Dynamic surface critical behavior of isotropic Heisenberg ferromagnets

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Abstract

The effects of free surfaces on the dynamic critical behavior of isotropic Heisenberg ferromagnets are studied via phenomenological scaling theory, field-theoretic renormalization group tools, and high-precision computer simulations. An appropriate semi-infinite extension of the stochastic model J is constructed, the boundary terms of the associated dynamic field theory are identified, its renormalization in $d \leq 6$ dimensions is clarified, and the boundary conditions it satisfies are given. Scaling laws are derived which relate the critical indices of the dynamic and static infrared singularities of surface quantities to familiar static bulk and surface exponents. Accurate computer-simulation data are presented for the dynamic surface structure factor; these are in conformity with the predicted scaling behavior and could be checked by appropriate scattering experiments.

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A key ingredient of modern theories of critical phenomena is the arrangement of microscopically different systems in universality classes \([1]\). First developed for static equilibrium bulk critical behavior, this classification scheme has subsequently been extended both to dynamic bulk critical behavior \([2]\) as well as to static surface critical behavior of semi-infinite systems at bulk critical points \([3,4]\).

Since distinct dynamics may have the same equilibrium distribution, each static bulk universality class generally splits up into several dynamic ones, represented by stochastic models called A, B, \ldots, J \([2]\). Likewise, to which static surface universality class a given system belongs is decided by its static bulk universality class and additional relevant surface properties. Hence each static surface universality class and each dynamic bulk universality class generally splits up into separate dynamic surface universality classes \([5,6]\).

Unfortunately, detailed investigations of dynamic surface critical behavior have remained scarce \([5–9]\) and largely focused on models with purely relaxational dynamics. Isotropic Heisenberg ferromagnets form an important class of systems, characterized by the presence of nondissipative (mode-coupling) terms and a conserved order parameter, whose dynamic surface critical behavior has not yet been investigated. To fill this gap, we shall use two different lines of approaches: (i) phenomenological scaling and the field-theoretic renormalization group (RG); (ii) computer-simulation studies of the dynamic surface structure function.

Building on (i), we shall conclude that the critical indices characterizing the dynamic surface critical behavior of such systems (which are \(O(3)\) symmetric both in the bulk and at the surface) can be expressed in terms of known static bulk and surface critical exponents. Recently developed highly efficient spin dynamics algorithms \([10,11]\) have enabled us to corroborate these findings numerically.

In the simulations we utilized a classical isotropic Heisenberg ferromagnet on a simple cubic lattice whose sites \(i = (i_1, i_2, i_3)\), \(i_1, i_2, i_3 = 0, \ldots, L - 1\), are occupied by spins \(S_i = (S_i^\alpha, \alpha = 1, 2, 3)\) of length \(|S_i| = 1\). Free boundary conditions apply along the \(i_3\) direction, and periodic ones along the others, so that the layers \(i_3 = 0\) and \(i_3 = L - 1\) are free surfaces. The dynamics is defined through

\[
\frac{dS_i}{dt} = \frac{\partial H_{\text{lat}}}{\partial S_i} \times S_i, \tag{1}
\]

with the Hamiltonian

\[
H_{\text{lat}} = -J \sum_{i, j \neq 0, L-1}^{(i, j)} S_i \cdot S_j - J_1 \sum_{i = j = 0, L-1}^{(i, j)} S_i \cdot S_j, \tag{2}
\]

whose nearest-neighbor bulk and surface bonds \(J\) and \(J_1\) (measured in units of temperature \(T\)) are ferromagnetic.

In the thermodynamic limit the model undergoes a continuous bulk phase transition whose critical behavior is representative of the \(O(3)\) universality class. Owing to the \(O(3)\) symmetry, the surface of such a \(d=3\)-dimensional system cannot spontaneously order for \(J_1/J < \infty\). Hence the surface transition that occurs at the bulk critical point \(T = T_c\) is the so-called ordinary one \([4]\). Its critical indices can be expressed in terms of two independent bulk exponents, e.g., \(\eta\) and \(\nu\), and one surface exponent, e.g., the correlation exponent \(\eta^{\text{ord}}\).

In our computer simulations, (1) is integrated numerically for a given set of more than 700 initial spin configurations generated by a Monte-Carlo simulation of the thermal equilibrium state \(\propto e^{-H_{\text{lat}}}\) \([10–12]\). The spin-spin cumulant
with \( r = (i_1-i_2, i_1'-i_2') \), \( z = i_3 \), and \( z' = i_3' \) is calculated, where \( t \) and \( t' \) are times to which the initial spin configuration at \( t = 0 \) has evolved according to (1). The average \( \langle . \rangle \) is taken over the set of initial configurations. Before turning to the results, let us discuss scaling.

Consider a \( d \)-dimensional analog of the above model in the thermodynamic limit \( L \to \infty \). According to scaling considerations [13,14] and RG work [15,16], the dynamic bulk critical exponent \( z \) is given by

\[
z = \begin{cases} \frac{(d+2-\eta)}{2} & \text{if } d \leq d^*_s = 6, \\ \frac{d}{4} & \text{if } d > 6. \end{cases}
\]  

(4)

Here \( d^*_s = 6 \) is the upper critical dimension of model \( J \), and the mean-field (MF) value \( \eta = 0 \) applies for \( d > d^*_s = 4 \), the static upper critical dimension.

Let \( 2 < d < 4 \), so that hyperscaling holds. A scaling ansatz for the cumulant (3) at \( T_c \) must comply with the scaling forms of (a) the bulk cumulant that (3) approaches as \( z, z' \to \infty \) with \( z-z' \) fixed, and (b) the static cumulant \( C(r; z, z'); 0) \). Both requirements impose strong restrictions. To see this, recall that the static critical behavior is captured by the semi-infinite 3-vector model with Hamiltonian

\[
\mathcal{H} = \int_{\mathbb{R}_+^d} \left[ \frac{1}{2} (\nabla \phi)^2 + \frac{\tau_0}{2} \phi^2 + \frac{u_0}{4!} |\phi|^4 \right] + \int_{\mathcal{B}} \frac{c_0}{2} \phi^2 ,
\]  

(5)

defined on the half-space \( \mathbb{R}_+^d \equiv \{ (x_\parallel, z) \in \mathbb{R}^d \mid z \geq 0 \} \) with boundary plane \( \mathcal{B} \) at \( z = 0 \). In this model there is ordinary surface critical behavior at bulk criticality if \( c_0 > c_{sp} \). At the corresponding ordinary fixed point \( c \), the renormalized analog of \( c_0-c_{sp} \), takes the value \( c = \infty \). This implies that the order-parameter field \( \phi \) asymptotically satisfies the Dirichlet boundary condition \( \phi|_{\mathcal{B}} = 0 \). The behavior of \( \phi(x) \) as \( x \equiv (x_\parallel, z) \) approaches the surface point \( x_{\mathcal{B}} \equiv (x_\parallel, 0) \) follows from the boundary operator expansion (BOE) [3]

\[
\phi(x) = D(z) \partial_n \phi(x_{\mathcal{B}}) + \ldots.
\]  

(6)

The scaling dimensions of the operators \( \phi \) and \( \partial_n \phi \) are \( (d-2+\eta)/2 \) and \( (d-2+\eta_{ord})/2 \), respectively, whence \( D(z) = D_0 z^{(\eta_{ord} - \eta)/2} \).

From requirement (b) we draw the important conclusion that \( \phi |_{x \in \mathcal{B}} \) and the surface operator \( \partial_n \phi \) ought to retain their scaling dimensions in the dynamic case. The reason is that for the locally scale invariant theory considered here the scaling dimension of any local scaling operator \( \mathcal{O}(x, t) \) cannot differ from its bulk value except for points \( x \) on the boundary [3] or at an initial condition [17]. However, the initial configurations \( \phi_{t=0} \) are drawn from the equilibrium distribution and should therefore not give rise to different scaling dimensions.

Requirement (a) tells us that the dependence on \( t \) must involve the usual bulk scaling variables, such as \( \text{tr}^{-4} \). Additional relevant or marginal dynamic surface scaling fields can be ruled out because (i) at the ordinary transition the surface does not act as an independent source of critical behavior [3] and (ii) the \( O(3) \) invariance of the interactions precludes a local violation of the order-parameter conservation at the surface. Hence, sufficiently close to \( T_c \), possible times scales generated by the surface should be much smaller than the characteristic bulk time scale. An appropriate scaling ansatz for \( C^{\alpha \beta} = \delta_{\alpha \beta} C \) at \( T = T_c \) thus is
The BOE (8) leads to \( \Upsilon (z, z'; t) \approx (zz')^{(\eta_{\text{ord}} - \eta)/2} \Upsilon_0 (t) \) in the limit \( z, z' \to 0 \). By consistency we must have

\[
\begin{align*}
\hat{C}_{11}(p, \omega) &= p^{\eta_{\text{ord}} - 1 - \eta} \sigma(\omega p^{-\eta}) , \\
\hat{C}_{11}(0, \omega) &= \text{const} \omega^{-\left(\frac{d+1-\eta_{\text{ord}}}{2}\right)} ,
\end{align*}
\]

where \( \hat{C}_{11}(p, \omega) \), the dynamic surface structure function, is the Fourier transform of \( C(r; 0, 0; t) \) with respect to \( r \) and \( t \).

For \( 4 < d < 6 \), the breakdown of hyperscaling (caused by the dangerous character of the irrelevant scaling field \( u \sim u_0 \)) must be taken into account. While static exponents like \( \eta \) and \( \eta_{\text{ord}} \) take their MF values 0 and 2, respectively, the value \( (d+2)/2 \) of \( \eta \) agrees with the MF value 3 of the magnetic shift exponent only for \( d = 4 \).

To put the above findings on a firmer basis, let us construct an appropriate semi-infinite extension of model J. We may assume that the surface-induced modifications of both the interactions and the dynamics are restricted to the immediate vicinity of the boundary \( \mathcal{B} \). Hence, for points with \( z > 0 \), we use the stochastic bulk equation \([18]\)

\[
\dot{\phi}(x, t) - \zeta = \lambda_0 \left( \nabla \delta \mathcal{H} / \delta \phi + f_0 \nabla \delta \mathcal{H} / \delta \phi \times \phi \right) ,
\]

where \( \zeta \) is a Gaussian random force with average \( \langle \zeta \rangle = 0 \) and

\[
\langle \zeta^\alpha(x, t) \zeta^\beta(x', t') \rangle = -\lambda_0 \delta^{\alpha\beta} \Delta \delta(x-x') \delta(t-t') .
\]

The derivative \( \delta \mathcal{H} / \delta \phi \) involves a contribution \( \delta(z)(c_0 - \partial_z) \phi \) implied by the boundary term of \( \delta \mathcal{H} \), which yields one obvious surface contribution to \([12]\). But there may be others, corresponding to local changes of the dynamics. As expounded in \([5]\), the requirements of detailed balance, locality, order-parameter conservation, absence of irrelevant and redundant operators, and here also \( O(3) \) symmetry, impose strong constraints, which are best dealt with on the level of the equivalent path-integral formulation (see, e.g., \([13]\)). To ensure detailed balance, the action must have the form

\[
\mathcal{J} = \int \int_0^\infty dt \{ \phi + \mathcal{R} \left[ \delta \mathcal{H} / \delta \phi - \delta \mathcal{R} / \delta \phi \right] \}) ,
\]

where \( \mathcal{J} \) comprises both volume and surface integrals, \( \phi \) is the usual auxiliary field needed in such a Lagrangian formulation, and a prepoint discretization in time is used.

The right-hand side of \([11]\) can be written as \( -\mathcal{R} \cdot \delta \mathcal{H} / \delta \phi \) with

\[
\mathcal{R}^{\alpha\beta} = -\lambda_0 \left( \delta^{\alpha\beta} \Delta + f_0 e^{\alpha\beta\gamma} \phi^\gamma \right) .
\]

To find out which surface terms must be included in \( \mathcal{J} \) and the associated boundary conditions, we proceed as in Refs. \([3, 4]\). As reaction operator in the action \([12]\) we use \([13]\), with the Laplacian \( \Delta \) replaced by \( -\hat{\nabla} \cdot \hat{\nabla} \) (where \( \hat{\nabla} \) acts to the left). Contributions to \( \mathcal{R}^{\alpha\beta} / \lambda_0 \) of the form \( e^{\alpha\beta\gamma} \delta(z) \) correspond to nonconservative dynamic surface terms \([3]\) and are ruled out by the presumed spin isotropy. As boundary conditions (valid in an operator sense \([3, 5]\)) we obtain
ensure self-adjointness of renormalization schemes: a massless one, RS
precession term yields a contribution
$\mu Z$ is a consequence of (18) [16]; it implies that the beta function $f$
The second, (15), means that
follows.

to all orders in $\tilde{\phi}$ of 
functions [19], including those involving the surface operators
may be gleaned from [16], which also tells us that single insertions of the composite operator

\begin{equation}
(\partial_n - c_0)\phi = 0 ,
\end{equation}

\begin{equation}
\partial_n \frac{\delta H}{\delta \phi} = \partial_n \big( \tau_0 + \frac{u_0}{6} |\phi|^2 - \Delta \big) \phi = 0 ,
\end{equation}

\begin{equation}
\partial_n \tilde{\phi} = 0 ,
\end{equation}

\begin{equation}
(\partial_n - c_0)\tilde{\phi} \hat{R} = \lambda_0 (c_0 - \partial_n) \big( \Delta \tilde{\phi} - f_0 \tilde{\phi} \times \phi \big) = 0 ,
\end{equation}

where $\partial_n$ is a derivative along the inner normal. The first, (14), is known from statics. The second, (15), means that $n \cdot j^\alpha$, the normal component of the current $j^\alpha = -\lambda_0 (\nabla \frac{\delta H}{\delta \phi} + f_0 e^{\alpha \beta \gamma} \phi^\beta \nabla \phi^\gamma)$, whose negative divergence gives the right-hand side of (10), vanishes at $B$. The precession term yields a contribution $\propto e^{\alpha \beta \gamma} \phi^\beta \partial_n \phi^\gamma$ which is zero by (14). The remaining two ensure self-adjointness of $\Delta$ and consistency with the fluctuation-dissipation theorem (FDT)

\begin{equation}
- \theta(t) \langle \phi^\alpha (x, t) \phi^\beta (x', 0) \rangle = \langle \phi^\alpha (x, t) (\tilde{\phi} \hat{R})^\beta (x', 0) \rangle .
\end{equation}

To study the ordinary transition, it is convenient to set $c_0 = \infty$. Then (14) and (17) simplify to Dirichlet boundary conditions for $\phi$ and $\tilde{\phi} \hat{R}$. In applying the RG, we consider two distinct renormalization schemes: a massless one, $RS_1$, based on the $\epsilon$ expansion about $d^*_t$, and a massive one, $RS_2$, in fixed dimension $d \leq 4$. Common to both is the form of the reparametrizations $\phi = Z^{1/2}_\phi \phi_{\text{ren}}, \tilde{\phi} = Z^{-1/2}_\phi \tilde{\phi}_{\text{ren}}, \partial_n \phi = [Z_\phi Z_{1, \infty}]^{1/2} \partial_n \phi_{\text{ren}}, \lambda_0 = \mu^{-1} Z_\lambda \lambda, \text{and } f_0 = \mu^{3-d/2} Z^{1/2}_\phi Z^{-1}_\lambda f$, where $\mu$ is either an arbitrary momentum scale ($RS_1$) or the renormalized mass ($RS_2$). That the $Z$-factors of $\tilde{\phi}$ and $\phi$ can be chosen reciprocal to each other follows from the fact that the bulk vertex function $V_{\phi \phi \phi \phi}^{(b)}(d)$ has no primitive uv divergence \( \propto \delta^4(t - t') \). The form of the $Z$-factor of $f$ is a consequence of (18), (17); it implies that the beta function $\beta_f \equiv \mu \partial_{\mu} f$ becomes $\beta_f = \frac{1}{2} (d - 6 - \eta_6 + 2 \eta_\lambda) f$, with $\eta_{6, \lambda} \equiv \mu \partial_{\mu} \ln Z_{6, \lambda}$. From the resulting exact relation $\eta^*_6 = \frac{1}{2} (6 - d + \eta^*_6)$ among the values $\eta^*_6 = \eta$ and $\eta^*_\lambda = 4 - 3$ at the infrared-stable fixed point, expression (4) for $\lambda$ follows.

Consider first $RS_1$ for $4 < d \leq 6$. For $u_0 = 0$, the theory is renormalizable and $Z_\phi = Z_{1, \infty} = 1$ to all orders in $f$. Only one bulk renormalization factor $Z_\lambda$ remains whose expansion to order $f^2$ may be gleaned from [16], which also tells us that single insertions of the composite operator $\tilde{\phi} \hat{R}$ appearing in $\tilde{\phi} \hat{R}$ additionally require a subtraction $\propto \Delta \tilde{\phi}$. Together with this latter counterterm, the above reparametrizations suffice to cure the uv singularities of the correlation and response functions [19], including those involving the surface operators $\partial_n \phi$ and $|\tilde{\phi}|_{z=0}$ and single insertions of $\tilde{\phi} \hat{R}$. The proof [20] utilizes power counting, the boundary conditions (14)–(17), and the FDT (18) [21]. The BOE (6) holds with $D(z) \sim z$.

If $u_0 \neq 0$ and $d < 4$, perturbative massless RG schemes are plagued by infrared singularities [22]. The usual escape via an $\epsilon$ expansion here is not possible because of the different upper critical dimensions 6 and 4 associated with $f_0$ and $u_0$. We therefore use $RS_2$. Writing $u_0 = \mu^{d-4} Z_\mu u$, we fix all static bulk and surface counterterms (mass shift $\tau_0 - \mu^2, Z_\phi, Z_{\phi u}, Z_{1, \infty}$) as in [23], Eqs. (3.3a-d), (710a,b)]. The remaining dynamic (bulk) counterterms ($Z_\lambda, \text{subtraction for } \tilde{\phi} \hat{R}$) can be fixed by appropriate (massive) normalization conditions for the dynamic bulk theory. From the resulting RG equations of the dynamic theory and well-established RG results for the static theory the BOE (6) and the scaling forms (7)–(8) follow.

Our simulation results are displayed in Figs. 1 and 2. They were obtained for $T = T_c, L = 60$, and a total integration time of about 5000$J$. The algorithm was parallelized and implemented on the ALiCE cluster at the BUGH Wuppertal, where the MPI (message passing interface) library
was used for communication between the processes. Finite-size effects turned out to be negligible for this choice of parameters.

![Graph](image)

**FIG. 1.** Structure function \( \hat{C}_{11}(0, \omega) \) for \( J_1/J = 0.3 \ (\times) \), 0.73 (+), and 1.0 (•). Error bars (one standard deviation) are smaller than the symbol sizes. The solid lines indicate the theoretically expected power law (4) for \( \omega \to 0 \).

In Fig. 1 the structure function \( \hat{C}_{11}(0, \omega) \) is shown for different values of \( J_1/J \) in comparison with (4). For the exponent \( (\frac{3}{4} + 1 - \eta_{\text{ord}})/3 \), we used the value 0.856 ± 0.005 that follows from the estimate \( \eta(d=3) = 2.482 \pm 0.002 \), obtained by substitution of the value \( \eta(d=3) = 0.036 \pm 0.004 \) into (4), and the current estimate \( \eta_{\text{ord}}(d=3) \) = 1.358 ± 0.012.

Depending on whether \( J_1/J \) is small (\( J_1/J = 0.3, \times \)) or larger (\( J_1/J = 1, \ast \)), the approach to the asymptotic power law (4) is from above or below. In the latter case, the asymptotic regime is not reached within the frequency range shown in Fig. 1. The best agreement with (4) over the largest frequency range is obtained for the intermediate value \( J_1/J = 0.73 \ (\ast) \).

Fig. 2 shows a scaling plot of \( \hat{C}_{11}(p, \omega) \) for \( p = (\frac{n \pi}{30}, 0, 0) \). The scaling regime in \( x \) shrinks as the mode index \( n \) is increased from \( 1(\times) \) to \( 4(\square) \). The shape of the scaling function in (8), for \( x < 1 \), is captured surprisingly well by

\[
\sigma(x) = \sigma_0 \left[ 1 + (x/x_0)^4 \right]^{(\eta_{\text{ord}}^{\text{ord}} - 1)/4},
\]

whose form is inspired by the known zero-loop result (5). The exponent at the square bracket is chosen so as to reproduce (2) in the limit \( x \to \infty \) (\( p \to 0 \) at fixed \( \omega \neq 0 \)). The amplitude \( \sigma_0 \) and the crossover parameter \( x_0 \) are used as fit parameters. The fit shown in Fig. 2 has been obtained from the data for \( n = 3 \) and \( x < 1 \).
with \( n = 1, \ldots, 4 \), are shown. Error bars (one standard deviation) are smaller than the symbol sizes. The solid line displays a fit to (19). The data for \( x \geq 1 \) are outside the scaling regime.

The agreement between the data displayed in Figs. 1 and 2 and the scaling laws (8) and (9) is quite satisfactory, albeit small deviations are seen to remain on closer inspection. Just as in [12], intermediate values of \( J_1/J (= 0.73) \) appear to be empirically optimal in that they yield the largest asymptotic scaling regime. Possible sources of deviations are (i) insufficient momentum resolution, (ii) insufficient frequency resolution, and (iii) corrections to scaling. Momentum resolution is intimately linked to the system size \( L \), which despite formidable progress in simulation techniques, still is a serious limiting factor. Frequency resolution is limited by the total integration time. From inspection of \( C_{11}(p, t) \) (not shown) we conclude that the integration time is sufficiently long. The frequency resolution \( \delta \omega/J \simeq 1.2 \times 10^{-3} \) available here rivals that of neutron scattering experiments [11]. Momentum resolution is more modest.

Corrections to scaling may have familiar static roots or be of genuine dynamic origin. Examples of the former category are corrections \( \sim (u-u^*) \) governed by the static Wegner exponent \( \omega_u \equiv \beta_u(u^*) \simeq 0.8 \), for \( d = 3 \) [24], and corrections due to the finiteness of \( c_0 \) (‘nonzero extrapolation length’) [4]. An example of the second category are Wegner-type corrections \( \sim (f-f^*) \), governed by \( \omega_f \equiv \beta_f(u^*, f^*) \), the dynamic analog of \( \omega_u \), whose \( \epsilon \) expansion about \( d=6 \) reads \( \omega_f = \epsilon + O(\epsilon^2) \) [16]. While we cannot rule out that corrections of the latter category are large, we are not aware of compelling reasons to expect this. Thus the mentioned corrections of static origin may well be the most important ones.

![Graph showing scaling function \( \sigma(x) \) according to (8). Data obtained for \( J_1/J = 0.73 \) and \( p = (\frac{4\pi}{30}, 0, 0) \), with \( n = 1, \ldots, 4 \), are shown. Error bars (one standard deviation) are smaller than the symbol sizes. The solid line displays a fit to (19). The data for \( x \geq 1 \) are outside the scaling regime.](image-url)
In summary, we have presented a detailed study of the surface critical behavior of isotropic Heisenberg ferromagnets based on phenomenological scaling and field-theoretical RG methods and corroborated our findings through high-precision simulations. Our results depicted in Figs. 1 and 2 may serve as guidelines for careful experimental tests. For these, one must choose ferromagnets for which dipolar forces (ignored here) can be trusted to be unimportant.

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