RECENT THEORETICAL ESTIMATES OF THE CRITICAL EXPONENTS

V. A. Rabinovich and Yu. E. Sheludyak UDC 536.425/44

It is shown that the latest estimates of the critical exponents obtained by different methods can be represented as fractions: $\eta = 1/32$ and $\nu = 17/27$. New formulas are given which reproduce the values of the critical exponents for systems with various dimensionalities and numbers of order parameters.

In the theory of critical phenomena normally six critical exponents are used: α, the exponent of the specific heat at constant volume c_V (the specific heat c_H in zero magnetic field H = 0); β, the exponent of the coexistence curve (magnetization); γ, the exponent of the isothermal compressibility (susceptibility); δ, the exponent in the dependence of the pressure on density on the critical isotherm (dependence of the magnetic field intensity on the magnetization); ν, the exponent for the correlation range; η, the exponent of the correlation function. The magnetic analogs of the thermodynamic quantities for a liquid–gas system are given in parentheses.

The critical exponents are related to each other by the equations [1]:

$$\alpha + 2\beta + \gamma = 2, \tag{1}$$

$$\gamma = \beta(\delta - 1), \tag{2}$$

$$\alpha = 2 - d\nu, \tag{3}$$

$$\gamma = (2 - \eta)\nu, \tag{4}$$

where d is the dimensionality of the system. Therefore, if two of the critical exponents are known, the relations (1) through (4) can be used to calculate the others.

Up until 1972, the only source of theoretical information on the values of the critical exponents of pure materials was the analysis of the series expansions of the lattice gas model (three-dimensional Ising model) [2]. For different lattices (simple cubic, bcc, fcc, and diamond) from 15 to 40 terms are known for the high and low-temperature series for the specific heat, magnetization, susceptibility, and spherical moments of the correlation function. The critical exponent α, β, γ, ν can be determined from these series.

The calculation of the coefficients of the series for the Ising model is a very complicated combinatorial problem and the results obtained pushed the limits of the computers in 1972 [2-8].

The method of obtaining the critical exponents from analysis of the series expansions is itself simple [9, 10]. Because the asymptotic behavior of a quantity given by a power series

$$f(x) = \sum_n a_n x^n; \tag{5}$$

is determined by a function of the form

$$f(x) = E(1 - yx)^{-\varepsilon}, \tag{6}$$

the n-th coefficient of the series is given by the expression

$$a_n = E\left(\frac{n+\varepsilon-1}{n}\right) y^n, \tag{7}$$

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where $y = x_c^{-1}$ is the radius of convergence of the series; $[(n+\varepsilon-1)/n] = [\varepsilon(\varepsilon+1)\ldots(\varepsilon+n-1)/n!]$ is the binomial coefficient.

The expansion parameter x in the Ising model is usually the variable $v = \mathrm{th}(J/kT)$ for $T \geq T_c$ and $u = \exp(-4J/kT)$ for $T \leq T_c$, where J is the interaction parameter for nearest neighbors and k is the Boltzmann constant.

The ratio of successive coefficients of the series (5) can be written as

$$r_n = \frac{a_n}{a_{n-1}} = \left(1 + \frac{\varepsilon - 1}{n}\right) y. \tag{8}$$

The limit of the sequence $\{r_n\}$ as $1/n \to 0$ determines the radius of convergence y of the series (the critical temperature). Expanding in y, we obtain from (8) a sequence of estimates of the critical exponent

$$\varepsilon_n = n(r_n y^{-1} - 1) + 1. \tag{9}$$

Having the values y and ε, we obtain from (7) a sequence of estimates of the critical amplitude

$$E_n = a_n \Big/ \left[\binom{n+\varepsilon-1}{n} y^n\right]. \tag{10}$$

Usually the value of ε_n depends on the number of terms in the series. Therefore it is necessary to extrapolate the sequence $\{\varepsilon_n\}$ to an infinite number of terms of the series

$$\varepsilon_n^{(m)} = \frac{1}{m}[n\varepsilon_n^{(m-1)} - (n-m)\varepsilon_{n-1}^{(m-1)}]. \tag{11}$$

Here m is the order of the extrapolation, and m = 0 corresponds to the original sequence $\{\varepsilon_n\}$.

The logarithmic derivative of the function f(x) is

$$F(x) = \frac{d \ln f(x)}{dx} = \frac{\varepsilon y}{1 - yx} = \sum_n b_n x^n. \tag{12}$$

From (7) and (12) we obtain a sequence of estimates of the critical exponent by the logarithmic derivative method

$$\varepsilon_n = b_n / y^{n+1}. \tag{13}$$

The Padé approximant of the function F(x) is a ratio of polynomials

$$\sum_{i=0}^{N+M+1} b_i x^i = \sum_{i=0}^{N} p_i x^i / (1 + \sum_{i=1}^{M} q_i x^i). \tag{14}$$

There are different methods of determining the critical exponents using the Padé approximant method. For example, one can form the Padé approximant to the series

$$F(x) = (y^{-1} - x)\frac{d \ln f(x)}{dx} = \sum_i b_i x^i \tag{15}$$

and obtain a table of values of the critical exponent ε by evaluating the approximants with $x = y^{-1}$.

The ratio and logarithmic derivative methods can be applied only to series whose coefficients form an ordered sequence of the same sign (high-temperature series for all lattices and low-temperature series for the diamond lattice). The Padé approximant method can also be used for series whose coefficients randomly oscillate in sign and magnitude (low-temperature series for simple cubic, fcc, and bcc lattices).

The values of the critical exponents of the three-dimensional Ising model obtained with these methods are, to a very good approximation

$$\alpha = 1/8; \quad \beta = 5/16; \quad \gamma = 5/4. \tag{16}$$

Application of these methods to the series for the two-dimensional Ising model gives results which are practically identical to the exact values: $\alpha = 0$ (logarithmic singularity); $\beta = 1/8$; $\gamma = 7/4$; $\delta = 15$; $\nu = 1$; $\eta = 1/4$.

This gives confidence that the values of the critical exponents (16) can be identified with the exact values for the lattice gas model. But there are two discrepancies which should be noted. The critical exponents from the low-temperature series expansion of the susceptibility $\gamma' = 1.26$-1.31 [11, 12] and are higher than the assumed value $\gamma = 1.25$; and the values of the correlation range exponent $\nu = 0.636$-0.642 [13-15] are above the value $\nu = 0.625$ which follows from the relations (3).

A new stage in the calculation of the critical exponents began with the work of Wilson [16], in which the critical exponents were determined by the renormalization group method for an n-component system to within terms of order ε^2. Here n is the number of components of the order parameter, and $\varepsilon = 4 - d$ is the expansion parameter. Detailed discussions of the renormalization group method are given in [1, 17, 18].

The work of Wilson not only provided a new direction for the calculation of the critical exponents, but also gave support to the hypothesis of the universality of critical phenomena; i.e., the values of the critical exponents do not depend on the nature of the material or the type of physical system, but depend only on the dimensionality d and the number of components n of the order parameter of the system. A pure material belongs to the class of three-dimensional systems $d = 3$ with a single-component order parameter $n = 1$. For this type of system Wilson's solution gives the following values of the critical exponents:

$$\alpha = 0{,}077; \quad \beta = 0{,}340; \quad \gamma = 1{,}244; \quad \nu = 0{,}626. \tag{17}$$

The significant discrepancy between the Wilson values and the values (16) indicated that further work was necessary on the determination of the critical exponents.

In later papers a different variant of the renormalization group was used, based on the field-theoretic approach to the problem of phase transitions.

The following values were obtained in [19, 20]

$$\alpha = 0{,}132; \quad \beta = 0{,}322; \quad \gamma = 1{,}224, \tag{18}$$

and in [21]

$$\alpha = 0{,}118; \quad \beta = 0{,}320; \quad \gamma = 1{,}242. \tag{19}$$

The most reliable values of the critical exponents using the renormalization group were obtained in [22]

$$\alpha = 0{,}1132; \quad \beta = 0{,}3243; \quad \gamma = 1{,}238 \tag{20}$$

and in [23, 24]

$$\alpha = 0{,}110; \quad \beta = 0{,}325; \quad \gamma = 1{,}2402. \tag{21}$$

Therefore the latest values of the critical exponents using the renormalization group (20) and (21) are consistent with one another, but differ by about 0.01 from the values (16) obtained from series expansions of the three-dimensional Ising model. This difference shook the confidence in the accuracy of the values of the critical exponents (16) and led to a series of new papers on the determination of the critical exponents from series expansions of the Ising model.

As is obvious from (9), (13), and (15), the values of the critical exponents from the series expansions depend on the choice of the radius of convergence of the series y. If the error in y is Δy, the error in ε_n by the ratio method is

$$\Delta\varepsilon_n \approx n\Delta y/y, \tag{22}$$

and extrapolation of the sequence of estimates to $1/n = 0$ leads to an increase rather than a decrease in the error of the critical exponent. Linear extrapolation of the sequence of estimates (9) gives the additional error

$$\Delta\varepsilon_n^{(1)} \approx (2n - 1)\frac{\Delta y}{y}, \tag{23}$$

and the second-order extrapolant differs from the extrapolation with the exact value of the critical temperature by the quantity

$$\Delta\varepsilon_n^{(2)} \approx 3(n - 1)\frac{\Delta y}{y}. \tag{24}$$

In [25] the critical exponents α and γ were obtained from analysis of the high-temperature series expansions for simple cubic, fcc, and bcc lattices, independently of the choice of the critical temperature. The essence of the method is that the function F(x) given by the series

$$F(x) = \sum_n c_n x^n = \sum_n \frac{a_n}{b_n} x^n, \tag{25}$$

where a_n and b_n are the series expansion coefficients of the functions

$$f_1(x) = E_1(1 - yx)^{-\varepsilon_1} = \sum_n a_n x^n; \tag{26}$$

$$f_2(x) = E_2(1 - yx)^{-\varepsilon_2} = \sum_n b_n x^n, \tag{27}$$

has the asymptotic form

$$F(x) \sim (1 - x)^{-(\varepsilon_1 - \varepsilon_2 + 1)}, \tag{28}$$

and the radius of convergence of the series (25) is y = 1.

The logarithmic derivative of any arbitrary function can serve as the function $f_2(x)$. In this case $\varepsilon_2 = 1$ and the series (25) gives a value of the critical exponent ε_1 independent of the critical temperature.

The values of the critical exponents obtained in [25] are below those quoted earlier: $\alpha = 1/8$ and $\gamma = 5/4$. The most ordered sequence of estimates is obtained for an fcc lattice, where extrapolation gives $\alpha = 0.111 \pm 0.001$; $\gamma = 1.244 \pm 0.0005$.

In [26] high-temperature series expansions were analyzed using a previously determined critical temperature. The results $\alpha = 0.110$ and $\gamma = 1.245$ are similar to the values obtained in [25], and the value $\nu = 0.638$ was obtained for the correlation range exponent.

Hence if we remove the error associated with an error in the critical temperature, the estimates of the critical exponents from series expansions converge on the values obtained using the renormalization group, but there remains a discrepancy of ~ 0.005 for γ and ~ 0.01 for ν.

In [27] the effect of a correction term to the asymptotic dependence on the critical exponents obtained from series expansions was considered. For a function of the form

$$f(x) = E(1 - yx)^{-\varepsilon}[1 + e(1 - yx)^{\Delta}] = \sum_n a_n x^n \tag{29}$$

the n-th coefficient of a power series expansion is given by the expression

$$a_n = Ey^n \left(\prod_{i=1}^{n} \frac{\varepsilon + i - 1}{i!}\right)\left(1 + e\prod_{i=1}^{n} \frac{\varepsilon - \Delta + i - 1}{\varepsilon + i - 1}\right). \tag{30}$$

From (30) we obtain an equation for the sequence of critical exponents obtained by the ratio method

$$\varepsilon_n = \varepsilon - \Delta \frac{e\varphi_{n-1}}{1 + e\varphi_{n-1}}, \tag{31}$$

where

$$\varphi_n = \frac{\varepsilon - \Delta}{\varepsilon} \frac{\varepsilon - \Delta + 1}{\varepsilon + 1} \cdots \frac{\varepsilon - \Delta + n - 1}{\varepsilon + n - 1}. \tag{32}$$

Comparing (31) for ε_n and ε_{n-1}, we obtain a final expression for the critical exponent by the ratio method and with the inclusion of the first correction term to the asymptotic dependence

$$\varepsilon = \varepsilon_n - \frac{(\varepsilon_{n-1} - \varepsilon_n)(\varepsilon - \Delta + n - 2)}{\Delta + \varepsilon_{n-1} - \varepsilon}, \tag{33}$$

where ε_n and ε_{n-1} are determined according to (9).

When there is a correction term to the asymptotic dependence, the convergence of the sequence of estimates of the critical exponent to the exact value is very slow. Linear extrapolation of the sequence (31) gives

$$\varepsilon_n^{(1)} - \varepsilon \approx (\varepsilon_n - \varepsilon)(1 - \Delta), \tag{34}$$

TABLE 1. Recent Theoretical Estimates of the Critical Exponents for a Three-Dimensional System with a One-Component Order Parameter

Method	Source	Year	α	β	γ	δ	ν	η
Renormalization gr.	[22]	1976	0,1132	0,3243	1,238	4,818	0,6289	0,0313
Renormalization gr.	[23]	1977	0,110	0,325	1,2402	4,816	0,6300	0,0315
Series expansions	[27]	1980	0,112	0,324	1,240	4,827	0,6293	0,0297
Series expansions	[31]	1982	0,113	0,3245	1,238	4,815	0,629	0,0318
Renormalization gr.	[34]	1984	0,1118	0,3246	1,2390	4,817	0,6294	0,0315
Average value			0,1120	0,3245	1,2390	4,818	0,6293	0,0312
Mean square deviat.			0,0012	0,0005	0,0010	0,005	0,0005	0,0007
Scatter of the estimates $\varepsilon_{max} - \varepsilon_{min}$			0,0032	0,001	0,0022	0,012	0,0011	0,0011

and the equation for the second-order extrapolants has the form

$$\varepsilon_n^{(2)} - \varepsilon \approx \left(\frac{\varepsilon_n^{(1)} + \varepsilon_{n-1}}{2} - \varepsilon\right)(1 - \Delta). \quad (35)$$

The analysis in [27] of the high-temperature series expansions for fcc-lattices with the inclusion of the correction term to the asymptotic dependence gives the results $\alpha = 0.112 \pm 0.002$ and $\gamma = 1.240 \pm 0.002$, and these values agree with the critical exponents obtained using the renormalization group method [22-24].

In [28] the high-temperature series expansions of the correlation function and susceptibility of bcc lattices were extended up to 21 terms and new values were obtained for the critical exponents: $\gamma = 1.239 \pm 0.002$ and $\nu = 0.631 \pm 0.003$.

The high-temperature series expansions for bcc lattices with 21 terms have been analyzed by many authors [29-32]. In [31] the first correction term to the asymptotic dependence was taken into account and the following values of the critical exponents were obtained: $\gamma = 1.238 \pm 0.003$; $\nu = 0.629 \pm 0.002$.

In [33] the high-temperature series expansion of the correlation function of an fcc lattice with 13 terms was analyzed and here too good agreement with the results of [22-24] was obtained: $\nu = 0.630 \pm 0.001$.

In [34] the renormalization group calculation for a simple-cubic lattice in the Ising model was done using the Monte Carlo method and the critical exponents $\nu = 0.6294$ and $\eta = 0.0315$ were obtained.

Hence the latest estimates of the critical exponents, obtained with different methods, are consistent among themselves, as can be seen from Table 1. The scatter of the estimates does not exceed the computational errors cited by the authors of ± 0.002 to ± 0.003, and the mean-square deviation ranges from 0.0005 to 0.0012 (for the exponent δ the deviation is three times as large, in view of Eq. (2)).

It would be difficult to believe that the excellent agreement of five independent sets of estimates of the critical exponents, obtained by different methods and on different models is accidental, and that the estimates have a systematic error. Therefore we can state that the critical exponents, which are the fundamental constants of the theory of critical phenomena, are known at present with an accuracy to the third decimal place:

$$\eta = 1/32; \quad \nu = 17/27; \quad \alpha = 1/9; \quad \beta = 187/576; \quad \gamma = 119/96; \quad \delta = 53/11. \quad (36)$$

We also note that the values obtained in [23, 24] for the critical exponents of three-dimensional systems with a two-component order parameter $n = 2$ ($\eta = 0.033 \pm 0.004$ and $\nu = 0.669 \pm 0.002$) and for three-dimensional systems with a three-component order parameter $n = 3$ ($\eta = 0.033 \pm 0.004$ and $\nu = 0.705 \pm 0.003$) are close to the fractions $\eta = 1/32$ and $\nu = 2/3$ for $n = 2$ and $\eta = 1/32$ and $\nu = 19/27$ for $n = 3$. The critical exponents η and ν for systems with dimensionalities $d = 2, 3, 4$ and number of order parameters $n = 1, 2, 3$ can be obtained from the proposed formulas:

$$\eta = \frac{4-d}{d^3 + d^2 - 4}; \quad \nu = \frac{2}{d} + \frac{(d-2)(d-4)(2-n)}{d^3}. \quad (37)$$

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