Phase boundaries near critical end points. III. Corrections to scaling and spherical models

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Thermodynamics in the vicinity of a critical end point is studied. Phenomenological arguments are used to show the presence of further critical nonanalyticities beyond the leading-order singularities found in papers I and II. These contributions are related to the universal correction-to-scaling features of the bulk thermodynamics on the critical λ line. The predictions are checked on exactly soluble spherical models with short- and long-range interactions.

I. INTRODUCTION

Papers I and II of this series of papers[1,2] are concerned with phase boundaries in the vicinity of a critical end point. The basic phase diagram (see Fig. 2 of I) arises in a thermodynamic space of three fields (g,T,h) where T is temperature, h is the ordering field, and g is the nonordering field. These fields can be, for example, the pressure, the magnetic field, or the chemical potential. In outline the phase diagram is as follows. For low values of g, only the noncritical spectator phase, α, is present. This phase appears whenever g is small. Increasing g, one finds a manifold σ, given by $g_\sigma(T,h)$ on which various phases coexist. On this manifold one has the following picture. For $h=0$ and low T, the phases α, β, and γ coexist on a triple line, τ. For $h\neq 0$, the phase α coexists either with and $\beta(h>0)$ or with $\gamma(h<0)$, while, for high T, α coexists with the single disordered phase $\beta\gamma$.

Increasing T along τ, one finds a point, $T=T_e$, $g=g_e$, $h=0$, where the triple line ends. This is the critical end point, at which the phases β and γ become mutually critical. This point is also the end of a critical λ line, $T=T_\lambda(g)$ in the $h=0$ manifold. This line separates the $\beta+\gamma$ phase (we will use this notation for the coexistence of the phases β and γ) from the $\beta\gamma$ phase above the manifold σ, i.e., $g>g_\sigma(T,h)$. The λ line also bounds the coexistence manifold ρ on which both β and γ coexist for $T<T_c(g)$.

In I, the question addressed was: what sort of singularities should be observed near the critical end point in the function $g_\sigma(T,h)$ which specifies the phase boundary σ? Using phenomenological and thermodynamic arguments it was suggested that $g_\sigma(T,h)$ should display characteristic nonanalyticities at the critical end point controlled by the bulk critical properties of the β,γ, and $\beta\gamma$ phases on the critical λ line.[1,3,4] If one puts

$$\hat{t}\equiv\frac{T-T_e}{T_0} \tag{1.1}$$

with T_0 being a convenient reference temperature, it is found

$$g_\sigma(T,h)=g_e+g_1\hat{t}-X_\pm\mid\hat{t}\mid^{2-\alpha}-Y_\pm\mid\hat{t}\mid^{\beta}\mid h\mid -\tfrac{1}{2}Z_\pm\mid\hat{t}\mid^{-\gamma}h^2+\Delta g(T,h) \tag{1.2}$$

when $h\to 0$ and $\hat{t}\to 0$. Here one has $Y_+=0$, while[5] α,β, and γ are the (universal) critical exponents related to the λ-line singularities and Δg contains singular terms of $O(h^3)$ and regular ones of $O(h^2)$. It was then demonstrated that various dimensionless ratios formed from the amplitudes $X_\pm,Y_\pm$, and $Z_\pm$ should be universal and related to the bulk λ line amplitude ratios by

$$\frac{X_+}{X_-}=\frac{A_+}{A_-}\ , \tag{1.3}$$

$$\frac{Z_+}{Z_-}=\frac{C_+}{C_-}\ , \tag{1.4}$$

$$\Xi_1\equiv\frac{X_+Z_+}{Y_-^2}=\frac{A_+C_+}{(2-\alpha)(1-\alpha)B^2}\ , \tag{1.5}$$

$$\Xi_2\equiv\frac{X_+Y_c^\delta}{Y^{\delta+1}}=\frac{\Delta^\delta A_+B_c^\delta}{(2-\alpha)^{\delta+1}(1-\alpha)B^{\delta+1}}\ , \tag{1.6}$$

where $A_\pm,C_\pm,B$, and B_c are the amplitudes for specific heat, susceptibility, spontaneous order parameter, and order parameter at criticality, respectively. Numerical values for the spherical and Ising models were presented.

The arguments in I were not rigorous. They assume that no new type of criticality arises at the end point and they ignore the droplet fluctuations that might induce such changes.[4] One should note that droplet fluctuations lead to singularities in the free energy as the phase boundary σ is approached.[4,6] In view of this, there is a useful check on the predictions of (1.3)–(1.6) on specific models. With this purpose,[2] the free energy of a d-dimensional lattice with N sites occupied by n-component spins $\mathbf{S}_i$ with $i=1,...,N$ was considered following Sarbach and Fisher,[7,8] in the thermodynamic $N\to\infty$ and spherical model $n\to\infty$ limits, the free energy per spin is given by

$$F(T,D,h) = \min_{m_2}\{ \tfrac{1}{2}k_BT[\mathcal{F}_d(\zeta) - \zeta I_d(\zeta)] + W(m_2) - hm\}, \quad (1.7)$$

where the spherical fields ζ is determined by the constraint and minimization equations [see Eqs. II(2.8) and (2.9), i.e., Eqs. (2.8) and (2.9) in of II], while

$$W = \tfrac{1}{2}\, Dm_2 + \tfrac{1}{4}\, Um_2^2 + \tfrac{1}{6}\, Vm_2^3, \quad (1.8)$$

where D plays the role of nonordering field. In order to realize tricriticality and critical end points one must have $U < 0$ and $V > 0$. In addition one has $h = |\mathbf{h}|$, while $m = <S>$ and $m_2 = <S^2>$ are the spherical model averages and the the functions of ζ are defined in the integrals

$$\mathcal{F}_d(\zeta) = \int a^d \frac{d^dk}{(2\pi)^d} \ln\{[\zeta + \hat{J}(k) - \hat{J}(0)]/2\pi k_BT\}, \quad (1.9)$$

$$I_d(\zeta) = \frac{\partial \mathcal{F}_d}{\partial \zeta}. \quad (1.10)$$

Here a is the lattice spacing and $\hat{J}(k)$ is the Fourier transform of the interaction $J(R)$ that can be short ranged ($\sigma = 2$) or long ranged with $J(R) \sim 1/R^{d+\sigma} (\sigma < 2)$ as $R \to \infty$. Specifically it was assumed that $\hat{J}(k)$ has an expansion about a unique maximum at $k = 0$ given by Eq. II(2.5).

It was shown that this model, studied in the tricritical regime by Sarbach and Fisher,[7,9] displays, for *all* dimensionalities, a critical line that ends at a critical end point for an appropriate choice of the parameters in the Hamiltonian. In particular it was shown, in the nonclassical regime specified by $d_- < d < d_+$ where $d_- = \sigma$, $d_+ = 2\sigma$, that the end point is present for $d_0 > d > d_-$, where $d_0 = \frac{3}{2}\sigma$, for any value of the parameters and for $d_+ > d > d_0$ when U is not too small. In these cases, the $\beta + \gamma$ to $\beta\gamma$ critical behavior specified by the critical exponents α, γ, β, and δ and amplitudes $C_\pm$, $A_\pm$, B, and B_c were computed and the phase boundary σ given by (1.1) and (1.2) was obtained. It was explicitly proved to have universal amplitude ratios as in (1.3)–(1.6).

For the borderline $d = d_+$ case the spherical model free energy contains confluent logarithms that diverge on the critical λ line. We analyze this special case fully in Appendix A.

For $d > d_+$ the spherical model exhibits classical critical behavior in leading order.[8] But, nonclassical corrections to scaling also appear. In view of this, one may ask if such corrections will generate singularities on the phase boundary near the end point. The aim of this paper is to investigate this question using the following strategy. First, we will note, as usual,[10] correction-to-scaling amplitudes related to the susceptibility, the specific heat, and the magnetization near the critical λ line, as well as, the magnetization at $T = T_c(g)$. Then, using pure thermodynamic arguments,[1] we will suggest that, besides the leading-order singularities shown in Eq. (1.2), the phase boundary exhibits further ones involving higher powers of $\hat{t}$ which are related to the critical singularities by universal amplitude ratios. Such behavior will be especially relevant as soon as α, β, or γ approach integer values or, if the leading amplitudes become too small or vanish. This is the case, for example, for the classical regime of the spherical model where the only singularities arise from the correction-to-scaling terms. In this case we explicitly check our predictions.

In outline the remainder of this paper is as follows. In Sec. II we analyze correction-to-scaling confluent singularities for thermodynamic functions, obtaining universal amplitude ratios. An appropriate extension of our early classical arguments[11] for determining phase boundaries by matching free energies of distinct phases is assessed in Sec. III. A complete study for the classical regime of the spherical model is performed in Sec. IV where we also obtain the singular behavior of the phase boundaries, closely following II.[2] Section V summarizes the conclusions briefly.

TABLE I. Comparison between theoretical values for the exponent θ and amplitude ratios for n (number of components) = 1, 2, 3. These values were extracted from Refs. 14–18.

n	θ	a_ξ/a_χ^+	a_c/a_χ^+
1	0.496 ± 0.005	0.64	8.6 ± 0.2
	0.492 ± 0.02	0.64 ± 0.05	8.5 ± 0.9
		0.7 ± 0.03	
2	0.524 ± 0.004	0.615 ± 0.005	5.95 ± 0.15
	0.522 ± 0.018	0.6 ± 0.04	5.9 ± 0.5
		0.6 ± 0.1	
3	0.5501 ± 0.0003	0.6 ± 0.01	4.6
	0.550 ± 0.016	0.59 ± 0.06	4.6 ± 0.05

II. CORRECTIONS TO SCALING AND CRITICALITY

Some years ago, it was realized both theoretically[10] and experimentally[12] that, in order to analyze data not very close to the critical point, corrections to scaling should be included. It is generally accepted that a physical quantity f_i should be written as[13]

TABLE II. Comparison between theoretical calculations for correction amplitude ratios. The calculations were performed with a renormalization-group approach in $d = 3$ dimensions (BBMN, Ref. 19), and in $d = 4 - \epsilon$ (assumed $\epsilon = 1$) expansion by Chang and Houghton (CH, Ref. 21) and Nicoll and Albright (NA, Refs. 20 and 22).

	a_c^+/a_c^-	a_χ^+/a_χ^-	a_m^-/a_χ^+
(BBMN)	0.96 ± 0.25	0.315 ± 0.013	0.90 ± 0.21
(CH)	1.0	0.23	1.16
(NA)	2.54	0.32	0.5

TABLE III. Comparison between theoretical (Refs. 19–22) and experimental estimates of some universal correction-to-scaling amplitude ratios.

	n	a_c^-/a_c^+	a_c^+/a_m	a_m/a_χ^+	a_m/a_χ^-
Theoretical	1	1.12 ± 0.29	1.10 ± 0.25	0.90 ± 0.21	0.29 ± 0.08
	3	1	0.333	0.6	0.35
Experimental					
SF_6 (Ref. 23)	1	—	—	0.7	—
Ar (Ref. 24)	1	—	—	0.15 ± 0.04	—
CO_2 (Refs. 25 and 26)	1	1.4	—	—	0.58
He_3 (Refs. 26 and 27)	1	—	—	0.42 ± 0.02	0.46
Xe (Refs. 23, 26, and 28)	1	—	—	1.4	1.5
He_4 (Ref. 26)	1	—	—	—	0.59
Ni (Ref. 29)	3	—	—	—	0.29
EuO (Ref. 30)	3	—	—	—	0.03
Pd_3Fe (Ref. 31)	3	—	—	—	0.37

$$f_i = A_i \mid \tilde{t} \mid^{-\lambda_i} (1 + a_i \mid \tilde{t} \mid^{\theta} + \cdots), \tag{2.1}$$

where $\tilde{t} = (T - T_\lambda)/T_\lambda$ is the reduced critical temperature T_λ, λ_i is the critical exponent, while a_i and θ describe the leading nonanalytic correction to scaling.

In practice analytic terms varying as $\tilde{t}, \tilde{t}^2, \ldots$, must also be included in the correction factor.

It is well known that the critical exponents λ_i and the dimensionless ratios involving leading amplitudes A_i are universal quantities. It has been suggested some time ago that ratios among the correction amplitudes a_i are universal.[10] Since then, many studies have been made to test this theory. A complete review in this sense can be found in Ref. 14 and summarized in Tables I, II, and III.

III. THERMODYNAMICS AND UNIVERSALITY

A. Corrections to scaling near the critical line

To characterize the behavior near the critical λ line in the space (T, g, h), using general scaling arguments, we postulate, following I, that the Gibbs free energy can be decomposed as

$$G_\pm(g,T,h) = G_0(g,T,h) - Q \mid \tilde{t} \mid^{2-\alpha} W_\pm \left(\frac{U\tilde{h}}{\mid \tilde{t} \mid^{\Delta}}, U_4 \mid \tilde{t} \mid^{\theta} \ \ldots \right), \tag{3.1}$$

where $+$ $(-)$ means disordered (ordered) phase and where the ellipsis means higher-order corrections to scaling with exponents $\theta_5, \theta_6, \cdots$. The first term, $G_0(g,T,h)$, represents an analytic background, and, the second, a singular term given in terms of two scaling fields

$$\tilde{t} \approx [T - T_\lambda(g)]/T_e, \quad \tilde{h} \approx h, \tag{3.2}$$

where $T = T_\lambda(g)$ locates the critical λ line while, T_e the end-point temperature, serves as a reference temperature, and the "$\approx$" symbol entails $T \to T_\lambda(g)$, and $h \to 0$. The functions $\tilde{t}$ and $\tilde{h}$ are presumed to be smooth functions of T, g, and h. In (3.1) α is the specific heat exponent, Δ is the gap exponent, and θ is leading-order correction-to-scaling exponent, Q, U, U_4, and U_5 are smooth functions of g, T, and h, and the scaling function

$$W_\pm^0(y,z) \equiv W_\pm(y,z,0,0,\ldots) \tag{3.3}$$

is well defined. For simplicity, it will be normalized by $W_+(0,0) \equiv 1$. The two branches of this function must satisfy matching conditions as $y \to \pm\infty$ and $z \to 0$ which ensures the analyticity and consequently we should have

$$\begin{aligned} W_\pm^0(y,z) &\approx \mid y \mid^{(2-\alpha)/\Delta} W_\pm(w_\infty h^{\theta/\Delta}, \ldots) \\ &\approx \mid y \mid^{(2-\alpha)/\Delta} W_\infty(1 + w_\infty h^{\theta/\Delta} + \cdots), \end{aligned} \tag{3.4}$$

where the ellipsis includes higher-order contributions in $\tilde{t}$ and h, while

$$w_\infty = \frac{U_4}{U^{\Delta/\theta}} \left. \frac{d\tilde{W}}{dx} \right|_0 \Big/ W_\infty . \tag{3.5}$$

In a standard way we can define various thermodynamic functions, namely, the specific heat at a constant field above and below $T_\lambda(g)$,

$$\mathcal{C}_-(g,T) \approx T_\lambda^{-1} A_\pm(g) \mid \tilde{t} \mid^{-\alpha} (1 + a_\pm \mid \tilde{t} \mid^{\theta} + \cdots), \tag{3.6}$$

the spontaneous order parameter

$$M_0(g,T) \approx B(g) \mid \tilde{t} \mid^{\beta} (1 + b \mid \tilde{t} \mid^{\theta} + \cdots),$$

$$\beta = 2 - \alpha - \Delta , \tag{3.7}$$

the critical isotherm at $T = T_c(g)$

$$\begin{aligned} \Delta M &= M(g, T_c, h) - M_c(g) \\ &\approx \pm B_c(g) \mid h \mid^{1/\delta} (1 + b_c h^{\theta/\Delta} + \cdots), \end{aligned} \tag{3.8}$$

and the susceptibility above and below $T_c(g)$

$$\chi(g,T) \approx C_\pm(g) \mid \tilde{t} \mid^{\gamma} (1 + c_\pm \mid \tilde{t} \mid^{\theta} + \cdots) . \tag{3.9}$$

From (3.1) and (3.4), the leading-order amplitudes $A_\pm, C_\pm, B$, and B_c are given in terms of $W_\pm(y, \cdots)$ by Eqs. I(3.8) and (3.9) while the correction-to-scaling amplitudes are found from

$$a_{\pm} = U_4 \frac{(2-\alpha+\theta)(1-\alpha+\theta)}{(2-\alpha)(1-\alpha)} \frac{dW_{\pm}}{dz}(0,0) \Big/ W_{\pm}(0,0),$$

$$c_{\pm} = U_4 \frac{d^3 W_{\pm}}{dy^2 dz}(0,0), \Big/ \frac{d^2 W_{\pm}}{dy^2}(0,0), \quad b = U_4 \frac{d^2 W}{dy\,dz}(0,0) \Big/ \frac{dW}{dy}(0,0), \quad b_c = \frac{(2-\alpha+\theta)}{(2-\alpha)} w_{\infty}. \tag{3.10}$$

Then we can introduce various dimensionless ratios of correction-to-scaling amplitudes. The following are convenient as seen in Sec. II:

$$\frac{a_+}{a_-} = \frac{dW_+}{dz} \Big/ \frac{dW_-}{dz}, \quad \frac{c_+}{c_-} = \frac{d^3 W_+}{dy^2 dz} \frac{d^2 W_-}{dy^2} \Big/ \frac{d^3 W_-}{dy^2 dz} \frac{d^2 W_+}{dy^2},$$

$$\frac{a_{\pm}}{c_{\pm}} = \frac{(2-\alpha+\theta)(1-\alpha+\theta)}{(2-\alpha)(1-\alpha)} \frac{dW_{\pm}}{dz}(0,0) \frac{d^2 W_{\pm}}{dy^2}(0,0) \Big/ W_{\pm}(0,0) \frac{d^3 W_{\pm}}{dy^2 dz}, \tag{3.11}$$

$$\frac{b}{c_{\pm}} = \frac{d^2 W_{\pm}}{dy\,dz}(0,0) \frac{d^2 W_{\pm}}{dy^2}(0,0) \Big/ \frac{dW}{dy}(0,0) \frac{d^3 W_{\pm}}{dy^2 dz}(0,0).$$

Note that, since they only depend on $W_{\pm}$ and its derivatives, they are universal quantities. This is in agreement with Aharony and Ahlers[19] who pointed out that such ratios should be universal. One can also note that the mixed amplitude ratio

$$\Theta_5 = \left(\frac{A_+}{C_+}\right)^{\theta/\beta\delta} \frac{b_c^2}{a_+ c_+} \tag{3.12}$$

should equally be universal. Of course, one could build additional amplitude ratios, involving higher-order derivatives, as well as other combinations of critical amplitudes and correction-to-scaling amplitudes, but since we want to apply these to the spherical model, we will focus on (3.10)–(3.12).

B. Phase Boundary

Following earlier assumptions in I and before,[1,3] we will assume that the noncritical α phase can be described by an analytical free energy $G_2(T,g,h)$ throughout the space of parameters except, perhaps, on the phase boundary σ given by $g_\sigma(T,h)$, and, more particularly, near the end point $T = T_e$ and $h = 0$. Following thermodynamic arguments of Gibbs[3] we can derive the phase boundary simply by equating $G_\alpha = G_{\beta\gamma}$. Although the droplet picture does not enable us to assume analytical continuation of the free energies G_α and $G_{\beta\gamma}$ beyond the boundary σ, as pointed out in I, the equality holds for continuity.[6]

Near the end point one can expand G_α as we did in Eq. I(4.1), obtaining

$$G_\alpha(g,T,h) = G_e + G_1^\alpha \Delta g + G_2^\alpha \hat{t} + G_3^\alpha h + \ldots, \tag{3.13}$$

on and below $g_\sigma(T,h)$ where

$$\Delta g = g - g_e \quad \text{and} \quad \hat{t} = (T - T_e)/T_e\ . \tag{3.14}$$

Now simply equating (3.13) and (3.1), the phase boundary without neglecting the leading correction to scaling yields the phase boundary in the form

$$g_\sigma(T,h) = g_0(T,h) - R(T,h)\,|\,\tilde{t}\,|^{2-\alpha}\, W_{\pm}\left(\frac{U\tilde{h}}{|\,\tilde{t}\,|^{\Delta}}, U_4 \tilde{t}^{\theta}\right). \tag{3.15}$$

Here we are not including higher-order correction-to-scaling terms that should come with exponents $\tilde{\theta}_5, \tilde{\theta}_6, \ldots$ [not the same of Eq. (3.1)]. We also have

$$R(T,h) = Q[g_\sigma; T, h]/(D_1 + D_2'\hat{t} + D_3' h + \cdots) \tag{3.16}$$

in which $D_1', D_2', D_3', R_1, R_2$, etc., are given by expansions of $G_0, Q, U, \tilde{h}$, and $\tilde{t}$ in powers of h, Δg, and $\hat{t}$ [see Eqs. I(4.4)–(4.8)].

C. Coexistence line

Let us now examine $g_\sigma(T,h)$, in some particular cases. First, consider the $h = 0$ surface. Then, when $\hat{t} \to 0$, Eq. (3.15) gives

$$g_\sigma(T) - g_0(T) \approx g_e + g_1 \hat{t} + \cdots - X_{\pm}\,|\,\hat{t}\,|^{2-\alpha} \times \left[1 + x_{\pm}\hat{t}^{\theta} + O\,|\,\hat{t}\,|^{1-\alpha}\right], \tag{3.17}$$

where the ellipsis denotes higher-order analytic terms, α is the specific heat exponent, and θ is the correction-to-scaling exponent given by Eq. (3.1) if we assume $\theta < 1$ and $\theta < 1 - \alpha$. Even though these assumptions are not always true, they cover the cases for which the correction to scaling is relevant.

In this case, the leading-order amplitudes $X_{\pm}$ are given by Eqs. (5.3)–(5.5) in I, namely,

$$X_{\pm} = R_e\,|\,e_0\,|^{2-\alpha}\, W_{\pm}(0,0) \tag{3.18}$$

with $R_e = R(T = T_e, h = 0)$ and the geometric factor

$$e_{v-1} \equiv 1 - v\left(\frac{dg_\sigma}{dT}\right)_e \left(\frac{dT_\lambda}{dg}\right)_e \tag{3.19}$$

while

$$x_\pm = U_4 \mid e_0 \mid^\theta \frac{dW_\pm}{dZ}(0,0) \Big/ W_\pm(0,0). \tag{3.20}$$

One may note that Eq. (3.17) confirms, as we stressed in I, that the singularity on the phase boundary is mainly due to the critical-line singularity.

It is clear that besides the universal relation (1.3) we now also have

$$\frac{x_+}{x_-} = \frac{a_+}{a_-} \tag{3.21}$$

which is determined purely by the bulk behavior on the critical line. Note that the factor e_0 in Eq. (3.20) drops out of the ratio x_+/x_-. In Tables I and II we listed some values for these ratios for the $d = 3$ Ising model.

D. Small fields

For a small field above T_e the phase boundary is given by

$$\begin{aligned} g_\sigma(T,h) - g_0(T,h) & \\ \approx Y_\pm \mid h \mid\mid \hat{t} \mid^\beta (1 + y_\pm \mid \hat{t} \mid^\theta + \cdots) & \\ -\tfrac{1}{2} Z_\pm h^2 \hat{t}^{-\gamma}(1 + z_\pm \mid \hat{t} \mid^\theta + \cdots) + O(h^4), & \end{aligned} \tag{3.22}$$

where $Y_+ = y_+ = 0$, by analyticity of G_+ in h through $h = 0$, while β and γ are the magnetization and susceptibility exponents, $Y_- \equiv Y$ and $Z_\pm$ are given in Eqs. I(5.8) and (5.9), and

$$y = U_{4e} \mid e_0 \mid^\theta \frac{d^2W_-}{dy\,dz}(0,0) \Big/ \frac{dW_-}{dy^2}(0,0), \tag{3.23}$$

$$z_\pm = U_{4e} \mid e_0 \mid^\theta \frac{d^3W_\pm}{dy^2dz}(0,0) \Big/ \frac{d^2W_\pm}{dy^2}.$$

Here $U_e = U(T = T_e, g = g_e)$ and $U_{4e} = U_4(T = T_e, g = g_e)$.

Now we can easily see that, besides the universal ratios (1.4) and (1.5) we also have that

$$\frac{z_+}{z_-} = \frac{c_+}{c_-}, \quad \frac{y}{z_\pm} = \frac{b}{c_\pm}, \tag{3.24}$$

should be universal. Some theoretical and experimental ratios are given in Tables II and III.

E. Field at criticality

Let us now consider the general locus

$$\frac{T - T_e}{g - g_e} = v\left(\frac{dT_c}{dg}\right)_e, \tag{3.25}$$

where $v = 0$ gives the $T = T_e$ isotherm plane while $v = 1$ specifies the critical line, $T = T_c(g)$ asymptotically. Now, we find

$$g_\sigma(h)_v - g_e = \{g_2 h - Y_c \mid h \mid^{(\delta+1)/\delta} [1 + y_c h^{\theta/\beta\delta} + O(h^{(\delta-1)/\delta}, h)]\} \Big/ e_{v-1}, \tag{3.26}$$

where we have supposed $\theta < \gamma$, which, since $\gamma \geq 1$, is certainly satisfied if $\theta < 1$. Here Y_c is given by [Eq. I(5.14)] and

$$y_c = \tilde{U}_{4e} R_e, \tag{3.27}$$

where $\tilde{U}_{4e} = \tilde{U}_4(T = T_e, g = g_e, h = 0)$.

In addition to the previous expression for Ξ_2 in (1.6) we have that

$$\begin{aligned} \Xi_5 &\equiv \left(\frac{X_+}{Z_+}\right)^{\theta/\beta\delta} \frac{y_c^2}{x_+ z_+} \\ &= \left(\frac{A_+}{(2-\alpha)(1-\alpha)C_+}\right)^{\theta/\beta\delta} \frac{(1-\alpha+\theta)\Delta^2}{(2-\alpha+\theta)} \frac{B_c^2}{a_+ c_+} \end{aligned} \tag{3.28}$$

is universal.

As mentioned such corrections will be relevant when $a_\pm \hat{t}^\theta$ is not small. Furthermore, in the classical regime ($\alpha = 0$, $\beta = \frac{1}{2}$, and $\gamma = 1$) , the correction $x_\pm \hat{t}^\theta$ will give the leading singularity in the expression for $g_\sigma(T)$. This is the case for the classical regime of the spherical model in its $d \geq 2\sigma$ that is studied in Sec. IV.

IV. SPHERICAL-MODEL CLASSICAL REGIME

A. The model

Let us now consider the spherical model introduced in Sec. I. The critical behavior of the model can be determined knowing $I_d(\zeta)$ with ζ given by the constraint, since $\zeta \equiv h/m = 0$ specifies the critical temperature, and so, we have $T_c(D)$ given by Eq. II(2.18). Since $\zeta \to 0$, in the disordered phase, as $h \to 0$ with $m(h \to 0) = 0$, the inverse of susceptibility $\chi^{-1} = \zeta$ will give the behavior in the critical vicinity. In II we obtained a complete phase diagram where we stressed that the critical or λ line ends in two possible ways: either at a tricritical point at the vertex of the parabola Eq. II(2.19) at $D = D_t$ and $T = T_t$; or at a critical end point when the λ line is cut by a first-order line separating the disordered and ordered phases from the noncritical α phase at $D = D_e < D_t$ and $T > T_t$.

It is then clear that the presence of the end point depends on the existence of the α phase at the tricritical locus. To analyze this location we will introduce, as in II

$$t = \frac{T - T_t}{T_t},$$

$$\bar{g} \equiv \frac{D - D_t}{V}, \tag{4.1}$$

$$m_2 = \tilde{m} + w(1 + t),$$

where $w = \mid U \mid /2V$. Now the free energy can be written as a sum of an analytical piece [see Eq. II(3.9)] and a singular part, namely,

$$\Delta F = \tfrac{1}{6}\,\tilde{m}^3 V + \tfrac{1}{2}\left[wt\tilde{m}^2 + (\bar{g} + w^2t^2)\tilde{m}\right] V - hm + \tfrac{1}{2}k_B T\left[\mathcal{F}_d(\zeta) - \zeta I_d(\zeta) - \mathcal{F}_d(0)\right] \ , \tag{4.2}$$

that vanishes identically on the λ line. Also the constraint and minimization relations are given by

$$\tilde{m} \equiv u^{-2} = m^2 + w(1+t)[I_d(\zeta) - I_d(0)], \tag{4.3}$$

$$v(\tilde{m}) = \tilde{m}^2 + 2t\tilde{m} + \bar{g} + t^2w^2. \tag{4.4}$$

Using (4.3) and (4.4) one can obtain the critical behavior for $d < d_+$ as given in II. Also the behavior for $d = d_+$ can be checked through explicit and exact expressions given in Appendix A. In the remainder of this section we will explore the case $d > d_+$, extracting the free-energy correction to scaling and its influence on the phase boundaries.

B. The phase diagram

For $d > d_+$ the singular behavior of the integral (1.9) appears only in higher orders than in II. If one assumes $\bar{d}_+ > d > d_+$ with $\bar{d}_+ = \min(3\sigma, 6)$

$$I_d(\zeta) = I_d^0\left[1 - q\zeta + p\zeta^{1+\theta} + O(\zeta^2)\right], \tag{4.5}$$

where the crucial parameters p and q are defined via

$$I_d^0 \hat{J}_\sigma^2 q = \theta(\tilde{\pi})^{\theta\sigma} \Big/ 2^{d-1}\pi^{d/2}\sigma\Gamma\left(\frac{d}{2}\right), \tag{4.6}$$

$$I_d^0 \hat{J}_\sigma^{2+\theta} p = 1 \Big/ 2^{d-1}\pi^{d/2-1}\sigma\Gamma\left(\frac{d}{2}\right)\sin(\theta\pi), \tag{4.7}$$

in which

$$\theta = (d - 2\sigma)/\sigma \ . \tag{4.8}$$

Note that θ is positive but less than unity for $d < \bar{d}_+$. For convenience a spherical Brillouin zone of ratio $|\,k\,| = \tilde{\pi}/a$ with $\tilde{\pi} \simeq \pi$ has been assumed.

The singular part of the free energy (1.7) will now come from (4.3) with

$$\Delta F = \bar{p}\bar{\zeta}^2\left(\frac{1}{2} - \frac{(1+\theta)}{(2+\theta)}\,\bar{\zeta}^\theta\right) \Big/ 8V^{1/2}\theta(1+\theta)\left(\frac{p}{q}\right)^{3\theta/2} , \tag{4.9}$$

and from the constraint (4.4), namely,

$$u^{-2}(\zeta) = \bar{p}^2\bar{\zeta}^2(1 - \bar{\zeta}^\theta)/16V\theta^2(1+\theta)^2\left(\frac{p}{q}\right)^{1/\theta} , \tag{4.10}$$

where $\bar{\zeta} \equiv (p/q)^{1/\theta}\zeta$. In addition a basic dimensionless parameter has been introduced, namely,

$$\bar{p} \equiv 2\theta(1+\theta)\left(\frac{U^2}{V}\right)^{1/2} q\left(\frac{q}{p}\right)^{1/\theta} \tag{4.11}$$

that is equivalent to Eq. II(3.2) and also coincides with (A4) in the limit $\theta \to 0$.

At the tricritical point where $t = \bar{g} = 0$, the minimization and constraint relations (4.4) can be used to eliminate $\tilde{m}$ and yield

$$4\theta(1+\theta) = \bar{p}\bar{\zeta}^{1/2}(1 - \bar{\zeta}^\theta) \ . \tag{4.12}$$

Besides the trivial $\bar{\zeta} = 0$ or tricritical solution, there is a second or α-phase solution $\bar{\zeta} = \bar{\zeta}_0$. The free energy of the tricritical point, namely,

$$\Delta F_t = \bar{p}\bar{\zeta}^2\left(1 - \frac{2(1+2\theta)}{2+\theta}\,\bar{\zeta}^\theta\right) \Big/ 24\theta(1+\theta)\left(\frac{p}{q}\right)^{3\theta/2} \tag{4.13}$$

vanishes when $\zeta = 0$ and, consequently the α phase and the end point will be present whenever $\Delta F_t \leq 0$ or $\bar{p} \geq \bar{p}_0$ with

$$\bar{p}_0(d) = \tfrac{8}{3}\,e^{3/4}\,\left(1 + \tfrac{33}{16}\,\theta\right). \tag{4.14}$$

One should notice that $\bar{p}_0(d)$ is continuous and analytical in the $d \geq d_+$ region [see $\bar{p}_0(d < d_+)$ in II and Appendix A here].

Precisely when $\bar{p} = \bar{p}_0$ the tricritical point and the critical end point coincide (see Fig. 4 in II). Owing to the presence of the α phase we must also locate the phase boundary separating the α phase from the $\beta\gamma$ phase. Such a first-order line ends, as usual, at a critical point, located by imposing the usual phenomenological condition that the three solutions of (4.4), namely, ζ_0, ζ_+, and ζ_- assume the same value. (As in II the critical point at the end of the $\alpha - \alpha\beta$ boundary is completely classical in character.)

Now, from the conditions

$$\begin{aligned} u(\tilde{m}) &= v(\tilde{m}), \\ u'(\tilde{m}) &= v'(\tilde{m}) = 2\tilde{m} + 2t \ , \\ u''(\tilde{m}) &= v''(\tilde{m}) = 2 \ , \end{aligned} \tag{4.15}$$

we obtain the equation

$$\bar{p}^2(1 - Z)^3 = K_\theta Z^{1-1/\theta} \ , \tag{4.16}$$

where $K_\theta \equiv [2(1+\theta)\theta^{3/2}/(1+t)]^2$ and $\bar{\zeta}^\theta \equiv Z/(1+\theta)$. This has a solution provided $K_\theta/\bar{p}^2$ is small enough and $\theta < 1$. In this case, the critical point locus is found from (4.14) to be described by

$$\begin{aligned} t = t_c &= \frac{-\tau_c}{1 - \tau_c}, \\ \tau_c &\equiv + \left[\left(\frac{1+2\theta}{1+\theta}\right)Z^2 - (2+\theta)Z + 1\right] \\ &\quad \times \left(\frac{p}{q}\right)^{1/\theta}\frac{pZ^{1/\theta - 1}}{\theta(1+\theta)^{1/\theta}} \ . \end{aligned} \tag{4.17}$$

Note that the condition $t_c = 0$ ($T_c = T_t$) yields the parameter-space locus $\bar{p} = \bar{p}_1(d)$ where

$$\bar{p}_1 \approx 5.0882(1+2.073\theta), \tag{4.18}$$

that is illustrated in Fig. 5 of II. Below T_t the critical point can also arise with $D_c = D_t$ at $\bar{g}_c = 0$ for $\bar{p} = p_2 < \bar{p}_1$. For lower D values, the critical point reaches the $\alpha - (\beta+\gamma)$ phase boundary at a special quadruple point at $\bar{p}-\bar{p}_3 < \bar{p}_2$. One can then learn from this analysis that the $d > d_+$ phase diagrams for different $\bar{p}$ values have the same qualitative behavior as those for $d < d_+$ ones.

Now that we can ensure the existence of an end point we may focus on the λ line neighborhood near the end point.

C. Free energy near the λ line

In order to obtain the phase boundary we will have to compute the free energy of the $\beta\gamma$, $\beta+\gamma$, and α phases near the λ line. To that end we introduce

$$\tilde{t} = \bar{g} + w^2 t^2 \tag{4.19}$$

which measures the deviation from the critical line. From Eqs. (4.3) and (4.4)–(4.8), the singular piece of the free energy is given by

$$\Delta F = \frac{w}{2} p(1+t)(2+\theta)^{-1}\zeta^{2+\theta} - \frac{(1+t)qw\tilde{t}^2}{4[1+2q(1+t)w^2 t]} - hm. \tag{4.20}$$

Now, assuming that $h \to 0$ so that $\zeta = \chi^{-1}$ and using Eq. (4.4), we find that the susceptibility diverges as

$$\chi_+ \approx \zeta^{-1} \approx C_+ \tilde{t}^{-1}(1 + c_+ \tilde{t}^{\theta}), \tag{4.21}$$

so $\gamma = 1$ as expected, with amplitudes

$$C_+ = 1 + 2qt(1+t)w^2, \tag{4.22}$$

$$c_+ = -2pt(1+t)w^2/C_+^{1+\theta}, \tag{4.23}$$

and consequently the singular part of the $\beta\gamma$ free energy is

$$\Delta F^s_{\beta\gamma} = -\frac{A_+}{2}\tilde{t}^2\left(1 + \frac{2a_+\tilde{t}^{\theta}}{(2+\theta)(1+\theta)}\right) - \tfrac{1}{2}C_+\tilde{t}^{-1}h^2(1+c_+\tilde{t}^{\theta}) \tag{4.24}$$

with

$$A_+ = -\frac{1}{2tC_+} \tag{4.25}$$

and

$$a_+ = -c_+ \tag{4.26}$$

if a small field is allowed. We might point out here that one has $\alpha = 0$ for $d > d_+$ and, consequently, the leading order "singular part" of the free energy varies as $\tilde{t}^2$; thus the separation from the analytic part is not obvious. A proper choice is, however, fundamental in order λ to preserve the universal leading-order amplitude ratios given by (1.3)–(1.6).

In zero field the ordered phase presents $\bar{\zeta} = 0$ and, consequently, $\Delta F_{\beta\_}$ is analytic with $A_- = a_- = 0$. As one allows $h \neq 0$, the ordered phase-free energy exhibits a singular part given by

$$\Delta F^s_{\beta+\gamma} = -mh - \tfrac{1}{2}C_-\tilde{t}^{-1}h^2, \tag{4.27}$$

where $C_- = C_+/2$ (classical behavior) while, since $\tilde{m} = m^2$ is nonzero, from Eq. (4.4), a spontaneous magnetization, namely,

$$m \approx B \mid \tilde{t} \mid^{\beta} [1 + O(\tilde{t})] \tag{4.28}$$

arises with, as we obtained in II, $\beta = \frac{1}{2}$ and $B = 1/(2wt)^{1/2}$, note, however, there is *no* correction-to-scaling terms $O(\tilde{t}^{\theta})$, in other words, $b = c_- = a_- = 0$.

Now, on the critical isotherm we find

$$m_c \approx B_c \mid h \mid^{1/3} (1 + b_c \mid h \mid^{2\theta/3}) \tag{4.29}$$

and

$$\Delta F_c \approx -\frac{3}{4} \mid h \mid^{4/3} \left(1 + \frac{2}{2+\theta}\, b_c \mid h \mid^{2\theta/3}\right) \tag{4.30}$$

with amplitudes

$$B_c = (C_+/2wt)^{1/3} \tag{4.31}$$

and

$$b_c = -(2wt/C_+)^{1+\theta/3}(1+t)wp/3 \; . \tag{4.32}$$

One might well note that the universal leading-order amplitude ratios given by [see also Eq. II(2.19)]

$$\frac{A_-}{A_+} = 0, \quad \frac{C_-}{C_+} = \frac{1}{2}, \tag{4.33}$$

$$\Theta_1 \equiv \frac{A_+ C_+}{B^2} = -\frac{1}{2} \; , \tag{4.34}$$

$$\Theta_2 \equiv \frac{A_+ B_c^{\delta}}{B^{\delta+1}} = -\frac{1}{2}, \tag{4.35}$$

are classical. Besides, correction-to-scaling amplitudes

$$\frac{a_-}{a_+} = \frac{a_-}{c_+} = \frac{b}{a_+} = \frac{b}{c_+} = 0 \; , \quad \frac{a_+}{c_+} = -1, \tag{4.36}$$

and

$$\Theta_5 = \left(\frac{A_+}{C_+}\right)^{2\theta/3} \frac{b_c^2}{a_+ c_+} = \frac{1}{9} \tag{4.37}$$

are, as expected, universal. Note that they are independent of (d,σ).

D. The α-phase free energy

As observed in the analysis of the phase diagram, the α phase is basically characterized by the nonvanishing of the spherical field ζ even when the critical λ line is approached. This phase should exhibit an analytic free energy as expected since it is a spectator phase as regards of the vicinity of the λ line. In order to ensure the absence of singularities, the free energy in the neighborhood of the end point should have a Taylor expansion in powers of $\hat{t} = t - t_e$ and $\hat{g} = g - g_e$ where (t_e, g_e) are the end-point values. Thus, we rewrite the free energy, as in Eq. II(5.1), but now with the parameters K_i and L_i given by

$$K_0 = -\tfrac{1}{4}V\Gamma w' q, \quad K_1 = \frac{1}{2}\,\frac{1}{2+\theta} \; - V\Gamma w' w q t,$$

$$K_2 = -\tfrac{1}{2}\Gamma w t(\tilde{t} + 1 + 2Vw'wqt)K_3$$
$$= -\frac{1}{6}\,\frac{(1+2\theta)}{(2+\theta)} \; - \frac{1}{2}\,V\Gamma q t w w', \qquad (4.38)$$

$$K_4 = -\tfrac{1}{4}\,V\Gamma w' q,$$

where $\Gamma = \theta/(2+\theta)$ and $w' = w(1+t)$ and

$$L_0 = \frac{1}{2}\,\frac{(1+\theta)}{(2+\theta)}\,\tilde{t}, \quad L_1 = \frac{wt(1+\theta)}{(2+\theta)},$$
$$L_2 = \frac{1}{2}\,\frac{(1+\theta)}{(2+\theta)}, \quad L_3 = L_4 = 0. \qquad (4.39)$$

Now, following II, the end-point location is obtained by taking $\tilde{t} = 0$ as well as $\Delta F_\alpha = 0$ that reproduces Eq. II(5.9) from II but with

$$b = -2\,(2\theta+1)/3\theta V w' q - 2wt, \qquad (4.40)$$
$$c = +2t/Vq(1+t) + 4w^2t^2. \qquad (4.41)$$

Now we can compute the end-point location. For small $\bar{p} - \bar{p}_0$, $\zeta_{\alpha,e}$ will also be small and consequently the end point is given by

$$m_{\alpha,e} \approx -2\,(2\theta+1)/3\theta V w q \;, \qquad (4.42)$$
$$\zeta_{\alpha,e} \approx 4\,(2\theta+1)^2/9Vw^2q^2 \;. \qquad (4.43)$$

Then, we can develop the expansion for the spectator α phase about the end point as in Eq. II(5.17). The coefficients Q_{ij} and R_{ij} will be well-behaved functions of V, w, p, and q that, for brevity, are not given here. It is not hard to see that to compute the leading singularities as well as the first correction in the phase boundary one does not actually need these coefficients provided $\theta < 1$. (It is clear that the cases with $\theta > 1$ can be analyzed in the same way but with greater complexity and less interest.)

Now that we have all the needed free energy functions, we can compute the phase boundaries and check for singularities.

E. A further amplitude ratio

The explicitly computed free energies for the $\beta\gamma$, $\beta+\gamma$, and the α phases can now be used to compute the phase boundary $D_\sigma(T,h)$ or $\bar{g}_\sigma(\hat{t},h)$ near the end point simply by equating the free energies. The procedure is explained in detail in I and II. In the presence of a small external field, the phase boundary is given by Eq. (3.22) with the amplitude ratios $x_-/x_+ = z_-/x_+ = y/x_+ = 0$, since $x_- = y = z_- = 0$. We can similarly check the behavior on the $T = T_e$ loci (3.25) following (3.26)–(3.28). Explicity we find

$$\Xi_5 \equiv \left(\frac{X_+}{Z_+}\right)^{2\theta/3} \frac{y_c^2}{x_+ z_+} = \frac{1}{2^{2(1+\theta/3)}}\,\frac{(1+\theta)}{(2+\theta)}, \qquad (4.44)$$

which verifies the predicted universality and relation to the bulk critical amplitudes on the λ line.

V. CONCLUSION

We have studied the bulk thermodynamics near a critical end point in order to examine the existence and nature of higher-order nonanalyticities. Using purely phenomenological arguments, first introduced in I, we predict in Sec. III that such behavior should be controlled by the correction-to-scaling universal bulk critical exponent, and amplitudes on the critical λ line. In order to demonstrate the relevance of such correction terms, we also summarize in Sec. II some universal features in correction to scaling, noting that the values of the universal amplitude ratio are even now not well-established numerically. Apart from this we must say that these corrections become more interesting when the leading-order singularities are "weak" (small amplitude and exponent) or absent.

Relevant bulk critical-point correction-to-scaling amplitude ratios are present in (3.11) and (3.12) and related to the phase-boundary-singularities amplitudes in (3.21), (3.24), and (3.28).

Then, in order to check these predictions against a specific model, we study in Sec. IV, as we did in II, the spherical model with short- and long-range interactions but now for dimensions exceeding to the upper critical dimension $d_+ = 2\sigma$. In this case the leading-order singularities are classical and the *non*classical correction to scaling play an important role.

Following the procedure introduced in II we find that the phase boundary between the spectator or α phase and the critical phase exhibits singularities as the end point is approached. The amplitude of these singularities combine to give universal ratios.

These ratios are directly related to universal bulk amplitude ratios evaluated on the λ line. The form of these relations are just those predicted in Sec. III, so confirming the phenomenological theory. One may remark that the spherical model is somewhat artificial; we cannot thus assert that a more realistic model might not contradict our heuristic predictions.

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APPENDIX A

It is well known[8] that at the borderline $d = d_+$, the spherical model exhibits logarithmic factors. In this appendix we will check this explicitly. Besides one can ask if the $d = d_+$ case yields the same $d < d_+$ behavior given qualitatively in Figs. 4 and 6 in II. In order to answer this question we have to compute $\bar{p}_0$, $\bar{p}_1$, and $\bar{p}_2$ which we do next.

For $d = d_+$, the integral $I_d(\zeta)$ can be computed, following the Appendix in II. From this the constraint condition (4.4) becomes

$$\tilde{m} = -w(1+t)\,\frac{\hat{p}}{4}\,\zeta\ln\left(\frac{\zeta+\hat{J}_\sigma\tilde{\pi}^\sigma}{\zeta}\right) + O(\zeta), \quad \text{(A1)}$$

where $O(\zeta)$ comes from higher-order terms in Eq. II(2.5), while

$$\hat{J}^{3/2}I_d^0\hat{p} = \left(\frac{1}{2}\right)^{2\sigma+1}\pi^\sigma\,\sigma\,\Gamma(\sigma). \quad \text{(A2)}$$

The free energy term in (4.3) becomes

$$\Delta F = \frac{(\hat{J}_\sigma\tilde{\pi}^2)^2}{16}\,\hat{p}\left[\ln(1+\bar{\zeta})+\bar{\zeta}^2\ln\left(1+\frac{1}{\bar{\zeta}}\right)-\bar{\zeta}\right] + O(\bar{\zeta}^2), \quad \text{(A3)}$$

where $\bar{\zeta} \equiv \zeta/\hat{J}_\sigma\tilde{\pi}^\sigma$. If $\hat{J}(k) = \hat{J}(0) - \hat{J}_\sigma \mid ka \mid^\sigma$, (A1) and (A2) should be exact.

At $t = \bar{g} = 0$, on the tricritical point, we may eliminate $\tilde{m}$ from (4.15) and (A1). A nonzero solution $\bar{\zeta} = \bar{\zeta}_0$ of this equation will be allowed if $\Delta\mathcal{F}_t(\bar{\zeta} = \bar{\zeta}_0) \le 0$ or, following procedure similar to that in Sec. IV, $\bar{p}(d = d_+) \ge \bar{p}_0$ where we have the definition

$$\bar{p} \equiv W\sqrt{\hat{J}_\sigma\tilde{\pi}^\sigma V}\;\hat{p} \quad \text{(A4)}$$

we obtain, numerically

$$\bar{p}_0 \simeq 5.11\,. \quad \text{(A5)}$$

Further information about the phase diagram is obtained from the critical-point analysis. Following II, we find that the phase boundary between the critical and noncritical phases is terminated by a critical point solution of

$$(1+t)^2\bar{p}^2 = 8C(\bar{\zeta})/\bar{\zeta}(1+\bar{\zeta}), \quad \text{(A6)}$$

where

$$C(\bar{\zeta}) = (1+\bar{\zeta})\ln\left(1+\frac{1}{\bar{\zeta}}\right) - 1. \quad \text{(A7)}$$

The new critical point is located at

$$t_c = \frac{\tau_c}{1-\tau_c},\quad \tau_c = \frac{\bar{b}}{8}\,\bar{p}\bar{\zeta}\left[\ln,\left(1+\frac{1}{\bar{\zeta}}\right) - C^2(\bar{\zeta})\right],$$
$$\bar{g}_c = \tfrac{1}{64}\,\bar{b}^2\bar{p}^2\bar{\zeta}^2(1+t)^2(1+\bar{\zeta})^{-1}C^3(\bar{\zeta})[2-C(\bar{\zeta})(1+\bar{\zeta})], \quad \text{(A8)}$$

where $\bar{b} \ge 1$ depends on $J(\hat{k}) = \hat{J}(0) - \hat{J}_\sigma \mid ka \mid^\sigma + E(k)$ and the equality would hold if one assumes $E = 0$ [in that case (A1) should be exact].

At $t_c = 0$, one has $\bar{p} = \bar{p}_1$ where

$$\bar{p}_1 \simeq 4.7183\,, \quad \text{(A9)}$$

and at $g_c = 0$, one has $\bar{p} = \bar{p}_2$ where

$$\bar{p}_2 \simeq 4.503\,. \quad \text{(A10)}$$

Now, on the basis of (A5), (A9), and (A10) we are allowed to claim that the $d = d_+$ case follows qualitatively the same $d < d_+$ phase diagrams.

It must be pointed out that the $\bar{p}$ values computed in this appendix differ from the $\theta \to 0$ limit of those obtained in Sec. IV ones. This difference depends on $O(\zeta^3)$ approximation used there.

Finally we can answer our prior question regarding the presence of logarithms in the free energy and consequently in the thermodynamics functions.

Following the standard procedure,[2] we find that the singular terms in the free energy should be given by

$$\Delta F_{\beta\gamma} = -\frac{A_+}{2}\,\tilde{t}^2 \mid \ln\tilde{t} \mid [1+O(\tilde{t}^2)] + \tfrac{1}{2}\,C_+\tilde{t}^{-1} \mid \ln\tilde{t} \mid \; h^2[1+(O(\ln\tilde{t})^{-1}), h^2/t^3] \quad \text{(A11)}$$

and

$$\Delta F_{\beta+\gamma} = -B \mid \tilde{t} \mid^\beta \mid h \mid [1+O(\mid h \mid / \mid \tilde{t} \mid^{3/2})], \quad \text{(A12)}$$

where $\beta\gamma$ (and $\beta+\gamma$) means $T > T_\lambda$ (and $T < T_\lambda$). At $T = T_\lambda$

$$\Delta F_c \approx -\tfrac{4}{3}B_c \;\mid h \mid^{4/3} \mid \ln h \mid^{1/3}, \quad \text{(A13)}$$

where A_+, C_+, B, and B_c are simply the $\gamma \to 1$ limits of Eqs. II(4.4), (4.6), (4.8), and (4.11) and, since no logarithmic factor is present in $F_{\beta\gamma}$, $A_- = 0$ and we cannot define a susceptibility (note that this is no longer true for $d > d_+$). From these amplitudes we can obtain universal amplitude ratios, for example,

$$\frac{A_-}{A_+} = 0\;,\qquad \Theta_1 \equiv \frac{A_+C_+}{B^2} = -\frac{1}{2}\;,\qquad \Theta_2 \equiv \frac{A_+B_c^\delta}{B^{\delta+1}} = -\frac{1}{2}\;. \quad \text{(A14)}$$

Related phase boundary ratios as given by Eqs. (1.3)–(1.6) can now be obtained. First, we rewrite Eq. (1.2) as

$$g_\sigma = g_e + g_1\hat{t} - X_\pm\hat{t}^2\ln \mid \hat{t} \mid - Y_\pm \mid \hat{t} \mid^{1/2} \mid h \mid - \tfrac{1}{2}Z_\pm \mid \hat{t} \mid^{-1}\ln \mid \hat{t} \mid h^2 + \Delta g(T,h), \quad \text{(A15)}$$

where we assumed the existence of logarithmic singularities. Next, by equating (3.13) to (A11), (A12), and (A13), one obtains that, even in this borderline case, the model exhibits phase-boundary ratios given by Eqs. (1.3)–(1.6). Note that the universality of such ratios are not obvious due to the presence of logarithmic terms.

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