

# Extended scaling behavior of the spatially anisotropic classical XY model in the crossover from three to two dimensions

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The bivariate high-temperature expansion of the spin-spin correlation function of the three-dimensional classical XY (planar rotator) model, with spatially anisotropic nearest-neighbor couplings, is extended from the tenth through the 21st order. The computation is carried out for the simple cubic lattice, in the absence of magnetic field, in the case in which the coupling strength along the  $z$  axis of the lattice is different from those along the  $x$  and the  $y$  axes. It is then possible to determine accurately the critical temperature as function of the parameter  $R$  which characterizes the coupling anisotropy and to check numerically the universality, with respect to  $R$ , of the critical exponents of the three-dimensional anisotropic system. The analysis of our data also shows that the main predictions of the generalized scaling theory for the crossover from the three-dimensional to the two-dimensional critical behavior are compatible with the series extrapolations.

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## I. INTRODUCTION

The three-dimensional (3D) layered magnetic spin systems, in which the strength of the interactions among the layers is much smaller than within the layers, are often referred to as quasi-two-dimensional. Although strictly two-dimensional (2D) magnetic systems do not exist in nature, their statistical mechanics can be studied by experimenting with diverse more mundane structures and in particular by exploring how quasi-two-dimensional systems<sup>1</sup> crossover, i.e., change their universality class, on going from the 3D to the 2D critical regime. From a more general standpoint, the study of spatially anisotropic systems also provides the simplest example of a wide variety of crossover phenomena<sup>2-6</sup> of different origin which may occur near criticality.

The simplest Hamiltonian, which can model a quasi-two-dimensional magnetic system, in the absence of a magnetic field, is that of an  $N$ -vector spin model with axially anisotropic couplings

$$H_{an}\{v\} = -NJ_1 \sum_{nn(xy)} \vec{v}(\vec{r}) \cdot \vec{v}(\vec{r}') - NJ_2 \sum_{nn(z)} \vec{v}(\vec{r}) \cdot \vec{v}(\vec{r}'). \quad (1)$$

We have indicated by  $\vec{v}(\vec{r})$  an  $N$ -component classical spin vector of unit length located at the site  $\vec{r}$  of a simple cubic (sc) lattice. The first sum in Eq. (1) is extended to the nearest-neighbor (nn) spin pairs within each horizontal ( $xy$ ) layer, while the second sum is over the nn spins in adjacent layers along the  $z$  direction. We shall denote by  $R=J_2/J_1$  the ratio of the interlayer to the intralayer coupling strength which characterizes the spatial anisotropy of the spin couplings and therefore is sometimes referred to as *anisotropy parameter*. The thermodynamic quantities of the model can be expressed as functions of the variables  $K_1=J_1/kT$  and  $K_2=J_2/kT$ , with  $k$  as the Boltzmann constant. One may, equivalently, choose either the pair of variables  $K_1$  and  $R$  or the pair  $K_2$  and  $\bar{R}=1/R$ . For  $R \rightarrow 0$ , the system becomes a stack of noninteracting spin layers. When  $R=1$ , the system

has directionally isotropic interactions. For  $R \rightarrow \infty$ , or equivalently for  $\bar{R} \rightarrow 0$ , it reduces to an array of noninteracting spin chains.

Only a few pioneering studies<sup>7-12</sup> of Hamiltonian (1) by high-temperature (HT) methods are presently available. They were aimed at the following:

(1) A numerical test of the critical universality<sup>13</sup> for the anisotropic system, in particular of the  $R$  independence of the critical exponents as long as  $R > 0$ .

(2) An investigation of the change in universality class of the critical transition as  $R \rightarrow 0$ , i.e., of the crossover from the sc to the square-lattice critical behavior.

They relied on HT series expansions, in terms of the two variables  $K_1$  and  $K_2$ , computed through 11th order<sup>8</sup> for  $N=1$  (the spin-1/2 Ising model) and through tenth order<sup>10</sup> for  $N=2$  (the planar rotator or XY model) or  $N=3$  (the classical Heisenberg model) on the sc lattice. The corresponding expansions for the face-centered-cubic lattice also reached the same orders. Altogether 78 coefficients were computed in the sc-lattice Ising case and 66 coefficients in the other cases but, unfortunately, no further coefficients were added since. In the Ising case, although rather short, the expansions are sufficiently well behaved that their extrapolations can support unambiguously the simplest theoretical expectations concerning the crossover. The accuracy of the first series analyses in the Ising case could be only marginally improved<sup>14</sup> by resorting to bivariate partial-differential approximants<sup>15,16</sup> (i.e., by approximately resumming the HT expansions in terms of the solution of a linear first-order *partial* differential equation with appropriately chosen bivariate polynomial coefficients) instead of using the conventional ratio or Padé approximant (PA) methods. The reason of this failure is that there is no substitute for significantly longer expansions. Later on, also several Monte Carlo simulations<sup>17,18</sup> were carried out in an attempt at further clarifying the crossover behavior of Ising systems, but the accuracy of the results is still subject to controversy for small positive  $R$ , i.e., in the region of main interest. On the other hand, for the models with  $N > 1$ , the earliest HT analyses were inconclusive, thus calling

for a substantial extension of the expansions. In particular, the crossover issue remained to be studied because even the existence of a critical point at nonzero temperature and the nature of the critical singularity in the 2D limit were not yet firmly assessed at the time of the first analyses. Also the successive simulation studies, carried out when the critical behaviors in 2D of the  $N=2$  model<sup>19</sup> (and of the  $N>2$  models<sup>20</sup>) were better understood, probably cannot yet be considered sufficiently accurate<sup>21,22</sup> or are not directly comparable<sup>23</sup> with the series analyses.

We have been motivated by this situation to devote our study to the  $N=2$  anisotropic model, taking advantage of our recent extensions through order 21 (i.e., from 66 to 253 series coefficients), of the bivariate HT expansions for the two-spin correlation function and its moments on the sc lattice. Another reason of interest into this model is that it has been suggested to provide an approximate description of layered high- $T_c$  superconductors.<sup>24</sup>

The paper is organized as follows. In Sec. II, we briefly mention the algorithm adopted and specify the results of our series computations. In Sec. III, we discuss some of the simplest predictions of the extended phenomenological scaling theory for the crossover from the 3D to the 2D [and from the 3D to the one-dimensional (1D)] critical behavior. We begin by reviewing in some detail the well studied  $N=1$  case only to recall the general ideas of this approach and to contrast its features with those of the less studied and more complex  $N \geq 2$  cases. In Sec. IV, we outline our numerical analysis of the expansions and compare the results with the theoretical expectations.

We should finally notice that, throughout this report, for reasons of clarity, we have used a notation sometimes different and heavier but more detailed and perhaps more explicit than that generally adopted in the earliest studies of the crossover phenomena.

## II. EXTENDED HIGH-TEMPERATURE EXPANSIONS

Our computation of the series coefficients was carried out using a computerized recursive algorithm based on the Schwinger-Dyson equations.<sup>25</sup> This method was initially applied only to the determination of single-variable HT expansions. Only recently, taking advantage of the great improvements of the computer performances of the last decades, it could be straightforwardly adapted<sup>26,27</sup> to derive also the more memory-demanding and computationally intensive bivariate expansions for a wide class of isotropic and anisotropic  $XY$  models with nn and next-to-nn interactions. It should be noted that in our approach only extended-integer exact arithmetic is used, thus avoiding all round-off errors which limited the precision of the preceding<sup>10</sup> floating-point computations. To give an idea of the performance of the algorithm, let us note that an ordinary single-processor desktop personal computer (pc) can complete, in less than a second, all tenth-order calculations for the anisotropic  $N=2$  case so far documented<sup>10</sup> in the literature. The calculation of the next nine orders takes a few days. To compute the last two orders, we have used a pc-cluster for a time equivalent to approximately six months of a single pc.

Fixing  $N=2$ , we have calculated the spin-spin correlations

$$C(\vec{0}, \vec{x}; N; K_1, R) = \langle \vec{v}(\vec{0}) \cdot \vec{v}(\vec{x}) \rangle, \quad (2)$$

for all values of  $\vec{x}$  for which the HT expansion coefficients are nontrivial within the maximum order reached. As usual, here  $\langle O \rangle = \text{Tr}(O \exp[-H_{an}]) / \text{Tr}(\exp[-H_{an}])$ .

In terms of Eq. (2), we have formed the expansions of the  $l$ th-order spherical moments of the correlation function:

$$m^{(l)}(N; K_1, R) = \sum_{\vec{x}} |\vec{x}|^l \langle \vec{v}(\vec{0}) \cdot \vec{v}(\vec{x}) \rangle \quad (3)$$

and, in particular, of the reduced ferromagnetic susceptibility defined as  $\chi(N; K_1, R) = m^{(0)}(N; K_1, R)$ .

The second-moment correlation length is expressed in terms of  $m^{(2)}(N; K_1, R)$  and  $\chi(N; K_1, R)$  as

$$[\xi(N; K_1, R)]^2 = m^{(2)}(N; K_1, R) / 2d\chi(N; K_1, R). \quad (4)$$

where  $d$  is the lattice dimensionality, i.e.,  $d=1$  for  $\vec{R}=0$ ,  $d=2$  for  $R=0$ , and  $d=3$  otherwise.

Usually, for the univariate HT expansions, the only accessible validation procedure of an extended computation is the comparison with the lower-order results that might be already known. In the case at hand, only the expansion coefficients of the second moment of the correlation function are tabulated through tenth order in Ref. 10, but they contain small round-off errors in the eighth figure at highest order. After correction of these errors they agree with our results. Of course, this is not a very stringent test of correctness. However, the extended expansions can be subjected, at all orders, to additional tests, some of which deriving from equations of Sec. III. First, we can check that, taking  $R=1$ , the coefficients of the single-variable expansions for the corresponding quantities of the isotropic 3D  $XY$  model, already known<sup>28</sup> through order 21, are reproduced. Moreover, we can observe that for  $R=0$  and  $\vec{R}=0$ , the expansions of  $\chi(N; K_1, R)$  and  $m^{(2)}(N; K_1, R)$  reduce, as they should, to those of the corresponding quantities in the 2D (Refs. 29 and 30) and the 1D  $XY$  model, respectively. Finally, we take advantage of Eqs. (15) and (23) of the next section, in the case of the susceptibility [or Eqs. (22) and (24) for the second moment], to pin down two more among the  $r+1$  series coefficients occurring at the  $r$ th order. The success of this variety of tests, through all orders we have computed, strengthens the confidence that our extensions of the bivariate expansions are correct.

Our data for the susceptibility and the second moment of the correlation function are tabulated in an appendix reported only in the arXiv version of this paper.

## III. DIMENSIONAL CROSSOVER

For all values of  $N$ , at fixed  $R>0$ , the 3D spin models described by Hamiltonian (1) display a conventional power-law critical transition. As the reduced deviation  $\tau(N; R) = 1 - K_1 / K_{1c}(N; R)$  from the critical point  $K_{1c}(N; R)$  of the 3D system with anisotropy parameter  $R$  tends to zero from above, for the susceptibility one has  $\chi(N; K_1, R) \sim [\tau(N; R)]^{-\gamma(N; R)}$ , while for the correlation length one has

$\xi(N; K_1, R) \sim [\tau(N; R)]^{-\nu(N; R)}$ . The universality hypothesis<sup>13</sup> dictates that, for a given value of  $N$ , the critical exponents  $\gamma(N; R)$  of the susceptibility and  $\nu(N; R)$  of the correlation length of the  $N$ -vector system with arbitrary finite anisotropy should be independent of  $R$  as long as  $R > 0$  and thus should coincide with the exponents  $\gamma(N; 1)$  and  $\nu(N; 1)$  of the isotropic system. The initial part of our analysis of the HT expansions in Secs. IV A and IV B will be devoted to the determination of the critical temperature and exponents as functions of  $R$  for  $R > 0$ , thus making it possible to test numerically the universality of the exponents with respect to  $R$ .

When  $R \rightarrow 0$  the sc lattice system crosses over to a stack of uncoupled square-lattice systems, and we expect that an anomalous behavior at criticality indicates a discontinuous change in universality class. The crossover behavior is described by a phenomenological scaling theory introduced in Ref. 4 and subsequently extended and clarified in Refs. 2, 5, and 6. This approach, whose validity has been verified in the mean-field approximation and in the spherical model,<sup>5,6</sup> is first outlined for  $N=1$  (the Ising model) in Sec. IV A and then generalized to cover also the case  $N \geq 2$  in Sec. IV B. The predictions of the scaling theory for  $N=2$  will finally be compared to the HT-based approximations in Sec. IV C.

An anomalous behavior is also expected to occur in the  $\bar{R} \rightarrow 0$  limit in which the sc lattice crosses over to the linear lattice.

#### A. $N=1$ model

For  $N=1$ , both the 3D and the 2D  $N$ -vector models display a power-law critical behavior. As a consequence, for all critical exponents  $\gamma(1; R)$ ,  $\nu(1; R)$ , ... of the 3D Ising model with anisotropy  $R$ , the  $R \rightarrow 0$  limit exists and yields the corresponding exponents  $\gamma(1; 0)$ ,  $\nu(1; 0)$ , ... of the 2D Ising model. Thus, for  $R=0$ , one can write

$$\chi(1; K_1, 0) \approx \chi_{as}(1; K_1, 0) \sim \tau^{-\gamma(1; 0)} \quad (5)$$

and

$$\xi(1; K_1, 0) \approx \xi_{as}(1; K_1, 0) \sim \tau^{-\nu(1; 0)} \quad (6)$$

in the critical region. For brevity, only in this subsection we have set  $\tau = \tau(1; 0) = 1 - K_1/K_{1c}(1; 0)$ . The crossover from the 3D to the 2D critical behavior, as  $R \rightarrow 0$ , can be described in terms of a direct generalization<sup>2-7</sup> of the usual phenomenological scaling hypothesis valid for isotropic systems. Specifically, it is assumed that, for sufficiently small  $\tau$  and  $R$ , the scaling form of the singular part  $f(1; \tau, h, R)$  of the free energy in a field  $h$  embodies also the anisotropy parameter  $R$  as follows:

$$f(1; \tau, h, R) \approx \tau^{2-\alpha(1; 0)} F(h \tau^{-\beta(1; 0) - \gamma(1; 0)}, R \tau^{-\phi}), \quad (7)$$

where  $F$  is a universal function. The exponents  $\alpha(1; 0)$  and  $\beta(1; 0)$  refer to the specific heat and the magnetization of the 2D Ising model. The quantity  $\phi$ , called *crossover exponent*, is universal and must coincide<sup>7,31-33</sup> with  $\gamma(1; 0)$ , the exponent of the susceptibility of the 2D Ising model. Taking two derivatives with respect to  $h$  in Eq. (7) one obtains that the susceptibility in zero field is given by

$$\chi(1; K_1, R) \approx A^{(0)} \tau^{-\gamma(1; 0)} X^{(0)}(B^{(0)} R \tau^{-\phi}), \quad (8)$$

where  $X^{(0)}(x)$ , called universal *susceptibility crossover-scaling function* is uniquely defined by choosing the normalization  $X^{(0)}(0) = dX^{(0)}(0)/dx = 1$ .  $A^{(0)}$  and  $B^{(0)}$  are nonuniversal scale factors. Here and in what follows, a superscript zero is attached to all quantities related to the zeroth moment of the correlation function.

Scaling forms (7) and (8) provide an interpolation between the critical behaviors in 2D (i.e., for  $R=0$ ) and in 3D for small nonvanishing  $R$  and thus can describe both of them. In particular, by the normalization of  $X^{(0)}(x)$ , Eq. (8) is consistent with the 2D critical behavior Eq. (5) of the susceptibility in 2D. On the other hand, the consistency of Eq. (8) with the 3D critical behavior  $\chi(1; K_1, R) \approx \tilde{A}^{(0)} [\tau(1; R)]^{-\gamma(1; R)}$  is achieved by assuming that  $X^{(0)}(x)$  is singular as  $K_1 \rightarrow K_{1c}(1; R)$  and, for  $x$  in a vicinity of  $\dot{x}$ , has the structure

$$X^{(0)}(x) \approx \frac{\dot{X}^{(0)}}{(1-x/\dot{x})^{\gamma(1; R)}}, \quad (9)$$

with

$$\dot{x} = B^{(0)} R [\tau_R(1; 0)]^{-\gamma(1; 0)} \quad (10)$$

and  $\tau_R(1; 0) = 1 - K_{1c}(1; R)/K_{1c}(1; 0)$ . Due to the universality of  $X^{(0)}(x)$ , also the constants  $\dot{X}^{(0)}$  and  $\dot{x}$  are universal.

For small positive  $R$ , the solution of Eq. (10) yields the reduced shift of the critical temperature of the 3D Ising system with anisotropy  $R$  from the critical temperature of its 2D limit, which has the following asymptotic behavior

$$K_{1c}(1; 0)/K_{1c}(1; R) - 1 \sim R^{1/\phi}, \quad (11)$$

with  $\phi = \gamma(1; 0)$ . Therefore this important result is a simple consequence of the crossover-scaling ansatz Eq. (8) and of Eq. (5), the critical behavior of  $\chi(1; K_1, 0)$ .

The validity of the extended scaling assumptions Eqs. (7) and (8) can be further tested by a numerical HT analysis of the asymptotic behavior as  $\tau \rightarrow 0$  of the successive partial derivatives

$$\Xi_s^{(0)}(1; K_1, 0) = \left( \frac{\partial^s \chi(1; K_1, R)}{\partial R^s} \right)_{R=0} \quad (12)$$

of  $\chi(1; K_1, R)$  with respect to  $R$ , evaluated in the  $R=0$  limit. The critical behavior of these quantities is defined by the asymptotic form

$$\Xi_s^{(0)}(1; K_1, 0) \approx C_s^{(0)}(1) \tau^{-\lambda_s} \quad (13)$$

as  $\tau \rightarrow 0$ . By the extended scaling hypothesis Eq. (8) the exponents of divergence  $\lambda_s$  should satisfy the relation

$$\lambda_s = \gamma(1; 0) + s\phi = (s+1)\gamma(1; 0). \quad (14)$$

For  $s=1$ , Eq. (14) can also be seen as an immediate consequence of the relation

$$\Xi_1^{(0)}(N; K_1, 0) = 2K_1 [\chi(N; K_1, 0)]^2 \quad (15)$$

proved in Ref. 7 for  $N$ -vector models with *arbitrary*  $N$ .

For  $N=1$  and  $s=2, 3$ , the validity of Eq. (14) is confirmed using the inequalities

$$8K_1^2[\chi(1;K_1,0)]^3 \geq \Xi_2^{(0)}(1;K_1,0) \geq 4K_1^2[\chi(1;K_1,0)]^3, \quad (16)$$

$$48K_1^3[\chi(1;K_1,0)]^4 \geq \Xi_3^{(0)}(1;K_1,0) \geq 8K_1^3[\chi(1;K_1,0)]^4. \quad (17)$$

A proof<sup>7</sup> of Eqs. (16) and (17) is based on classical correlation inequalities known to hold in the  $N=1$  case. Some generalization of Eqs. (16) and (17) might still be valid also for models with  $N>1$ .

For the  $l$ th moment of the correlation function, one can assume the validity of the extended scaling form

$$m^{(l)}(1;K_1,R) \approx A^{(l)}\tau^{-\gamma(1;0)-l\nu(1;0)}X^{(l)}(B^{(l)}R\tau^{-\gamma(1;0)}). \quad (18)$$

As a consequence, a generalization of Eq. (14) is thus obtained also for the exponents of divergence  $\mu_s$  of the successive  $R$  derivatives

$$\Xi_s^{(2)}(1;K_1,0) = \left( \frac{\partial^s m^{(2)}(1;K_1,R)}{\partial R^s} \right)_{R=0} \quad (19)$$

of the second moment of the correlation function  $m^{(2)}(1;K_1,R)$ , which are defined by the asymptotic behavior

$$\Xi_s^{(2)}(1;K_1,0) \approx C_s^{(2)}(1)\tau^{-\mu_s} \quad (20)$$

as  $\tau \rightarrow 0$ . From Eq. (18) it follows that the exponents  $\mu_s$  should satisfy the relation

$$\mu_s = 2\nu(1;0) + (s+1)\gamma(1;0). \quad (21)$$

For  $s=1$ , the validity of Eq. (21) is immediately proved<sup>7</sup> by using an analog of Eq. (15) for the second moment  $m^{(2)}(N;K_1,R)$  of the correlation function:

$$\begin{aligned} \Xi_1^{(2)}(N;K_1,0) &= 2K_1\{[\chi(N;K_1,0)]^2 + 2\chi(N;K_1,0)m^{(2)}(N;K_1,0)\}. \end{aligned} \quad (22)$$

Notice that, as for Eq. (15), also the validity of Eq. (22) is not limited to the  $N=1$  model.

For  $s=2$  and 3, inequalities analogous to Eqs. (16) and (17) can be derived<sup>7</sup> also for  $\Xi_s^{(2)}(1;K_1,0)$ , thus justifying Eq. (20). A numerical test<sup>7,10,11</sup> of Eqs. (13), (14), (20), and (21) gave support to the crossover-scaling ansatz for  $N=1$ .

As a final remark, let us point out that, using the variables  $K_2$  and  $\bar{R}=1/R$ , more convenient in the  $R \rightarrow \infty$  limit in which the system becomes an array of one-dimensional spin chains, also the following relations, valid for arbitrary  $N$ , are obtained:

$$\left( \frac{\partial \chi(N;K_2,\bar{R})}{\partial \bar{R}} \right)_{\bar{R}=0} = 4K_2[\chi(N;K_2,0)]^2, \quad (23)$$

$$\begin{aligned} &\left( \frac{\partial m^{(2)}(N;K_2,\bar{R})}{\partial \bar{R}} \right)_{\bar{R}=0} \\ &= 4K_2\{[\chi(N;K_2,0)]^2 + 2\chi(N;K_2,0)m^{(2)}(N;K_2,0)\}. \end{aligned} \quad (24)$$

Here  $\chi(N;K_2,0)$  and  $m^{(2)}(N;K_2,0)$  indicate, respectively, the susceptibility and the second moment of the correlation function of the anisotropic  $N$ -vector model for  $\bar{R}=0$ , i.e., in 1D. Equations (15) and (22)–(24) are quite helpful also to validate the computation of the bivariate series expansion.

It is now also clear<sup>5,6</sup> how to compute an expansion of the universal susceptibility crossover-scaling function  $X^{(0)}(x)$  in powers of  $x$ . Observing that the critical amplitudes  $C_s^{(0)}(1)$  in Eq. (13) are expressed in terms of  $X^{(0)}(x)$  as

$$C_s^{(0)} = A^{(0)}(B^{(0)})^s \left( \frac{d^s X^{(0)}(x)}{dx^s} \right)_{x=0} \quad (25)$$

and that the dependence on the nonuniversal quantities  $A^{(0)}$  and  $B^{(0)}$  disappears from the ratios

$$Q_s = \frac{C_{s-1}^{(0)}C_{s+1}^{(0)}}{[C_s^{(0)}]^2}, \quad (26)$$

the expansion of  $X^{(0)}(x)$  for small  $x$  can be written in the form

$$\begin{aligned} X^{(0)}(x) &= 1 + x + \frac{Q_1}{2}x^2 + \frac{Q_1Q_2}{3!}x^3 + \frac{Q_1^2Q_2^2Q_3}{4!}x^4 \\ &+ \frac{Q_1^4Q_2^3Q_3^2Q_4}{5!}x^5 + \frac{Q_1^5Q_2^4Q_3^3Q_4^2Q_5}{6!}x^6 \dots \end{aligned} \quad (27)$$

which is universal, i.e., the coefficients are independent of the lattice structure. The calculation of  $X^{(0)}(x)$  can be numerically extended to the whole interval  $[0,\bar{x}]$  by Padé approximants. This approximation can be shown to yield an asymptotic description of the properties of  $\chi(1;K_1,R)$  which, in the range of validity of the crossover-scaling ansatz, is consistent with those obtained from other approaches.

### B. $N \geq 2$ models

A slightly different formulation of the extended phenomenological scaling is necessary in the  $N \geq 2$  cases that will be considered in this subsection simply because the asymptotic relations Eqs. (7) and (8), and therefore Eqs. (11), (13), and (20) cannot be valid anymore. Before introducing this issue, it is convenient to make a brief digression to recall how the critical behavior in 2D has been characterized<sup>19</sup> in the  $N=2$  case. As  $K_1 \rightarrow K_{1c}(2;0)$  from below, the divergence of the correlation length of the 2D XY model is dominated by an exponential singularity

$$\xi(2;K_1,0) \approx \xi_{as}(2;K_1,0) = D \exp[b\tau^{-\sigma}]. \quad (28)$$

In this and the following sections, for brevity, we have set  $\tau = \tau(2;0) = 1 - K_1/K_{1c}(2;0)$ . The universal exponent  $\sigma$  is expected to take the value  $\sigma=1/2$ , while  $b$  is a nonuniversal positive constant. The critical behavior of the singular part of the free energy is predicted to be



$$f_{sing}(2;K_1,0) \approx f_{as}(2;K_1,0) = \tilde{F}[\xi_{as}(2;K_1,0)]^{-2}, \quad (29)$$

with  $\tilde{F}$  as a nonuniversal amplitude, while for the susceptibility one has

$$\chi(2;K_1,0) \approx \chi_{as}(2;K_1,0) = A^{(0)} \tau^{-\theta\sigma} \exp\{[2 - \eta(2;0)]b\tau^{-\sigma}\} \quad (30)$$

as  $K_1 \rightarrow K_{1c}(2;0)$  from below. For  $K_1 > K_{1c}(2;0)$  both  $\xi$  and  $\chi$  are infinite. The quantity  $\eta(2;0)=1/4$  is the exponent characterizing the large-distance behavior at criticality of the spin-spin correlation function for the 2D XY model. In Eq. (30), the presence of a multiplicative correction to the leading singular behavior by a power of the logarithm of  $\xi$  (equivalently by a power of  $\tau^{-\sigma}$ ) and the value of the exponent  $\theta$  are still controversial. A rediscussion<sup>34</sup> of the renormalization-group approach indicates that  $\theta=0$ , while a recent high-order HT study<sup>30</sup> and a high-precision Monte Carlo study<sup>35</sup> support the estimate  $\theta \approx 1/16$ . However, the precise value of  $\theta$  is practically irrelevant in our discussion of scaling. The numerical value of the susceptibility critical amplitude  $A^{(0)}$  depends on the value assumed for  $\theta$ , but it is also irrelevant in the determination of the crossover-scaling function  $X^{(0)}(x)$ .

Let us now return to the scaling issue and make the natural assumption that the crossover-scaling ansatz, introduced in the Ising case for the singular part of the free energy in an external field of modulus  $h$ , can be simply generalized to the XY model case as follows:

$$f(2; \tau, h, R) \approx [\xi_{as}(2;K_1,0)]^{-2} F\{h\xi_{as}(2;K_1,0) \times [\chi_{as}(2;K_1,0)]^{1/2}, R\chi_{as}(2;K_1,0)\} \quad (31)$$

for sufficiently small positive  $R$  and  $\tau$ . Taking two derivatives with respect to the field, we get the generalized scaling form for the susceptibility in zero field

$$\chi(2;K_1,R) \approx \chi_{as}(2;K_1,0) X^{(0)}[B^{(0)}R\chi_{as}(2;K_1,0)]. \quad (32)$$

Here  $X^{(0)}(x)$  is a universal crossover-scaling function that can be uniquely defined assuming that  $X^{(0)}(0)=dX^{(0)}(0)/dx=1$ .  $B^{(0)}$  is a nonuniversal scale factor.

The generalized crossover-scaling forms (31) and (32) are immediately shown to reduce to Eqs. (7) and (8) in the  $N=1$  case by using Eqs. (5) and (6) and the scaling laws. However, for  $N=2$ , these forms have the additional virtue of correctly allowing for the fact that the critical singularities in 2D are not powerlike since the exponents  $\gamma(2;R)$  and  $\nu(2;R)$  [as well as  $\alpha(2;R)$  and  $\beta(2;R)$ ] are ill-defined in the  $R \rightarrow 0$  limit and also no crossover exponent  $\phi$  exists.

By the normalization of  $X^{(0)}(x)$ , scaling form (32) is consistent with the 2D critical behavior; since for  $R=0$  and  $\tau \rightarrow 0$ , one has  $\chi(2;K_1,0) \approx \chi_{as}(2;K_1,0)$ . On the other hand, for small but nonvanishing  $R$ , the conventional 3D critical behavior  $\chi(2;K_1,R) \sim \tilde{A} \tau^{-\gamma(2;R)}$  as  $\tau(2;R) \rightarrow 0$  is recovered by assuming that  $X^{(0)}(x)$  has the same singularity structure as in Eq. (9), i.e., that  $X^{(0)}(x) \approx \dot{X}^{(0)}/(1-x/\dot{x})^{\gamma(2;R)}$ , when  $x$  is in a neighborhood of  $\dot{x}$ , with

$$\dot{x} = B^{(0)}R\chi_{as}[2;K_{1c}(2;R),0]. \quad (33)$$

As in the  $N=1$  case, by solving Eq. (33), we can obtain the small- $R$  asymptotic behavior of the reduced critical-temperature shift of the anisotropic 3D model from its 2D limiting value

$$K_{1c}(2;0)/K_{1c}(2;R) - 1 \approx V/[\ln(R/W)]^2. \quad (34)$$

Here  $V=[2-\eta(2;0)]^2 b^2$  and  $W=\dot{x}/BA^{(0)}$  are nonuniversal constants. The higher-order corrections to the leading behavior in Eq. (34) are also expressed in terms of inverse powers of  $|\ln R|$  and possibly of  $\ln|\ln R|$ , depending on the value of the exponent  $\theta$ . It is interesting to point out that the original argument<sup>36,37</sup> for Eq. (34) relied on approximate renormalization-group ideas rather than being a simple consequence of the generalization of the crossover-scaling ansatz and of the exponentially singular critical behavior of the XY model.

As a further immediate consequence of our scaling assumption Eq. (32), the divergence of the successive  $R$  derivatives of the susceptibility turns out to have the structure

$$\begin{aligned} \Xi_s^{(0)}(2;K_1,0) &\approx C_s^{(0)}(2)[\chi_{as}(2;K_1,0)]^{s+1} \\ &\sim \tau^{\theta\sigma(s+1)} \exp\{[2 - \eta(2;0)]b(s+1)\tau^{-\sigma}\} \end{aligned} \quad (35)$$

as  $\tau \rightarrow 0$ , which can be seen as a natural generalization of Eq. (13). For  $s=1$ , the validity of Eq. (35) is an obvious consequence of Eq. (15). For  $s=2$  and 3, it might follow from some extension of the inequalities Eqs. (16) and (17). Equation (35) will be numerically tested in Sec. IV C by studying the behavior of  $\Xi_s^{(0)}(2;K_1,0)$  as  $K_1 \rightarrow K_{1c}(2;0)$  for the first six values of  $s$ .

By assuming for the second moment  $m^{(2)}(2;K_1,R)$  of the correlation function the crossover-scaling form

$$m^{(2)}(2;K_1,R) \approx m_{as}^{(2)}(2;K_1,0) X^{(2)}[B^{(2)}R\chi_{as}(2;K_1,0)], \quad (36)$$

where  $m_{as}^{(2)}(2;K_1,0)=4[\xi_{as}(2;K_1,0)]^2\chi_{as}(2;K_1,0)$ , the analog of Eq. (20) is obtained

$$\Xi_s^{(2)}(2;K_1,0) \approx C_s^{(2)}(2)[\xi_{as}(2;K_1,0)]^2[\chi_{as}(2;K_1,0)]^{s+1}. \quad (37)$$

By Eq. (22), this equation is certainly valid for  $s=1$ , and we shall suppose that it is true also for  $s>1$ . Also Eq. (37) will be tested numerically in Sec. IV C by the same method used for Eq. (35).

The HT expansions of  $\Xi_s^{(0)}(2;K_1,0)$  and  $\Xi_s^{(2)}(2;K_1,0)$  can be immediately read from our tables of the series coefficients of  $\chi(2;K_1,K_2)$  and  $m^{(2)}(2;K_1,K_2)$ , respectively. The expansion in powers of  $x$  of the universal scaling function  $X^{(0)}(x)$  can be computed by the same procedure already outlined for the  $N=1$  case.

A generalized scaling assumption can be made also to describe the crossover of the 3D system to a set of one-dimensional noninteracting XY chains as  $R \rightarrow \infty$ . It is now convenient to shift to the variables  $K_2$  and  $\bar{R}=1/R$ . One has simply to observe that in this case  $K_{2c}(2;\bar{R}) \rightarrow \infty$  as  $\bar{R} \rightarrow 0$

and that, at criticality, the divergence of the susceptibility in one dimension is

$$\chi(2;K_2,0) \approx \chi_{as}(2;K_2,0) = \bar{A}^{(0)}K_2^2. \quad (38)$$

Then it is natural to introduce a universal susceptibility scaling function  $\bar{X}^{(0)}(x)$ , normalized like  $X^{(0)}(x)$  and with the same singularity structure and assume that

$$\chi(2;K_2,\bar{R}) \approx \chi_{as}(2;K_2,0)\bar{X}^{(0)}[\bar{B}^{(0)}\bar{R}\chi_{as}(2;K_2,0)]. \quad (39)$$

It follows that

$$K_{2c}(2;\bar{R}) \sim \bar{R}^{-1/2} \quad (40)$$

as  $\bar{R} \rightarrow 0$ . Moreover, predictions for the  $\bar{R}$  derivatives of the susceptibility, similar to those mentioned above for the  $R$  derivatives, are easily obtained along the same lines.

Let us finally point out that generalized crossover-scaling assumptions of the same form as Eqs. (31) and (32) can be written down also for the  $N$ -vector spin models with  $N > 2$ . The main difference is that for these models,  $K_{1c}(N;R) \rightarrow \infty$  as  $R \rightarrow 0$  and that, in 2D, the critical divergence of the correlation-function moments and of the correlation length is exponential in  $K_1$ . As a result, we can conclude that for small  $R$ , we have  $K_{1c}(N;R) \sim |\ln R|$ , by the same scaling arguments used above. Here, we shall not further investigate the models with  $N > 2$ , but only note that a general discussion<sup>38</sup> of the numerical difficulties of the HT-expansion approach to the  $N$ -vector models in 2D suggests that a HT study of the crossover might also meet with similar problems caused by the unphysical singularities in the complex inverse-temperature plane revealed by a large- $N$  study.<sup>39</sup>

#### IV. NUMERICAL ANALYSIS

We shall now turn to an analysis of our HT expansions to study the crossover behavior Eq. (34) of the critical inverse-temperature  $K_{1c}(2;R)$  as  $R \rightarrow 0$  or  $R \rightarrow \infty$ , to check the universality with respect to  $R$  of the critical exponents of the anisotropic system, to test the validity of the consequences Eqs. (34), (35), (37), and (40) of the crossover-scaling assumptions Eqs. (32), (36), and (39) and finally to obtain an approximation of the susceptibility scaling function  $X^{(0)}(x)$ .

##### A. Estimates of the critical temperature as function of $R$

Let us first study the behavior of the susceptibility  $\chi(2;K_1,R)$  as function of  $K_1$  at fixed values of  $R$  to determine the critical locus. We shall later use these results to bias the computation of the critical exponents of the susceptibility and of the correlation length and verify that they satisfy the universality hypothesis, as long as  $R > 0$ . For simplicity, we have analyzed the behavior of our expansions as functions of  $K_1$  at fixed values of  $R$  (or as functions of  $K_2$  at fixed values of  $\bar{R}$ ), using the conventional *single-variable* methods<sup>16</sup> of series analysis, namely, PAs or inhomogeneous differential approximants (DAs). It may be helpful to recall that in the DA approach a (single-variable) power series is resummed by expressing it as the solution of a linear (first- or higher-

order) differential equation with polynomial coefficients and inhomogeneous term, appropriately defined in terms of the coefficients of the given series. We believe that taking advantage of the large number of series coefficients presently available, also more complex methods of series analysis, such as multivariate PAs (Ref. 40) or partial-differential approximants,<sup>15</sup> become now worth exploring. However, we have not yet thoroughly pursued these approaches.

In our computation of the critical temperature, for  $R > 0.05$ , we have used second-order DAs and have considered the class of  $[k,l,m;n]$  DAs restricted by the conditions:  $13 \leq k+l+m+n \leq 19$  with  $k \geq 3; l \geq 3; m \geq 3$ . Among these, we have selected the DAs with the additional properties of being defect-free, i.e., having sufficiently isolated physical singularities, and of being near-diagonal, i.e., such that  $|k-l|, |l-m| \leq 2, 1 < n < 4$ . Finally, we have not “biased” the DAs, i.e., we have not discarded the approximants yielding critical exponents with values outside appropriate limits. Here we are using the standard notation in which  $k, l, m, n$  denote the degrees of the polynomial coefficients and of the inhomogeneous term of the differential equation defining the DA. These rather technical specifications are given only to make our results completely reproducible. However, we have always made sure that our final estimates, within a fraction of their uncertainties, are essentially independent of the precise definition of the DA class examined. At a given value of  $R$ , our central estimate of  $K_{1c}(2;R)$  is the sample mean of the locations of the singularities in this class of DAs, taken after dropping evident outliers. A small multiple of the spread of the reduced sample is taken as an estimate of the uncertainty. Possible residual unsaturated trends of the central estimates, as the number of series coefficients used in the calculation is increased, have been accounted for by attaching generous error bars to the final estimates. Sometimes we have made small corrections of these central estimates (always well within the uncertainties) suggested by a comparison with the sequence of Zinn-Justin modified-ratio<sup>16,41</sup> estimates.

Coming to the numerical results, let us first note that, for  $R=1$ , our estimate  $K_{1c}(2;1)=0.22710(3)$  compares well both with our older estimate<sup>28</sup>  $K_{1c}(2;1)=0.227095(10)$  obtained from HT expansions of order 21 for the isotropic 3D  $XY$  system and with the much more precise<sup>42</sup> recent determination  $K_{1c}(2;1)=0.2270827(5)$ , obtained from a high-accuracy Monte Carlo simulation.

The determination of the line of critical points  $K_{1c}(2;R)$  for very small values of  $R$ , as required for a numerical test of the predicted crossover behavior Eq. (34), is a delicate task both by series study and by simulation. The progressive decoupling of the horizontal layers as  $R \rightarrow 0$  makes a reliable extrapolation of the susceptibility to its genuinely 3D critical behavior possible only from a closer and closer vicinity of the critical point. (See also the comments to Fig. 5 in the next subsection.) As a consequence, the precision of the estimates of the location of the critical point and of the critical exponents tends to deteriorate as  $R \rightarrow 0$ . We have observed that, for  $R \leq 0.05$ , a reasonable increasing behavior of  $K_{1c}(2;R)$  is still obtained simply by assuming what will be actually borne out by our analysis, namely, that the critical exponent of the susceptibility is universal, to a good approximation, all along the critical locus for  $R > 0$  and thus by

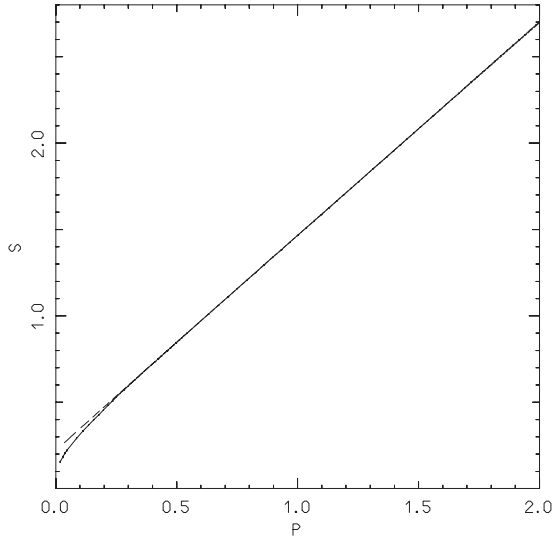


FIG. 1. The quantity  $S = K_{1c}(2;0)/K_{1c}(2;R) - 1$ , which represents the reduced shift of the critical temperature of the system with anisotropy  $R$  from its 2D limit, is plotted vs  $P = R^{2/3}$ . A continuous line interpolates our estimates, whose error bars are smaller than the width of the line, except for very small  $R$ . The dashed line (hardly visible except for small  $R$ ), which is superimposed to the continuous one, is the result of a fit of the expression  $f(R) = aR^g + c$  to our data for  $0.05 < R < 3.4$ . The values of the fit parameters are  $a \approx 1.245$ ,  $g \approx 0.661$ , and  $c \approx 0.221$ .

imposing also a “weak” bias on this exponent when computing  $K_{1c}(2;R)$ . This simply amounts to discard from the sample of our data the critical temperature estimates obtained from DAs whose exponent at the singularity differs by more than 10% from the expected value of  $\gamma(2;1)$ . Even after this simple improvement of the analysis, for  $R < R_{\min} \approx 0.0015$ , our expansions do not anymore seem to be long enough to locate the critical point with acceptable accuracy. Therefore we shall not report estimates for  $R < R_{\min}$ . Our results for the reduced shift  $S = K_{1c}(2;0)/K_{1c}(2;R) - 1$  of the critical temperature from its 2D limiting value are plotted vs  $R^{2/3}$  in Fig. 1. The value  $K_{1c}(2;0) = 0.56000(5)$  of the critical inverse temperature of the 2D XY model on the square lattice has been taken from recent<sup>29,30,35</sup> high-precision studies. A short list of our numerical DA estimates of  $K_{1c}(2;R)$  for  $0.005 \leq R \leq 3.4$  can be found in Table I.

It should be noticed that the critical curve must be separately symmetric under the transformations  $K_1 \rightarrow -K_1$  and

TABLE I. Estimates of the critical inverse temperatures of the anisotropic system for various values of  $R$ . Only the two smallest- $R$  estimates are biased, the remaining ones being unbiased.

$R$	$K_{1c}(2;R)$	$R$	$K_{1c}(2;R)$	$R$	$K_{1c}(2;R)$
3.4	0.13901(6)	1.3	0.20727(3)	0.15	0.3562(3)
3.0	0.14724(6)	1.0	0.22710(3)	0.1	0.3776(5)
2.6	0.15693(6)	0.8	0.24394(3)	0.075	0.391(2)
2.2	0.16861(5)	0.6	0.26537(3)	0.05	0.409(3)
1.9	0.17914(5)	0.4	0.29460(6)	0.0125	0.454(4)
1.6	0.19176(4)	0.2	0.3395(2)	0.005	0.473(4)

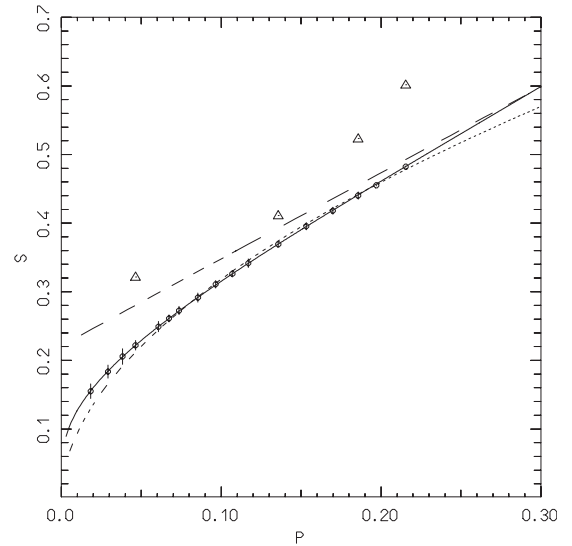


FIG. 2. A blowup of the lower left corner of Fig. 1, showing the plot of the reduced critical-temperature shift  $S = K_{1c}(2;0)/K_{1c}(2;R) - 1$  vs  $P = R^{2/3}$ . The continuous line is a fit of the expression  $V/[\ln(R/W)]^2$  to our estimates of  $S$  (circles) for  $0.005 < R < 0.15$ . The values of the parameters are  $V \approx 11.34$  and  $W \approx 12.7$ . The short-dashed line is the result of a fit of the expression  $\tilde{f}(R) = aR^{g'}$ , with  $a \approx 1.08$  and  $g' \approx 0.354$ , to the same set of data. The long-dashed line is the result of the same fit as in Fig. 1 of the expression  $f(R) = aR^g + c$ , with parameters  $a \approx 1.245$ ,  $g \approx 0.661$ , and  $c \approx 0.221$ , to all data for  $0.05 \leq R \leq 3.4$ . The triangles are small- $R$  estimates of  $S$  taken from the simulation of Ref. 21.

$K_2 \rightarrow -K_2$ . Therefore the ferromagnetic phase diagram, so far represented, should be completed by the remaining branches of the critical locus.

In Fig. 1 we have also shown that  $S$  has a very simple dependence on  $R$ , valid to a high accuracy over a wide range of intermediate-large (but not too large) values of  $R$ . The expression  $f(R) = aR^g + c$ , with  $a \approx 1.245$ ,  $g \approx 0.661$ , and  $c \approx 0.221$  interpolates quite accurately our data points for  $S$  in the interval  $0.025 < R < 2.9$ , visibly departing from them only for small  $R$ , i.e., in the region where the crossover is expected to occur. The value of the exponent  $g$  justifies our choice to plot  $S$  vs  $R^{2/3}$ . It would be interesting to look for an analytic explanation of this purely empirical remark.

It is interesting to remember that a not very different  $R^{4/7}$  law was conjectured<sup>43</sup> to describe the  $R$  dependence of the critical temperature over the region  $0.01 < R < 0.7$ , while for  $R > 0.7$ , a linear law was proposed. This suggestion was based on a self-consistent mean-field approximation, which is probably not very accurate for small  $R$  and is certainly inaccurate for intermediate-large  $R$ .

Let us now turn to the small- $R$  region to study the features of the crossover behavior. Figure 2 is a blowup of the lower left corner of Fig. 1 showing our estimates of the critical temperature for  $R < 0.13$ . We can notice that they clearly depart from the simple  $R^{2/3}$  behavior indicated by a long-dashed line. A continuous line indicates the result of a fit of the asymptotic expression  $V/[\ln(R/W)]^2$  of Eq. (34) predicted by the crossover-scaling theory to describe the behavior of the reduced temperature shift in the crossover region.



Restricting the fit to the critical-temperature estimates which fall within the window ( $0.0025, R_{\max}=0.1$ ), we determine the values of the parameters  $V \approx 11.34$  and  $W \approx 12.7$ . In the same figure, for comparison, we have reported also some old Monte Carlo estimates<sup>21</sup> of  $K_{1c}(2;R)$  in the small  $R$  range. In spite of their order-of-magnitude agreement with our series estimates, these simulation data seem to suggest a qualitatively different behavior as  $R \rightarrow 0$ . We must therefore suppose that they are affected by large errors (unfortunately not assessed in Ref. 21) from underestimated finite-size effects because the volume of the simulated system was small (at most  $20^3$ ) and no finite-size-scaling analysis was performed. A more recent simulation,<sup>22</sup> also carried out with  $20^3$  sized systems and extending to much smaller values of  $R$ , is likely to suffer from similar problems although its results seem to show a better agreement with ours.

Some remarks have to be made on Fig. 2. First, one should be aware that a logarithmic behavior is quite difficult to identify numerically by using data which refer to only a two-decade variation in the independent variable since, over a restricted range, it can also be well represented as a power-law behavior with a small exponent. Moreover the choice of the window of values of  $R$  to be studied is a delicate issue because the upper end of the window should be sufficiently small that both the crossover-scaling assumptions and the asymptotic behavior Eq. (34) apply with small corrections, while the lower end should be sufficiently large that our estimates of the critical temperature are not too uncertain. In our case the value of  $R_{\max}$  can be varied by a factor of two or more, still obtaining good fits of the same functional form, with not very different values of the parameters  $V$  and  $W$ . Finally, we observe that the best-fit value of  $V$  is not very different from its expected value  $[2 - \eta(2;0)]^2 b^2 \approx 9.5$ , while the value of  $W$  is much larger. It is reasonable to interpret these results as an indication that  $R_{\min}$  is still too large and therefore the higher-order corrections to asymptotic form (34), suppressed only by inverse powers of  $|\ln R|$ , are still important so that  $V$  and  $W$  can only be effective parameters. To conclude, in spite of the notable extension of the HT expansions we have analyzed, these results still can give only a suggestive indication that our estimates of the critical temperature for small  $R$  are compatible with the predicted asymptotic behavior Eq. (34).

On the other hand, one might wish to describe also this crossover behavior by a power law and fit an expression  $\tilde{f}(R) = aR^{g'}$ , of the same form as Eq. (11) valid in the  $N=1$  case, to the same small- $R$  sample of our data points. We then find the following values of the parameters:  $a \approx 1.08$  and  $g' \approx 0.354$ . We have displayed also this fit in Fig. 2. Thus, if for consistency we describe also the critical behavior of the 2D  $XY$  model in terms of conventional power laws, this result suggests an unusually large susceptibility exponent, i.e.,  $\gamma(2;0) = 1/g' \approx 2.8$ . We can also observe that, subdividing the small- $R$  range into two intervals, this kind of fit would yield a smaller exponent  $g'$  in the leftmost interval. This suggests that even smaller values of the exponent  $g'$  (and thus larger values of the susceptibility exponent) are likely to be found if it were possible to further reduce both ends of the window of values of  $R$  under consideration, for example, by

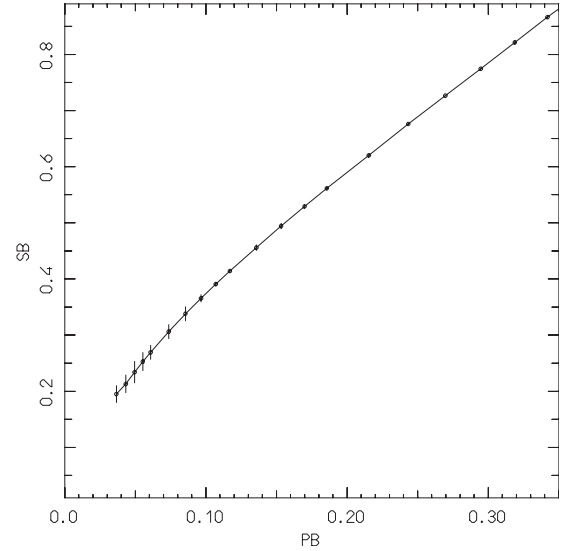


FIG. 3. A plot of  $SB = 1/2K_{2c}(2;\bar{R})$  (circles) vs  $PB = \bar{R}^{2/3}$  in the small  $\bar{R}$  region. A continuous line interpolates our estimates.

using future significantly longer HT expansions. It is then reasonable to believe that this power-law crossover is only apparent because the exponent is  $R$  dependent and vanishes as  $R \rightarrow 0$  and hence that we are actually representing a genuine logarithmic behavior as a power-law behavior.

In Fig. 3, we have plotted  $[2K_{2c}(2;\bar{R})]^{-1}$  vs  $\bar{R}^{2/3}$ . The behavior of the curve as  $\bar{R} \rightarrow 0$  also gives some support to the validity of Eq. (40) and therefore it confirms the generalized scaling approach to the crossover from 3D to 1D.

### B. Universality of the critical exponents with respect to $R$

Unfortunately, so far we have computed expansions only for the sc lattice structure and therefore our verification of the universality of certain quantities does not include their lattice independence but is limited to a test of their independence on  $R$ .

In the range  $R > 0.05$ , in which our computation of the critical temperature was completely unbiased, we have also evaluated both the critical exponents  $\gamma(2;R)$  and  $\nu(2;R)$  by using second-order DAs, chosen in the above specified class and biased with our estimates of  $K_{1c}(2;R)$ . We have also determined, by simple first-order DAs, the ratio of the logarithmic derivatives of  $m^{(2)}(N;K_1,R)/K_1$  and  $\chi(N;K_1,R)$ , whose value at  $K_{1c}(2;R)$  yields the ratio  $\nu(2;R)/\gamma(2;R)$ . In Fig. 4, we have plotted vs  $R$  our estimates of these exponents and of their ratio normalized to our estimates of  $\gamma(2;1) = 1.328(10)$ ,  $\nu(2;1) = 0.679(8)$ , and  $\nu(2;1)/\gamma(2;1) = 0.5099(6)$ , respectively. The central values of our estimates of the normalized exponents and of the exponent ratio are very near to unity and fairly independent of  $R$  within  $\approx 0.5\%$ , over a range wider than that shown in the figure, except for very small or large  $R$ , due to the expected crossover. These results support the universality with respect to  $R$  of the critical behavior for the anisotropic 3D model. It is fair to note that, while the deviations of our exponent estimates for the anisotropic system from those for the  $R=1$  system are uni-



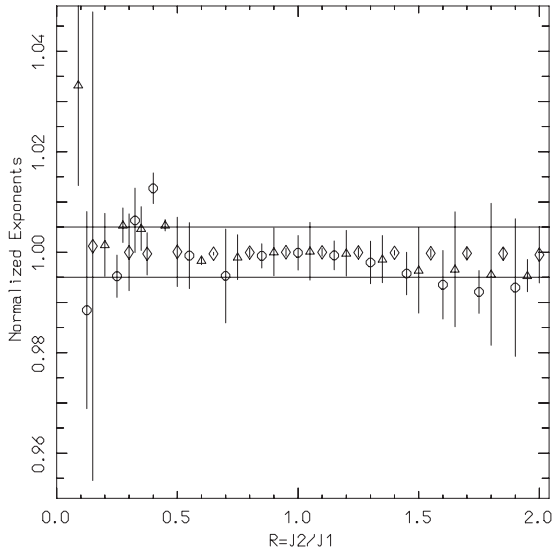


FIG. 4. Estimates of the exponents  $\gamma(2;R)$  (circles),  $\nu(2;R)$  (triangles), and of the ratios  $\nu(2;R)/\gamma(2;R)$  (rhombs) plotted vs the anisotropy parameter  $R$ . All these quantities are computed by DAs biased with the critical temperature and they are normalized to our estimates of their values at  $R=1$ . The horizontal lines are bands of 0.5% deviation from our estimates of  $\gamma(2;1)$ ,  $\nu(2;1)$ , and  $\gamma(2;1)/\nu(2;1)$ .

formly very small, our estimates of  $\gamma(2;1)$  and  $\nu(2;1)$  are larger, by  $\approx 1\%$ , than the most recent<sup>41,44</sup> estimates  $\gamma(2;1) = 1.3178(2)$  and  $\nu(2;1) = 0.67155(27)$ . On the contrary, the deviation of our estimates of the exponent ratio from its recent determination  $\nu(2;1)/\gamma(2;1) = 0.5096(3)$  is quite small. Substantially longer series or improved methods of exponent determination<sup>26,41,44</sup> might be necessary to remove the discrepancy in the exponent estimates, which certainly can be ascribed to the residual influence of the corrections to scaling.

In Fig. 5 we have plotted, for various fixed values of  $R$ , the effective exponent<sup>4,45</sup>  $\gamma_{eff}(2;K_1,R)$  of the susceptibility

$$\gamma_{eff}(2;K_1,R) = - \frac{d \ln \chi(2;K_1,R)}{d \ln \tau(2;R)}. \quad (41)$$

Roughly speaking, this quantity represents the local value of the critical exponent which would be inferred by a measure of the susceptibility in a neighborhood of  $K_1$  and only in the critical limit it coincides with the asymptotic critical exponent. By showing how the local critical behavior changes, this quantity is helpful to describe the crossover phenomena. The curves shown in the figure are obtained simply by forming the highest-order, defect-free, diagonal, or near-diagonal PAs of the HT expansion of the right-hand side of Eq. (41). The figure illustrates the narrowing down of the genuinely 3D critical region as  $R \rightarrow 0$  that was already discussed in the preceding subsection. More precisely, when  $R$  is not too small, the effective exponent is approximately independent of the temperature and stays close to its 3D asymptotic value. On the other hand, going to sufficiently small  $R$ , the effective exponent becomes increasingly temperature sensitive: in most of the HT temperature range it takes rather large values,

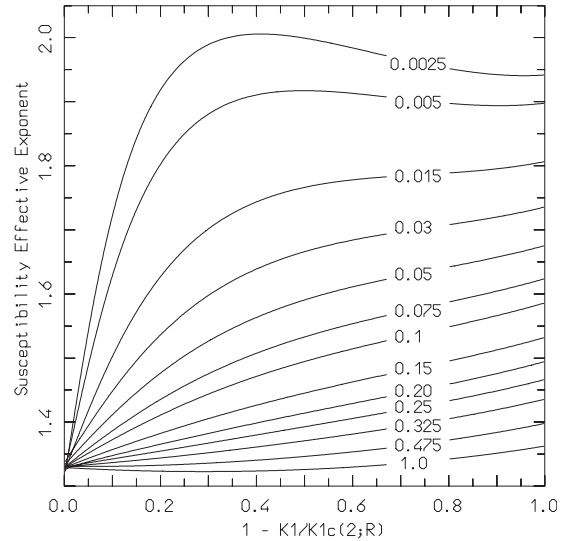


FIG. 5. The effective exponent  $\gamma_{eff}(2;K_1,R)$ , computed by PAs, for the susceptibility of the anisotropic system is plotted vs  $\tau(2;R) = 1 - K_1/K_{1c}(2;R)$  for various fixed values of  $R$  indicated on the corresponding curves.

which somehow reflect the exponential 2D critical singularity, and only as  $K_1$  gets very close to the critical value, it approaches the 3D asymptotic value.

In Fig. 6 we have plotted, for various fixed values of  $\bar{R}$ , the effective exponent  $\gamma_{eff}(2;K_2,\bar{R})$  of the susceptibility, defined in strict analogy with Eq. (41) to describe the crossover from 3D to 1D. Also in this case, the curves indicate a transition from a region of very high values of the effective exponent, reflecting the critical divergence of the susceptibility of the 1D system, to the asymptotic region where the 3D critical behavior is attained.

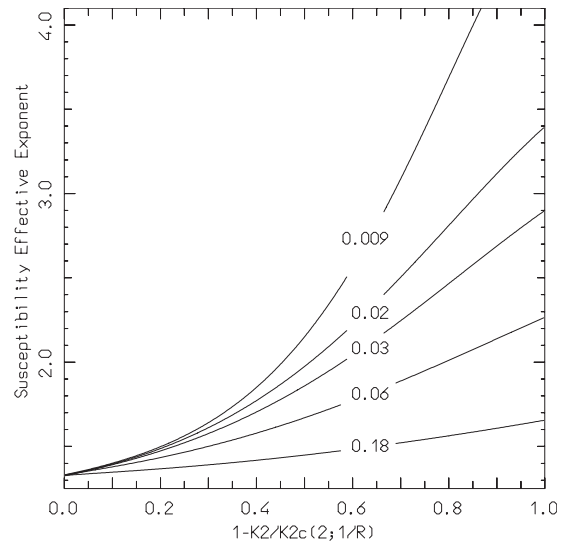


FIG. 6. The effective exponent  $\gamma_{eff}(2;K_2,\bar{R})$ , computed by PAs, for the susceptibility of the anisotropic system vs  $\tau(2;\bar{R}) = 1 - K_2/K_{2c}(2;\bar{R})$  for various fixed values of  $\bar{R}$  indicated on the corresponding curves.

TABLE II. Estimates, by first-order DAs, of the critical values  $G_s^{(0)}$  of the normalized ratios  $G_s^{(0)}(K_1)$  as  $K_1 \rightarrow K_{1c}(2;0)$ .

Critical value	$G_1^{(0)}$	$G_2^{(0)}$	$G_3^{(0)}$	$G_4^{(0)}$	$G_5^{(0)}$	$G_6^{(0)}$
1	1.00(1)	1.01(1)	1.00(2)	1.02(8)	0.95(15)	
Critical value	$G_1^{(2)}$	$G_2^{(2)}$	$G_3^{(2)}$	$G_4^{(2)}$	$G_5^{(2)}$	$G_6^{(2)}$
	1.04(5)	0.99(4)	0.99(1)	0.99(1)	0.99(3)	0.98(13)

### C. Critical behavior of $\Xi_0^{(0)}(2;K_1,0)$ : An approximation of the susceptibility crossover-scaling function $X^{(0)}(x)$

As sensitive and specific indicators to test the critical behavior Eq. (35) of the successive  $R$  derivatives of the susceptibility  $\Xi_s^{(0)}(2;K_1,0)$ , we have formed the normalized ratios of their logarithmic derivatives

$$G_s^{(0)}(K_1) = \frac{1}{s+1} \frac{d \ln[\Xi_s^{(0)}(2;K_1,0)]/dK_1}{d \ln[\Xi_0^{(0)}(2;K_1,0)]/dK_1}. \quad (42)$$

If Eq. (35), showing the critical behavior of  $\Xi_s^{(0)}(2;K_1,0)$ , is valid, the quantities  $G_s^{(0)}(K_1)$  are expected to tend to unity, as  $\tau \rightarrow 0$ , independently of  $s$ . This result is obvious for  $s=1$ , thanks to the exact relation Eq. (15), but for  $s > 1$  it ought to be numerically tested. We have used near-diagonal first-order DAs of the HT expansions of  $G_s^{(0)}(K_1)$  to estimate the limits of these quantities as  $K_1 \rightarrow K_{1c}(2;0)$ . Our results, summarized in Table II, support the validity of the asymptotic relation Eq. (35) to a good approximation when  $s=2,3,4,5,6$  and therefore lend support to the validity of the generalized crossover-scaling assumption Eq. (32). In general, it should not be surprising that the precision of these, as well as of the following estimates, is smaller than that reported in previous studies of much shorter series in the  $N=1$  case, in which the critical singularities are powerlike, because of the more complex structure of the critical singularity in the 2D XY model. One should also notice that the number of nontrivial expansion coefficients of the  $R$  derivatives of the moments of the correlation function and hence the precision of the numerical approximation for the quantities related to them, decreases as  $s$  increases. Therefore these tests are less reliable for values of  $s$  larger than those examined here.

A completely parallel study of the indicator  $G_s^{(2)}(K_1)$ , a strict analog of  $G_s^{(0)}(K_1)$  for the quantity  $\Xi_s^{(2)}(2;K_1,0)/[\xi(2;K_1,0)]^2$ , which can be associated to the  $R$  derivatives of the second moment of the correlation function, also leads to results in agreement with Eq. (37), albeit slightly less precise, because of the known slower convergence of the second moment expansion. Thus also the validity of Eq. (36) is confirmed. Our estimates of the limits of the quantities  $G_s^{(2)}(K_1)$  as  $K_1 \rightarrow K_{1c}(2;0)$  are also reported in Table II.

Let us now turn to the study of the universal crossover-scaling function  $X^{(0)}(x)$  of the susceptibility, following the procedure<sup>5,6</sup> described above in detail for the  $N=1$  case at the end of Sec. III A. As a first step, we have to determine the critical amplitudes  $C_s^{(0)}(2)$  of  $\Xi_s^{(0)}(2;K_1,0)$ , defined in Eq. (35) by the limit of the *effective amplitudes*  $C_s^{(0)}(2;K_1,0) = \Xi_s^{(0)}(2;K_1,0)/\chi^s(2;K_1,0)$  as  $K_1 \rightarrow K_{1c}(2;0)$ .

TABLE III. Estimates of the universal ratios  $Q_s$  computed by extrapolating first-order DAs of the effective ratios in Eq. (43).

$Q_1$	$Q_2$	$Q_3$	$Q_4$	$Q_5$	$Q_6$
1.584(6)	1.436(2)	1.287(9)	1.24(1)	1.18(1)	1.12(9)

The amplitudes  $C_s^{(0)}(2)$  are then used to form the universal ratios  $Q_s$ , defined by Eq. (26). Alternatively, the ratios  $Q_s$  can also be determined directly and perhaps more accurately by extrapolating the HT expansions of the *effective ratios*

$$Q_s(2;K_1,0) = \frac{\Xi_{s-1}^{(0)}(2;K_1,0)\Xi_{s+1}^{(0)}(2;K_1,0)}{[\Xi_s^{(0)}(2;K_1,0)]^2} \quad (43)$$

to  $K_1 = K_{1c}(2;0)$ . The estimates so obtained for the universal quantities  $Q_s = \lim_{K_1 \rightarrow K_{1c}} Q_s(2;K_1,0)$  are reported in Table III.

The coefficients of the small- $x$  expansion of  $X^{(0)}(x)$  are finally expressed in terms of the  $Q_s$ , as indicated in Eq. (27)

$$X^{(0)}(x) = 1 + x + 0.792(3)x^2 + 0.600(5)x^3 + 0.44(1)x^4 + 0.32(1)x^5 + 0.23(2)x^6 + 0.16(3)x^7 + \dots \quad (44)$$

Having assumed that  $X^{(0)}(x)$  is singular at  $\dot{x}$  and has the form  $X^{(0)}(x) \approx \dot{X}^{(0)}/(1-x/\dot{x})^{\gamma(2;R)}$  in a vicinity of  $\dot{x}$ , we can give a reasonably good estimate of  $\dot{x}$  by locating the nearest pole of the highest-order defect-free near-diagonal PAs of the expansion of  $[X^{(0)}(x)]^{1/\gamma(2;R)}$ . Choosing  $\gamma(2;R) = 1.3178(2)$  and allowing for the uncertainties of the expansion coefficients in Eq. (44) and the spread of the PA singularities, we can estimate  $\dot{x} = 1.475(15)$  and  $\dot{X}^{(0)} = 1.154(15)$ . A direct estimate of  $\dot{x}$ , by extrapolating to  $R=0$  the argument  $BR\chi_{as}(2;K_{1c}(2;R),0)$  of the scaling function, fails to yield a more accurate result because of the extrapolation uncertainties.

Let us represent the scaling function simply as  $X^{(0)}(x) = P(x/\dot{x})(1-x/\dot{x})^{-\gamma(2;R)}$ , where  $P(x/\dot{x})$  is some function interpolating between the small  $x$  and the large  $x$  behavior of  $X^{(0)}(x)$  and therefore taking the values  $P(0)=1$  and  $P(1) = \dot{X}^{(0)}$ . It turns out that the simple linear expression  $P(x/\dot{x}) = 1 + (\dot{X}^{(0)} - 1)x/\dot{x}$  is a quite accurate approximation of the regularized scaling function  $X^{(0)}(x)(1-x/\dot{x})^{\gamma(2;R)}$ . We have then used this approximate form of the crossover-scaling function to compute the effective exponent

$$\gamma_{eff}(2;R) = \frac{K_{1c}(2;R)}{K_{1c}(2;0)} \frac{\tau(2;R)}{[\tau(2;0)]^{\sigma+1}} b\sigma \left[ 1 + z \left( \frac{P'(z)}{P(z)} + \frac{\gamma(2;R)}{1-z} \right) \right], \quad (45)$$

with  $z = x/\dot{x}$ . The effective exponent computed using Eq. (45) is plotted vs  $\tau(2;R)$  in Fig. 7, in which we have shown the curves corresponding to the eight smallest values of  $R$  chosen in Fig. 5. The agreement between Figs. 5 and 7 can be considered as another satisfactory confirmation of the validity of the crossover-scaling ansatz if one observes that the former is a good PA representation of the effective exponent

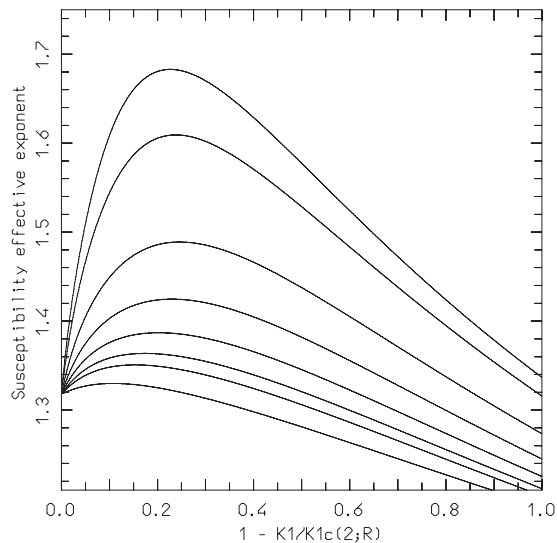


FIG. 7. The effective exponent  $\gamma_{eff}(2; K_1, R)$  of the susceptibility as obtained from the scaling form (45) plotted vs  $\tau(2; R) = 1 - K_1/K_{1c}(2; R)$ . From top to bottom  $R=0.0025, 0.005, 0.015, 0.03, 0.05, 0.075, 0.1, 0.15$ . These values of  $R$  coincide with the eight smallest values used in Fig. 5.

on the whole interval  $0 < K_1 < K_{1c}(2; R)$ , whereas the curves of Fig. 7 can be quantitatively reliable only in the small range of validity of the crossover-scaling form (32), for example, when  $\tau(2; R) \leq 0.05$  and  $R \leq 0.05$ .

## V. CONCLUSIONS

We have added 187 coefficients to the already known 66 coefficients of the bivariate HT expansion for the spin-spin

correlation function of the 3D XY model, with directionally anisotropic couplings, on the sc lattice. Analyzing these data by PA and DA methods, we have determined to a good precision the critical locus of the system in the ferromagnetic region and checked to a fair accuracy the universality of the critical exponents of the susceptibility and the correlation length with respect to the anisotropy parameter  $R$ . We have also shown that the main predictions of the extended scaling theory for the crossover from the 3D to the 2D critical regime, concerning both the behavior of the line of critical points  $K_{1c}(2; R)$  in the limit of small  $R$  and the critical divergence of the successive  $R$  derivatives, at  $R=0$ , of the susceptibility and of the second moment of the correlation function are compatible with the numerical extrapolations of our extended expansions. Finally, combining the HT expansions with the crossover-scaling ansatz, we have obtained a concrete approximate representation of the crossover-scaling function  $X^{(0)}(x)$  for the susceptibility and have shown that it reproduces, in an appropriately restricted temperature range, the effective exponent as computed by PAs on the HT side of the critical point.

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