Rapid Communications

Intrinsic jump character of first-order quantum phase transitions

Qiang Luo,[1,*] Jize Zhao,[2,†] and Xiaoqun Wang[3,4,‡]

[1]*Department of Physics, Renmin University of China, Beijing 100872, China*

[2]*School of Physical Science and Technology & Key Laboratory for Magnetism and Magnetic Materials of the MoE, Lanzhou University, Lanzhou 730000, China*

[3]*Key Laboratory of Artificial Structures and Quantum Control (Ministry of Education), School of Physics and Astronomy, Tsung-Dao Lee Institute, Shanghai Jiao Tong University, Shanghai 200240, China*

[4]*Beijing Computational Science Research Center, Beijing 100084, China*

(Received 25 June 2019; published 26 September 2019)

We find that the first-order quantum phase transitions (QPTs) are characterized by intrinsic jumps of relevant operators while the continuous ones are not. Based on such an observation, we propose a bond reversal method where a quantity $\mathcal{D}$, the difference of bond strength (DBS), is introduced to judge whether or not a QPT is of first order. This method is first applied to an exactly solvable spin-1/2 *XXZ* Heisenberg chain and a quantum Ising chain with a longitudinal field where distinct jumps of $\mathcal{D}$ appear at the first-order transition points for both cases. We then use it to study the topological QPT of a cross-coupled ($J_\times$) spin ladder where the Haldane–rung-singlet transition switches from being continuous to exhibiting a first-order character at $J_{\times,I} \simeq 0.30(2)$. Finally, we study a recently proposed one-dimensional analogy of a deconfined quantum critical point connecting two ordered phases in a spin-1/2 chain. We rule out the possibility of a weakly first-order QPT because the DBS is smooth when crossing the transition point. Moreover, we affirm that such a transition belongs to the Gaussian universality class with a central charge $c = 1$.

DOI: 10.1103/PhysRevB.100.121111

Introduction. Understanding how strongly correlated systems order into different phases as well as the transitions among them remains one of the most fundamental and significant problems in modern condensed matter physics [1–3]. In particular, the quantum phase transitions (QPTs), which occur at zero temperature, are omnipresent phenomena and could in general be classified into two types. One is continuous when the ground state of the system changes continuously at the transition point, accompanied by a diverging correlation length and vanishing energy gap. The other is, instead, of first order when the order parameter and other relevant observables display discontinuity across the transition point. While traditional continuous QPTs are well described by the Landau-Ginzburg-Wilson (LGW) theory, recent years have witnessed some exceptions such as topological QPTs [4–6] and deconfined quantum critical points (DQCPs) [7–10] that are beyond the scope of the LGW paradigm. The topological QPT may take place between two disordered phases, thus it cannot be detected by local order parameters [11,12]. What is more, it could be either continuous or of first order upon a fine-tuned interaction strength [13–16]. The DQCP was proposed by Senthil *et al.* [7,8] whereby a continuous QPT occurs between two spontaneously symmetry breaking (SSB) phases and the critical point implies an emergent symmetry. The *J*-*Q* model [9] is such an example where extensive numerical studies provide evidence for a continuous (or weakly first-order) transition between a Néel phase and a valence bond solid (VBS) phase [17–19].

In contrast to continuous QPTs, first-order QPTs are less studied so far despite appearing frequently in quantum many-body systems. Remarkably, a first-order QPT called a photon-blockade breakdown was observed experimentally in a driven circuit quantum electrodynamics system [20]. The finite-size scaling of gap and various probes borrowed from quantum information sciences near the transition points of the first-order QPTs have been discussed until recently [21–25]. Therefore, it is of vital importance to devise appropriate tools for a proper characterization of their dominating features.

Let us consider a Hamiltonian of the form [1]

$$\mathcal{H}(\lambda) = \mathcal{H}_0 + \lambda \mathcal{H}_I, \tag{1}$$

where λ is a driving parameter. If $\mathcal{H}_0$ and $\mathcal{H}_I$ commute, then both of them could be simultaneously diagonalized and eigenfunctions are independent of λ. This means that the spectra of $\mathcal{H}_0$ and $\mathcal{H}_I$ are irrelevant of λ, while the total ground-state energy $E_g(\lambda) = \langle \mathcal{H}(\lambda) \rangle$ could vary linearly with λ. Consequently, there can be a level-crossing point λ_t where the ground-state energy per site $e_g(\lambda) = (1/L)E_g(\lambda) = e_0 + \lambda e_I$ as a function of λ exhibits nonanalyticity. Here, L is the number of lattice sites. It should be aware that continuous QPTs could also occur and we move the discussion to the Supplemental Material (SM) [26]. Taking the derivative of $e_g(\lambda)$ with respect to λ, a jump of e_I at λ_t will appear, indicating a first-order QPT. The jump also reflects the structural change of the ground-state wave function. Because of the continuity of energy $e_g(\lambda)$, a similar jump for e_0 is also expected to

*qiangluo@ruc.edu.cn
†zhaojz@lzu.edu.cn
‡xiaoqunwang@sjtu.edu.cn

eliminate the singularity. To detect the transition point λ_t, a quantity $\mathcal{D}$, dubbed the difference of bond strength (DBS), is introduced to magnify the jump behaviors. It is defined as

$$\mathcal{D} = e_0 - \mathrm{sgn}(\lambda_t) e_I, \tag{2}$$

where the minus sign reflects the spirit of the bond reversal method. Nevertheless, in most systems the two terms $\mathcal{H}_0$ and $\mathcal{H}_I$ do not commute, resulting in a cumbersome expression of $e_g(\lambda)$ vs λ. However, the main spirit remains unchanged in that the jump character of $\mathcal{D}$ faithfully inherits the discontinuity of first-order QPTs.

In what follows we will first illustrate the bond reversal method in two different but thoroughly studied one-dimensional (1D) spin models that possess first-order QPTs: (i) a celebrated spin-1/2 Heisenberg *XXZ* chain for which all the energy as well as the DBS $\mathcal{D}$ can be calculated analytically and (ii) a quantum Ising chain with both longitudinal and transverse fields which does not host an exact solution but the transition line is well known. Having established the cornerstone of our method, we then apply it to (iii) a topological QPT of a cross-coupled spin ladder and (iv) a recently proposed spin-1/2 chain with DQCP, both of which are beyond the scope of the conventional LGW paradigm. All the models are studied by the density-matrix renormalization group (DMRG) method [32–35], which is a powerful tool for dealing with quantum-mechanical problems in 1D systems. We utilize the periodic boundary condition (PBC) for the first two cases to have a better comparison with the analytical results. For the latter cases, however, we turn to the open boundary condition (OBC) which is beneficial to large-scale numerical calculations.

XXZ chain. The 1D spin-1/2 Heisenberg *XXZ* chain has long served as the workhorse for the study of quantum magnetism [36]. Its Hamiltonian is given by

$$\mathcal{H} = \sum_{i=1}^{L} \frac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + \Delta S_i^z S_{i+1}^z, \tag{3}$$

where $S_i^{\pm} = S_i^x \pm i S_i^y$ is the raising/lowering operator at site i and Δ is the anisotropic parameter. In particular, in the region $-1 < \Delta \leqslant 1$ the ground state is a Luttinger liquid (LL) with a gapless excitation spectrum. The ground-state energy per site e_g in the thermodynamic limit (TDL) $L \to \infty$ can be calculated as [37–39]

$$e_g^{\mathrm{LL}}(\Delta) = \frac{\Delta}{4} - \frac{\sin \pi\upsilon}{\pi} \int_0^{\infty} \left(1 - \frac{\tanh \upsilon x}{\tanh x}\right) dx, \tag{4}$$

with $\Delta = \cos \pi\upsilon$. Beyond the critical region it presents a long-range ferromagnetic (FM) or antiferromagnetic (AFM) order, exhibiting in correspondence to the FM point $\Delta = -1$ a first-order QPT, and a continuous one belonging to the Kosterlitz-Thouless (KT) universality class at the AFM point $\Delta = 1$. In the FM phase ($\Delta < -1$), the spins are parallel along the z direction, resulting in $e_g^{\mathrm{FM}} = \Delta/4$. The spin-spin correlation functions could be obtained by the Hellmann-Feynman theorem. In the LL phase, however, no simple expressions for the correlation functions are available except for some rational υ values [40]. Historically, the explicit expressions of the correlation functions [26] were first given by Jimbo and Miwa in 1996 [41], and then simplified by Kato *et al.* several years later [42]. According to Eq. (2), the DBS is defined as $\mathcal{D}_L = \langle S_{L/2}^z S_{L/2+1}^z \rangle + 2\langle S_{L/2}^x S_{L/2+1}^x \rangle$.

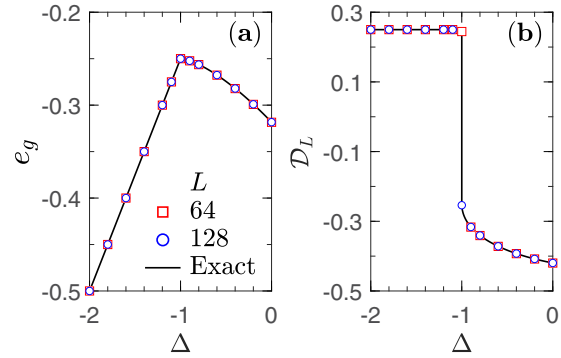

FIG. 1. (a) The ground-state energy e_g for $L = 64$ (red rhombus), 128 (blue circle), and TDL (black line). (b) The same setup as (a) for DBS $\mathcal{D}_L$.

At $\Delta = -1$ the Hamiltonian Eq. (3) possesses a hidden FM $SU(2)$ symmetry, resulting in a ground-state manifold of degenerate $SU(2)$ multiplets corresponding to the largest total spin. The model is not conformal invariant and dramatic changes in its entanglement behaviors occur [43–46]. In Fig. 1(a) we show the ground-state energy e_g around the transition point $\Delta = -1$. A vivid cusp of the energy curve could be spotted at $\Delta = -1$, while it turns to be a jump of $\mathcal{D}_L$ in Fig. 1(b). This gives clearly a first glance of the jump character of $\mathcal{D}$ in the first-order QPT [26].

Quantum Ising chain with longitudinal field. The 1D quantum Ising chain is integrable and its exact solution was presented by Pfeuty in 1970 [47]. It owns a continuous QPT of the Ising universality class separating a FM and a paramagnetic phase at the critical value of the transverse field $h_z(\geqslant 0)$ [48]. What is more, an emergent E_8 symmetry was experimentally verified around the critical point [49]. By introducing a longitudinal field h_x the model is no longer integrable except for a specially fine-tuned weak longitudinal field [50]. The total Hamiltonian is thus given by

$$\mathcal{H} = -\sum_{i=1}^{L} \left(\sigma_i^x \sigma_{i+1}^x + h_z \sigma_i^z + h_x \sigma_i^x\right), \tag{5}$$

where $\hat{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ are the Pauli matrices. In the FM phase ($h_z < 1$) of the magnetic phase diagram [24,51,52], a first-order QPT with a discontinuity of the magnetization, $M_x = \frac{1}{L}\sum_i \langle \sigma_i^x \rangle$, takes place at $h_x = 0$. Specifically, let $h_z = 1/2$, and we have the exact ground-state energy $e_{g,0} = -\frac{3}{4\pi} E(\sqrt{6\sqrt{2}}/3) \approx -1.0635$, where $E(\cdot)$ is the complete elliptic integral of the second kind [47]. As can be seen from Fig. 2(a), there is a pinnacle at $h_x = 0$ in the energy curve, and the symmetric feature is reminiscent of $\mathbb{Z}_2^x$ symmetry. The DBS is defined as $\mathcal{D}_L = \langle \sigma_{L/2}^x \rangle - \langle (\sigma_{L/2}^x \sigma_{L/2+1}^x + h_z \sigma_{L/2}^z) \rangle$, which is merely a shift of M_x by $e_{g,0}$ currently. In this occasion $\mathcal{D}_L$ plays the role of the order parameter M_x and it is no wonder that it exhibits a jump at $h_x = 0$ [see Fig. 2(b)]. In general, since DBS has an ambiguous relation with the order parameter, it is thus well founded to regard this jump as a signal for a first-order QPT [26].

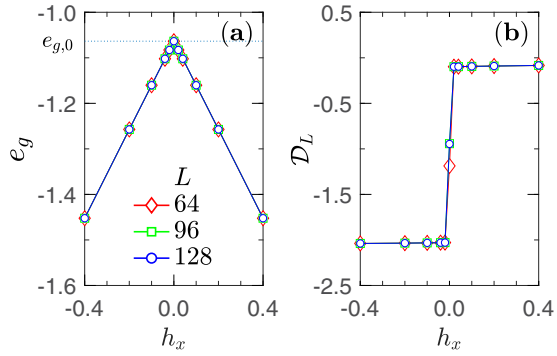

FIG. 2. (a) The ground-state energy e_g for $L = 64$ (red rhombus), 96 (green square), and 128 (blue circle). (b) The same setup as (a) for DBS $\mathcal{D}_L$.

Cross-coupled spin ladder. The role of frustration in quasi-1D magnetic materials has attracted numerous attention [36] ever since the discovery of high-temperature superconductivity in the 1980's [53]. The cross-coupled spin ladder [13,54,55], in particular, is one of the most outstanding models which is not only of theoretical importance [56–58] but also experimentally accessible [59]. The Hamiltonian of the model reads as follows,

$$\mathcal{H} = J_\parallel \sum_{i=1}^{L} \sum_{\alpha=1,2} \mathbf{S}_{i,\alpha} \cdot \mathbf{S}_{i+1,\alpha} + J_\perp \sum_{i=1}^{L} \mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2} \times J_\times \sum_{i=1}^{L} (\mathbf{S}_{i,1} \cdot \mathbf{S}_{i+1,2} + \mathbf{S}_{i,2} \cdot \mathbf{S}_{i+1,1}), \quad (6)$$

where $\mathbf{S}_{i,\alpha}$ denotes a spin-1/2 operator at site i of the α th leg. $J_\parallel (= 1)$ and $J_\perp$ are the nearest-neighbor (NN) interactions along the leg and rung directions, respectively. $J_\times > 0$ is the antiferromagnetic cross-coupled interaction.

Whereas a continuous QPT with a central charge $c = 2$ occurs at $J_\perp = 0$ in the absence of $J_\times$ [60], there have been contentious results for the past decade disputing the existence of nonzero $J_\times$. On the one hand, a columnar dimerized phase was predicted between the Haldane phase and the rung-singlet phase in a narrow parameter region at a weak cross-coupled interaction $J_\times$ [61]. Though some clues for the dimerized phase appear at the finite-size case [62,63], it is now generally believed that there is actually no such phase [64–68]. On the other hand, when $J_\times = 1$, the Hamiltonian of Eq. (6) undergoes a first-order QPT at $J_{\perp,t} = 1.401\,484$ [54]. Due to the dual symmetry of Eq. (6) [69], we shall just concentrate on the case where $J_\times$ is below the dual line $J_\times = 1$. Though various numerical calculations have firmly established that such a first-order QPT remains present for deviations away from the dual line as large as $J_\times = 0.6$, a unanimous conclusion has not been drawn on whether the first-order QPT could extend to all loci of the phase boundary or just end at a nonzero inflection point $J_{\times,I}$. At weak interchain couplings, an early analytic result predicted that the transition is always of first order [70], and later a numerical calculation of the same group yielded the conclusion [65]. Meanwhile, in the work of Wang [13], it is found that the first-order QPT is dismissed at $J_{\times,I} = 0.287$, and a continuous QPT down to

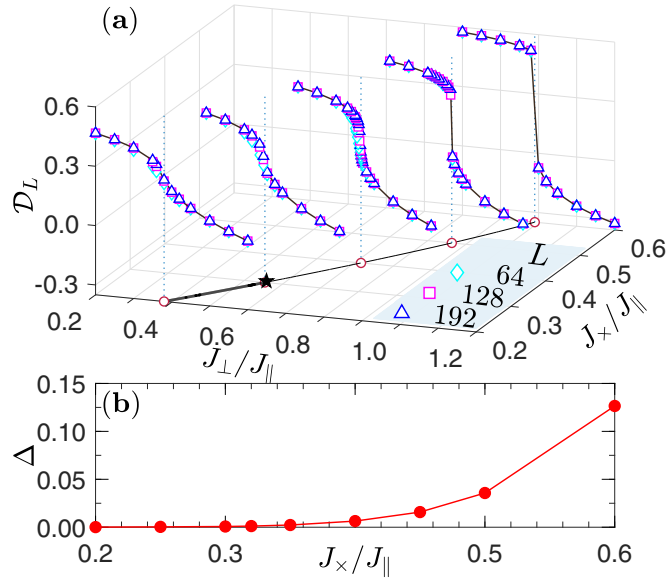

FIG. 3. (a) The DBS $\mathcal{D}_L$ for $L = 64$ (cyan rhombus), 128 (magenta square), and 192 (blue triangular) of different $J_\times$'s. The solid lines are guides for the eyes. In the bottom projection plane, the thick black line and the thin black line are the continuous and first-order phase boundaries, respectively. The pentagram (★) marks the inflection point. (b) The Haldane gap Δ along the phase boundary.

the vanishing interchain couplings takes over afterward. It is worth mentioning that the fact that a continuous QPT occurs at $J_\times = 0.2$ has been checked by the tensor network approach [68] and the quantum Monte Carlo method [55]. In view of the ambiguity, it is our purpose to determine the inflection point $J_{\times,I}$ accurately by the bond reversal method.

During each calculation we shall fix $J_\times$ and vary $J_\perp$ of Eq. (6). We thus define the DBS as $\mathcal{D}_L = \mathcal{R}_L - \mathcal{L}_L$, where $\mathcal{R}_L = \langle (S^z_{L/2,1} S^z_{L/2,2} + S^z_{L/2+1,1} S^z_{L/2+1,2}) \rangle$ and $\mathcal{L}_L = \langle (S^z_{L/2,1} + S^z_{L/2,2})(S^z_{L/2+1,1} + S^z_{L/2+1,2}) \rangle$ in a plaquette in the spirit of Eq. (2). In Fig. 3(a) we show the curvatures of DBS for different $J_\times$'s from 0.2 to 0.6. Here, we keep as many as 2000 states typically in our DMRG calculation and extend to 3000 states when necessary. For $J_\times = 0.5$ and 0.6, there is a jump of DBS in each case, indicating that a first-order QPT occurs. For other cases that are smaller than $J_\times = 0.4$, however, the curves are rather smooth and no conspicuous jumps are encountered. This is strong evidence that the transitions here are not of first order but continuous with a central charge $c = 2$ [26]. Whereas the curvatures of DBS for $J_\times = 0.4$ seem to be smooth, a jump which is a signal for a first-order QPT appears for a large enough system size [26]. We also calculate the energy gap of the Haldane phase, i.e., $\Delta_L = E_g(S^z_{\text{tot}} = 2) - E_g(S^z_{\text{tot}} = 0)$, and the results are shown in Fig. 3(b). It could be found that the gap is infinitesimal within our numerical precision when $J_\times \lesssim 0.30$, and it opens exponentially afterward. After a series of careful calculations we thus conclude that the inflection point $J_{\times,I}$ has a finite value of 0.30(2).

Spin-1/2 chain with DQCP. Whereas the DQCP was originally proposed in two-dimensional systems [7,8], the 1D analogy of DQCP was constructed quite recently [71] and

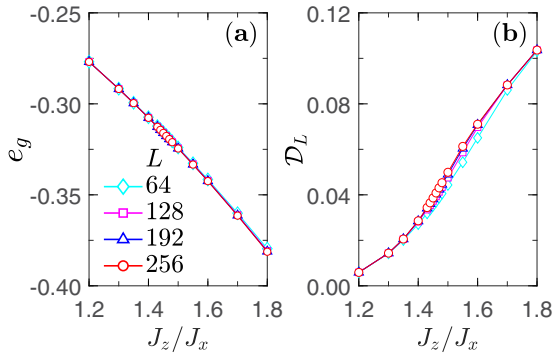

FIG. 4. (a) The ground-state energy e_g for $L = 64$ (cyan rhombus), 128 (magenta square), 192 (blue triangular), and 256 (red circle). (b) The same setup as (a) for DBS $\mathcal{D}_L$.

it has been studied by several parallel works on frustrated spin-1/2 chains with discrete symmetries [72–74]. For concreteness, we consider the following anisotropic model,

$$\mathcal{H} = \sum_{i=1}^{L} \sum_{\upsilon=x,z} -J_\upsilon S_i^\upsilon S_{i+1}^\upsilon + K_\upsilon S_i^\upsilon S_{i+2}^\upsilon, \tag{7}$$

where $J_\upsilon, K_\upsilon > 0$ so that the NN interactions are ferromagnetic while the second-NN interactions are antiferromagnetic. We shall treat the NN interaction $J_x = 1$ and fix the second-NN interaction $K = K_{x/z} = 1/2$ so that the only adjustable parameter is $J_z(>0)$. When J_z is not very large, the ground state of Eq. (7) could be continuously connected to that of the Majumdar-Ghosh point [75] where $J_z = 1$. This phase is the well-known dimerized VBS phase which breaks translational symmetry. On the contrary, in the regime where J_z is dominant, the spins align parallely along their z directions, resulting in a zFM phase with breaking $\mathbb{Z}_2^z$ symmetry. In the original work of Jiang *et al.* [71], the VBS-zFM transition was argued to be continuous, a transition which is at odds with the LGW theory where a direct transition between two states breaking irrelevant symmetries should be of first order. The critical point $J_{z,c}$ is called DQCP in analogy with its two-dimensional counterpart, and a continuous $O(2) \times O(2)$ symmetry emerges [71]. The model Eq. (7) has been studied by the matrix product state (MPS) which works directly in the TDL in two independent calculations [72,73]. Both order parameters of the SSB phases have a tiny but finite jump around the critical point. Notwithstanding, such a discontinuity is argued to be an artifact of the MPS method. In fact, the weakly first-order phase transition is hardly distinguishable from a continuous one [17–19], and thus meticulous calculations should be carried out to check the type of transition. We therefore resort to the DMRG method where up to 2000 states are kept to revisit this problem.

To begin with, we calculate the ground-state energy, and the energy curves shown in Fig. 4(a) are rather smooth. The DBS $\mathcal{D}_L = \langle S^z_{L/2} S^z_{L/2+1} - S^x_{L/2} S^x_{L/2+1} \rangle$ [see Fig. 4(b)] is continuous likewise when tuning J_z and no overt jump could be observed in the curves. This implies that the transition is indeed not a first-order one.

Because of the OBC utilized in our simulations, the VBS phase only has a unique ground state while the zFM phase still has twofold degeneracy. We define the energy gaps $\Delta_{1,2} = E_{1,2} - E_g$ as the total energy difference between the first/second excited states $E_{1,2}$ and the ground state E_g. In Fig. 5(a) we show energy gaps $\Delta_{1,2}$ vs J_z. With increasing J_z, Δ_1 decreases all the way and vanishes rapidly when crossing the critical point. For Δ_2, however, there is a minimum $\Delta^{\rm m}_{2,L}$ at each length L around the critical point. As shown in the inset, the $\Delta^{\rm m}_{2,L}$'s follow a linear scaling versus $1/L$ and the gap at TDL is 0.0000(4), indicating the closure of the energy gap at the critical point. Because of the linear scaling ansatz, the critical point is conformal invariant [76]. The von Neumann entropy (vNE) $\mathcal{S}_L$ is calculated by the minimal entangled ground state and the final result is shown in Fig. 5(b). A hump appears near the critical point, and this is more evidence of a continuous QPT. We fit the maxima of vNE $\mathcal{S}_L$ as a function of length L, $\mathcal{S}^{\rm m}_L = \frac{c}{6} \ln(\frac{2L}{\pi}) + c'$, where c is the central charge and c' is a nonuniversal constant [77]. We find that $c \simeq 1.02(5)$ at the critical point.

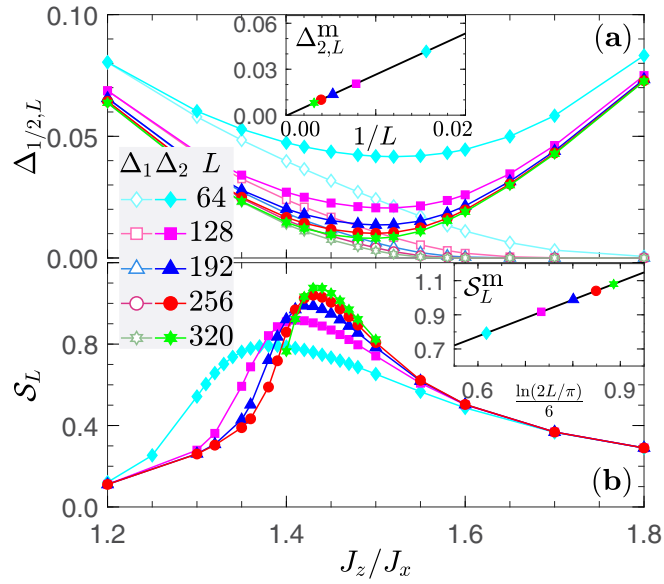

FIG. 5. (a) The first two energy gaps Δ_1 (open symbols) and Δ_2 (solid symbols). The inset shows a linear extrapolation of Δ_2 to TDL. (b) Evolution of vNE $\mathcal{S}_L$. Inset: Logarithmic extrapolation of peaks of $\mathcal{S}_L$ at different length L's.

We now calculate the critical point $J_{z,c}$ and critical exponents of the order parameters. The VBS phase is characterized by the difference of the adjacent bond strength, i.e., $M_L^{\rm VBS} = |\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle - \langle \mathbf{S}_{i-1} \cdot \mathbf{S}_i \rangle|$. The zFM phase has a nonzero local moment at each site and thus $M_L^{z\rm FM} = |\langle S_i^z \rangle|$. In practice, we could set $i = L/2$ to minimize the finite-size effect. Also, when calculating the $M_L^{z\rm FM}$, a finite pinning field of order 1 is added at the boundaries of the open chain so as to select a determinate ground state. Theoretically, the order parameter M_L vs J_z with the length L follows [78],

$$M_L(J_z) \simeq L^{-\beta/\nu} f_M(|J_z - J_{z,c}|L^{1/\nu}), \tag{8}$$

where the critical exponent ν describes the divergence of the correlation length and β is the critical exponent of the order parameter such that $M \sim |J_z - J_{z,c}|^\beta$ near the critical point $J_{z,c}$.

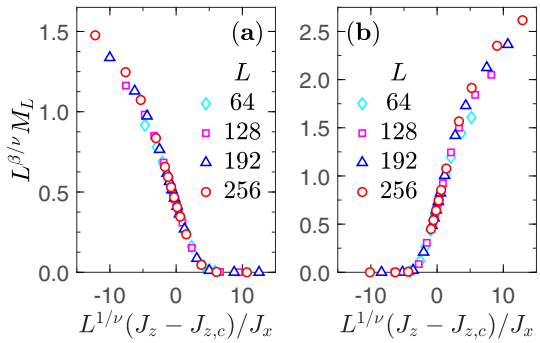

FIG. 6. The FSS of the order parameters (a) M_L^{VBS} and (b) $M_L^{z\mathrm{FM}}$. The critical point $J_{z,c}$ and critical exponents β and ν are shown in Table I.

In Fig. 6 we apply the finite-size scaling (FSS) method to the VBS [Fig. 6(a)] and zFM [Fig. 6(b)] phases in the range of $J_z \in [1.20, 1.80]$. The scaling results are fairly good when J_z is close to the critical point $J_{z,c}$. Some data, however, deviate from the scaling function when J_z is far away from $J_{z,c}$. The best fitting values of the critical point $J_{z,c}$ and critical exponents are presented in Table I. The overall critical point $J_{z,c} \simeq 1.4646(6)$, which is fairly consistent with previous work by Huang *et al* [73]. The critical exponents are almost identical for both order parameters, in agreement with the property of the DQCP [71]. The final results are $\beta = 0.53(3)$ and $\nu = 1.55(6)$. Interestingly, we find the quantity $2\nu(1 - 2\beta/\nu)$ is roughly equal to 1, as predicted from the Luttinger theory where both order parameters could be expressed by a sole Luttinger parameter [71,72]. We also check the cases where $K \neq 1/2$ [26] and indeed find that the critical exponents change with K. Together with the central charge $c \approx 1$, we could say that the VBS-zFM transition belongs to the Gaussian universality class and the critical point shows some similarities with the LL phase.

Conclusions. In this Rapid Communication, we propose a bond reversal method to determine a first-order quantum phase transition (QPT) by a quantity $\mathcal{D}$ called the difference of bond strength (DBS). A first-order QPT could be detected by a jump in DBS and the discontinuity point is exactly the transition point. The method is rather efficient and could be easily implemented in almost every numerical method. We use it to study two unconventional QPTs which are both beyond the scope of the Landau-Ginzburg-Wilson theory. For the cross-coupled ($J_\times$) spin ladder, we clarify that a continuous QPT indeed occurs at weak interchain couplings, and the inflection point separating the continuous and first-order QPTs is $J_{\times,I} \simeq 0.30(2)$. For a recently proposed spin-1/2 chain which owns two spontaneously symmetry breaking phases, we confirm that the transition is continuous because the DBS is fairly smooth and the energy gap vanishes when crossing the critical point. After a careful finite-size scaling analysis, we find that the transition belongs to the Gaussian universality class with the central charge $c = 1$.

TABLE I. Extracted critical point $J_{z,c}$ and corresponding critical exponents β and ν for the continuous VBS-zFM phase transition.

Phase	$J_{z,c}$	β/ν	$1/\nu$	β	ν	$2(\nu - 2\beta)$
VBS	1.4647(3)	0.344(2)	0.64(2)	0.53(2)	1.55(5)	0.98
zFM	1.4645(5)	0.350(3)	0.65(3)	0.54(2)	1.54(7)	0.92

Note added. Recently, we became aware of a work on a spin-1/2 chain with DQCP that supports our findings [79].

Acknowledgments. We thank S. Hu and S. Jiang for fruitful discussions. Q.L. was financially supported by the Outstanding Innovative Talents Cultivation Funded Programs 2017 of Renmin University of China. J.Z. was supported by the the National Natural Science Foundation of China (Grant No. 11874188) and the Fundamental Research Funds for the Central Universities. X.W. was supported by the National Program on Key Research Project (Grant No. 2016YFA0300501) and by the National Natural Science Foundation of China (Grants No. 11574200 and No. 11974244).

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