



Critical exponents and equation of state of three-dimensional spin models

M. Campostrini^a, M. Hasenbusch^b, A. Pelissetto^c, P. Rossi^a and E. Vicari^a

^aDipartimento di Fisica dell'Università di Pisa and I.N.F.N., I-56126 Pisa, Italy

^bInstitut für Physik, Humboldt-Universität zu Berlin, Invalidenstr. 110, D-10115 Berlin, Germany

^cDipartimento di Fisica dell'Università di Roma I and I.N.F.N., I-00185 Roma, Italy

Three-dimensional spin models of the Ising and XY universality classes are studied by a combination of high-temperature expansions and Monte Carlo simulations. Critical exponents are determined to very high precision. Scaling amplitude ratios are computed via the critical equation of state. Our results are compared with other theoretical computations and with experiments, with special emphasis on the λ transition of ^4He .

1. INTRODUCTION

The notion of universality is central to the modern understanding of critical phenomena. It is therefore very important to compare high-precision theoretical and experimental determinations of universal quantities, such as critical exponents or universal ratios of amplitudes, for systems belonging to the same universality class.

Critical exponents and amplitudes parametrize the singular behavior of thermodynamical quantities in the vicinity of a critical point. In the high-temperature (symmetric) phase $t > 0$, $C_H \approx A^+ |t|^{-\alpha}$, $\chi \approx C^+ |t|^{-\gamma}$, $\xi \approx f^+ |t|^{-\nu}$, where $t = (T - T_c)/T_c$ is the reduced temperature, C_H is the specific heat, χ is the magnetic susceptibility, and ξ is the correlation length. In the low-temperature (broken) phase $t < 0$, $H \rightarrow 0$, $C_H \approx A^- |t|^{-\alpha}$, $\chi \approx C^- |t|^{-\gamma}$, $\xi \approx f^- |t|^{-\nu}$ (in the case of Ising), $M \approx B |t|^\beta$, where M is the magnetization. On the critical isotherm $t = 0$, $H \neq 0$, $\chi \approx C^c |H|^{-\gamma/\beta\delta}$, $\xi \approx f^c |H|^{-\nu/\beta\delta}$. At the critical point $t = 0$, $H = 0$ at nonzero momentum, the two-point function behaves like $\tilde{G}(q) \approx Dq^{\eta-2}$.

The *critical exponents* are universal, and are independent of the phase; they are related by the scaling and hyperscaling relations. The amplitudes are not universal, and their value depends on the phase; it is however possible to define *universal ratios of amplitudes*, which are independent of the normalization of H , M , and T .

The universality classes of Ising and XY in

three dimensions have been the subject of many theoretical studies. Nonetheless, we believe that further refinement is worthwhile: many critical phenomena in nature fall into these classes, and the precision of experiments is ever improving; moreover, several theoretical techniques can be applied and compared to each other.

High-temperature (HT) series expansion is one of the oldest and most successful approaches to the study of critical phenomena. We are extending the length of the series available for wide families of models belonging to the classes of universality we are interested in; so far we computed the two-point function of the three-dimensional Ising class to 25th order on the bcc lattice, and four-, six-... point functions to 21st, 19th... order [1]. Work is in progress on the sc lattice and on the XY class.

The precision of the results which can be extracted from long HT series is mainly limited by the presence of confluent corrections with noninteger exponents. Let us consider, e.g., the magnetic susceptibility χ ; near the critical temperature, it behaves like

$$\chi = Ct^{-\gamma} (1 + a_{0,1}t + a_{0,2}t^2 + \dots + a_{1,1}t^\Delta + a_{1,2}t^{2\Delta} + \dots + a_{2,1}t^{\Delta_2} + \dots).$$

While the exponents Δ , Δ_2 , ... are universal, the coefficients a are model dependent. For the models we are interested in, $\Delta \sim 0.5$ and $\Delta_2 \gtrsim 2\Delta$; therefore it is very helpful to select one-parameter

families of models, and tune the irrelevant parameter λ to the special value λ^* for which $a_{1,1} = 0$; we will call such models “improved”.

Monte Carlo (MC) algorithms and finite-size scaling techniques are very effective in the determination of λ^* and β_c , but not as effective in the computation of critical exponents or other universal quantities. On the other hand, the analysis of HT series is very effective in computing universal quantities, but not in computing λ^* and β_c .

The strength of the two methods can be combined by computing λ^* and β_c by MC, and feeding the resulting values into the analysis of HT series (by “biasing” the analysis); this greatly improves the quality of the results.

In order to keep systematic errors under control, we always select several different families of models in the same universality class and check that they give compatible results for universal quantities.

2. CRITICAL EXPONENTS

Without further discussion, we present in Table 1 a selection of results for the critical exponents γ , ν , and η of the three-dimensional Ising model; for other exponents, see Ref. [2]. We compare the most precise theoretical results and experiments. IHT denotes our results [2]; HT is a “traditional” HT determination [3]; MC are Monte Carlo results [4]; FT are results from a g expansion in fixed dimension [5]. Experimental results are LV for liquid-vapor transitions; BM for binary mixtures; MS for uniaxial magnetic systems; MI for micellar systems; cf. Refs. [2] and [6] for bibliographical details. The agreement between the different determinations is overall satisfactory.

On the theoretical side, similar techniques can be applied to the XY model, with results of comparable quality. The experimental situation is quite different: one extremely precise experiment on the λ transition of ^4He [7] overshadows the field. We present results for the critical exponents γ , η , and α (we remind that $d\nu = 2 - \alpha$) in Table 2 (cf. footnote 2 in Ref. [8] for discussion of the experimental results). Theoretical results are taken from Refs. [9] (IHT), [8] (IHT*), [3] (HT),

Table 1

Comparison of determinations of critical exponents of the three-dimensional Ising model.

	γ	ν	η
IHT	1.2371(4)	0.63002(23)	0.0364(4)
HT	1.2384(6)	0.6308(5)	
MC	1.2367(11)	0.6296(7)	0.0358(9)
FT	1.2405(15)	0.6300(15)	0.032(3)
LV	1.233(10)		0.042(6)
BM	1.228(39)	0.628(8)	0.0300(15)
MS	1.25(2)	0.64(1)	
MI	1.237(7)	0.630(12)	0.039(4)

Table 2

Comparison of determinations of critical exponents of the three-dimensional XY model.

	γ	η	α
^4He			-0.01056(38)
IHT	1.3179(11)	0.0381(3)	-0.0150(17)
IHT*	1.3177(5)	0.0380(4)	-0.0146(8)
HT	1.322(3)	0.039(7)	-0.022(6)
MC	1.3177(10)	0.0380(5)	-0.0148(15)
FT	1.3169(20)	0.0354(25)	-0.011(4)

[8] (MC), and [5] (FT). There is disagreement between IHT* and experiment; it would be interesting to improve further the theoretical computation, and to have an independent confirmation of the experimental measurement.

3. CRITICAL EQUATION OF STATE

The critical equation of state is a relation between thermodynamical quantities which is valid in both phases in the neighborhood of the critical point (cf., e.g., Ref. [10]).

In order to determine the critical equation of state, we start from the effective potential (Helmholtz free energy)

$$\mathcal{F}(M) = MH - \frac{1}{V} \log Z(H).$$

In the high-temperature phase, \mathcal{F} can be expanded in powers of M^2 around $M = 0$. By choosing appropriately the normalizations of the renormalized quantities, and using the “second

moment” mass m as mass scale, we can write

$$\Delta\mathcal{F} \equiv \mathcal{F}(M) - \mathcal{F}(0) = \frac{m^d}{g_4} A(z),$$

$$A(z) = \frac{1}{2}z^2 + \frac{1}{4!}z^4 + \sum_{j \geq 3} \frac{1}{(2j)!} r_{2j} z^{2j},$$

where z is the (rescaled) zero-momentum vacuum expectation value of the renormalized field, $r_{2j} = g_{2j}/g_4^{j-1}$, and g_{2j} is the renormalized zero-momentum $2j$ -point coupling constant. The (universal) critical limit of g_4 and r_{2j} can be computed from the HT expansion of the zero-momentum $2j$ -point Green’s function; for the Ising model, we obtain [2]

$$g_4 = 23.49(4), \quad r_6 = 2.048(5),$$

$$r_8 = 2.28(8), \quad r_{10} = -13(4).$$

The equation of state can now be written as

$$H(M, t) = \frac{\partial \mathcal{F}}{\partial M} \propto t^{\beta\delta} \frac{dA}{dz} = t^{\beta\delta} F(z), \quad (1)$$

$$z \propto Mt^{-\beta};$$

The analyticity properties of $F(z)$ are constrained by Griffiths’ analyticity conditions on $H(M, t)$.

It is possible to implement all analyticity and scaling properties of the critical equation of state introducing a parametric representation [11]

$$M = m_0 R^\beta \theta,$$

$$t = R(1 - \theta^2),$$

$$H = h_0 R^{\beta\delta} h(\theta), \quad h(\theta) = \theta + O(\theta^3).$$

The following correspondences should be noticed:

$$\theta = 0 \longrightarrow t > 0, M = 0;$$

$$\theta = 1 \longrightarrow t = 0;$$

$$\theta = \theta_0 \longrightarrow t < 0, M = M_0,$$

where θ_0 is the first positive zero of $h(\theta)$. The analytic properties of the equation of state are reproduced if $h(\theta)$ is analytic in the interval $[0, \theta_0]$.

Combining the parametric representation with Eq. (1), we obtain

$$z = \rho \theta^2 (1 - \theta^2)^{-\beta},$$

$$h(\theta) = \rho^{-1} (1 - \theta^2)^{\beta\delta} F(z(\theta)).$$

Table 3

Comparison of determinations of universal ratios of amplitudes of the three-dimensional Ising model.

	U_0	Q_c	U_ξ
IHT	0.530(3)	0.3330(10)	1.961(7)
HT+LT	0.523(9)	0.324(6)	1.96(1)
MC	0.560(10)	0.328(5)	1.95(2)
MC	0.550(12)		
FT	0.540(11)	0.331(9)	2.013(28)
BM	0.56(2)	0.33(5)	1.93(7)
MS	0.51(3)		1.92(15)
LV	0.538(17)	0.35(4)	

In the Ising case, corresponding to the breaking of a discrete symmetry, θ_0 is a simple zero of $h(\theta)$. We approximate $h(\theta)$ with an odd polynomial in θ , fixing its coefficients from the small- z expansion of $F(z)$. ρ is a free parameter; as long as we keep the parametric representation exact its value is immaterial, but it becomes significant once we make approximations. ρ can be used to optimize the approximation, and it can be determined from a global stationarity condition [2].

We use the values of $\beta, \delta, r_6, r_8, r_{10}$ obtained by IHT to compute successive approximations to $h(\theta)$; we check the stability of the values of several universal amplitude ratios in order to select the best approximation. Among the many amplitude ratios which can be computed from $h(\theta)$, we report in Table 3 $U_0 = A^+/A^-$, $Q_c = B^2(f^+)^3/C^+$, $U_\xi = f^+/f^-$; many more ratios can be found in Ref. [2]. HT+LT is a combination of HT and low-temperature expansion [12,13]; the other theoretical determinations are the same discussed for the critical exponents, and are taken from Refs. [2] (IHT), [14,15] (MC), and [16–18] (FT). For experimental data, see Refs. [2] and [6]. The agreement between the different determinations is again satisfactory.

In the XY case, corresponding to the breaking of a continuous symmetry, θ_0 is a double zero of $h(\theta)$. We therefore set

$$h(\theta) = \theta(1 - \theta^2/\theta_0^2)^2(1 + c_2\theta^2 + c_4\theta^4 \dots).$$

We fix θ_0, c_2, \dots from the small- z expansion of

Table 4

Comparison of determinations of the universal ratio $U_0 = A^+/A^-$ of the three-dimensional XY model.

	A^+/A^-
${}^4\text{He}$	1.0442
IHT+ ${}^4\text{He}$	1.055(3)
IHT*	1.062(4)
FT	1.056(4)
ε -exp	1.029(13)

$F(z)$, and ρ from the requirement $h(\theta) \approx (\theta_0 - \theta)^2$ for $\theta \rightarrow \theta_0$.

Only the ratio A^+/A^- is measured experimentally to high precision [7]. We report a selection of theoretical determinations: IHT+ ${}^4\text{He}$ is our IHT computation, using as input for α the experimental value $\alpha = -0.01285(38)$ [19]; IHT* is a complete IHT computation, without experimental input [8]; FT is a g expansion in fixed dimension [16]; ε -exp is obtained by ε expansion [17]. The value of A^+/A^- is strongly correlated with the value of α , and all disagreement between IHT* and experiment can be reconduced to the discrepancy in α .

4. CONCLUSIONS

The study of HT series of “improved” models, with parameters determined by MC simulations, allowed us to compute with high precision the universal quantities (critical exponents and effective potential) characterizing the critical behavior of the symmetric phase.

Suitable approximation schemes allow the reconstruction of the critical equation of state starting from the symmetric phase; many universal amplitude ratios can be computed.

For the Ising universality class, theoretical computations are much more precise than experiments. On the other hand, for the XY class, some very precise experimental results for α and A^+/A^- have been obtained [7]. There is disagreement with the most precise theoretical results [8]. A new-generation experiment is in preparation [20]; it would be interesting to improve further the theoretical computations as well.

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