

Random-Length Random Walks and Finite-Size Scaling in High Dimensions

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We address a long-standing debate regarding the finite-size scaling (FSS) of the Ising model in high dimensions, by introducing a *random-length random walk* model, which we then study rigorously. We prove that this model exhibits the same universal FSS behavior previously conjectured for the self-avoiding walk and Ising model on finite boxes in high-dimensional lattices. Our results show that the mean walk length of the random walk model controls the scaling behavior of the corresponding Green's function. We numerically demonstrate the universality of our rigorous findings by extensive Monte Carlo simulations of the Ising model and self-avoiding walk on five-dimensional hypercubic lattices with free and periodic boundaries.

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Finite-size scaling (FSS) [1,2] is a fundamental theory which characterizes the asymptotic approach of finite systems to the thermodynamic limit, close to a continuous phase transition. While critical systems above the upper critical dimension d_c exhibit simple mean-field behavior in the thermodynamic limit [3], their FSS behavior above d_c is surprisingly subtle and the subject of long-standing debate; see, e.g., Refs. [4–10]. In this work, we clarify a number of these subtleties by introducing a simple model, which can be studied rigorously.

The n -vector model [11], which describes interacting spin systems on a lattice, plays a central role in various areas of physics such as statistical mechanics and condensed matter physics. Prominent examples are the self-avoiding walk (SAW) ($n \rightarrow 0$) in polymer physics, and the Ising ($n = 1$) and XY ($n = 2$) models of ferromagnetism. The latter can be related to the Bose-Hubbard model [12] which describes bosonic atoms in an optical lattice.

On an infinite hypercubic lattice \mathbb{Z}^d , it is known rigorously [13,14] that for sufficiently large dimension d , the two-point functions of the critical Ising and SAW models exhibit the same scaling behavior as the Green's function of the simple random walk (SRW). On finite lattices this connection breaks down because the SRW is recurrent, implying that its Green's function does not exist.

In this Letter, we argue that if one considers random walks with an appropriate random (finite) length \mathcal{N} , then the Green's function displays the same finite-size scaling as the two-point functions of the SAW and Ising models, defined on boxes in \mathbb{Z}^d of linear size L . For this random-length random walk (RLRW) model, one can prove [15] that if $d \geq 3$ and $\langle \mathcal{N} \rangle \asymp L^\mu$ with $\mu \geq 2$, then the Green's function scales as

$$g(\mathbf{x}) \asymp \begin{cases} \|\mathbf{x}\|^{2-d}, & \|\mathbf{x}\| \leq O(L^{(d-\mu)/(d-2)}) \\ L^{\mu-d}, & \|\mathbf{x}\| \geq O(L^{(d-\mu)/(d-2)}). \end{cases} \quad (1)$$

In words, if $\mu > 2$, $g(\mathbf{x})$ exhibits the standard infinite-lattice asymptotic decay $\|\mathbf{x}\|^{2-d}$ at moderate values of \mathbf{x} , but then enters a plateau of order $L^{\mu-d}$ which persists to the boundary. Since a typical RLRW will explore distances of order $\sqrt{\langle \mathcal{N} \rangle}$ from the origin, no plateau exists for $\mu < 2$ because typical walks will be too short to feel the boundary; in this case $g(\mathbf{x})$ decays significantly faster [15] than $\|\mathbf{x}\|^{2-d}$ for $\|\mathbf{x}\| \gg \sqrt{\langle \mathcal{N} \rangle}$.

The above scaling behavior of the Green's function holds on boxes with both free and periodic boundaries. As a consequence of this scaling [16], one can prove [15] that the corresponding susceptibility scales as

$$\chi \asymp L^\mu, \quad \text{for any } \mu > 0. \quad (2)$$

The mean walk length of the SAW, restricted to a finite box in \mathbb{Z}^d , depends strongly on the boundary conditions imposed. For a given choice of SAW boundary conditions, one can consider a RLRW where $\langle \mathcal{N} \rangle$ is chosen to scale in the same way as it does for the SAW. Our numerical results below strongly suggest that the scaling of the Green's function of this RLRW model, given by Eq. (1), then correctly predicts the two-point function scaling of the corresponding SAW model. We therefore conclude that the SAW two-point function is only affected by geometry via its effect on the mean walk length. These observations are seen to hold not only at the thermodynamic critical point, but also at general pseudocritical points. We numerically demonstrate the universality of these predictions by

showing that they also correctly describe the FSS behavior of the Ising two-point function.

These observations shed light on a number of open questions regarding the FSS behavior of the Ising model above d_c . For periodic boundary conditions (PBCs) at criticality, the scaling of the Ising two-point function has been actively debated in Refs. [6–8]. The known [17] behavior of the mean walk length of the SAW on the complete graph [18], together with extensive Monte Carlo simulations in five dimensions, suggest that on high-dimensional tori at criticality we have $\langle \mathcal{N} \rangle_{\text{SAW}} \asymp L^{d/2}$. We therefore predict that the critical SAW and Ising two-point functions should be given by Eq. (1) with $\mu = d/2$. This prediction is in agreement with the conjectured behavior of the critical Ising two-point function given in Ref. [19], and is in excellent agreement with the numerical results presented in Ref. [6].

For free boundary conditions (FBCs), the possible existence of the FSS behavior $\chi \asymp L^{d/2}$ at *pseudocritical* points is the subject of ongoing debate [4,7,10]. Specifically, denoting by T_L the temperature which maximizes $\chi(T, L)$ on a box of size L , it was observed numerically in Ref. [10] that $\chi(T_L, L)$ has the same $L^{d/2}$ scaling observed at criticality for periodic systems. The results in Ref. [7] are in agreement with this observation; however, the more recent work Ref. [4] refuted this claim, and numerically observed only the standard mean-field scaling L^2 . From Eq. (2), we see that one *can* observe $\chi \asymp L^{d/2}$ in a RLRW model in which the mean walk length scales as $L^{d/2}$. Universality then suggests that this scaling should also be observable in the SAW and Ising models, at appropriate pseudocritical points. Our numerical results below confirm this.

Random-length random walk.—Let $(S_t)_{t \in \mathbb{N}}$ be a simple random walk on a box of side length L in \mathbb{Z}^d , centered at the origin. Let \mathcal{N} be an \mathbb{N} -valued random variable, independent of each choice of step in $(S_t)_{t \in \mathbb{N}}$. We refer to $(S_t)_{t=0}^{\mathcal{N}}$ as the corresponding RLRW. We study its Green's function

$$g_{\text{RLRW}}(\mathbf{x}) := \mathbb{E} \left(\sum_{n=0}^{\mathcal{N}} P(S_n = \mathbf{x}) \right),$$

which is the expected number of visits to \mathbf{x} , and the corresponding susceptibility $\chi_{\text{RLRW}} := \sum_{\mathbf{x}} g_{\text{RLRW}}(\mathbf{x})$. Here, $P(S_n = \mathbf{x})$ denotes the probability that the RLRW is at site \mathbf{x} after n steps.

Consider a RLRW with mean walk length $N := \langle \mathcal{N} \rangle \asymp L^\mu$ on a $d \geq 3$ dimensional hypercubic lattice, with either periodic or free boundary conditions. If $\mu \geq 2$, it can then be proved [15] that the Green's function exhibits the piecewise asymptotic behavior in Eq. (1). In particular, the case $\mu > 2$ shows the existence of a macroscopic plateau of order $L^{\mu-d}$ for large distances, while this plateau is absent for $0 < \mu < 2$. The case $\mu = 2$ is marginal.

Numerical setup for n -vector models.—We study the two-point function $g_{\text{Ising}}(\mathbf{x}) := \mathbb{E}(s_0 s_{\mathbf{x}})$ for the zero-field ferromagnetic Ising model, defined by the Hamiltonian $\mathcal{H} = -\sum_{ij} \mathbf{s}_i \cdot \mathbf{s}_j$. Here, $\mathbf{s}_i = \pm 1$ denotes the spin at site i of a hypercubic lattice of side length L , and the sum is over nearest neighbors. We simulate the Ising model at fugacities $z := \tanh(\beta)$, where β is the inverse Ising temperature, via the worm algorithm introduced in Ref. [20].

We also investigate the SAW on a box with linear size L in the variable length ensemble. We study the two-point function $g_{\text{SAW}}(\mathbf{x}) := \sum_{\omega: 0 \rightarrow \mathbf{x}} z^{|\omega|}$, where the sum is over all SAWs starting at the origin 0 and ending at \mathbf{x} . We simulated this ensemble using an irreversible version of the Berretti-Sokal algorithm [21,22]. For both models we study the corresponding susceptibility, defined by $\chi_{\text{Ising/SAW}} := \sum_{\mathbf{x}} g_{\text{Ising/SAW}}(\mathbf{x})$.

We study our models on hypercubic lattices, in the case of both free and periodic boundary conditions. The Ising model was simulated at the estimated location of the infinite-volume critical point $z_{c, \text{Ising}, 5\text{D}} = 0.113\,915\,0(5)$ [9] in five dimensions, and the simulations for the SAW were performed at the estimated infinite-volume critical point $z_{c, \text{SAW}, 5\text{D}} = 0.113\,140\,84(1)$ [22]. We also simulated the FSS behavior at pseudocritical points $z_L = z_c - aL^{-\lambda}$ for various $a \in \mathbb{R}$ and $\lambda > 0$. We simulated linear system sizes up to $L = 71$ in the Ising model and $L = 201$ for the SAW. To estimate the exponent value for a generic observable Y we performed least-squares fits to the ansatz $Y = a_Y L^{b_Y} + c_Y$. A detailed analysis of autocorrelation times can be found in Ref. [23] for the worm algorithm and in Ref. [22] for the irreversible Berretti-Sokal algorithm.

Universal scaling at criticality.—We now argue that Eqs. (1) and (2) correctly predict the FSS behavior of the two-point functions and the susceptibility of the critical SAW and Ising model, with either FBCs or PBCs.

We first study the periodic case. It is expected that models on high-dimensional tori should exhibit the same scaling as the corresponding model on the complete graph. It was proved in Ref. [17] that, on the complete graph, N_{SAW} scales at criticality like the square root of the number of vertices. On five-dimensional tori, our fits for N_{SAW} at criticality lead to the exponent value 2.50(1), in excellent agreement with the complete graph prediction of $d/2$. Combining this scaling for N_{SAW} with our results for the RLRW, the two-point functions of the critical Ising and SAW models on high-dimensional tori are then predicted to display the scaling in Eq. (1) with $\mu = d/2$. Figure 1(a) verifies this prediction, showing an excellent data collapse for appropriately scaled versions of the two-point functions of the Ising and SAW models onto the scaling variable $y := \|\mathbf{x}\|/L^{(d-\mu)/(d-2)}$ with $\mu = d/2$. As a corollary of this two-point function scaling, we obtain $\chi \asymp L^{d/2}$, in agreement with the numerical studies for the Ising model in

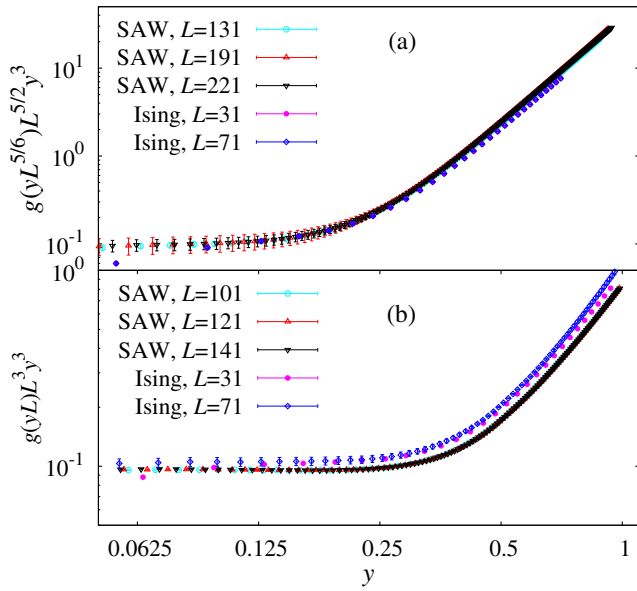


FIG. 1. Appropriate scaled two-point functions of the Ising model and SAW on five-dimensional hypercubic lattices with *periodic* boundaries onto the scaling variable $y = \|\mathbf{x}\|/L^{(d-\mu)/(d-2)}$. (a) Anomalous FSS scaling at z_c onto the ansatz in Eq. (1) with $\mu = d/2$. When $\|\mathbf{x}\| \approx L/2$, the two-point functions display the anomalous FSS behavior $g(\mathbf{x}) \asymp L^{-d/2}$, in contrast to the standard mean field prediction $g(\mathbf{x}) \asymp L^{2-d}$. (b) Standard mean-field scaling at the pseudocritical point $z_L = z_c - aL^{-2}$ onto the ansatz in Eq. (1) with $\mu = 2$. In contrast to the critical PBC case, the two-point functions display the standard mean-field scaling behavior $g(\mathbf{x}) \asymp L^{2-d}$ when $\|\mathbf{x}\| \approx L/2$.

Refs. [24,25], and with our direct exponent estimates for $d = 5$ of 2.50(1) for χ_{SAW} , and 2.51(2) for χ_{Ising} .

On free boundaries at criticality, our fits for N_{SAW} lead to the exponent value 2.00(1), strongly suggesting that $N_{\text{SAW}} \asymp L^2$. Combining this scaling for N_{SAW} with our results for the RLRW, the two-point functions of the critical Ising and SAW models on high-dimensional boxes with free boundaries are then predicted to display the scaling in Eq. (1) with $\mu = 2$. Figure 2(a) verifies this prediction, showing an excellent data collapse for the two-point functions of the critical Ising and SAW models onto the ansatz in Eq. (1) with $\mu = 2$. Equation (2) then predicts $\chi \asymp L^2$, in agreement with the numerical study of the Ising model in Ref. [9], and with our direct exponent estimates for $d = 5$ of 2.01(8) for the Ising model and 1.99(1) for the SAW.

Universal scaling at pseudocritical points.—We now turn to the actively debated question [4,7,10] of whether one can observe the scaling behavior $\chi \asymp L^{d/2}$, corresponding to critical PBC behavior, on free boundaries at pseudocritical points. This also motivates the reverse question, of whether it is possible to observe the standard mean-field behavior $\chi \asymp L^2$, corresponding to critical FBC behavior, at pseudocritical points on periodic boundaries.

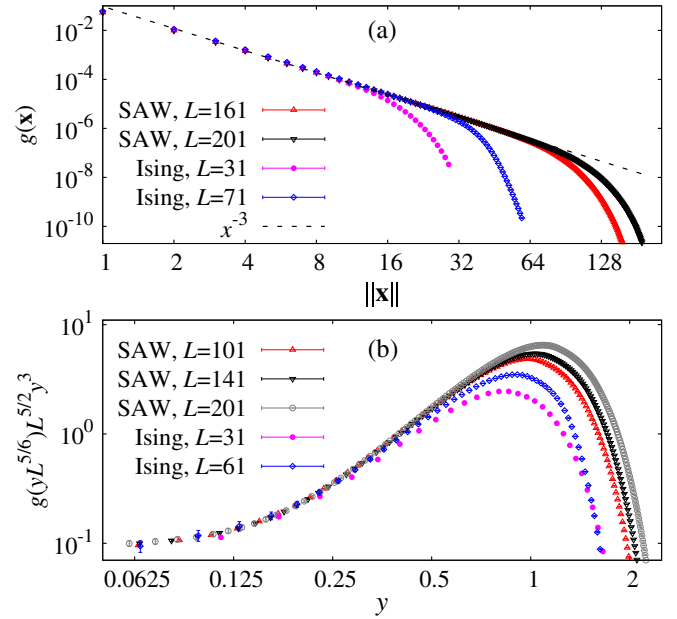


FIG. 2. Two-point functions of the Ising model and SAW on five-dimensional hypercubic lattices with *free* boundaries. (a) Standard mean-field scaling $g(\mathbf{x}) \asymp \|\mathbf{x}\|^{2-d}$ at z_c . (b) Anomalous FSS at the pseudocritical point $\tilde{z}_L = z_c + aL^{-2}$ onto the scaling variable $y = \|\mathbf{x}\|/L^{(d-\mu)/(d-2)}$ with $\mu = d/2$. The two-point functions collapse except at distances close to the boundary. This shows that $g(\mathbf{x})$ displays the same FSS behavior as on periodic boundaries at criticality.

The above results for the RLRW suggest that the FSS behavior of the SAW two-point function should only depend on the boundary conditions through their effect on N . We now numerically verify that this is indeed the case, and that analogous results also hold for the Ising model.

For periodic boundaries, we study FSS at pseudocritical points $z_L(\lambda) = z_c - aL^{-\lambda}$, with a chosen positive so that the walk lengths are *decreased* compared with criticality. On the complete graph, it can be shown [15] that at a pseudocritical point $z_V(\zeta) = z_c - aV^{-\zeta}$ we have $N_{\text{SAW}} \asymp V^{1/2}$ if $\zeta \geq 1/2$, while $N_{\text{SAW}} \asymp V^\zeta$ if $\zeta \leq 1/2$. Considering a RLRW on a high-dimensional torus, whose mean walk length scales in this way, the Green's function and susceptibility then scale as in Eqs. (1) and (2) with $\mu = \zeta d = \lambda$ for any $0 < \lambda \leq d/2$, and $\mu = d/2$ for $\lambda \geq d/2$. By universality, we then expect the same behavior to hold for both the SAW and the Ising model at the pseudocritical point $z_L(\lambda)$ on high-dimensional tori.

Taking $\lambda = 2$, the above argument predicts that the pseudocritical two-point functions display the mean-field behavior $g(\mathbf{x}) \asymp \|\mathbf{x}\|^{2-d}$. Figure 1(b) shows an appropriately scaled version of the two-point functions of the Ising model and SAW onto the ansatz in Eq. (1) with $\mu = 2$. The excellent data collapse provides strong evidence for the predicted existence of standard mean-field behavior at $z_L(2)$.

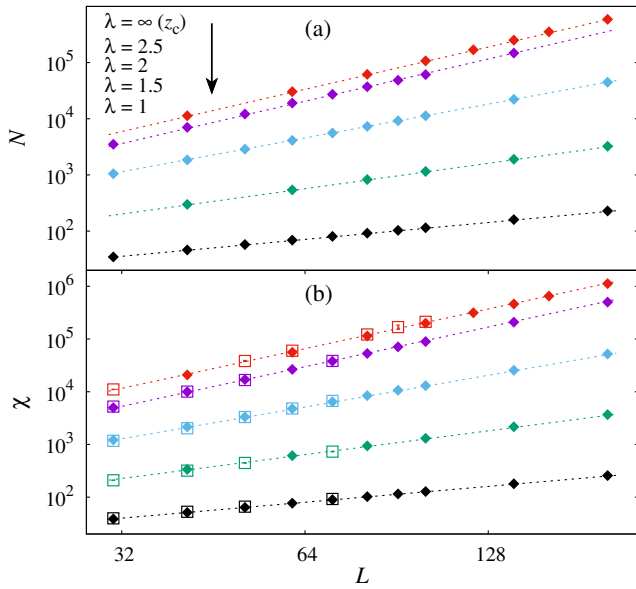


FIG. 3. FSS behavior of the mean walk length N_{SAW} (a) and the susceptibility $\chi_{\text{Ising,SAW}}$ (b) with *periodic* boundary conditions in five dimensions. The diamonds (squares) display SAW (Ising) data. To emphasize universality, the Ising and SAW data were translated onto the same curve. In each figure, the line on the top corresponds to the critical scaling behavior $N, \chi \asymp L^{d/2}$. The remaining lines (top to bottom) correspond to the scaling behavior $N, \chi \asymp L^\lambda$ at pseudocritical points $z_L(\lambda) = z_c - aL^\lambda$ ($a > 0$) with $\lambda = 2.5, 2, 1.5, 1$.

We emphasize that, despite appearances, the two-point functions in Fig. 1(a) and (b) do not display the same FSS behavior. In particular, it follows from the scaling ansatz in Eq. (1) that if $\|\mathbf{x}\| \approx L/2$, then the critical two-point functions scale as $g(\mathbf{x}) \asymp L^{-d/2}$, while $g(\mathbf{x}) \asymp L^{2-d}$ at $z_L(2)$.

Considering more general values of λ , Fig. 3(a) shows the scaling of N_{SAW} at $z_L(\lambda)$ on five-dimensional tori for $\lambda = 1, 1.5, 2, 2.5$. Our fits lead to the exponent values 0.998(2) for $\lambda = 1$, 1.499(2) for $\lambda = 1.5$, 2.01(1) for $\lambda = 2$, and 2.47(4) for $\lambda = 2.5$, in excellent agreement with the corresponding results on the complete graph. Figure 3(b) then shows the scaling behavior of the susceptibility for $\lambda = 1, 1.5, 2, 2.5$. Our fits for the SAW lead to the exponent values 1.005(6) for $\lambda = 1$, 1.503(5) for $\lambda = 1.5$, 2.00(1) for $\lambda = 2$, 2.46(5) for $\lambda = 2.5$. For the Ising model, our fits lead to 1.00(1) for $\lambda = 1$, 1.51(2) for $\lambda = 1.5$, 2.05(7) for $\lambda = 2$, and 2.4(1) for $\lambda = 2.5$. These estimates are all in excellent agreement with above predictions.

Finally, we consider pseudocritical behavior with free boundary conditions. There has been considerable debate [4,7,10] concerning the existence of critical PBC FSS behavior on lattices with FBC at a pseudocritical point which maximizes $\chi(T, L)$ on a box of linear size L . It has been numerically established that this pseudocritical point has shift exponent $\lambda = 2$ [4,7,10]. A simple methodology to gauge the possibility of observing $\chi \asymp L^{d/2}$ at such a pseudocritical point is to define a sequence a_L such that

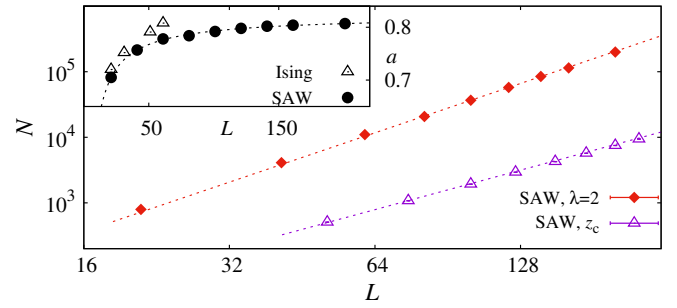


FIG. 4. FSS behavior of the mean walk length N_{SAW} with *free* boundary conditions in five dimensions. The inset shows the convergence of a_L in the SAW (circles) and Ising model (triangles).

$\chi_{\text{FBC}, \tilde{z}_L}(L) = \chi_{\text{PBC}, z_c}(L)$ with $\tilde{z}_L := z_c + a_L L^{-2}$, and to then show that a_L converges. If such a convergent sequence exists, this approach forces $\chi_{\text{FBC}, \tilde{z}_L}$ to scale as $L^{d/2}$, where $z_L = z_c + a_\infty L^{-2}$. The inset of Fig. 4 shows the sequence a_L in the Ising and SAW models. For the SAW, the series a_L clearly appears to converge, and our fits predict $a_{\text{SAW}, \infty} = 0.824(2)$. The Ising data are roughly consistent with the SAW data, albeit over a much smaller range of L values.

Fitting the FBC data for N_{SAW} at \tilde{z}_L produces an exponent estimate of 2.48(6), suggesting that $N_{\text{SAW}} \asymp L^{d/2}$, compared with $N_{\text{SAW}} \asymp L^2$ at z_c ; see Fig. 4. Universality then suggests that the Ising and SAW two-point functions should follow Eq. (1) with $\mu = d/2$. Figure 2(b) shows the appropriately rescaled two-point functions. We observe excellent data collapse, except at distances close to the boundary. This strong boundary effect may explain the apparent discrepancies [4,7,10] in determining the correct scaling behavior for the pseudocritical Ising model with FBCs. Regardless, we conclude from Fig. 2(b) that the anomalous FSS behavior, observed on periodic boundaries at criticality, *can* be observed on free boundaries, in agreement with Refs. [7,10].

Discussion.—In this Letter, we have introduced a random-length random walk model to clarify a number of open questions regarding the FSS behavior of the Ising model above d_c . For periodic boundaries, by combining the RLRW model with the scaling of the mean walk length of the SAW on the complete graph, we were able to predict the asymptotic scaling of the Ising and SAW two-point functions on high-dimensional tori at a family of pseudocritical points $z_L(\lambda) = z_c - aL^{-\lambda}$, and showed that the scaling exponents vary continuously with λ when $0 < \lambda \leq d/2$. As special cases, at z_c we recovered the behavior conjectured in Ref. [19], while at $z_L(2)$ we showed the Ising two-point function displays standard mean-field behavior.

On free boundaries, combining the RLRW model with the numerical scaling of N_{SAW} predicts that the critical Ising two-point function displays standard mean-field decay. It follows that the susceptibility scales as L^2 , in agreement with the numerical observation in Ref. [9]. We

also studied the actively debated FSS behavior at the pseudocritical point $z_L = z_c + aL^{-2}$. We established that the Ising two-point function displays the same FSS behavior as on periodic boundaries at criticality, in agreement with the numerical observations in Refs. [7,10].

Recently, three-dimensional quantum spin models, which are related to the corresponding four-dimensional classical counterpart [26], have been the subject of intensive theoretical, experimental and numerical studies [27–29]. Our work has focused on the FSS behavior of the n -vector model above $d_c = 4$. Although at d_c the situation is likely complicated by logarithmic corrections, we believe that our results for $d > d_c$ are a necessary first step in understanding the correct scaling behavior for applications to three-dimensional quantum spin models.

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