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Phase transitions and critical behaviors of XXZ ladders

Chengxiang Ding

School of Science and Engineering of Mathematics and Physics, Anhui University of Technology, Maanshan, Anhui 243002, People's Republic of China
E-mail: dingcx@ahut.edu.cn

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Abstract. We study the phase transitions and critical behaviors of the two-leg dimerized XXZ ladders by extensive Monte Carlo simulations and finite-size scaling analysis. For the Heisenberg model on the staggered ladder, we verify that the phase transition between the two topological phases belongs to the four-state Potts universality class; for the XY case ($\Delta = 0.5$), the phase diagram is similar to the Heisenberg case, but the critical behavior belongs to a new universality class; for the Ising case ($\Delta = 1.5$), we find three topological phases, in which one of them has both the topological orders and the local magnetic order; the two phase transitions associated with these phases also belong to the Ising universality class. On the columnar ladder, we have not found any phase transition for all the three cases. Furthermore, we find that the magnetic field can also induce phase transitions for both the staggered and columnar models, and the topological phases are in certain magnetic plateaux. For the staggered model, we study the phase transition associated with the plateau of zero magnetization; we find that the critical behavior of the string order parameter belongs to the 2D classical Ising model, and the scaling behavior of the uniform magnetization is different from the Dzhaparidze–Nersesyan–Pokrovsky–Talapov universality class. For the columnar model, we study the phase transition associated with the plateau whose magnetization is half of the saturation value, which has fractional quantized Berry phase; in this case, the conventional string order parameters are not applicable as order parameters, we determine the critical point of this phase transition by the scaling behavior of the uniform magnetization which is also different from the Dzhaparidze–Nersesyan–Pokrovsky–Talapov universality class.

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Keywords: quantum Monte Carlo simulations, quantum phase transitions, spin chains, ladders and planes, topological phases of matter

Contents

1. Introduction

In the Landau–Ginzburg theory [1], phase transition is associated with certain type of spontaneous symmetry breaking, and the universality class of the continuous transition is determined by the symmetry of order parameter and the dimension of space. However, recently several new types of phase transitions which go beyond the Landau paradigm have been found, such as the quantum deconfined phase transition [2–5], the spin liquid [8], and the topological phase transitions [9].

For the critical behaviors of these new types of phase transitions, the universality classes can not be simply speculated from the symmetry, although it is closely related to the symmetry. For example, the universality of the phase transition from superfluid to spin liquid has an obviously different critical exponent η from that of the ordinary XY universality class, which is called XY* universality class [10]. This is also the case for the topological phase transition, which is not characterized by any type of symmetry breaking. The topological phase transition are characterized by the change of certain type of topological number, such as the Chern number, the Berry phase [6], or the winding number [7]; it is not described by any type of local order parameter but certain type of nonlocal topological order. Typical examples can be found in quantum Hall states [11], the spin liquid [8], and the Kitaev spin systems [12].

Specifically, in the study of topological phase transitions of one dimensional quantum system, the string orders are introduced [13], which is widely used in both integrable and nonintegrable systems. For example, the topological phase transitions in cluster Ising models [14, 15], the Haldane phase and the related phase transitions in one dimensional bond-alternating Heisenberg chain [16], the spin ladders [18–21], and so forth.

Although the ground state of the uniform Heisenberg chain is the gapless Luttinger liquid, however, once the bond alternating is introduced, it becomes the gapped Haldane phase, and the related phase transitions belongs to the Gaussian universality class [16]. This indicate that bond alternating may introduce interesting topological phases and phase transitions, this is also the case for the Heisenberg ladders. Although the columnar dimerized ladder is always gapped thus no phase transitions [17], however, the gap can be closed in the staggered ladder [17], and the phase transition is between two types of topological string orders, which belongs to the four-state Potts universality class [18, 19]. Once more complicated interactions or magnetic field is introduced the topological phase transitions can be more complicated and interesting. For example, the ferromagnetic interaction can close the gap of columnar dimerized ladder, and a phase transition between the Haldane phase and a dimer phase is found [22]. The magnetic field can also induce phase transitions in the Heisenberg ladder, including the uniform field [24–26] and staggered field [27]. Specially, the magnetic field may induce magnetic plateaus, which may corresponds to fractional quantization of the Berry phase [28].

In this paper, we study the topological phase transitions of the two-leg XXZ ladder with bond-alternating by the quantum Monte Carlo simulations and finite-size scaling analysis. For the zero-field case of the staggered ladder, we not only confirm the four-state Potts universality class of the topological phase transition of the Heisenberg model ($\Delta = 1$), but also find a new universality class for the XY case ($\Delta = 0.5$) and several topological transitions which belong to the Ising universality class for the Ising case ($\Delta = 1.5$). For the nonzero-field case, we not only confirm the existence of magnetic plateaus, especially the half saturated plateau ($m = 0.25$) in the columnar ladder, but also study the critical properties of the phase transitions associated with the phases of these plateaus.

2. The model and method

As shown in figure 1, the Hamiltonian of the two-leg XXZ model in a magnetic field is written as

$$\mathcal{H} = J_{ij} \sum_{i=1}^{L} \sum_{j=1}^{2} \vec{S}_{i,j} \cdot \vec{S}_{i+1,j} + J_{\perp} \sum_{i=1}^{L} \vec{S}_{i,1} \cdot \vec{S}_{i,2} - h \sum_{i=1}^{L} \sum_{j=1}^{2} S^{z}_{i,j} \tag{1}$$

where $\vec{S}_i \cdot \vec{S}_j = S^x_i S^x_j + S^y_i S^y_j + \Delta S^z_i S^z_j$, and the periodic condition is applied in the leg direction, i.e. $\vec{S}_{L+1,j} = \vec{S}_{1,j}$. The coupling constant J_{ij} can be $J[1 + (-1)^{i+j}\delta]$ for the staggered model and $J[1 + (-1)^{i}\delta]$ for the columnar model, as shown in figure 1. In this paper, we fix $J = 1$ and $\delta = 0.5$; $J_{\perp}$, Δ, and h are tuning parameters.

To simulate the system, we use the stochastic series expansion (SSE) quantum Monte Carlo method with the direct loop algorithm [29]. In order to improve the efficiency, the Suwa–Todo algorithm [30] is adopted, which is an algorithm without detailed balance. The combination of the two algorithms enable us to simulate the model with large system size that reaches $L = 160$, thus enough to extrapolate the critical behaviors of the model. The SSE method is a finite-temperature method, but our purpose is to study the zero-temperature behaviors of the system, therefore, in the

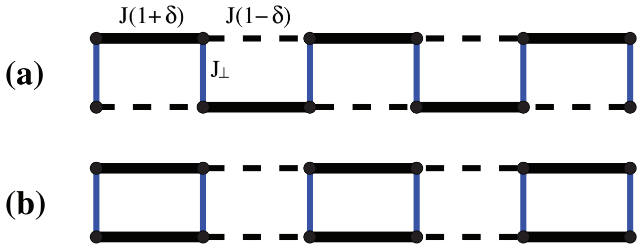

Figure 1. (a) The staggered model; (b) the columnar model.

simulations we set $T = 0.5/L$; the zero-temperature properties are obtained by taking the finite-size scaling, i.e. $T \to 0$ as $L \to \infty$.

The sampled variables include the two types of string order parameters S_e and S_o, the local order parameters m_u and m_s, and the Binder ratios of them

$$S_o = \langle \mathcal{S}_o \rangle, \quad Q_o = \frac{\langle \mathcal{S}_o \rangle^2}{\langle \mathcal{S}_o^2 \rangle}, \tag{2}$$

$$S_e = \langle \mathcal{S}_e \rangle, \quad Q_e = \frac{\langle \mathcal{S}_e \rangle^2}{\langle \mathcal{S}_e^2 \rangle}, \tag{3}$$

$$m_u = \langle \mathcal{M}_u \rangle, \quad Q_u = \frac{\langle \mathcal{M}_u^2 \rangle^2}{\langle \mathcal{M}_u^4 \rangle}, \tag{4}$$

$$m_s = \langle \mathcal{M}_s \rangle, \quad Q_s = \frac{\langle \mathcal{M}_s^2 \rangle^2}{\langle \mathcal{M}_s^4 \rangle}, \tag{5}$$

where $\mathcal{S}_o$, $\mathcal{S}_e$, $\mathcal{M}_u$, and $\mathcal{M}_s$ are defined as

$$\mathcal{S}_o = -\lim_{|n-m|\to\infty} S_n^{o,z} \cdot \exp\left[\mathrm{i}\pi \sum_{l=n+1}^{m-1} S_l^{o,z}\right] \cdot S_m^{o,z}, \tag{6}$$

$$\mathcal{S}_e = -\lim_{|n-m|\to\infty} S_n^{e,z} \cdot \exp\left[\mathrm{i}\pi \sum_{l=n+1}^{m-1} S_l^{e,z}\right] \cdot S_m^{e,z}, \tag{7}$$

$$\mathcal{M}_u = \left| \frac{1}{N} \sum_{i,j} S_{i,j}^z \right|, \tag{8}$$

$$\mathcal{M}_s = \left| \frac{1}{N} \sum_{i,j} (-1)^{i+j} S_{i,j}^z \right|, \tag{9}$$

with $S_l^{o,z} = S_{l,1}^z + S_{l,2}^z$, $S_l^{e,z} = S_{l,1}^z + S_{l+1,2}^z$, and $N = 2L$ the number of sites of the ladder. Because we are simulating the finite system, thus in practice we let the length from n to m be $L/2$.

In order to get the critical exponent, we can use the finite-size scaling theory. In the vicinity of the critical point, the Binder ratio satisfies the following form

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$$Q = Q_0 + \sum_{k=1} a_k(p - p_c)^k L^{ky_t} + \cdots + \sum_{i=1} b_i L^{y_i}, \tag{10}$$

where p is the tuning parameter, i.e. p can be $J_\perp$ or h, and $p_c = J_{\perp c}$ or h_c is the critical point of the phase transition. y_t is the thermal exponent in the renormalization, it is related to the critical exponent ν with $y_t = 1/\nu$, where ν describes the divergence of the correlation length ξ, i.e. $\xi \sim |p - p_c|^{-\nu}$. $y_i < 0$ is the irrelevant exponent in the renormalization, and the corresponding items are the corrections to scaling. Q_0, a_k and b_i are unknown parameters.

At the critical point, the order parameters satisfy the following formulas

$$S = L^{2[y_h-(d+z)]}(a + bL^{y_i}), \tag{11}$$

$$m_u = aL^{y_m-(d+z)}(a + bL^{y_i}), \tag{12}$$

$$m_s = aL^{y_s-(d+z)}(a + bL^{y_i}), \tag{13}$$

where S is the string order parameters S_e or S_o, d is the space dimension of the system, in current paper, it is 1. $z = 1$ is the dynamical critical exponent of the XXZ model. y_h, y_m, or y_s is the magnetic exponent in the renormalization, it is related to the critical exponent β with y_h, y_m, or $y_s = d + z - \beta/\nu$, where β describes the asymptotic behavior of the order parameters, i.e. $S \sim |p - p_c|^{2\beta}$, $m_u \sim |p - p_c|^{\beta}$, or $m_s \sim |p - p_c|^{\beta}$; β is different for different order parameter of a given phase transition.

By fitting the data according to equations (10)–(13), we can get the critical point and the critical exponent y_t, y_m, and y_h, thus determine the universality class of the phase transition.

3. Results

3.1. The cases with no magnetic field

Firstly, we pay attention to the critical behaviors of the Heisenberg case, i.e. $\Delta = 1$, and in the simulations, we set $\delta = 0.5$. This case has ever been studied by the method of exact diagonalization [19], however, because the system size is too small, the results are not accurate enough. Here, we study it by extensive Monte Carlo method. It is confirmed that there is a phase transition between the two topological phases, as shown in figure 2, the system is in a topological phase with S_o order when $J_\perp < J_{\perp c} \approx 1.23$ but S_e order when $J_\perp > J_{\perp c}$. Analytical work [31] based on mean-field method shows that the S_o ordered phase has a winding number $N_w = 1$ and the S_o order phase has a winding number $N_w = 0$.

The critical point can be located by the Binder ratio Q_o or Q_e, as shown in figure 3. In order to get an accurate estimation of this critical point and also the critical exponent y_t, we do extensive simulations in the vicinity of $J_{\perp c}$, which is in a very small range of $J_\perp$; the largest system size reaches $L = 160$. The data of Q_e is shown in figure 4; fitting the data according to equation (10) with $L_{\min} = 24$, we get $J_{\perp c} = 1.226\,53(8)$ and $y_t = 1.40(1)$. The critical point we get coincides with that in [32], which is obtained by the scaling behaviors of the Berry phase and Berry connection based on path-integral quantum Monte Carlo simulations. For the critical exponent y_t, it should be noted that the estimated value has small deviation from the theoretical prediction $y_t = 1.5$, the reason is the logarithmic correction to scaling [33]. In the theoretical prediction [18], the universality class of the model belongs to the four-state Potts model, owing to the $Z_2 \times Z_2$ hidden symmetry [31]; the four-state Potts is one of the cases of the conformal field theory [34] with central charge $c = 1$, the marginal operator in this $c = 1$ space leads to the logarithmic corrections [35] and certain uncertainty in determining the universality class, except the Baxter–Wu model [36–38]. In the finite-size scaling analysis, if the logarithmic correction is not included, the result of y_t generally has some deviation from the exact value [32, 33, 39]. One may expect the result can be much better if the logarithmic correction is included, however, a meaningful data fitting with logarithmic correction need very large system size, which will be very difficult in practice; for example, in [39] although the system size reaches $L = 256$, the error bar is still too large. Therefore, in current paper we do not pursue this aspect.

In order to determine the critical exponent y_h, we simulate at the estimated critical point $J_{\perp c}$ and fitting the data of S_o and S_e (as shown in figure 5) according to equation (11), the best estimation gives $y_h = 1.87(1)$, this result coincides with the theoretical result $y_h = 1.875$.

In summary, for the Heisenberg case with no magnetic field and $\delta = 0.5$, we give very accurate result of the critical point $J_{\perp c} = 1.226\,53(8)$, and confirm that the phase transition is in the universality class of four-state Potts model.

Secondly, by the same way, we simulate the XY case with $\Delta = 0.5$, in this case the phase transition is also between the two types of topological phases, as shown in figure 6. Fitting the data according to equation (10), we get the critical point $J_{\perp c} = 1.2204(5)$ and the critical exponent $y_t = 0.99(2)$. Furthermore, we simulate at this critical point, the data of S_e and S_o are shown in figure 7; fitting the data according to equation (11), we get the critical exponent $y_h = 1.76(1)$ from S_e and $y_h = 1.753(5)$ from S_o. From these estimated values of critical exponents, we know the phase transition belongs to a new universality class that is different from the four-state Potts model.

Thirdly, we study the Ising case, with $\Delta = 1.5$; in this case, the phase diagram is much different from the Heisenberg case and XY case, as shown in figure 8. There are two phase transitions between three ordered phases; when $J_\perp < J_{\perp c1} \approx 1.0$, the system has S_o topological order; when $J_\perp > J_{\perp c2} \approx 1.4$, the system has S_e topological order; when $J_{\perp c1} < J_\perp < J_{\perp c2}$, the system has both S_o and S_e topological orders, and also the symmetry breaking order m_s. Furthermore, we do extensive simulations in the vicinity of the critical points and fit the data according to equation (10), we get $J_{\perp c1} = 1.033(1)$ and $y_t = 1.01(2)$ for the first phase transition, and $J_{\perp c2} = 1.443(1)$ and $y_t = 0.99(2)$ for the second phase transition. In the estimated critical points, we do further simulations and fit the data according to equation (11) or (13); at the critical point $J_{\perp c1}$, we get $y_h = 1.87(1)$ from S_e and $y_s = 1.872(7)$ from m_s; at the critical point $J_{\perp c2}$, we get $y_h = 1.871(8)$ from S_o and $y_s = 1.88(1)$ from m_s; all of the results are consistent with the magnetic exponent of Ising model, which is 15/8. From the estimations of y_t, y_h, and y_s, we conclude that the two phase transitions belongs to the Ising universality class.

At last of this section,we summarize the phase transitions and universality classes of the two-leg staggered XXZ ladder that we studied in figure 9.

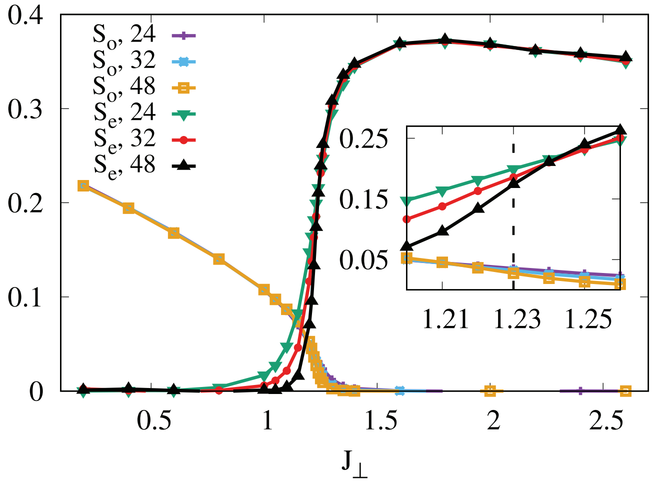

Figure 2. Order parameters of the Heisenberg model on the staggered ladder, with $\delta = 0.5$; the inset is a zoom into the region around the critical point.

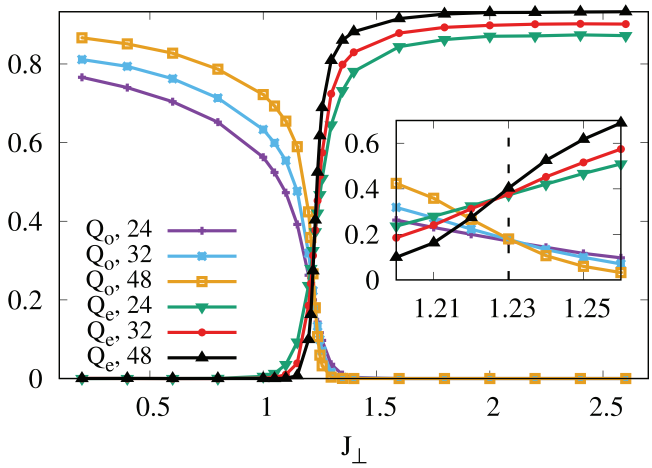

Figure 3. Binder ratio of the Heisenberg model on the staggered ladder, with $\delta = 0.5$; the inset is a zoom into the region around the critical point.

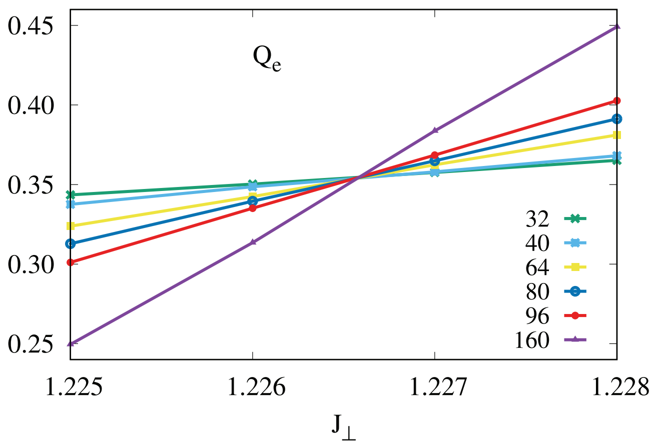

Figure 4. (a) Binder ratio Q_e of the Heisenberg model on the staggered ladder, with $\delta = 0.5$.

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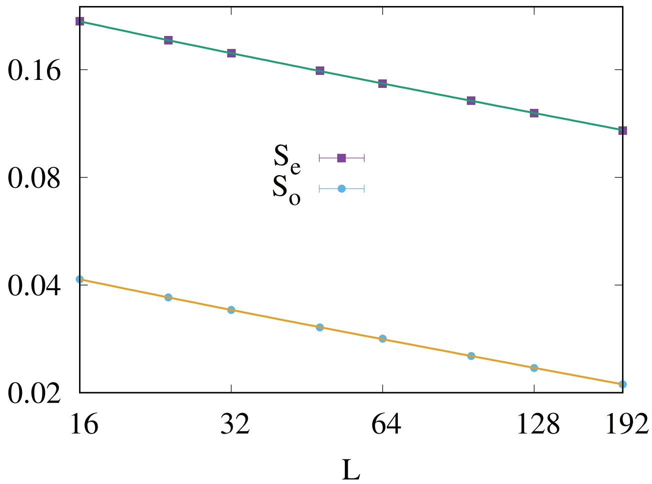

Figure 5. Log–log plot of the critical behaviors of the order parameters of Heisenberg model on the two-leg staggered ladder, with $\delta = 0.5$ and $J_\perp = J_{\perp c} = 1.226\,53(8)$.

For the two-leg columnar ladder, the Heisenberg model is always gapped, thus there is no phase transitions [17]; for the XY case and Ising case, we have not find any phase transition either.

3.2. In the presence of magnetic field

When the magnetic field is included, phase transition exists in both the staggered model and columnar model; some of the phases are in the magnetic plateaux. As shown in figure 10, there are two plateaux with $m_u = 0$ and $m_u = 0.5$ (saturated magnetization) for the staggered Heisenberg model with $\delta = 0.5$ and $J_\perp = 0.2$. In the figure, it is very clear that in phase I, the system has zero magnetization and zero S_e but non-zero S_o; in phase II, both S_e and S_o are zero. In order to study the critical behaviors of the phase transition from I to II, we do extensive simulation in the vicinity of the transition point; both the Binder ratios Q_o and Q_m can give the critical point, which is $h_c = 1.0606(12)$, and the critical exponent is $y_t = 1.03(4)$, which coincides with that of Ising model. Furthermore, fitting the data of S_o at the critical point according to equation (11), we get $y_h = 1.87(1)$, which confirms the Ising universality class of this phase transition. Fitting of the data of m_u according to equation (12), we get $y_m = 1.25(2)$, which is obviously different from that of Ising model (i.e. 15/8); this is not strange, because in phase II, although the magnetization m_u is nonzero, it does not means the phase has any symmetry breaking, thus there is no reason to expect $y_m = 15/8$.

The critical behavior of the field-induced second-order transitions of the uniform XXZ chain is described by

$$(m_u - m_{uc})^2 \sim h^2 - h_c^2, \tag{14}$$

which is called Dzhaparidze–Nersesyan–Pokrovsky–Talapov universality class [23, 24]. In equation (14), m_{uc} is the value of the magnetization of the plateau, for the uniform chain $m_{uc} = 0.5$ is the saturated value, and $h_c = 1 + \Delta$ is the critical value of the field. Equation (14) means that as h approaching the critical value h_c, $|m_u - m_{uc}|$ scales as

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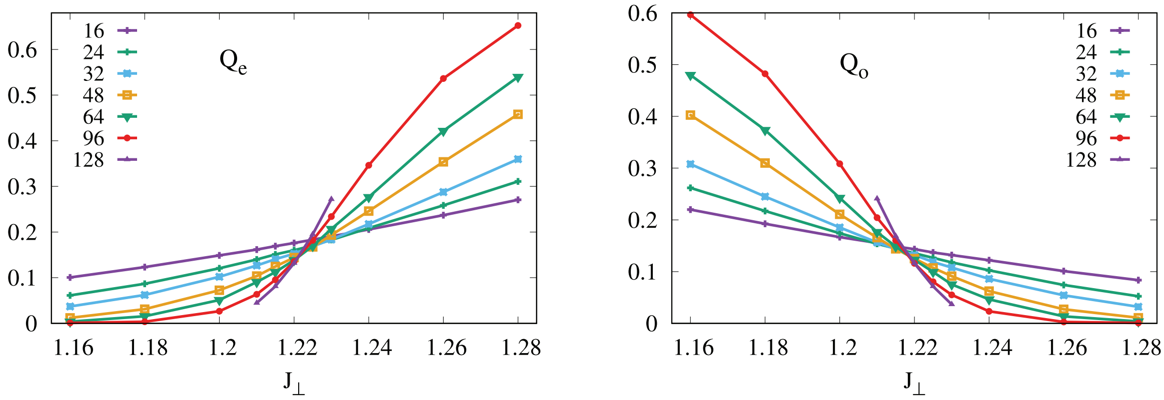

Figure 6. Binder ratio of the staggered XXZ ladder on the staggered ladder, with $\delta = 0.5$ and $\Delta = 0.5$.

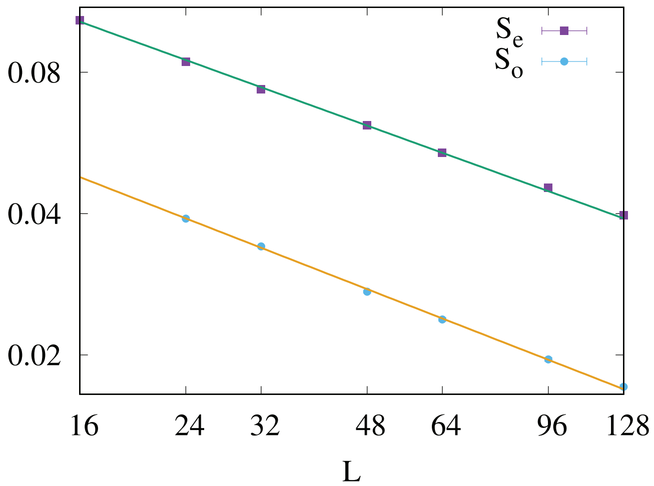

Figure 7. Log–log plot of the critical behaviors of the order parameters of the XXZ model on the staggered ladder, with $\delta = 0.5$ and $\Delta = 0.5$.

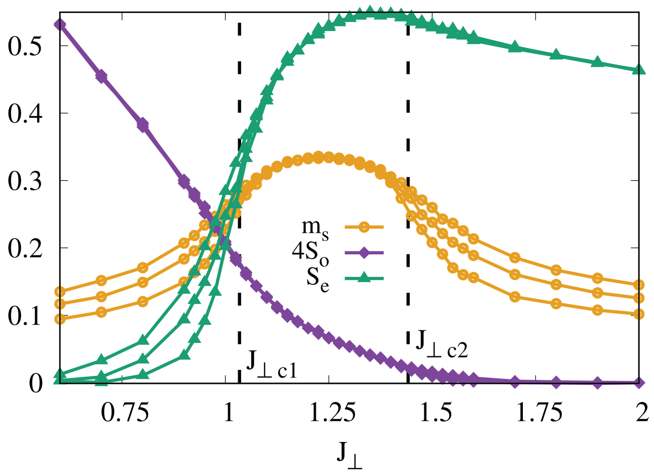

Figure 8. Order parameters of the staggered XXZ ladder, with $\delta = 0.5$ and $\Delta = 1.5$.

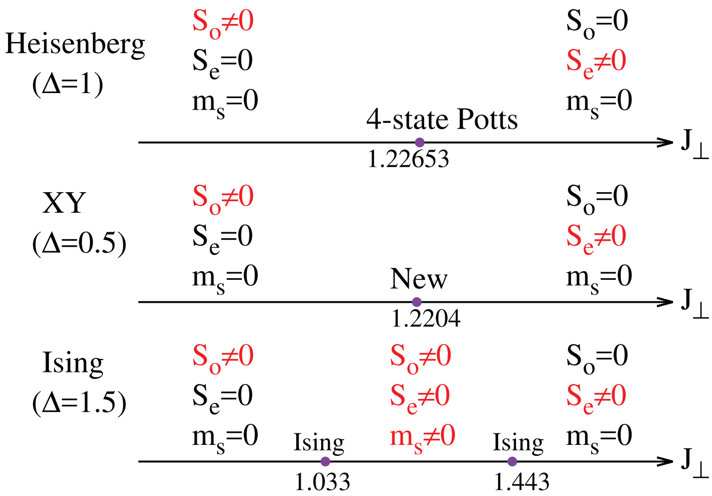

Figure 9. Phase transitions and universality classes of the staggered XXZ ladder, with $\delta = 0.5$; the dots are the critical points. The 'New' universality of the XY case has critical exponents $y_t = 1$ and $y_h \approx 1.75$.

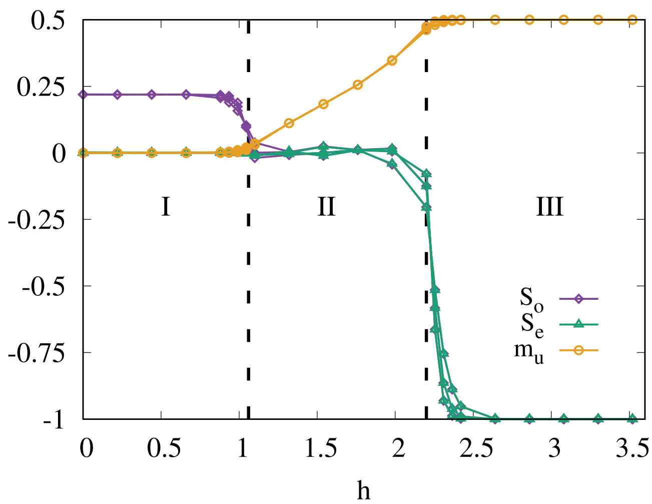

Figure 10. Order parameters of the Heisenberg model on the staggered ladder, with $\delta = 0.5$ and $J_\perp = 0.2$. In phase III, $m_u = 0.5$ is the saturated magnetization.

$$|m_u - m_{uc}| \sim (h - h_c)^{1/2}, \tag{15}$$

this means the critical exponent $\beta = 1/2$, thus the renormalization exponent $y_m = 2 - \beta/\nu = 1.5$. This is different from the result of the staggered ladder, we also numerically verify this conclusion by the finite-size scaling; as shown in figure 11, the slope of the log–log line of the critical value of $|m_u - m_{u_c}|$ versus L for the staggered ladder is obviously different from that of the uniform Heisenberg chain. Therefore, the field-induced second-order phase transition of the staggered ladder does not belong to the Dzhaparidze–Nersesyan–Pokrovsky–Talapov universality class. Note that the field-induced phase transition in the XXZ chain is between a gapless phase and a gapped phase, while the field-induced phase transition in the XXZ ladder is between two gapped phases, thus the universality classes can be different.

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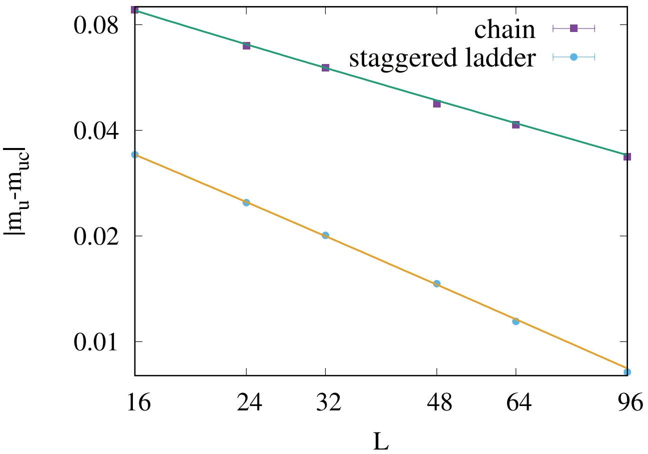

Figure 11. Uniform magnetization of the Heisenberg chain and staggered ladder. For the chain, $h_c = 1 + \Delta = 2$, $m_{uc} = 1$; for the staggered ladder, $\delta = 0.5$, $J_\perp = 1$, $h_c = 1.0606(12)$, $m_{uc} = 0$.

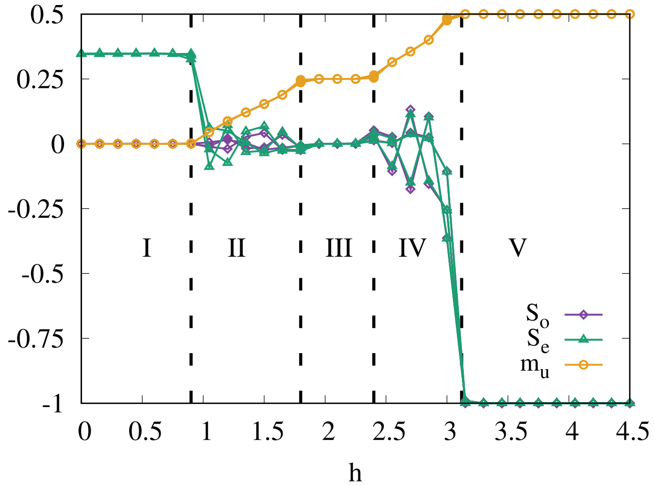

Figure 12. Order parameters of the Heisenberg model on the columnar ladder, with $\delta = 0.5$ and $J_\perp = 1$. In phase V, $m_u = 0.5$ is the saturated magnetization; in phase III, $m_u = 0.25$ is the half saturated magnetization.

For the columnar ladder, as shown in figure 12, the magnetic field also induces a topological phase transition from the phase I with S_e order to phase II. However, instead of study the critical behavior of this phase transition, here we pay attention to another phase transition, i.e. the phase transition from phase III to phase IV. Phase III is in a plateau of magnetization with $m_u = 0.25$ (half saturation), and this phase is said to have a fractional quantization Berry phase, which is $\pi/2$ instead of π [28], thus it is very interesting to study the critical behavior associated with this phase. However, as shown in the figure both the III and IV phases have zero value of S_e and S_o, although in phase IV S_e and S_o show much stronger fluctuation than that in phase III, therefore S_e and S_o are not applicable to be the order parameters here. However, the value of m_u shows substantial changes from phase III to phase IV, thus here we use the value of $m_u - 0.25$ as a detector of this phase transition, the critical point and the critical exponent y_t can be determined by the corresponding Binder ratio, which are $h_c = 2.4076(8)$

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and $y_t = 0.99(1)$. We also simulate at the critical point, finite-size scaling analysis of m_u gives $y_m = 1.24(1)$, this coincides with the result of the aforementioned staggered model; it also does not belong to the Dzhaparidze–Nersesyan–Pokrovsky–Talapov universality class.

4. Conclusion and discussion

In summary, we have studied the phase transitions and critical behaviors of the dimerized XXZ ladders, mainly about the staggered cases. For the Heisenberg model on the two-leg staggered ladder, we confirm the four-state Potts universality class of the phase transition, which is between two types of topological phases. For the XY case ($\Delta = 0.5$), the phase transition is also between the two topological phases, but the universality class is a new one that is different from the four-state Potts model. For the Ising case ($\Delta = 1.5$), the phase transitions are also studied, we find two topological phase transitions which belong to the Ising universality class.

We also studied the field-induced phase transitions in both the staggered and columnar models. For the staggered ladder, we find that the critical behavior of the string order parameter belongs to the 2D classical Ising model, and the scaling behavior of the uniform magnetization is different from the Dzhaparidze–Nersesyan–Pokrovsky–Talapov universality class.

For the columnar model, the conventional string orders are not applicable as the order parameters; the critical point is determined by the critical behavior of the uniform magnetization which is also different from the Dzhaparidze–Nersesyan–Pokrovsky–Talapov universality class. In this case, it is an interesting question whether we can define a topological order parameter like but different to the conventional string orders S_o or S_e, however, currently we are not clear about what this order parameter is, we leave this question for further study.

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