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Correlation length and the scaling parameter in the Renormalization Group / Dolcini, Fabrizio; Ferrari, L.; Rioli, A.; DEGLI ESPOSTI BOSCHI, C.. - In: PHYSICAL REVIEW E. - ISSN 1063-651X. - STAMPA. - 57:3(1998), pp. 2594-2601. [10.1103/PhysRevE.57.2594]

*Availability:*

This version is available at: 11583/2303464 since:

*Publisher:*

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*Published*

DOI:10.1103/PhysRevE.57.2594

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## Correlation length and the scaling parameter in the renormalization group

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(Received 21 July 1997; revised manuscript received 1 October 1997)

The basic procedure of renormalization group theory is used to split the free energy into a Kadanoff block formation part, and a renormalized block-block interaction part. The study of this redistribution as a function of the scaling parameter  $s$  shows that there is a *stationarity* value  $s^*$  of  $s$ , which turns out to have the same *critical* behavior as the correlation length. It is suggested that  $s^*$  can be used as an appropriate measure and definition of the correlation length, even for noncritical regions. The calculation of  $s^*$  is thereby performed explicitly for the Gaussian, and numerically for the  $S^4$  model. A sharp separation between noncorrelated and correlated regimes is also found for the Gaussian model, well above the critical temperature. For the  $S^4$  model, the results suggest that  $\xi$  is characterized by a high-temperature Gaussian branch and by a genuine  $S^4$  branch at low temperatures, connected by a “plateau” in the intermediate region. [S1063-651X(98)03303-0]

PACS number(s): 05.70.Jk, 64.60.Ak

### I. INTRODUCTION

On a physical ground, the correlation length  $\xi$  is identified as the decay scale of the exponential tail of the correlation function  $G_2(r)$ . However, except for very special cases like the Ising model in one-dimension,  $G_2(r)$  develops an exponential tail only in the asymptotic regime, that is, only when  $\xi$  is large compared to the ultraviolet cutoff scale. On a more formal ground, the standard definition of  $\xi$  is

$$\xi_{st}^2 \propto \langle r^2 \rangle, \quad (1)$$

where  $\langle r^2 \rangle$  is the second moment of the normalized  $G_2(r)$ . From Eq. (1), the asymptotic meaning of  $\xi$  is recovered, and the calculation can be extended to any regime. The standard definition  $\xi_{st}$  of correlation length has the advantage of allowing for a direct comparison with experimental data, since  $\langle r^2 \rangle$  can be extracted from scattering measurements through the structure factor. In the present paper we aim to show that, by means of renormalization group theory (RGT), it is possible to introduce a further definition of correlation length, in terms of the scaling parameter  $s$ . In practice, we will find a stationarity condition which yields a special value  $s^*$  of  $s$ , proportional to  $\xi$  in the asymptotic regime. We will use  $s^*$  to study the crossover between the Gaussian behavior and the  $S^4$  behavior of  $\xi$ , under the assumption that  $\xi$  is large even in the crossover region (this means that the quartic coupling constant is to be taken small enough). In the high-temperature region where  $\xi$  is small, it is found that  $s^*$  and  $\xi_{st}$  do behave differently. In particular,  $s^*$  exhibits some effects due to short wavelength features which are absent in the square rooted second moment of  $G_2$ . This point will be reconsidered in Sec. V. We now give a brief description of the asymptotic relationship between the scaling parameter  $s$  and the correlation length.

In a real-space picture  $s$  can be interpreted as the side of a Kadanoff block of interacting spins (measured in units of the lattice spacing). The renormalization procedure yields a re-

lation between the original parameters of the Hamiltonian (identified by the vector  $\vec{\mu}_0$ ) and the rescaled parameters  $\vec{\mu}_s$  [1]:

$$\vec{\mu}_s = \vec{F}(\vec{\mu}_0, s). \quad (2)$$

Accordingly, the original free energy per spin  $f(\vec{\mu}_0)$  can be written as the sum of two terms [2]:

$$f(\vec{\mu}_0) = \frac{f(\vec{\mu}_s)}{s^d} + f_{\text{res}}(\vec{\mu}_0, s), \quad (3)$$

where  $d$  is the system's dimension. In the standard approach, one is especially interested in the behavior of  $\vec{\mu}_s$  in the neighborhood of a fixed point  $\vec{\mu}^*$  of transformation (2). This behavior is dominated by the *relevant* fields  $\{\Phi_{ij}\}$  and by the corresponding eigenvalues  $\{\lambda_{ij}\}$ . The vector  $\vec{\mu}_s$  can be reexpressed in terms of the  $\{\Phi_{ij}\}$ 's, then inserted into Eq. (3) in order to determine the scaling properties of the *singular* part  $f_{\text{sing}}$  of the free energy, close to the fixed points [3]. The next conclusive step is to express the scaling relations among the various *physical* exponents in terms of the eigenvalues  $\{\lambda_{ij}\}$ . A crucial point for this purpose is the arbitrariness of the scaling parameter  $s$ : we can therefore assert that the importance of  $s$  in RGT lies on its *mathematical* role, and that there is no manifest reason for the Kadanoff blocks to be anything but a useful mind picture. In the present work we suggest an approach to the renormalizative techniques which aims to impart a more *physical* role to  $s$  and to the Kadanoff blocks as well. A renormalization operation (RO) will now be regarded to as a way of splitting the available free energy  $f(\vec{\mu}_0)$  into two components: the first term on the right-hand side of Eq. (3) can be interpreted as the part of free energy coming from the (rescaled) block-block interaction,  $f(\vec{\mu}_s)$  being the “effective” free energy of the rescaled system; the residual term  $f_{\text{res}}$  on the right-hand side is thereby the free energy of the noninteracting blocks, that is, the free energy of “formation” of the blocks themselves [4]. We stress that

both  $f(\vec{\mu}_s)/s^d$  and  $f_{\text{res}}(\vec{\mu}_0, s)$  do depend on  $s$  (i.e., on the Kadanoff block side), while their sum  $f(\vec{\mu}_0)$  obviously does not. We will study redistribution (3) on varying  $s$ , and find that there is a particular value  $s^*$  of  $s$  (i.e., a particular size of the Kadanoff block) which makes the energy redistribution *stationary*; that is

$$\left. \frac{d}{ds} \left( \frac{f(\vec{\mu}_s)}{s^d} \right) \right|_{s=s^*} = - \left. \frac{df_{\text{res}}}{ds} \right|_{s=s^*} = 0. \quad (4)$$

Such a stationarity point  $s^*$  turns out to have the same *critical* behavior as the correlation length of the system:

$$s^* \propto \xi \quad (\xi \text{ large}). \quad (5)$$

This relation will be directly proved in Sec. II for any kind of Gaussian-like system, and widely generalized in Sec. III for systems located close enough to a Wilsonian fixed point. So far Eq. (5) is nothing but a *mathematical* outcome. However, there is a *physical* argument suggesting that  $s^*$  should actually play the role of a correlation length *in any case*. Indeed we will show that Eq. (4) is a criterion of thermodynamical stability, since  $s^*$  turns out to correspond to the minimum free energy of formation of the Kadanoff blocks. Thus  $s^*$  is a measure of the optimal linear size of the Kadanoff blocks, with respect to the condition of thermal equilibrium.

The technical part of the present paper is mainly concerned with the calculation of  $s^*$ . In Sec. II we start with the Gaussian model. Even in this ‘‘elementary’’ case we find a nontrivial result, that is, a finite temperature  $T_+$  above which  $s^* = 1$  (the Kadanoff blocks coincide with a *single* spin), and below which  $s^*$  start to increase with decreasing temperature. In Sec. IV we approach the  $S^4$  model. From the results obtained we argue that  $s^*$  should display, on a log-log plot, a ‘‘plateau’’ connecting a Gaussian branch to the genuine  $S^4$  branch at lower temperatures.

## II. GENERAL FORMALISM AND THE GAUSSIAN MODEL

Consider a physical system modeled on a  $d$ -dimensional hypercubic lattice and described by a set  $\{S_{\vec{r}}\}$  of coordinates associated with the sites of the lattice ( $\vec{r} = \vec{m}a$ ,  $\vec{m}$  being a vector of integers and  $a$  the spacing). Suppose that the Hamiltonian of the system is the following:

$$H_N(\{S_{\vec{r}}\}) = \frac{J}{2} \sum_{\vec{r}} \sum_{i=1}^d (S_{\vec{r}+\vec{a}_i} - S_{\vec{r}})^2 + \frac{R}{2} \sum_{\vec{r}} S_{\vec{r}}^2 + U \sum_{\vec{r}} S_{\vec{r}}^4 - \mathcal{H} \sum_{\vec{r}} S_{\vec{r}}, \quad (6)$$

where  $U(>0)$  and  $R$  are two independent parameters and  $\mathcal{H}$  is a uniform external field. The Hamiltonian (multiplied by  $\beta$ ) in  $\vec{q}$ -space turns out to be

$$\beta H_N(\{S_{\vec{q}}\}) = \frac{1}{N} \sum_{\vec{q} \in B} \frac{u_2(\vec{q})}{2} |S_{\vec{q}}|^2 + \frac{u_0}{N^{3-d}} \sum_{q_1 \dots q_4 \in B} S_{q_1}^- S_{q_2}^- S_{q_3}^- S_{q_4}^- \delta_{\sum \vec{q}_i, \vec{0}} - h_0 S_{\vec{q}=\vec{0}}, \quad (7)$$

where  $S_{\vec{q}}^- = \pi \sqrt{\beta J} \sum_{\vec{r}} S_{\vec{r}}^- e^{-i(\pi/a)\vec{q} \cdot \vec{r}}$  is the one-component field (for simplicity);  $N$  is the number of spins;  $u_2(\vec{q})$  is an analytic function of  $\vec{q}$ , whose coefficient of  $\vec{q}^2$  is equal to 1;  $u_0 = U/(\pi^4 \beta J^2)$  is a dimensionless coupling constant; and  $h_0 = (\mathcal{H}/\pi) \sqrt{\beta/J}$  is the dimensionless external field.

The Gaussian model is characterized by the absence of any coupling among the  $\{S_{\vec{q}}\}$ 's [ $u_0 = 0$  in Eq. (7)]. In zero external field, we have

$$\beta H^{(G)}(\{S_{\vec{q}}\}) = \frac{1}{N} \sum_{\vec{q} \in B} \frac{u_2(\vec{q})}{2} |S_{\vec{q}}|^2, \quad (8)$$

where  $u_2(\vec{q})$  is a dimensionless regular function, usually depending on even powers of the dimensionless wave vector  $\vec{q}$ :

$$u_2(q) = r_0 + q^2 + a_0 q^4 + b_0 q^6 + \dots \quad (9)$$

The parameters  $\{r_0, a_0, b_0, \dots\}$  are all *scaling fields*; the critical surface is characterized by  $r_0 = 0$ , where  $r_0$  is associated to the reduced temperature  $\theta = [(T - T_c)/T_c]$ . The calculation of the correlation length for the Gaussian model is a standard exercise:

$$\xi \sim \frac{1}{\sqrt{r_0}} \quad (\xi \gg a). \quad (10)$$

Let us now turn to the energy redistribution (3). We will examine how the available free energy  $f(\vec{\mu}_0)$  shares between the two components with a varying of the scaling parameter  $s$ . Let us focus, for example, on  $f_{\text{res}}$ ; the details about this calculation can be found in Ref. [4] (see also Ref. [5]). The resulting expression is exact and reads

$$\frac{f_{\text{res}}^{(G)}(\{r_0, a_0 \dots\}; s)}{K_B T} = \frac{g_d}{2^{d+1}} \int_{\text{out}_s} d^d \vec{q} \ln[\gamma u_2(q)] - \frac{\ln s}{s^d}, \quad (11)$$

where  $\gamma = (J/K_B T)(\pi/2)$  is a dimensionless parameter;  $\text{out}_s$  is a *hyperspherical* shell ( $\vec{q} \in \text{out}_s \Leftrightarrow 1/s < |\vec{q}| < 1$ ); and  $g_d = [\pi^{d/2}/2^d \Gamma(1 + d/2)]$  is the ratio between the volume of the cube and the volume of the sphere in  $d$ -dimension. The factor  $g_d$  is due to the change of shape (*cube*  $\rightarrow$  *sphere*), the latter being far more practical for calculations. It is generally accepted that details about geometrical shapes of the Brillouin zone ( $B$ ) do not influence (once the thermodynamic limit is performed) the values of *intensive* quantities. Thus one can use *extensive* quantities defined either on a hypercubic  $B$  or on a hyperspherical one, provided that they are afterwards divided by the correct number of degrees of freedom (DOF) they refer to. That is why, if the Brillouin spacing is  $2/\bar{N}$ , where  $N = \bar{N}^d$  is the number of DOF actu-

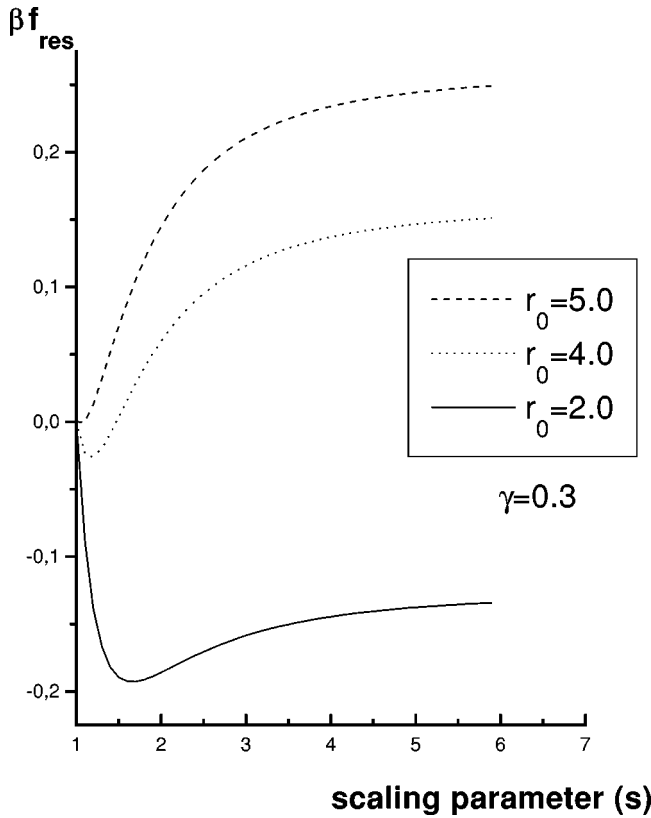


FIG. 1. Standard Gaussian model: behavior of  $\beta f_{\text{res}}$  as a function of  $s$ .

ally present in a hypercubic zone, a hyperspheric zone  $B$  inscribed in it will contain  $Ng_d$  DOF.

Let us start with the standard Gaussian model, that is,

$$u_2(q) = r_0 + q^2; \tag{12}$$

in  $d=3$  dimensions one has

$$\begin{aligned} \frac{f_{\text{res}}^{(G)}(r_0; s)}{K_B T} &= \frac{1}{2} \ln[\gamma(1+r_0)] - \frac{1}{3} + r_0 \left(1 - \frac{1}{s}\right) \\ &\quad - \frac{1}{2s^3} \{ \ln[\gamma(1+r_0s^2)] - \frac{2}{3} \} \\ &\quad - r_0^{3/2} (\arctan \sqrt{r_0} - \arctan \sqrt{r_0s}), \end{aligned} \tag{13}$$

whose plot is shown in Fig. 1 as a function of  $s$ .

As long as  $r_0$  is large (high temperatures), the curve is an increasing function at  $s$ . But, if we lower  $r_0$  down to a special value  $r_+ = (e^{2/3}/\gamma) - 1$ , the curve starts displaying a stationary minimum point, denoted by  $s^*$ , which depends on  $r_0$ . In particular,  $s^*$  diverges for  $r_0 \rightarrow 0^+$  (i.e.,  $T \rightarrow T_c^+$ ). One can easily calculate the dependence of  $s^*$  on  $r_0$ , with the result

$$s^* = \frac{c_3}{\sqrt{r_0}} \quad (s^* \gg 1), \tag{14}$$

where  $c_3 = [(e^{2/3}/\gamma) - 1]^{1/2}$ . For  $c_3$  to be real, the temperature must be bounded from below, that is,

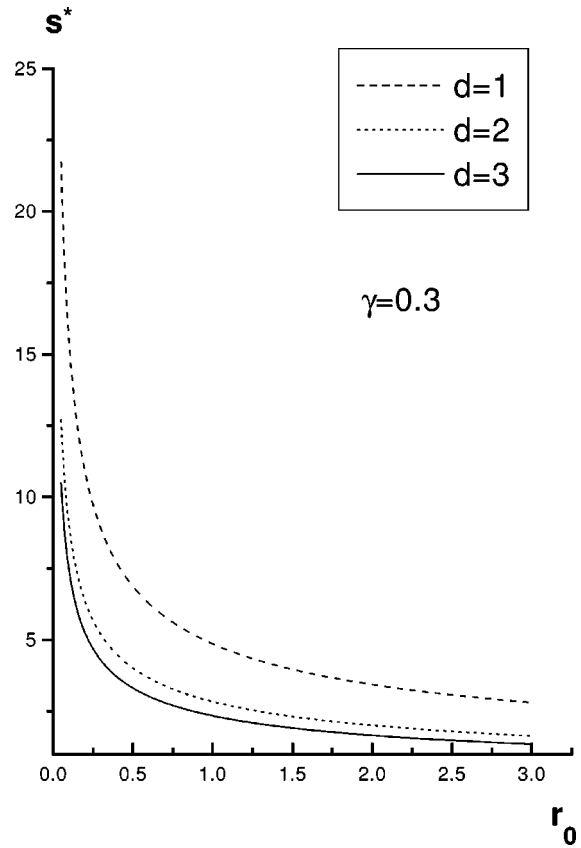


FIG. 2. Standard Gaussian model: behavior of  $s^*$  in any dimension.

$$\frac{e^{2/3}}{\gamma} - 1 > 0 \Leftrightarrow T > T_{\text{inf}} = \frac{J}{K_B} \frac{\pi}{2e^{2/3}}.$$

However, as  $T_0 = qJ/K_B$  ( $q$  being the number of first neighbors) is the critical temperature for a mean-field theory of an Ising-like system (cf. Ref. [6]), and as  $T_c = T_0$  for a Gaussian model, one can argue that

$$T_c > T_{\text{inf}}.$$

Since we explore the range of temperatures  $T \geq T_c$ , it is clear that  $c_3$  is real for all our purposes. The singular behavior of  $s^*$  is characterized by the same exponent ( $=\frac{1}{2}$ ) as the correlation length [cf. Eq. (10)]. Quite similar results are obtained in one and two dimensions (see Fig. 2), with a general coefficient

$$c_d = \left( \frac{e^{2/d}}{\gamma} - 1 \right)^{1/2}. \tag{15}$$

One can also introduce some new parameters into Eq. (9) such as a quartic coupling constant

$$u_2(q) = r_0 + q^2 + a_0 q^4. \tag{16}$$

Qualitatively the results for  $f_{\text{res}}$  are very similar to those in Fig. 1. In particular, as  $r_0 \rightarrow 0$ , the minimum point  $s^*$  behaves now in the following manner:

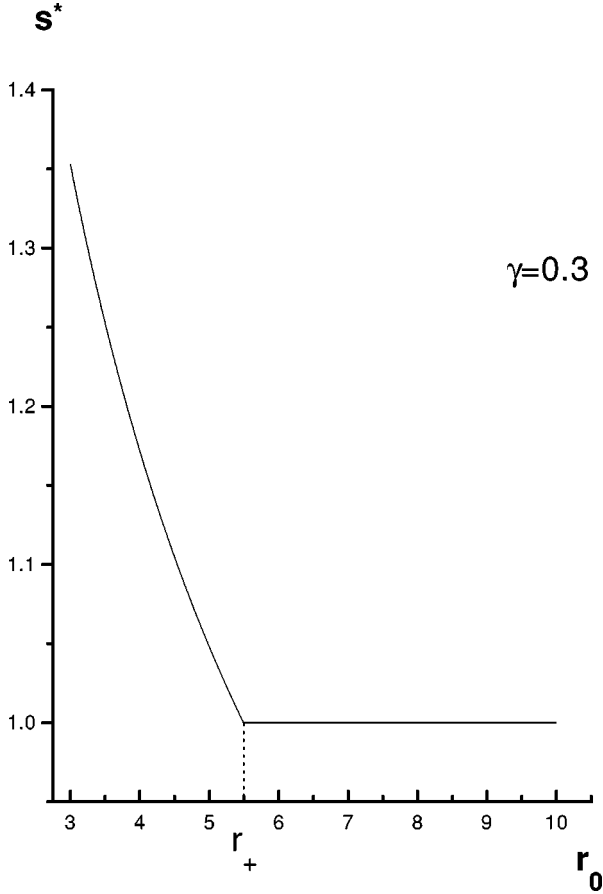


FIG. 3. Behavior of  $s^*$  at high temperatures for the Gaussian model in three dimensions: the value  $r_+$  separates the *correlated region* ( $r_0 < r_+$ ) from the *completely uncorrelated region* ( $r_0 > r_+$ ).

$$s^* \sim \frac{c_d}{\sqrt{r_0}} \left( 1 - \frac{r_0 a_0}{c_d^4} \right)^{1/2}.$$

Now let us turn to Fig. 1; as already noted, the stationary point  $s^*$  “vanishes” (i.e., it reaches the minimal value  $s^* = 1$ ) at a *finite* temperature  $T_+$ , defined by the equation

$$\frac{e^{2/3}}{\gamma(T_+)} - 1 = r_0(T_+).$$

This means that the components of the system are completely uncorrelated down to  $T_+$ . According to our picture, this is just the temperature below which the system starts getting arranged into Kadanoff blocks (see Fig. 3). This behavior seems to have the same formal features as a high-temperature pretransition (we will come back to this point in Sec. V).

### III. NEAR WILSON'S FIXED POINTS

We now wish to study the energy redistribution (3) close to a Wilson fixed point. The use of a widely general formalism will provide some insights which support the validity of relation (5) for much more general models than the Gaussian one. From RGT, one knows that the flow equations in the parameters space have an autonomous form  $d\vec{\mu}/dt = \vec{\mu}(\vec{\mu})$ ,

with  $t = \ln s$  and  $\vec{\mu} \equiv \vec{\mu}_s$ . Let us now expand  $\vec{u}(\vec{\mu})$  about a fixed point  $\vec{\mu}^*$  [defined by  $\vec{u}(\vec{\mu}^*) = \vec{0}$ ],

$$\vec{u}(\vec{\mu}) = \mathcal{T} \cdot \delta\vec{\mu} + O(\|\delta\vec{\mu}\|^2) \quad \mathcal{T}_{i,j} = \frac{\partial u_i}{\partial \mu_j}, \quad (17)$$

where  $\delta\vec{\mu} = \vec{\mu} - \vec{\mu}^*$ . The solution of the linearized flow equation is

$$\delta\vec{\mu}(t) = \sum_j \vec{Y}_j \Phi_{0j} e^{\lambda_j t}, \quad (18)$$

where the  $\vec{Y}_j$ 's are the right eigenvectors of the matrix  $\mathcal{T}$ , with eigenvalues  $\{\lambda_j\}$ , and the  $\Phi_{0j}$ 's are the scaling fields at  $t=0$ .

Let us now turn to relation (3). As the total free energy is independent of  $s$ , the stationary points of the energy redistribution are also found by

$$\frac{d}{ds} \left( \frac{f(\vec{\mu}_s)}{s^d} \right) = 0. \quad (19)$$

We implicitly assume that Eq. (19) admits a solution. Our results on the Gaussian model suggest that this is the case; for other specific models this should be directly verified (see, for example, Sec. IV). Recalling that  $t = \ln s$ , Eq. (19) is also equivalent to

$$\vec{\nabla}_{\vec{\mu}} f[\vec{\mu}(t)] \cdot \vec{u}[\vec{\mu}(t)] = f[\vec{\mu}(t)] d, \quad (20)$$

where  $\vec{\nabla}_{\vec{\mu}} f = [(\partial f / \partial \mu_1), (\partial f / \partial \mu_2), \dots]$ .

Let us now take  $\vec{\mu}_0$  in the neighborhood of a Wilsonian fixed point  $\vec{\mu}^*$ . In this case, one can write

$$f(\vec{\mu}) = f(\vec{\mu}^*) + \vec{\nabla}_{\vec{\mu}} f(\vec{\mu}^*) \cdot \delta\vec{\mu} + O(\|\delta\vec{\mu}\|^2), \quad (21)$$

$$\vec{\nabla}_{\vec{\mu}} f(\vec{\mu}) = \vec{\nabla}_{\vec{\mu}} f(\vec{\mu}^*) + O(\|\delta\vec{\mu}\|), \quad (22)$$

provided that

$$\lim_{\vec{\mu} \rightarrow \vec{\mu}^*} f(\vec{\mu}) \quad \text{and} \quad \lim_{\vec{\mu} \rightarrow \vec{\mu}^*} \vec{\nabla}_{\vec{\mu}} f(\vec{\mu})$$

are *finite*. Replacing (21), (22), and (17) into Eq. (20), and equating powers of  $\|\delta\vec{\mu}\|$  we have from Eq. (20)

$$\sum_j [\vec{\nabla}_{\vec{\mu}} f(\vec{\mu})]_{\vec{\mu}^*} \cdot \vec{Y}_j (\lambda_j - d) \Phi_{0j} e^{\lambda_j t} = f(\vec{\mu}^*) d. \quad (23)$$

We cannot be sure that this is always the case, since  $\vec{\mu}^*$  is a *critical* point, and  $f$  would develop a singularity at some order; such a hypothesis is to be verified in every single case; for example, in the usual Gaussian model one has  $\vec{\mu} = (r_0, h_0)$ ,  $\vec{\mu}^* = (0, 0)$ , and

$$\frac{\partial f}{\partial r}(\vec{\mu}^*) \propto \frac{K_B T_c}{2^{d+1}} \int_B \frac{d^d \vec{x}}{x^2},$$

where  $B$  is the Brillouin zone. The integral only converges for  $d > 2$ . However, for any Gaussian-like model we have

already proved (by direct calculations) that actually  $s^* \sim \xi$  in any dimension (see Sec. II). Introducing the quantities

$$L_j \equiv [\vec{\nabla}_{\vec{\mu}} \ln |f(\vec{\mu})|]_{\vec{\mu}^*} \cdot \vec{Y}_j, \quad (24)$$

Eq. (23) reads

$$\sum_j L_j (\lambda_j - d) \Phi_{0j} e^{\lambda_j t} = d. \quad (25)$$

Suppose now that there are only two relevant fields, say  $\Phi_1$  and  $\Phi_2$ . This means

$$\lambda_1, \lambda_2 > 0, \quad \lambda_j < 0 \quad \forall j \geq 3. \quad (26)$$

Since the relevant fields measure the distance from the critical surface, they are usually associated with

$$\Phi_{01} \propto \theta = \frac{T - T_c}{T_c} \quad \text{reduced temperature,} \quad (27)$$

$$\Phi_{02} \propto h \quad \text{magnetic field.} \quad (28)$$

We are interested in the situation of zero external magnetic field:  $\Phi_{02} = 0$ ; in this case Eq. (25) yields

$$L_1 (\lambda_1 - d) \Phi_{01} s^{*\lambda_1} + \sum_{j \geq 3} L_j (\lambda_j - d) \Phi_{0j} s^{*\lambda_j} = d.$$

On assuming that  $L_1 \neq 0$  and  $\lambda_1 \neq d$ , we obtain

$$s^{*\lambda_1} = \frac{d - \sum_{j \geq 3} L_j (\lambda_j - d) \Phi_{0j} s^{*\lambda_j}}{L_1 (\lambda_1 - d) \Phi_{01}}. \quad (29)$$

For small enough irrelevant fields,  $s^*$  is an increasing function of  $\Phi_{01}^{-1}$ . Moreover, as all the  $\{\lambda_j\}$ 's with  $j \geq 3$  are negative, the contribution of the right side of the numerator in Eq. (29) becomes negligible with respect to  $d$ . We thus obtain, from Eq. (29),

$$s^* \sim \left( \frac{1}{\Phi_{01}} \right)^{1/\lambda_1} = \left( \frac{1}{\theta} \right)^\nu \sim \xi, \quad (30)$$

where the second equality follows from the standard relation  $\lambda_1 = 1/\nu$ . The validity of Eq. (5) is thereby extended to all cases for which  $f(\vec{\mu}^*)$  and  $\vec{\nabla}_{\vec{\mu}} f(\vec{\mu}^*)$  are finite, provided that the Hamiltonian of our system is located close enough to the Wilsonian fixed point. This imparts a wide deal of generality to the relationship between the stationary point  $s^*$  and the correlation length. For the discussions in what follows, it is useful to express the second derivative of the interaction free energy with respect to  $s$  in  $s^*$ :

$$\begin{aligned} & \left( \frac{d^2}{ds^2} \frac{f(\vec{\mu})}{s^d} \right)_{s=s^*} \\ &= \frac{f(\vec{\mu}^*)}{(s^*)^{d+2}} \left[ \sum_j L_j \Phi_{0j} (\lambda_j^2 - d^2) (s^*)^{\lambda_j - d^2} \right]. \end{aligned} \quad (31)$$

#### IV. $S^4$ MODEL

The  $S^4$  model Hamiltonian is defined through Eq. (7) as

$$\beta H(\{S_{\vec{q}}\}) = \beta H^{(G)}(\{S_{\vec{q}}\}) + u_0 V_4(\{S_{\vec{q}}\}), \quad (32)$$

where  $H^{(G)}$  is the standard Gaussian model [cf. Eq. (8) and (12)], and

$$V_4(\{S_{\vec{q}}\}) = \frac{1}{N^3} \sum_{\vec{q}_1, \vec{q}_2, \vec{q}_3, \vec{q}_4 \in B} S_{\vec{q}_1}^- S_{\vec{q}_2}^- S_{\vec{q}_3}^- S_{\vec{q}_4}^- \delta_{\Sigma_{\vec{q}_i}, \vec{0}}. \quad (33)$$

If we (perturbatively) apply a RO to the Hamiltonian (32), to first order in  $u_0$  we obtain, following Ref. [7]:

$$\begin{aligned} \beta H'(\{S_{\vec{q}}\}) &= \frac{1}{N'} \sum'_{\vec{q} \in B} |S_{\vec{q}}|^2 \frac{s^2}{2} \left( r_0 + \frac{q^2}{s^2} \right. \\ &\quad \left. + \frac{3u_0}{2^{d-2}} \int_{\text{out}_s} \frac{d^d \vec{q}}{r_0 + q^2} \right) \\ &\quad + \frac{s^{4-d} u_0}{N'^3} \sum'_{\vec{q}_1, \dots, \vec{q}_4 \in B} S_{\vec{q}_1}^- S_{\vec{q}_2}^- S_{\vec{q}_3}^- S_{\vec{q}_4}^- \delta_{\Sigma_{\vec{q}_i}, \vec{0}}, \end{aligned} \quad (34)$$

with  $N' = N/s^d$ . The prime in the sums refers to the usual rescaled spacing in the Brillouin zone. Note that the quartic coefficient of Hamiltonian (34) does not contain the  $u_0^2$  term, which leads to the correct fixed point according to the Wilson theory [1]. However, the main aim of Wilson's method is to prove the *universality* of systems. Hence one usually applies the RO *iteratively*, searching for a *fixed point*. In order for this scheme to be appropriately defined, the parameter space is to be large enough (actually infinite dimensional): one therefore has to extend the renormalization transformation to a more general functional form than Eq. (32), containing all even order terms  $S^{2n}$  and any momentum dependence as well. The existence of a nontrivial fixed point is proved, and the universality follows as a consequence. The price to be paid for this crucial result is to deal with the  $\varepsilon$  expansion ( $\varepsilon = 4 - d$ ).

Our purpose is different: once a Hamiltonian  $H$  is given, the renormalization is used here to ‘‘create’’ an effective system; we then examine how the energy redistribution depends on the scaling parameter  $s$ , no matter whether the parameter space is or is not enlarged by the RO itself: our method requires a *single* RO, since our aim is not universality. In fact, we stick to model (32), which is described by a finite number of parameters (actually two), and which belongs to a discrete-dimensional space ( $d=3$  for example). The  $S^4$  model is not considered here as representative of a universality class, but as an actual mathematical model whose precritical features are the point of interest which we address.

Equation (34) leads to a fairly simple expression for the residual free energy, to first order in  $u_0$  (see Ref. [4] and, for further details, Ref. [5]):

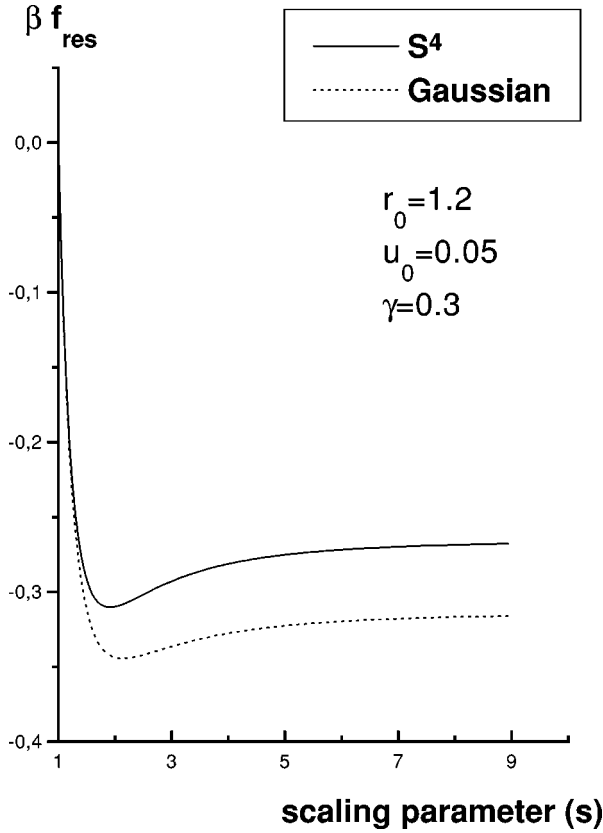


FIG. 4. The  $S^4$  model: behavior of  $\beta f_{\text{res}}$  as a function of  $s$ .

$$\frac{f_{\text{res}}(r_0; u_0; s)}{K_B T} = \frac{f_{\text{res}}^{(G)}(r_0; s)}{K_B T} + 3u_0 \left( \frac{g_d}{2^d} \int_{\text{out}, r_0+q^2} \frac{d^d \vec{q}}{q^2} \right)^2, \quad (35)$$

where  $f_{\text{res}}^{(G)}$  is given by Eq. (11). In the case  $d=3$ , Eq. (35) becomes

$$\frac{f_{\text{res}}(r_0; u_0; s)}{K_B T} = \frac{f_{\text{res}}^{(G)}(r_0; s)}{K_B T} + 27u_0 \left( 1 - \frac{1}{s} - \sqrt{r_0} (\arctan s \sqrt{r_0} - \arctan \sqrt{r_0}) \right)^2, \quad (36)$$

where  $f_{\text{res}}^{(G)}$  in  $d=3$  is given by Eq. (13). The function  $f_{\text{res}}$  [Eq. (36)] versus  $s$  is plotted in Fig. 4.

From Eq. (36), we obtain the equation for  $s^*$ :

$$\frac{3}{2} \ln(1 + r_0 s^{*2}) - K + 54u_0 \frac{s^{*2}}{(1 + r_0 s^{*2})} \left( 1 - \frac{1}{s^*} - \sqrt{r_0} (\arctan s^* \sqrt{r_0} - \arctan \sqrt{r_0}) \right) = 0, \quad (37)$$

where  $K = 1 - \frac{3}{2} \ln \gamma$  is a constant. The function  $s^* = s^*(r_0; u_0)$  was evaluated numerically, using the method of bisection [8]. We have studied how  $s^*$  depends on  $r_0$ , for a fixed value of  $u_0$ . The result is plotted in Fig. 5. As we can

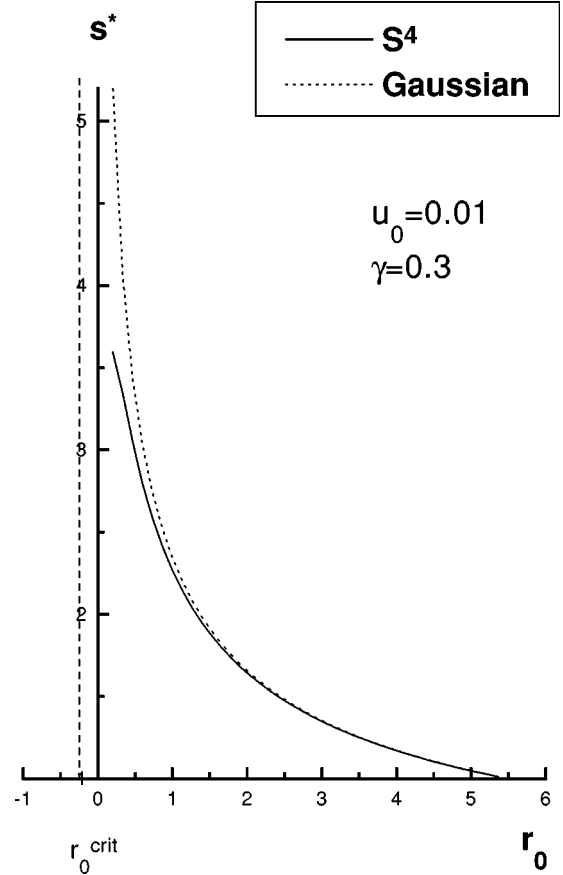


FIG. 5. Plot of the stationarity point  $s^*$  as a function of  $r_0$  at a fixed  $u_0$ .

see, the curve of the  $S^4$  model lies *below* the Gaussian one, in agreement with the splitting of the critical point down to negative values of  $r_0$ .

In Fig. 5,  $r_0$  ranges above a value  $r_{0\text{MIN}} > 0$ . This lower bound depends sensitively on the perturbative order of  $u_0$ . We wish to consider; for example, if we stop to first order, for  $r_{0\text{MIN}}$  we choose a minimal value of  $r_0$  for which the  $u_0$  contribution in Eq. (36) can be regarded to as an actual first-order perturbation of the unperturbed Gaussian part  $f_{\text{res}}^{(G)}$ . In practice, this yields  $r_{0\text{MIN}} \approx 20/25u_0$ . For a given value of  $u_0$ ,  $r_{0\text{MIN}}$  can be lowered by including higher-order terms of the expansion. Anyway  $r_{0\text{MIN}}$  will always be *positive*. This is inherent in the perturbative technique of the Gaussian averages that we used, which only makes sense if  $r_0 > 0$ . This technique was also used by Wilson in deriving the RGT equations (cf. Ref. [1]). However, those equations have no singularities in  $r_0 = 0$ , and can be extended to the region  $r_0 < 0$ . In contrast, our calculations involve expressions containing  $\sqrt{r_0}$ . So they cannot be straightforwardly extended to the case  $r_0 < 0$ . On converting Fig. 5 into a log-log plot, one obtains the result given in Fig. 6, that displays an interesting feature: the curve turns out to have a *concave* shape at low  $r_0$ . This might look surprising, since we know (from Sec. III) that in the very neighborhood of  $r_0^{\text{crit}}$  where  $s^* \propto (r_0 - r_0^{\text{crit}})^{-\nu}$ , the exponent  $\nu$  is *greater* than the Gaussian one (actually  $\nu = 0.631 \dots$  in three-dimensions). In a log-log plot, this means that the ultimate slope of the curve must be greater than the Gaussian one. The simplest way to match the

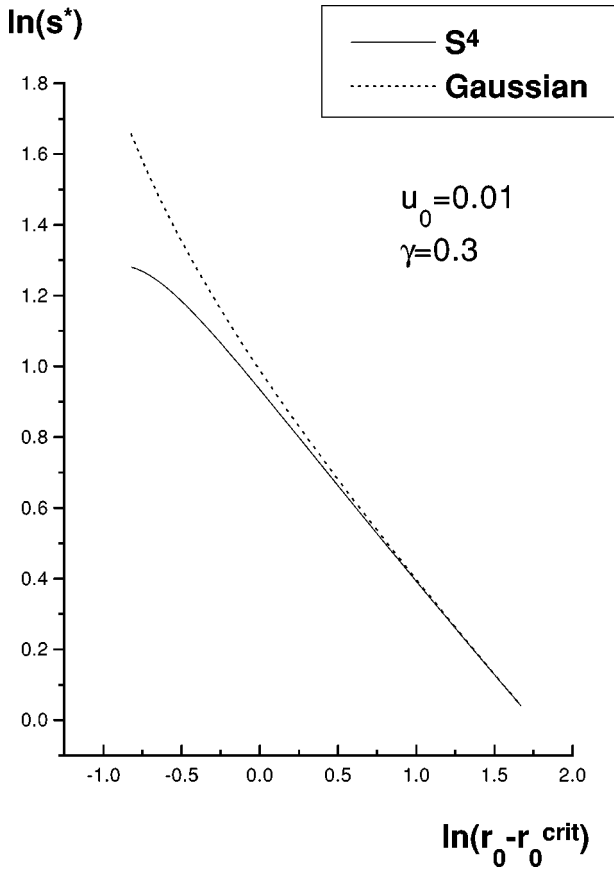


FIG. 6. A log-log plot of  $s^*$  as a function of  $r_0 - r_0^{\text{crit}}$  (the Gaussian curve is not a straight line here, because the value of  $r_0^{\text{crit}}$  refers to the  $S^4$  model).

curve in Fig. 6 with a larger linear slope at lower temperatures is an inflection point. If so, the actual critical behavior should appear just after a plateau of the log-log plot of the correlation length, as though the correlation length “took a breath” just above the *Gaussian* region, before approaching the  $S^4$  divergence (see Fig. 7).

In order to support this possibility, one needs to enter the region  $r_0^{\text{crit}} < r_0 < 0$ . However, the preceding expression, obtained for  $r_0 > 0$ , are singular in  $r_0 = 0$  [see Eq. (37)], and they cannot be extended to negative values of  $r_0$  as they stand. Instead, we can use the general results of Sec. III for which RGT itself provides manageable expressions just close to the critical point. In particular, we refer to Eq. (29), showing that the corrections to the asymptotic slope of  $s^*$  are due to the irrelevant fields (for  $h = 0$ ). To first order in  $u_0$  and  $\varepsilon = 4 - d$ , it can be shown (see Ref. [4]) that the sign of the correction to the asymptotic slope of  $s^*$  is determined by the sign of the quantity  $(u_0 - \varepsilon/144)$  (the irrelevant field). Hence, for  $u_0 > \varepsilon/144$ , the correction is *positive*, which supports the existence of the inflection point as sketched in Fig. 7. In the opposite case, the *negative* correction might prelude to a more complicated matching. Just to obtain an insight, we have studied the sign of  $(u_0 - 1/144)$  ( $d = 3$ ) in the case of an Ising model on a cubic lattice. By transforming this problem into a  $S^4$  model (see Sec. 20 of Ref. [9]),  $u_0$  turns out to be greater than  $\frac{1}{144}$ , in the region  $r_0 < 0$ . So we may reasonably support the qualitative behavior in Fig. 7 for a wide class of model systems. In addition, we verified by means of Eq. (31)

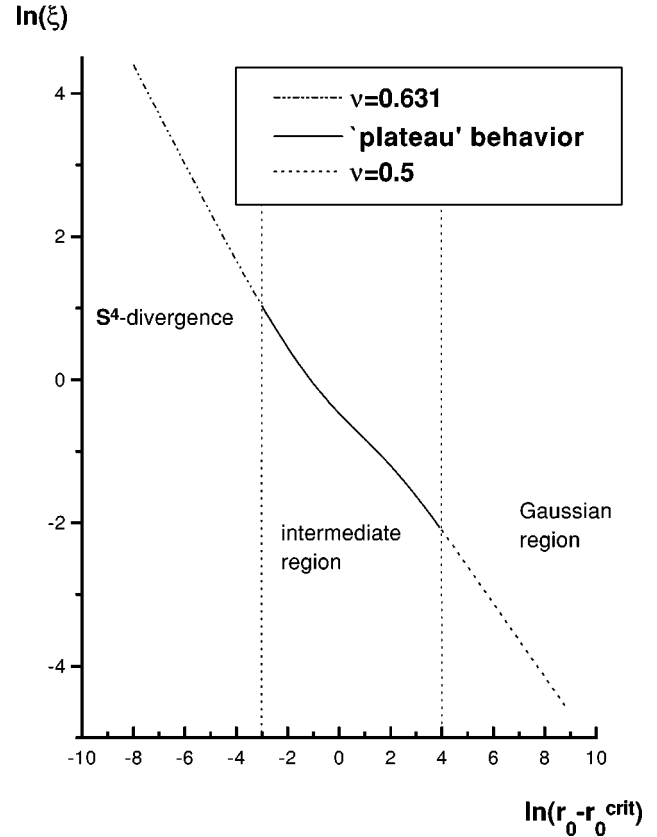


FIG. 7. The correlation length should exhibit a “plateau” behavior before entering the region of the universal  $S^4$  divergence, marked by  $\nu = 0.631$ .

that  $s^*$  is a *maximum* point for the interaction free energy, that is, a *minimum* of  $f_{\text{res}}$  [see Eq. (4)]. Hence, even close to the asymptotic region, we can identify  $s^*$  as the optimal linear size of the Kadanoff blocks in thermal equilibrium, in analogy with the case  $r_0 > 0$ .

## V. CONCLUSIONS

The aim of the present paper was to explore the possibility that RGT can be fruitfully used even in regions where the *nonuniversal* features of the model become important. Hence our study is intermediate between the “standard” RGT and more sophisticated renormalizative techniques, such as the hierarchical reference theory [10]. At present, we limited our analysis to the correlation length as to the most relevant quantity for any preliminary approach.

It is a mathematical result that the stationarity condition (4) on the RGT energy redistribution (3) does determine a special value  $s^*$  of the scaling parameter  $s$  (fixing the Kadanoff block’s size) which turns out to have the same *critical* behavior as the correlation length  $\xi$  [Eq. (5)]. As our study highlighted, the system seems to arrange into blocks whose size makes their “formation energy” *minimal*, and their mutual interaction energy *maximal*. The scaling parameter  $s$  might therefore be regarded as a thermodynamic parameter, whose equilibrium value (that is the mean size of the Kadanoff blocks) is  $s^*$ . As for the thermodynamic fluctuations of  $s$  around  $s^*$ , we notice (see Fig. 1) that the plot of  $f_{\text{res}}$  spreads out as the critical conditions are approached. In



particular, it can be shown that the *relative* fluctuations diverge when the critical temperature is reached. This looks reasonable in a statistical thermodynamic picture, because the number of Kadanoff blocks (i.e., the statistical population) becomes smaller and smaller in such a limit. More details on the fluctuations of  $s$  will be given in a forthcoming paper.

The method just outlined was originally developed in order to calculate the correlation length for nontrivial models—like the  $S^4$  model—in regions that are not strictly critical. In particular we deal with the crossover between the Gaussian and the  $S^4$  regimes, under the assumption that  $\xi$  is sufficiently large in this region too. A nontrivial result is that, to first order in  $u_0$ , the correlation length of Ising models that can be mapped into a  $S^4$  model is expected to develop an inflection point connecting a quasi-Gaussian behavior at high temperatures to the  $S^4$  divergence at low temperature (see Fig. 6). Moreover, the plot in Fig. 5 indicates that the Gaussian critical temperature ( $r_0=0$ ) should be probably *included* just into the plateau region around the inflection point. In a sense, the plateau looks like a “memory” of the Gaussian criticality. This point should deserve further attention in view of phenomenological applications. As for the experimental evidence of the predicted behavior of  $\xi$  (see Fig. 7), encouraging results have been found in the precritical region of simple liquids (see, in particular, Fig. 2 of Ref. [11]) where the data for  $\xi$  in krypton seem to indicate a bending down of the log-log plot reminiscent of our curve in Fig. 6.

Another unexpected result was obtained just in the “trivial” Gaussian case. In Fig. 3 it is shown that the stationarity point  $s^*$  reaches the minimal possible value  $s^*=1$  at a *finite* temperature  $T_+$ . Figure 1 shows that, above  $T_+$ , the minimum of  $f_{\text{res}}$  just corresponds to  $s=1$ . According to a thermodynamic interpretation,  $s^*$  should thereby remain equal to the value 1 for any temperature above  $T_+$ . The preceding result suggests that there is a sharp separation between correlated and noncorrelated regions, marked by  $T_+$ . It can be also shown that, on mapping an Ising model into a Gaussian model,  $s^*$  decreases with  $T$  *continuously*, down to a lower limiting value  $s^*(T=\infty)>1$ . These effects are due to the *temperature-dependent* factor  $c_d(T)$  [Eq. (15)], that marks the difference between the standard definition  $\xi_{\text{st}}$  [Eq. (1)] of the correlation length and the optimal Kadanoff block’s size  $\xi_{\text{Kad}} \propto s^*$ . In the Gaussian regime, one has, in fact,  $\xi_{\text{Kad}} \propto c_d(T) \langle r^2 \rangle^{1/2} \propto c_d(T) \xi_{\text{st}}$ . The difference between  $\xi_{\text{Kad}}$  and  $\xi_{\text{st}}$  is relevant just in the high-temperature regime in which the notion of the correlation length itself becomes elusive. However, if one believes that no *physical* length scale can be smaller than the lattice parameter (or any related cutoff scale), one should note that  $\xi_{\text{Kad}}$  fulfills this requirement, while  $\xi_{\text{st}}$  does not.

#### ACKNOWLEDGMENTS

We are grateful to Dr. G. Morandi for useful and stimulating discussions. This work was partially supported by the Italian Ministry of Technology and Scientific Research.

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