

Topological charge scaling at a quantum phase transition

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We reexamine the Kosterlitz-Thouless phase transition in the ground state $|\Psi_0\rangle$ of an antiferromagnetic spin- $\frac{1}{2}$ Heisenberg chain with nearest- and next-nearest-neighbor interactions λ from a different perspective: After defining winding number (topological charge) W in the basis of resonating valence bond states, the finite-size scaling of $\langle\Psi_0|W|\Psi_0\rangle$, $\langle\Psi_0|W|\partial_\lambda\Psi_0\rangle$, $\langle\partial_\lambda\Psi_0|W|\partial_\lambda\Psi_0\rangle$ leads to the accurate value of critical coupling $\lambda_c = 0.2412 \pm 0.0007$ and to the value of subleading critical exponent $\nu = 2.000 \pm 0.001$. This approach should be useful when examining the topological phase transitions in all systems described in the basis of resonating valence bonds.

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Introduction. At a quantum phase transition (QPT) properties of the ground state of the quantum system change drastically due to quantum fluctuations, which are most clearly pronounced at zero temperature. Although many approaches have been proposed to examine QPTs, to locate critical points, and to calculate the values of critical exponents, an important question still remains: *Is it possible to explore the critical behavior of a system at QPT by examining the change of its ground state $|\Psi_0\rangle$ in a critical region, especially when there is no possibility to identify an order parameter nor to establish a pattern related to symmetry breaking?* Still, there exists a quest for new approaches, based on scaling and renormalization to search for and characterize QPTs.

Recently, mostly due to the interplay between information theory and quantum many-body physics, new possibilities have emerged for the study of QPTs. One of the latest observations was that the fidelity f , understood as an overlap between the system ground states calculated for the slightly shifted values of the parameter λ whose change leads the system towards QPT, may be used to find it; see, e.g., Refs. [1,2]. Later on, this approach was extended to the fidelity susceptibility, $\chi_F = \langle\partial_\lambda\Psi_0|\partial_\lambda\Psi_0\rangle$, and the phase transition was to be seen as a shift of the maximum in the dependencies of f and χ_F on the parameter λ . However, some difficulties were encountered with finite-size scaling (FSS) of the fidelity susceptibility χ_F for topological QPTs: It was unclear whether the maxima of χ_F obey FSS, and some attempts were made to interpret the emerging discrepancies [3] as logarithmic corrections to scaling. It turned out recently [4] that the maximum of χ_F is shifted relative to the Kosterlitz-Thouless (KT) quantum critical point λ_c by a universal constant $\frac{B^2}{36}$ towards the *gapped* phase in which the correlation length ξ falls exponentially, $\xi(\lambda) \sim \exp(B/\sqrt{|\lambda - \lambda_c|})$. For this reason, the maximum in question does not scale with the system size L as expected—see, e.g., Eq. (5) in Ref. [5] or Eq. (7) in what follows—and the change of its position with the change of the system size L cannot be used to find the critical properties of the system

within FSS of fidelity susceptibility. On the other hand, the exponential decay of the correlation length near the critical coupling λ_c causes the numerical investigation of KT transition to be hard, since one has to examine rather large system (hundreds of spins) to avoid finite-size effects.

In this Letter, we address the problem of precise determination of the critical coupling and some critical exponents at a topological quantum phase transition and show that the FSS method may be used for small systems to locate such a quantum critical point and to determine the critical exponents, despite the shift of the maximum mentioned earlier.

The model under consideration and its essential properties. Our answer to the question posed in the Introduction is based on the reexamination of the quantum phase transition in the known [6–8] one-dimensional (1D) spin- $\frac{1}{2}$ Heisenberg antiferromagnet with nearest-neighbor interactions, set equal to 1, and next-nearest-neighbor interactions, set equal to λ . The Hamiltonian reads

$$H = \sum_i S_i S_{i+1} + \lambda \sum_i S_i S_{i+2}. \quad (1)$$

The ground state of this system depends on λ : for $\lambda < \lambda_c = 0.241167$ it is similar to the ground state of a 1D antiferromagnet with nearest-neighbor interactions (spin liquid phase), i.e., it is critical with the correlation function decaying in a power-like way, $\sim \sqrt{\ln(r)}/r$, where r stands for spin-spin separation. Excitations are gapless: the finite-size triplet gap scales like $1/L$ (also with logarithmic correction). For $\lambda > \lambda_c$, the system displays a different ground state (dimerized phase): the correlation function decays exponentially, $\sim \exp[-r/\xi(\lambda)]$, with the distance, and the triplet gap remains open in the thermodynamic limit. The transition between these phases is known to be of Kosterlitz-Thouless type.

Resonating valence bond (RVB) basis and winding numbers. Using the RVB basis sheds additional light on the critical properties of the considered system. Recall then, briefly, the essential features of RVB approach [9,10] to quantum spin- $\frac{1}{2}$

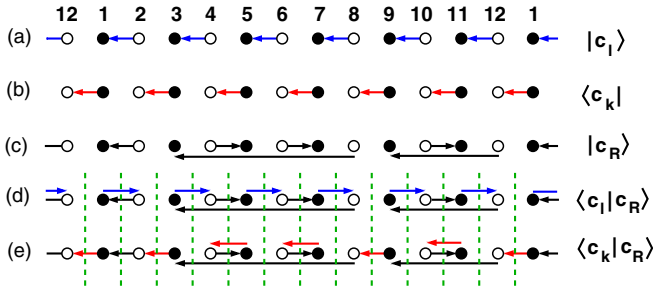


FIG. 1. Examples of calculating the winding numbers for two states $|c_l\rangle$ [blue, (a)] and $|c_k\rangle$ [red, (b)] with respect to the reference state $|c_R\rangle$ [black, (c)] in a 12-spin system. The system with periodic boundary conditions is represented as a line. The winding number $W_{lR} = 0$ is assigned to the transition graph $\langle c_l|c_R\rangle$ (d) since the number of singlets cut by green line modulo 2 is equal to 0 (see text). In (e) the number of singlets modulo 2 crossed by the green line equals 1 and consequently $W_{kR} = 1$.

systems: Matrix elements of the Hamiltonian are calculated not in the Ising basis but in the (complete) nonorthogonal basis $|c_k\rangle$ taken from an overcomplete set of *singlet coverings*:

$$\langle c_k|\mathbf{S}_i \cdot \mathbf{S}_j|c_l\rangle = (-1)^d \left(\pm \frac{3}{4} \right) \langle c_k|c_l\rangle; \quad (2)$$

$\langle c_k|c_l\rangle = 2^{\mathcal{N}(c_k, c_l) - \mathcal{N}_s}$ with $\mathcal{N}(c_k, c_l)$ being the number of loops arising when the coverings $\langle c_k|$ and $|c_l\rangle$ are drawn simultaneously on the same lattice (“transition graph”) and $\mathcal{N}_s = \frac{L}{2}$ stands for the number of singlets in the system. All singlets belonging to $|c_k\rangle$ are oriented; d denotes the number of *disoriented* ones one meets while moving along the loop in $\langle c_k|c_l\rangle$ containing i and j . Finally, $+\frac{3}{4}$ is taken if there is an even number of dimers between i to j , $-\frac{3}{4}$ in the opposite case. To find the ground state of Hamiltonian (1), one solves the generalized eigenproblem $H|\Psi_0\rangle = E_0 C|\Psi_0\rangle$, with C being the matrix formed from the scalar products $\langle c_k|c_l\rangle$.

The procedure of finding the ground state in the nonorthogonal RVB basis has an advantage that can be seen when one uses periodic boundary conditions and maps the periodicity of the Hamiltonian onto a regular polygon. The L (even number) vertices of this polygon represent L interacting Heisenberg spins $\frac{1}{2}$ and the L edges represent interactions between spins. Such a bipartite system of spins has $C_{L/2}^{L/2} / (\frac{L}{2} + 1)$ linearly independent RVB basis states—see, e.g., Ref. [9]—and each of them may be characterized by its *topological* winding number W (topological charge). To accomplish this, one chooses any basis state $|c_R\rangle$ as a reference state, as noticed in Ref. [11] (see definition on page 3) and obtains the winding number assigned to any other basis state $|c_l\rangle$ from the transition graph $\langle c_l|c_R\rangle$ [11] in the following way. The polygon, representing the spin system (vertices denote spins, edges denote interactions between them) divides the plane into two disjoint areas; one draws lines (green dashed in Fig. 1) connecting these areas and crossing each edge of the polygon. Eventually, after drawing the transition graph $\langle c_l|c_R\rangle$ on the polygon, one counts how many singlets are cut by the green-dashed lines connecting the inside and outside of the polygon (see Fig. 1). Note that the number of singlets cut by *any* green-dashed line modulo 2 equals 0 for Fig. 1(d) and 1 for Fig. 1(e). We therefore assign $W_{lR} = 0$ and $W_{kR} = 1$ to the basis states $|c_l\rangle$

and $|c_k\rangle$ with respect to the state $|c_R\rangle$. Taking other basis states as reference states and carrying out the similar procedure, one finds the matrix of winding numbers W_{pq} between all basis states.

The set of all basis states, after applying this definition, splits into two disjoint subsets (sectors) A and B regardless of the choice of the reference state $|c_R\rangle$: Each of the linearly independent basis states belongs to one of them. For indices which number basis states within one sector it holds that $W_{\alpha\alpha'} = W_{\beta\beta'} = 0$, while for different sectors one has $W_{\alpha\beta} = W_{\beta\alpha} = 1$ for $\alpha, \alpha' \in A$ and $\beta, \beta' \in B$. This division leads to the block antidiagonal form of the matrix W_{kl} ; see an example for $L = 8$ in the Supplemental Material [12]. The basis states belonging to the same sector can be transformed into each other by a sequence of *local* singlet moves. The transition graph resulting from a *local* move does not wind around the entire system with periodic boundary conditions. The basis functions from different sectors are not topologically equivalent: one can not pass from a basis state belonging to one topological sector to a basis state belonging to another sector by making only local singlet moves; at least one move is required for which the transition graph winds around the entire system. It means that the resonances between basis states from different sectors extend throughout the whole system (they are *global* ones), whereas for basis states from the same sector only *local* resonances exist. The global resonances are not topologically equivalent to the local ones.

In what follows, we apply the above observation to examine resonances present in the ground state of the system under consideration and show that their change from global to local ones while changing λ makes it possible to determine λ_c and critical exponents after applying the FSS technique. For this purpose, we consider how the following quantities depend on λ for systems of various sizes L :

- (i) $\eta_T(\lambda) = \langle \Psi_0(\lambda)|W|\Psi_0(\lambda)\rangle$ (topological charge),
- (ii) $\chi_l(\lambda) = \frac{\chi_T(\lambda)}{L} = \frac{1}{L} \langle \partial_\lambda \Psi_0(\lambda)|W|\partial_\lambda \Psi_0(\lambda)\rangle$ (we will henceforth call it topological fidelity susceptibility), and
- (iii) $\beta_l(\lambda) = \frac{\beta_T(\lambda)}{L} = \frac{1}{L} \langle \Psi_0(\lambda)|W|\partial_\lambda \Psi_0(\lambda)\rangle$ (we will henceforth call it topological connection).

The mean value of the Hermitian operator W (topological charge) informs us how large is the component of the vector $W|\Psi\rangle$ along $|\Psi\rangle$, i.e., what part of the state $|\Psi\rangle$ is composed of the basis functions belonging to different topological sectors. If there were present only local (global) resonances in this state, this value would be 0 (1). If, however, local and global resonances are present, this value will be between 0 and 1. Similarly, the value of $\chi_T(\lambda)$, being the inner product between $|\Psi_\lambda\rangle$ and $W|\Psi_\lambda\rangle$, tells us what amount of $W|\Psi_\lambda\rangle$ points in the direction of $|\Psi_\lambda\rangle$, i.e., what part of the fidelity susceptibility $\langle \partial_\lambda \Psi|\partial_\lambda \Psi\rangle$ is composed of the basis functions belonging to different topological sectors. Eventually, β_l reveals what part of the change of $|\Psi\rangle$, with λ remaining parallel to $|\Psi\rangle$ itself, is composed of basis functions belonging to different topological sectors. Thus, the change of η_T , χ_T , and β_l with λ enables the examination how the proportion changes between the basis states belonging to different topological sectors in a given state of the system. This is equivalent to the change of the ratio between local and global resonances in this state. As we will see further, η_T , χ_T , and β_l are subject to the finite-size scaling laws.

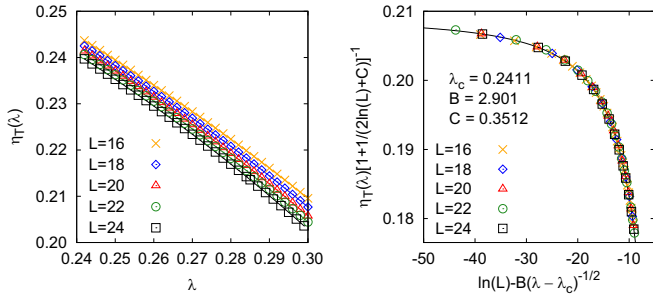


FIG. 2. Topological charge η_T dependence on λ above the transition ($\lambda_c = 0.2411$) before (left) and after (right) rescaling, according to Eq. (5), for systems up to 24 spins.

Finite-size scaling of the topological charge and calculation of the critical coupling in the system. Expressing the ground state in the RVB basis $|c_i\rangle$ and taking into account that for the system under consideration all the coefficients $\alpha_i(\lambda)$ in this expansion may be chosen to be *real numbers*, we find that

$$\eta_T(\lambda) = \sum_{k,l} \alpha_k(\lambda) \alpha_l(\lambda) W_{kl} \langle c_k | c_l \rangle. \quad (3)$$

Let us now assume that $\eta_T(\lambda, L)$ calculated for finite systems approaches, similarly to the spin stiffness (see Ref. [8] page 52 and Ref. [13]), its infinite size value with a logarithmic size correction, i.e.,

$$\eta_T(\lambda_c, L) = \eta_T(\lambda_c, \infty) \left(1 + \frac{1}{2 \ln(L) + C} \right), \quad (4)$$

and C is a system dependent parameter. Subsequently, using the FSS hypothesis and taking into account that above the transition correlation length ξ does not fall in a power-like manner, but rather exponentially [$\xi(\lambda) \sim \exp(B/\sqrt{|\lambda - \lambda_c|})$], leads [8] to the conclusion that

$$\eta_T(\lambda, L) \left(1 + \frac{1}{2 \ln(L) + C} \right)^{-1} = \Lambda \left(\ln(L) - \frac{B}{\sqrt{|\lambda - \lambda_c|}} \right), \quad (5)$$

with Λ being some universal scaling function. In Fig. 2 it is shown that the scaling given by Eq. (5) does occur: we observe the collapse of $\eta_T(\lambda)$ calculated for different values of L onto a single curve for $\lambda_c = 0.2411$, $B = 2.901$ and $C = 0.3512$. The value of B is related to the KT transition width. The transition in the considered system is much *broader* than that undergoing in the 1D Bose-Hubbard model ($B = 0.261$), in the XXZ spin- $\frac{3}{2}$ model ($B = 1.61$) [4], or in the 2D XY model ($B = 1.5$) [14]. This is also the reason why the maximum of χ_T is shifted quite far from λ_c .

Finite-size scaling of topological fidelity susceptibility. One can calculate the topological fidelity susceptibility $\langle \partial_\lambda \Psi_0(\lambda) | W | \partial_\lambda \Psi_0(\lambda) \rangle$ from Eq. (3) by replacing the coefficients α_k and α_l by their numerical derivatives with respect to λ . Its dependence on λ in systems up to $L = 24$ spins is shown in Fig. 3 (top left). Notice the two gray areas in this figure marked by A1 and A2.

The enlarged A1 area (right top of Fig. 3) shows the maximum of χ_T/L for 24 spins. From the position of this maximum, we can independently determine the numerical value of parameter B for the second time using the main

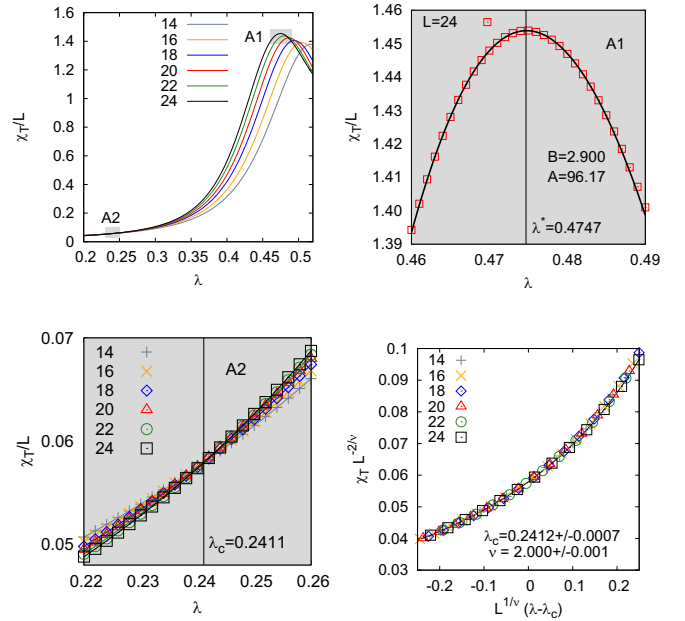


FIG. 3. Top left: Topological fidelity susceptibility for systems up to 24 spins versus λ . Top right: Enlarged maximum for 24 spins (grey area A1). Red squares: calculated values of χ_T/L ; black line: fit to Eq. (6). Bottom: Enlarged grey area A2 shows topological fidelity susceptibility before (left) and after rescaling (right) for systems with $L = 16-24$ spins. The scaling collapse leads to the optimal values of λ_c and exponent ν . The errors were estimated by finding the collapse several times, taking the numerical data with Gaussian noise with standard deviation equal to the accuracy of numerical differentiation while calculating χ_T .

result of Ref. [4]: The maximum of fidelity susceptibility χ_F should be shifted with respect to λ_c by the universal constant $\frac{B^2}{36}$. To prove this, the authors of Ref. [4] assumed that the singular part of the fidelity $\langle \Psi_0(\lambda_1) | \Psi_0(\lambda_2) \rangle$ near the critical point is a homogeneous function with respect to $\xi(\lambda_1)$ and $\xi(\lambda_2)$ and scales as [4] $\langle \Psi_0(\lambda_1) | \Psi_0(\lambda_2) \rangle = b^{-1} \Theta \left(\frac{\xi(\lambda_1)}{b}, \frac{\xi(\lambda_2)}{b} \right)$, with Θ being some universal function and b a scaling factor. From the definition of fidelity susceptibility, from this form of the scaling hypothesis, and from the exponential dependence of $\xi(\lambda)$, it follows that close to the critical point the fidelity susceptibility χ_F/L is given by

$$\chi_F(\lambda)/L = A \frac{\exp(-B/\sqrt{|\lambda - \lambda_c|})}{|\lambda - \lambda_c|^3}. \quad (6)$$

Let us now assume that χ_T , being a part of χ_F , is subjected to the same scaling. Then we can find B for the second time by fitting the calculated values of χ_T/L for 24 spins near its maximum to Eq. (6). The continuous line (in black) resulting from this fitting is shown on the right top of Fig. 3. The numerical value of $B = 2.900$ determined by this method agrees well with the B value obtained from topological charge scaling ($B = 2.901$). The slight difference of the last digit may be due to the fact that the system of 24 spins was treated as if it were an infinite one.

If we look more closely at the A2 area (left bottom of Fig. 3), we will see the crossing of χ_T/L calculated for systems from $L = 14$ to $L = 24$ spins for some value of λ_c . To

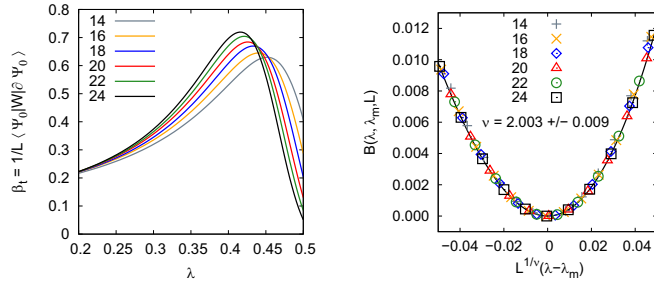


FIG. 4. Left: The topological connection $\frac{1}{L} \langle \Psi_0(\lambda) | W | \partial_\lambda \Psi_0(\lambda) \rangle$ versus λ before rescaling. Right: The value of the function $B(\lambda, \lambda_m, L)$ defined by Eq. (8) versus $L^{1/\nu}(\lambda - \lambda_m)$ for system sizes $L = 14$ – 24 . As expected from the finite-size scaling ansatz, the data for different system sizes collapse on a single curve for $\nu = 2.003$ (right). The error is estimated as explained in the caption of Fig. 3.

find this value and the critical exponent ν , one takes into account the argument that the topological fidelity susceptibility, $\chi_T(\lambda)$, after appropriate rescaling of arguments and function values, for different system sizes should collapse onto the same curve. Let us assume that the topological fidelity susceptibility $\chi_T(\lambda)$ at the critical point scales as the fidelity susceptibility $\chi_F(\lambda)$ [1,5,15]:

$$\chi_T(\lambda)/L = L^{2/\nu-1} \Phi(L^{1/\nu}(\lambda - \lambda_c)), \quad (7)$$

with Φ being a universal scaling function. The data from the left bottom of Fig. 3 have been plotted on the right side using rescaled values of each of the arguments $L^{1/\nu}(\lambda - \lambda_c)$ and the function $\chi_F(\lambda)L^{-2/\nu}$. Collapse occurs for $\lambda_c = 0.2412 \pm 0.0002$ and $\nu = 2.000 \pm 0.001$. The singular part of $\chi_T(\lambda)$ should scale as $|\lambda - \lambda_c|^{2-\nu}$ [5,15]. Since $\nu = 2$, this scaling behavior is subleading and the presence of χ_T peak is a result of the dependence $\xi(\lambda) \sim \exp(B/\sqrt{|\lambda - \lambda_c|})$. The value of $\nu = 2$ also results directly from Eq. (7), because then χ_T/L

does not depend on L , which leads to the crossing of χ_T curves for different L at the critical point.

Topological connection scaling. Let us now determine the subleading exponent ν for the second time from the FSS of the topological connection $\frac{1}{L} \langle \Psi_0(\lambda) | W | \partial_\lambda \Psi_0(\lambda) \rangle = \frac{1}{L} \sum_{k,l} \alpha_k \frac{\partial \alpha_l}{\partial \lambda} W_{kl} \langle c_k | c_l \rangle$. The topological connection dependence on λ displays a well-marked peak for some $\lambda_m(L) > \lambda_c$. This maximum shifts towards λ_c with increasing L [see Fig. 4 (left)], and the value of $\beta_t(\lambda_m)$ diverges logarithmically with L : $\beta_t(\lambda_m) \propto 0.170 \ln L$. Similar dependence was reported [16] for the phase transition in the ground state of the quantum XY chain. This logarithmic divergence suggests [17] that it is possible to extract a critical exponent ν from the scaling of the function

$$B(\lambda, \lambda_m, L) = (1 - e^{\beta_t(\lambda(L)) - \beta_t(\lambda_m(L))}) \propto L^{1/\nu} [\lambda(L) - \lambda_m(L)]; \quad (8)$$

$\lambda_m(L)$ stands for the peak position for a given L (Fig. 4 left) and $\beta_t(\lambda(L))$ for the topological connection near λ_c for a given L . All data for systems with different L collapse onto a single curve as shown in Fig. 4 (right), after taking $\lambda_c = 0.2411$ for $\nu = 2.003 \pm 0.009$.

Summary. The topological charge η_T , the topological susceptibility χ_T , and the topological connection β_t obey the finite-size scaling. The scaling occurs for relatively small systems. Treated as a test, this made it possible to determine accurately the critical coupling λ_c and subleading exponent ν in a well-known topological phase transition in a spin- $\frac{1}{2}$ Heisenberg chain with nearest- and next-nearest-neighbor interactions. We hope that the presented results will stimulate further exploration of topological critical phenomena in other *resonating valence bond* systems in which there is no possibility to define an order parameter.

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