# High-precision estimates of critical quantities by means of improved Hamiltonians

Massimo Campostrini, Paolo Rossi, Ettore Vicari
*Dipartimento di Fisica and INFN – Sezione di Pisa*
*Università degli Studi di Pisa*
*I-56127 Pisa, ITALY*

Martin Hasenbusch
*Institut für Physik*
*Humboldt-Universität zu Berlin*
*D-10115 Berlin, GERMANY*

Andrea Pelissetto
*Dipartimento di Fisica and INFN – Sezione di Roma I*
*Università degli Studi di Roma "La Sapienza"*
*I-00185 Roma, ITALY*

December 12, 2000

**Abstract**

Three-dimensional spin models of the Ising and XY universality classes are studied by a combination of high-temperature expansions and Monte Carlo simulations applied to improved Hamiltonians. The critical exponents and the critical equation of state are determined to very high precision.

# 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 amplitude ratios, for systems belonging to the same universality class.

There exist several different methods for determining critical quantities. One may study lattice models by means of high-temperature (HT) expansions or Monte Carlo (MC) simulations, or may consider continuum models and apply the well-known methods of perturbative field theory. All these methods require some extrapolation: in HT studies one wishes to determine the behavior at the critical point $\beta_c$ from a perturbative series around $\beta = 0$; in MC studies that use finite-size scaling methods, an extrapolation $L \to \infty$ is needed; in perturbative field-theory calculations one must compute the value for $g = g^*$, $g^*$ being the fixed point, from a perturbative series in powers of $g$. The accuracy of these extrapolations depends on the analytic behavior of the considered functions at $\beta_c$ or $g^*$, which, in turn, is determined by the renormalization-group (RG) theory. The complex structure of the critical behavior, characterized by a multitude of subleading exponents $\omega_i$, gives rise to nonanalyticities at the critical (or fixed) point that make the extrapolations difficult and often introduce large and dangerously undetectable systematic errors. We will not review here the field-theoretical case and we address the reader to Refs. [1–4] and we will only discuss HT and MC methods.

The precision of the results which can be extracted from the analysis of HT series and from MC simulations is mainly limited by the presence of confluent corrections with noninteger exponents. Let us consider, e.g., the magnetic susceptibility $\chi(L, T)$ in a finite box $L^d$, as a function of the reduced temperature $t$. The analyses of HT expansions aim to determine the infinite-volume asymptotic behavior for $t \to 0$, which is

$$\chi(\infty, t) \;\; = \;\; C t^{-\gamma}(1 + a_{0,1} t + ... + a_{1,1} t^{\Delta} + a_{1,2} t^{2\Delta} + ... + a_{2,1} t^{\Delta_2} + ...), \tag{1}$$

where $\Delta$, $\Delta_2$, ... are universal exponents. Analogously, MC simulations may try to determine the volume dependence of $\chi(L, t)$ at the critical point (or, in more sophisticated and efficient approaches, for a sequence of temperatures $t(L)$ approaching $t = 0$ as $L \to \infty$):

$$\chi(L, 0) \;\; = \;\; \hat{C} L^{\gamma/\nu}(1 + \hat{a}_{1,1} L^{-\Delta/\nu} + \hat{a}_{1,2} L^{-2\Delta/\nu} + ... + \hat{a}_{2,1} L^{-\Delta_2/\nu} + ...). \tag{2}$$

In both calculations the corrections with exponents $\Delta$ or $\Delta/\nu$ are one of the most important sources of systematic errors. To overcome these problems one may use improved models, that is models for which the leading correction to scaling vanishes, i.e. $a_{1,1} = \hat{a}_{1,1} = 0$. Such models can be determined by considering a one-parameter family of theories belonging to the given universality class, depending, say, on $\lambda$, and by tuning the irrelevant parameter $\lambda$ to the special value $\lambda^\star$ for which $a_{1,1} = \hat{a}_{1,1} = 0$; we will call such models "improved".

MC algorithms and finite-size scaling techniques are very effective in the determination of $\lambda^\star$ and $\beta_c$, 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 $\lambda^\star$ and $\beta_c$.

The strength of the two methods can be combined by computing $\lambda^\star$ and $\beta_c$ 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.

| | Ising | | | XY | | |
|---|---|---|---|---|---|---|
| | $\gamma$ | $\nu$ | $\eta$ | $\gamma$ | $\eta$ | $\alpha$ |
| IHT$^\star$ | 1.2372(3) | 0.6301(2) | 0.0364(4) | 1.3177(5) | 0.0380(4) | −0.0146(8) |
| IHT | 1.2371(4) | 0.6300(2) | 0.0364(4) | 1.3179(11) | 0.0381(3) | −0.0150(17) |
| HT | 1.2375(6) | 0.6302(4) | | 1.322(3) | 0.039(7) | −0.022(6) |
| MC | 1.2367(11) | 0.6296(7) | 0.0358(9) | 1.3177(10) | 0.0380(5) | −0.0148(15) |
| FT(a) | 1.2396(13) | 0.6304(13) | 0.0335(25) | 1.3169(20) | 0.0354(25) | −0.011(4) |
| FT(b) | 1.2403(8) | 0.6303(8) | 0.0335(6) | 1.3164(8) | 0.0349(8) | −0.0112(21) |

Table 1: Critical exponents of the three-dimensional Ising and XY models.

In order to keep systematic errors under control, one may consider 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 2 a selection of results for the critical exponents $\gamma$, $\nu$, and $\eta$ of the three-dimensional Ising model; for other exponents, see Ref. [5]. IHT denotes the results of Ref. [5], where three different improved models were considered. IHT$^\star$ is a new determination in which we bias the analyses by using the MC estimate of $\beta_c$, as we did in Ref. [6] for the XY model. HT is a "traditional" HT determination [7] obtained by analyzing the 25th-order series for the Ising model obtained in Ref. [8] by means of biased approximants; MC are Monte Carlo results for the $\phi^4$ improved Hamiltonians [9] (see also Ref. [10]); FT are results from the field-theoretical expansion in fixed dimension: results (a) are taken from Ref. [11], results (b) from Ref. [12]. Other results can be found in Ref. [13]. The agreement among the different determinations is overall satisfactory, although small systematic deviations are observed between the lattice (IHT and MC) results and the field-theoretic estimates. We suspect that the error estimates of Ref. [12] are quite too optimistic.

Similar techniques can be applied to the XY model, with results of comparable quality. We present results for the critical exponents $\gamma$, $\eta$, and $\alpha$ (we remind that $d\nu = 2 - \alpha$) in Table 2. They are taken from Refs. [14] (IHT), [6] (IHT$^\star$), [15] (HT), [6] (MC), [11] (FT(a)), and [12] (FT(b)). Other results can be found in Ref. [13]. These results should be compared with the precise experimental estimate [16] $\alpha = -0.01056(38)$ obtain from a Space Shuttle experiment for the $\lambda$ transition of $^4$He (cf. footnote 2 in Ref. [6] for discussion of the experimental results). There is disagreement between IHT$^\star$ 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 equation of state relates the thermodynamical quantities $M$, $H$, and $T$. It is easily accessible experimentally and thus it is important to have predictions for its behavior in the critical limit.

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

$$\mathcal{F}(M,t) = MH - \frac{1}{V}\log Z(H,t). \tag{3}$$

In the critical limit $\mathcal{F}(M,t)$ obeys a general scaling law:

$$\Delta\mathcal{F} \equiv \mathcal{F}(M) - \mathcal{F}(0) = t^{d\nu}\widehat{F}_{\rm sing}(Mt^{-\beta}). \tag{4}$$

In the HT phase, $\mathcal{F}$ can be expanded in powers of $M^2$ around $M = 0$. We can write

$$\Delta\mathcal{F} \equiv \mathcal{F}(M) - \mathcal{F}(0) = \frac{m^d}{g_4}A(z), \tag{5}$$

$$A(z) = \frac{1}{2}z^2 + \frac{1}{4!}z^4 + \sum_{j\geq 3}\frac{1}{(2j)!}r_{2j}z^{2j}, \tag{6}$$

where $z \propto Mt^{-\beta}$—the normalization is fixed by Eq. (6)—, $m$ is the second-moment mass, and $g_4$ is the renormalized zero-momentum four-point coupling constant. In the critical limit, $t \to 0$, $M \to 0$ at $z$ fixed, the function $A(z)$ is universal. 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 functions. For the Ising model, we obtain [5]

$$g_4 = 23.54(4), \qquad r_6 = 2.048(5),$$
$$r_8 = 2.28(8), \qquad r_{10} = -13(4).$$

By using (6), the equation of state can now be written as

$$H(M,t) = \frac{\partial\mathcal{F}}{\partial M} \propto t^{\beta\delta}\frac{dA}{dz} \equiv t^{\beta\delta}F(z), \tag{7}$$

Equivalently, one can write

$$H(M,t) = aM^\delta f(x), \tag{8}$$

where $x \propto tM^{-1/\beta}$ is normalized so that $x = -1$ corresponds to the coexistence curve and $a$ is fixed by the normalization condition $f(0) = 1$. The advantage of this representation is that by varying $x$ for $x > -1$ one obtains the full equation of state, while, by using $F(z)$ an analytic continuation in the complex plane is needed to reach the coexistence curve. The analyticity properties of $F(z)$ and $f(x)$ are constrained by Griffiths' analyticity.

It is possible to implement all analyticity and scaling properties of the critical equation of state introducing a parametric representation [17–19]

$$M = m_0 R^\beta \theta,$$
$$t = R(1-\theta^2),$$
$$H = h_0 R^{\beta\delta} h(\theta),$$

| | $U_0$ | $U_2$ | $Q_c$ | $U_\xi$ |
|---|---|---|---|---|
| IHT | 0.530(3) | 4.77(2) | 0.3330(10) | 1.961(7) |
| HT+LT | 0.523(9) | 4.95(15) | 0.324(6) | 1.96(1) |
| MC | 0.560(10) | 4.75(3) | 0.328(5) | 1.95(2) |
| MC | 0.550(12) | | | |
| FT | 0.540(11) | 4.72(17) | 0.331(9) | 2.013(28) |

Table 2: Universal amplitude ratios for the three-dimensional Ising model.

where $h(\theta)$ is normalized as $h(\theta) = \theta + O(\theta^3)$. Note that $\theta = 0$ corresponds to the HT phase $t > 0, M = 0$, $\theta = 1$ to the critical isotherm $t = 0$, and $\theta = \theta_0$, where $\theta_0$ is the first positive zero of $h(\theta)$, to the coexistence curve. The analytic properties of the equation of state are reproduced if $h(\theta)$ is analytic in the interval $[0, \theta_0)$. Given $h(\theta)$ the equation of state is easily obtained:

$$f(x) = \theta^{-\delta}\frac{h(\theta)}{h(1)}, \qquad\qquad x = \frac{1-\theta^2}{\theta_0^2 - 1}\left(\frac{\theta_0}{\theta}\right)^{1/\beta}. \tag{9}$$

Approximate representations of the equation of state are obtained by approximating $h(\theta)$ be an odd polynomial in $\theta$, i.e.

$$h(\theta) = \theta + \sum_{n=1}^{k} h_{2n+1}\theta^{2n+1}. \tag{10}$$

In Ref. [5] the coefficients were determined by using IHT results for the constants $r_{2n}$ and a variational condition. More precisely, one first uses the $(k-1)$ estimates of $r_6$, ..., $r_{2k+2}$ to fix $h_5$, ..., $h_{2k+1}$ in terms of $h_3$—in Ref. [5] the variable $\rho^2 = 6(\gamma + h_3)$ was used— and then requires physical results to be stationary with respect to variations of $h_3$. The idea behind this method is that in the exact case the function $h(\theta)$ is not uniquely defined: There exists a one-parameter family of equivalent $h(\theta)$. Thus, one parameter in $h(\theta)$ can be fixed at will. Whenever we approximate $h(\theta)$ this is no longer true. What we can require is that physical results have the weakest possible dependence on the parameter.

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. In Table 3 we report the results of Ref. [5] for the following amplitude ratios: $U_0 = A^+/A^-$, $U_2 = C^+/C^-$, $Q_c = B^2(f^+)^3/C^+$, $U_\xi = f^+/f^-$. The amplitudes are defined in terms of the critical behavior for $t \to 0^\pm$ of the specific heat $C_H = A^\pm|t|^{-\alpha}$, of the second-moment correlation length $\xi = f^\pm|t|^{-\nu}$, of the susceptibility $\chi = C^\pm|t|^{-\gamma}$, and of the spontaneous magnetization $M = B(-t)^\beta$. We compare these estimates with results obtained using different methods. HT+LT is a combination of HT and low-temperature expansions [20, 21]; the other theoretical determinations are the same discussed for the critical exponents, and are taken from Refs. [5] (IHT), [22, 23] (MC), and [24–26] (FT). The agreement among the different determinations is again satisfactory.

In the XY case, there are Goldstone singularities at the coexistence curve. In three dimensions, the leading singular behavior is correctly reproduced if $h(\theta) \sim (\theta - \theta_0)^2$. We may therefore set

$$h(\theta) = \theta(1 - \theta^2/\theta_0^2)^2 \left(1 + \sum_{n=1}^{k} c_n \theta^n\right). \qquad (11)$$

The constant $\theta_0$ and the $k$ coefficients $c_n$ are fixed [6, 14] by requiring the approximation to reproduce the $(k+1)$ parameters $r_6, \ldots, r_{2k+4}$.

Only the ratio $U_0 = A^+/A^-$ is measured experimentally to high precision. [16] Such a ratio has been determined in Ref. [6] using the equation of state and the IHT$^\star$ estimate of $\alpha$: They obtain $U_0 = 1.062(4)$. This result disagrees with the experimental estimate $U_0 = 1.0442$. However, the estimate of $U_0$ is strongly correlated to that of $\alpha$. Indeed, by using a slightly lower value of $\alpha$, $\alpha = -0.01285(38)$, Ref. [27] found $U_0 = 1.055(3)$. Thus, the disagreement between the estimate of Ref. [6] and experiment can be reconduced to the discrepancy in $\alpha$. Other estimates of $\alpha$ have been obtained by using the fixed-dimension expansion, [24] $U_0 = 1.056$, and the $\epsilon$-expansion, [25] $U_0 = 1.029(13)$.

# 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 equation of state—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 $\alpha$ and $A^+/A^-$ have been obtained. [16] There is disagreement with the most precise theoretical results. [6] A new-generation experiment is in preparation [28]; it would be interesting to improve further the theoretical computations as well.

# References


[1] B. G. Nickel, in *Phase Transitions*, ed. by M. Lévy, J. C. Le Guillou, and J. Zinn-Justin (Plenum, New York and London, 1982).

[2] A. Pelissetto and E. Vicari, *Nucl. Phys.* B **519**, 626 (1998).

[3] P. Calabrese, M. Caselle, A. Celi, A. Pelissetto, and E. Vicari, *J. Phys.* A **33**, 8155 (2000).

[4] M. Caselle, A. Pelissetto, and E. Vicari, hep-th/0010228.

[5] M. Campostrini, A. Pelissetto, P. Rossi, and E. Vicari, *Phys. Rev.* E **60**, 3526 (1999).

[6] M. Campostrini, M. Hasenbusch, A. Pelissetto, P. Rossi, and E. Vicari, cond-mat/0010360.

[7] P. Butera and M. Comi, *Phys. Rev.* B **62**, 14837 (2000).

[8] M. Campostrini, cond-mat/0005130.

[9] M. Hasenbusch, *J. Phys.* A **32**, 4851 (1999).

[10] M. Hasenbusch, K. Pinn, and S. Vinti, *Phys. Rev.* B **59**, 11471 (1999).

[11] R. Guida and J. Zinn-Justin, *J. Phys.* A **31**, 8103 (1998).

[12] F. Jasch and H. Kleinert, cond-mat/9906246v2.

[13] A. Pelissetto and E. Vicari, cond-mat/0012164.

[14] M. Campostrini, A. Pelissetto, P. Rossi, and E. Vicari, *Phys. Rev.* B **61**, 5905 (2000).

[15] P. Butera and M. Comi, *Phys. Rev.* B **56**, 8212 (1997).

[16] J. A. Lipa *et al.*, *Phys. Rev. Lett.* **76**, 944 (1996); **84**, 4894 (2000).

[17] P. Schofield, *Phys. Rev. Lett.* **22**, 606 (1969).

[18] P. Schofield, J. D. Lister, and J. T. Ho, *Phys. Rev. Lett.* **23**, 1098 (1969).

[19] R. Guida and J. Zinn-Justin, *Nucl. Phys.* B **489**, 626 (1997).

[20] A. J. Liu and M. E. Fisher, *Physica* A **156**, 35 (1989).

[21] M. E. Fisher and S.-Y. Zinn, *J. Phys.* A **31**, L629 (1998).

[22] M. Caselle and M. Hasenbusch, *J. Phys.* A **30**, 4963 (1997).

[23] M. Hasenbusch and K. Pinn, *J. Phys.* A **31**, 6157 (1998).

[24] S. A. Larin, M. Mönnigman, M. Strösser, and V. Dohm, *Phys. Rev.* B **58**, 3394 (1998).

[25] C. Bagnuls, C. Bervillier, D. I. Meiron, and B. G. Nickel, *Phys. Rev.* B **35**, 3585 (1987).

[26] G. Münster and J. Heitger, *Nucl. Phys.* B **424**, 582 (1994); C. Gutsfeld, J. Küster, and G. Münster, *Nucl. Phys.* B **479**, 654 (1996).

[27] M. Campostrini, A. Pelissetto, P. Rossi, and E. Vicari, *Phys. Rev.* B **62**, 5843 (2000).

[28] J. A. Nissen, D. R. Swanson, Z. K. Geng, V. Dohm, U. E. Israelsson, M. J. DiPirro, and J. A. Lipa, Low Temp. Phys. **24**, 86 (1998).