Third-harmonic exponent in three-dimensional *N*-vector models

Martino De Prato,[1,*] Andrea Pelissetto,[2,†] and Ettore Vicari[3,‡]
[1]*Dipartimento di Fisica, Università di Roma Tre, and INFN, I-00146 Roma, Italy*
[2]*Dipartimento di Fisica, Università di Roma La Sapienza, and INFN, I-00185 Roma, Italy*
[3]*Dipartimento di Fisica, Università di Pisa, and INFN, I-56127 Pisa, Italy*

(Received 8 February 2003; revised manuscript received 21 May 2003; published 5 September 2003)

We compute the crossover exponent associated with the spin-3 operator in three-dimensional $O(N)$ models. A six-loop field-theoretical calculation in the fixed-dimension approach and a five-loop calculation in ϵ expansion give $\phi_3=0.600(10)$ for the experimentally relevant case $N=2$ (XY model). The corresponding exponent $\beta_3=1.414(10)$ is compared with the experimental estimates obtained in materials undergoing a normal-incommensurate structural transition and in liquid crystals at the smectic-*A*–hexatic-*B* phase transition, finding good agreement.

DOI: 10.1103/PhysRevB.68.092403 PACS number(s): 05.70.Jk, 64.60.Fr, 75.40.Cx, 61.30.−v

I. INTRODUCTION

In nature many physical systems undergo phase transitions belonging to the universality classes of the $O(N)$ vector models. In particular, the XY model, corresponding to $N=2$, describes the λ transition in ^{4}He, (anti)ferromagnets with easy-plane anisotropy, density-wave systems, etc.; see Ref. 1 for a review. The critical exponents associated with the order parameter have been accurately measured both experimentally and theoretically.[1] Moreover, in some XY systems it is also possible to measure experimentally the critical exponents associated with secondary order parameters. This is the case of liquid crystals,[2–4] of normal-incommensurate transitions,[5–7] and of graphite-intercalation compounds.[8]

The most relevant exponent is the second-harmonic one that has been recently computed to high precision using field-theoretical methods in Refs. 9 and 10. The ϵ expansion gives $\phi_2=1.174(12)$, while the fixed-dimension expansion gives $\phi_2=1.184(12)$. The fourth-harmonic crossover exponent was reported in Refs. 11 and 10: $\phi_4=-0.077(3)$ (ϵ expansion) and $\phi_4=-0.069(5)$ (fixed-dimension expansion). Here, we wish to determine the third-harmonic exponent by means of a six-loop perturbative calculation in the fixed-dimension approach and of a five-loop calculation in ϵ expansion, extending previous three-loop determinations.[12,13,3] Such a calculation is also relevant for some crossover phenomena, in which the XY symmetry is reduced to that of the three-state Potts model, as it happens in cubic magnets in the presence of stress or of appropriate magnetic fields.[14,15]

In the field-theoretical approach one starts from the usual ϕ^4 Hamiltonian

$$\mathcal{H}=\int d^dx\left[\frac{1}{2}(\partial_\mu\phi)^2+\frac{1}{2}r\phi^2+\frac{1}{4!}u(\phi^2)^2\right],\qquad(1)$$

where $\phi_a(x)$ is an N-component real field. The XY model corresponds to $N=2$, but here we will keep N generic. Secondary order parameters are associated with operators $\mathcal{O}^{(l)}$ that are polynomials of order l in the fields and that transform irreducibly under the spin-l representation of the $O(N)$ group. In particular, the third-harmonic operator is

$$\mathcal{O}^{(3)}_{abc}=\phi_a\phi_b\phi_c-\frac{\phi^2}{N+2}(\phi_a\delta_{bc}+\phi_b\delta_{ac}+\phi_c\delta_{ab}).\qquad(2)$$

We wish now to compute the crossover exponent ϕ_3 associated with $\mathcal{O}^{(3)}_{abc}$ and the corresponding exponents β_3 and γ_3 given by

$$\beta_3=2-\alpha-\phi_3,$$
$$\gamma_3=-2+\alpha+2\phi_3.\qquad(3)$$

The exponents β_3 and γ_3 describe, respectively, the critical (singular) behavior of the average $\langle\mathcal{O}^{(3)}(x)\rangle\sim|t|^{\beta_3}$ and of the susceptibility $\chi_{\mathcal{O}}\equiv\Sigma_x\langle\mathcal{O}^{(3)}(0)\mathcal{O}^{(3)}(x)\rangle_c\sim|t|^{-\gamma_3}$.

Let us first present the fixed-dimension calculation. We determine the renormalization function $Z_3(g)$ from the one-particle irreducible three-point function $\Gamma_3^{(3)}(0)$ with an insertion of the operator $\mathcal{O}^{(3)}_{abc}$ at zero external momenta, i.e., we set

$$\Gamma_3^{(3)}(0)\equiv\langle\mathcal{O}^{(3)}_{abc}\phi_a\phi_b\phi_c\rangle^{1PI}=AZ_3^{-1}(g),\qquad(4)$$

where A is a numerical coefficient that ensures that $Z_3(0)=1$, and g is the four-point renormalized coupling. Then, we compute the renormalization-group function

$$\eta_3(g)\equiv\left.\frac{\partial\ln Z_3}{\partial\ln m}\right|_u=\beta(g)\frac{d\ln Z_3}{dg},\qquad(5)$$

and $\eta_3=\eta_3(g^*)$, where g^* is the fixed-point value of g. Finally, the renormalization-group scaling relation (valid in d dimensions)

$$\phi_3=\left(\eta_3+3-\frac{d}{2}-\frac{3}{2}\eta\right)\nu\qquad(6)$$

allows us to determine ϕ_3.

The calculation of $\Gamma_3^{(3)}(0)$ to six loops is rather cumbersome since it requires the evaluation of a few thousand Feynman diagrams. We use a symbolic manipulation program in MATHEMATICA. It generates the diagrams,[16] computes the symmetry factor of each of them using the algorithm discussed in Ref. 17, and finally determines the group factors by a straightforward application of the Feynman rules. We use the numerical results compiled in Ref. 17 for the integrals associated with each diagram. Indeed, it is easy to realize that each graph contributing to the one-particle irreducible correlation function appearing in Eq. (4) can be interpreted (as far as the Feynman integral is concerned, symmetry and group factor of course differ) as a diagram contributing to the four-point function. It is enough to add an external line to the vertex corresponding to the insertion. In order to check the calculation, we determine more generally $\langle P_{def}\phi^a\phi^b\phi^c\rangle^{1PI}$, where $P_{def}\equiv(\phi^d\phi^e\phi^f)$, and verify the zero-momentum identity

$$\frac{u}{6}\left\langle\left(\sum_m P_{mmf}\right)\phi^a\phi^b\phi^c\right\rangle^{1PI}=\langle\phi^f\phi^a\phi^b\phi^c\rangle^{1PI}, \qquad (7)$$

which follows from the equations of motion. This is a strong check of our computation. Finally, we obtain

$$\begin{aligned}\eta_3(\bar{g})=&-\frac{6}{N+8}\bar{g}+\frac{2(N+10)}{(N+8)^2}\bar{g}^2-\frac{128.736+15.4900\,N-0.650238\,N^2}{(N+8)^3}\bar{g}^3\\&+\frac{1148.68+191.005\,N+1.82163\,N^2+0.283028\,N^3}{(N+8)^4}\bar{g}^4\\&-\frac{12606.9+2550.46\,N+64.4818\,N^2-2.34060\,N^3-0.152501\,N^4}{(N+8)^5}\bar{g}^5\\&+\frac{161373.+38736.8\,N+1874.23\,N^2-5.98451\,N^3+1.88168\,N^4+0.094179\,N^5}{(N+8)^6}\bar{g}^6+O(\bar{g}^7),\end{aligned} \qquad (8)$$

where, as usual, we have introduced the rescaled coupling $\bar{g}$ defined by

$$g=\frac{48\pi}{8+N}\bar{g}. \qquad (9)$$

Here g is the usual four-point renormalized coupling normalized so that $g=u/m$ (m is the renormalized mass) at tree level.

We have repeated the calculation in ϵ expansion in the minimal subtraction scheme to five loops. The computation is analogous. Symmetry and group factor coincide with those compute before, while for the divergent part of the Feynman integrals we use the results reported in Ref. 18. We obtain

$$\begin{aligned}\eta_3(\epsilon)=&-\frac{6}{N+8}\epsilon+\frac{3(N+2)(N-2)}{(N+8)^3}\epsilon^2+\frac{(N+2)(1705.97+244.849\,N+44.0753\,N^2+1.5\,N^3)}{(N+8)^5}\epsilon^3-\frac{(N+2)}{(N+8)^7}(256540\\&+79763.8\,N+10638.6\,N^2+130.68\,N^3-15.3532\,N^4+1.05309\,N^5)\epsilon^4+\frac{(N+2)}{(N+8)^9}(5.84399\times10^7+2.81169\times10^7\,N\\&+5.88038\times10^6\,N^2+627841\,N^3+39530.4\,N^4+940.222\,N^5-30.6634\,N^6+0.058929\,N^7)\epsilon^5+O(\epsilon^6),\end{aligned} \qquad (10)$$

where $\epsilon=4-d$. At three loops this expansion is consistent with the results reported in Ref. 19.

Field-theoretical perturbative expansions are divergent, and thus, in order to obtain accurate results, an appropriate resummation is required. We use the method of Ref. 20 that takes into account the large-order behavior of the perturbative expansion; see, e.g., Ref. 21. Mean values and error bars are computed using the algorithm of Ref. 11.

Let us now analyze the perturbative series, starting from the six-loop ones. Given the expansion of $\eta_3(\bar{g})$, we determine the perturbative expansion of $\phi_3(\bar{g})$, $\beta_3(\bar{g})$, and $\gamma_3(\bar{g})$ using relations (3) and (6) with $d=3$. Then, we resum the perturbative series and compute them at $\bar{g}=\bar{g}^*$.[22] For $N=2$ we obtain $\phi_3=0.5963(21)$, $0.5968(2)$, $\beta_3=1.398(8)$, $1.405(3)$, $\gamma_3=-0.800(7)$, $-0.808(13)$, where for each exponent we report the estimate obtained from the direct analysis and from the analysis of the series of the inverse. The two estimates obtained for each exponent agree within error bars, but, with the quoted errors, scaling relations (3) are not well satisfied. For instance, using $\nu=0.67155(27)$ (Ref. 23) and $\beta_3=1.403(8)$ we obtain $\phi_3=0.611(8)$, while using the same value of ν and $\gamma_3=-0.803(13)$ we have ϕ_3

TABLE I. Critical exponents associated with the spin-3 operator $O^{(3)}_{abc}$.

	Fixed dimension			ϵ expansion		
N	ϕ_3	β_3	γ_3	ϕ_3	β_3	γ_3
0	0.445(11)	1.331(11)	$-0.89(2)$	0.434(5)	1.342(5)	$-0.909(10)$
2	0.601(10)	1.413(10)	$-0.81(2)$	0.599(15)	1.415(15)	$-0.815(31)$
3	0.678(18)	1.455(18)	$-0.78(4)$	0.681(30)	1.452(30)	$-0.771(60)$
4	0.760(23)	1.487(23)	$-0.73(4)$	0.764(34)	1.483(34)	$-0.72(7)$
5	0.814(14)	1.484(14)	$-0.67(3)$	0.813(19)	1.485(19)	$-0.67(4)$
8	0.971(33)	1.519(33)	$-0.55(7)$	0.950(50)	1.540(50)	$-0.59(10)$
16	1.193(12)	1.540(12)	$-0.35(2)$	1.17(9)	1.57(9)	$-0.40(17)$
∞	$\frac{3}{2}$	$\frac{3}{2}$	0	$\frac{3}{2}$	$\frac{3}{2}$	0

$=0.606(6)$. These two estimates are slightly higher than those obtained from the analysis of $\phi_3(g)$ and $1/\phi_3(g)$. Clearly, the errors are somewhat underestimated, a phenomenon that is probably connected with the nonanalyticity[24–26] of the renormalization-group functions at the fixed point $\overline{g}^*$.

In order to obtain a conservative estimate, we have thus decided to take as estimate of ϕ_3 the weighted average of the direct estimates and of the estimates obtained using β_3 and γ_3 together with scaling relations (3). The error is such to include all estimates. The other exponents are dealt with analogously.[27] The final results for several values of N are reported in Table I.

The same analysis has been repeated by using the five-loop ϵ-expansion series. The results are reported in Table I. They are in perfect agreement with the fixed-dimension ones, providing an important check to our final results. Note that in many cases the difference is much less than the reported errors, confirming that our errors are very conservative. For the relevant case $N=2$, the estimates of ϕ_3 obtained using the two expansions are essentially identical. As final estimate we take $\phi_3=0.600(10)$.

Let us compare these results with previous ones for $N=2$. Reference 3 reports $\beta_3=3\beta+3\nu x_3$, where $x_3\approx 0.174$ from the ϵ expansion[28] and $x_3\approx 0.276$ from the fixed-dimension expansion. It follows $\beta_3\approx 1.397$ and $\beta_3\approx 1.602$ in the two cases. These results are reasonably close to ours. The exponent β_3 has been determined at the smectic-A–hexatic-B phase transition in liquid crystals, obtaining[2,3] $\beta_3\approx 4.8\beta\approx 1.66$, using $\beta=0.3485(4)$ (Ref. 23). Such an exponent has also been measured in some materials exhibiting a structural normal-incommensurate phase transition. From the analysis of x-ray scattering data in erbium Ref. 6 obtains $\beta_3=1.8(3)$, while two different experiments in Rb_2ZnCl_4 give, respectively, $\beta_3=1.80(5)$ (Ref. 5) and $\beta_3=1.50(4)$ (Ref. 7). Keeping into account that the experimental errors seem to be underestimated, there is reasonable agreement with our results. The exponent $\delta^*\equiv\beta/\phi_3$ was measured at the trigonal-to-pseudotetragonal transition in [111]-stressed $SrTiO_3$ obtaining[14] $\delta^*=0.62(10)$. Such an estimate is in good agreement with our prediction $\delta^*=0.58(1)$. Finally, we should mention that our results are also relevant for polymer physics. Indeed, we can derive from the estimates obtained for $N=0$ the partition-function exponent p for nonuniform[29] star polymers with three arms. Using $\phi_3=0.440(10)$, we obtain $p=3(\gamma+\nu)/2+\phi_3=3.01(1)$, where we used $\gamma=1.1575(6)$ (Ref. 30).

*Email address: deprato@fis.uniroma3.it
†Email address: Andrea.Pelissetto@roma1.infn.it
‡Email address: vicari@df.unipi.it

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resulting list was compared with that presented in Ref. 17, finding full agreement. Then, the relevant diagrams for $\Gamma_3^{(3)}(0)$ were obtained as follows: (i) We consider each four-point graph H; (ii) Then, we consider all vertices V of H with at least an external line; for each V we generate a graph G_i, such that the insertion is in V and one external line of H in V is deleted; (iii) Finally, we check which of the diagrams G_i are unrelated by symmetry.

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