# Critical confluent corrections: Universality and estimates of amplitude ratios from field theory at d = 3

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We estimate, at d = 3, from  $\phi^4$  field theory the universal ratios of confluent critical correction amplitudes relative to the correlation length, the susceptibility, and the specific heat above  $T_c$ . Our central values are comparable to these available from analysis of high-temperature series and the  $\epsilon$  expansion. Furthermore, experiments in progress on a binary mixture are in good agreement with one of our results, the ratio of the confluent corrections for the specific heat and susceptibility which have not been previously estimated. We also present, in detail, a derivation of the universality of these quantities in the framework of field theory.

#### I. INTRODUCTION

Systems which exhibit a second-order phase transition at a critical temperature  $T_c$  have special properties which are responsible for singularities in some functions of the reduced temperature  $\tau = (T - T_c)/T_c$ .

Let us denote by  $f_i(\tau)$  these functions. In the vicinity of  $T_c(\tau \rightarrow 0^{\pm})$  they behave as<sup>1</sup>

$$f_{i}(\tau) \sim_{\tau \to 0^{\pm}} f_{i}^{(0)^{\pm}} |\tau|^{-\lambda_{i}} \times (1 + a_{f_{i}} |\tau|^{\Delta_{1}} + b_{f_{i}} |\tau|^{\Delta_{2}} + \dots + \mathfrak{N}) , \quad (1.1)$$

where  $\mathfrak{N}$  is the nonsingular terms. The  $\lambda_i$  are the critical exponents,  $f_i^{(0)\pm}$  the critical amplitudes,  $a_{f_i}$ and  $b_{f_i}$  the amplitudes of the first and second confluent corrections;  $\Delta_1$  is the leading subcritical exponent; terms analytic in  $\tau$  have been omitted. If one deals only with the  $\phi^4$  theory, and neglects cutoff corrections, then  $\Delta_2 = 2\Delta_1$ . Following the universality hypothesis<sup>2</sup> systems are grouped into classes. Within each class, in addition to scaling laws, the critical and subcritical exponents together with some combinations of critical amplitudes are universal numbers. These classes are characterized by the dimensionalities of both the order parameter and space (n and d). While some efforts have been devoted towards the determination of universal combinations of amplitudes<sup>3,4</sup> very little is known concerning the confluent amplitudes.

The knowledge of these amplitudes would be very useful for the analysis of the various experimental data<sup>5</sup> and high-temperature (HT) series.<sup>6</sup> Following

the HT series we expect the ratio of two such amplitudes (susceptibility and correlation length) to be universal (extended universality<sup>7,8</sup>). The field-theory technique is an efficient tool for studying the universality and calculating perturbatively any quantity of interest for critical phenomena.<sup>9</sup> Recently the  $\epsilon$  expansion ( $\epsilon = 4 - d$ ) for amplitude corrections<sup>10</sup> was calculated up to order  $\epsilon^2$ , but it is hard to assess the reliability of the numbers obtained at  $\epsilon = 1$ .

In order to eliminate some disadvantages of using noninteger dimension, Parisi<sup>11</sup> suggested that the kloop contributions at fixed dimensions be computed directly. Following this scheme, Nickel *et al.*<sup>12</sup> have performed, up to sixth order, the calculations at d = 3for  $\phi^4$  theory. Their results, together with the resummation method based on the large order behavior<sup>13</sup> provide us with an opportunity to reach various universal quantities attached to corrections, with a good accuracy.

As this perturbative expansion was calculated in the massive renormalized theory, it has not been possible as yet to investigate the amplitudes below  $T_c$ . In this paper, we have considered the corrections above  $T_c$  for the magnetic susceptibility ( $\chi$ ), the correlation length ( $\xi$ ), and the singular part of the specific heat ( $C_s$ ). To be more precise, let us introduce the notation used: we calculate the ratios  $a_{\xi}^+/a_{\chi}^+, a_c^+/a_{\xi}^+$  (and  $a_c^+/a_{\chi}^+$ ) such that, as  $\tau \to 0+$ , we have

$$\xi \simeq \xi_0^+ t^{-\nu} (1 + a_{\xi}^+ t^{\omega\nu} + \cdots) \quad , \tag{1.2}$$

$$\chi \simeq \Gamma t^{-\gamma} (1 + a_{\chi}^{+} t^{\omega \nu} + \cdots) \quad , \tag{1.3}$$

$$C_{S} \simeq \frac{A^{+}}{\alpha} t^{-\alpha} (1 + \alpha a_{C}^{+} t^{\omega \nu} + \cdots) \quad , \qquad (1.4)$$

in which  $\nu$ ,  $\gamma$ ,  $\alpha$  are the usual critical exponents, and

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 $\omega$  is the derivative of the Wilson's function at the fixed point.

First, in Sec. II we present a derivation of the universality of the various correction amplitude ratios in the framework of the massive renormalized field theory. We have tried to be as explicit as possible because of the fact that universality was hitherto considered essentially only in the zero-mass renormalized theory.<sup>4,9</sup> The derivation of universality in field theory consists in showing that (i) the cutoff dependence disappears from the critical behavior—this is accomplished by the use of the renormalized theory. (ii) Expected universal quantities do not depend on the bare coupling constant. (iii) The renormalization scheme does not affect the final result.

Following these general considerations, we give in Sec. III the expressions for quantities that we have estimated.

Finally, in Sec. IV, we discuss, without mathematical details, the results obtained from the resummation method used.

#### **II. UNIVERSALITY AND MASSIVE FIELD THEORY**

The theoretical background of this part can be found in many review papers.<sup>9,14</sup> The starting point of the renormalized field-theory approach to critical phenomena is the Landau-Ginsburg-Wilson Hamiltonian

$$\mathcal{K}/k_B T = \int d^d x \left\{ \frac{1}{2} \left[ -\vec{\varphi}_0(x) \cdot \Delta \vec{\varphi}_0(x) + m_0^2 \vec{\varphi}_0^2(x) \right] + \frac{g_0}{4!} \left[ \vec{\varphi}_0^2(x) \right]^2 \right\} , \qquad (2.1)$$

which is used to define the probability distribution of the variable  $\vec{\varphi_0} = \{\varphi_0^i, i = 1, 2, \dots, n\}$  whose mean value is the order parameter. The subscript "0" means that the form (2.1) is the continuous limit of a realistic model (e.g., lattice model) and indicates the "physical variables" which will be related to the renormalized quantities.

In Eq. (2.1),  $\Delta$  denotes the Laplace operator

$$\Delta = \sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2} \quad ,$$

and d is the dimension of space. Because of the noncontinuous character of the physics, we have to keep in mind that the integrals over the d-dimensional space are a continuous limit of a discrete sum. This can be taken into account by integrating only over  $\vec{k}$ momenta (conjugated to  $\vec{x}$  in a Fourier transform) such that

$$0 \le \left| \overline{\mathbf{k}} \right| \le \Lambda$$
 , (2.2)

the cutoff  $\Lambda$  being fixed and finite. We are interested in the critical behavior of the one-particle irreduci-

ble vertex functions

 $\Gamma_0^{(L,N)}(q_1,\ldots,q_L;p_1,\ldots,p_N;m_0,g_0,\Lambda)$ 

which are related to the correlation functions

$$G_0^{(L,N)}(y_1, \dots, y_L; x_1, \dots, x_N; m_0, g_0) = \langle \varphi_0^2(y_1) \cdots \varphi_0^2(y_L) \varphi_0(x_1) \cdots \varphi_0(x_N) \rangle \quad (2.3)$$

calculated with the Hamiltonian (2.1).

The critical behavior appears as the bare mass  $m_0$  goes to its critical value  $m_{0c}$  defined by

$$\Gamma_0^{(0,2)}(0;m_{0c},g_0,\Lambda) = 0 \quad . \tag{2.4}$$

As  $m_0$  goes to  $m_{0c}$  singularities appear in the vertex functions, and the naive perturbation theory in powers of  $g_0$  breaks down since the effective expansion parameter becomes infinite, but the explicit dependence on  $\Lambda$  can be forgotten ( $\Lambda^{-1} \equiv 0$ ). The irrelevance of this length scale in the critical domain motivates the use of the renormalized theory.<sup>9, 11, 15</sup>

Hence, following the standard procedure, we introduce new (renormalized) variables  $\varphi$ , u, and m which are defined from the bare ones  $\varphi_0$ ,  $g_0$ , and  $m_0$ through

$$\varphi_0 = Z_3^{1/2} \varphi$$
 , (2.5a)

$$g_0 = um^{\epsilon} Z_1 / Z_3^2$$
 , (2.5b)

$$m^2 = Z_3 m_0^2 + \delta m^2 \quad , \tag{2.5c}$$

$$\rho_0^2 = Z_3 / Z_4 \varphi^2 \quad , \tag{2.5d}$$

so that in the limit  $\Lambda \rightarrow \infty$  the bare and renormalized vertex functions [for  $(L,N) \neq (0,0)$ , (1,0), and (2,0)] are related as follows:

$$\lim_{\Lambda \to \infty} \Gamma_0^{L,N}(\{q\};\{p\};m_0,g_0,\Lambda) = Z_3^{-N/2}(u) \left(\frac{Z_4(u)}{Z_3(u)}\right)^{-L} \Gamma^{L,N}(\{q\};\{p\};m,u)$$
(2.6)

The  $Z_i$ 's are arbitrary functions which depend on the dimensionless coupling constant u. These functions are given by some renormalization conditions on the  $\Gamma^{L,N}$ . In the renormalized theory the critical domain is defined by [see Eqs. (2.4) and (2.6)]

$$m^{2}Z_{3}^{-1}(u)\mathfrak{F}^{(0,2)}(u) \to 0$$
(2.7)

in which, using simple dimensional arguments

$$\mathfrak{F}^{(L,N)}(u) = \frac{\Gamma^{L,N}(m,u)}{m^{D_{LN}}} \equiv \Gamma^{L,N}(1,u) \quad . \tag{2.8}$$

 $D_{LN}$  being the classical dimension of  $\Gamma^{L,N}$ , namely,

$$D_{LN} = d - \frac{N}{2}(d-2) - 2L \qquad (2.9)$$

We shall now show that, provided the exponent  $\eta$ 

verifies the inequalities

$$0 < \eta < 2 \tag{2.10}$$

and that  $\mathfrak{F}^{(L,N)}(u)$  are well-defined functions for any value of u, then the limit (2.7) corresponds to  $m \rightarrow 0$ .

Equation (2.5b) indicates the existence of a special value  $u^*$  of u since  $m \rightarrow 0$  and  $g_0$  is fixed. This fixed point  $u^*$  is the zero of the function  $\beta(u)$ , namely,

$$\beta(u) = -\epsilon \left[ \frac{d}{du} \ln \left( \frac{uZ_1}{Z_3^2} \right) \right]^{-1} .$$
 (2.11)

Near  $u^*$ , an expansion of this function reads

$$\frac{1}{\beta(u)} = \frac{1}{\omega(u-u^*)} + \sum_{n=0}^{\infty} \rho^{(n)} (u-u^*)^n \quad (2.12)$$

Using this expansion and Eq. (2.5b) the integration of Eq. (2.11) leads to

$$\Delta u \equiv u - u^*$$
  
=  $m^{\omega} \left(\frac{A_1}{g_0}\right)^{\omega/\epsilon} \left[1 - \rho^{(0)} \omega m^{\omega} \left(\frac{A_1}{g_0}\right)^{\omega/\epsilon} + \cdots\right], \quad (2.13)$ 

where  $A_1$  enters as a constant of integration. This result shows that, if  $\omega$  is positive, u goes to  $u^*$  when m goes to zero as expected.

We now define the following functions:

$$\gamma_k(u) = \beta(u) \frac{d}{du} \ln Z_k(u), \quad k = 3, 4$$
, (2.14)

with

$$\gamma_k(u) = \sum_{n=0}^{\infty} \gamma_k^{(n)} \Delta u^n \quad . \tag{2.15}$$

Then as previously we find near  $u^*$ 

$$Z_{k}(u) = \Delta u^{\gamma_{k}^{(0)}/\omega} A_{k} \left[ 1 + \left( \frac{\gamma_{k}^{(1)}}{\omega} + \gamma_{k}^{(0)} \rho^{(0)} \right) \Delta u + \cdots \right] .$$
(2.16)

with

$$\gamma_3^{(0)} \equiv \eta \quad , \tag{2.17a}$$

$$\gamma_4^{(0)} \equiv \eta_4 \quad . \tag{2.17b}$$

Together with Eq. (2.13) the result (2.16) shows that the limit (2.7) is given by  $m \rightarrow 0$  provided that (2.10) holds.

The critical behavior of the bare theory then requires the study of the right-hand side of Eq. (2.6) as u goes to  $u^*$ . The part which comes from the functions  $Z_k$  is given by (2.16) and (2.13). Simple dimensional arguments for the  $\Gamma^{L,N}(\{0\},\{0\};m,u)$ and a Taylor expansion around  $u^*$ , yield

$$\Gamma^{(L,N)}(\{0\};\{0\};m,u) = m^{D_{LN}} \mathfrak{F}^{(L,N)}\left(1 + \frac{d}{du} \ln \mathfrak{F}^{(L,N)}(u) \Big|_{u=u} \Delta u + \cdots\right)$$
(2.18)

in which  $\mathfrak{F}^{(L,N)}$  stands for  $\mathfrak{F}^{(L,N)}(u^*)$ .

It is then straightforward to establish the following behavior of the bare vertex functions, as *m* goes to zero:

$$\Gamma_{0}^{L,N}(\{0\};\{0\};m_{0},g_{0},\Lambda) \underset{m \to 0^{+}}{\sim} Dm^{\{D_{LN}+2L-(N/2)\eta-L/\nu\}} \times \left\{ 1 + \left[ \left(L - \frac{N}{2}\right) \frac{\gamma_{3}^{(1)}}{\omega} - \frac{L\gamma_{4}^{(1)}}{\omega} + \frac{d}{du} \ln \mathfrak{F}^{(L,N)}(u) \right]_{u=u^{*}} m^{\omega} \left(\frac{A_{1}}{g_{0}}\right)^{\omega/\epsilon} + \cdots \right\}$$
(2.19)

in which we have introduced the exponent  $\nu$ 

$$\nu = (2 - \eta + \eta_4)^{-1}$$
(2.20)
and the constant

$$\mathfrak{D} = \left(\frac{A_3}{A_4}\right)^L \frac{\mathfrak{F}^{(L,N)}}{A_3^{N/2}} \left(\frac{A_1}{g_0}\right)^{[-(N/2)\eta + L(2-1/\nu)]^{1/\epsilon}}$$
(2.21)

Equation (2.19) is not yet the final result. The renormalized mass must be expressed in terms of the variable  $t = m_0^2 - m_{0c}^2 \left[ -\tau + O(\tau^2) \right]$  in order to obtain the expected asymptotic expansion [Eq. (1.1)]. The relation between the variables *m* and  $m_0$  can be obtained from Eqs. (2.5) and (2.6). Instead we shall replace one of these equations by an equivalent differential form: the Callan-Symanzik equation which is

$$\left(m\frac{\partial}{\partial m} + \beta(u)\frac{\partial}{\partial u} - \frac{N}{2}\gamma_{3}(u) - L\left[\gamma_{4}(u) - \gamma_{3}(u)\right]\right)\Gamma^{(L,N)}(q_{1}, \ldots, q_{L}; \{p\}; m, u)$$

$$= m\frac{\partial m_{0}^{2}}{\partial m}\left|_{g_{0}}\frac{Z_{3}}{Z_{4}}\Gamma^{(L+1,N)}(q_{1}, \ldots, q_{L}, 0; \{p\}; m, u)\right| \qquad (2.22)$$

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For N = 2, L = 0, and p = 0 this equation, together with Eq. (2.6), leads to

$$\frac{\partial m_0^2}{\partial m} = (2 - \gamma_3) \frac{Z_4}{Z_3} \frac{\mathfrak{F}^{(0,2)}(u)}{\mathfrak{F}^{(1,2)}(u)} m \left[ 1 + \frac{\beta}{2 - \gamma_3} \frac{d}{du} \ln \mathfrak{F}^{(0,2)}(u) \right] .$$
(2.23)

After some obvious manipulations which use Eqs. (2.13) and (2.16) one obtains the relation that we were looking for, namely,

$$m = (Xt)^{\nu} \left[ 1 - \frac{\nu}{\omega\nu + 1} C \left( \frac{A_1}{g_0} \right)^{\omega\nu/\epsilon} (Xt)^{\omega\nu} + \cdots \right] , \qquad (2.24)$$

where

$$C = \frac{\gamma_4^{(1)} - \gamma_3^{(1)}}{\omega} - \frac{\gamma_3^{(1)}}{2 - \eta} + \frac{d}{du} \ln \frac{\mathfrak{F}^{(0,2)}(u)}{\mathfrak{F}^{(1,2)}(u)} \bigg|_{u = u^*} + \frac{\omega}{2 - \eta} \frac{d}{du} \ln \mathfrak{F}^{(0,2)}(u) \bigg|_{u = u^*} ,$$
  

$$X = \frac{A_3}{\gamma A_4} \left( \frac{A_1}{g_0} \right)^{(2 - 1/\nu)/\epsilon} \frac{\mathfrak{F}^{(1,2)}}{\mathfrak{F}^{(0,2)}} .$$
(2.25)

The exponent  $\gamma$  comes from the scaling law

$$\gamma = \nu(2-\eta) \quad . \tag{2.26}$$

We are now ready to write the general form of the asymptotic behavior of the bare vertex functions in terms of the critical variable t. Using Eqs. (2.19) and (2.24), we have

$$\Gamma_{0}^{(L,N)} \sim (\gamma X)^{L} Y^{N}(Xt)^{\{\nu[D_{LN}-(N/2)\eta+2L\}-L\}} \left[ \frac{\mathfrak{F}^{(0,2)}}{\mathfrak{F}^{(1,2)}} \right]^{L} \mathfrak{F}^{(L,N)} \left[ 1 + K_{LN}(Xt)^{\omega\nu} \left( \frac{A_{1}}{g_{0}} \right)^{\omega\nu/\epsilon} + \cdots \right] , \qquad (2.27)$$

with  $Y = (A_1/g_0)^{-\eta/\epsilon}(1/A_3)$  and X given in Eq. (2.25).

Finally  $K_{LN}$  can be expressed as

$$K_{LN} = \left(L - \frac{N}{2}\right) \frac{\gamma_3^{(1)}}{\omega} - L \frac{\gamma_4^{(1)}}{\omega} + \frac{d}{du} \ln \mathfrak{F}^{(L,N)}(u) \bigg|_{u^*} - \left(D_{LN} + 2L - \frac{N}{2}\eta - \frac{L}{\nu}\right) \frac{\nu}{\omega\nu + 1} C \quad , \tag{2.28}$$

C being also given in Eqs. (2.25).

Following Ref. 4 we observe that, for the leading amplitudes, defined for different values of L and N in Eq. (2.27), any combination among them which eliminates the factors X and Y is independent of  $g_0$  and is therefore a candidate for an universal quantity. Similarly for the amplitudes of the confluent terms we see that any ratio of two of them (for two different vetex functions) is also independent of  $g_0$  since the same subleading exponent governs the behavior of all these terms.

In order to be complete we must investigate the arbitrariness introduced by the renormalization scheme. Any renormalized theory has to give back the same bare theory Eqs. (2.5) and (2.6). Thus, two renormalized theories, characterized by  $\Gamma^{(L,N)}$  and  $\tilde{\Gamma}^{(L,N)}$ , are related through

$$\Gamma^{(L,N)}(\{q\},\{p\};m,u) = \zeta_3^{(N/2-L)}\zeta_4^L \tilde{\Gamma}^{(L,N)}(\{q\},\{p\};\tilde{m},\tilde{u}) , \qquad (2.29)$$

$$m^{\epsilon} \frac{uZ_{1}(u)}{[Z_{3}(u)]^{2}} = \tilde{m}^{\epsilon} \frac{\tilde{u}Z_{1}(\tilde{u})}{[\tilde{Z}_{3}(\tilde{u})]^{2}} , \qquad (2.30)$$

and

$$m^{2}\left(1 - \frac{\delta m^{2}}{m^{2}}(u)\right) = \zeta_{3}\tilde{m}^{2}\left(1 - \frac{\delta \tilde{m}^{2}}{\tilde{m}^{2}}(\tilde{u})\right) , \qquad (2.31)$$

with

$$\zeta_k = \frac{Z_k(u)}{\tilde{Z}_k(\tilde{u})} \quad .$$

Equations (2.30) and (2.31) may be written equivalently

$$\tilde{u} = U(u) \tag{2.33}$$

and

$$\tilde{m} = \lambda(u)m \quad (2.34)$$

where U and  $\lambda$  are known and nonsingular functions of u when the two different renormalization schemes are precisely specified. In other words, these functions define the change of the renormalization scheme. We must then look at the change introduced by the transformations (2.33) and (2.34) on the amplitudes of interest to us. Since these latter are quantities calculated at the fixed point we consider the transformation for u in the vicinity of  $u^*$ .

It is easy to find the following relation, between  $\beta(u)$  and  $\tilde{\beta}(\tilde{u})$ 

$$\tilde{\beta}(\tilde{u}) = \frac{dU}{du} \frac{\beta(u)}{1 + \beta(u)(d/du) \ln\lambda(u)}$$
(2.35)

which shows that when  $u \to u^*$  then  $\tilde{u} \to \tilde{u}^*$ . Following this relation one obtains readily the universality of the exponents:  $\omega$ ,  $\eta$ , and  $\eta_4$ , and the transformations<sup>16</sup>:

$$\gamma_k^{(1)} = \frac{dU}{du} \tilde{\gamma}_k^{(1)} + \omega \left[ \tilde{\gamma}_k^{(0)} \frac{d\ln\lambda}{du} \bigg|_{u^*} + \frac{d\ln\zeta_k}{du} \bigg|_{u^*} \right] , \qquad (2.36)$$

$$\mathfrak{F}^{(L,N)} = \left(\frac{dU}{du}\right)_{u^*}^{[(L-N/2)\eta-L\eta_4]\omega} \left(\frac{A_3}{\tilde{A}_3}\right)^{N/2-L} \left(\frac{A_4}{\tilde{A}_4}\right)^L \lambda^{D_{LN}} \tilde{\mathfrak{F}}^{(L,N)} , \qquad (2.37)$$

$$\frac{d}{du}\ln\mathfrak{F}^{(L,N)}(u)\Big|_{u^*} = \frac{dU}{du}\frac{d}{d\tilde{u}}\ln\tilde{\mathfrak{F}}^{(L,N)}(\tilde{u})\Big|_{\tilde{u}^*} + \left(\frac{N}{2} - L\right)\frac{d}{du}\ln\zeta_3\Big|_{u^*} + L\frac{d}{du}\ln\zeta_4\Big|_{u^*} + D_{LN}\frac{d\ln\lambda}{du}\Big|_{u^*} \quad (2.38)$$

In the derivation of Eqs. (2.37) and (2.38), we also used the definitions (2.8) and (2.16). It is then simple to show that

$$\frac{K_{L_1N_1}}{K_{L_2N_2}} = \frac{\tilde{K}_{L_1N_1}}{\tilde{K}_{L_2N_2}} \quad . \tag{2.39}$$

This result ends the derivation of the universality of the ratio of confluent corrections amplitudes in two vertex functions. Let us note that the change in the renormalization scheme is not absorbed in a change of the quantities X and Y for confluent corrections as is the case for the leading amplitudes.<sup>4</sup>

## III. AMPLITUDE CORRECTION RATIOS FOR x, $\xi$ , AND $C_S$

Nickel, Meiron, and Baker<sup>12</sup> calculated directly at d = 3 the functions  $Z_k$  (k = 1, 3, 4) and  $\beta$ , as power series in the coupling constant, corresponding to the following renormalization condition for the renormalized vertex functions:

$$\Gamma^{(0,2)}(0;m,u) = m^2 , \qquad (3.1a)$$

$$\frac{d}{dp^2} \Gamma^{(0,2)}(p;m,u) |_{p=0} = 1 \quad , \tag{3.1b}$$

$$\Gamma^{(0,4)}(\{0\}; m, u) = m^{\epsilon} u , \qquad (3.1c)$$

$$\Gamma^{(1,2)}(0, \{0\}; m, u) = 1 \quad . \tag{3.1d}$$

This allows us, using the result of Sec. II, to derive the amplitudes of the confluent terms for the susceptibility  $\chi$  and the correlation length  $\xi$  above  $T_c$ . Equations (3.1) lead to

$$\mathfrak{F}^{(1,2)}(u) = \mathfrak{F}^{(0,2)}(u) \equiv 1 \quad . \tag{3.2}$$

The susceptibility is defined as

$$\chi^{-1} = \Gamma_0^{(0,2)}(0, m_0, g_0) \equiv Z_3^{-1} m^2 \quad , \tag{3.3}$$

and the correlation length as the second moment of the correlation function:

$$\xi^{-2} = \frac{\Gamma_0^{(0,2)}(0;m_0,g_0)}{(d/dp^2)\Gamma_0^{(0,2)}(p;m_0,g_0)|_{p=0}} \equiv m^2 \quad . \tag{3.4}$$

It then follows from the Sec. II and relations (3.2) that the universal ratio for confluent corrections of  $\xi$  and  $\chi$  is expressed by

$$\frac{a_{\chi}^{+}}{a_{\xi}^{+}} = 2 - \eta + \frac{\gamma_{3}^{(1)}(\omega\nu + 1)}{\omega\nu[(\gamma_{4}^{(1)} - \gamma_{3}^{(1)})/\omega - \gamma_{3}^{(1)}/(2 - \eta)]}$$
(3.5)

where we recall that

$$\gamma_k^{(1)} = \frac{d}{du} \gamma_k(u) \Big|_{u^*} \quad . \tag{3.6}$$

The functions  $\gamma_k(u)$  (k = 3, 4) are defined in Eqs. (2.14) and their series have been calculated up to sixth order<sup>17</sup> in a coupling constant v related to u

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through

$$u = D v \quad , \tag{3.7}$$

$$D = \frac{6}{(n+8)} \frac{(2\pi)^d}{\pi^{d/2} \Gamma_E(2-d/2)} , \qquad (3.8)$$

where  $\Gamma_E(z)$  denotes the standard gamma function. Since *D* is a constant, we can replace *u* by *v* in (3.5). The quantities  $\eta$ , v,  $\omega$ , and  $v^*$  have been already calculated by Le Guillou and Zinn-Justin<sup>13</sup> so that it remains to resum the  $\gamma_k^{(1)}$ 's.

The ratio (3.5) is the only ratio which can be obtained directly from Ref. 12. The renormalization scheme is not adapted to go below  $T_c$  since the limit m = 0 is not defined and the functions  $\mathfrak{F}^{(L,N)}(u)$  have not been investigated apart from the particular cases L = 0, N = 2 and L = 1, N = 2 [Eq. (3.2)].

Nevertheless, in Ref. 18 the authors have extracted the function  $\Gamma_0^{(2,0)}$  from the work of Baker, Meiron, and Nickel, finding

$$\Gamma_0^{(2,0)}(\{0\}; m, g_0) = \frac{6Z_5^{-1}(\lambda)}{g_0} \quad . \tag{3.9}$$

The coupling constant  $\lambda$  is related to v through the

relation

$$v = -(n+8)\frac{Z_3^{d/2}}{Z_1}\lambda \quad . \tag{3.10}$$

The series in power of  $\lambda$  is given by Eq. (19) of Ref. 18. [One of the present authors (C.B.) apologizes for a misprint in this equation: in the first line read 4.849 instead of 4.89.]

The function  $\Gamma_0^{(2,0)}$  is related to the specific heat C  $C = -\Gamma_0^{(2,0)} \qquad (3.11)$ 

To obtain the critical behavior of C we cannot use the result of Sec. II for L = 2 and N = 0 owing to the additive character of the renormalization for  $\Gamma^{(2,0)}$ , but we may derive the singular part  $C_S$  of the specific heat from the critical behavior of  $\Gamma_0^{(3,0)}$  which is considered in the Sec. II.

We know that

$$\Gamma_0^{(3,0)}(m,g_0) = \frac{\partial}{\partial m_0^2} \Gamma^{(2,0)}(m,g_0) \big|_{g_0} \quad (3.12)$$

An integration over  $m_0$  (i.e., *t*) of the critical behavior of  $\Gamma_0^{(3,0)}$ , then gives back the singular part of the specific heat. Thus the corresponding confluent correction term  $a_c^+$ , defined in Eq. (1.4) at d = 3, reads

$$a_{C}^{+} = \frac{(XA_{1}/g_{0}^{e})^{\omega\nu}}{\omega\nu - \alpha} \left[ \frac{3(\gamma_{4}^{(1)} - \gamma_{3}^{(1)})\nu(\omega+1)}{\omega(\omega\nu+1)} - \frac{3\gamma_{3}^{(1)}(\nu-1)}{(2-\eta)(\omega\nu+1)} - \frac{d}{du} \ln \mathfrak{F}^{(3,0)}(u) \Big|_{u^{*}} \right] .$$
(3.13)

In order to express  $\mathfrak{F}^{(3,0)}(u)$  in term of known functions, we use Eqs. (3.7)-(3.10), (3.12), (2.5), and (2.6b) to find

$$\mathfrak{F}^{(3,0)}(u) = -\frac{\pi^{d/2}\Gamma_E(2-d/2)(d-4)}{2(2\pi)^d} \frac{(Z_4)^2}{(Z_3)^{d/2}} \left(\frac{Z_5^{-1}}{\lambda}\right) \left[1 + \lambda \frac{d}{d\lambda} \ln\left(\frac{Z_5^{-1}}{\lambda}\right)\right]$$
(3.14)

Thus we can obtain two other universal ratios  $a_C^+/a_{\xi}^+$ and  $a_C^+/a_{\chi}^+$  with only one more function to resum, namely  $(d/du)[\ln \mathfrak{F}^{(3,0)}(u)|_{u=u}^*]$ .

### IV. RESUMMATION AND DISCUSSION OF THE RESULTS

The series of interest for us have been summed using a method developed and discussed at length by Le Guillou and Zinn-Justin.<sup>13</sup> We shall just recall, at a practical level, how the free parameters necessary to the method are introduced. The reader interested in a theoretical justification of such a technique can refer to the work cited above.

Let us denote by  $S(v) = \sum_k S_k v^k$  a renormalized perturbation series that we deal with. At large order K we know<sup>19</sup> that

$$S_{K} \sim K! (-a)^{K} K^{o_{0}} c \tag{4.1}$$

in which a is independent of the series in contrast to  $b_0$  and c. The quantity a depends only on the spatial dimensionality d and on the form of the Hamiltonian. In our case and for d = 3 we have

$$a = \frac{9}{n+8} \left( 0.147\,774\,22 \right) \ . \tag{4.2}$$

The free parameters (b and  $\mu$ ) are introduced through the following transformations on the initial series S(v) to give resummed quantities  $S_{b,\mu}(v)$ : (i) Define first the series at order L by

$$\tilde{S}_b(x) = \sum_{k}^{L} \frac{S_k}{\Gamma_E(k+b+1)} x^k \quad .$$

(ii) Introduce a new expansion parameter

$$u(x) = \frac{(1+ax)^{1/2}-1}{(1+ax)^{1/2}+1} ,$$

with a given in Eq. (4.2).

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(iii) Call  $\overline{S}_{b,\mu}(u)$  the sum (term by term) of the

series in powers of u obtained from the series  $S_b(x)$ [in which x is replaced by its expansion in u from point (ii)] multiplied by the series of the function  $(1-u)^{\mu}$ , all these transformations are carried up to order L.

(iv) Finally consider

$$S_{b,\mu}(v) = \int_0^\infty dx \; \frac{e^{-x} x^b}{[1-u(vx)]^{\mu}} \bar{S}_{b,\mu}[u(vx)]$$

 $S_{b,\mu}(v)$  would give S(v) for any value of b and  $\mu$ provided that one deals with an infinite number of terms in the initial series. In the case of restriction to a finite number of terms (L orders) we learn from Ref. 13 that S(v) would be approximated optimally for some particular range of values for b and  $\mu$ . This fact necessitates the use of criteria for the determination of the error estimates. Since our series are shorter (five orders for  $\gamma_{3}^{(1)}$ ,  $\gamma_{4}^{(1)}$  and four for

 $(d/du)[\mathfrak{F}^{(3,0)}(u)]$  than those considered in the references cited above we have adopted some different criteria. We want to show now that they lead to reliable error estimates for the quantities of interest in the present paper.

If we were interested in a central value for a series to a given order, then the best choice for parameters b and  $\mu$  would be that which gives the best convergence for the series. This choice at each order L supplies values which vary smoothly with L. In order to determine the upper and lower bounds of the error estimates we have looked at the oscillatory (OC) and smooth (SC) curves in L for a large range of values of b and  $\mu$ . We have retained as the range of the uncertainty, the amplitude of the last oscillation of the smallest OC which encloses at least a SC.

The central value is then given by the best convergent SC provided that the OC are symmetrically disposed with respect to it (see Fig. 1 and 2). When



FIG. 1. Typical oscillating and smooth curves obtained for  $-(d/dv)\gamma_4|_{u=v}$  for n=1 and  $v^*=1.416$  as a function of the order L. The solid and dashed curves correspond, respectively, to the summation of the direct series, and of the inverse series. Different values for the free parameters b and  $\mu$  are labeled as follows: +b=3,  $\mu=-3$ ; 0 b=7.5,  $\mu=-3$ ;  $\bullet b=5.5$ ,  $\mu=2$ ;  $\Box$ b=9,  $\mu=0$ . The values obtained by the Padé approximant applied to the sequence of estimates at b and  $\mu$  fixed for the whole range of variation of these parameters is indicated by an arrow. The error estimate chosen for n = 1 and  $v^* = 1.416$  is drawn.



FIG. 2.  $-(d/dv)\gamma_4|_{v=v}$  obtained from the inverse series for n = 1,  $v^* = 1.416$ . The symbols correspond to, for  $\mu = 2$ : + b = 3.5, 0 = 4.5, \* b = 5.5,  $\Delta b = 6.5$  and  $\Box b = 9$ ,  $\mu = 0$ .

that is not the case, the last value of the SC is not related to the central value but gives the upper or lower, bound of the error bar according to the asymmetry (see Fig. 3).

To be more explicit let us consider the characteristic cases that we have encountered.

For the quantity  $(d/dv)\gamma_4|_{v=v} * (\equiv \gamma_4^{(1)})$  at  $\mu = -3$ , we found at least one OC which encloses at least one SC. In Fig. 1 we present the OC and SC which have the best convergence. We note that for the inverse series the selected OC and SC correspond to different values of  $\mu$  and lead to the same determination of  $\gamma_4^{(1)}$  as obtained from the direct series. Let us stress the fact that in all cases we have considered the direct and inverse series to check the consistency of the choice. In order to lighten Fig. 1 we present in Fig. 2 the evolution of the OC for the  $\gamma_4^{(1)}$  obtained from the inverse series as b is varied. We have adopted the OC with b = 5.5 as the result of a compromise between the best convergent OC, the best enclosure of a SC and the agreement (see Fig. 1) with this analysis applied to the inverse series data. In Fig. 2 only one SC appears although there are others (for different values of  $\mu$ ) but they would be so close to one another when drawn that they would be indistinguishable. The unsatisfactory behavior for the series  $\gamma_3$  which is already responsible of the relatively large uncertainty in the value of  $\eta$  has led us to sum as a global quantity the combination ( $\gamma_4^{(1)} - \gamma_3^{(1)}$ ) which naturally arises in the confluent correction terms. We present in Fig. 3 some curves to illustrate this case which appears to be the most tricky. We find a situation in which the asymmetry goes upward and that is why the error estimate is shifted upward.

It is clear that all the above considerations are based on a careful inspection of many curves for different values of b and  $\mu$ . The above criteria have thus been applied to the resummation at corresponding  $v^*$  (Ref. 13) of the unknown quantities of interest for n = 1, 2, and 3.



FIG. 3. Oscillations displayed in the resummation of the series  $-(d/dv)[\gamma_4(v) - \gamma_3(v)]|_{v=v}^*$  are not symmetrically disposed with regard to the smooth curves (asymetric case). This figure corresponds to n = 1 and  $v^* = 1.416$ . The solid and dashed curves represent, respectively, the direct and inverse resummed series. The parameters b and  $\mu$  are labeled as follows: + b = 1.5,  $\mu = -1$ ;  $\bigcirc b = 8$ ,  $\mu = -1$ ;  $\bigcirc b = 4.5$ ,  $\mu = 3$ ; \* b = 4.5,  $\mu = 3$ ;  $\Delta b = 9$ ,  $\mu = 1$ . The error estimate chosen is indicated.

Taking into account the uncertainties in  $v^*$ , in the critical exponents and in  $\omega$  from Ref. 13 we obtain the values of the universal ratios presented in Table I. One of these ratios  $(a_{\xi}^+/a_{\chi}^+)$  has been investigated already from high-temperature expansion for n = 1 (Ref. 7) and n = 2 (Ref. 20); and from an  $\epsilon$  expan-

TABLE I. Values of the ratios of confluent critical amplitudes obtained from field theory at d = 3, for different values of the number (*n*) of components of the order parameter.

Ratios $(v^*)$	$\frac{1}{(1.416 \pm 0.005)}$	2 (1.406 ± 0.004)	$3 \\ (1.391 \pm 0.004)$
$a_{\xi}^{+}/a_{\chi}^{+}$ $a_{C}^{+}/a_{\xi}^{+}$ $a_{C}^{+}/a_{\chi}^{+}$	$0.65 \pm 0.05$	$0.60 \pm 0.04$	$0.59 \pm 0.06$
	13.2 ± 1	9.8 ± 0.6	7.8 ± 0.6
	8.5 ± 0.9	5.9 ± 0.5	4.6 ± 0.5

sion up to  $\epsilon^2$  (Ref. 10). As it can be seen in Table II, the agreement is good with HT series. It is remarkable that the  $\epsilon$  expansion gives such a good estimation when we perform a naive sum.

The ratios relative to the specific heat have been calculated only at the leading order in  $\epsilon$  by Aharony

TABLE II. Values of ratio  $a_{\xi}^{-}/a_{x}^{+}$  obtained from the high-temperature expansion (HTE) and the  $\epsilon$  expansion ( $\epsilon_{exp}$ ) for n = 1, 2, 3. For this latter case, the series is known up to  $\epsilon^{2}$ . The numbers presented in this table correspond to the Padé approximants ([2,0],[1,1],[0,2]).

Method n HTE	$1 \\ 0.70 \pm 0.03$	$2 \\ 0.6 \pm 0.1$	3
[2,0]	0.65	0.63	0.62
$\epsilon_{\rm exp}$ [1,1]	0.43	0.42	0.42
[0,2]	0.71	0.67	0.64

and Ahlers.<sup>5</sup> They obtained

$$a_C^+/a_X^+ = 2(n+8)/(n+2) + O(\epsilon)$$
,

$$a_{C}^{+}/a_{E}^{+} = 4(n+8)/(n+2) + O(\epsilon)$$
.

An experiment<sup>21</sup> in progress on a binary mixture

(water-triethylamine) has permitted a determination of  $a_C/a_x$  as

$$\frac{a_c^+}{a_x^+} = 7.9 \pm 1.2 \quad . \tag{4.3}$$

This result is in a very good agreement with ours.

- <sup>1</sup>See, for example, F. J. Wegner, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. VI.
- <sup>2</sup>See, for example, L. P. Kadanoff, in *Critical Phenomena*, edited by M. S. Green (Academic, New York, 1971).
- <sup>3</sup>A. Aharony and P. C. Hohenberg, Phys. Rev. B <u>13</u>, 3081 (1976).
- <sup>4</sup>C. Bervillier, Phys. Rev. B <u>14</u>, 4964 (1976).
- <sup>5</sup>A. Aharony and G. Ahlers, Phys. Rev. Lett. <u>44</u>, 782 (1980); and see also G. Ahlers, Rev. Mod. Phys. <u>52</u>, 489 (1980).
- <sup>6</sup>B. G. Nickel (unpublished).
- <sup>7</sup>M. Ferer, Phys. Rev. B <u>16</u>, 491 (1977) (for d = 3, n = 1).
- <sup>8</sup>D. S. Ritchie and D. D. Betts, Phys. Rev. B <u>11</u>, 2559 (1975) (for d = 2).
- <sup>9</sup>E. Brézin, J. C. Le Guillou, and J. Zinn-Justin, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. VI.
- <sup>10</sup>M. C. Chang and A. Houghton, Phys. Rev. Lett. <u>44</u>, 785 (1980); and Phys. Rev. B 21, 1881 (1980).
- <sup>11</sup>G. Parisi (unpublished); J. Stat. Phys. <u>23</u>, 49 (1980).

- <sup>12</sup>B. G. Nickel, D. I. Meiron, and G. A. Baker, Jr. (unpublished).
- <sup>13</sup>J. C. Le Guillou and J. Zinn-Justin, Phys. Rev. B <u>21</u>, 3976 (1980).
- <sup>14</sup>K. G. Wilson and K. Kogut, Phys. Rep. C <u>12</u>, 75 (1974); A. Aharony, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. VI and other papers in this volume.
- <sup>15</sup>J. Zinn-Justin (unpublished).
- <sup>16</sup>It is useful to note that for the leading amplitudes, universal combinations follow the relation  $dU/du \simeq \lambda^{\omega} (\tilde{A}_1/A_1)^{\omega}$ .
- <sup>17</sup>G. A. Baker, Jr., B. G. Nickel, and D. I. Meiron, Phys. Rev. B <u>17</u>, 1365 (1978).
- <sup>18</sup>C. Bervillier and C. Godrèche, Phys. Rev. B <u>21</u>, 5427 (1980).
- <sup>19</sup>E. Brézin, J. C. Le Guillou, and J. Zinn-Justin, Phys. Rev. D <u>15</u>, 1544 (1977).
- <sup>20</sup>J. Rogiers, M. Ferer, and E. R. Scaggs, Phys. Rev. B <u>19</u>, 1644 (1979).
- <sup>21</sup>A. Bourgou and D. Beysens (unpublished).