Field theory and anisotropy of cubic ferromagnet near Curie point

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(Dated: January 5, 2016)

Abstract

Critical fluctuations are known to change the effective anisotropy of cubic ferromagnet near the Curie point. If the crystal undergoes phase transition into orthorhombic phase and the initial anisotropy is not too strong, effective anisotropy acquires at T_c the universal value $A^* = v^*/u^*$ where u^* and v^* are coordinates of the cubic fixed point entering the scaling equation of state and expressions for nonlinear susceptibilities. In the paper, the numerical value of the anisotropy parameter A at the critical point is estimated using the ϵ -expansion and pseudo- ϵ expansion techniques. Pade resummation of six-loop pseudo- ϵ expansions for u^* , v^* and A^* leads to the estimate $A^* = 0.13$ close to that extracted from the five-loop ϵ -expansion but differing considerably from the value $A^* = 0.089$ given by the analysis of six-loop expansions of the β functions themselves. This discrepancy is discussed and its roots are cleared up.

Key words: cubic model, effective anisotropy, renormalization group, ϵ expansion, pseudo- ϵ expansion

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Approaching the critical point thermal fluctuations of magnetization become so strong that lead to the appreciable temperature dependence of effective anisotropy of the cubic ferromagnet. To be precise, the crystalline anisotropy of the nonlinear susceptibilities of different orders is meant here. If the crystal undergoes a phase transition to the orthorhombic phase and its initial anisotropy is not too strong, under $T \rightarrow T_c$ the magnetic subsystem either becomes isotropic [1] or its anisotropy A goes to a universal value which does not depend on magnitude of A far from the Curie point. For large initial values of A fluctuations make the critical behavior of the system unstable and the first-order phase transition occurs [2–4]. Which one of the above-described modes is realized in the critical region depends on the number of the order parameter components (dimensionality) n. For $n < n_c$ the system goes to the isotropic critical asymptote, while under $n > n_c$ it remains anisotropic at the Curie point [5].

It is clear that the numerical value of the boundary dimensionality n_c is of prime physical interest since it determines how real cubic (n = 3) and tetragonal (n = 2)ferromagnets will behave in the vicinity of T_c . The renormalization group (RG) analysis in the lower-orders of the perturbation theory [3, 6, 7] as well as some lattice calculations [8] have shown that the n_c likely lies between 3 and 4. However, further studies including the resummation of the three-loop RG expansions [9, 10] and multiloop RG calculations for 3D [11–13] and $(4 - \epsilon)$ -dimensional [14] models changed this estimate to $n_c < 3$ [9–21]. In particular, detailed 3D RG analysis [13], processing in different ways of the five-loop ϵ -expansions [13, 17] and addressing the pseudo- ϵ expansion technique led to $n_c = 2.89$, $n_c = 2.855$, $n_c = 2.87$, and $n_c = 2.862$, respectively. It means that cubic ferromagnets undergoing the second-order phase transitions should belong to the special – cubic – universality class, i. e. to possess a nonzero anisotropy at the Curie point and to have their own specific set of critical exponents.

On the other hand, the value of n_c is very close to the physical value n = 3 and thus the cubic fixed point should be located near the Heisenberg fixed point at the phase diagram of RG equations. As a result, the critical exponents corresponding to these points should almost coincide with each other. The idea about degree of their closeness can be obtained by comparing, e. g., the most reliable values of the susceptibility exponent γ for Heisenberg fixed point and the cubic one; they are equal to 1.3895(50) [22] and 1.390(6) [13], respectively. It is quite clear that measuring of critical exponents in experiments it is impossible to determine what kind of the critical behavior is realized in cubic ferromagnets.

Nevertheless, to determine by means of physical and computer experiments in what way the system with cubic symmetry behaves near the Curie point is still possible but in order to do this one should study the nonlinear susceptibilities of different orders $\chi^{(2k)}$ [23]. As the RG analysis has shown, the anisotropy of the nonlinear susceptibility $\chi^{(4)}$ in the critical region may be as large as 5% what allows to definitely consider it as a measurable quantity [23]. At the same time, this result can not be perceived as quite reliable because it was obtained by processing of the series for β functions of 3D cubic model with coefficients that are not small and the expansions themselves are known to be divergent.

In such situation it is natural to address the alternative theoretical schemes which would allow to find the anisotropy of susceptibility $\chi^{(4)}$ under $T \to T_c$ and to confirm or to correct the estimate mentioned above. The ϵ -expansion should be considered as the most popular among such schemes; it is widely used for evaluation of critical exponents and of other universal parameters of critical behavior. The second field-theoretical approach being rather perspective in the indicated sense is the pseudo- ϵ expansion technique proposed many years ago by B. Nickel(see reference [19] in the paper [24]). This technique has demonstrated its exceptional efficiency when used to estimate the universal characteristics of not only the 3D [19, 22, 24–29] but also of two-dimensional systems [24, 30–34] for which the known RG expansions are shorter and more strongly divergent. Application of the pseudo- ϵ expansion approach accelerates the convergence of the iterations and smoothes the oscillations of numerical estimates so markedly, that in many cases for getting reliable quantitative results it turns sufficient to use simple Pade approximants or even to directly sum up the corresponding series.

Below, we find the value of the anisotropy of cubic ferromagnets near the Curie point using ϵ -expansion and pseudo- ϵ expansion methods, compare the numbers given by three versions of field-theoretical RG machinery mentioned above, and discuss the results obtained.

So, in the critical region the expansion of the free energy of the cubic model in powers of magnetization components M_{α} can be written down in the form:

$$F(M_{\alpha},m) = F(0,m) + \frac{1}{2}m^{2-\eta}M_{\alpha}^{2} + m^{1-2\eta}(u_{4} + v_{4}\delta_{\alpha\beta})M_{\alpha}^{2}M_{\beta}^{2} + \dots,$$
(1)

where m is an inverse correlation length, η being the Fisher exponent, and u_4 and v_4 are dimensionless renormalized coupling constants taking under $T \to T_c$ the universal values. In particular, the fourth-order nonlinear susceptibility which is of interest for us can be expressed via these couplings:

$$\chi^{(4)}_{\alpha\beta\gamma\delta} = \frac{\partial^3 M_\alpha}{\partial H_\beta \partial H_\gamma \partial H_\delta} \bigg|_{H=0}.$$
 (2)

Of special interest are the values of the nonlinear susceptibility for two highly symmetric directions corresponding to the orientation of the external field along the cubic axis $(\chi_c^{(4)})$ and the space diagonal $(\chi_d^{(4)})$ of the unit cell. For these directions the difference between the values of the $\chi^{(4)}$ is maximal, i. e. the cubic anisotropy is most pronounced. As is easily to show,

$$\chi_c^{(4)} = -24 \frac{\chi^2}{m^3} (u_4 + v_4), \qquad \chi_d^{(4)} = -24 \frac{\chi^2}{m^3} \left(u_4 + \frac{v_4}{3} \right), \qquad (3)$$

where χ is a linear susceptibility. A role of natural characteristic of the nonlinear susceptibility anisotropy plays the ratio

$$\delta^{(4)} = \frac{|\chi_c^{(4)} - \chi_d^{(4)}|}{\chi_c^{(4)}}.$$
(4)

This ratio

$$\delta^{(4)} = \frac{2v_4}{3(u_4 + v_4)} \tag{5}$$

and can be expressed in terms of the anisotropy parameter

$$A = \frac{v_4}{u_4}.\tag{6}$$

Its value at the Curie point A^* we will find in this paper.

The fluctuation Hamiltonian of the cubic model has the form:

$$H = \frac{1}{2} \int d^D x \left[m_0^2 \varphi_\alpha^2 + (\nabla \varphi_\alpha)^2 + \frac{u_0}{12} \varphi_\alpha^2 \varphi_\beta^2 + \frac{v_0}{12} \varphi_\alpha^4 \right],\tag{7}$$

where φ_{α} is *n*-component field of the order parameter fluctuations, a bare mass squared $m_o^2 \sim T - T_c^{(0)}$, and $T_c^{(0)}$ – the phase transition temperature in the mean-field approximation. The asymptotic value of the anisotropy parameter in the critical region A^* is determined by the coordinates of the cubic fixed point of RG equations u_4^* and v_4^* . For $D = 4 - \epsilon$ they are known today in the five-loop approximation [14]. Corresponding ϵ -expansions for the physically interesting case n = 3 are as follows:

$$u^* = 1.22222222\epsilon + 0.49291267\epsilon^2 - 0.4899848\epsilon^3 + 0.5912287\epsilon^4 - 1.429021\epsilon^5, \quad (8)$$

$$v^* = -0.40740741\epsilon + 0.19783570\epsilon^2 + 0.2270881\epsilon^3 + 0.1855026\epsilon^4 - 0.6908416\epsilon^5, \quad (9)$$

where $u^* = (11/2\pi)u_4^*$, $v^* = (11/2\pi)v_4^*$. As is seen, expansions (8) and (9) have an irregular structure (non-alternating), their coefficients are not small and rapidly begin to grow with the number of the series term. No wonder that the use of different resummation methods including those based on the Borel transformation does not lead in this case to more or less satisfactory results. Starting from the series for the coupling constants, it is possible, however, to obtain the ϵ -expansion for the anisotropy parameter itself

$$A^* = -\frac{1}{3} + 0.29629630\epsilon - 0.0673269\epsilon^2 + 0.458956\epsilon^3 - 1.31038\epsilon^4,$$
(10)

which, being also divergent, has an advantage over (8) and (9) because it is alternating. Since the higher-order coefficients of (10) strongly grow up, it is reasonable to apply the Borel transformation for the processing of this series, with the subsequent analytic continuation of the Borel transform with a help of Pade approximants [L/M]. The results of the resummation of (10) using this technique are presented in Table 1. Although the estimates obtained are considerably scattered, the most likely value of the A^* , i. e. that given by the diagonal approximant [2/2], is close to the interval where the results of the six-loop RG analysis are grouped. Indeed, the resummation of the series for β functions of the three-dimensional cubic model leads to $u_4^* = 0.755 \pm 0.010$, $v_4^* = 0.067 \pm 0.014$ [13] what, in its turn, yields $A^* = 0.089 \pm 0.018$. On the other hand, the distinction of the obtained numbers – 0.089 and 0.124 – is not so small to completely ignore it. This distinction should have origins. The specific feature of the ϵ -expansion for A^* may be referred to as one of them: under the physical value of ϵ first two terms of the series (10) almost cancel each other what effectively shortens this series and drastically worsens its approximating properties. Since ϵ -expansions for the coupling constants also have computationally unfavorable structure we conclude that the method of ϵ -expansion does not allow to estimate with sufficient accuracy the magnitude of the anisotropy of cubic ferromagnets in the critical region.

In such a situation it is reasonable to address the other version of the RG perturbation theory – the technique of pseudo- ϵ expansion. The key idea of this method is to introduce, starting from the three-dimensional RG expansions, a formal small parameter τ having inserted it into linear terms of the series for β functions and to calculate observables as power series in τ . Their numerical values may be then obtained putting $\tau = 1$. So, we start from the six-loop RG expansions for the cubic model [13]. Iterating the equations

$$\beta_u(u,v) = 0, \qquad \qquad \beta_v(u,v) = 0 \tag{11}$$

by the way just described, for the coordinates of the cubic fixed point under n = 3 we obtain

$$u^* = 1.2222222\tau + 0.3323342\tau^2 - 0.122585\tau^3$$
$$-0.065595\tau^4 - 0.061083\tau^5 + 0.01269\tau^6, \tag{12}$$

$$v^* = -0.4074074\tau + 0.1306486\tau^2 + 0.232337\tau^3 + 0.128399\tau^4 + 0.050252\tau^5 + 0.02224\tau^6.$$
(13)

These series have a structure much more attractive than that of the ϵ -expansions (8), (9). Their higher-order coefficients are small and decrease in modulo with increasing the number of the series term. It may be expected that even direct summation of (12) and (13) will give acceptable results. Indeed, substituting into the expansion (12) $\tau = 1$,

we get $u^* = 1.318$, the number which is close to the most reliable – six-loop – RG estimate $u^* = 1.321$ [13]. For the second coupling constant an analogous procedure gives $v^* = 0.1565$. This value considerably differs from its six-loop RG counterpart $v^* = 0.117$ [13] yielding, however, for the anisotropy parameter the value 0.119 differing only slightly from that extracted from the ϵ -expansion for A^* .

Let's try to refine the estimates provided by the pseudo- ϵ expansion approach with a help of Pade approximants. Pade triangles for the expansions (12), (13) are shown in Tables 2 and 3. It is seen that, although three higher-order approximants for u^* including [3/2] have dangerous poles, the iteration procedure in general steadily converges to the value 1.322 that is very close to the six-loop RG estimate $u^* = 1.321$ [13]. This value will be accepted as an ultimate. The structure of the content of Table 3 is also regular in the sense that the higher-order Pade approximants yield the estimates of v^* differing from the asymptotic value $v^* = 0.1817$ by no more than $0.03 \div 0.04$. Having found the coordinates of the cubic fixed point we get $A^* = 0.1375$. This number is certainly of interest: it strongly differs from the six-loop RG estimate $A^* = 0.117/1.321 = 0.0886$ and is appreciably greater than the value $A^* = 0.119$ obtained by direct summation of pseudo- ϵ expansions for u^* and v^* .

Further we will find an alternative estimate of the anisotropy parameter in the critical region. It can be done by constructing the pseudo- ϵ expansion directly for the A^* . Combining (12) and (13), we obtain:

$$A^* = -\frac{1}{3} + 0.197531\tau + 0.102951\tau^2 + 0.078982\tau^3 + 0.023907\tau^4 + 0.03847\tau^5.$$
(14)

The coefficients of this series apart from the last one decrease in modulo, the last coefficient is small and, therefore, the expansion (14) is suitable for getting numerical estimates. The results of its summation by means of Pade approximants are presented in Table 4. As is seen, two of the highest-order approximants – [4/1] and [1/4]– have dangerous poles while the asymptotic value $A^* = 0.1304$ is close to the number 0.1375 obtained above. Taking an average of these values and considering their difference as a natural estimate of the accuracy of the approximation scheme employed, we can assume that $A^* = 0.134 \pm 0.004$. On the other hand, pseudo- ϵ expansions for v^* and A^* have unfavorable feature: their first terms are negative and biggest in modulo, so the numerical results are obtained as small differences of big numbers. It certainly reduces their accuracy. Therefore we accept more conservative estimate as a final one:

$$A^* = 0.13 \pm 0.01,\tag{15}$$

which seems to us realistic.

So, the pseudo- ϵ expansion method leads to the value of the anisotropy parameter which 1.5 times greater than its RG analogue $A^* = 0.089$. How can one explain such a significant difference of two field-theoretical estimates obtained within the highest-order available – six-loop – approximation? One of the possible reasons has already been mentioned: the numerical value of A^* is much smaller than the coefficients of the first terms of the series employed, and it is calculated as a small difference of big numbers. This smallness, in its turn, is related to the fact that the boundary dimensionality of the order parameter n_c is close to 3. If n_c coincided with the physical value of n, then the anisotropy parameter would be equal to zero at the critical point. Since the difference $3 - n_c$ is numerically small $(0.1 \div 0.15)$, the value of A^* turns out to be small as well. However, precisely for this difference various field-theoretical schemes provide significantly different estimates. For example, the processing of the six-loop 3D RG expansions for β functions of the cubic model by means of the "conform-Borel" technique leads to $3 - n_c = 0.11$ [13], while the values of this difference obtained by the resummation of the pseudo- ϵ and ϵ expansions for n_c equal 0.138 [19] and 0.145 [17], respectively. Since the first of the above mentioned numbers differs from the others by tenths of percents, it is not surprising that a difference of values A^* , obtained within the same iteration schemes, turns out to be so significant.

In conclusion we note that if one accepts the value of A^* found above, the anisotropy of the nonlinear susceptibility at the Curie point

$$\delta^{(4)} = \frac{2A}{3(1+A)} \tag{16}$$

will grow up almost to 8%. This makes the arguments in favor of the possibility of experimental detection of the anisotropic critical behavior in cubic ferromagnets [23] even more convincing.

The work was supported by the Saint Petersburg State University (project 11.38.636.2013) and by the Russian Foundation for Basic Research (grant 15-02-04687).

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TABLE I: The Pade-Borel triangle for the ϵ -expansion (10) of the universal value of the anisotropy parameter A^* . Approximant [1/2] has "dangerous" pole, so the corresponding number in the table is missing.

$M \setminus L$	0	1	2	3	4
0	-0.3333	-0.0370	-0.1044	0.3546	-0.9558
1	-0.2063	-0.0882	-0.0482	0.0314	
2	-0.1737	-	0.1241		
3	-0.1568	-0.1110			
4	-0.1489				

TABLE II: The Pade triangle for the pseudo- ϵ expansion (12) of the coupling constant u^* . Approximants [3/1], [3/2] and [2/2] have poles close to 1, therefore the corresponding estimates are not reliable; in the table they are bracketed. The bottom line (RoC) indicates the rate and the character of convergence of Pade estimates to the asymptotic value. Here Pade estimate of k-th order is the number given by corresponding diagonal approximant [L/L] or by a half of the sum of the values given by approximants [L/L-1] and [L-1/L] when a diagonal approximant is absent. The resulting value of $u^* = 1.3218$ is obtained by averaging over three working approximants [4/1], [2/3], and [1/4].

$M \setminus L$	0	1	2	3	4	5
0	1.2222	1.5546	1.4320	1.3664	1.3053	1.3180
1	1.6787	1.4650	1.2909	(0.4782)	1.3158	
2	1.3545	1.3832	(0.9025)	(1.2483)		
3	1.3868	1.3629	1.3197			
4	1.3004	1.3300				
5	1.3472					
RoC	1.2222	1.6166	1.4650	1.3371	(0.9025)	1.3218

TABLE III: The Pade triangle for pseudo- ϵ expansion (13) of the coupling constant v^* . Approximant [1/1] has a pole close to 1, corresponding estimate is unreliable and it is bracketed in the table. The convergence of Pade estimates to the asymptotic value is illustrated by the bottom line (RoC). Here the Pade estimate of k-th order is the number obtained in the same manner as in the case of the constants u^* (see Table 2).

$M \setminus L$	0	1	2	3	4	5
0	-0.4074	-0.2768	-0.0444	0.0840	0.1342	0.1565
1	-0.3085	(-0.5753)	0.2426	0.1665	0.1741	
2	-0.2043	0.0416	0.1507	0.1729		
3	-0.1505	0.1905	0.1906			
4	-0.1149	0.1906				
5	-0.0900					
RoC	-0.4074	-0.2926	(-0.5753)	0.1416	0.1507	0.1817

TABLE IV: The Pade triangle for the pseudo- ϵ expansion (14) of the anisotropy parameter in the Curie point. Approximants [2/1], [1/2], [4/1] and [1/4] have dangerous poles, corresponding estimates are not reliable and therefore are given in brackets. The bottom line (RoC) shows the character of convergence of Pade estimates to the asymptotic value. Here the Pade estimate of *k*-th order is the same as in Tables 2 and 3.

$M \setminus L$	0	1	2	3	4	5
0	-0.33333	-0.13580	-0.03285	0.04613	0.07004	0.10851
1	-0.20930	0.07921	(0.30639)	0.08042	(0.00689)	
2	-0.14798	(0.25821)	0.13630	0.13044		
3	-0.10880	0.06129	0.13035			
4	-0.08417	(0.34520)				
5	-0.06592					
RoC	-0.33333	-0.17255	0.07921	(0.28230)	0.13630	0.13039