Classical-to-critical crossovers from field theory

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We extend the previous determinations of nonasymptotic critical behavior of Phys. Rev B32, 7209 (1985) and B35, 3585 (1987) to accurate expressions of the complete classical-to-critical crossover (in the 3-d field theory) in terms of the temperature-like scaling field (i.e., along the critical isochore) for: 1) the correlation length, the susceptibility and the specific heat in the homogeneous phase for the \( n \)-vector model (\( n = 1 \) to 3) and 2) for the spontaneous magnetization (coexistence curve), the susceptibility and the specific heat in the inhomogeneous phase for the Ising model (\( n = 1 \)). The present calculations include the seventh loop order of Murray and Nickel (1991) and closely account for the up-to-date estimates of universal asymptotic critical quantities (exponents and amplitude combinations) provided by Guida and Zinn-Justin [J. Phys. A31, 8103 (1998)].

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I. INTRODUCTION

The asymptotic critical behavior, characterized by universal quantities (exponents and amplitude combinations), is now theoretically well established \([6,7]\) with accuracy \([\Box]\). However, the comparison of the theoretical results with experimental or numerical data is made easier when the theoretical expressions are extended into regimes where the asymptotic pure scaling breaks down \([\Box]\) (calculations done far away from the critical point, characterized by nonuniversalities and including eventually crossover phenomena, see reviews \([\Box]\)). This extension has appeared necessary notably when measurements on colloids \([\Box]\), but also on complex systems such as ionic fluids \([\Box]\) or polymers \([\Box]\), seemed to yield strong nonuniversalities in approaching the critical point. Indeed theoretical studies have suggested that, in some cases, those nonuniversalities could be due to a phenomenon of “retarded criticality” which characterizes measurements done outside the asymptotic critical domain \([\Box]\). Several recent theoretical (and/or numerical) studies have as well explicitly considered the evolution of effective exponents with emphasis on their monotonic or non-monotonic character \([\Box]\). Furthermore the description of the classical-to-critical crossover for Ising systems is not yet clear-cut \([\Box]\). For these reasons and because our preceding determination of nonasymptotic critical behavior from field theory \([\Box]\) did not yield continuous functions covering an entire crossover region, it seems to us useful to consider again those calculations in order to (see also \([\Box]\)):

1. extend them to a complete account of the classical-to-critical crossover which characterizes the framework of field theory \([\Box]\).

2. include the seventh order series for the critical exponents determined by Murray and Nickel \([\Box]\) in order to account as closely as possible for the up-to-date estimates of universal asymptotic critical quantities (exponents and amplitude combinations) provided by Guida and Zinn-Justin \([\Box]\) (referred to in the following as GZ).

In the previous work \([\Box]\), and contrary to an initial attempt \([\Box]\) regarding the homogeneous phase (\( n = 1 \)), we provided only continuous expressions of \( t \) valid for \( t \lesssim 10^{-2} \) (\( t \) is the temperature-like scaling field which is proportional to the absolute value of the reduced critical temperature \([T - T_c]/T_c\)). The crossover was not completely described because it was thought at that time that the field theoretical framework had a range of validity strictly limited to the first correction to scaling term. Consequently, the practical limit of physical validity of the functions was imposed by the range of \( t \) where the second correction to scaling term specific to field theory becomes non negligible and this occurs \([\Box]\) about \( t \simeq 10^{-2} \). Since then, it has appeared that the range of validity of field theory could be much larger

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than that and even could cover the entire classical-to-critical crossover region [16] that it describes. Somehow it is interesting to give expressions valid in the entire crossover region if only because it may be compared to other kinds of classical-to-critical crossovers either experimental [11] or from numerical studies [11,20,22,29,30] which, under some particular conditions, are identical [18,34,23,1] to the field theoretical form (but see also our comment in [23]).

For technical reasons, in the preceding work [13,14] we did not constrain our theoretical expressions to include very closely the estimates of universal asymptotic quantities of that time (with their error bars) so that uncertainties were underestimated and then our estimates of the correction amplitude ratios were, presumably, also not firmly determined. Moreover small errors existed in the preceding study of the inhomogeneous phase [10] (as indicated elsewhere [18,34,23,1]) which have been eliminated from the present work (nevertheless, we have explicitly verified (see fig. 1 of ref. [33]) that the errors have had no important consequence on the final results as it could be clearly deduced from a comparison of our estimates of universal amplitude-combinations [7] with those of Guida and Zinn-Justin [34,3]).

II. PRINCIPLE OF THE CALCULATIONS

A. Brief reminder

As in the preceding work [13,14], and using the same resummation method, we have considered the correlation length \( \xi (t) \) (in the homogeneous phase \( T > T_c \) for the \( n \)-vector model with \( n = 1 \) to 3), the susceptibility \( \chi (t) \) and the specific heat \( C(t) \) (in the homogeneous phase \( T > T_c \) with \( n = 1 \) to 3 and in the inhomogeneous phase \( T < T_c \) with \( n = 1 \)) and the coexistence curve (spontaneous magnetization) \( M(t) \) (in the inhomogeneous phase with \( n = 1 \)).

For practical reasons, it is useful to fix our notations relative to the actual asymptotic critical behaviors (i.e., in terms of the physical variable \( \tau = \frac{T - T_c}{T_c} \rightarrow 0^\pm \) instead of \( t \rightarrow 0 \), see also section [13,14]):

\[
\xi (\tau) = \xi_0^\pm |\tau|^{-\nu} \left[ 1 + a_\xi^\pm |\tau|^\Delta + O (|\tau|^{2\Delta}) \right] \tag{1a}
\]

\[
\chi (\tau) = \Gamma^\pm |\tau|^{-\gamma} \left[ 1 + a_\chi^\pm |\tau|^\Delta + O (|\tau|^{2\Delta}) \right] \tag{1b}
\]

\[
C (\tau) = \frac{A^\pm}{\alpha} |\tau|^{-\alpha} \left[ 1 + a_C^\pm |\tau|^\Delta + O (|\tau|^{2\Delta}) \right] + B_{cr} \tag{1c}
\]

\[
M (\tau) = B |\tau|^\beta \left[ 1 + a_M |\tau|^\Delta + O (|\tau|^{2\Delta}) \right] \tag{1d}
\]

in which \( \alpha, \beta, \gamma \) and \( \nu \) are the critical exponents, \( \Delta \) (also denoted by \( \theta = \omega \nu \) by GZ) is the correction exponent, \( \xi_0^\pm, \Gamma^\pm, A^\pm \) and \( B \) are the leading critical amplitudes and \( a_\xi^\pm, a_\chi^\pm, a_C^\pm, a_M \) are the (confluent) first-correction amplitudes, finally \( B_{cr} \) is a critical background. One usually restricts the consideration of the critical singularities to small values of \( t \propto |\tau| \) as it is implicitly assumed in Eqs. (1). The obtention of nonasymptotic critical behavior supposes the explicit consideration of non-necessarily small values of \( t \).

Let us suppose that we want to calculate the susceptibility \( \chi \) as function of the (non-necessarily small) temperature-like scaling field \( t \). Calculations of such a nonasymptotic critical behavior from (the massive) field theory (in three dimensions) [3,7] present the following features (additional details may also be found elsewhere [3,7]):

1. the function \( \chi(t) \) is primarily performed under the implicit form because the quantities \( \chi \) and \( t \) are primarily given as perturbation series in powers of the renormalized coupling parameter \( g \) (up to fifth [36] or sixth [17] order): the functions \( \chi(g) \) and \( t(g) \) are resummed for \( g \) varying in the range \( [0, g^*] \) where \( g^* \) is the zero of the Wilson function (or the “\( \beta \)-function”) \( W(g) \) also primarily given as power series of \( g \) (up to sixth order [37]: \( g^* \) is the fixed point value of \( g \)).

2. The consideration of discontinuous values of \( g \) is a compelling need of the numerical resummation procedure. Consequently fitting an ad hoc function of \( t \) to the calculated points eliminates the auxiliary variable \( g \) and provides us with the final expression of \( \chi(t) \) as the explicit continuous function of \( t \) we are looking for in the range \( |t| \in [0, +\infty[ \).

3. The actual calculation of the quantities of interest \( [\chi(g)] \) for values of \( g \) close to \( g^* \), at which point they are singular (due to the critical singularity we expect to closely reproduce), requires expressing them under an integral representation like:

\[
\chi(g) = \chi(y_0) \exp \left[ - \int_{y_0}^{g} dx \frac{\gamma(x)}{v(x) W(x)} \right] \tag{2}
\]
in which \( \gamma (g) \) and \( v (g) \) are not singular at \( g^* \) and are primarily given as power series of \( g \) (up to seventh order \( 28 \)). Especially, \( \gamma (g^*) \) and \( v (g^*) \) provide the field theoretical estimates of the critical exponents \( \gamma \) and \( \nu \). Only the elementary series \( \gamma (g) \), \( v (g) \) and \( W (g) \) are resummed using the sophisticated method mentioned in the following step [the value \( y_0 \) is chosen small enough to allow a direct simple summation of the series \( \chi (y_0) \)].

4. To sum perturbation series like \( \gamma (g) \), \( v (g) \) or \( W (g) \) for a given value of \( g \) a Borel–Leroy transformation is used, combined with a conformal mapping. An estimation of the error is deduced from the observation of the convergence properties of the series when varying the free parameters of the transformation. This leads us to fix those parameters (resummation criteria) in such a way as to obtain a combination of the error bounds on e.g., \( \gamma (g) \), \( v (g) \) and \( W (g) \) which gives a kind of envelope for \( \chi (g) \) via two functions \( \chi_{\text{max}} (g) \) and \( \chi_{\text{min}} (g) \) (and similarly for \( t (g) \)).

5. Since the critical singularities are similar in the two phases of the transition, the calculations in the inhomogeneous phase \( (T < T_c) \) do not require the consideration of new series for the exponents compared to the homogeneous phase \( (T > T_c) \). Hence the same three series \( \gamma (g) \), \( v (g) \) and \( W (g) \) express the critical singularities via integrals similar to that given in \( 2 \), only new critical amplitude functions of \( g \) (hence not singular at \( g^* \)) must be calculated \( 26 \) and summed using the transformation mentioned in step \( 3 \).

B. Improvements to the previous work and presentation of the results

1. The fitting procedure

In the present work, the fitting procedure of step \( 2 \) of section \( \text{II.A} \) is performed in the entire range of values of \( g \in [0, g^*] \). Consequently the entire classical-to-critical crossover specific to the field theoretical framework is completely accounted for by our final functions [see Eqs. \( (3) \) and tables \( \text{I–IV} \)]. This is illustrated, for the Ising model \( (n = 1) \), by fig. \( \text{I} \) which displays the evolution of two effective exponents \( \gamma_{\text{eff}} (t) \) and \( \alpha_{\text{eff}} (t) \), which are defined as for example [see Eqs. \( (3) \)]:

\[
\gamma_{\text{eff}} (t) = - \frac{d \ln \chi (t)}{d \ln t}
\]

(3)

Fig. \( \text{I} \) shows the effective exponents (calculated from the crossover functions of tables \( \text{I} \) and \( \text{II} \)) which interpolate between critical and classical (mean field) values following a form of crossover dictated by the framework of field theory. Indeed the (massless or critical, i.e., for \( t = 0 \)) scalar field theory in three dimensions is defined on a special trajectory of the renormalization group (a renormalized trajectory \( 26 \) [RT]) which takes its origin at the Gaussian fixed point (characterized by classical values of the “critical” exponents) and joins the Wilson-Fisher fixed point (where the critical exponents take on their critical values according to the universality class considered). Of course, the crossover so induced is not universal, it is specific of the framework used. In fact, strictly speaking, only the extreme asymptotic moving away from the Wilson-Fisher fixed point induced by small non-zero values of \( t \) is universal (critical exponents and critical amplitude combinations), even the first-correction amplitude (defined in the close vicinity of the fixed point when \( t \) is not very small) is not universal. For example, in the present work, a specific definite sign of the first correction amplitude is imposed due to the RT chosen, however in actual systems that kind of correction may well be of the opposite sign and even absent \( 12 \). Fortunately, nonuniversal does not mean necessarily absent in actual critical behaviors. It may well occur that actual systems (or models) display, more or less partially, the kind of crossover behaviors. It may well occur that actual systems (or models) display, more or less partially, the kind of crossover behaviors. It may well occur that actual systems (or models) display, more or less partially, the kind of crossover behaviors.
in which $\Delta$ is the correction exponent. We have adjusted each of the parameters $Z$, $e$, $\{X_i, Y_i\}$ ($i = 1, \cdots, K$), $S_1$, $S_2$, $X_6$ and $\Delta$ so as to fit the discretized evolutions of the quantities considered ($\xi$, $\chi$, $C$, $M_S$) as continuous functions of the temperature-like variable $t$ in the range $t \in [10^{-17}, 10^{14}]$. Of course, there are some external constraints on the values of these parameters which facilitate their adjustment:

1. The exponents $e$ and $\Delta$ must take on values already known from the resummation of the corresponding elementary series.

2. The amplitude $Z$ is easily determined with few points corresponding to very small values of $t$.

3. To make it easy to get a close reproduction of the crossover towards the classical behavior when $t \to \infty$, there are constraints:
   - on $S_1$, so that we have (see, for example, Eqs. (A9, A10) of S. Caracciolo et al. [21]):
     \[
     D(t) \rightarrow_{t \to \infty} \frac{1}{2}
     \]
     this leads to:
     \[
     S_1 = S_2 \left(\frac{3}{2} - \Delta\right)
     \] (7)
   - on one of the couple $\{X_i, Y_i\}$’s by imposing that a known classical behavior is reached in the limit $t \to \infty$ then it comes:
     \[
     e + \frac{1}{2} \sum_{i=1}^{K} Y_i = e_c
     \] (8)
     \[
     Z \prod_{i=1}^{K} (X_i)^{Y_i} = Z_c
     \] (9)
     with $e_c$ and $Z_c$ the classical values of the critical exponents and amplitude respectively. This leads to the constraints for one of the $\{X_i, Y_i\}$’s:
     \[
     Y_{i_0} = 2(e_c - e) - \sum_{i \neq i_0} Y_i
     \] (10)
     \[
     X_{i_0} = \left[\frac{Z_c}{Z} \prod_{i \neq i_0} (X_i)^{-Y_i}\right]^{1/Y_{i_0}}
     \] (11)
     with the classical values $e_c = 1, \frac{1}{2}, \frac{1}{2}$ or 0 and $Z_c = 2, 1, \sqrt{6}$ or $B_c - X_6$ for respectively the susceptibility, the correlation length, the coexistence curve and the specific heat [$X_6$ is the additive critical part of the specific heat and $B_c$ its classical value; $B_c = 3$ in the inhomogeneous phase ($T < T_c$), while $B_c = 0$ in the homogeneous phase ($T > T_c$)].

With the above prescriptions, we have been able to reproduce the original calculated points with a maximum (local in $t$) of relative deviation less than $10^{-4}$ (in the worst case and for a limited number of functions especially in the inhomogeneous phase). However, globally (mean value of the local deviations over the entire range of $t$), the adjustment is much better for all the quantities.

The results of those adjustments to the discrete calculated points are given in tables I–IV.

We emphasize that the large number of digits displayed in the tables lays no claim to a better accuracy than in the work of GZ, it is simply required to obtain a careful fit of the crossover functions to the discontinuous points primarily calculated from the available perturbative series.
2. The resummation criteria

In our preceding work \[\text{[6,7]},\] the resummation criteria of step \[3\] of section \[\Pi A\] which gave the bounds “max” and “min” were not chosen so as to closely reproduce the uncertainty of the (at that time up-to-date) estimates of universal asymptotic critical quantities (exponents and amplitude combinations). They simply proceeded from a primary analysis of the convergences of the elementary series \[\text{i.e., } \gamma (g), \nu (g), \text{ etc.} \ldots\] resulting from the (unique) resummation technique considered. This makes a notable difference because a given function brings several elements into play [see, e.g., Eq. \((3)\)] introducing a possible frustration of the individual resummation criteria. Moreover, when one determines the error bar for an individual quantity, one often rounds it up because several resummation methods may have been considered yielding answers slightly different from each other. Since the various asymptotic critical behaviors of the functions of interest \((\chi (t), \text{ etc.} \ldots)\) result from the combination of a small number of elementary series \[\text{[39]}\] (namely: \(\gamma (g), \nu (g), W (g) \text{ and a few amplitude functions}), the individual criteria were combined in our preceding work \[\text{[6,7]}\] so as to provide an envelope of the error accounting automatically for correlations (frustrations) between the error bounds. This has induced some underestimation of the errors when the universal critical exponents or amplitude combinations were (re)-considered from the final expressions of the functions compared to their independent estimates.

The spirit of the present work is different. We have constrained the resummation criteria of the elementary series so as to get as closely as possible the GZ estimates for the universal quantities despite the possible frustrations of the error bounds mentioned above. Thus we have taken into account the extensions up to seven loops of the series for the critical exponents given by Murray and Nickel \[\text{[28]}\]. For the reasons indicated just above, and also because the error estimates of the amplitude combinations of GZ are deduced from the analysis of the parameter dependence in the equation of state \[\text{[34]}\] (they have not been obtained from the direct analysis of specific series for the quantities of interest), we have encountered some difficulties in fixing the resummation criteria for some amplitude series (it is likely that GZ have overestimated the error for some quantities). In addition, in doing so and concerning the amplitudes we have introduced an imbalance between the error estimates of the two phases. Indeed our criteria are adjusted so as to get universal ratios (or combinations) of amplitudes which, structurally in the present work, express themselves as series strictly defined in the inhomogeneous phase. On the contrary, the resummation criteria in the homogeneous phase (for only one amplitude function) have been fixed without constraint. Consequently, the resulting error estimates of the correction amplitudes that we presently obtain are larger than in the previous work of refs. \[\text{[6,7]}\] and notably in the inhomogeneous phase case; they are presumably overestimated (see below and part \[\Pi B\]).

Table \[\text{[III]}\] shows our estimates of the critical exponents (resulting from our resummation criteria) compared to the GZ estimates. One may observe some very small differences due to the fact that, in the present work, the scaling relations are automatically satisfied for each bound “max” or “min” (see step \[3\] of section \[\Pi A\]) while only the central values of the GZ exponent estimates satisfy the scaling relations (the apparent errors for \(\gamma, \nu, B\) have been determined independently \[\text{[3]}\]). Table \[\text{[III]}\] shows how much the respective estimates meet the scaling relations in both cases. Tables \[\text{VI} \text{ and VII}\] display the values of the universal combinations of leading critical amplitudes as they are accounted for by our crossover functions. The degree of agreement with GZ is graphically illustrated by figs \[\text{[III]}\].

From tables \[\text{[IV}, \text{V}\] one may observe that our bounds on the correction exponent \(\Delta\) differ from GZ. This is due to the correlation of errors mentioned above. Indeed, we have never considered \(\Delta\) as an independent constituent of the asymptotic critical behavior. Instead it has been (numerically) deduced from the resummation criteria associated with the elementary series \(\nu (g)\) and \(W (g)\) because of the definition \(\Delta = \omega \nu\) with:

\[
\omega = \frac{dW (g)}{dg} \bigg|_{g=g^*} \quad \nu = \nu (g^*)
\]

The resummation criteria for the elementary series \(W (g)\) have been chosen so as to yield estimates on the bounds on \(g^*\) very close to those of GZ (see table \[\text{VIII}\]).

Similarly, the present determinations of \(\Delta\) (and the uncertainties on) the first correction-to-scaling terms displayed in tables \[\text{IX} \text{ and X}\] differ from our preceding work \[\text{[6,7]}\] essentially because of our systematic account for the up-to-date estimates of the leading amplitude combinations (see tables \[\text{VI} \text{ and VII}\]). Notice the likely unrealistic smallness of the correction amplitude \(a_M\) in the case “min”. This confirms our probable overestimation of the error on the correction terms (see part \[\Pi B\]).

It is worth indicating that the values displayed in tables \[\text{IX} \text{ and X}\] are not obtained from the crossover functions of tables \[\text{[IV}, \text{V}\] by simply using the expression [see Eq. \((3)\)]:

\[
a_F = \sum_{i=1}^{K} X_i Y_i
\]

5
which would be the right expression if the correction exponent in Eq. (4) was the actual correction exponent $\Delta$ instead of the effective exponent $D(t)$ of Eq. (5). To get the values displayed in tables IX and X we have made specific fits of the functions $F(t)$ of Eq. (4) to the theoretical points with $D(t) = \Delta$ in ranges of values of $t < 10^{-2}$ (as in the preceding work [5,6]).

III. PRACTICAL USE OF THE CROSSOVER FUNCTIONS

As already said above, the structural form of the classical-to-critical crossover that we produce here is not universal, it is peculiar to the field theoretical framework which corresponds to having performed a limit (the continuum limit) in the renormalization group (RG) theory [40]. The approximation induces the idea that, strictly speaking, the “nonasymptotic” calculations would, in fact, be only valid in the close vicinity of $T_c$. Hence, we do not expect our functions to reproduce the experimental data in the entire range $t \in [0, +\infty]$. However, the width $L$ of the domain of agreement between experiments and field theory is not universal: it could actually be reduced (purely and simply) to the strict asymptotic critical region (pure scaling laws) or include exclusively the first correction to scaling, but, fortunately it may sometimes be much larger and could even cover the entire crossover region! It is our aim to allow experimentalists to determine the width $L$ of the domain of agreement. Notice that, we do not aim at determining (or providing) all the ingredients needed to describe the variety of classical-to-critical crossovers that may be produced by actual systems, this would be too difficult (due to the infinite variety of nonuniversal contributions). Simply, we think our calculation accurate enough to allow the determination of $L$ for any system allowing, in some sense, the determination of subclasses of universality.

As already explained [5–7], the comparison of the theoretical functions with experimental data involves a very small number of adjustable parameters:

1. Non-universal global factors,

2. The proportionality factor $\theta$ between the temperature like scaling field $t$ and $\tau = \frac{T - T_c}{T_c}$ (neglecting higher analytical contributions in $\tau$ which may sometimes be non-negligible [10] but are out of the scope of our present aim):

$$t = \theta |\tau|$$  

(15)

3. Additive regular background terms for the specific heat,

4. Eventually $T_c$.

For example the comparison with experimental measurements of the susceptibility $\chi$ may be made as follows:

$$\chi_0 \chi_{th}(\theta |\tau|) = \chi_{exp}(|\tau|)$$  

(16)

in which $\chi_{exp}(|\tau|)$ represents the experimental data and $\chi_{th}(t)$ our function for one [41] of the two bounds “max” and “min”. One generally expects theoretically that $\chi_0$ and $\theta$ take on the same values [42] for the two sets of measurements above and below $T_c$ provided that the range of values of $\tau$ is not too large. The fact that $\chi_0$ must be unchanged is the consequence of the universality of the ratio $\frac{\Gamma_+}{\Gamma_-}$ with as $\tau \to 0$:

$$\chi_{exp}(|\tau|) \approx \Gamma_0^\pm |\tau|^{-\gamma} \left(1 + \Gamma_1^\pm |\tau|^{\Delta_\pm} + \cdots\right)$$  

(17)

in which $\Gamma_0^\pm$ and $\Gamma_1^\pm$ are related to our previous definition [Eq. (11)] as follows:

$$\Gamma_0^\pm = \chi_0 \theta^{-\gamma} \Gamma^\pm$$  

(18)

$$\Gamma_1^\pm = \theta^{-\Delta_\pm} a^\pm$$  

(19)

As for the stability of $\theta$ this is because the ratio $\frac{\Gamma_+}{\Gamma_-}$ is universal. The values of the universal amplitude combinations included in our calculated functions are given in tables VI, VII, IX and X.
A. Redefinition of the role of $\theta$

If one introduces $\theta$ literally as in Eq. (15), then the fitted leading critical amplitude involves two adjustable parameters. This is not very suitable. For practical use, we propose to introduce the adjustable parameters as follows (compare with eq (4)):

$$\chi_{\text{exp}}^{-1} (|\tau|) = \chi_0 \left[ Z |\tau|^\gamma \prod_{i=1}^K \left( 1 + X_i t^{D(t)} \right)^{Y_i} + X_6 \right]$$  \hfill (20)

t = \theta |\tau| \hfill (21)

in which $\theta$ is no longer involved in the pure scaling part of the critical behavior ($Z |\tau|^\gamma$). So introduced, $\theta$ is a nonuniversal parameter which exclusively controls the magnitude of the corrections to scaling. Hence we can progressively adjust the theoretical functions to the data starting from the data close to the critical point with $\theta = 0$ and then introducing more and more data with $\theta \neq 0$ (notice that $\theta \geq 0$) up to the point where consistency is lost.

The domain $\mathcal{L}$ of $\tau$ where the experimental data and the field theory agree may involve correction-to-scaling terms higher than the first one and this is why it is interesting to have the theoretical expression under the form of a complete classical-to-critical crossover \cite{14}.

Consistency test: If we consider a supplementary set of measurements like the specific heat above and below $T_c$, then, by virtue of universality, one must obtain again the same value for $\theta$ with a good fit in a range of values of $\tau$ similar to that considered with $\chi$. For the specific heat, it comes:

$$C_0 C_{th} (\theta |\tau|) + B_0 (\tau) = C_{\text{exp}} (|\tau|)$$  \hfill (22)

in which $B_0 (\tau)$ is an additive non critical (i.e., regular or analytic in $\tau$) background and $C_0$ a nonuniversal multiplicative factor which must be the same in the two phases.

Let us emphasize that the field theoretical form obtained for $C_{th} (t)$ involves a specific critical additive background term which reproduces the famous “classical jump” of the specific heat [see fig. \[4\)]. Of course, the magnitude of this jump is not universal but in the case where an actual system would reproduce the entire classical-to-critical crossover of field theory, then it should also exhibit this jump (up to the global additive background $B_0(\tau)$ analytic in $\tau$).

If, in addition to $C$ and $\chi$, we also possess coexistence curve data, we would have a stronger constraint since then no other adjustable parameter would be required to fit those new data. Indeed in the relation:

$$M_0 M_{th} (\theta |\tau|) = M_{\text{exp}} (|\tau|)$$  \hfill (23)

everything is fixed since $M_0$ is related to $C_0$ and $\chi_0$ due to the universal amplitude combination \cite{14} $R_C$ and $\theta$ must have the same value whatever the quantity considered.

If we had simultaneously also access to experimental measurements of the correlation length $\xi$, then the constraint would be even stronger since again the theory must agree with the data without new adjustable parameter.

In order to facilitate the use of the crossover functions displayed in table \[\[4\], text-files of Fortran code are provided \[\[15\].

B. Account for the error bounds

We have accounted for the error estimates by providing two sets (“max” and “min”) of functions. In general the accuracy of the experimental measurements are much smaller than in the present theoretical calculation so that it is not very important to make a difference between the two sets of functions. One or the other choice would provide essentially the same quality of the adjustment in the fitting procedure.

Sometimes accounting for the difference between the bounds “max” and “min” may have some importance so that neither one or the other agrees with the measurements but a mixing of the two would. In such a case we propose to introduce the mixing via the introduction of a supplementary adjustable parameter $E$.

Let us define a new theoretical function as follows

$$F_E (t) = [F_{\text{max}} (t)]^E \cdot [F_{\text{min}} (t)]^{1-E}$$  \hfill (24)

which, regarding the definition of the effective exponents corresponds to the linear weighting:

$$e_{\text{eff}} (t) = E \cdot e_{\text{eff}}^{\text{max}} (t) + (1 - E) \cdot e_{\text{eff}}^{\text{min}} (t)$$  \hfill (25)
then the introduction of the other adjustable parameters, such as $\theta$ for example, within $F_E(t)$ is unchanged compare
to the description given above.

As said in part it is likely that the close account of the GZ estimates has led us to overestimate the uncertainty on the correction terms so that it seems to us useful to provide also the reader with functions reproducing the complete classical-to-critical crossover according to the resummation criteria of the previous (but corrected, see work of refs although (or rather because), this time, the error are underestimated. This is why we provide two additional text-files of Fortran code corresponding to the former resummation criteria applied to the corrected series (without the seventh order of ref.).

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field theory at $d = 3$. II. The ordered-phase case” Phys. Rev. B35, 3585 (1987).”, hep-th/0006187.

[34] R. Guida and J. Zinn-Justin, Nucl. Phys. B489, 626 (1997).

[35] C. Bagnuls and C. Bervillier, in “Fluctuating Paths and Fields”, p. 401, Ed. by W. Janke, A. Pelster, H.-J. Schmidt, M. Bachmann (World Scientific, Singapore, 2001).

[36] C. Bervillier and C. Godrêche, Phys. Rev. B21, 5427 (1980).

[37] B. G. Nickel, D. I. Meiron and G. A. Baker, Jr., “Compilation of 2-pt and 4-pt graphs for continuous spin models”, Guelph University preprint, unpublished (1977). May be obtained via the web site http://www.physik.fu-berlin.de/~kleinert/kleinerreb8/programs/programs.html.

[38] J. H. Chen, M. E. Fisher and B. G. Nickel, Phys. Rev. Lett. 48, 630 (1982). C. Bagnuls and C. Bervillier, Phys. Rev. B41, 402 (1990); Phys. Lett. A195, 163 (1994). M. Hasenbusch, J. Phys. A34, 8221 (2001). M. Campostrini, M. Hasenbusch, A. Pelissetto, P. Rossi and E. Vicari, Int. J. Mod. Phys. Vol. A16, 2009 (2001). For negative corrections see also: A. Liu and M. E. Fisher, J. Stat. Phys. 58, 431 (1990). L. Schäfer, Phys. Rev. E50, 3517 (1994). A. D. Sokal, Europhys. Lett. 27, 661 (1994).

[39] That is precisely how universal combinations of amplitudes and scaling relations between exponents occur in the field theoretical framework.

[40] Only one family of corrections to scaling (controlled by the unique exponent $\Delta$) is accounted for.

[41] Or a combination of the two bounds see section IIIH.

[42] Generally speaking this is true, but $\theta$ may be nil because there exist systems which do not approach the Ising fixed point along the RG trajectory which links the Gaussian and Ising fixed points. For example some models may have correction-to-scaling terms strictly different from those accounted for by field theory. Also some may have “negative” correction-to-scaling terms. See [38].

[43] The comparison is made easier than with functions having a limited range of applicability.

[44] A. Aharony and P. C. Hohenberg, Phys. Rev. B13, 3081 (1976). C. Bervillier, Phys. Rev. B14, 4964 (1976).

[45] See EPAPS Document No. xxxxxxxxx. Two sets of two files each are provided: first, utdfns1.txt and utdfnsN.txt which contain the fortran code for the up-to-date crossover functions of respectively tables I and II (Ising like systems in the two phases) in one hand and tables III and IV ($n$-vector-like system in the homogeneous phase) in the other hand and second, functions1.txt and functionsN.txt which contain the fortran code for the preceding (corrected, see [33]) work of refs [6,7]. In each case the file contains its own instructions for use. This document may be retrieve via the EPAPS homepage (http://www.aip.org/pubservs/epaps.html) or from ftp.aip.org in the directory /epaps/. See the EPAPS homepage for more information.
FIG. 1. Respective evolutions (calculated from the crossover functions of tables I and II) of the effective exponents $\gamma_{\text{eff}}(t)$ and $\alpha_{\text{eff}}(t)$ in the two phases: the homogeneous (continuous line) and the inhomogeneous (dashed line) phases. Notice, in this latter case, the moving down of $\gamma_{\text{eff}}(t)$ below the classical value ($= 1.0$) in the regime of high values of $t$. This nonmonotonic feature of $\gamma_{\text{eff}}(t)$ in the inhomogeneous phase is in agreement with Refs. [18, 19] and has been numerically observed in Refs. [17, 20].
FIG. 2. The two bounds “max” (continuous lines) and “min” (short-dashed line) have been determined so as to reproduce as closely as possible the GZ estimates. This is illustrated here with the effective exponents calculated from the crossover functions for $n = 1$ determined in the present work (see tables I and II). For each exponent, a partial magnification (A) of the critical region is provided to show the agreement with the GZ estimates. A similar partial magnification (B) is also provided to show the difference with our preceding work of [6,7] (long-dashed lines). (For other values of $n$, see table V.)
FIG. 3. The two bounds “max” (continuous line) and “min” (short-dashed line), determined so as to reproduce as closely as possible the GZ estimates, account also for the universal amplitude combinations. This is illustrated here with the ratio $\Gamma^+/\Gamma^-$ [see Eq. (1b)] calculated from the crossover functions for $n = 1$ determined in the present work (see tables I, II and VI). The illustration could have been made as well with the two other universal quantities of table VI.
FIG. 4. The field theoretical form of the specific heat exhibits the classical “jump”.
TABLE I. Numerical values of the parameters of the generic crossover function $F(t)$ [Eqs. (4,5)] corresponding to the three quantities calculated in the homogeneous phase ($T > T_c$ and for $n = 1$): the correlation length $\xi$, the susceptibility $\chi$ and the specific heat $C$. For each parameter two values are provided which correspond to the bounds “max” (upper line) and “min” (lower line) of the error treatment. These bounds have been determined so as to reproduce as closely as possible the error estimates of GZ on the asymptotic universal quantities (see tables V and VI and text for more details) and provide the “$\min$” bounds of the error treatment. These bounds have been determined so as to reproduce as closely as possible the error estimates of GZ on the asymptotic universal quantities (see tables V and VI and text for more details) and provide two exclusive sets of functions $F_{\text{max}}$ and $F_{\text{min}}$. The first row of the table displays the estimate of the universal value of the leading critical amplitude $\alpha$ common to all the quantities for the respective bounds “max” and “min”. The values of the parameters have been determined by a careful adjustment of $F(t)$ to the discrete evolution of the respective quantities primarily calculated by resummation of perturbation series using a Borel-Leroy + conformal mapping method. The specific notations of the two leading parameters $\epsilon$ (universal critical exponent) and $Z$ (leading critical amplitude) are recalled for each quantity [see Eq. (1)]. The symbol “$-$” means that the term is absent.

| $n = 1$, homogeneous phase: $\Delta$ | “max”: 0.49862 | “min”: 0.50516 |
|-------------------------------------|-----------------|-----------------|
| $\xi^{-1}$                         | $\chi^{-1}$     | $C$             |
| $e$                                 | $\nu$           | $\gamma$       | $-\alpha$ | $-0.1049675$ | $-0.11271$ |
| $2.150817$                          | $2.091612$      | $3.75927$       | $3.660588$ | $1.871810$   | $1.580112$ |
| $S_1$                               | $32.24878$      | $34.05096$      | $30.37745$ | $33.65919$   |
| $S_2$                               | $32.20434$      | $34.00404$      | $30.33559$ | $33.83377$   |
| $X_1$                               | $10.48005$      | $2.853295$      | $31.94041$ | $3.476590$   |
| $Y_1$                               | $-0.5247187$    | $-0.31016527$   | $-2.547260 \times 10^{-2}$ | $0.2200185$ |
| $X_2$                               | $10.41513$      | $1.257832$      | $9.400643$ |
| $Y_2$                               | $28.75634$      | $11.51061$      | $7.017899$ |
| $X_3$                               | $0.3775152$     | $-8.204163 \times 10^{-3}$ | $-8.344217 \times 10^{-3}$ | $-9.616869 \times 10^{-3}$ |
| $Y_3$                               | $2.315848$      | $8.313963$      | $33.06508$ |
| $X_4$                               | $2.014284$      | $30.25994$      | $0.2462918$ |
| $Y_4$                               | $-1.307939 \times 10^{-2}$ | $-0.163456$ | $-3.258311$ |
| $X_5$                               | $39.95028$      | $-0.1745266$    | $-7.002609 \times 10^{-5}$ |
| $Y_5$                               | $53.07176$      | $-0.072117 \times 10^{-2}$ | $1.508835 \times 10^{-2}$ | $-4.048544$ |
| $X_6$                               | $-0.1030731$    | $-3.027917 \times 10^{-2}$ | $-3.548035$ |
TABLE II. Same as table I for the coexistence curve $M_S$, the susceptibility $\chi$ and the specific heat $C$ calculated in the inhomogeneous phase ($T < T_c$ and for $n = 1$). Notice that for each bound, the critical exponents $\gamma$, $\alpha$ and the subcritical exponent $\Delta$ take on the same values as in table I (as it must according to the theory). An indication on the accuracy of the $X$ value as in table I and differs slightly for the bound "max".

\[
\begin{array}{cccc}
\text{M}_S & \chi^{-1} & C \\
\hline
\varepsilon & \beta & 0.3270735 & 1.2408875 & -0.1049675 \\
& 0.3244954 & 1.239830 & -0.11271 \\
Z & B & 0.93804691 & 18.386609 & 3.3664988 \\
& 0.93700952 & 17.160196 & 3.048086 \\
S_1 & & 35.738988 & 2.3395295 & 1.6036462 \\
& & 11.312578 & 231.57111 & 4.7885026 \\
S_2 & & 35.689736 & 2.3363054 & 1.6014362 \\
& & 11.371253 & 232.78025 & 4.8133395 \\
X_1 & & 303.21696 & 76.549557 & 79.538017 \\
& & 241.51662 & 23.010983 & 123.82899 \\
Y_1 & & -1.7687565 \times 10^{-3} & -3.4865628 & 7.8643478 \times 10^{-2} \\
& & -5.7056933 \times 10^{-2} & 0.88915951 & -0.26171236 \\
X_2 & & 9.3779630 & 59.838911 & 4.0631542 \times 10^{-2} \\
& & 13.371447 & 61.975912 & 0.42099375 \\
Y_2 & & 0.17204103 & -16.395572 & 9.152242 \times 10^{-5} \\
& & 0.20926322 & 4.0096724 & -3.6312569 \times 10^{-3} \\
X_3 & & 1.3921229 & 3.6904512 & 16.574905 \\
& & 248.39869 & 316.29079 & 10.791900 \\
Y_3 & & 6.0877711 \times 10^{-3} & 4.7894058 \times 10^{-2} & -0.28063252 \\
& & -7.7226529 \times 10^{-3} & -0.15361387 & 7.2072941 \times 10^{-2} \\
X_4 & & 30.597947 & 63.029796 & 14.361662 \\
& & 82.917148 & 50.582996 & 86.921949 \\
Y_4 & & 0.17144092 & 19.215714 & 0.13070258 \\
& & 0.15795660 & -5.2595105 & 0.41499782 \\
X_5 & & 6.3064180 & 9.3807398 & 19.477188 \\
& & 4.7939978 & 2.5999921 & 0.57982484 \\
Y_5 & & -1.9479626 \times 10^{-3} & 0.13675156 & 0.28112994 \\
& & 4.8568967 \times 10^{-2} & 3.7692433 \times 10^{-2} & 3.6928566 \times 10^{-3} \\
X_6 & & -4.0481532 & -3.5480350 & \\
\end{array}
\]
TABLE III. Same as table I for the correlation length $\xi$, the susceptibility $\chi$ and the specific heat $C$ calculated in the homogeneous phase ($T > T_c$ and for $n = 2$). Comparing with tables II and IV one may notice the correlation of the value of the parameter $X_6$ (the critical background of the specific heat) with the values of leading amplitude $A^+ / \alpha$ and of $\alpha$: when $\alpha$ vanishes, $A^+$ and $\alpha X_6$ take on opposite values so as to transform the power law behavior $|t|^{-\alpha}$ into the logarithmic singularity $\ln|t|$.

| $n = 2$, homogeneous phase: $\Delta$ | $\max$: 0.52551 | $\min$: 0.52986 |
|-------------------------------------|----------------|----------------|

| $\xi^{-1}$ | $\chi^{-1}$ | $C$ |
|------------|-------------|-----|
| $c$        | $\nu$       | $\gamma$ | $-\alpha$ | $A^+$ / $\alpha$ |
| 0.67181082 | 0.66878932  | 1.3188985 | $-\alpha$ | $1.5440 \times 10^{-2}$ |
| 2.6289918  | 2.5496125   | 5.5612909 | $\frac{A^+}{\alpha}$ | $-55.881907$ |
| $Z_n$ (or $\xi_0^{-1}$) | $\left(\Gamma^+\right)^{-1}$ | 5.3464216 | $\frac{A^+}{\alpha}$ | $-121.13056$ |
| $S_1$      | 15.963748   | 96.831346 | 4.0480920 |
|            | 33.474847   | 60.160224 | 28.884078 |
| $S_2$      | 16.381644   | 99.366178 | 4.1540622 |
|            | 34.505171   | 62.011900 | 29.773102 |
| $X_1$      | 28.529734   | 16.310867 | 1.1911602 |
|            | 111.52736   | 11.716728 | 37.837491 |
| $Y_1$      | $-9.0963764 \times 10^{-2}$ | $-0.57358194$ | $5.5704053 \times 10^{-2}$ |
|            | $-2.8491431 \times 10^{-2}$ | $-4.1213479 \times 10^{-2}$ | $3.5434706$ |
| $X_2$      | 9.1112497   | 3.6615694 | 1.2675164 |
|            | 13.427180   | 15.104245 | 59.951524 |
| $Y_2$      | $-0.22311836$ | $5.6950360 \times 10^{-2}$ | $-5.8499557 \times 10^{-2}$ |
|            | $-15.783043$ | $-0.53630510$ | $-1.7677012 \times 10^{-2}$ |
| $X_3$      | 0.11326011  | 0.32669257 | 27.562173 |
|            | 24.100833   | 3.1051883 | 1.3847300 |
| $Y_3$      | $3.8347877 \times 10^{-4}$ | $-4.8535318 \times 10^{-4}$ | $-7.7243929 \times 10^{-3}$ |
|            | $1.8612028 \times 10^{-3}$ | $-3.8536260 \times 10^{-2}$ | $2.2769060 \times 10^{-4}$ |
| $X_4$      | 72.907613   | 430.16727 | 46.806723 |
|            | 13.360107   | 239.95179 | 37.714084 |
| $Y_4$      | $-5.0166740 \times 10^{-2}$ | $-6.7793463 \times 10^{-3}$ | $-2.0360103 \times 10^{-2}$ |
|            | $15.603262$ | $-1.3735564 \times 10^{-2}$ | $-3.5387612$ |
| $X_5$      | 10.299474   |    —     |    —     |
|            | 7.396058    |    —     |    —     |
| $Y_5$      | $2.0243740 \times 10^{-2}$ |    —     |    —     |
|            | $-0.13116817$ |    —     |    —     |
| $X_6$      |    —     |    —     | 50.158572 |
|            |    —     |    —     | 115.95104 |
TABLE IV. Same as table I for the correlation length $\xi$, the susceptibility $\chi$ and the specific heat $C$ calculated in the homogeneous phase ($T > T_c$ and for $n = 3$).

\[ n = 3, \text{homogeneous phase: } \Delta \begin{array}{c} \text{"max": 0.55227} \\ \text{"min": 0.55702} \end{array} \]

| $\xi^{-1}$ | $\chi^{-1}$ | $C$ |
|------------|-------------|-----|
| $c$        | $\nu$       | $\gamma$ | $-\alpha$ | 0.132720 |
| 0.71090629 | 0.70856062  | 1.3946000 | 1.3845100 | 0.11143582 |
| $Z$        | $(\xi^+)^{-1}$ | $(\Gamma^+)^{-1}$ | $\Delta^+$ | $-20.228436$ |
| 3.1722403  | 2.9632572   | 7.9856105 | 7.2687650 | $-18.976690$ |
| $S_1$      | $\frac{1}{10}$ | 31.477107 | 72.301387 | 17.216585 |
| 78.590543  | 52.048362   | 33.213159 | 76.289014 | 18.166416 |
| $S_2$      | $\frac{1}{10}$ | 83.342746 | 55.195616 | 102484.48 |
| $X_1$      | 394.95293 | 13.735280 | 389.17897 |
| 10.931307  | 0.15890396 | $-5.2545625 \times 10^{-3}$ | $-0.75390860$ | $-3.0498190 \times 10^{-3}$ |
| $Y_1$      | 16.025379  | 1.1525134 \times 10^{-3} | 0.19945718 |
| 0.15078920 | 1.3616777  | 4.7607464 \times 10^{-2} |
| $X_2$      | 3.2123716  | 11.028433 | 1179.5468 |
| 2.8641031 \times 10^{-3} | 0.46960131 | $-4.7495792 \times 10^{-2}$ | $3.2528813 \times 10^{-4}$ |
| $X_3$      | 11.387266  | 1.3862969 | 12.991689 |
| 505.9921   | 12.528570  | $-0.35982658$ | $-0.49056204$ | $-0.16565010$ |
| $X_4$      | 78.0895588 | 437.65747 | 65.185231 |
| 11.021201  | 312.81912  | $-5.6692560 \times 10^{-2}$ | $-1.4330672 \times 10^{-2}$ | $-0.10948246$ |
| $Y_4$      | 16.378555  | $-1.8816147 \times 10^{-2}$ | $-0.35127870$ |
| 0.19582193 | 2.8188361  | 0.97748668 | 11.698778 |
| $Y_5$      | $-2.9029786 \times 10^{-3}$ | $-7.8502947 \times 10^{-3}$ | 1.2417093 \times 10^{-2} |
| $X_6$      | —          | —          | 8.2684338 |
|           | —          | —          | 9.1558605 |
TABLE V. Above: Values of the (universal) critical exponents as they are accounted for by the crossover functions defined in tables I–IV. The numbers given in parenthesis correspond to the GZ respective error-bound estimates. Below: the scaling relations structurally satisfied for each bound of the crossover functions defined in tables I–IV (the expected theoretical values are zero). Due to the practical necessity of using a small number of predefined criteria in the (unique) resummation method used, the scaling relations are (automatically) better satisfied in the present work than in the final upper and lower bounds of GZ (the numbers in parenthesis correspond to their bound estimates which have not particularly been determined so as to satisfy the scaling relations).

| n  | γ         | ν         | α          | β          |
|----|-----------|-----------|------------|------------|
| 1  | 1.240875  | 0.631678  | 0.1049675  | 0.3270735  |
|    | (1.2409)  | (0.6317)  | (0.105)    | (0.3272)   |
|    | 1.23830   | 0.6290975 | 0.11271    | 0.3244954  |
|    | (1.2383)  | (0.6291)  | (0.113)    | (0.3244)   |
| 2  | 1.3188985 | 0.67181082| −0.01544   | −0.00637   |
|    | (1.3189)  | (0.6718)  | (−0.015)   | (−0.007)   |
|    | 1.3148952 | 0.66878932| −0.013270  | −0.00637   |
|    | (1.3149)  | (0.6688)  | (−0.132)   | (−0.007)   |
| 3  | 1.39460   | 0.71090629| −0.13270   | −0.11143582|
|    | (1.3945)  | (0.7108)  | (−0.132)   | (−0.112)   |
|    | 1.38451   | 0.70381062| −0.11143582| −0.11143582|
|    | (1.3845)  | (0.7038)  | (−0.112)   | (−0.112)   |

TABLE VI. Values of universal combinations of leading critical amplitudes for thermodynamic quantities combining calculations in the two phases, hence for \( n = 1 \) only (from the crossover functions of tables I and II). The two superposed numbers correspond to the respective bounds “max” (upper line) and “min” (lower line). In parenthesis are the respective bounds of the GZ estimates.

| A' / A- | \( \Gamma^+ / \Gamma^- \) | \( R^+_x = A^+ \Gamma^+ / B^2 \) |
|---------|---------------------------|----------------------------------|
| 0.55601 (0.556) | 4.89100 (4.89) | 0.05940 (0.0594) |
| 0.51826 (0.518) | 4.68783 (4.69) | 0.05541 (0.0554) |

TABLE VII. Values of the universal quantity \( R^+_x = \xi_0 a \binom{A^+}{3} \) combining calculations in the homogeneous phase only, hence for three values of \( n \) (from the crossover functions of tables I, III and IV). The two superposed numbers correspond to the respective bounds “max” (upper line) and “min” (lower line). In parenthesis are rounded forms of the same estimates.

| n  | \( R^+_x \)         | \( R^+_x \)         | \( R^+_x \)         |
|----|---------------------|---------------------|---------------------|
| 1  | 0.27029 (0.2696±0.0007) | 0.36212 (0.3609±0.0012) | 0.43813 (0.4357±0.0025) |
| 2  | 0.36212 (0.3609±0.0012) | 0.35974 (0.3600±0.0012) | 0.43316 (0.4357±0.0025) |
| 3  | 0.43813 (0.4357±0.0025) | 0.43316 (0.4357±0.0025) | 0.43316 (0.4357±0.0025) |
TABLE VIII. Bounds on the fixed point values of the renormalized coupling $g$ defined as the zero of the Wilson function $W(g)$. The resummation criteria for $W(g)$ have been chosen so as to yield values of $g^*$ as close as possible to the GZ estimates given in parenthesis. The two superposed numbers correspond to the respective bounds “max” (upper line) and “min” (lower line).

| $n$ | 1         | 2         | 3         |
|-----|-----------|-----------|-----------|
| $g^*$ | 1.41512 (1.415) | 1.40602 (1.406) | 1.39401 (1.394) |
|      | 1.40687 (1.407) | 1.40004 (1.400) | 1.38605 (1.386) |

TABLE IX. Values of the universal ratios of the amplitudes of the first correction to scaling for thermodynamic quantities combining calculations in the two phases, hence for $n = 1$ only (not obtained from the crossover functions, see text). Same presentation as in table VII.

| $a_+^\chi/a_\chi$ | $a_+^C/a_\chi$ | $a_M/a_\chi$ |
|---------------------|-----------------|--------------|
| 0.243 (0.215±0.029) | 0.893 (1.36±0.47) | 0.743 (0.40±0.35) |
| 0.186                | 1.823            |              |

TABLE X. Values of the universal ratios of the amplitudes of the first correction to scaling for the quantities calculated in the homogeneous phase (not obtained from the crossover functions, see text). Same presentation as in table VII.

| $a_+^\xi/a_\chi$ | $a_+^C/a_\chi$ | $a_+^\xi/a_\chi$ |
|-------------------|-----------------|-------------------|
| 0.699 (0.68±0.02) | 0.642 (0.636±0.006) | 0.625 (0.612±0.014) |
| 0.659 (0.68±0.02) | 0.630 (0.636±0.006) | 0.598 (0.582±0.014) |
| 8.89 (8.68±0.23)  | 6.09 (5.97±0.13)  | 4.63 (4.58±0.06)  |
| 8.43 (8.68±0.23)  | 5.84 (5.97±0.13)  | 4.52 (4.58±0.06)  |

19
APPENDIX A: COMPUTER PROGRAM IN FORTRAN FOR THE ISING MODEL IN THE TWO PHASES (UP-TO-DATE CRITERIA)

program utdFTcross1
  c***************************************************************************
  c up-to-date *
  c Crossover functions up to seven loop orders *
  c from Murray-Nickel (1991) and *
  c accounting for the recent analysis by Guida *
  c and Zinn-Justin [J Phys A31, 8103 (1998)] *
  c***************************************************************************
  c For Ising-like systems (n=1) above & below Tc *
  c***************************************************************************
  c see the companion paper:
  c "Classical-to-critical crossovers from field theory" by C. Bagnuls and C. Bervillier
  c***************************************************************************
  c The important subroutine is
  c fns(res,iphase,ibound,ifn,tau,theta,ikont)
  c res is the return value of the subroutine
  c iphase controls the phase:
  c iphase=1 corresponds to T>Tc
  c iphase=2 corresponds to T<Tc
  c ibound controls the type of function chosen:
  c ibound=1 corresponds to T>Tc if iphase=1
  c ibound=2 corresponds to T<Tc if iphase=2
  c ibound=3 gives the specific heat
  c ibound=4 controls the accuracy of the theoretical calculation:
  c ibound=1 corresponds to "max"
  c ibound=2 corresponds to "min"
  c tau is |T-Tc|/Tc
  c theta is the adjustable parameter which relates the scaling field t to tau:
  c in principle t=theta*tau but for practical use we have separated the asymptotic
  c pure scaling from the correction-to-scaling contributions, see the companion paper,
  c for theta=1 one recovers the pure theoretical
  c functions of the scaling field t)
  c ikont is an integer which allows to choose the nature of res
  c if ikont=0 then res gives the functions as indicated above
  c if ikont=1 then res corresponds to the effective exponent associated to the function
  c chosen according to the criteria described above.
  c All the functions are for Ising-like model (n=1)
  C***************************************************************************
  implicit double precision (a-h,o-z)
  C***************************************************************************
  C Evolution of the functions and of the effective exponents *
  C in terms of the pure scaling field t *
  C (i.e., theta=1) *
  C***************************************************************************
  C***
  C Selection of the function
  C***
    iphase=2 ! controls the phase: 1=T>Tc, 2=T<Tc
    ibound=1 ! controls the accuracy bound : 1=max, 2=min
    ifn=3 ! controls the fn: 1=xi, 2=chi, 3=c; for T<Tc, 1=coex curve
C***
C End of selection
C***
C***
C Files for saving the results
C***

open(29,FILE='expeff.dat')
open(30,FILE='Funct.dat')
theta=1 ! gives the theoretical evolution in terms of the scaling field t
  t=1.d-9
  do 30 i=1,45
    call fns(f3,iphase,ibound,ifn,t,theta,0) !Call of the function with ikont=0
    write(30,666) t,f3
    call fns(exp2,iphase,ibound,ifn,t,theta,1) ! Call of the effective exponent with ikont=1
    print *, t,f3,exp2
    alogt=dlog10(t)
    write(29,666) alogt,exp2 ! Ready for a Log-Lin plot
    t=t*2
  30 continue
  close(29)
  close(30)
stop

666 format(2(G13.6,1x))
end

C***
C Theoretical functions for n=1
C***

SUBROUTINE fns(res,i,j,k,t,theta,ikont)

C*************************************************
C if ikont=0: res gives the function
C if ikont=1: res gives the effective exponent
C Table f contains the values of the functions' parameters.
C At the end of each set a comment allows to distinguish the
c kind of function concerned.
C For each set, the first value is the critical exponent value
C (or minus this value for the specific heat), the second value
C is the inverse of the critical amplitude for xi and chi, the
c critical amplitude for aim and c, the third value is the critical
C background which is non zero only for c.
C The two values of the subcritical exponent delta corresponding to the two
C bounds "max" and "min" are contained in the table del
C*************************************************

implicit double precision (a-h,o-z)
dimension del(2),x(5),y(5)
dimension f(15,3,2,2)
data del/0.49862,0.50516/
data F/0.631678,2.150817,0.,32.24878,32.20434,11.02452,
  #-.5247187,10.41513,0.3775152,2.315848,-1.307939D-02,
  #39.95028,-1.307939D-02,0.,0., !ximax T>Tc (corr length)
  #1.2408875,3.75927,0.,34.05096,34.00404,23.27915,,-0.3101657,
  #1.257832,-8.204169D-03,3.31963,,-0.1634056,0.,0.,0.,0.,
  #-.1049675,1.871810,-4.048544,30.37745,30.33593,33.31814,3.476590,
  #9.400643,-8.344217D-03,33.06508,,-3.258311,0.,0.,0.,0.,
  #0.6290975,2.091612,0.,17.48596,17.57665,10.48005,,-0.1283214,
  #28.75634,,-9.207901D-02,2.014284,,-6.897436D-03,53.07716,
  #3.027917D-02,0.,0., !ximin T>Tc (corr length)
  #1.23830,3.660588,0.,13.38814,13.45758,2.853295,,-2.547260D-02,
  #11.51061,,-0.2766098,30.25994,,-0.1745266,0.,0.,0.,0., !chimax T>Tc (suscept)
  #1.23830,3.660588,0.,13.38814,13.45758,2.853295,,-2.547260D-02,
  #11.51061,,-0.2766098,30.25994,,-0.1745266,0.,0.,0.,0., !chimin T>Tc (suscept)
d=del(j) ! correction exponent  
e=F(1,k,j,i) ! asymptotic exponent  
z=f(2,k,j,i) ! asymptotic amplitude  
x6=f(3,k,j,i) ! additive critical background  
s1=f(4,k,j,i)  
s2=f(5,k,j,i)  
kmax=0
1 do 1 ii=1,5
   x(iii)=f(2*ii+4,k,j,i) ! definitions of the Xi's and Yi's
   if(x(iii).eq.0.) go to 2
   y(iii)=f(2*ii+5,k,j,i) 
kmax=kmax+1
2 continue
if(ikont.eq.0) then ! calculation of the function
   res=Z*t**e
   if(theta.eq.0.) then ! If theta=0
      res=res+x6 ! there is no correction-to-scaling
   else
      tt=theta*t
      D=D-1+(S1*dsqrt(tt)+1)/(S2*dsqrt(tt)+1)
      trr=(tt)**D
      do 3 kk=1,kmax
         res=res*(1+X(kk)*trr)**Y(kk)
      res=res+x6
      return
   end if
22
if(ikont.eq.1) then ! calculation of the effective exponent
   if(theta.eq.0.) then ! If theta=0
      e=e
   else
      end if
end if
   if(k.eq.3) res=-res ! the effective exponent
   return ! reduces to the constant
   tt=theta*t
C*********
C definitions of constants
C*********
"
D = D - 1 + (S1*dqrt(tt)+1)/(S2*dqrt(tt)+1)
trr = (tt)**D
Dp = (S1 - S2)/(2*dqrt(tt)*(S2*dqrt(tt)+1)**2)
res = 0.
do 4 kk = 1, kmax
res = res + X(kk)*Y(kk)/(1 + X(kk)*trr)
res = res * (Dp*tt*DLOG(tt)+D)*trr
res = res + e
if(k.eq.3) res = -res ! the exponent changes sign for c
return
end if
print *, "Error, ikont is ", ikont, ", but must be 0 or 1."
stop
end

program utdFTcrossN
C******************************************************************************
c up-to-date *
c Crossover functions up to seven loop orders *
c from Murray-Nickel (1991) and *
c accounting for the recent analysis by Guida *
c and Zinn-Justin [J Phys A31, 8103 (1998)] *
c******************************************************************************
c For N-vector-like systems (n=1, 2, 3) *
c in the homogeneous phase only *
c******************************************************************************
c see the companion paper: *
C "Classical-to-critical crossovers from field theory" by C. Bagnuls and C. Bervillier *
c******************************************************************************
c The important subroutine is 
c fns(res,iN,ibound,ifn,tau,theta,ikont) 
c res is the return value of the subroutine 
c iN controls the value of n: 
c iN=1 corresponds to n=1 
c iN=2 corresponds to n=2 
c iN=3 corresponds to n=3 
c ifn controls the type of function chosen: 
c ifn=1 gives the inverse correlation length 
c ifn=2 gives the inverse susceptibility 
c ifn=3 gives the specific heat 
c ibound controls the accuracy of the theoretical calculation: 
c ibound=1 corresponds to "max" 
c ibound=2 corresponds to "min" 
c tau is |T-Tc|/Tc 
c theta is the adjustable parameter which relates the scaling field t to tau: 
c (in principle t=theta*tau but for practical use we have separated the asymptotic 
 pure scaling from the correction-to-scaling contributions, see the companion paper, 
 for theta=1 one recovers the pure theoretical 
 functions of the scaling field t) 
c ikont is an integer which allows to choose the nature of res 
c if ikont=0 then res gives the functions as indicated above 
c if ikont=1 then res corresponds to the effective exponent associated to the function 
 chosen according to the criteria described above. 
c******************************************************************************
implicit double precision (a-h,o-z)
C******************************************************************************
C Evolution of the functions and of the effective exponents *
C in terms of the pure scaling field t *
C (i.e., theta=1) *
C******************************************************************************
C***
C Selection of the function 
C***
iN=2  ! controls the value of n: 1, 2, or 3
ibound=1! controls the accuracy bound : 1=max, 2=min
ifn=3  ! controls the fn: 1=xi, 2=chi, 3=c
C***
C Files for saving the results
C***

open(29,FILE='expeff.dat')
open(30,FILE='Funct.dat')
theta=1 ! gives the theoretical evolution in terms of the scaling field t
t=1.d-9
do 30 i=1,45
  call fns(f3,IN,ibound,ifn,t,theta,0) !Call of the function with ikont=0
  write(30,666) t,f3
  call fns(exp2,IN,ibound,ifn,t,theta,1) ! Call of the effective exponent with ikont=1
  alogt=dlog10(t)
  write(29,666) alogt,exp2 ! Ready for a Log-Lin plot
  t=t*2
30 continue
close(29)
close(30)
stop

666 format(2(G13.6,1x))
end

C***
C Theoretical functions for n-vector-like systems
C***

SUBROUTINE fns(res,i,j,k,t,theta,ikont)
c*************************************************
c if ikont=0: res gives the function
    c if ikont=1: res gives the effective exponent
    c Table f contains the values of the functions' parameters.
    c At the end of each set a comment allows to distinguish the
    c kind of function concerned.
    c For each set, the first value is the critical exponent value
    c (or minus this value for the specific heat), the second value
    c is the inverse of the critical amplitude for xi and chi, the
    c critical amplitude for c, the third value is the critical
    c background which is non zero only for c.
    c The six values of the subcritical exponent delta corresponding to the two
    c bounds "max" and "min" for each value of n are contained in the table del
  implicit double precision (a-h,o-z)
  dimension del(2,3),x(5),y(5)
  dimension f(15,3,2,3)
data del/0.49862,0.50516,0.52551,0.52986,0.55227,0.55702/
data F/0.631678,2.150817,0.,32.24878,32.20434,11.02452,#-0.5247187,10.41513,0.3775152,2.315848,-1.307939D-02,39.95028,-1.030731D-01,0.,0.,0.0.
#1.2408875,3.75927,0.,34.05096,34.00404,23.27915, -0.31016527, 
#1.257832,-8.204163D-03,8.313963,-0.1634056,0.,0.,0., 
#-1.049675,1.871810,-4.048544,30.37745,30.33559,33.31814,3.476590, 
#9.400643,-8.344217D-03,33.06508,-3.258311,0.,0.,0., 
#0.6290975,2.091612,0.,17.48596,17.57665,10.48005, -0.1283214, 
#28.75634,-9.269701D-02,2.014284, -6.897436D-03,53.07716, 
#-3.027917D-02,0.,0.,0.0., 
#1.23830,3.660588,0.,13.38814,13.45758,2.853295,-2.547260D-02, 
#11.51061,-0.2766008,30.25994,-0.1745266,0.,0.,0.,0.0., 
#1.23830,3.660588,0.,13.38814,13.45758,2.853295,-2.547260D-02, 
#11.51061,-0.2766008,30.25994,-0.1745266,0.,0.,0.,0.0.,
C definitions of constants

if(i.gt.3.or.i.lt.1) then
  print *, "Error, n=",i," is not available. Sorry. (0<n<4)"
  stop
end if

d=del(j,i)  ! correction exponent

  e=F(1,k,j,i)  ! asymptotic exponent

  z=f(2,k,j,i)  ! asymptotic amplitude

  x6=f(3,k,j,i)  ! additive critical background

  s1=f(4,k,j,i)

  s2=f(5,k,j,i)

kmax=0

do 1 ii=1,5
  x(ii)=f(2*ii+4,k,j,i)  ! definitions of the Xi's and Yi's
  if(x(ii).eq.0.) go to 2
  y(ii)=f(2*ii+5,k,j,i)

  kmax=kmax+1
1 26

C*********
C definitions of constants
C*********

if(i.gt.3.or.i.lt.1) then
  print *, "Error, n=",i," is not available. Sorry. (0<n<4)"
  stop
end if

d=del(j,i)  ! correction exponent

  e=F(1,k,j,i)  ! asymptotic exponent

  z=f(2,k,j,i)  ! asymptotic amplitude

  x6=f(3,k,j,i)  ! additive critical background

  s1=f(4,k,j,i)

  s2=f(5,k,j,i)

kmax=0

do 1 ii=1,5
  x(ii)=f(2*ii+4,k,j,i)  ! definitions of the Xi's and Yi's
  if(x(ii).eq.0.) go to 2
  y(ii)=f(2*ii+5,k,j,i)

  kmax=kmax+1
1 26
continue
if(ikont.eq.0) then ! calculation of the function
    res=Z*t**e
    if(theta.eq.0.) then ! If theta=0
        res=res+x6 ! there is no correction-to-scaling
        return ! only the pure scaling form
    end if ! survives
end if !

tt=theta*t
D=D-1+(S1*dsqrt(tt)+1)/(S2*dsqrt(tt)+1)
trr=(tt)**D

3 do 3 kk=1,kmax
    res=res*(1+X(kk)*trr)**Y(kk)
    res=res+x6
return
end if

if(ikont.eq.1) then ! calculation of the effective exponent
    if(theta.eq.0) then ! If theta=0
        res=e ! then
    end if ! critical exponent
    tt=theta*t
    D=D-1+(S1*dsqrt(tt)+1)/(S2*dsqrt(tt)+1)
trr=(tt)**D
    Dp=(S1-S2)/(2*dsqrt(tt)*(S2*dsqrt(tt)+1)**2)
    res=0.
    do 4 kk=1,kmax
        res=res+X(kk)*Y(kk)/(1+X(kk)*trr)
        res=res*(Dp*tt*DLOG(tt)+D)*trr
        res=res+e
    if(k.eq.3) res=-res ! the exponent changes sign for c
    return
end if
print *, "Error, ikont is ",ikont, ", but must be 0 or 1."
stop
end
APPENDIX C: COMPUTER PROGRAM IN FORTRAN
FOR THE ISING MODEL IN THE TWO PHASES
(FORMER CRITERIA, CORRECTED SERIES)

program FTcross1
  c***************************************************************
  c former corrected
  c Crossover functions up to six loop orders
  c after correction of the errors for the
  c inhomogeneous phase
  c***************************************************************
  c For Ising-like systems (n=1) above & below Tc
  c***************************************************************
  c see the companion paper:
  c "Classical-to-critical crossovers from field theory" by C. Bagnuls and C. Bervillier
  c***************************************************************
  c The important subroutine is
  c fns(res,iphase.ibound,ifn,tau,theta,ikont)
  c res is the return value of the subroutine
  c iphase controls the phase:
  c iphase=1 corresponds to T>Tc
  c iphase=2 corresponds to T<Tc
  c ifn controls the type of function chosen:
  c ifn=1 gives the inverse correlation length for T>Tc if iphase=1
  c otherwise (iphase=2) it gives the coexistence curve
  c ifn=2 gives the inverse susceptibility
  c ifn=3 gives the specific heat
  c ibound controls the accuracy of the theoretical calculation:
  c ibound=1 corresponds to "max"
  c ibound=2 corresponds to "min"
  c tau is |T-Tc|/Tc
  c theta is the adjustable parameter which relates the scaling field t to tau:
  c (in principle t=theta*tau but for practical use we have separated the asymptotic
  c pure scaling from the correction-to-scaling contributions, see the companion paper,
  c for theta=1 one recovers the pure theoretical
  c functions of the scaling field t)
  c ikont is an integer which allows to choose the nature of res
  c if ikont=0 then res gives the functions as indicated above
  c if ikont=1 then res corresponds to the effective exponent associated to the function
  c chosen according to the criteria described above.
  c All the functions are for Ising-like model (n=1)
  C******************************************************
  implicit double precision (a-h,o-z)
  C***************************************************************
  C Evolution of the functions and of the effective exponents
  C in terms of the pure scaling field t
  C (i.e., theta=1)
  C***************************************************************
  C
  C***
  C Selection of the function
  C***
  iphase=2 ! controls the phase: 1=T>Tc, 2=T<Tc
  ibound=1 ! controls the accuracy bound : 1=max, 2=min
  ifn=3   ! controls the fn: 1=xi, 2=chi, 3=c; for T<Tc, 1=coex curve
  C***
C End of selection
C***
C Files for saving the results
C***
open(29,FILE='expeff.dat')
open(30,FILE='Funct.dat')
theta=1 ! gives the theoretical evolution in terms of the scaling field t
t=1.d-9
do 30 i=1,45
call fns(f3,iphase,ibound,ifn,t,theta,0) !Call of the function with ikont=0
write(30,666) t,f3
call fns(exp2,iphase,ibound,ifn,t,theta,1) ! Call of the effective exponent with ikont=1
print *, t,f3,exp2
alogt=dlog10(t)
write(29,666) alogt,exp2 ! Ready for a Log-Lin plot
t=t*2
30 continue
close(29)
close(30)
stop
666 format(2(G13.6,1x))
end
C***
C Theoretical functions for n=1
C***
SUBROUTINE fns(res,i,j,k,t,theta,ikont)
!*************************************************
! if ikont=0: res gives the function
! if ikont=1: res gives the effective exponent
! Table f contains the values of the functions' parameters.
! At the end of each set a comment allows to distinguish the
! kind of function concerned.
! For each set, the first value is the critical exponent value
! (or minus this value for the specific heat), the second value
! is the inverse of the critical amplitude for xi and chi, the
! critical amplitude for aim and c, the third value is the critical
! background which is non zero only for c.
! The two values of the subcritical exponent delta corresponding to the two
! bounds "max" and "min" are contained in the table del
!*************************************************
implicit double precision (a-h,o-z)
dimension del(2),x(5),y(5)
dimension f(15,3,2,2)
data del/0.49125,0.50031/
data F/0.630501,2.12411,0.,16.87409,16.72772,23.51302,-0.2154827,
#0.6009808,-1.955281D-03,5.460931,-4.356399D-02,0.,0.,0.,0.,
#1.24194,3.80403,0.,10.7784,10.6849,18.2831,-0.447952,0.211862,
#-1.12883D-03,2.82005,-3.47989D-02,0.,0.,0.,0.,
#-1.108496,1.74928,-3.87997,22077.0,21885.5,8.15287,-8.12340D-03,
#36.4432,0.223350,395.406,1.76520D-03,0.,0.,0.,0.,
#0.629121,2.09256,0.,1.793553,1.794109,32.37368,-0.1214804,
#1.124729,-0.1263489,2.192044,-1.041270D-02,0.,0.,0.,0.,
#1.239485,3.706359,0.,1.229767,1.230149,2.198050,-2.015454D-02,
#24.55992,-0.2546755,10.44460,-0.2041400,0.,0.,0.,0.,
#-1.112636,1.58819,-3.57607,69.75599,69.7762,11.38361,
#-1.004983D-01,11.37558,8.030914D-02,33.34772,0.2454611,0.,0.,0.,
#0.,
!ximax T>Tc (corr length)
!chimax T>Tc (suscept)
!cmax T>Tc (specif heat)
!xmin T>Tc (corr length)
!chimin T>Tc (suscept)
!cmin T>Tc (specif heat)
C definitions of constants

C*********
d=del(j) ! correction exponent
e=F(1,k,j,i) ! asymptotic exponent
z=f(2,k,j,i) ! asymptotic amplitude
x6=f(3,k,j,i) ! additive critical background
s1=f(4,k,j,i)
s2=f(5,k,j,i)
kmax=0
do 1 ii=1,5
  x(ii)=f(2*ii+4,k,j,i) ! definitions of the Xi's and Yi's
  if(x(ii).eq.0.) go to 2
  y(ii)=f(2*ii+5,k,j,i)
1 kmax=kmax+1
2 continue
if(ikont.eq.0) then ! calculation of the function
  res=Z*t**e
  if(theta.eq.0.) then ! If theta=0
    res=res+x6 ! there is no correction-to-scaling
    return ! only the pure scaling form
  end if ! survives
  tt=theta*t
  D=D-1+(S1*dsqrt(tt)+1)/(S2*dsqrt(tt)+1)
  trr=(tt)**D
  do 3 kk=1,kmax
    res=res*(1+X(kk)*trr)**Y(kk)
    res=res+X6
 3 return
end if ! calculation of the effective exponent
if(ikont.eq.1) then
  tt=theta*t
  D=D-1+(S1*dsqrt(tt)+1)/(S2*dsqrt(tt)+1)
  trr=(tt)**D
  do 3 kk=1,kmax
    res=res*(1+X(kk)*trr)**Y(kk)
    res=res+X6
 3 return
end if ! calculation of the effective exponent
if(k.eq.3) then
  res=-res ! the effective exponent reduces to the constant
  end if ! critical exponent
  tt=theta*t
  D=D-1+(S1*dsqrt(tt)+1)/(S2*dsqrt(tt)+1)
  trr=(tt)**D
  Dp=(S1-S2)/(2*dsqrt(tt)**(S2*dsqrt(tt)+1)**2)
  res=0.
  do 4 kk=1,kmax

res = res + X(kk)*Y(kk)/(1+X(kk)*ttr)
res = res * (Dp*tt*DLOG(tt)+D)*ttr
res = res + e
if (k.eq.3) res = -res  ! the exponent changes sign for c
end if
print *, "Error, ikont is ",ikont," , but must be 0 or 1."
stop
end
program FTcrossN

C******************************************************************************
C former *
C Crossover functions up to six loop orders *
C******************************************************************************
C For N-vector-like systems (n=1, 2, 3) *
C in the homogeneous phase only *
C******************************************************************************
C see the companion paper: *
C "Classical-to-critical crossovers from field theory" by C. Bagnuls and C. Bervillier *
C******************************************************************************
C The important subroutine is
C fns(res,iN,ibound,ifn,tau,theta,ikont)
C res is the return value of the subroutine
C iN controls the value of n:
C iN=1 corresponds to n=1
C iN=2 corresponds to n=2
C iN=3 corresponds to n=3
C ifn controls the type of function chosen:
C ifn=1 gives the inverse correlation length
C ifn=2 gives the inverse susceptibility
C ifn=3 gives the specific heat
C ibound controls the accuracy of the theoretical calculation:
C ibound=1 corresponds to "max"
C ibound=2 corresponds to "min"
C tau is |T-Tc|/Tc
C theta is the adjustable parameter which relates the scaling field t to tau:
C (in principle t=theta*tau but for practical use we have separated the asymptotic
C pure scaling from the correction-to-scaling contributions, see the companion paper,
C for theta=1 one recovers the pure theoretical
C functions of the scaling field t)
C ikont is an integer which allows to choose the nature of res
C if ikont=0 then res gives the functions as indicated above
C if ikont=1 then res corresponds to the effective exponent associated to the function
C chosen according to the criteria described above.
C******************************************************************************
implicit double precision (a-h,o-z)
C******************************************************************************
C Evolution of the functions and of the effective exponents *
C in terms of the pure scaling field t *
C******************************************************************************
C***
C Selection of the function
C***
   iN=2     ! controls the value of n: 1, 2, or 3
   ibound=1 ! controls the accuracy bound : 1=max, 2=min
   ifn=3    ! controls the fn: 1=xi, 2=chi, 3=c
C***
C End of selection
C***
C***
C Files for saving the results
C***

open(29,FILE='expeff.dat')
open(30,FILE='Funct.dat')
theta=1 ! gives the theoretical evolution in terms of the scaling field t

t=1.d-9

do 30 i=1,45
  call fns(f3,iN,ibound,ifn,t,theta,0) ! Call of the function with ikont=0
  write(30,666) t,f3
  call fns(exp2,iN,ibound,ifn,t,theta,1) ! Call of the effective exponent with ikont=1
  print *, t,f3,exp2
  alogt=dlog10(t)
  write(29,666) alogt,exp2 ! Ready for a Log-Lin plot
  t=t*2
 30 continue

close(29)
close(30)

stop

666 format(2(G13.6,1x))

end

C***
C Theoretical functions for n-vector-like systems
C***

SUBROUTINE fns(res,i,j,k,t,theta,ikont)

! **************************************************
! if ikont=0: res gives the function
! if ikont=1: res gives the effective exponent
! Table f contains the values of the functions' parameters.
! At the end of each set a comment allows to distinguish the
! kind of function concerned.
! For each set, the first value is the critical exponent value
! (or minus this value for the specific heat), the second value
! is the inverse of the critical amplitude for xi and chi, the
! critical amplitude for c, the third value is the critical
! background which is non zero only for c.
! The six values of the subcritical exponent delta corresponding to the two
! bounds "max" and "min" for each value of n are contained in the table del
! **************************************************

implicit double precision (a-h,o-z)
dimension del(2,3),x(5),y(5)
dimension f(15,3,2,3)
data del/0.49125,0.50031,0.52012,0.52737,0.54975,0.55043/
data F/0.630501,2.12411,0.,16.87409,16.72772,23.51302,-0.2154827,
#0.6009808,-1.955281D-03,5.460931,-4.356399D-02,0.,0.,0.,0.,
#1.24194,3.80403,0.,10.7784,10.6849,18.2831,-0.447952,0.211862,
#-1.12883D-03,2.82005,-3.47989D-02,0.,0.,0.,0.,
#-1.08496,1.74928,-3.87997,22.077,-0.21885,5.8.15287,-8.12340D-03,
#36.4432,0.223350,395.406,1.76520D-03,0.,0.,0.,
#0.629121,2.09256,0.,1.79355,3.1794109,32.37368,-0.1214804,
#11.42729,-0.126349,2.192044,-1.041270D-02,0.,0.,0.,0.,
#1.239485,3.706359,0.,1.229767,1.230149,2.198050,-2.015454D-02,
#24.55992,-0.2546755,10.44460,-0.2041400,33.34772,0.2454611,0.,0.,
#-1.12636,1.58819,-3.57607,69.75599,69.7762,11.38361,
#-1.004983D-01,11.37558,8.03093D-02,33.34772,0.2454611,0.,0.,0.,
#0.,
#0.669848,2.578296,0.,28.84310,29.43534,15.75544,-0.2585115,
#5.012764,-4.34325D-02,77.73647,-3.775196D-02,0.,0.,0.,0.,
!xmax T>Tc n=1 (corr length)
!chimax T>Tc n=1 (suscept)
!cmax T>Tc n=1 (specif heat)
!xmin T>Tc n=1 (corr length)
!chimin T>Tc n=1 (suscept)
!cmin T>Tc n=1 (specif heat)
!xmax T>Tc n=2 (corr length)
| x1  | y1  | z1  | x2  | y2  | z2  |
|-----|-----|-----|-----|-----|-----|
| 1.31792 | 5.51529 | 0.63 | 8357 | 65.1464 | 16.9739 | -0.508216 |
| 1.85577 | -1.44706 | 0.27 | 33240 | -1.03476 | 0.124704 | -9.67699D-03 |
| 9.48805 | 1.53795 | 0.92 | 36121 | 45.8256 | 46.2262 | 21.93721 |
| 4.63085 | 1.62941 | 0.35 | 686347 | -0.151815 | 3.70188 | 4.02903 |

**C definitions of constants**

```fortran
if(i.gt.3.or.i.lt.1) then
  print *, "Error, n=",i,"is not available. Sorry. (0<n<4)"
  stop
end if

d=del(j,i) ! correction exponent
e=F(1,k,j,i) ! asymptotic exponent
z=f(2,k,j,i) ! asymptotic amplitude
x6=f(3,k,j,i) ! additive critical background
s1=f(4,k,j,i)
s2=f(5,k,j,i)
kmax=0
do 1 ii=1,5
  x(ii)=f(2*ii+4,k,j,i) ! definitions of the Xi's and Yi's
  if(x(ii).eq.0.) go to 2
  y(ii)=f(2*ii+5,k,j,i)
  kmax=kmax+1
  continue
  if(ikont.eq.0) then
    res=Z**e
    if(theta.eq.0) then
      res=res+x6
    else
      res=theta**e
    end if
  else
    res=theta**e
end if
```

!chimax T>Tc n=2 (suscept)
!cmax T>Tc n=2 (specif heat)
!ximin T>Tc n=2 (corr length)
!chimin T>Tc n=2 (suscept)
!ximax T>Tc n=3 (corr length)
!chimax T>Tc n=3 (suscept)
!cmax T>Tc n=3 (specif heat)
!ximin T>Tc n=3 (corr length)
!chimin T>Tc n=3 (suscept)
!cmin T>Tc n=3 (suscept)
tt=theta*t
D=D-1+(S1*dsqrt(tt)+1)/(S2*dsqrt(tt)+1)
trr=(tt)**D
do 3 kk=1,kmax
  res=res*(1+X(kk)*trr)**Y(kk)
  res=res+X6
  return
end if
if(ikont.eq.1) then ! calculation of the effective exponent
  if(theta.eq.0) then ! If theta=0
    res=e ! then
  else if(k.eq.3) res=-res ! the effective exponent
    return ! reduces to the constant
  end if ! critical exponent
  tt=theta*t
  D=D-1+(S1*dsqrt(tt)+1)/(S2*dsqrt(tt)+1)
  trr=(tt)**D
  Dp=(S1-S2)/(2*dsqrt(tt)*(S2*dsqrt(tt)+1)**2)
  res=0.
do 4 kk=1,kmax
  res=res+X(kk)*Y(kk)/(1+X(kk)*trr)
  res=res*(Dp*tt*DLOG(tt)+D)*trr
  res=res+e
  if(k.eq.3) res=-res ! the exponent changes sign for c
  return
end if
print *, "Error, ikont is ",ikont, ", but must be 0 or 1."
stop
end