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FREE ENERGY AND NON-LINEAR SUSCEPTIBILITIES OF $O(n)$-SYMMETRIC SYSTEMS AT CRITICALITY

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Renormalized coupling constants g_6 and g_8 entering the small-field expansion of the free energy and determining the system non-linear susceptibilities are calculated for the 3D n-vector model in the four-loop and three-loop approximations, respectively. Four-loop expansion for g_6 of the 2D Ising model is also found. The Padé–Borel–Leroy technique is used for resummation of these renormalization-group series, and numerical estimates for universal critical values of g_6 and g_8 are obtained.

Higher-order renormalized coupling constants g_{2k} for the basic models of phase transitions became the target of intensive theoretical studies in recent years (see, e.g., [1, 2] and references therein). These constants enter the small-field expansion of the free energy and scaling equation of state, determine the system nonlinear susceptibilities and thus play a key role at criticality. Along with critical exponents, they are universal, i.e., possess, under $T \to T_c$, numerical values which depend only on the space dimensionality and the symmetry of the order parameter. Calculation of the universal critical values of g_6, g_8, etc., for the 3D Ising model by various methods showed that the field-theoretical renormalization-group (RG) approach in fixed dimensions yields the most accurate numerical estimates. It is a consequence of a rapid convergence of the iteration schemes originating from RG expansions [3, 4]. It is natural, therefore, to use the field theory for calculation of renormalized higher-order coupling constants for more general, $O(n)$-symmetric model and for the Ising model in two dimensions. In the report, the 3D RG expansions of the renormalized coupling constants g_6 and g_8 for arbitrary n will be presented along with the 2D RG series for g_6 at $n = 1$ and numerical estimates for their universal critical values will be obtained.

The 3D $O(n)$-symmetric model is described at criticality by Euclidean field theory with the Hamiltonian

$$H = \int d^3x \left[\frac{1}{2}(m_0^2 \varphi_\alpha^2 + (\nabla\varphi_\alpha)^2) + \lambda(\varphi_\alpha^2)^2 \right], \tag{1}$$

where m_0^2 is proportional to $T - T_c^{(0)}$, $T_c^{(0)}$ being the phase transition temperature in the absence of the order parameter fluctuations. The fluctuations give rise to many-point correlations $\langle\varphi(x_1)\varphi(x_2)...\varphi(x_{2k})\rangle$ and, correspondingly, to higher-order terms in the expansion of the free energy in powers of the magnetization M:

$$F(M,m) = F(0,m) + \sum_{k=1}^{\infty} g_{2k} m^{3-k(1+\eta)} M^{2k}, \tag{2}$$

where m is a renormalized mass, η is a Fisher exponent, and g_{2k} are dimensionless coupling constants. Let, as usually, $g_2 = 1/2$. Then g_4, g_6, g_8,... will acquire, under $T \to T_c$, the universal values.

The asymptotic critical values of g_4, $g_4^*(n)$, determining critical exponents and other universal quantities, have been found from the 6-loop expansion for RG β-function [1, 5–7]; they are known with rather high accuracy. To estimate the universal values g_6^* and g_8^* of the higher-order couplings, we calculate corresponding RG series and perform their resummation by means of the Pad$\acute{e}$–Borel–Leroy technique. The RG series for g_6 and g_8 are obtained from conventional Feynman graph expansions for the 6-point and 8-point vertices in terms of the bare coupling constant λ. In its turn, λ is expressed perturbatively via the renormalized coupling constant g_4. Substituting then the series for λ into the «bare» expansions, we obtain the RG expansions for g_6 and g_8.

As was earlier shown [3, 8], the 1-, 2-, 3-, and 4-loop contributions to g_6 are formed by 1, 3, 16, and 94 one-particle irreducible Feynman graphs, respectively. In this case, the calculations just described give [9]:

$$g_6 = \frac{9}{\pi} g_4^3 \Bigg[\frac{n+26}{27} - \frac{17\,n + 226}{81\pi} g_4 + (0.000999164\,n^2 + 0.14768927\,n + 1.24127452) g_4^2 - (-0.00000949\,n^3 + 0.00783129\,n^2 + 0.34565683\,n + 2.14825455) g_4^3 \Bigg]. \tag{3}$$

In the case of g_8, the 1-, 2-, and 3-loop contributions are given by 1, 5, and 36 graphs, respectively [8]. Corresponding RG expansion is found to be [9]:

$$g_8 = -\frac{81}{2\pi} g_4^4 \Bigg[\frac{n+80}{81} - \frac{81\,n^2 + 7114\,n + 134960}{13122\pi} g_4 + (0.00943497\,n^2 + 0.60941312\,n + 7.15615323) g_4^2 \Bigg]. \tag{4}$$

Being a field-theoretical perturbative expansions these series are divergent (asymptotic). To get reasonable numerical estimates for g_6^* and g_8^* some procedure of making them convergent should be applied. The Borel–Leroy transformation

$$f(x) = \sum_{i=0}^{\infty} c_i x^i = \int_0^{\infty} t^b e^{-t} F(xt) dt, \qquad F(y) = \sum_{i=0}^{\infty} \frac{c_i}{(i+b)!} y^i. \tag{5}$$

can play a role of such a procedure. Since the RG series considered turns out to be alternating, the analytical continuation of the Borel–Leroy transform may be then performed by using Padé approximants [L/M].

For g_6 we have the 4-loop RG expansion and can construct, in principle, three different Padé approximants: [2/1], [1/2], and [0/3]. To obtain proper approximation schemes, however, only diagonal [L/L] and near-diagonal Padé approximants should be employed. That's why further we limit ourselves with approximants [2/1] and [1/2]. Moreover, the diagonal Padé approximant [1/1] will be also dealt with although this corresponds to the usage of the lower-order, 3-loop approximation.

The algorithm of estimating g_6^* we use here is as follows. Since the Taylor expansion for the free energy contains as coefficients the ratios $R_{2k} = g_{2k}/g_4^{k-1}$ we work with the RG series for R_6. It is resummed in three different ways based on the Padé approximants just mentioned. The Borel–Leroy integral is evaluated as a function of the parameter b under $g_4 = g_4^*(n)$. For the fixed point coordinate $g_4^*(n)$ the values extracted from the six-loop RG expansion are adopted [1, 5]. The optimal value of b providing the fastest convergence of the iteration scheme is then determined. It is deduced from the condition that the Padé approximants employed should give, for $b = b_{opt}$, the values of R_6^* which are as close as possible to each other. Finally, the average over three estimates for R_6^* is found and claimed to be a numerical value of this universal ratio.

The results of our calculations of g_6^* are presented in the Table. It contains numerical estimates resulting from the 4-loop RG expansion (column 3) and their analogs given by the Padé–Borel resummed 3-loop RG series [1] (column 4). As is seen, with increasing n the difference between the 4-loop and 3-loop estimates rapidly diminishes: being small (0.9 %) even for $n = 1$, it becomes negligible at $n = 10$ and practically disappears for $n \geq 14$. Such a behaviour is quite natural since with increasing n the approximating properties of RG series for g_6 become better [1, 9].

How close to the exact values of g_6^* may the numbers in column 3 be? To clear up this point, let us compare our 4-loop estimate for R_6^* at $n = 1$ with those obtained recently by an analysis of the 5-loop scaling equation of state for the 3D Ising model [4, 10]. R. Guida and J. Zinn-Justin have obtained $R_6^* = 1.644$ and, taking into account some additional information, $R_6^* = 1.643$, while our estimate is $R_6^* = 1.648$. Keeping in mind that the exact value of R_6^* should lie between the 4-loop and 5-loop estimates (the RG series is alternating), our estimate can differ from the exact number by no more than 0.3 %. Since for $n > 1$ the RG

Table. Our estimates of universal critical values of the renormalized sextic coupling constant for the 3D n-vector model (column 3). The fixed point coordinates g^* are taken from [5] ($1 \leq n \leq 3$) and [1] ($4 \leq n \leq 40$). The g_6^* estimates extracted from the Pade–Borel resummed 3-loop RG expansion (column 4), from the exact RG equations (column 5), obtained by the lattice calculations (column 6), resulting from a constrained analysis of the ϵ-expansions (column 7), and given by the $1/n$-expansion (column 8) are presented for comparison

n	g^*	g_6^*	$g_6^*[1]$	$g_6^*[11]$	$g_6^*[12]$	$g_6^*[2]$	g_6^* $(1/n)$
	2	3	4	5	6	7	8
1	1.415	1.608	1.622	1.52	1.92(24)	1.609(9)	
2	1.406	1.228	1.236	1.14	1.27(25)	1.21(7)	
3	1.392	0.951	0.956	0.88	0.93(20)	0.931(46)	
4	1.3745	0.747	0.751	0.68	0.62(15)	0.725(29)	1.6449
5	1.3565	0.596	0.599				1.0528
6	1.3385	0.483	0.485				0.7311
8	1.3045	0.329	0.331			0.319(4)	0.4112
10	1.2745	0.235	0.236				0.2632
12	1.2487	0.174	0.175				0.1828
16	1.2077	0.105	0.105			0.1032(4)	0.1028
20	1.1773	0.0693	0.0694				0.0658
24	1.1542	0.0487	0.0488				0.0457
32	1.1218	0.0276	0.0276			0.0275(1)	0.0257
40	1.1003	0.0176	0.0176				0.0164

expansion (3) should provide better numerical estimates than in the Ising case, this value (0.3 %) represents an upper bound for the deviation of the numbers in column 3 of the Table from their exact counterparts.

It is interesting to compare our estimates with those obtained by other methods. Since 1994, the universal values of the sextic coupling constant for the 3D $O(n)$-symmetric model were estimated by solving the exact RG equations [11], by lattice calculations [12], and by a constrained analysis of the ϵ-expansion [2]; corresponding results are collected in columns 5, 6, and 7 of the Table respectively. As is seen, they are, in general, in accord with ours. For large n, our estimates are consistent also with those given by the $1/n$-expansion which are presented in column 8.

The RG expansion for the octic coupling constant g_8 turns out to be worse than the series (3) from the point of view of their summability. Indeed, the series (4) diverges considerably stronger and is one term shorter than that for g_6. It implies that the only Pade approximant — [1/1] — may be really used in a course of the resummation of this series. In the Ising case $n = 1$, such a simple Pade–Borel procedure, when applied to the 3-loop RG expansion for g_8, was found to lead to rather crude numerical estimates [8]. As our analysis shows, with increasing n the situation becomes better but, nevertheless, the RG estimates for $g_8^*(n)$ remain much less accurate than those obtained for the sextic coupling constant. Corresponding numerical results are presented elsewhere [9].

For the 2D Ising model the four-loop calculations lead to the following RG expansion for the renormalized sextic coupling constant [13]:

$$g_6 = \frac{36}{\pi}\, g_4^3 \left(1 - 3.2234882\, g_4 + 14.957539\, g_4^2 - 85.7810\, g_4^3\right). \qquad (6)$$

This series is resummed in a manner quite similar to that used in three dimensions. For the fixed point coordinate the value $g_4^* = 0.6125$ [14–16] is accepted which was extracted from lengthy high-temperature expansions and is believed to be the most accurate estimate for g_4^* available nowadays. As our calculations show, for $b = b_{opt}$ all three working Padé approximants yield practically the same value of g_6^*. It is as follows:

$$g_6^* = 1.10. \qquad (7)$$

To estimate an (apparent) accuracy of this number we analyze the sensitivity of estimates given by RG expansion (6) to the type of resummation. The results produced by Padé approximant $[2/1]$ turn out to be most strongly dependent on the parameter b. This situation resembles that for 3D $O(n)$-symmetric model where Padé approximants of $[L-1/1]$ type for β-function and critical exponents lead to numerical estimates demonstrating appreciable variation with b while for diagonal and near-diagonal approximants the dependence of the results on the shift parameter is practically absent $[1, 5]$. In our case, Padé approximants $[1/1]$ and $[1/2]$ generate such «stable» approximations for g_6^*. For b varying from 0 to 15 (i.e., for any reasonable b) the magnitude of g_6^* averaged over these two approximations is found to remain within the segment (1.044, 1.142) [13]. Hence, the value (7) is believed to differ from the exact one by no more than 5%. Very good agreement between our estimate and those obtained recently from the high-temperature expansions [14] ($g_6^* = 1.104$) and by matching of corresponding ϵ-expansion with the exact results known for $D = 1$ and $D = 0$ [2] may be considered as an argument in favor of this belief.

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