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Critical limit and anisotropy in the two-point correlation function of three-dimensional $O(N)$ models

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PACS. 75.10Hk – Classical spin models.

Abstract. – In three-dimensional $O(N)$ models, we investigate the low-momentum behavior of the two-point Green’s function $G(x)$ in the critical region of the symmetric phase. We consider physical systems whose criticality is characterized by a rotational-invariant fixed point. In non-rotational invariant physical systems with $O(N)$-invariant interactions, the vanishing of space-anisotropy approaching the rotational-invariant fixed point is described by a critical exponent $\rho$, which is universal and is related to the leading irrelevant operator breaking rotational invariance. At $N = \infty$ one finds $\rho = 2$. We show that, for all values of $N \geq 0$, $\rho \simeq 2$. Non-Gaussian corrections to the universal low-momentum behavior of $G(x)$ are evaluated, and found to be very small.

Three-dimensional $O(N)$ models describe many important critical phenomena in nature. We just mention that the case $N = 3$ describes the critical properties of ferromagnetic materials. The case $N = 2$ is related to the helium superfluid transition. The case $N = 1$ (i.e. Ising-like systems) describes liquid-vapor transitions in classical fluids or critical binary fluids. Finally, the limit $N \rightarrow 0$ is related to dilute polymers. The critical behavior of the two-point correlation function $G(x)$ of the order parameter is related to the phenomenon of critical scattering observed in many experiments, e.g., neutron scattering in ferromagnetic materials, light and X-rays in liquid-gas systems.

We will specifically consider systems with an $O(N)$-invariant Hamiltonian in the symmetric phase, i.e. where the $O(N)$ symmetry is unbroken. Furthermore, we will only consider systems with a rotationally symmetric fixed point. Interesting members of this class are systems defined on highly symmetric lattices, i.e. Bravais or two-point base lattices with a tetrahedral or larger discrete rotational symmetry.

In the critical region of the symmetric phase and at low momentum, experiments show that $G(x)$ is well approximated by a Gaussian behavior, i.e.

$$\frac{\tilde{G}(0)}{G(k)} \simeq 1 + \frac{k^2}{M_G^2},$$

(1)

where $M_G$ is a mass scale defined at zero momentum, i.e. $M_G \equiv 1/\xi_G$ and $\xi_G$ is the second moment correlation length.
Our aim is to estimate the deviations from eq. (1) in the critical region of the symmetric phase, i.e. for $0 < T/T_c - 1 \ll 1$, and in the low-momentum regime $k^2 \lesssim M_G^2$. We focus on two quite different sources of deviations: i) Non rotationally invariant scaling violations, reflecting a microscopic anisotropy in the space distribution of the spins (assuming that no anisotropy is generated by their interaction). This phenomenon may be relevant, for example, in the study of ferromagnetic materials, where the atoms lie on the sites of a lattice, and anisotropy may be observed in neutron scattering experiments. In these systems anisotropy vanishes in the critical limit, and $G(x)$ approaches a rotationally invariant form. ii) Scaling corrections to eq. (1), depending on the ratio $k^2/M_G^2$, and reflecting the non-Gaussian nature of the fixed point.

Several approaches have been considered in order to study the critical behavior of the two-point function $G(x)$. In lattice $O(N)$ non-linear $\sigma$ models, we have calculated the strong-coupling expansion of $G(x)$ up to 15th order on the cubic lattice and 21st order on the diamond lattice within the corresponding nearest-neighbor formulations. We have analyzed the first few non-trivial terms of the $1/N$-expansion, $\epsilon$-expansion and of the $g$-expansion (i.e. expansion in the coupling at fixed dimensions $d = 3$) of the two-point function within the corresponding $\phi^4$ formulation of $O(N)$ models.

Anisotropy of $G(x)$, for the class of systems we are considering, vanishes at the rotationally invariant fixed point, with a behavior governed by a universal critical exponent $\rho$. Non-spherical moments (i.e. those which vanish when calculated on spherical functions) of $G(x)$ are depressed with respect to spherical moments carrying the same naive physical dimensions by a factor $\xi^{-\rho}$. From a field-theoretical point of view, anisotropy in space is due to non rotationally invariant (but $O(N)$ symmetric) irrelevant operators in the effective Hamiltonian, whose presence depends essentially on the symmetries of the physical system, or of the lattice formulation. The exponent $\rho$ is related to the critical effective dimension of the leading irrelevant operator breaking rotational invariance. On cubic-like lattices the leading operator has canonical dimension $d + 2$. In the large-$N$ limit, where the canonical dimensions determine the scaling properties, one then finds $\rho = 2$. We show $\rho$ remains close to its canonical value for all values of $N \geq 0$. We mention that for the two-dimensional Ising model the exact result $\rho = 2$ holds.

We will present rather accurate determinations of the scaling corrections to the Gaussian behavior (1), which substantially improve earlier analyses [1]-[5]. The experimental observation that scaling corrections to the Gaussian behavior (1) are very small is confirmed.

The technical details of our study will be reported in a separate extended paper. Here we only describe the general features of our analysis and the main numerical results.

For definiteness let us consider the cubic lattice version of the models. We parametrize the two-point spin-spin function by a multipole expansion in the form

$$\beta^{-1}G^{-1}(k, M_G) = \sum_{l=0}^{\infty} g_{2l}(y, M_G)Q_{2l}(k), \quad (2)$$

where $y \equiv k^2/M_G^2$, and $Q_{2l}(k)$ are homogeneous functions of momenta of degree $2l$ which are invariant under the symmetries of the lattice. Their expressions can be obtained from the fully symmetric traceless tensors of rank $2l$, $T^{\alpha_1\ldots\alpha_2}_{2l}(k)$, by considering all the cubic-invariant combinations. Odd rank terms are absent in the expansion (2) because of the parity symmetry. The first non-trivial function is

$$Q_4(k) = \sum_{\mu} k^4_{\mu} - \frac{3}{5} \left( \sum_{\mu} k^2_{\mu} \right)^2. \quad (3)$$

$Q_4(k)$ corresponds to the leading irrelevant operator that breaks rotational invariance in the
low-momentum expansion of the Hamiltonian. In the continuum notation this operator has the form $s(x) \cdot Q_4(\partial)s(x)$, and has canonical dimension five in $d = 3$.

The scaling limit of eq. (2) corresponds to taking $M_G \to 0$ while keeping the ratio $k/M_G$ finite. Hence we can parametrize the low-momentum behavior of $G^{-1}(k, M_G)$ in the critical region by

$$\beta^{-1} G^{-1}(k, M_G) = Z^{-1} \tilde{g}_0(y) M_G^2 + \ldots + Z_4 Q_4(k/M_G) \tilde{g}_4(y) M_G^4 + O(M_G^6),$$

where we have dropped rotationally invariant $O(M_G^4)$ terms which we are not interested in, and we have introduced the quantities

$$Z^{-1} = \frac{g_0(0, M_G)}{M_G^2}, \quad Z_4 = g_4(0, M_G),$$

which, in the limit $M_G \to 0$, absorb all non-analytical dependence on $M_G$ of the corresponding terms. The functions $\tilde{g}_0(y)$ and $\tilde{g}_4(y)$ are universal, i.e. they do not depend on the specific form of the lattice Hamiltonian. They possess a regular expansion around $y = 0$:

$$\tilde{g}_0(y) = 1 + y + \sum_{i=2}^{\infty} c_i y^i,$$

$$\tilde{g}_4(y) = 1 + \sum_{i=1}^{\infty} d_i y^i.$$  \hspace{1cm} (6)

(7)

In the limit $N \to \infty$, the models are strictly Gaussian and therefore all the coefficients $c_i$ and $d_i$ are zero.

We consider the spherical moments $m_{2j} = \sum_x |x|^{2j} G(x)$, and the leading non-spherical moments $q_{4j} = \sum_x |x|^{2j} Q_4(x)G(x)$ which vanish if $G(x)$ is rotationally invariant. The critical exponent $\rho$, describing the vanishing of anisotropy, and the coefficients $c_i$ and $d_i$ of the low-momentum expansion of $\tilde{g}_0(y)$ and $\tilde{g}_4(y)$, can be determined by studying appropriate combinations of the above moments in the critical limit. In the critical region

$$\frac{q_{4m}}{m_{4+2m}} \sim \frac{1}{\xi^\sigma},$$

where $q_{2m}$ and $m_{4+2m}$ have the same naive physical dimensions.

In the case of non-Gaussian fixed points, like those corresponding to the theory at finite $N$, the operator $s(x) \cdot Q_4(\partial)s(x)$ develops an anomalous dimension $\sigma$, which causes a departure from the Gaussian value of $\rho$, i.e. $\rho = 2 + \sigma$. $\sigma$ may be extracted by evaluating the ratio $Z_4 z_4/M_G^6 \sim M_G^\sigma$. In turn this combination is easily estimated by taking the moment ratio $q_{4,0}/m_{2} \sim M_G^\sigma$. Strong-coupling estimates of $\sigma$ have been obtained by analyzing and comparing the available strong-coupling series of $q_{4,0}$ and $m_2$ on both cubic and diamond lattices. Universality between cubic and diamond lattice is substantially verified, although the analysis on the diamond lattice turns out to be less precise.

The exponent $\sigma$ can also be estimated by other expansions. We have calculated $\sigma$ to $O(1/N)$ in the $1/N$-expansion:

$$\sigma = \frac{32}{21 \pi^2 N} + O\left(\frac{1}{N^2}\right),$$

(9)

to $O(\epsilon^2)$ in the $\epsilon$-expansion:

$$\sigma = \frac{7}{20} \frac{(N + 2)}{(N + 8)^2} \epsilon^2 + O(\epsilon^3),$$

(10)
and to $O(g^3)$ in the $g$-expansion:

$$
\sigma = \bar{g}^2 \frac{5408}{25515} \frac{(N + 2)}{(N + 8)^2} (1 + \bar{g} \times 0.0450) + O(\bar{g}^4),
$$

(11)

where $\bar{g}$ is the rescaled coupling: $\bar{g} = g(N + 8)/48\pi$. In order to get a reliable quantitative estimate from the perturbative $g$-expansion, one should perform a resummation of the series and then evaluate it at the fixed point value of the coupling $\bar{g}^*$. However, one may obtain an indicative estimate of $\sigma$ by evaluating the available series (11) at $\bar{g}^*$. Estimates of $\bar{g}^*$ by various approaches can be found in the literature (see, for example, ref. [6]).

Our results are summarized in table I, where we show results from the strong-coupling analysis and from eqs. (9), (10) and (11) for the physically interesting values of $N$. We consider also large values of $N$ in order to verify the large-$N$ behavior (9). The errors displayed in the strong-coupling estimates should give an idea of the spread of the results from the various Padé-type and integral approximants we considered in our analysis. The global comparison is satisfactory. For $O(N)$ models, the values of $\sigma$ are very small in the whole range $N \geq 0$, thus indicating an essentially Gaussian behavior of this critical exponent.

We have studied the non-Gaussian corrections to $\hat{g}_0(y)$ in the low-momentum regime, and those of $\hat{g}_4(y)$, by calculations to $O(1/N)$ in the $1/N$-expansion, $O(\epsilon^3)$ in the $\epsilon$-expansion, $O(g^4)$ in the $g$-expansion, and by the analysis of the strong-coupling expansion of $G(x)$.

In table II we report our strong-coupling estimates for $c_2$, $c_3$ and $d_4$ on both cubic and diamond lattice, obtained by evaluating at $\beta_c$ appropriate approximants (such as Padé and first-order integral approximants) of the strong-coupling series of corresponding estimators. One may notice that universality between cubic and diamond lattice is always confirmed. The good precision of our strong-coupling estimates has been achieved essentially for two reasons: long series are available, and, even more important, improved estimators have been employed. We indeed took special care in the choice of estimators for the physical quantities $c_i$ and $d_i$. This is very important from a practical point view: better estimators can greatly improve the stability of the extrapolation to the critical point. Our search for optimal estimators was guided by the knowledge of the large-$N$ limit. We chose estimators which are perfect for $N = \infty$, i.e. do not present off-critical corrections to their critical value $c_i = d_i = 0$ in the symmetric phase.

Estimates from the $g$-expansion and $\epsilon$-expansion, which are reported in table II, have been obtained by tentative resumptions of the available series based on the method outlined.
in ref. [7]. The relatively few terms of the series do not allow a reliable estimate of the corresponding uncertainty. For the $g$-expansion, a check of stability would suggest an apparent uncertainty $\lesssim 20\%$ at small values of $N$, which decreases with increasing $N$. The comparison of the results from all the approaches we have considered is definitely good.

All calculations agree in indicating that the inequality

$$c_i \ll c_2 \ll 1 \quad \text{for} \quad i \geq 3$$

(12)

is satisfied for all $N$. This show that, in the critical region of the symmetric phase, the two-point Green’s function is substantially Gaussian in a large region around $k^2$, i.e. for $|k^2/M_0^2| \lesssim 1$, for all $N$ from zero to infinity. Another important consequence of the relation (12) is the possibility of evaluating the zero of $\tilde{g}_0(y)$ closest to the origin, $y_0$, to a rather good approximation by the relationship $-y_0 \simeq 1 + c_2$. The quantity $-y_0$ in turn is the scaling limit of the ratio of the second moment correlation length with the “true” correlation length obtained from the damping factor in the exponential long-distance behavior of $G(x)$. Direct calculations of this ratio confirm the above approximate relation for $y_0$. Similar results have been obtained in the two-dimensional O($N$) models [8].

In general, models defined on non-Bravais lattices such as the diamond lattice are not parity-invariant, and odd-rank operators are allowed in the corresponding expansion of the effective Hamiltonian. We finally discuss how space-parity violating terms, when they exist, vanish approaching the rotationally invariant fixed point. This fact should be described by a critical exponent $\rho_p$ which should be universal in systems breaking parity at a microscopic level, such as ferromagnetic materials having the structure of a diamond lattice. $\rho_p$ can be evaluated on the nearest-neighbor formulation of O($N$) models on the diamond lattice, which is not parity invariant. In the corresponding Gaussian theory, or the large-$N$ limit of O($N$) models, one has $\rho_p = 3$. In general, for finite $N$, $\rho_p$ may differ from its Gaussian value. The

<table>
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<tr>
<th>$N$</th>
<th>cubic</th>
<th>$c_2$</th>
<th>$c_3$</th>
<th>$d_1$</th>
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<td>$1.0(1) \times 10^{-5}$</td>
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<td>$1.1 \times 10^{-5}$</td>
<td>$-1.3 \times 10^{-4}$</td>
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<tr>
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<td>$\epsilon$-exp.</td>
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<td></td>
<td>diamond</td>
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<td>$1.0(2) \times 10^{-5}$</td>
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<td>$1.3 \times 10^{-5}$</td>
<td>$-1.6 \times 10^{-4}$</td>
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<tr>
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<td>$1.1(1) \times 10^{-5}$</td>
<td>$-2.3(2) \times 10^{-4}$</td>
</tr>
<tr>
<td></td>
<td>diamond</td>
<td>$-4.1(4) \times 10^{-4}$</td>
<td>$1.0(2) \times 10^{-5}$</td>
<td>$-3(1) \times 10^{-4}$</td>
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<td>$1.3 \times 10^{-5}$</td>
<td>$-1.7 \times 10^{-4}$</td>
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<td>$0.9 \times 10^{-5}$</td>
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<tr>
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<td>$1.1(3) \times 10^{-5}$</td>
<td>$-2.6(3) \times 10^{-4}$</td>
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strong-coupling analysis of the odd moments of $G(x)$ on the diamond lattice shows that the correction to the Gaussian value of $\rho_p$ is very small. We estimated that $0 \leq \rho_p - 3 < 0.01$ for all $N \geq 0$.

REFERENCES