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On critical behavior of phase transitions in certain antiferromagnets with complicated ordering

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Within the four-loop ε expansion, we study the critical behavior of certain antiferromagnets with complicated ordering. We show that an anisotropic stable fixed point governs the phase transitions with new critical exponents. This is supported by the estimate of critical dimensionality $N_c^C = 1.445(20)$ obtained from six loops via the exact relation $N_c^C = \frac{1}{2}N_c^R$ established for the real and complex hypercubic models.

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It is known that the critical properties of phase transitions in certain antiferromagnets involving an increase of the unit cell in one or more directions at the critical temperature can be described by a generalized $2N$-component ($N \geq 2$) Ginzburg-Landau model with three independent quartic terms

$$H = \int d^{\,D}x \Big[\frac{1}{2}\sum_{i=1}^{2N}(m_0^2\,\varphi_i^2 + \boldsymbol{\nabla}\varphi_i\boldsymbol{\nabla}\varphi_i) + \\ + \frac{u_0}{4!}\Big(\sum_{i=1}^{2N}\varphi_i^2\Big)^2 + \frac{v_0}{4!}\sum_{i=1}^{2N}\varphi_i^4 + 2\frac{z_0}{4!}\sum_{i=1}^{N}\varphi_{2i-1}^2\varphi_{2i}^2\Big] \quad (1)$$

associated with the isotropic, cubic, and tetragonal interactions, respectively [1]. Here φ_i is the real vector order parameter in $D = 4-\varepsilon$ dimensions and m_0^2 is proportional to the deviation from the mean-field transition point. When $N = 2$, Hamiltonian (1) describes the antiferromagnetic phase transitions in $TbAu_2$ and DyC_2 and the structural phase transition in NbO_2 crystal[2)]. Another physically important case $N = 3$ is relevant to the antiferromagnetic phase transitions in such substances as K_2IrCl_6, TbD_2, MnS_2, and Nd. All these phase transitions are known from experiments to be of second order[3)] (see Ref. [5] and references therein). However, the experimental data were insufficiently accurate to provide reliable values of critical exponents and the obtained estimates [6 – 8] were found to differ significantly from the theoretically expected numbers.

For the first time the magnetic and structural phase transitions described by model (1) were studied in the framework of the renormalization group (RG) by Mukamel and Krinsky within the lowest orders in ε [1, 4]. A three-dimensionally stable fixed point (FP) with coordinates $u^* > 0$, $v^* = z^* > 0$ was predicted[4)]. That point was shown to determine a new universality class with a specific set of critical exponents. However, for the physically important case $N = 2$, the critical exponents of this unique stable FP turned out to be exactly the same as those of the $O(4)$-symmetric one.

For the years an alternative analysis of critical behavior of the model, the RG approach in three dimensions, was carried out within the two-and three-loop approximations [9, 10]. Those investigations gave the same qualitative predictions: the unique stable FP does exist on the 3D RG flow diagram. By using different resummation procedures, the critical exponents computed at this point proved to be close to those of the Bose FP ($u = 0$, $v = z > 0$) rather than the isotropic ($O(N)$-symmetric; $u > 0$, $v = z = 0$) one. It was also shown that the unique and the Bose FPs are very close to each other, so that they may interchange their stability in the next orders of RG approximation [10].

Recently, the critical properties of the model were analyzed in third order in ε [11, 12]. Investigation of the FP stability and calculation of the critical dimensionality N_c of the order parameter, separating two different regimes of critical behavior[5)], confirmed that model (1) has the unique stable FP at $N = 2$ and $N = 3$. However,

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[2)] The phase transitions in helical magnets Tb, Dy, and Ho belong to the same class of universality [2].

[3)] An interesting type of multisublattice antiferromagnets, such as MnO, CoO, FeO, and NiO, was studied in Ref. [3, 4]. It was shown, in the leading orders in ε, that the phase transitions in these substances are of first order.

[4)] Following Mukamel [1], we call this point "unique".

[5)] When $N > N_c$ the unique FP is stable in 3D while for $N < N_c$ the stable FP is the isotropic one.

the twofold degeneracy of the stability matrix eigenvalues at the one-loop level was observed for this FP [12]. That degeneracy was shown to cause a substantial decrease of the accuracy expected within the three-loop approximation and powers of $\sqrt{\varepsilon}$ to appear in the expansions[6]. So, computational difficulties were shown to grow faster than the amount of essential information one may extract from high-loop approximations. That resulted in the conclusion that the ε-expansion method is not quite effective for the given model.

Another problem associated with model (1) is the question whether the unique FP is really stable in 3D, thus leading to a new class of universality, or its stability is only an effect of insufficient accuracy of the RG approximations used. Indeed, there are general nonperturbative theoretical arguments indicating that the only stable FP in 3D may be the Bose one and the phase transitions of interest should be governed by that stable FP [14]. However, up to now this assertion found no confirmation within the RG approach. In such a situation it is highly desirable to extend already known ε expansions for the stability matrix eigenvalues, critical exponents, and the critical dimensionality in order to apply more sophisticated resummation technique to longer expansions.

In this Letter we, firstly, avoid the problem of the eigenvalues degeneracy in model (1) by analyzing the critical behavior of an equivalent complex N^C-component order parameter model with the effective Hamiltonian

$$H = \int d^D x \Big[\frac{1}{2}(m_0^2 \psi_i \psi_i^* + \boldsymbol{\nabla}\psi_i \boldsymbol{\nabla}\psi_i^*) + \\ + \frac{u_0}{4!}\, \psi_i \psi_i^* \psi_j \psi_j^* + \frac{v_0}{4!}\, \psi_i \psi_i \psi_i^* \psi_i^* \Big] \qquad (2)$$

comprising the isotropic and cubic interactions[7]. Note that this Hamiltonian also describes the real hypercubic model [16] if ψ_i is thought to be the real N^R-component order parameter. The model (2) comes out exactly from model (1) at $v_0 = z_0$ and it is free from the eigenvalues degeneracy. Secondly, we examine the existence of the anisotropic stable FP in model (2) on the basis of the higher-order ε expansion. Namely, using dimensional regularization and the minimal subtraction scheme [17], we derive the four-loop RG functions as power series in ε and analyze the FP stability. For the first time, we give realistic numerical estimates for the stability matrix eigenvalues using the Borel transformation with a conformal mapping [18]. This allows us to carry out the careful analysis of the stability of all the FPs of the model. We state the exact relation $N_c^C = \frac{1}{2} N_c^R$ between the critical (marginal) spin dimensionalities of the real and complex hypercubic models and obtain the estimate $N_c^C = 1.445(20)$ using six-loop results of Ref. [19]. We show that the anisotropic (complex cubic; $u \neq 0$, $v \neq 0$) stable FP of model (2), being the counterpart of the unique point in model (1), does exist on 3D RG flow diagram at $N^C > N_c^C$. For this stable FP we give more accurate critical exponents estimates in comparison with the previous three-loop results [12] by applying the summation technique of Ref. [20] to the longer series.

The four-loop ε expansion for the β-functions of model (2) were recently obtained by the present authors in Ref. [21]. From the system of equations $\beta_u(u^*, v^*) = 0$, $\beta_v(u^*, v^*) = 0$ one can calculate formal series for the four FPs: the trivial Gaussian one and nontrivial isotropic, Bose, and complex cubic FPs. Instead of presenting here the FPs themselves, which have no direct physical meaning, we present the eigenvalues of the stability matrix

$$\Omega = \begin{pmatrix} \dfrac{\partial \beta_u(u,v)}{\partial u} & \dfrac{\partial \beta_u(u,v)}{\partial v} \\ \dfrac{\partial \beta_v(u,v)}{\partial u} & \dfrac{\partial \beta_v(u,v)}{\partial v} \end{pmatrix} \qquad (3)$$

taken at the most intriguing Bose and complex cubic FPs. They are

$$\omega_1^B = -\frac{1}{2}\varepsilon + \frac{6}{20}\varepsilon^2 + \frac{1}{8}\left[-\frac{257}{125} - \frac{384}{125}\zeta(3)\right]\varepsilon^3 + \\ + \frac{1}{16}\left[\frac{5109}{1250} + \frac{624}{125}\zeta(3) - \frac{576}{125}\zeta(4) + \frac{3648}{125}\zeta(5)\right]\varepsilon^4,$$

$$\omega_2^B = \frac{1}{10}\varepsilon - \frac{14}{100}\varepsilon^2 + \frac{1}{8}\left[\frac{311}{625} + \frac{768}{625}\zeta(3)\right]\varepsilon^3 + \\ + \frac{1}{16}\left[-\frac{61}{250} + \frac{3752}{3125}\zeta(3) + \frac{1152}{625}\zeta(4) - \frac{4864}{625}\zeta(5)\right]\varepsilon^4, \qquad (4)$$

at the Bose FP and for $N^C = 2$

$$\omega_1^{CC} = -\frac{1}{2}\varepsilon + \frac{13}{48}\varepsilon^2 + \frac{1}{8}\left[-\frac{65}{36} - \frac{7}{3}\zeta(3)\right]\varepsilon^3 + \\ + \frac{1}{16}\left[\frac{1679}{432} + \frac{169}{36}\zeta(3) - \frac{7}{2}\zeta(4) + \frac{365}{18}\zeta(5)\right]\varepsilon^4,$$

[6] Similar phenomenon was observed earlier in studying the impure Ising model (see Refs. [13]). Half-integer powers in ε arising in that model have different origin but also lead to the loss of accuracy.

[7] The model with the complex vector order parameter was considered by Dzyaloshinskii [15] in studying the phase transitions in DyC_2, $TbAu_2$ ($N^C = 2$) and TbD_2, MnS_2, and Nd ($N^C = 3$).

Table 1

Eigenvalue exponent estimates for the Bose (BFP) and the complex cubic (CCFP) FPs at $N^C = 2$ and $N^C = 3$ obtained in the four-loop order in ε ($\varepsilon = 1$) using the Borel transformation with a conformal mapping

Type of FP	$N^C = 2$		$N^C = 3$	
	ω_1	ω_2	ω_1	ω_2
BFP	−0.395(25)	0.004(5)	−0.395(25)	0.004(5)
CCFP	−0.392(30)	−0.029(20)	−0.400(30)	−0.015(6)

$$\omega_2^{CC} = -\frac{1}{12}\varepsilon^2 + \frac{1}{8}\left[\frac{5}{18} + \frac{5}{6}\zeta(3)\right]\varepsilon^3 + \\ + \frac{1}{16}\left[\frac{181}{144} - \frac{145}{72}\zeta(3) + \frac{5}{4}\zeta(4) - \frac{50}{9}\zeta(5)\right]\varepsilon^4 \qquad (5)$$

and $N^C = 3$

$$\omega_1^{CC} = -\frac{1}{2}\varepsilon + \frac{58}{220}\varepsilon^2 + \\ + \frac{1}{8}\left[-\frac{19533}{15125} - \frac{14832}{6655}\zeta(3)\right]\varepsilon^3 + \\ + \frac{1}{16}\left[\frac{310518757}{91506250} + \frac{1644864}{1830125}\zeta(3) - \right. \\ \left. - \frac{22248}{6655}\zeta(4) + \frac{283056}{14641}\zeta(5)\right]\varepsilon^4,$$

$$\omega_2^{CC} = -\frac{1}{22}\varepsilon + \frac{2}{2420}\varepsilon^2 + \\ + \frac{1}{8}\left[\frac{90363}{166375} - \frac{3408}{73205}\zeta(3)\right]\varepsilon^3 + \\ + \frac{1}{16}\left[\frac{1151231173}{1006568750} - \frac{50696504}{20131375}\zeta(3) - \right. \qquad (6) \\ \left. - \frac{5112}{73205}\zeta(4) + \frac{107344}{161051}\zeta(5)\right]\varepsilon^4$$

at the complex cubic one, where $\zeta(3)$, $\zeta(4)$, and $\zeta(5)$ are the Riemann ζ functions.

It is known that RG series are at best asymptotic. An appropriate resummation procedure has to be applied in order to extract reliable physical information from them. To obtain the eigenvalue estimates we have used an approach based on the Borel transformation modified with a conformal mapping [18, 20]. If both eigenvalues of matrix (3) are negative, the associated FP is infrared stable and the critical behavior of experimental systems undergoing second-order phase transitions is determined only by that stable point. For the Bose and the complex cubic FPs our numerical results are presented in Table 1. It is seen that the complex cubic FP is absolutely stable in $D = 3$ ($\varepsilon = 1$), while the Bose point appears to be of the "saddle" type. However ω_2's of either points are very small at the four-loop level, thus implying that these points may swap their stability in the next order of RG approximation. We can compare ω_2 at the complex cubic FP quoted in Table 1 with the three-loop results of Ref. [9] obtained in the framework of RG approach directly in 3D. Those estimates $\omega_2 = -0.010$ for $N^C = 2$ and $\omega_2 = -0.011$ for $N^C = 3$ are solidly consistent with ours.

The four-loop ε expansion for the critical dimensionality of the order parameter of model (2) reads

$$N_c^C = 2 - \varepsilon + \frac{5}{24}\Big[6\zeta(3) - 1\Big]\varepsilon^2 + \\ + \frac{1}{144}\Big[45\zeta(3) + 135\zeta(4) - 600\zeta(5) - 1\Big]\varepsilon^3.$$

Instead of processing this expression numerically, we state the exact relation $N_c^C = \frac{1}{2}N_c^R$, which is independent on the order of approximation used. In fact, the critical dimensionality N_c^C for the complex cubic model is determined as that value of N^C, at which the complex cubic FP coincides with the isotropic one. In the same way, the critical dimensionality N_c^R is defined for the real cubic model. Both systems exhibit effectively the isotropic critical behavior at $N^C = N_c^C$ and $N^R = N_c^R$. So, because the complex $O(2N^C)$-symmetric model is equivalent to the real $O(N^R)$-symmetric one, the relation $2N_c^C = N_c^R$ holds true. For $N^C > N_c^C$ the complex cubic FP of model (2) should be stable in 3D.

The five-loop ε expansion for N_c^R was recently obtained in Ref. [22]. Resummation of that series gave the estimate $N_c^R = 2.894(40)$ (see Ref. [23]). Therefore we conclude that $N_c^C = 1.447(20)$ from the five-loops. Practically the same estimate $N_c^C = 1.435(25)$ follows from a constrained analysis of N_c^R taking into account $N_c^R = 2$ in two dimensions [19]. From the recent pseudo-ε expansion analysis of the real hypercubic model [24] one can extract $N_c^C = 1.431(3)$. However the most accurate estimate $N_c^C = 1.445(20)$ results from the

Table 2

Critical exponents for the isotropic (IFP), the Bose (BFP), and the complex cubic (CCFP) FPs at $N^C = 2$ and $N^C = 3$ calculated in the four-loop order in ε ($\varepsilon = 1$) using the Borel transformation with a conformal mapping

Type of FP	$N^C = 2$			$N^C = 3$		
	η	ν	γ	η	ν	γ
IFP	0.0343(20)	0.725(15)	1.429(20)	0.0317(10)	0.775(15)	1.524(25)
BFP	0.0348(10)	0.664(7)	1.309(10)	0.0348(10)	0.664(7)	1.309(10)
CCFP	0.0343(20)	0.715(10)	1.404(25)	0.0345(15)	0.702(10)	1.390(25)

value $N_c^R = 2.89(4)$ obtained on the basis of the numerical analysis of the four-loop [23] and the six-loop [19] 3D RG expansions for the β-functions of the real hypercubic model.

Finally, we have computed the four-loop ε series for the critical exponents. At the stable complex cubic FP they are

$$\eta = \frac{\varepsilon^2}{48} + \frac{5}{288}\varepsilon^3 - \frac{21\zeta(3) - 13}{1728}\varepsilon^4,$$

$$\gamma^{-1} = 1 - \frac{\varepsilon}{4} - \frac{7}{96}\varepsilon^2 + \frac{84\zeta(3) - 1}{1152}\varepsilon^3 - \\ - \frac{1420\zeta(3) - 1512\zeta(4) + 5840\zeta(5) - 2059}{27648}\varepsilon^4, \qquad (7)$$

for $N^C = 2$ and

$$\eta = \frac{5}{242}\varepsilon^2 + \frac{177}{10648}\varepsilon^3 - \frac{59328\zeta(3) - 50083}{5153632}\varepsilon^4,$$

$$\gamma^{-1} = 1 - \frac{3}{11}\varepsilon - \frac{7}{242}\varepsilon^2 + \frac{912\zeta(3) + 3905}{58564}\varepsilon^3 - \\ - \frac{207682\zeta(3) - 15048\zeta(4) + 30320\zeta(5) - 151817}{1288408}\varepsilon^4, \qquad (8)$$

for $N^C = 3$. Other critical exponents can be found through the known scaling relations. The numerical estimates obtained are collected in Table 2. The critical exponents for the isotropic and the Bose FPs are also presented, for comparison. We can compare our results with the available experimental data. For example, in the case of the structural transition in the NbO_2 crystal the critical exponent of spontaneous polarization was measured in Ref. [7], $0.33 < \beta < 0.44$. Our estimate $\beta = 0.371$ obtained using the data of Table 2 and scaling relations lies in that interval.

In summary, the four-loop ε-expansion analysis of the Ginzburg-Landau model with cubic anisotropy and complex vector order parameter relevant to the phase transitions in certain antiferromagnets with complicated ordering has been carried out. Investigation of the global structure of RG flows for the physically significant cases $N^C = 2$ and $N^C = 3$ leads to the conclusion that the anisotropic complex cubic FP is absolutely stable in 3D. Therefore the critical thermodynamics of the phase transitions in the NbO_2 crystal and in the antiferromagnets $TbAu_2$, DyC_2, $K_2\,IrCl_6$, TbD_2, MnS_2 should govern by this stable point with a specific set of critical exponents, in the frame of the given approximation. The critical dimensionality $N_c^C = 1.445(20)$ obtained from six loops supports this conclusion. At the complex cubic FP, the critical exponents were calculated using the Borel summation technique in combination with a conformal mapping. For the structural phase transition in NbO_2 and for the antiferromagnetic phase transitions in $TbAu_2$ and DyC_2 they were shown to be close to the critical exponents of the $O(4)$-symmetric model. In contrast to this, the critical exponents for the antiferromagnetic phase transitions in K_2IrCl_6, TbD_2, MnS_2 and Nd turned out to be close to the Bose ones.

Although our calculations show that the complex cubic FP, rather than the Bose one, is stable at the four-loop level, the eigenvalues ω_2 of both points are very small. Therefore the situation is very close to marginal, and the FPs might change their stability to opposite in the next order of perturbation theory, so that the Bose point would occur stable. This conjecture is in agreement with the recent six-loop RG study of three-coupling-constant model (1) directly in three dimensions [25]. The authors argue the global stability of the Bose FP, although the numerical estimate $\omega_2 = -0.007(8)$ of the smallest stability matrix eigenvalue of the Bose point appears to be very small and the apparent accuracy of the analysis does not exclude the opposite sign for ω_2. In this situation it would be very desirable to compare the critical exponents values obtained theoretically with values that could be determined from experiments, in order to verdict which of the two FPs is really stable in physical space. Finally, it would be also useful to investigate certain universal amplitude ratios of the model because they vary much more among different universality

classes than exponents do and might be more effective as a diagnostic tool.

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