Classical-to-critical crossovers from field theory

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We extend our previous determinations of nonasymptotic critical behavior of Phys. Rev. B **32**, 7209 (1985) and **35**, 3585 (1987) to accurate expressions of the complete classical-to-critical crossover (in three-dimensional field theory) in terms of the temperaturelike 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) 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 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. A **31**, 8103 (1998)].

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I. INTRODUCTION

Asymptotic critical behavior characterized by universal quantities (exponents and amplitude combinations) is now theoretically well established [1,2] with accuracy [3]. 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 [4–7] (calculations done far away from the critical point, characterized by nonuniversalities and including eventually crossover phenomena; see the reviews [1,8–11]). This extension appeared necessary notably when measurements on colloids [12], but also on complex systems such as ionic fluids [13] and polymers [14], 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 the phenomenon of "retarded criticality" which characterizes measurements done outside the asymptotic critical domain [15,16]. Several recent theoretical (and/or numerical) studies have also explicitly considered the evolution of effective exponents with emphasis on their monotonic or nonmonotonic character [11,17–21]. Furthermore, although recent work [22] satisfactorily compares experimental data on ^{3}He with the renormalization-group- (RG-) based φ^4 model following the scheme developed by Dohm and co-workers [23], the description of the classical-to-critical crossover for Ising systems is not yet clear-cut [24,25]. For these reasons and because our previous determination of nonasymptotic critical behavior from field theory [6,7] 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 [18,26,27]) (1) extend them to a complete account of the classical-to-critical crossover which characterizes the framework of field theory [28,29], and (2) include the seventh order series for the critical exponents determined by Murray and Nickel [30] 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 [3] (referred to in the following as GZ).

In the previous work [6,7], and contrary to an initial attempt [5] regarding the homogeneous phase ($n=1$), we provided only continuous expressions for t valid for $t \lesssim 10^{-2}$ (t is the temperaturelike 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 at about $t \simeq 10^{-2}$ [6,7]. Since then, it has appeared that the range of validity of field theory could be much larger than that and even could cover the entire classical-to-critical crossover region [16] that it describes. Thus it is interesting to give expressions valid in the entire crossover region if only because they may be compared to other kinds of classical-to-critical crossover, either experimental [10] or from numerical studies [11,20,24,31,32], which, under some particular conditions, are identical [18,19,26,31,33] to the field theoretical form (but see also our comment in [25]).

For technical reasons, in the previous work [6,7] we did not constrain our theoretical expressions to include very closely the estimates of universal asymptotic critical quantities of that time (with their error bars) so that uncertainties were underestimated and thus our estimates of the correction amplitude ratios were, presumably, also not firmly determined. Moreover, small errors existed in the previous study of the inhomogeneous phase [7] (as indicated elsewhere [18,34,35]) which have been eliminated from the present

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work. Nevertheless, we explicitly verified (see Fig. 1 of Ref. [35]) that the errors had no important consequence on the final results, as can be clearly deduced from a comparison of our estimates of universal amplitude combinations [7] with those of Guida and Zinn-Justin [36,3].

II. PRINCIPLE OF THE CALCULATIONS

A. Brief reminder

As in the previous work [6,7], 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 notation relative to the actual asymptotic critical behaviors [i.e., in terms of the physical variable $\tau=(T-T_c)/T_c\to 0^{\pm}$ instead of $t\to 0$; see also Sec. III]:

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

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

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

$$M(\tau)=B|\tau|^{\beta}[1+a_{M}|\tau|^{\Delta}+O(|\tau|^{2\Delta})], \tag{1d}$$

in which α, β, γ, and ν are the critical exponents, Δ (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 $a_{\xi}^{\pm}$, $a_{\chi}^{\pm}$, $a_{C}^{\pm}$, and a_M are the (confluent) first-correction amplitudes; finally, B_{cr} is a critical background. One usually restricts consideration of the critical singularities to small values of $t\propto|\tau|$ as is implicitly assumed in Eqs. (1). Obtaining nonasymptotic critical behavior supposes the explicit consideration of not necessarily small values of t.

Let us suppose that we want to calculate the susceptibility χ as a function of the (not necessarily small) temperaturelike scaling field t. Calculations of such a nonasymptotic critical behavior from (the massive) field theory (in three dimensions) [5–7] present the following features (additional details may also be found elsewhere [37]).

(1) The function $\chi(t)$ is primarily determined in implicit form because the quantities χ and t are primarily given as perturbation series in powers of the renormalized coupling parameter g (up to fifth [38,6] or sixth [7] 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 "β function") $W(g)$, also primarily given as a power series of g (up to sixth order [39]; 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 [like $\chi(g)$] 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

$$\chi(g)=\chi(y_0)\exp\left[-\int_{y_0}^{g}dx\,\frac{\gamma(x)}{\upsilon(x)W(x)}\right], \tag{2}$$

in which $\gamma(g)$ and $\upsilon(g)$ are not singular at g^* and are primarily given as power series of g (up to seventh order [30]). In particular, $\gamma(g^*)$ and $\upsilon(g^*)$ provide field theoretical estimates of the critical exponents γ and ν. Only the elementary series $\gamma(g)$, $\upsilon(g)$, 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 $\gamma(g)$, $\upsilon(g)$, 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 the free parameters of the transformation are varied. 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., $\gamma(g)$, $\upsilon(g)$, and $W(g)$, which gives a kind of envelope for $\chi(g)$ via two functions $\chi_{\max}(g)$ and $\chi_{\min}(g)$ [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 consideration of new series for the exponents compared to the homogeneous phase ($T>T_c$). Hence the same three series $\gamma(g)$, $\upsilon(g)$, and $W(g)$ express the critical singularities via integrals similar to that given in Eq. (2); only new critical amplitude functions of g (hence not singular at g^*) must be calculated [38,7] and summed using the transformation mentioned in step 4.

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 Sec. IIA 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. (4),(5) and Tables I–IV]. This is illustrated, for the Ising model ($n=1$), by Fig. 1, which displays the evolution of two effective exponents $\gamma_{\rm eff}(t)$ and $\alpha_{\rm eff}(t)$, which are defined as, for example [see Eqs. (1)],

$$\gamma_{\rm eff}(t)=-\frac{d\ln\chi(t)}{d\ln t}. \tag{3}$$

Figure 1 shows the effective exponents (calculated from the crossover functions of Tables I and II) which interpolate between critical and classical (mean field) values following a

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 ξ, the susceptibility χ, 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 the text for more details) and provide two exclusive sets of functions $F_{\max}$ and $F_{\min}$. The first row of the table displays the estimate of the universal value of the correction exponent Δ 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 e (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, Δ at ''max''=0.498 62, at ''min''=0.505 16					
	ξ^{-1}		χ^{-1}		C
e ν	0.631 678	γ	1.240 887 5	$-\alpha$	−0.104 967 5
	0.629 0975		1.238 30		−0.112 71
Z $(\xi_0^+)^{-1}$	2.150 817	$(\Gamma^+)^{-1}$	3.759 27	A^+/α	1.871 810
	2.091 612		3.660 588		1.580 112
S_1	32.248 78		34.050 96		30.377 45
	17.485 96		13.388 14		33.659 19
S_2	32.204 34		34.004 04		30.335 59
	17.576 65		13.457 58		33.833 77
X_1	11.024 52		23.279 15		33.318 14
	10.480 05		2.853 295		31.940 41
Y_1	−0.524 718 7		−0.310 165 27		3.476 590
	−0.128 321 4		$-2.547\,260\times10^{-2}$		0.220 018 5
X_2	10.415 13		1.257 832		9.400 643
	28.756 34		11.510 61		7.017 899
Y_2	0.377 515 2		$-8.204\,163\times10^{-3}$		$-8.344\,217\times10^{-3}$
	$-9.269\,701\times10^{-2}$		−0.276 600 8		$-9.616\,869\times10^{-3}$
X_3	2.315 848		8.313 963		33.065 08
	2.014 284		30.259 94		0.246 291 8
Y_3	$-1.307\,939\times10^{-2}$		−0.163 405 6		−3.258 311
	$-6.897\,436\times10^{-3}$		−0.174 526 6		$-7.002\,609\times10^{-5}$
X_4	39.950 28		–		–
	53.077 16				76.393 66
Y_4	−0.103 073 1		–		–
	$-3.027\,917\times10^{-2}$				$1.508\,835\times10^{-2}$
X_6	–		–		−4.048 544
					−3.548 035

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 [28] (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 to the framework used. In fact, strictly speaking, only the extreme asymptotic moving away from the Wilson-Fisher fixed point induced by small nonzero 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 [40]. 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 calculated from field theory [16,18,19,26,31,33]. See Sec. III for a practical use of the crossover functions.

Let us now give some technical information about the fitting procedure of step 2 of Sec. II A that must be applied twice for each quantity considered because of the two error bounds ''max'' and ''min'' (see Secs. II A and II B 2 for the meaning of these bounds).

TABLE II. Same as Table I for the coexistence curve M_S, the susceptibility χ, 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 γ,α and the subcritical exponent Δ take on the same values as in Table I (as they must according to the theory). An indication of the accuracy of the present work is provided by the parameter X_6 (the critical background of the specific heat) which should take on the same value as in Table I and differs slightly for the bound "max."

$n=1$, inhomogeneous phase, Δ at "max"=0.498 62, at "min"=0.505 16					
	M_S		χ^{-1}		C
e β	0.327 073 5	γ	1.240 887 5	$-\alpha$	−0.104 967 5
	0.324 495 4		1.238 30		−0.112 71
Z B	0.938 046 91	$(gG^-)^{-1}$	18.386 609	A^-/α	3.366 498 8
	0.937 009 52		17.160 196		3.048 908 6
S_1	35.738 988		2.339 529 5		1.603 646 2
	11.312 578		231.579 11		4.788 502 6
S_2	35.689 736		2.336 305 4		1.601 43 62
	11.371 253		232.780 25		4.813 339 5
X_1	303.216 96		76.549 557		79.538 017
	241.516 62		23.010 983		123.828 99
Y_1	$-1.768\,756\,5\times10^{-3}$		−3.486 562 8		$7.864\,347\,8\times10^{-2}$
	$-5.705\,693\,3\times10^{-2}$		0.889 159 51		−0.261 712 36
X_2	9.377 963 0		59.838 911		$4.063\,154\,2\times10^{-2}$
	13.371 447		61.975 912		0.420 993 75
Y_2	0.172 041 03		−16.395 572		$9.152\,242\,4\times10^{-5}$
	0.209 263 22		4.009 672 4		$-3.631\,256\,9\times10^{-3}$
X_3	1.392 122 9		3.690 451 2		16.574 905
	248.398 69		316.290 79		10.791 900
Y_3	$6.087\,771\,1\times10^{-3}$		$4.789\,405\,8\times10^{-2}$		−0.280 632 52
	$-7.722\,652\,9\times10^{-3}$		−0.153 613 87		$7.207\,294\,1\times10^{-2}$
X_4	30.597 947		63.029 796		14.361 662
	82.917 148		50.582 996		86.921 949
Y_4	0.171 440 92		19.215 714		0.130 702 58
	0.157 956 60		−5.259 510 5		0.414 997 82
X_5	6.506 418 0		9.380 739 8		19.477 188
	4.793 997 8		2.590 992 1		0.579 824 84
Y_5	$-1.947\,962\,6\times10^{-3}$		0.136 751 56		0.281 129 94
	$4.856\,896\,7\times10^{-2}$		$3.769\,243\,3\times10^{-2}$		$3.692\,856\,6\times10^{-3}$
X_6	–		–		−4.048 153 2
					−3.548 035 0

In order to analytically reproduce the functions calculated point by point, we use the following general form [5]:

$$F(t)=Zt^{e}\prod_{i=1}^{K}(1+X_i t^{D(t)})^{Y_i}+X_6 \tag{4}$$

in which K is the maximum number of factors (in a preliminary work [5] we had $K=3$; in the present work K can be as large as 5), and with

$$D(t)=\Delta-1+\frac{S_1\sqrt{t}+1}{S_2\sqrt{t}+1}, \tag{5}$$

in which Δ is the correction exponent. We have adjusted each of the parameters Z, e, $\{X_i,Y_i\}$ $(i=1,...,K)$, S_1, S_2, X_6, and Δ so as to fit the discretized evolution of the quantities considered (ξ,χ,C,M_S) as continuous functions of the temperaturelike 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 Δ 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 toward the classical behavior when $t\to\infty$, there are the following constraints.

(a) On S_1, so that we have [see, for example, Eqs. (A9) and (A10) of [21]]

$$D(t)\overset{t\to\infty}{\to}1/2. \tag{6}$$

This leads to

TABLE III. Same as Table I for the correlation length ξ, the susceptibility χ, and the specific heat C calculated in the homogeneous phase ($T>T_c$ and for $n=2$). Comparing with Tables I 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^+/α and of α: when α vanishes, A^+ and αX_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, Δ at ''max''=0.525 51, at ''min''=0.529 86					
	ξ^{-1}		χ^{-1}		C
$e\ \nu$	0.671 810 82	γ	1.318 898 5	$-\alpha$	$1.544\,0\times10^{-2}$
	0.668 789 32		1.314 895 2		6.370×10^{-3}
$Z\ (\xi_0^+)^{-1}$	2.628 991 8	$(\Gamma^+)^{-1}$	5.561 290 9	A^+/α	−55.881 907
	2.549 612 5		5.346 421 6		−121.130 56
S_1	15.963 748		96.831 346		4.048 092 0
	33.474 847		60.160 224		28.884 078
S_2	16.381 644		99.366 178		4.154 062 2
	34.505 171		62.011 900		29.773 102
X_1	28.529 734		16.310 867		1.191 160 2
	111.527 36		11.716 728		37.837 491
Y_1	$-9.096\,376\,4\times10^{-2}$		−0.573 581 94		$5.570\,405\,3\times10^{-2}$
	$-2.849\,143\,1\times10^{-2}$		$-4.121\,347\,9\times10^{-2}$		3.543 470 6
X_2	9.111 249 7		3.661 569 4		1.267 516 4
	13.427 180		15.104 245		59.951 524
Y_2	−0.223 118 36		$5.695\,036\,0\times10^{-2}$		$-5.849\,955\,7\times10^{-2}$
	−15.783 043		−0.536 305 10		$-1.767\,701\,2\times10^{-2}$
X_3	0.113 260 11		0.326 692 57		27.562 173
	24.100 833		3.105 188 3		1.384 730 0
Y_3	$3.834\,787\,7\times10^{-4}$		$-4.853\,531\,8\times10^{-4}$		$-7.724\,392\,9\times10^{-3}$
	$1.861\,202\,8\times10^{-3}$		$-3.853\,626\,0\times10^{-2}$		$2.276\,906\,0\times10^{-4}$
X_4	72.907 613		430.167 27		46.806 723
	13.360 107		239.951 79		37.714 984
Y_4	$-5.016\,674\,0\times10^{-2}$		$-6.779\,346\,3\times10^{-3}$		$-2.036\,010\,3\times10^{-2}$
	15.603 262		$-1.373\,556\,4\times10^{-2}$		−3.538 761 2
X_5	10.299 474		–		–
	7.396 055 8				
Y_5	$2.024\,374\,0\times10^{-2}$		–		–
	−0.131 168 17				
X_6	–		–		50.158 572
					115.951 04

$$S_1=S_2\left(\frac{3}{2}-\Delta\right). \tag{7}$$

(b) On one of the couple $\{X_i, Y_i\}$ by requiring that a known classical behavior is reached in the limit $t\to\infty$. Thus

$$e+\frac{1}{2}\sum_{i=1}^{K} Y_i=e_c, \tag{8}$$

$$Z\prod_{i=1}^{K}(X_i)^{Y_i}=Z_c, \tag{9}$$

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:

$$Y_{i_0}=2(e_c-e)-\sum_{i\neq i_0} Y_i, \tag{10}$$

$$X_{i_0}=\left[\frac{Z_c}{Z}\prod_{i\neq i_0}(X_i)^{-Y_i}\right]^{1/Y_{i_0}}, \tag{11}$$

with the classical values $e_c=1$, 1/2, 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) relative deviation less than 10^{-4} (in the worst case and for a limited number of functions especially in the inhomoge-

TABLE IV. Same as Table I for the correlation length ξ, the susceptibility χ, and the specific heat C calculated in the homogeneous phase ($T>T_c$ and for $n=3$).

$n=3$, homogeneous phase, Δ at ''max''=0.552 27, at ''min''=0.557 02					
	ξ^{-1}		χ^{-1}		C
$e\ \nu$	0.710 906 29	γ	1.394 600 0	$-\alpha$	0.132 720
	0.703 810 62		1.384 510 0		0.111 435 82
$Z\ (\xi_0^+)^{-1}$	3.172 240 3	$(\Gamma^+)^{-1}$	7.985 610 5	A^+/α	−20.228 436
	2.963 257 2		7.268 765 0		−18.976 690
S_1	31.477 107		72.301 387		17.216 858
	78.590 543		52.048 362		96 640.818
S_2	33.213 159		76.289 014		18.166 416
	83.342 746		55.195 616		102 484.48
X_1	394.952 93		13.735 280		389.178 97
	10.931 307		0.158 903 96		52.385 639
Y_1	$-5.254\,562\,5\times10^{-3}$		−0.753 908 60		$-3.049\,819\,0\times10^{-3}$
	16.025 379		$1.152\,513\,4\times10^{-3}$		0.199 457 18
X_2	0.150 789 20		1.361 677 7		$4.760\,746\,4\times10^{-2}$
	3.212 371 6		11.028 433		1179.5468
Y_2	$2.864\,103\,1\times10^{-3}$		0.469 601 31		$3.252\,881\,3\times10^{-4}$
	−0.113 559 93		$-4.749\,579\,2\times10^{-2}$		$1.306\,210\,4\times10^{-3}$
X_3	11.387 266		1.386 296 9		12.991 689
	505.595 21		12.528 570		22.441 166
Y_3	−0.359 826 58		−0.490 562 04		−0.165 650 10
	$-6.979\,372\,6\times10^{-3}$		−0.696 010 28		−0.134 399 92
X_4	78.089 588		437.657 47		65.185 231
	11.021 201		312.819 12		36.340 773
Y_4	$-5.669\,256\,0\times10^{-2}$		$-1.433\,067\,2\times10^{-2}$		−0.109 482 46
	−16.378 555		$-1.881\,614\,7\times10^{-2}$		−0.351 278 70
X_5	0.195 821 93		–		1.708 027 7
	2.818 836 1		0.977 486 68		11.698 778
Y_5	$-2.902\,978\,6\times10^{-3}$		–		$1.241\,709\,3\times10^{-2}$
	$6.609\,431\,3\times10^{-2}$		$-7.850\,294\,7\times10^{-3}$		$6.204\,359\,5\times10^{-2}$
X_6	–		–		8.268 433 8
					9.155 860 5

neous phase). However, globally (the mean value of the local deviations over the entire range of t), the adjustment is much better for all the quantities.

The results of these 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 previous work [6,7], the resummation criteria of step 4 of Sec. II 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 [i.e., $\gamma(g)$, $\nu(g)$, etc.] 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. (2)] 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 [$\chi(t)$, etc.] result from the combination of a small number of elementary series [41] [namely, $\gamma(g)$, $\nu(g)$, $W(g)$, and a few amplitude functions], the individual criteria were combined in our preceding work [6,7] so as to provide an envelope of the error, accounting automatically for correlations (frustrations) between the error bounds. This 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

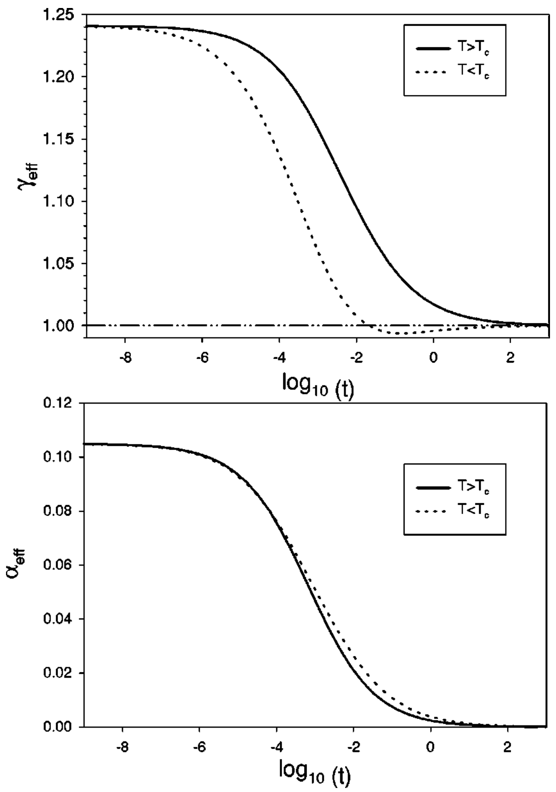

FIG. 1. Respective evolutions (calculated from the crossover functions of Tables I and II) of the effective exponents $\gamma_{\mathrm{eff}}(t)$ and $\alpha_{\mathrm{eff}}(t)$ in the two phases: the homogeneous (continuous line) and the inhomogeneous (dashed line) phases. Notice, in this latter case, the moving down of $\gamma_{\mathrm{eff}}(t)$ below the classical value $(=1.0)$ in the regime of high values of t. This nonmonotonic feature of $\gamma_{\mathrm{eff}}(t)$ in the inhomogeneous phase is in agreement with Refs. [18,19] and has been numerically observed in Refs. [17,32].

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 [30]. 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 [36] (they were not 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 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. [6,7] and notably in the inhomogeneous phase case; they are presumably overestimated (see below and Sec. III B).

Table V 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 4 of Sec. II A) while only the central values of the GZ exponent estimates satisfy the scaling relations (the apparent errors for γ, ν, β have been determined independently [3]). Table V shows how for the respective estimates meet the scaling relations in both cases. Tables VI 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 the GZ results is graphically illustrated by Figs. 2 and 3.

From Tables I–IV one may observe that our bounds on the correction exponent Δ differ from those of GZ. This is due to the correlation of errors mentioned above. Indeed, we have never considered Δ 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

$$\omega=\left.\frac{dW(g)}{dg}\right|_{g=g^{*}}, \tag{12}$$

$$\nu=\nu(g^{*}). \tag{13}$$

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 VIII).

Similarly, the present determinations of (and the uncertainties in) the first correction-to-scaling terms displayed in Tables IX and X differ from our previous work [6,7] essentially because of our systematic account for the up-to-date estimates of the leading amplitude combinations (see Tables VI 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 Sec. III B).

It is worth indicating that the values displayed in Tables IX and X are not obtained from the crossover functions of Tables I–IV by simply using the expression [see Eq. (4)]

$$a_F=\sum_{i=1}^{K} X_i Y_i , \tag{14}$$

which would be the right expression if the correction exponent in Eq. (4) were the actual correction exponent Δ 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 previous work [6,7]).

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 parentheses 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 parentheses correspond to their bound estimates, which have not been determined particularly so as to satisfy the scaling relations).

	Critical exponent values			
n	γ	ν	α	β
1	1.240 887 5 (1.2409)	0.631 678 (0.6317)	0.104 967 5 (0.105)	0.327 073 5 (0.3272)
	1.238 30 (1.2383)	0.629 097 5 (0.6291)	0.112 71 (0.113)	0.324 495 4 (0.3244)
2	1.318 898 5 (1.3189)	0.671 810 82 (0.6718)	−0.015 44 (−0.015)	—
	1.314 895 2 (1.3149)	0.668 789 32 (0.6688)	−0.006 37 (−0.007)	
3	1.394 60 (1.3945)	0.710 906 29 (0.7108)	−0.132 720 (−0.132)	—
	1.384 51 (1.3845)	0.703 810 62 (0.7038)	−0.111 435 82 (−0.112)	

	Scaling relations (should be zero)	
	$\lvert\alpha-2+3\nu\rvert$	$\lvert\alpha+2\beta+\gamma-2\rvert$
1	1.5×10^{-6} (1.0×10^{-4})	2.0×10^{-6} (3.0×10^{-4})
	2.5×10^{-6} (3.0×10^{-4})	8.0×10^{-7} (1.0×10^{-4})
2	7.5×10^{-6} (4.0×10^{-4})	—
	2.0×10^{-6} (6.0×10^{-4})	
3	1.1×10^{-6} (4.0×10^{-4})	
	4.0×10^{-6} (6.0×10^{-4})	

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 renormalization group theory [42]. 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 $\mathcal{L}$ 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 $\mathcal{L}$ 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 $\mathcal{L}$ for any system allowing, in some sense, the determination of subclasses of universality.

TABLE VI. Values of universal combinations of leading critical amplitudes for thermodynamic quantities combining calculations in the two phase; hence for $n=1$ only (from the crossover functions of Tables I and II). The two numbers in each column correspond to the bounds "max" (upper line) and "min" (lower line). In parentheses are the corresponding bounds of the GZ estimates.

A^+/A^-	Γ^+/Γ^-	$R_C^+=A^+\Gamma^+/B^2$
0.556 01 (0.556)	4.891 00 (4.89)	0.059 40 (0.0594)
0.518 26 (0.518)	4.687 83 (4.69)	0.055 41 (0.0554)

As already explained [5–7], the comparison of the theoretical functions with experimental data involves a very small number of adjustable parameters: (1) nonuniversal global factors; (2) the proportionality factor θ between the temperaturelike scaling field t and $\tau=(T-T_c)/T_c$ (neglecting higher analytical contributions in τ which may sometimes be non-negligible [10] but are out of the scope of our present aim)

$$t=\theta|\tau|; \tag{15}$$

(3) additive regular background terms for the specific heat; and (4) eventually T_c.

For example, the comparison with experimental measurements of the susceptibility χ may be made as follows:

$$\chi_0\chi_{\rm th}(\theta|\tau|)=\chi_{\rm expt}(|\tau|) \tag{16}$$

in which $\chi_{\rm expt}(|\tau|)$ represents the experimental data and $\chi_{\rm th}(t)$ our function for one [43] of the two bounds "max" and "min." One generally expects theoretically that χ_0 and θ will take on the same values [44] for the two sets of mea-

TABLE VII. Values of the universal quantity $R_\xi^+ = \xi_0^+ (A^+)^{1/3}$ 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 numbers in columns 2, 4, and 6 correspond to the bounds "max" (upper line) and "min" (lower line). In parentheses are rounded off forms of the same estimates.

n	1		2		3	
R_ξ^+	0.270 29 0.268 99	(0.2696 ± 0.0007)	0.362 12 0.359 74	(0.3609 ± 0.0012)	0.438 13 0.433 16	(0.4357 ± 0.0025)

surements above and below T_c provided that the range of values of τ is not too large. The fact that χ_0 must be unchanged is a consequence of the universality of the ratio Γ_0^+/Γ_0^- with, as $\tau \to 0^\pm$,

$$\chi_{\mathrm{expt}}(|\tau|) \simeq \Gamma_0^\pm |\tau|^{-\gamma}(1 + \Gamma_1^\pm |\tau|^\Delta + \cdots), \tag{17}$$

in which $\Gamma_0^\pm$ and $\Gamma_1^\pm$ are related to our previous definition [Eq. (1b)] as follows:

$$\Gamma_0^\pm = \chi_0 \theta^{-\gamma} \Gamma^\pm, \tag{18}$$

$$\Gamma_1^\pm = \theta^{-\Delta} a_\chi^\pm . \tag{19}$$

As for the stability of θ, this is because the ratio Γ_1^+/Γ_1^- 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 θ

If one introduces θ literally as in Eq. (15), then the fitted leading critical amplitude involves two adjustable param-

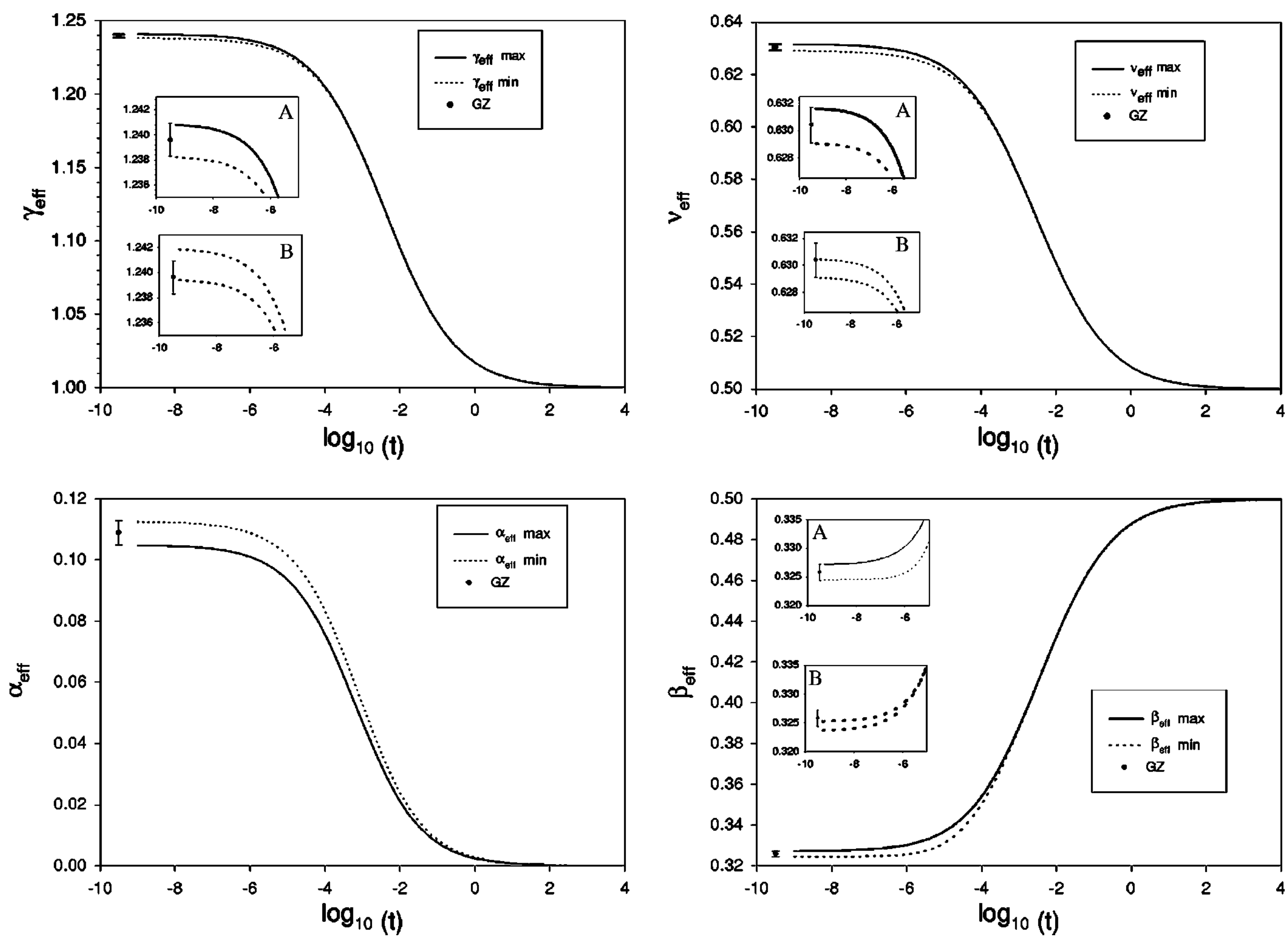

FIG. 2. The two bounds "max" (continuous lines) and "min" (short-dashed lines) have been determined so as to reproduce as closely as possible the GZ estimates. This is illustrated here with the effective exponents calculated from the crossover functions for $n=1$ determined in the present work (see Tables 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 from our preceding work of [6,7] (long-dashed lines). (For other values of n, see Table V.)

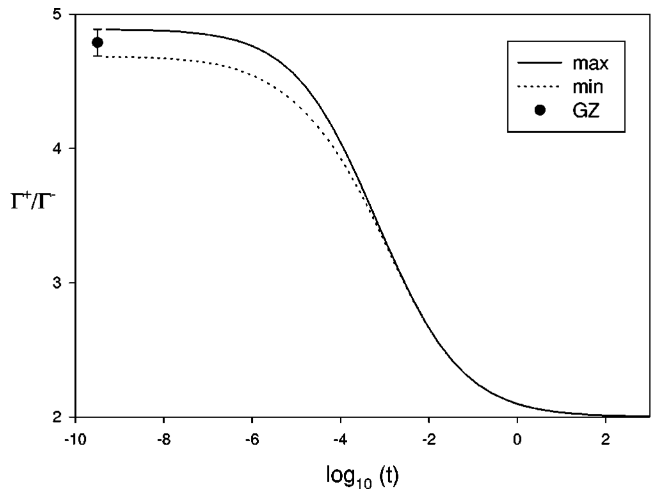

FIG. 3. The two bounds ''max'' (continuous line) and ''min'' (short-dashed line), determined so as to reproduce as closely as possible the GZ estimates, account also for the universal amplitude combinations. This is illustrated here with the ratio Γ^+/Γ^- [see Eq. (1b)] calculated from the crossover 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.

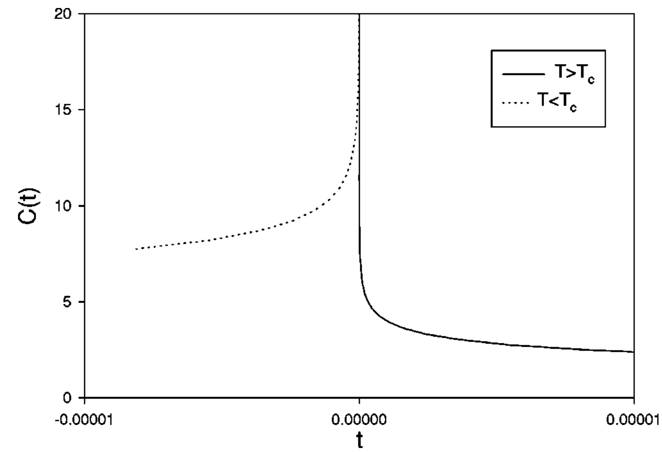

FIG. 4. The field theoretical form of the specific heat exhibits the classical ''jump.''

eters. This is not very suitable. For practical use, we propose to introduce the adjustable parameters as follows [compare with Eq. (4)]:

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

$$t=\theta|\tau|, \qquad (21)$$

in which θ is no longer involved in the pure scaling part of the critical behavior $(Z|\tau|^{\gamma})$. So introduced, *θ 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 $\theta\geqslant 0$) up to the point where consistency is lost.

The domain $\mathcal{L}$ of τ 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 in the form of a complete classical-to-critical crossover [45].

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 θ with a good fit in a range of values of τ similar to that considered with χ. For the specific heat,

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

in which $B_0(\tau)$ is an additive noncritical (i.e., regular or analytic in τ) 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 $C_{\text{th}}(t)$ 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 τ].

If, in addition to C and χ, we also possess coexistence curve data, we have a stronger constraint since then no other adjustable parameter is required to fit these new data. Indeed, in the relation

$$M_0 M_{\text{th}}(\theta|\tau|)=M_{\text{expt}}(|\tau|) \qquad (23)$$

everything is fixed since M_0 is related to C_0 and χ_0 due to the universal amplitude combination [46] R_C and θ must have the same value whatever the quantity considered.

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 parentheses. The two values correspond to the bounds ''max'' (upper line) and ''min'' (lower line).

n	1	2	3
g^*	1.415 12 (1.415)	1.406 02 (1.406)	1.394 01 (1.394)
	1.406 87 (1.407)	1.400 04 (1.400)	1.386 05 (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_χ^+/a_χ^-		a_C^+/a_C^-		a_M/a_χ^+	
0.243	(0.215±0.029)	0.893	(1.36±0.47)	0.743	(0.40±0.35)
0.186		1.823		0.048	

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.

n	1		2		3	
a_{ξ}^{+}/a_{χ}^{+}	0.699 0.659	(0.68 ± 0.02)	0.642 0.630	(0.636 ± 0.006)	0.625 0.598	(0.612 ± 0.014)
a_{C}^{+}/a_{χ}^{+}	8.89 8.43	(8.68 ± 0.23)	6.09 5.84	(5.97 ± 0.13)	4.63 4.52	(4.58 ± 0.06)

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

In order to facilitate the use of the crossover functions displayed in Tables I–IV, text files of FORTRAN code are provided [47].

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 is 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 nor 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:

$$F_{E}(t)=[F_{\max}(t)]^{E}[F_{\min}(t)]^{1-E}, \tag{24}$$

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

$$e_{\rm eff}(t)=E e_{\rm eff}^{\max}(t)+(1-E)e_{\rm eff}^{\min}(t). \tag{25}$$

Then the introduction of the other adjustable parameters, such as θ for example, within $F_E(t)$ is unchanged compared to the description given above except that the additive X_6 term mentioned in Eq. (20) is obviously excluded from $F_{\max}$ and $F_{\min}$ and treated as a new adjustable additive parameter.

As we said in Sec. II B 2 it is likely that the close account of the GZ estimates has led us to overestimate the uncertainty in the correction terms so that it seems to us useful to provide the reader also with functions reproducing the complete classical-to-critical crossover according to the resummation criteria of the previous (but corrected, see [35]) work of Refs. [6,7] although (or rather because) this time the errors are underestimated. This is why we provide two additional text files of FORTRAN code [47] corresponding to the former resummation criteria applied to the corrected series (without the seventh order of Ref. [30]).

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

[42] Only one family of corrections to scaling (controlled by the unique exponent Δ) is accounted for.

[43] Or a combination of the two bounds; see Sec. III B.

[44] Generally speaking this is true, but θ may be nil because there exist systems which do not approach the Ising fixed point along the RG trajectory that 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 [40].

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

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[47] See EPAPS Document No. E-PLEEE8-65-138206. Two sets of two files each are provided: first, utdfunctions1.txt and utdfunctionsN.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) on one hand and Tables I, III, and IV (n-vector-like systems in the homogeneous phase) on the other hand, and, second, functions1.txt and functionsN.txt which contain the FORTRAN code for the previous (corrected, see [35]) work of Refs. [6,7]. In each case the file contains its own instructions for use. This document may be retrieved 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.