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2001 J. Phys. A: Math. Gen. 34 L347

(http://iopscience.iop.org/0305-4470/34/23/102)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **34** (2001) L347–L353 www.iop.org/Journals/ja PII: S0305-4470(01)21167-6

LETTER TO THE EDITOR

Critical thermodynamics of three-dimensional MN-component field model with cubic anisotropy from higher-loop ε expansion

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Received 11 January 2001, in final form 6 April 2001

Abstract

The critical thermodynamics of an MN-component field model with cubic anisotropy relevant to the phase transitions in certain crystals with complicated ordering is studied within the four-loop ε expansion using the minimal subtraction scheme. Investigation of the global structure of RG flows for the physically significant cases $M = 2$, $N = 2$ and $M = 2$, $N = 3$ shows that the model has an anisotropic stable fixed point with new critical exponents. The critical dimensionality of the order parameter is proved to be equal to $N_c^C = 1.445(20)$, that is exactly half its counterpart in the real hypercubic model.

PACS numbers: 0570, 6150

We study the critical behaviour of an MN-component field model with cubic anisotropy having a number of interesting applications to phase transitions in three-dimensional simple and complicated systems. The effective Ginzburg–Landau Hamiltonian of the model reads

$$H = \int \mathrm{d}^d x \left[\frac{1}{2} \sum_{\alpha=1}^{N} (m_0^2 \, |\vec{\varphi}^\alpha|^2 + |\nabla \vec{\varphi}^\alpha|^2) + \frac{u_0}{4!} \left(\sum_{\alpha=1}^{N} |\vec{\varphi}^\alpha|^2 \right)^2 + \frac{v_0}{4!} \sum_{\alpha=1}^{N} |\vec{\varphi}^\alpha|^4 \right] \tag{1}$$

where each vector field $\vec{\varphi}^\alpha$ has M real components[3] φ_i^α, $i = 1, \ldots, M$ and $d = 4 - \varepsilon$ is the spatial dimensionality. Here $m_0^2 \sim (T - T_c)$ and m_0, u_0, v_0 are the 'bare' mass and coupling constants, respectively.

For $M = N = 2$ the Hamiltonian (1) describes the structural phase transition in the NbO_2 crystal and the antiferromagnetic phase transitions in $TbAu_2$ and DyC_2. Another physically important case $M = 2$, $N = 3$ is relevant to the antiferromagnetic phase transitions in

[3] For $M = 1$ and 2 the model (1) is merely the N-component cubic model determined either by the real or by the complex order parameter field, respectively.

K_2IrCl_6, TbD_2 and Nd materials [1]. The magnetic and structural phase transitions in a cubic crystal are governed by the model (1) at $M = 1$ and $N = 3$ [2]. In the replica limit $N \to 0$ ($M = 1$) the Hamiltonian (1) is known to determine the critical properties of weakly disordered quenched systems undergoing second-order phase transitions [3] with a specific set of critical exponents [4]. Finally, the case $M = 1$ and $N \to \infty$ corresponds to the Ising model with equilibrium magnetic impurities [5]. In this limit the Ising critical exponents take Fisher-renormalized values [6]. Since static critical phenomena in a cubic crystal as well as in randomly diluted Ising spin systems are well understood [7–11][4], we will focus here on the critical behaviour of the above-mentioned multisublattice antiferromagnets. This is the case of $M = 2$ and $N = 2,\ 3$ in the fluctuation Hamiltonian (1).

For the first time, magnetic and structural phase transitions in crystals with complicated ordering described by the model (1) were studied by Mukamel and Krinsky within the lowest orders in ε [1]. A stable fixed point ('unique' point), different from the isotropic ($O(MN)$-symmetric) or the Bose ($O(MN)$-symmetric, $MN = 2$) one[5], was predicted in $d = 3$. The point was shown to determine a new universality class with a specific set of critical exponents. However, for the physically important case $M = N = 2$, the critical exponents of the unique fixed point turned out to be the same as those of the O(4)-symmetric one within the two-loop approximation.

Later an alternative analysis of critical behaviour of the model, the RG approach in fixed dimension, was carried out within the two- and three-loop approximations [13, 14]. Those investigations gave the same qualitative predictions: the unique stable fixed point does exist on the three-dimensional RG flow diagram. However, the critical exponents computed at this point with the use of different resummation procedures proved to be close to those of the Bose fixed point rather than the isotropic one. It was also shown that the unique and the Bose fixed points are very close to each other on the diagram of RG flows, so that they may interchange their stability in the next orders of RG approximations [14].

Recently, the critical properties of the model were analysed in third order in ε [15, 16]. Investigation of the fixed point stability and calculation of the critical dimensionality N_c of the order parameter, separating two different regimes of critical behaviour, confirmed that the model (1) possesses the anisotropic (complex cubic; $M = 2$ and $u \neq 0$, $v \neq 0$) stable fixed point for $N = 2$ and 3. The realistic critical exponent estimates for the unique stable fixed point were obtained in [16] using the summation technique of [17]. The values appeared to be close to those of the isotropic point in contradiction to the numerical results given by RG directly in three dimensions [13, 14]. Such a distinction may be accounted for by the too short three-loop ε series used.

It is worthy of note that the existence of an anisotropic stable fixed point on the three-dimensional RG flow diagram contradicts the nonperturbative considerations [18]. Indeed, according to those considerations the only stable fixed point in three dimensions may be the Bose one and it is that point which governs the critical thermodynamics in the phase transitions of interest. The point is that the model (1) describes N interacting Bose systems. As was shown by Sak [19], the interaction term can be represented as the product of the energy operators of various two-component subsystems. It was also found that one (the smallest) of the eigenvalue exponents characterizing the evolution of this term under the renormalization group in a neighbourhood of the Bose fixed point is proportional to the specific heat exponent α. Since α is believed to be negative at that point, and that is confirmed experimentally [20] and theoretically [21], the interaction is irrelevant. Consequently, the Bose fixed point should

[4] For a six-loop study of the critical behaviour of the random Ising model see [12].

[5] Note that the isotropic or the Heisenberg fixed point can be determined as the point having the coordinates $u > 0$, $v = 0$ on the RG flow diagram, whereas for the Bose fixed point one has $u = 0$, $v > 0$.

be stable in three dimensions. However, the RG approach, applied to the model (1), has not yet confirmed this conclusion. It is therefore highly desirable to extend already known ε expansions for the stability matrix eigenvalues, critical exponents and critical dimensionality in order to apply more sophisticated resummation techniques to longer expansions.

Therefore, the aim of this Letter is to extend the existing three-loop ε expansions of the model to the four-loop order and to study more carefully the predictions of the RG method regarding the critical phenomena in the substances of interest. Namely, on the basis of the four-loop expansions for the RG functions obtained using dimensional regularization and the minimal subtraction scheme [22, 23], we analyse the stability of the fixed points and calculate the critical dimensionality of the order parameter. We show that the anisotropic stable fixed point does exist on the three-dimensional RG flow diagram. For this point, we give more accurate critical exponent estimates, in comparison with the previous three-loop results [16], by applying a new summation approach [17] to the four-loop series.

The four-loop ε expansions for the β-functions of the model are as follows:

$$
\begin{aligned}
\beta_u = {} & \varepsilon u - u^2 - \frac{4}{N+4}uv + \frac{1}{(N+4)^2}[3u^3(3N+7) + 44u^2v + 10uv^2] \\
& - \frac{1}{(N+4)^3}\left[\frac{u^4}{4}(48\zeta(3)(5N+11) + 33N^2 + 461N + 740) + u^3v(384\zeta(3)\right. \\
& \left. +79N + 659) + \frac{u^2v^2}{2}(288\zeta(3) + 3N + 1078) + 141uv^3\right] - \frac{1}{(N+4)^4} \\
& \times\left[\frac{u^5}{12}(-48\zeta(3)(63N^2 + 382N + 583) + 144\zeta(4)(5N^2 + 31N + 44)\right. \\
& -480\zeta(5)(4N^2 + 55N + 93) + 5N^3 - 3160N^2 - 20\,114N - 24\,581) \\
& -\frac{2u^4v}{3}(12\zeta(3)(3N^2 + 276N + 1214) - 36\zeta(4) \times (19N + 85) \\
& +\zeta(5)(2400N + 23\,040) - 28N^2 + 3957N + 15\,967) - \frac{u^3v^2}{3}(72\zeta(3) \\
& \times(19N + 426) - 4032\zeta(4) + 39\,840\zeta(5) + 1302N + 46\,447) \\
& +\frac{2u^2v^3}{3}(60\zeta(3)(N - 84) - 792\zeta(4) - 4800\zeta(5) - 125N - 12809) \\
& \left. -\frac{uv^4}{2}(400\zeta(3) + 768\zeta(4) + 3851)\right]
\end{aligned} \qquad (2)
$$

$$
\begin{aligned}
\beta_v = {} & \varepsilon v - \frac{1}{N+4}(6uv + 5v^2) + \frac{1}{(N+4)^2}\left[u^2v(5N+41) + 80uv^2 + 30v^3\right] \\
& - \frac{1}{(N+4)^3}\left[\frac{u^3v}{2}(96\zeta(3)(N+7) - 13N^2 + 184N + 821)\right. \\
& +\frac{u^2v^2}{4}(4032\zeta(3) + 59N + 5183) + uv^3(768\zeta(3) + 1093) \\
& \left. +\frac{v^4}{2}(384\zeta(3) + 617)\right] - \frac{1}{(N+4)^4}\left[\frac{u^4v}{4}(48\zeta(3)\right. \\
& \times(N^3 - 12N^2 - 140N - 567) + 144\zeta(4)(2N^2 + 17N + 45) \\
& -3360\zeta(5)(3N + 13) - 29N^3 - 28N^2 - 6958N - 19\,679) \\
& +\frac{u^3v^2}{3}(12\zeta(3)(9N^2 - 591N - 7028) + \zeta(4) \times (3528N + 21\,240)
\end{aligned}
$$

Table 1. Eigenvalue exponent estimates obtained for the Bose (BFP) and the complex cubic (CCFP) fixed points at $N = 2$ and 3 within the four-loop approximation in ε ($\varepsilon = 1$) using Borel transformation with a conformal mapping.

Type of fixed point	$N = 2$		$N = 3$	
	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)

$$
-480\zeta(5)(10N+287)+61N^2-5173N-66\,764)
-\frac{u^2v^3}{3}\times(1800\zeta(3)(N+62)-144\zeta(4)(8N+203)
+172\,800\zeta(5)+56N+93\,701)-4uv^4(5090\zeta(3)-1296\zeta(4)+7600\zeta(5)
+4503)+\frac{v^5}{2}(-8224\zeta(3)+1920\zeta(4)-12\,160\zeta(5)-7975)\Big] \tag{3}
$$

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

From the system of equations $\beta_u(u^*, v^*) = 0$ and $\beta_v(u^*, v^*) = 0$, we found formal series for the four fixed points: trivial Gaussian and nontrivial isotropic, Bose and complex cubic. Then we calculated the eigenvalues of the stability matrix

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

taken at the most intriguing Bose and complex cubic fixed points. The corresponding numerical estimates are obtained using an approach based on the Borel transformation

$$
F(\varepsilon; a, b) = \sum_{k=0}^{\infty} A_k(\lambda) \int_0^{\infty} \mathrm{e}^{-\frac{x}{a\varepsilon}} \left(\frac{x}{a\varepsilon}\right)^b \mathrm{d}\left(\frac{x}{a\varepsilon}\right) \frac{z^k(x)}{[1-z(x)]^{2\lambda}} \tag{4}
$$

modified with a conformal mapping $z = \frac{\sqrt{x+1}-1}{\sqrt{x+1}+1}$ [24], which does not require the knowledge of the exact asymptotic high-order behaviour of the series [17]. The parameter λ is chosen from the condition of the most rapid convergence of series (4), that is by minimizing the quantity $\left|1 - \frac{F_l(\varepsilon;a,b)}{F_{l-1}(\varepsilon;a,b)}\right|$, where l is the step of truncation and $F_l(\varepsilon; a, b)$ is the l-partial sum for $F(\varepsilon; a, b)$. If the real parts of both eigenvalues are negative, the associated fixed point is infrared stable and the critical behaviour of experimental systems undergoing second-order transitions is determined only by that stable point. For the Bose and the complex cubic fixed points our numerical results are presented in table 1. It is seen that the complex cubic fixed point is absolutely stable in $d = 3$ ($\varepsilon = 1$), while the Bose point appears to be of the 'saddle' type[6]. However, the ω_2 of either point is very small at the four-loop level, thus implying that these points may swap their stability in the next order of the RG approximation.

In addition to the eigenvalues, we calculated the critical dimensionality N_c^C of the order parameter from the condition of vanishing ω_2 for the complex cubic fixed point. The four-loop expansion is

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

[6] We say the fixed point is of the 'saddle' type provided the eigenvalue exponents ω_1 and ω_2 are of opposite signs in the (u, v) plane.

Table 2. Critical exponents calculated for the isotropic (IFP), the Bose (BFP) and the complex cubic (CCFP) fixed points at $N = 2$ and 3 within the four-loop approximation in ε ($\varepsilon = 1$) using Borel transformation with a conformal mapping.

Type of fixed point	$N = 2$			$N = 3$		
	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)

Instead of processing this expression numerically, we established the exact relation $N_c^C = \frac{1}{2}N_c^R$, which is independent on the order of approximation used[7]. 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 fixed point coincides with the isotropic one. The same assertion holds for the cubic model with the real N^R-component order parameter. So, because of the relation $O(2N^C) = O(N^R)$, the relation $2N_c^C = N_c^R$ should hold too.

The five-loop ε-expansion for N_c^R was recently obtained in [7]. Resummation of that series gave the estimate $N_c^R = 2.894(40)$ [9]. 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 [10]. From the recent pseudo-ε expansion analysis of the real hypercubic model [11] one can extract $N_c^C = 1.431(3)$. However the most accurate estimate $N_c^C = 1.445(20)$ results from the value $N_c^R = 2.89(4)$ obtained on the basis of the numerical analysis of the four-loop [9] and the six-loop [10] three-dimensional RG expansions for the β-functions of the real hypercubic model. Since $N_c^C < 2$, the phase transitions in the NbO_2 crystal and in the antiferromagnets $TbAu_2$, DyC_2, K_2IrCl_6, TbD_2 and Nd are of second order and their critical thermodynamics should be controlled by the complex cubic fixed point with a specific set of critical exponents, in the frame of the given approximation. The corresponding four-loop critical exponent estimates are displayed in table 2. The critical exponent estimates obtained for the isotropic and the Bose fixed points are also presented in the table, for comparison.

In conclusion, the four-loop ε-expansion analysis of the generalized MN-component Ginzburg–Landau model with cubic anisotropy describing phase transitions in certain real antiferromagnets with complicated ordering has been carried out with the use of the minimal subtraction scheme. Investigation of the global structure of RG flows for the physically significant cases $M = 2$, $N = 2$ and $M = 2$, $N = 3$ has shown that the complex cubic rather than the Bose fixed point is absolutely stable in three dimensions. The critical dimensionality $N_c^C = 1.445(20)$ of the order parameter obtained from six loops has confirmed this conclusion. For the stable complex cubic fixed point, reasonable estimates of critical exponents were obtained 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 and Nd turned out to be close to the Bose ones. Although our results seem to be substantially consistent with other predictions of the RG approach, still there is a definite contradiction with the general nonperturbative theoretical arguments [18] mentioned in the introduction. One can hope, however, that the five-loop contributions being taken into

[7] Here N_c^C and N_c^R are the critical (marginal) spin dimensionalities in the complex ($M = 2$) and in the real ($M = 1$) hypercubic model, respectively.

account will eliminate this controversy. Indeed, the present calculations have shown that, although the complex cubic fixed point, rather than the Bose one, is stable at the four-loop level, the eigenvalues ω_2 of both fixed points are very small. Therefore the situation is very close to marginal, and the points might change their stability to the opposite in the next order of perturbation theory, so the Bose point would turn out to be stable. There is a hope that comparison of the critical exponent values obtained theoretically for different fixed points with those values determined from experiments or, probably, from Monte Carlo simulations would indicate which fixed point is really stable in three dimensions. Finally, it would also be desirable 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.

We are grateful to Professor M Henkel for helpful remarks and to Dr E Blagoeva for communicating her results mentioned in [15]. One of the authors (KBV) acknowledges useful discussions with Dr B N Shalaev. This work was supported by the Russian Foundation for Basic Research, grant no 01-02-17048, and by the Ministry of Education of the Russian Federation, grant no E00-3.2-132.

Note added. More recently, the six-loop RG functions of the model of interest have been calculated within the alternative three-dimensional RG approach [12, 25]. Although the authors argue the global stability of the Bose fixed point, the numerical estimate of the smallest stability matrix eigenvalue of the Bose fixed point, which governs the RG flows near this point, appears to be very small, $\omega_2 = -0.007(8)$ [25], and the apparent accuracy of the analysis does not exclude the opposite sign for ω_2. This result agrees well with our conclusions.

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