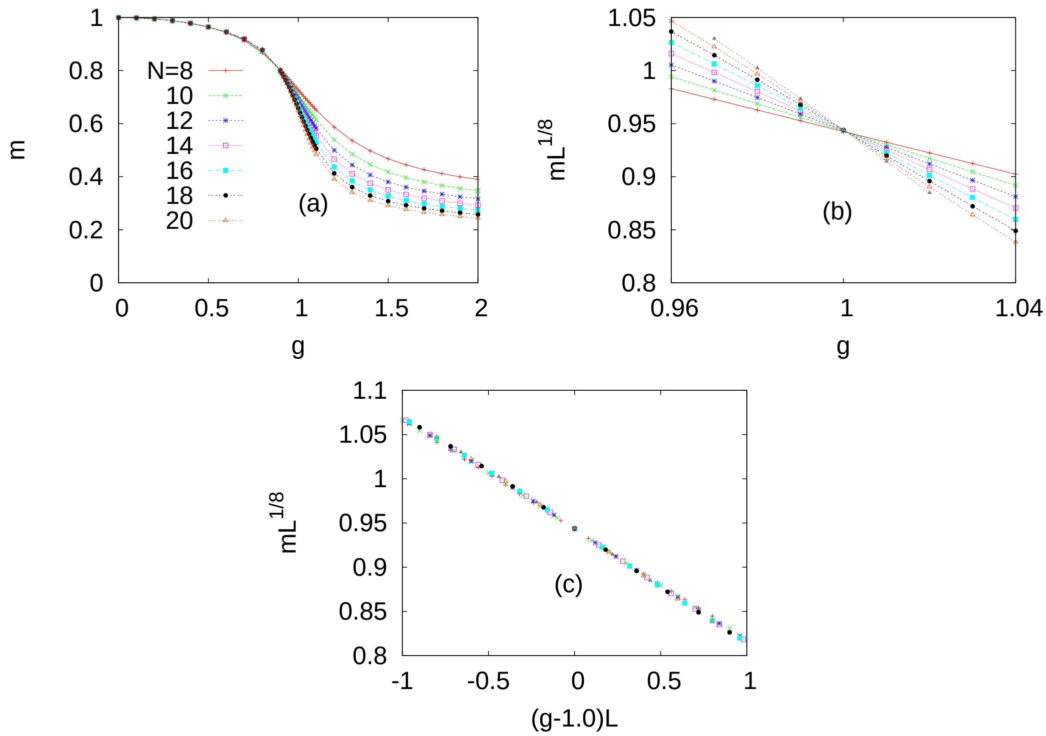

Fig. 1. (Color online) Spontaneous magnetization m and its scaling plots. In (a), the change of m with respect to g implies a phase transition at $g_c \approx 1$ from ordered to disordered states. The crossing at $g = g_c = 1$ in (b) and the scaling collapse in (c) yield the critical exponents $\beta = 1/8$ and $\nu = 1$, consistent with the 2D classical Ising model.

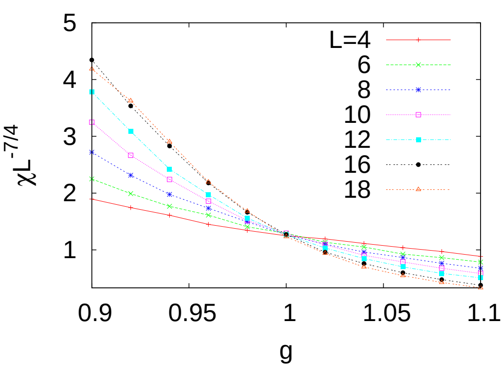

Fig. 2. (Color online) Finite-size scaling of the magnetic susceptibility χ in the z-direction. The existence of a unique crossing point indicates that $g_c = 1$ and $\gamma/\nu = 7/4$.

when we plot $mL^{\beta/\nu}$ versus $(g - g_c)\, L^{1/\nu}$, data points collapse into a single smooth curve with $\nu = 1$, as shown in Fig. 1(c). The exponents $\beta = 1/8$ and $\nu = 1$ estimated above, of course, agree with the 2D classical Ising model. It is remarkable that small systems can be used, via finite-size scalings, to reveal the phase transition, which, in principle, can be defined in the thermodynamic limit.

We next apply the finite-size scaling method to the response function, *i.e.*, the magnetic susceptibility χ, for an external magnetic field in the z-direction:

$$\chi = \frac{1}{L} \frac{d \left\langle \sum_i \sigma_i^z \right\rangle_B}{dB} \bigg|_{B \to +0}, \tag{9}$$

where B is the external magnetic field applied in the z-direction. The finite-size scaling form is written as

$$\chi = L^{\gamma/\nu} \bar{\chi} \left((g - g_c)\, L^{1/\nu} \right), \tag{10}$$

where γ is the critical exponent describing the divergence $\chi \sim |g - g_c|^{-\gamma}$. With $\gamma/\nu = 7/4$, $\chi L^{-\gamma/\nu}$ for different sizes cross at $g = 1$, as shown in Fig. 2. The crossing point agrees with our result $g_c = 1$ obtained above from the spontaneous magnetization. Again, $\gamma/\nu = 7/4$ is consistent with the corresponding value for the 2D classical Ising model.

Similarly, the transverse susceptibility χ_x is obtained from the second derivative of the energy with respect to g:

$$\chi_x = \frac{1}{L} \frac{d \left\langle \sum_i \sigma_i^x \right\rangle_g}{dg}. \tag{11}$$

Since g is analogous to T in classical systems, we expect $g\chi_x$ to be equivalent to the specific heat in the 2D classical Ising model. When we plot $g\chi_x$ as a function of g, peaks exist near $g \approx 1$, as displayed in Fig. 3(a). Through the use of the diagonalized form of

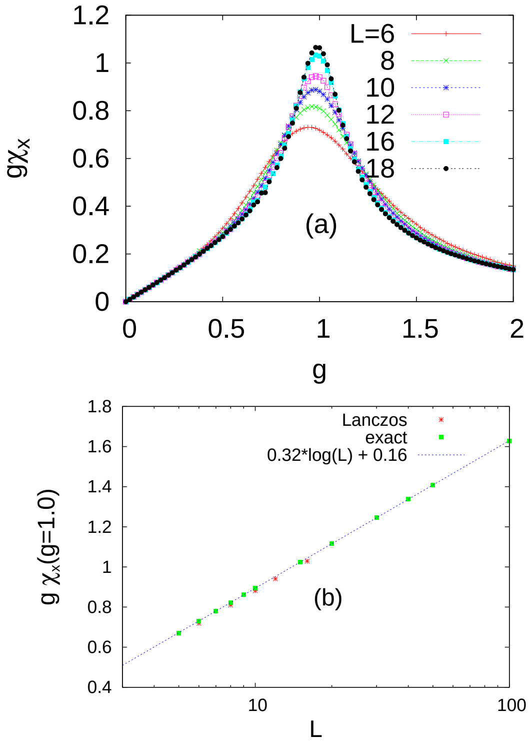

Fig. 3. (Color online) (a) Transverse susceptibility χ_x is shown in the form of $g\chi_x$ versus g. $g\chi_x$ shows a peak at $g \approx 1$ in (a), and the peak heights at $g = 1$ are shown to fit well to the logarithmic divergence form in (b), analogous to the specific heat in the 2D classical Ising model. For comparison, we also plot exactly obtained values of the peak heights in (b), as well as the curve for the least-squares fit.

the Hamiltonian in Eq. (2) with the ground-state energy $E_G = -1/2 \sum_k \epsilon_k$, it is straightforward to obtain

$$g\chi_x = -g\frac{d^2 E_G}{dg^2} = g \sum_{k \neq 0} \frac{1-\cos^2 k}{(1+g^2-2g\cos k)^{\frac{3}{2}}}. \qquad (12)$$

Since the summation in Eq. (12) can be approximated as an integral over k for sufficiently large systems, it is clear that the logarithmic divergence occurs when $k \to 0$ at $g = 1$, which is, indeed, the case shown in Fig. 3(b) for both the analytic and the numerical results. The logarithmic divergence $g\chi_x$ is also consistent with the well-known divergence of the specific heat in 2D [3], yielding the specific heat exponent $\alpha = 0$.

In standard statistical physics, the histogram of the magnetization is often used to detect the nature of a phase transitions. We rewrite the expectation value of $(1/L)\sum_i \sigma_i^z$ as

$$\frac{1}{L}\left\langle \sum_i \sigma_i^z \right\rangle = \sum_n |a_n|^2 m_n \equiv \sum_m P(m)m, \qquad (13)$$

and the probability $P(m)$ for the system to have magnetization m is used as the histogram in classical cases.

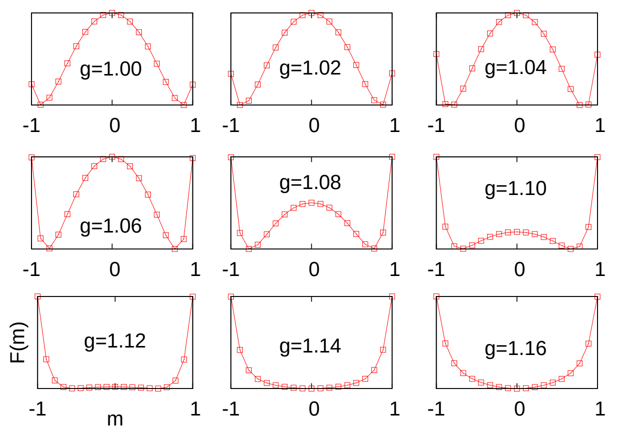

Fig. 4. (Color online) Free-energy-like function $F(m) \equiv -\log P(m)$ with the probability $P(m)$ for the system to have a magnetization m is displayed for various values of g for $L = 18$. As g increases, $F(m)$ changes from a double-well to to a single-well form continuously.

The free-energy-like function is then defined as

$$F(m) \equiv -\log P(m), \qquad (14)$$

which is shown in Fig. 4 at various values of g for the size $L = 18$. Upon increasing g, the value of m at the minimum approaches zero, indicating the continuous nature of the phase transition.

III. SUMMARY

In summary, we have investigated the quantum phase transition in the 1D quantum Ising model. Ground states have been obtained via the modified Lanczos method, and the standard finite-size scaling method has been applied. As we expected from well-known existing studies, all measured quantities, including the magnetization and the response functions, indicate that the quantum phase transition belongs to the 2D classical Ising universality class with exponents $\alpha = 0$, $\beta = 1/8$, $\gamma = 7/4$, and $\nu = 1$. We emphasize that although numerical calculations have been performed in very small chains up to 20 spins at most, the modified Lanczos method combined with the finite-size scaling method can be very useful for investigating quantum phase transitions. As future works, we are planning to study the finite-temperature behaviors, *i.e.*, the quantum critical region in the 1D quantum Ising model and the phase transition on irregular network structures.

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