Special Transition and Extraordinary Phase on the Surface of a Two-Dimensional Quantum Heisenberg Antiferromagnet

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Abstract

Continuous phase transitions exhibit richer critical phenomena on the surface than in the bulk, because distinct surface universality classes can be realized at the same bulk critical point by tuning the surface interactions. The exploration of surface critical behavior provides a window looking into higher-dimensional boundary conformal field theories. In this work, we study the surface critical behavior of a two-dimensional (2D) quantum critical Heisenberg model by tuning the surface coupling strength, and discover a direct special transition on the surface from the ordinary phase into an extraordinary phase. The extraordinary phase has a long-range antiferromagnetic order on the surface, in sharp contrast to the logarithmically decaying spin correlations in the 3D classical O(3) model. The special transition point has a new set of critical exponents, $y_s = 0.86(4)$ and $\eta_\parallel = -0.32(1)$, which are distinct from the special transition of the classical O(3) model and indicate a new surface universality class of the 3D O(3) Wilson-Fisher theory.

1 Introduction

Exotic states of matter and unconventional phase transitions are the central topics of condensed matter and statistical physics. As the system undergoes a continuous phase transition in the bulk, its boundary also exhibits critical behavior [1, 2]. The surface critical behavior falls into different universality classes, which are are controlled by the surface interactions and are richer than the corresponding bulk criticality. They correspond to the fixed points of the renormalization group transformation of the surface coupling parameters, and are captured by the conformally invariant boundary conditions of the boundary conformal field theory (BCFT) [3–5]. Therefore, the investigation of possible surface critical universality provides a window looking into the BCFT in complement to the bootstrap and holographic approaches [6, 7].

The surface criticality has attracted renewed interest recently, which was partly motivated by the study of the gapless edge states of topological phases. A new surface universality class of the (2+1)-dimensional O(3) Wilson-Fisher quantum critical point (QCP) was observed in quantum antiferromagnetic (AF) Heisenberg models with gapless edge states composed of dangling spin-1/2 sites [8–11], but the necessity of the edge states was also questioned by the observation of similar surface critical exponents in spin-1 models [12], which do not have gapless edge states.

The surface critical behavior of the classical O(N) models was believed to be well-documented in the literature [1, 2, 13, 14]. In the three-dimensional (3D) Ising model ($N = 1$), the surface

criticality is controlled by the ratio of the surface and the bulk coupling parameters, $\kappa = J_s/J$. For κ smaller than a critical value κ_c, the surface criticality is only induced by the bulk phase transition at $T_{c,b}$ and belongs to the ordinary class. When $\kappa > \kappa_c$, the surface forms a long-range order below a critical temperature $T_{c,s} > T_{c,b}$. In this case, the surface is already ordered at $T_{c,b}$ but shows extra weak singularities, which is dubbed the extraordinary transition. At $\kappa = \kappa_c$, $T_{c,s}$ merges with $T_{c,b}$, leading to a special transition on the surface. These surface universality classes are characterized by a set of critical exponents.

The surface criticality of the 3D $O(N)$ models with $N \geq 2$ are more subtle, because the 2D surface itself cannot have long-range order for $T > T_{c,b}$ due to the celebrated Mermin-Wagner-Hohenberg theorem. In the 3D $O(2)$ model, the surface undergoes a Berezinskii-Kosterlitz-Thouless transition at $T_{c,s} > T_{c,b}$ for $\kappa > \kappa_c$ and develops a quasi-long-range order for $T < T_{c,s}$, but the nature of the surface extraordinary phase at $T_{c,b}$ remained elusive [13]. In the 3D $O(3)$ model, there is not any phase transition on the surface above $T_{c,b}$, thus it was not expected to show any special or extraordinary transitions, even though there was preliminary numerical evidence of a possible special transition in the strong coupling regime on the surface [13].

Motivated by the numerical evidence of a nonordinary transition in the (2+1)D $O(3)$ models, a recent theoretical work [15, 16] proposed that the spin fluctuations on the surface is marginally irrelevant for $2 \leq N \leq N_c < \infty$ due to its coupling to the bulk critical state. The spin correlation on the surface is predicted to decay logarithmically, $C_{\parallel}(r) \propto [\log(r/r_0)]^{-q_{\parallel}}$. Therefore, such surface critical behavior is dubbed the extraordinary-log phase.

Guided by this proposal, the surface criticality of the 3D classical $O(2)$ and $O(3)$ models have been numerically revisited recently [17, 18]. It is found that increasing the surface coupling strength leads to a special transition from the ordinary phase to an extraordinary phase in both models, and the spin correlation in the extraordinary phase decays logarithmically, which is consistent with the postulated extraordinary-log phase. The anomalous dimension of the magnetic order at the special transition of the $O(3)$ model is numerically close to that in the (2+1)D quantum Heisenberg models with dangling spins [17].

In a different theoretical approach [19], a spin-1/2 Heisenberg chain coupled to the ordinary surface of a (2+1)D $O(3)$ QCP was studied with the non-Abelian bosonization and the renormalization group analysis. It is shown that the Luttinger liquid phase of the spin chain is destabilized by its coupling to the bulk and gives way to either an AF order or a valence bond solid (VBS) order, and there is a direct surface transition in between. The nonordinary surface critical state found in numerical simulations [8–11] was argued to correspond to the AF phase with a vanishingly small order parameter [1].

In this work, we reexamine the spin-1/2 quantum Heisenberg model on a dimerized square lattice, which is shown in Fig. 1 (a). At the bulk QCP, it was found to show the nonordinary critical behavior on the surface formed by cutting the strong bonds and exposing dangling spins, and show the ordinary critical behavior otherwise [9]. Starting from the ordinary phase of the nondangling surface, we show that increasing the surface coupling leads to a special transition into an extraordinary phase, which is illustrated in the surface phase diagram in Fig. 1 (b). The extraordinary phase has a long-range AF order on the surface, in sharp contrast to the extraordinary-log phase of the 3D classical $O(2)$ and $O(3)$ models. Moreover, we find that the critical exponents at the special transition are distinct from those at the special transition of the 3D classical $O(3)$ model [17], thus indicate a new surface universality class of the 3D $O(3)$ Wilson-Fisher theory.

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[1]Our further numerical study of the Heisenberg model with a dangling spin chain will be presented elsewhere.
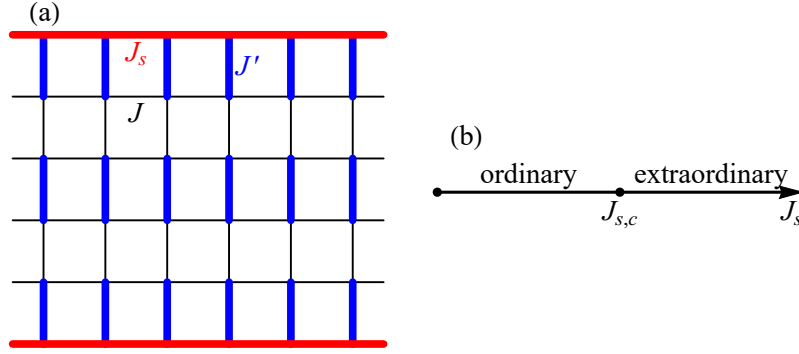
Figure 1: (a) The dimerized square lattice Heisenberg model with two open boundaries. J' and J are the coupling parameters of the strong (blue) and the weak (black) bonds in the bulk, repectively. J_s is the coupling in the surface layer (red bonds). (b) Schematic phase diagram of the surface critical behavior at the bulk quantum critical point. A special transition is found at $J_{s,c} = 6.38(3)$ from the ordinary phase for $J_s < J_{s,c}$ to the extraordinary phase with a long-range antiferromagnetic order for $J_s > J_{s,c}$.

2 Model and method

We study the spin-1/2 quantum Heisenberg model on the dimerized square lattice shown in Fig. 1 (a) with the open boundary condition in one direction and the periodic boundary condition in the other direction. The Hamiltonian is given by

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle ij \rangle'} \mathbf{S}_i \cdot \mathbf{S}_j + J_s \sum_{\langle ij \rangle_s} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}$$

where J' and J correspond to the strong (blue) and the weak (black) bonds in the bulk, and J_s is the coupling parameter in the surface layer (red bonds). We set $J = 1$ as the unit of energy. This model undergoes a quantum phase transition in the bulk at $J'_c = 1.90951(1)$, which belongs to the 3D O(3) universality class [20–22]. For $J_s \simeq 1$, the surface shows the ordinary critical behavior [9]. On the other hand, for $J_s \gg 1$, the surface layer may be treated as a spin-1/2 Heisenberg chain with relatively weak coupling to the critical bulk state. We shall study the phase diagram of the surface critical behavior controlled by J_s in this work.

We adopt the projective quantum Monte Carlo algorithm in the valence bond basis [23, 24]. All simulations are performed at the bulk QCP. The largest system size in the simulations is $L = 160$. 10^7 times of Monte Carlo sampling are taken for each data point.

The surface spin correlation function $C_\parallel(L/2)$ and the static spin structure factors are calculated to characterize the surface critical behavior. Here,

$$C_\parallel(r) = \frac{1}{L} \sum_x \langle \mathbf{S}_{x+r} \cdot \mathbf{S}_x \rangle, \tag{2}$$

in which both spins reside in the same surface layer. The surface spin structure factor is defined by

$$S(q) = \frac{1}{L} \sum_{x,x'} e^{iq(x-x')} \langle \mathbf{S}_x \cdot \mathbf{S}_{x'} \rangle, \tag{3}$$

in which $q = \pi$ or $\pi + \delta q$ ($\delta q = 2\pi/L$). The surface correlation length ξ_s is defined by

$$\xi_s = \frac{1}{2\sin(\pi/L)} \sqrt{\frac{S(\pi)}{S(\pi + \delta q)} - 1}. \tag{4}$$

The special transition and the nature of the extraordinary phase are derived from the finite-size scaling analysis of the above variables, which will be presented in detail in the following sections.

3 Results

3.1 Special transition
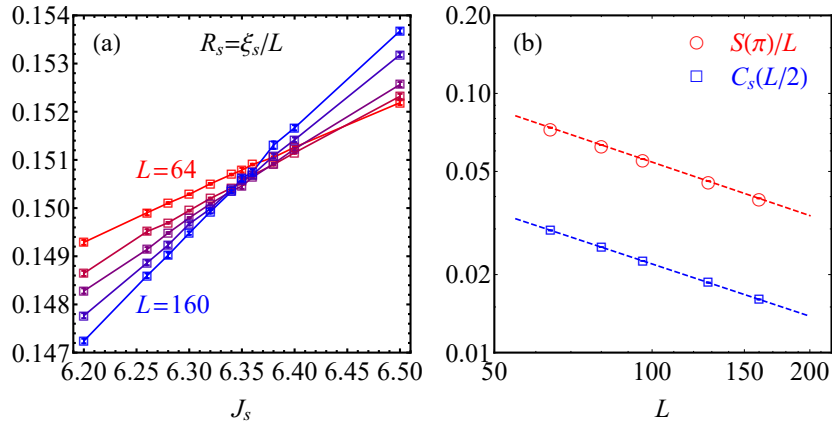
Figure 2: (a) The surface correlation ratio $R_s = \xi_s/L$ versus J_s for different lattice sizes. Solid lines are guide to the eye. (b) Log-log plot of $C_s(L/2)$ and $S(\pi)/L$ versus L at the special transition $J_{s,c}$. Dashed lines are fitting according to Eqs. (7) and (8).

Table 1: Details of the finite-size scaling analysis of the surface correlation ratio $R_s = \xi_s/L$ near the special transition according to Eq. (5) with $k_{\max} = 2$. The correction-to-scaling exponents are set to be $\omega_1 = 1$ and $\omega_2 = 2$. The standard errors of the fitting parameters are obtained from the fitting procedure.

$L_{\min}$	$J_{s,c}$	y_s	R_0	χ^2/d.o.f
48	6.373(14)	0.863(37)	0.1522(5)	0.61
56	6.382(25)	0.863(40)	0.1526(9)	0.64
64	6.383(26)	0.862(42)	0.1526(10)	0.65

We first show that increasing the surface coupling strength J_s induces a special transition on the surface by examining the surface correlation ratio, $R_s = \xi_s/L$, which is plotted in Fig. 2 (a). In the ordinary phase, R_s decreases with increasing system size L, which is consistent with previous numerical results [8]. In contrast, R_s is found to increase with L in the large J_s regime, which indicates stronger spin correlations on the surface. The crossing point of different lattice sizes shown in Fig. 2 (a) indicates a special transition. If the transition is continuous with a scale-invariant critical point, the dimensionless ratio R_s should take the following finite-size scaling form [25,26],

$$R_s = \tilde{R}\left((J_s - J_{s,c})L^{y_s}\right) + \sum_i b_i L^{-\omega_i}$$

$$= R_0 + \sum_{k=1}^{k_{\max}} a_k (J_s - J_{s,c})^k L^{k y_s} + \sum_i b_i L^{-\omega_i}, \tag{5}$$
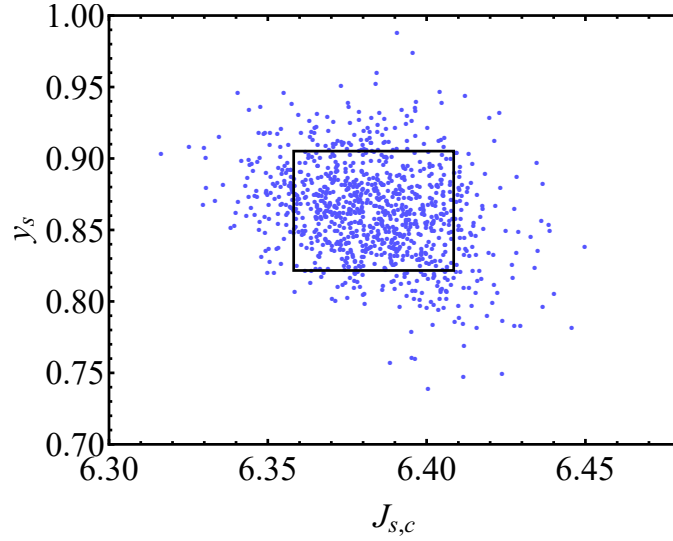
Figure 3: The scattered fitting parameters $J_{s,c}$ and y_s extracted from 1000 sets of randomly generated R_s data for $L_{\min} = 64$. The standard deviations (indicated by the black lines) serve as estimates of the statistical errors.

in which $y_s > 0$ is the scaling dimension of the relevant perturbation at the special transition, and ω_i's are the correction-to-scaling exponents. We set $\omega_1 = 1$ and $\omega_2 = 2$ in the following analysis. $\tilde{R}$ is the universal scaling function. In the second line of Eq. (5), $\tilde{R}$ is expanded as a polynomial near the critical point. The critical point $J_{s,c}$ and the exponent y_s, together with the coefficients R_0, a_k's, b_1 and b_2 are fitting parameters in the data collapse analysis. The finite-size scaling correction is found to be quite strong, thus we gradually increase the smallest system size $L_{\min}$ adopted in the analysis and achieve stable fitting for $L_{\min} \geq 48$. The results are listed in Table 1. Alternatively, the statistical errors of the fitting parameters can also be estimated with the following re-sampling method. A number of new data sets of R_s are randomly generated from the original data and the error bars assuming a normal distribution, and fitted with the same data collapse scaling procedure. The extracted fitting parameters are scattered around those from the original data (see Fig. 3 for $L_{\min} = 64$), and their standard deviations are taken as the statistical errors of the fitting parameters. our final estimates are $J_{s,c} = 6.38(3)$, $y_s = 0.86(4)$, and $R_0 = 0.153(1)$.

Table 2: Finite-size scaling analysis of $C_s(L/2)$ and $S(\pi)/L$ at the surface special transition according to Eqs. (7) and (8).

	$L_{\min}$	$\eta_\parallel$	χ^2/d.o.f
$C_s(L/2)$	64	-0.3317(8)	1.91
	80	-0.3302(10)	1.02
$S(\pi)/L$	64	-0.31447(9)	0.22
	80	-0.31435(14)	0.21

The staggered surface spin correlation function

$$C_s(L/2) = (-1)^{L/2} C_\parallel(L/2) \tag{6}$$

and the spin structure factor $S(\pi)/L$ at the special transition $J_{s,c}$ are shown in Fig. 2 (b). They

are fitted according to the following finite-size scaling formulas,

$$C_s(L/2) \propto L^{-1-\eta_\parallel}, \tag{7}$$

$$S(\pi)/L \propto L^{-1-\eta_\parallel}, \tag{8}$$

in which $\eta_\parallel$ is the anomalous dimension of the surface AF order parameter. By eliminating data of smaller lattice sizes progressively, we achieve stable fitting of both quantities for $L_{\min} \geq 64$, which are listed in Table 2. The slight difference of the exponents extracted from the two quantities might be attributed to scaling corrections not included in the fitting procedure, and serves as an estimate of the systematic error in the scaling analysis. Our final estimate of the exponent $\eta_\parallel$ is $\eta_\parallel = -0.32(1)$.

In summary, the universality class of the special transition of the dimerized quantum Heisenberg model is described by the critical exponents

$$y_s = 0.86(4), \tag{9}$$

$$\eta_\parallel = -0.32(1). \tag{10}$$

Both exponents are drastically different from those obtained at the special transition of the 3D classical O(3) model [17]: $y_s = 0.36(1)$ and $\eta_\parallel = -0.473(2)$. Therefore, the special transition found in this work belongs to a new surface universality class of the 3D O(3) Wilson-Fisher theory.

3.2 Extraordinary phase

We then study the nature of the extraordinary phase for $J_s > J_{s,c}$. In light of the proposals that the surface spin correlation in the extraordinary phase may either decay logarithmically [15] or have long-range AF order [19], we examine both possibilities in the following analysis.

The data of $C_s(L/2)$ and $S(\pi)/L$ at $J_s = 10$ and 16 are shown in Fig. 4, both of which are deep in the extraordinary phase. We first consider the extraordinary-log scaling form proposed in Ref. [15]. Suppose that the surface spin correlation decays logarithmically,

$$C_s(r) \propto [\ln(r/r_0)]^{-q_\parallel}, \tag{11}$$

in which r_0 is a nonuniversal constant, then the structure factor $S(\pi)/L$ would decay logarithmically as a function of the lattice size L with the same exponent $q_\parallel$,

$$S(\pi)/L \propto [\ln(L/L_0)]^{-q_\parallel}, \tag{12}$$

with another nonuniversal constant L_0. We find that $C_s(L/2)$ and $S(\pi)/L$ can be fitted pretty well with the logarithmic form as shown in Figs. 4 (a) and (b) and Table 3. However, the extracted exponents $q_\parallel$ from $C_s(L/2)$ and $S(\pi)/L$ are different from each other and vary significantly with J_s. Such inconsistency and non-universality indicate that the surface spin correlations cannot be captured by the extraordinary-log scaling.

We thus turn to the possibility of a true long-range AF order on the surface. Suppose $C_s(r)$ can be captured by a polynomial of $1/r$ as $r \to \infty$,

$$C_s(r) = m_s^2 + c_1 r^{-1} + c_2 r^{-2} + c_3 r^{-3}, \tag{13}$$

then $S(\pi)/L$ is given by

$$S(\pi)/L = m_s^2 + c_1' L^{-1} + c_1'' L^{-1} \ln L + c_2' L^{-2}, \tag{14}$$

in which the $L^{-1} \ln L$ term comes from summing over the r^{-1} term in $C_s(r)$. The order parameter squared m_s^2 can estimated by extrapolating $C_s(L/2)$ and $S(\pi)/L$ to the thermodynamic

Table 3: Extraordinary-log fitting of $C_s(L/2)$ and $S(\pi)/L$ at $J_s = 10$ and 16 according to Eqs. (11) and (12).

$C_s(L/2)$	$L_{\min}$	$q_{\parallel}$	r_0	$\chi^2/$d.o.f
$J_s = 10$	48	1.80(6)	0.57(8)	1.62
	64	1.85(13)	0.51(16)	1.88
	72	1.85(20)	0.51(26)	2.26
$J_s = 16$	48	0.824(23)	3.64(25)	3.04
	64	0.942(27)	2.50(22)	0.58
	72	0.95(5)	2.4(4)	0.68
$S(\pi)/L$	$L_{\min}$	$q_{\parallel}$	L_0	$\chi^2/$d.o.f
$J_s = 10$	48	4.09(9)	0.074(11)	3.46
	64	3.83(13)	0.116(27)	2.61
	72	3.73(19)	0.14(5)	2.83
$J_s = 16$	48	2.63(4)	0.77(6)	4.82
	64	2.47(6)	1.03(11)	2.58
	72	2.36(5)	1.27(13)	1.27

limit, $m_s^2 = \lim_{L\to\infty} C_s(L/2) = \lim_{L\to\infty} S(\pi)/L$. The orders of expansion in Eqs. (13) and (14) are restricted to keep the same number of fitting parameters. Fitting to the data of $C_s(L/2)$ and $S(\pi)/L$, the results are shown in Figs. 4 (c) and (d). The two quantities yield consistent estimate of m_s^2 within one standard deviation, which justifies the above fitting procedure and indicates a long-range AF order. More data with $6 \leq J_s \leq 16$ are presented in Fig. 5, and the extrapolated m_s^2 are shown in Fig. 6. The value of m_s^2 decreases with decreasing J_s and becomes vanishingly small with large relative error bars near the special transition point $J_{s,c}$. A simple power-law fitting

$$m_s^2 \propto (J_s - J_{s,c})^{2\beta_{\parallel}} \tag{15}$$

gives an estimate of the critical point $J_{s,c} = 6.42(4)$, which is consistent with the previous estimate from the correlation ratio R_s. Therefore, we conclude that the surface has long-range AF order throughout the extraordinary phase $J_s > J_{s,c}$. In principle, one can also extract β from fitting Eq. (15); however, currently our data of m_s^2 are not precise enough to give a reliable result of $\beta_{\parallel}$ by such way, instead, we give $\beta_{\parallel}$ by the scaling law $\beta_{\parallel} = (1 + \eta_{\parallel})/2y_s$, which is $\beta_{\parallel} = 0.40(3)$.

4 Conclusion and Discussions

In summary, we have found a special transition on the surface of a 2D quantum critical Heisenberg model between the ordinary phase and an extraordinary phase by tuning the coupling strength in the surface layer. The extraordinary phase has a long-range AF order, in sharp contrast to the extraordinary-log phase found in the 3D classical O(3) model. The critical exponents at the special transition are drastically different from those at the special transition of the classical O(3) model, thus indicate a new surface universality class of the 3D O(3) Wilson-Fisher theory.

The surface AF order observed in the extraordinary phase may be attributed to the long-range effective interactions induced by the critical fluctuations in the bulk, in the same spirit as the AF order proposed for a dangling spin chain coupled to the bulk in Ref. [19]. The AF order in the dangling-chain model is also confirmed numerically recently, which will be
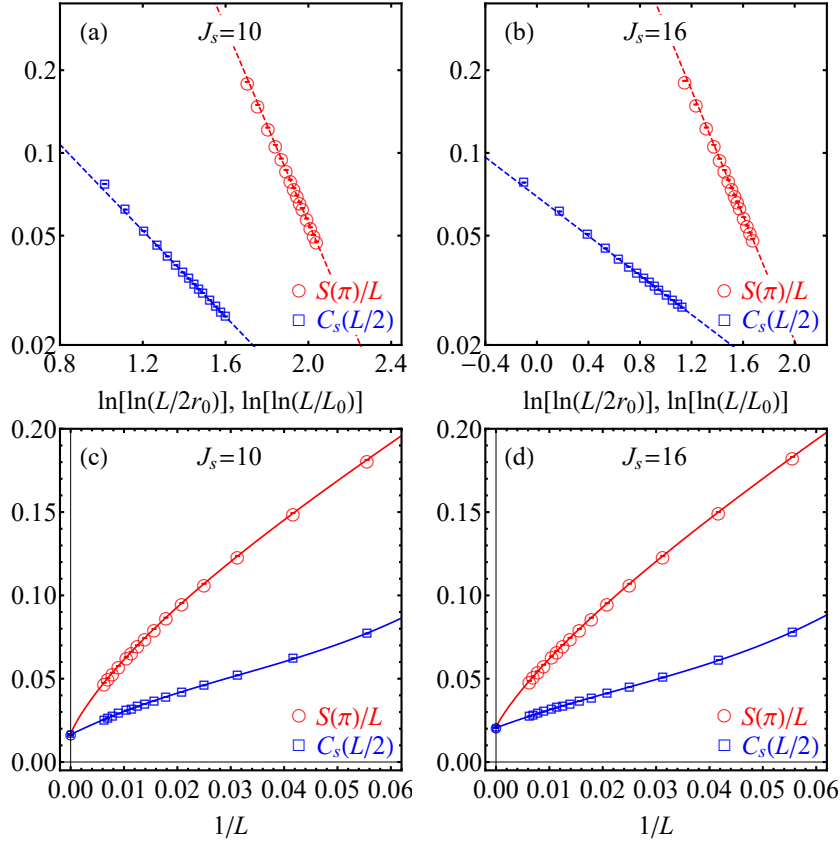
Figure 4: Finite-size scaling of $C_s(L/2)$ and $S(\pi)/L$ at (a,c) $J_s = 10$ and (b,d) $J_s = 16$, both of which are deep in the extraordinary phase. (a,b) $C_s(L/2)$ and $S(\pi)/L$ (in logarithmic scale) versus $\ln[\ln(L/2r_0)]$ and $\ln[\ln(L/L_0)]$, respectively. The nonuniversal constants r_0 and L_0 are presented in Table 3. Dashed lines are fitting with the logarithmic form in Eqs. (11) and (12). Their slopes indicate that the exponent $q_\parallel$ extracted from the two quantities are significantly different. (c,d) $C_s(L/2)$ and $S(\pi)/L$ versus $1/L$. Lines are fitting according to Eqs. (13) and (14).

reported elsewhere [2]. However, the model studied in this work is different from the dangling-chain model. Here, the first two layers at the surface may be treated as a dangling ladder, which is weakly coupled to the bulk. The ladder in itself has a spin gap due to the interchain coupling, and the weak coupling to the bulk leads to the ordinary surface critical behavior. When the AF interaction in the surface layer is strong, we may start from the Luttinger liquid phase of two decoupled chains and treat the interchain coupling and the coupling to the bulk as perturbations. With the bosonization and the renormalization group analysis, we find that there is a phase with long-range AF order on the surface, and an ordinary-AF transition. The details will be presented elsewhere [3].

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[2]C. Ding and L. Zhang, in preparation.

[3]H.-H. Song and L. Zhang, in preparation.
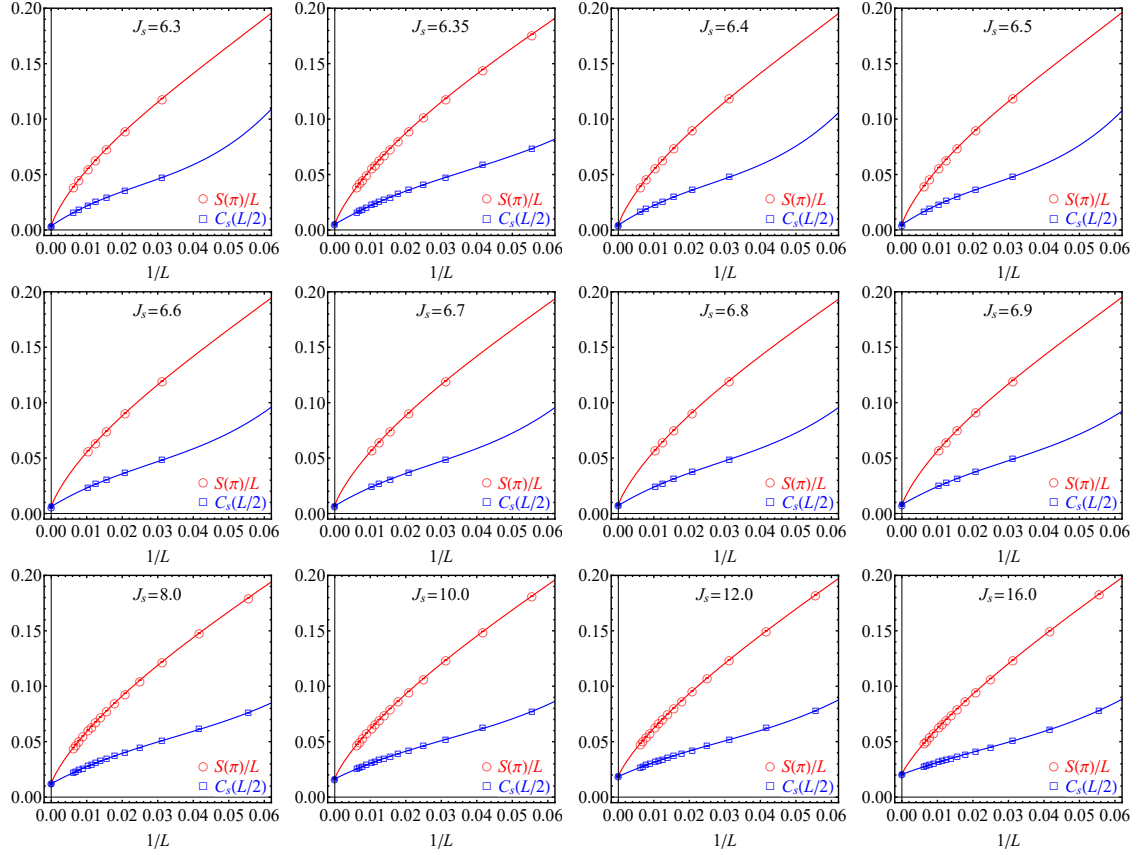
Figure 5: Finite-size scaling of $C_s(L/2)$ and $S(\pi)/L$ for various surface coupling parameter J_s. Lines are fitting according to Eqs. (13) and (14).
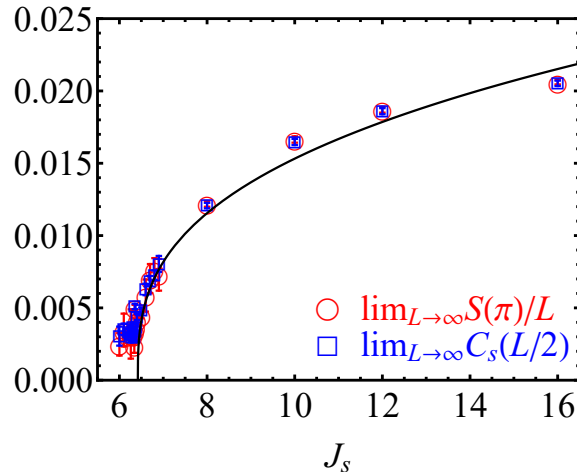
Figure 6: The extrapolated m_s^2 from $C_s(L/2)$ (blue squares) and $S(\pi)/L$ (red circles) versus J_s. The solid line is the power-law fitting with Eq. (15).

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