

Critical energy-density profile near walls

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We examine critical adsorption for semi-infinite thermodynamic systems of the Ising universality class when they are in contact with a wall of the so-called normal surface universality class in spatial dimension $d = 3$ and in the mean-field limit. We apply local-functional theory and Monte Carlo simulations in order to quantitatively determine the properties of the energy density as the primary scaling density characterizing the critical behaviors of Ising systems besides the order parameter. Our results apply to the critical isochore, near two-phase coexistence, and along the critical isotherm if the surface and the weak bulk magnetic fields are either collinear or anticollinear. In the latter case, we also consider the order parameter, which so far has yet to be examined along these lines. We find the interface between the surface and the bulk phases at macroscopic distances from the surface, i.e., the surface is “wet.” It turns out that in this case the usual property of monotonicity of primary scaling densities with respect to the temperature or magnetic field scaling variable does not hold for the energy density due to the presence of this interface.

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I. INTRODUCTION

We consider the semi-infinite Ising model in contact with a wall belonging to the so-called normal surface universality class [1,2], in the fixed-point case that the surface magnetic field $|h_1| = \infty$ is infinitely strong. Near the bulk critical point the delimiting surface exerts on the Ising system a perturbation of the entire system at the length scale of the bulk correlation length ξ in the direction normal to the wall. One of the important examples of such inhomogeneous fluid structures is the phenomenon of critical adsorption [3]. Fisher and de Gennes predicted the corresponding characteristic behavior of the order parameter (such as the magnetization m or the fluid density ρ) which is described by a universal scaling function [3]. Near the phase boundary and along the critical isochore the scaling of the magnetization near the bulk critical point, at zero bulk field h , is given by $m(z; t, h = 0) \simeq m_b(t, 0)P_{\pm}(z/\xi_{\pm})$, where $P_{\pm}(\cdot)$ are corresponding universal scaling functions, $m_b(t, 0) \simeq B|t|^{\beta}$, where B is the nonuniversal amplitude of the spontaneous bulk magnetization m_b , $t =$

$(T - T_c/T_c)$ is the reduced temperature, β is a standard critical exponent, z is the normal distance from the wall, and ξ_{\pm} is the bulk correlation length above and below T_c , respectively [4–12] (depending on whether T_c is an upper or lower critical point of demixing of a binary liquid mixture). Similarly, we denote $\xi_{<} = \xi(t = 0, h)$ for $hh_1 < 0$ and $\xi_{>} = \xi(t = 0, h)$ for $hh_1 > 0$. Universal scaling functions $P_c^>(x_{>})$ and $P_c^<(x_{<})$ describe the behavior of the order parameter along the critical isotherm (see Fig. 1), $m^>(z; t = 0, h) = m_b(0, h)P_c^>(z/\xi_{>})$ when $hh_1 > 0$ and $m^<(z; t = 0, h) = m_b(0, h)P_c^<(z/\xi_{<})$ for $hh_1 < 0$, assuming $|h| \rightarrow 0$ and the usual conditions for the continuum limit, such as $z \rightarrow \infty$ and $\xi \rightarrow \infty$ (i.e., large compared to all microscopic length scales) with $x_{\leq} = z/\xi_{\leq}$ finite, where $\xi_{\leq}(t = 0, h) \approx \xi_c^{\leq}|h|^{-\nu/(\beta\delta)}$ and $x_{\pm} = z/\xi_{\pm}$ for $\xi_{\pm}(t \rightarrow \pm 0, h = 0) \approx \xi_0^{\pm}|t|^{-\nu}$.

The paradigmatic discrete lattice model we refer to is the ferromagnetic Ising model. Typically, local observables investigated in such a model are sums of products of neighboring spins or the sum of the spins, such as the local magnetization itself as introduced above. The other kind of quantity, which is often in the focus, is the energy density $\sum_{\mathbf{r}, \mathbf{r}'} J(\mathbf{r} - \mathbf{r}')s(\mathbf{r})s(\mathbf{r}')$, where we associate a spin $s(\mathbf{r}) = \pm 1$ with each site of the lattice and where $J(\mathbf{r} - \mathbf{r}')$ is a short-ranged pair interaction.

While the examination of the local order parameter stimulated much experimental [13–19] and theoretical analyses

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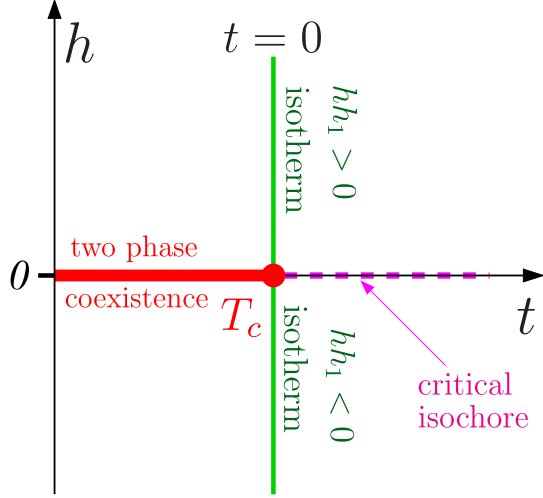


FIG. 1. Phase diagram in the (t, h) plane of the Ising system with the critical isochore ($t > 0, h = 0$), two-phase coexistence ($t < 0$), and critical isotherm $t = 0$ associated with the two branches $hh_1 > 0$ and $hh_1 < 0$.

[4–11], in higher spatial dimensions ($d = 3, 4$) the study of the energy density—along the above-mentioned critical loci and for the present choice of boundary conditions (BCs)—is lacking so far.

It is natural that the first nonclassical results for the energy density are related to the integrable two-dimensional (2D) Ising model. Moreover, the 2D model is conformally invariant in the scaling limit at the bulk critical point. This facilitates the application of conformal field theory [20] and Schramm-Loewner evolution techniques [21]. The energy density in the half plane along the critical isochore (i.e., zero bulk magnetic field $h = 0$ and $t > 0$, see Fig. 1) and near two-phase coexistence was obtained by Mikheev-Fisher’s theory for variable boundary conditions, including as limiting cases the normal and the ordinary surface universality classes [22–25]. Independently, the energy density has been recently obtained by using the transfer-matrix technique [26]. Conformal field theory was used to determine the 2D energy density and its correlation functions for various boundary conditions [20]. Recently, a rigorous approach in terms of discrete fermionic correlators was used in order to determine the energy density in the scaling limit of free and normal boundary conditions at the bulk critical point [27], for which full conformal invariance of the correlation function was shown to hold. Additionally, this approach also enables one to specify the lattice specific constant associated with the hyperbolic metric factor [27]. The critical behavior of the energy density near the ordinary transition has been studied in Ref. [28], where it has been demonstrated that the critical exponents associated with the energy density (near the ordinary transition) can be entirely expressed in terms of bulk exponents.

II. SCALING OF THE ENERGY DENSITY AND MAGNETIZATION

The energy density plays an essential role in Ising systems when establishing free-energy functionals on the basis of the

complete list of primary scaling densities, instead of using the magnetization only [23,24]. The energy density is a necessary theoretical prerequisite for determining the (specific) heat capacity, which is important as an experimentally measurable quantity.

The purpose of the present study is to analyze the energy density for $d \geq 3$ along the critical loci indicated in Fig. 1.

Scaling theory suggests that the behavior of the excess energy density is described by a universal scaling function, such that for the critical isochore ($t > 0, h = 0$) and near two-phase coexistence ($t < 0, h = 0$) close to the bulk critical point one has

$$\Delta \varepsilon_{\pm}(z; t, h = 0) = |t|^{1-\alpha} \Delta \tilde{\varepsilon}_{\pm}(x_{\pm}), \quad (1)$$

where $x_{\pm} = z/\xi_{\pm}$ are the corresponding scaling variables for $t > 0$ and $t < 0$, respectively, $\Delta \tilde{\varepsilon}_{\pm}(x_{\pm}) =: \tilde{\varepsilon}_{\pm}(x_{\pm}) - \varepsilon_{\text{bulk}}$ are universal scaling functions up to multiplicative nonuniversal constants C_0^{\pm} , such that $\Delta \tilde{\varepsilon}_{\pm}(x_{\pm}) = C_0^{\pm} \Phi_{\pm}^{\varepsilon}(x_{\pm})$ with the universal scaling function $\Phi_{\pm}^{\varepsilon}(x_{\pm})$, and α is the specific heat critical bulk exponent.

Similarly, the energy density along the critical isotherm is governed by the scaling law

$$\Delta \varepsilon_c^{\leq}(z; t = 0, h) = |h|^{\frac{1-\alpha}{\beta\delta}} \Delta \tilde{\varepsilon}_c^{\leq}(x_{\leq}), \quad x_{\leq} = z/\xi_{\leq}(t = 0, h), \quad (2)$$

where $\Delta \tilde{\varepsilon}_c^{\leq}$ is a universal scaling function up to a multiplicative nonuniversal constant C_c^{\leq} for $hh_1 > 0$ like $\Delta \tilde{\varepsilon}_c^{\leq}$ with the nonuniversal constant C_c^{\leq} referring to the case $hh_1 < 0$. Again, we shall present only the universal parts of Eq. (2) via the scaling functions $\Phi_{c, >}^{\varepsilon}$ and $\Phi_{c, <}^{\varepsilon}$ such that $\Delta \tilde{\varepsilon}_c^{\leq} = C_c^{\leq} \Phi_{c, \leq}^{\varepsilon}(x_{\leq})$.

Additionally, we consider the universal scaling function $P_c^{\leq}(x_{\leq})$ in the case that the bulk field h and the surface field h_1 are anticollinear, i.e., $hh_1 < 0$, which leads to the formation of an interface. This also helps to elucidate the unusual behavior of the universal energy-density scaling function $\Phi_{c, <}^{\varepsilon}$.

The local-functional method [29] is based on the free-energy functional

$$\mathcal{F}[m] = \int_0^{\infty} \mathcal{A}(m, \dot{m}; t, h) dz + f_1(m_1, h_1), \quad (3)$$

where $\dot{m} \equiv dm/dz$ and $m_1 \equiv m(z = 0)$. The surface contribution is taken into account via $f_1(m_1, h_1) = -h_1 m_1 + \dots$ and contains the symmetry-breaking surface field h_1 . The integrand $\mathcal{A}(m, \dot{m}; t, h)$ is assumed to take the form

$$\mathcal{A}(m, \dot{m}; t, h) = \{\mathcal{G}(\Lambda(m; t, h)\dot{m}) + 1\}W(m; t, h), \quad (4a)$$

with the auxiliary free energy function

$$W(m; t, h) = \Phi(m, t) - \Phi(m_b, t) - h(m - m_b), \quad (4b)$$

where $\Phi(m, t)$ is the bulk Helmholtz free energy density. The function $\mathcal{G}(\cdot)$ is endowed with several features following from requisites settled in Refs. [29,30]. It is an outstanding characteristic feature that for semi-infinite systems the function $\mathcal{G}(x)$ does not enter any pertinent formulas after minimizing the functional given by Eqs. (3) and (4) due to the fact that for the planar semi-infinite geometry the argument of \mathcal{G} becomes constant, that is, $\mathcal{G}(x \rightarrow -1)$ [12,31].

Generally, below the upper critical dimension ($d < d_c = 4$) the bulk quantities take on the scaling forms

$$W(m, t, 0) \approx |m|^{\delta+1} Y_{\pm}[m/(B|t|^{\beta})] \quad (5)$$

and

$$\frac{\xi_{\pm}^2}{2\chi} = |m|^{-\eta\nu/\beta} Z_{\pm}[m/(B|t|^{\beta})], \quad (6)$$

where χ is the magnetic susceptibility. These scaling forms are valid in the scaling limits $t \rightarrow 0^{\pm}$ and $m \rightarrow 0$ so that $m/|t|^{\beta}$ is finite, with η as the critical exponent of the bulk correlation function in common notation. The scaling functions in Eqs. (5) and (6) are distinguished by the following expansion properties [29], following from the analyticity of $\Phi(m; t)$ and $\xi(m; t)$ across the entire one-phase region but excluding the bulk critical point,

$$Y_{\pm}(y \rightarrow \pm\infty) = \frac{A_{\pm}|By|^{-(\delta+1)}}{(2-\alpha)(1-\alpha)} + \sum_{n=0}^{\infty} Y_{\infty,n}(\pm 1)|y|^{-n/\beta}, \quad (7)$$

where $y := \frac{m}{B|t|^{\beta}}$. A_{\pm} are nonuniversal amplitudes associated with the bulk specific heat $C_b \simeq A_{\pm}|t|^{-\alpha}$, while a similar expansion holds for $Z_{\pm}(y)$, but without the first term.

Analyticity along the critical isochore ($t > 0, h = 0$) implies

$$Y_{+}(y \rightarrow \pm\infty) = |y|^{-(1+\delta)} \sum_{n=0}^{\infty} Y_{0,2n} y^{2n}. \quad (8)$$

An analogous expansion is valid for $Z_{+}(y)$. The asymptotic behavior near two-phase coexistence is given by

$$Y_{-}(y \rightarrow 1) \approx (y \mp 1)^2 \sum_{n=0}^{\infty} Y_{1,n}(\pm 1)^n (y \mp 1)^n. \quad (9)$$

There is a similar expansion for $Z_{-}(y)$ [32].

Within the present model the excess energy density $\Delta\varepsilon(z, t, h)$ is defined in terms of the first temperature derivative of the surface tension Σ between the confining wall (or inert vapor phase, \cdot) and the fluid (ω), which yields $\sum[\cdot|\omega] \equiv \min_{[m]} \mathcal{F}[m] = 2 \int_0^{\infty} W(m) dz + f_1(m_1, h_1)$ so that

$$\frac{\partial \sum[\cdot|\omega]}{\partial t} = \int_0^{\infty} \Delta\varepsilon_{\pm}(z; t, h) dz. \quad (10)$$

The last equation leads to the local-functional expression for the excess energy density,

$$\Delta\varepsilon_{\pm}(z; t, h) = \frac{2}{\Lambda_{\pm}(m)} \frac{\partial}{\partial t} [\Lambda_{\pm}(m) W(m)],$$

$$\Lambda_{\pm}(m) \equiv \frac{\xi_{\pm}(m)}{\sqrt{2\chi(m)W(m)}}. \quad (11)$$

In order to substantiate the case of the critical isotherm for $hh_1 < 0$ we have also calculated the universal scaling function of the order parameter $P_c^<(x_<)$ defined in the Introduction. Minimizing the functional given by Eqs. (3) and (4) provides the first integral in the scaling limit $z \rightarrow \infty$ and $\xi_< \rightarrow \infty$

with $x_< = z/\xi_<$ finite. This determines $P_c^<$ via the following implicit equations,

$$x_< = z/\xi_< = \sqrt{\frac{\delta(\delta+1)}{2}} \int_{-P_c^<}^{\infty} \frac{u^{\frac{\gamma-2\nu}{2\beta}} du}{\sqrt{u^{1+\delta} + (1+\delta)u + \delta}},$$

for $-\infty < P_c^< \leq 0$, (12a)

and

$$x_< = z/\xi_< + x_{\text{inf}c} = \sqrt{\frac{\delta(\delta+1)}{2}} \int_0^{P_c^<} \frac{u^{\frac{\gamma-2\nu}{2\beta}} du}{\sqrt{u^{1+\delta} - (1+\delta)u + \delta}},$$

for $0 \leq P_c^< < 1$, (12b)

where $x_{\text{inf}c}$ is the position of the interface defined by the condition $P_c^<(x_{\text{inf}c}) \equiv 0$ and given explicitly by

$$x_{\text{inf}c} = \sqrt{\frac{\delta(\delta+1)}{2}} \int_0^{\infty} \frac{u^{\frac{\gamma-2\nu}{2\beta}} du}{\sqrt{u^{1+\delta} + (1+\delta)u + \delta}}. \quad (13)$$

Before expounding the mean-field and the three-dimensional results for the universal energy-density scaling functions $\Phi_{\pm}^{\varepsilon}(x_{\pm})$, $\Phi_{c,<}^{\varepsilon}(x_<)$, and $\Phi_{c,>}^{\varepsilon}(x_>)$ based on Eq. (11), and before analyzing the universal profiles $P_c^<(x_<)$ obtained from Eqs. (12) and (13), we first construe their *general* asymptotic properties following from analytical requirements imposed onto the functions $Y_{\pm}(y)$ and $Z_{\pm}(y)$ given in Eqs. (7)–(9).

III. SHORT-DISTANCE BEHAVIOR

Along the critical isochore the asymptotic behavior of the energy density $\Delta\varepsilon_{\pm}(x_{\pm})$ for small distances from the wall is dominated by a *single* diverging term which is determined by the energy-density scaling dimension $x_{\varepsilon} = (1-\alpha)/\nu$,

$$\Phi_{\pm}^{\varepsilon}(x_{\pm} \rightarrow 0) \approx \mp B^{\delta+1} \left(Y_{\infty,1} + \frac{Z_{\infty,1} Y_{\infty,0}}{Z_{\infty,0}} \right) (c_{\pm})^{\frac{1-\alpha}{\beta}} x_{\pm}^{-\frac{1-\alpha}{\nu}}, \quad (14)$$

where c_{\pm} are universal amplitudes emerging in the short-distance expansion of the universal profiles $P_{\pm}(x_{\pm})$ [8,12]. Apart from the leading term as given in Eq. (14), there is an infinite number of continuous subdominant terms of two kinds: $[\Phi_{\pm}^{\varepsilon}(x_{\pm} \rightarrow 0)]_{n,1} \propto (c_{\pm})^{-\frac{n}{\beta}} x_{\pm}^{\frac{n}{\nu}}$ and $[\Phi_{\pm}^{\varepsilon}(x_{\pm} \rightarrow 0)]_{n,2} \propto (c_{\pm})^{-\frac{\alpha+n}{\beta}} x_{\pm}^{\frac{\alpha+n}{\nu}}$. It is interesting that close to the surface of the ordinary surface universality class the energy density behaves as a linear combination of two powers $z^{\frac{1}{\nu}}$ and $z^{\frac{1+\alpha}{\nu}}$ in the lowest approximation [28], which correspond exactly to the first two terms of continuous expansions within the local-functional theory (LFT) as discussed just above.

These findings are in accord with the general expectation [33] that an *arbitrary* scaling density Ψ near the surface should exhibit the asymptotic behavior

$$\Psi(x_{\pm} \rightarrow 0) \propto x_{\pm}^{-x_{\Psi}}, \quad (15)$$

where x_{Ψ} is the corresponding scaling dimension of Ψ . The spontaneous magnetization vanishes $\propto x^{\frac{\beta_1-\beta}{\nu}}$ with the surface critical exponent β_1 . In the limit $h_1 \rightarrow \infty$ the crossover to the normal universality class occurs, for which $\beta_1 = 0$ [1,34]

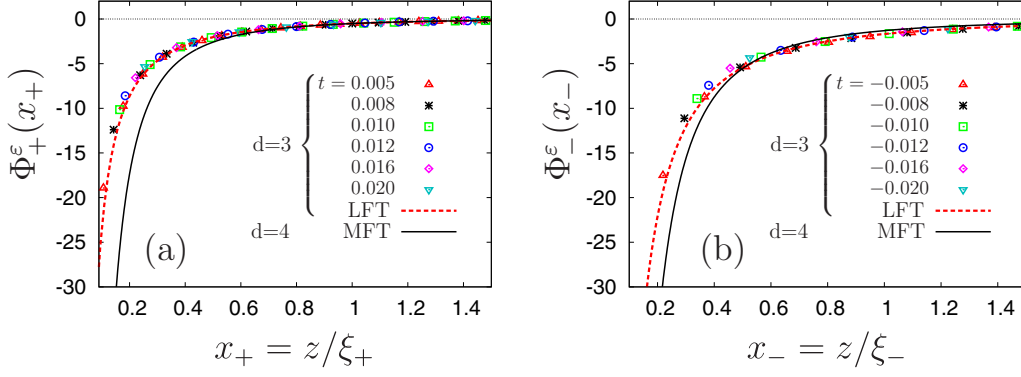


FIG. 2. Universal part of the excess energy density Φ_\pm^ϵ [see Eq. (1) and below] along the critical isochore provided by LFT in $d = 3$ (red dashed line) and MFT [black solid line, Eq. (22)] in comparison with the MC data in $d = 3$ (symbols), rescaled by nonuniversal factors so that the plotted symbols correspond to $\Phi_\pm^\epsilon(x_\pm) = \frac{1}{C_0^\pm} \Delta\tilde{\epsilon}_\pm$, where $C_0^- = 4.236$, $C_0^+ = 4.260$ (see the section “Monte Carlo simulations” and Table I for further details): (a) Φ_+^ϵ as a function of the scaling variable $x_+ = z/\xi_+$ for six values of the reduced temperature $t = 0.005, \dots, 0.02$; (b) Φ_-^ϵ as a function of the scaling variable $x_- = z/\xi_-$ for six values of the reduced temperature $t = -0.005, \dots, -0.02$. Here and in other figures, error bars are of the size of the symbols. The numerical data do scale and form universal scaling functions, which do not depend on t separately.

The short-distance behavior of the energy density along the critical isotherm is the same for both cases $hh_1 > 0$ and $hh_1 < 0$,

$$\Phi_{c,\leq}^\epsilon(x_{\leq} \rightarrow 0) \approx (\tilde{C}_c^{\leq})^{\frac{1-\alpha}{\beta}} x_{\leq}^{-\frac{1-\alpha}{\nu}}, \quad (16)$$

where \tilde{C}_c^{\leq} are universal constants associated with the short-distance expansion of the order-parameter scaling function $P_c^{\leq}(x_{\leq})$, as shown below in the case $hh_1 < 0$. Equation (16), which refers to the critical isotherm, confirms the validity of the general behavior as discussed in Eq. (15).

The short-distance expansion of the universal order-parameter scaling function $P_c^<(x_<)$ follows from the asymptotic solution of Eq. (12a),

$$P_c^<(x_< \rightarrow 0) \approx (\tilde{C}_c^<)^{\frac{1-\alpha}{\beta}} (x_<)^{-\frac{\beta}{\nu}}, \quad (17)$$

showing the power-law divergence of the type provided in Eq. (15), controlled by the order-parameter scaling dimension $x_\psi = \beta/\nu$. Equation (17) defines the universal constant $\tilde{C}_c^<$, which has also appeared above in Eq. (16). The universal constants $\tilde{C}_c^<$ and $\tilde{C}_c^>$ are not related in any way with the nonuniversal constants $C_c^<$ and $C_c^>$ which were introduced earlier [see Eq. (7) and below it]. A similar behavior holds also for $P_c^>(x_> \rightarrow 0)$, rendering $\tilde{C}_c^>$.

IV. LARGE-DISTANCE BEHAVIOR

The behavior of the universal energy-density scaling functions $\Phi_+^\epsilon(x_+ \rightarrow \infty)$ and $\Phi_-^\epsilon(x_- \rightarrow \infty)$, although characterized by exponential decays, is not the same along the isochore ($t > 0, h = 0$) and near two-phase coexistence ($t < 0, h = 0$).

For $T > T_c$ the energy-density expansion is described only by *even powers* of the exponential function e^{-x} ,

$$\Delta\tilde{\epsilon}_+(x_+ \rightarrow \infty) \approx \sum_{n=1}^{\infty} l_n e^{-2nx_+}, \quad (18)$$

where we quote only the first two expansion coefficients $l_1 = -\beta B^{1+\delta} Y_{0,1} [(1-\delta) + \frac{\eta\nu}{\beta}] (P_{+,1}^\infty)^2$ and $l_2 = -\beta B^{1+\delta} [(3-\delta) Y_{0,2} + \frac{Y_{0,1} Z_{0,1}}{Z_{0,0}} (2 + \frac{\eta\nu}{\beta}) + \frac{Y_{0,1} Z_{0,2}}{Z_{0,0}} (4 + \frac{\eta\nu}{\beta}) + \frac{Y_{0,3} Z_{0,3}}{Z_{0,0}} (\frac{\eta\nu}{\beta})] P_{+,1}^2$.

For $T < T_c$ the asymptotic expansion of the energy density comprises both even and odd powers of the exponential function,

$$\Delta\tilde{\epsilon}_-(x_- \rightarrow \infty) \approx \sum_{n=1}^{\infty} m_n e^{-nx_-}. \quad (19)$$

Here, we provide only the leading expansion terms $m_1 = -2\beta B^{1+\delta} Y_{1,0} P_{-,1}^\infty$ and $m_2 = -\beta B^{1+\delta} [3Y_{1,1} + \frac{Y_{1,0} Z_{1,1}}{Z_{1,0}} (2 + \frac{\eta\nu}{\beta}) + 2(\delta + 2) Y_{1,0}] P_{-,1}^2$.

Large-distance expansions of the energy densities along the *critical isotherm* are governed by exponential decays

$$\Phi_{c,\leq}^\epsilon(x_{\leq} \rightarrow \infty) \approx \pm \frac{1-\alpha}{\beta} P_{c,1}^\infty e^{-x_{\leq}} + \dots, \quad (20)$$

where the $>$ sign refers to $\Phi_{c,>}^\epsilon$ and the $<$ sign to $\Phi_{c,<}^\epsilon$. $P_{c,1}^\infty$ is the universal amplitude turning up originally within the large-distance expansion of the universal scaling functions $P_c^<(x_<)$ and $P_c^>(x_>)$ of the order parameter. Undertaking the asymptotic analysis of Eq. (12b), in the limit $x \rightarrow \infty$ we obtain

$$P_c^<(x_< \rightarrow \infty) = 1 - P_{c,1}^\infty e^{-x_<} + \dots, \quad (21)$$

with $P_{c,1}^\infty$ as a universal amplitude.

V. MEAN-FIELD RESULTS $d \geq 4$

Mean-field theory ($d \geq 4$) follows from the LFT if the bulk Helmholtz free energy introduced by Eq. (4b) takes on the Landau-Ginzburg form with $\xi^2/(2\chi)$ [Eq. (6)] being constant with respect to both variables t and h . In the case of the critical isochore ($t > 0, h = 0$) and near two-phase coexistence

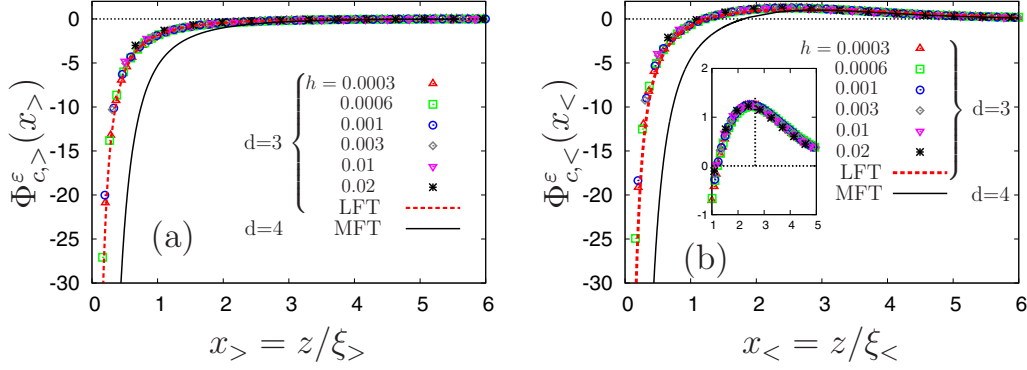


FIG. 3. Universal part of the excess energy density $\Phi_{c,\leq}^\epsilon(x_{\leq})$ [see Eq. (2) and below] along the isotherm as a function of the scaling variable $x_{\leq} = z/\xi_{\leq}$ for six values of the bulk field h , provided by LFT (red dashed line) and MFT [black solid line, Eqs. (23) and (26)] in comparison with MC data in $d = 3$ (symbols), rescaled by nonuniversal factors so that the plotted symbols correspond to $\Phi_{c,\leq}^\epsilon = \frac{1}{C_c^\leq} \Delta \tilde{\epsilon}_c^\leq(x_{\leq})$, where ($C_c^> = 1.747$, $\xi_c^> = 0.469$) and ($C_c^< = 1.886$, $\xi_c^< = 0.474$) for (a) $hh_1 > 0$ and (b) $hh_1 < 0$ (see Table I). In the inset of (b) the vertical dashed line indicates the interface position x_{inf} . The numerical data do scale and form universal scaling functions, which do not depend on h separately.

($t < 0$, $h = 0$) we obtain from the expression in Eq. (11)

$$\Phi_+^\epsilon(x_+) = \frac{3}{\sinh^2(x_+)} \quad (22a)$$

and

$$\Phi_-^\epsilon(x_-) = \frac{3}{2} \left[\coth^2\left(\frac{x_-}{2}\right) - 1 \right], \quad d \geq 4. \quad (22b)$$

In Fig. 2 we plot the results for the rescaled energy density along the critical isochore and near two-phase coexistence, as obtained within mean-field theory (MFT) [Eq. (22)], together with LFT and Monte Carlo (MC) results in $d = 3$, which are rescaled by using nonuniversal scaling factors.

Along the critical isotherm and for $hh_1 > 0$ the universal scaling function of the energy density $\Phi_{c,>}^\epsilon(x_>)$ takes the form

$$\Phi_{c,>}^\epsilon(x_>) = -\frac{3[1 + \sqrt{2} \sinh[x_> + \sinh^{-1}(\sqrt{2})]]}{[\sqrt{2} - \sinh[x_> + \sinh^{-1}(\sqrt{2})]]^2}, \quad d \geq 4, \quad hh_1 > 0, \quad (23)$$

which is plotted in Fig. 3(a) together with the results for $d = 3$.

Along the critical isotherm, but for $hh_1 < 0$, there is a competition between surface-induced order and the bulk order such that the emerging interface in between can depin from the nearby wall. Assigning mean-field exponents in Eq. (13) we obtain for the interface position

$$x_{\text{inf}}^{\text{MF}} = \ln(4 + 3\sqrt{2} + 2\sqrt{6} + 3\sqrt{3}) \simeq 2.90896. \quad (24)$$

Equation (12) yields for the universal order-parameter profile

$$P_{c,\text{MF}}^<(x_<) = -\frac{5 + 2\sqrt{6} + 4(2 + \sqrt{6})e^{x_<} - e^{2x_<}}{(e^{x_<} - 1)(5 + 2\sqrt{6} + e^{x_<})}, \quad x_< < x_{\text{inf}}^{\text{MF}}, \quad (25a)$$

and

$$P_{c,\text{MF}}^<(x_<) = 1 - \frac{6(3\sqrt{2} - 4)e^{x_<}}{12\sqrt{2} - 17 + e^{x_<}(6\sqrt{2} - 8 + e^{x_<})}, \quad x_< > x_{\text{inf}}^{\text{MF}}, \quad (25b)$$

The mean-field result of $P_{c,\text{MF}}^<$ is given in Fig. 4(b) together with $P_{c,\text{MF}}^>$ [12] for comparison. Employing Eq. (11) and the scaling law in Eq. (2) we obtain the universal scaling functions $\Phi_{c,>}^\epsilon$ [Eq. (23)] and $\Phi_{c,<}^\epsilon$ of the energy density along the critical isotherm,

$$\Phi_{c,<}^\epsilon(x_<) = \frac{6e^{x_<}[-22 - 9\sqrt{6} - 2(5 + 2\sqrt{6})e^{x_<} + (2 + \sqrt{6})e^{2x_<}]}{(e^{x_<} - 1)^2(5 + 2\sqrt{6} + e^{x_<})^2}, \quad x_< < x_{\text{inf}}^{\text{MF}}, \quad hh_1 < 0, \quad (26a)$$

and

$$\Phi_{c,<}^\epsilon(x_<) = \frac{6e^{x_<}[140 - 99\sqrt{2} + e^{x_<}(24\sqrt{2} - 34) + (3\sqrt{2} - 4)e^{2x_<}]}{[-17 + 12\sqrt{2} + e^{x_<}(-8 + 6\sqrt{2} + e^{x_<})]^2}, \quad x_< > x_{\text{inf}}^{\text{MF}}, \quad hh_1 < 0. \quad (26b)$$

We plot the scaling functions $\Phi_{c,>}^\epsilon$ and $\Phi_{c,<}^\epsilon$ for $d \geq 4$ in Figs. 3(a) and 3(b), respectively, as solid lines, together with

the results of the LFT and the MC calculations. In Fig. 3, already at the mean-field level, one sees that, contrary to

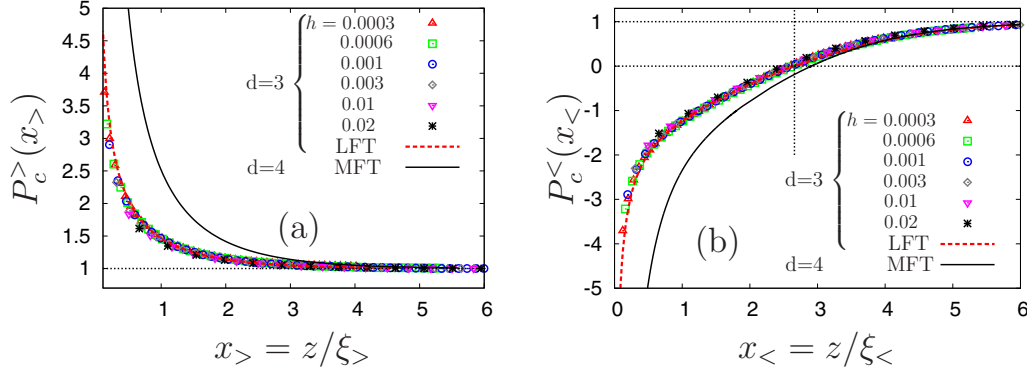


FIG. 4. Universal scaling functions $P_c^{\leq}(x_{\leq})$ of the order-parameter profiles along the isotherm as a function of the scaling variable $x_{\leq} = z/\xi_{\leq}$ for six values of the bulk field h , provided by LFT (red dashed line) and MFT (black solid line) in comparison with MC data [symbols, rescaled by nonuniversal factors such as with $\xi_{>}^z = 0.469$ and $\xi_{<}^z = 0.474$ in $P_c^{\leq}(x_{\leq})$]: (a) $hh_1 > 0$ and (b) $hh_1 < 0$. In (b) the vertical dotted line indicates the interface position $x_{\text{inf}} = 2.65905$.

all other primary scaling densities, $\Phi_{c,<}^{\varepsilon}$ is a nonmonotonic function due to the depinning of the emerging interface in the case $hh_1 < 0$, exhibiting a maximum exactly at the position $x = x_{\text{inf}}$ of the interface. The presence of the interface in the system is clearly evident from the behavior of the order-parameter scaling function $P_c^<(x_<)$ in Fig. 4(b).

VI. RESULTS IN $d = 3$

In order to derive reliable, quantitative predictions for the scaling functions $\Phi_{\pm}^{\varepsilon}(x_{\pm})$, $\Phi_{c,\leq}^{\varepsilon}(x_{\leq})$, and $P_c^<(x_<)$ in $d = 3$, one needs adequate values of the nonclassical bulk critical exponents entering into Eqs. (1)–(3) and (11)–(13). In Eq. (11) correct expressions for the non-mean-field scaling functions $Y_{\pm}(y)$ and $Z_{\pm}(y)$ must be provided. The appropriate way to represent the scaling functions in our study is based on Schofield’s parametric models [35] and its generalizations [29,36]. Based on the requirement to provide the most satisfactory fits to the bulk data, the latter models render at the same time the scaling functions $Y_{\pm}(y)$ and $Z_{\pm}(y)$ such that they indeed exhibit their analyticity properties, as borne out by Eqs. (7)–(9). The “linear” parametric mode, which we currently use, implements a satisfactory fit to the universal bulk amplitude relations, provided the values of the parameters introduced in Ref. [12] are chosen as $b^2 = 1.30$ and $a_2 = 0.28$. For the bulk critical exponents we choose $\beta = 0.328$ and $\nu = 0.632$.

The resulting scaling functions $\Phi_{\pm}^{\varepsilon}(x_{\pm})$ are plotted in Figs. 2(a) and 2(b) together with the corresponding MC data. The results of the pertinent calculations in $d = 3$ for $\Phi_{c,>}^{\varepsilon}(x_>)$ are shown together with the corresponding MC data in Fig. 3(a). The analytic mean-field result [Eq. (23)] for the latter quantity is shown in the same figure by a solid black line. The universal scaling function $\Phi_{c,<}^{\varepsilon}(x_<)$ along the critical isotherm for $hh_1 < 0$ has been calculated in $d = 3$ by LFT and MC as well as via MFT [Eq. (26)]. These results are shown in Fig. 3(b).

Local-functional results for the universal scaling functions $P_c^>(x_>)$ and $P_c^<(x_<)$ are given in Figs. 4(a) and 4(b) together with corresponding MC data. The analytically calculated universal scaling function $P_c^>$ [12], given here for the reason

of completeness, is compared here with respect to the MC data. Based on the results obtained in the mean-field limit $d = 4$ and in $d = 3$ we can report their qualitative agreement across the dimensions; moreover, we find excellent data collapse of the 3D MC data onto the theoretical master curve for $d = 3$. All primary scaling densities associated with critical adsorption, such as the universal profiles $P_c^>(x_>)$ considered in Ref. [12] together with the universal density profiles $\Phi_{\pm}^{\varepsilon}(x_{\pm})$, $\Phi_{c,>}^{\varepsilon}(x_>)$, and $P_c^<(x_<)$ scrutinized here, are monotonic functions of their scaling variable. An exception to this observation is the universal energy density $\Phi_{c,<}^{\varepsilon}(x_<)$ along the critical isotherm for $hh_1 < 0$, both in $d = 3$ and in the mean-field limit. The calculations of $P_c^<(x_<)$ in this study yield the interface depinning at $x_{\text{inf}} = 2.65906$ in $d = 3$ and at $x_{\text{inf}}^{\text{MF}} = 2.90896$. We recall that by definition one has $P_c^<(x_{\text{inf}}) \equiv 0$. The value $x_{\text{inf}} = 2.65905$ is computed by using Eq. (13) and it is indicated in Figs. 3(b) and 4(b) by vertical dashed lines. It turns out that for both $d = 3$ and $d = 4$ the scaling function $\Phi_{c,<}^{\varepsilon}(x_<)$ exhibits a maximum at x_{inf} , i.e., at the point where the order parameter changes sign (which is a natural choice for the interface position—albeit not mandatory).

VII. MONTE CARLO SIMULATIONS

We consider the Ising model with the bulk field h on a simple cubic lattice with spacing a . All distances are measured in units of a and therefore they are dimensionless. The system size is $L_{\parallel} \times L_{\parallel} \times L_{\perp}$. On each lattice site $\mathbf{r} = (i, j, k)$ with the coordinates $1 \leq i \leq L_{\parallel}$, $1 \leq j \leq L_{\parallel}$, and $1 \leq k \leq L_{\perp}$ a classical spin $s_{\mathbf{r}} = \pm 1$ is located. The Hamiltonian of the model is given by

$$\mathcal{H} = -J \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} s_{\mathbf{r}} s_{\mathbf{r}'} - h \sum_{\langle \mathbf{r} \rangle} s_{\mathbf{r}} - h_1 \sum_{\langle \text{bot} \rangle} s_{\mathbf{r}} - h_1 \sum_{\langle \text{top} \rangle} s_{\mathbf{r}}, \quad (27)$$

where the sum $\langle \mathbf{r}, \mathbf{r}' \rangle$ is taken over all pairs of nearest-neighbor spins on the lattice, the sum $\langle \mathbf{r} \rangle$ is taken over all spins on the lattice, and the sums $\langle \text{bot} \rangle$ and $\langle \text{top} \rangle$ run over the bottom layer $k = 1$ and the top layer $k = L_{\perp}$ of spins, respectively. For the computations along the critical isotherm we apply infinitely strong values $h_1 = +\infty$ of the surface fields in the

case of collinear fields (i.e., $hh_1 > 0$) and $h_1 = -\infty$ for the case of anticollinear fields (i.e., $hh_1 < 0$) while the value $h > 0$ of the bulk field $h > 0$ is always positive. Here and in the following, we measure the energy and the bulk and surface fields in units of J . We take the bottom wall to be located at point $1/2$ (i.e., half of a lattice spacing in vertical direction below the bottom layer). Therefore, the distance z from the wall for the layer k is $z = k - 1/2$. The layer order parameter at distance z (which is half integer, $z = 1/2, 3/2, 5/2, \dots$) from the wall is

$$m(z) = \frac{1}{L_{\parallel}^2} \sum_{\langle k=z+1/2 \rangle} s_{\mathbf{r}}, \quad (28)$$

where the sum $\langle k = z + 1/2 \rangle$ is taken over the corresponding layer $k = 1, 2, 3, \dots$ of spins. The energy density $\varepsilon(z)$ per site at distance z is

$$\varepsilon(z) = \frac{1}{2L_{\parallel}^2} \sum_{\langle k=z+1/2 \rangle} \sum_{|\mathbf{r}-\mathbf{r}'|=1} s_{\mathbf{r}}s_{\mathbf{r}'}, \quad (29)$$

where the sum $\langle k = z + 1/2 \rangle$ is taken over the layer k of spins at $\mathbf{r} = (i, j, k)$ and at the distance $z = k - 1/2$ from the wall, the second sum is taken over all six nearest neighbors \mathbf{r}' of the spin with the coordinates $(i \pm 1, j, k)$, $(i, j \pm 1, k)$, and $(i, j, k \pm 1)$. We have performed MC simulations for the system of size $L_{\parallel} \times L_{\parallel} \times L_{\perp} = 100 \times 100 \times 1000$ using the hybrid MC method [37]. Each MC step consists of a Wolff cluster update [38] which is followed by $L_{\parallel}^2 L_{\perp}$ single-spin Metropolis updates. The thermalization consists of 2×10^4 MC steps and the thermal averaging is performed over 10^5 MC steps. The reduced temperature is $t = (T - T_c)/T_c = (\beta_c - \beta)/\beta$ where the critical value of the inverse temperature $\beta = 1/T$ is $\beta_c \simeq 0.221\,654\,55(3)$ [39]. The values of the bulk critical exponents are $\alpha = 0.1097(6)$, $\beta = 0.326\,52(15)$ (not to be mixed up with $\beta = 1/T$), $\gamma = 1.2372(3)$, $\nu = 0.6301(2)$, $\eta = 0.0364(4)$, $\delta = 4.789\,23(400)$, and $\Delta = \beta\delta = 2 - \alpha - \beta = 1.5638(7)$ [40]. A more recent, and probably more accurate, value for $\nu = 0.630\,02(10)$ is provided in Ref. [41] but we use the value $0.6301(2)$ in order to stay consistent with other critical indices.

In order to obtain the wall-induced deviation of the energy density from the bulk behavior,

$$\Delta\varepsilon(z, t, h) = \varepsilon(z, t, h) - \varepsilon_{\text{bulk}}(t, h), \quad (30)$$

and in order to obtain the normalized order-parameter profile along the critical isotherm $\beta = \beta_c$ (before scaling becomes manifest),

$$P_c(z, t, h) = \frac{m(z, t, h)}{m_{\text{bulk}}(t, h)}, \quad (31)$$

one needs to know the bulk energy density $\varepsilon_{\text{bulk}}$ and the bulk magnetization m_{bulk} . In order to compute $\varepsilon_{\text{bulk}}$ and m_{bulk} along the isochore ($t, h = 0$) and the critical isotherm ($t = 0, h$) we have carried out additional simulations for a cubic system of the size 256^3 with periodic boundary conditions in all three directions, which are performed with the same number of MC steps as stated above. Then we compute $\Delta\tilde{\varepsilon}_{\pm}$ and $\Delta\tilde{\varepsilon}_c^{\leq}$ by using Eqs. (1) and (2). In the case under study, there are two sources of nonuniversal contributions. The total energy density comprises nonuniversal prefactors C_0^{\pm} multiplying the

TABLE I. Nonuniversal amplitudes $C_0^-, C_0^+, \xi_c^{\leq}, \xi_c^{\geq}, C_c^{\leq}$, and C_c^{\geq} which are obtained upon rescaling the MC scaling functions Φ_{\pm}^{ε} , Φ_{\pm}^{ε} , $P_c^{\leq}, P_c^{\geq}, \Phi_{c,\leq}^{\varepsilon}$, and $\Phi_{c,\geq}^{\varepsilon}$ such that the deviation between the 3D MC and LFT results are minimized. The asterisk * indicates that in the course of the fitting procedures for $\Phi_{c,\leq}^{\varepsilon}$ and $\Phi_{c,\geq}^{\varepsilon}$ (with the entries $C_c^{\leq} = 1.886^*$ and $C_c^{\geq} = 1.747^*$) the amplitudes $\xi_c^{\leq} = 0.474$ and $\xi_c^{\geq} = 0.469$, which are obtained from P_c^{\leq} and P_c^{\geq} , have been kept fixed.

Quantity	Φ_{-}^{ε}	Φ_{+}^{ε}	P_c^{\leq}	P_c^{\geq}	$\Phi_{c,\leq}^{\varepsilon}$	$\Phi_{c,\geq}^{\varepsilon}$
Scaled by	C_0^-	C_0^+	ξ_c^{\leq}	ξ_c^{\geq}	C_c^{\leq}	C_c^{\geq}
Values in $d = 3$	4.236	4.260	0.474	0.469	1.886*	1.747*

universal scaling functions Φ_{\pm}^{ε} : $\Delta\tilde{\varepsilon}(x_{\pm}) = C_0^{\pm}\Phi_{\pm}^{\varepsilon}(x_{\pm})$. The LFT reported results *only* for the universal scaling function Φ_{\pm}^{ε} , while the original MC data provided the total energy-density function $\Delta\tilde{\varepsilon}(x_{\pm})$, comprising the nonuniversal constants C_0^{\pm} . The second source of nonuniversality is due to the definition of the scaling variables x_{\pm} , involving metric factors via the nonuniversal amplitudes of the critical correlation length. For the present Ising model the critical amplitudes of the correlation length are $\xi_0^- \simeq 0.243(1)$ and $\xi_0^+ \simeq 0.501(2)$ in units of the lattice constant [42]. These factors stretch or compress the shape of the scaling functions without affecting their otherwise intrinsic universal properties, i.e., the functional form of the scaling functions.

In order to insist on agreement between the MC data $\Delta\tilde{\varepsilon}_{\pm}$ and the LFT data Φ_{\pm}^{ε} , we rescale the MC data according to $\frac{1}{C_0^{\pm}}\Delta\tilde{\varepsilon}_{\pm}(x_{\pm})$ with nonuniversal, dimensionless parameters C_0^{\pm} . First, we perform the fit for the two branches \pm separately. Explicitly, we compute the sum of the squares of the deviations (for practical reasons on a logarithmic scale) $\chi_{\pm}^2(C_0^{\pm}) = \sum_{\{x_{\pm}\}} [\ln |\Phi_{\pm}^{\varepsilon}(x_{\pm})| - \ln |\Delta\tilde{\varepsilon}_{\pm}(x_{\pm})/C_0^{\pm}|]^2$, as a function of the scaling factor C_0^{\pm} . The above sum $\{x_{\pm}\}$ has been taken over MC data points with arguments $0.5 \leq x_{\pm} < 2.5$. The value $C_0^- = 4.236$ minimizes $\chi_{-}^2(C_0^-)$. We repeat the same procedure for the $+$ branch $\chi_{+}^2(C_0^+) = \sum_{\{x_{+}\}} [\ln |\Phi_{+}^{\varepsilon}(x_{+})| - \ln |\Delta\tilde{\varepsilon}_{+}(x_{+})/C_0^+|]^2$, as a function of the scaling factor C_0^+ . The sum $\{x_{+}\}$ has been taken over MC data points with arguments $0.5 \leq x_{+} < 2.5$, leading to the result $C_0^+ = 4.260$. These values are collected in Table I.

For the standard Ising model the nonuniversal amplitude of the critical correlation length as a function of the bulk field has been determined as $\xi_c = 0.278(2)$ by resorting to universal bulk amplitude ratios [43]. For the bulk system one expects $\xi_c^{\leq} \equiv \xi_c^{\geq} \equiv \xi_c$ because the distinction between the upper and the lower branch of the critical isotherm vanishes at criticality. It turns out to be impossible to obtain agreement between the LFT and the MC results by using this value of the critical amplitude. MC simulations for a so-called improved Ising model (which is not equivalent to the standard Ising model but belongs to the same universality class) provide $\xi_c = 0.3048(9)$ [44]. (Since ξ_c is a nonuniversal quantity, these two values for ξ_c are not expected to be equal.) To the best of our knowledge, *direct* MC results for ξ_c for the standard Ising model on the simple cubic lattice are not available.

In order to nonetheless obtain agreement between the MC data and the LFT data, we have repeated the above procedure for the order-parameter scaling function by using the scaling factor $\xi_c^<$ and the expression $\chi_z^2(\xi_c^<) = \sum_{\{x_<\}} [\ln [P_c^<(x_<)] - \ln [P_c^<(z/\xi_c^<(h))]]^2$ where the sum $\{x_<\}$ has been taken over all MC data points for $hh_1 < 0$ with arguments $0.5 \leq x_< < 2$. This renders the value $\xi_c^< = 0.474$. For the other branch $hh_1 > 0$, minimizing $\chi_z^2(\xi_c^>) = \sum_{\{x_>\}} [\ln [P_c^>(x_>)] - \ln [P_c^>(z/\xi_c^>(h))]]^2$, where the sum $\{x_>\}$ has been taken over the same interval $0.5 \leq x_> < 2$, leads to the value $\xi_c^> = 0.469$, which is very close to $\xi_c^< = 0.474$ (see Table I). For $\Phi_{c,\leq}^<$ and $\Phi_{c,\leq}^>$ we rescale the MC data with two nonuniversal, dimensionless parameters $C_c^<$ and $C_c^>$. As before, for the branch $hh_1 < 0$ we compute the sum of the squares of the deviations $\chi_z^2(C_c^<) = \sum_{\{x_<\}} [\ln |\Phi_{c,<}^e(x_<)| - \ln |\Delta \tilde{\epsilon}_c^<(z/\xi_c^<(h))/C_c^<|]^2$ as a function of the scaling factor $C_c^<$. The above sum $\{x_<\}$ has been taken over the same interval $0.5 < x_< < 2$ as for P_c^{\leq} . The minimization renders $C_c^< = 1.886$. The analogous minimization of $\chi_z^2(C_c^>)$ within the same interval $0.5 < x_> < 2$ provides $C_c^> = 1.747$ (see Table I). In the course of this procedure, the previously obtained values $\xi_c^> = 0.469$ and $\xi_c^< = 0.474$ of the amplitudes are used.

Along the lines ($t < 0, h = 0$) and ($t > 0, h = 0$) the metric factors ξ_0^\pm , which enter into the definition of the scaling variables $x_\pm = z/\xi_\pm$, are the same quantities within LFT and MC. But in the case of the critical isotherm associated with

the definition of the scaling variables $x_< = z/\xi_<(h)$ and $x_> = z/\xi_>(h)$, where $\xi_<(h) = \xi_c^<|h|^{-\frac{v}{\beta\delta}}$ for $hh_1 < 0$ and $\xi_>(h) = \xi_c^>|h|^{-\frac{v}{\beta\delta}}$ for $hh_1 > 0$, we have used the metric factors ξ_c^{\leq} as fitting parameters and have found that the values $\xi_c^< = 0.474$ and $\xi_c^> = 0.469$ minimize the deviation of the LFT from the MC results. *A posteriori* these two values support the above expectation $\xi_c^< = \xi_c^>$. These values are approximately $0.474/0.278 \simeq 1.7$ times larger than the previously reported value $\xi_c \simeq 0.278$ obtained via universal bulk critical amplitude ratios. This signals that the values of ξ_c^{\leq} need clarification and should be studied independently by carrying out dedicated MC simulations.

VIII. CONCLUSION

Critical adsorption of Ising systems within the so-called normal surface universality class has been examined for the off-critical energy density in dimensions $d \geq 3$ by using local-functional theory and MC simulations. The mean-field results ($d \geq 4$) and the results in $d = 3$ turn out to be *qualitatively* similar. Within the case $d = 3$ excellent *quantitative* agreement has been achieved (with rescaling support) between the LFT and the MC data. Along the critical isotherm, due to the emergence of an interface in the system, monotonicity of the energy-density profiles is violated if the surface and the weak bulk magnetic fields are anticollinear.

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