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Large-Scale Structure of Fluctuating Order Parameter Field

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An effective free energy for a fluctuating system is investigated using an exact (local) renormalization group (RG) equation. This equation accounts for the fluctuation interaction in a reduced manner (at Fisher exponent $\eta = 0$) and leads to a physical solution branch which gives realistic estimations for the free energy and nice critical exponents. It is shown that in spite of the monotonic character of the effective free energy in the critical region, all vertices should be taken into account in the effective Ginzburg–Landau–Wilson functional. The large-scale structure of the fluctuating field at a second-order phase transition is studied utilizing the calculated free energy and localized nonlinear excitations are found with profiles rather like those previously obtained in a model approach.

KEY WORDS: Nonlinear excitations; critical region; renormalization group (RG); fluctuations.

INTRODUCTION

It is well known just from the mean field theory that a first-order phase transition is anticipated by nonlinear excitations which can be interpreted as nucleation centers in the paraphase. The kinetics of the first-order phase transition in different physical systems has been the subject of intensive studies (see for review refs. 1–10 and references in these papers). As a rule, the ordering of a metastable disordered phase is due to the fluctuation production and finally to the growth of the nucleus of the stable phase. In a first-order phase transition there is a change in some order parameter φ between these two phases which lowers the free energy as the new phase forms. The corresponding local free energy density $F(\varphi)$ must have a metastable minimum at $\varphi = 0$ and be energetically favorable for $\varphi = \varphi_0 \neq 0$.

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However, the free energy is transformed due to the fluctuations. This change is especially essential in the critical region at a second-order transition. It is well known from the theory of critical phenomena that the fluctuations manifest themselves by renormalization of critical exponents.[11-13] The renormalization group method allows one not only to perform purely numerical calculations of critical exponents, but also to predict some qualitatively new effects which could not be obtained within conventional approaches, e.g., within the Landau theory approximation. Among them are qualitative effects, such as the fluctuation-induced first-order phase transition (see, for example, refs. 14–17). This effect takes place in some anisotropic systems where the renormalized free energy $F(\varphi)$ undergoes transformations which are typical for the first-order phase transition.

Recently nucleation centers were found in a fluctuation-induced first-order transition.[18] However, in any case, the free energy is transformed due to fluctuations in the critical region. One can expect that even in the situation when the fluctuations are not strong enough to change the transition order they manifest themselves somehow. It was shown[19] that localized nonlinear excitations are possible in this situation, too. This effect was found using a very simple model of the phase transition.[19,20] Let us recollect it briefly.

The isotropic Landau–Ginzburg–Wilson functional

$$\mathbf{H} = \tfrac{1}{2} \int d\mathbf{r}\, [(\nabla\varphi)^2 + \bar{F}(\varphi)] \tag{1}$$

was considered with arbitrary function $\bar{F}(\varphi)$ having a representation in series form

$$\bar{F}(\varphi) = \sum_{k=1}^{\infty} u_{2k}(\varphi^2)^k \tag{2}$$

To make the model exactly solvable all integrals of the $\int d\mathbf{r}\, \varphi^{2k}(\mathbf{r})$ type were replaced by the powers of the integral $a = \int d\mathbf{r}\, \varphi^2(\mathbf{r})$, i.e.,

$$\int d\mathbf{r}\, \varphi^{2k}(\mathbf{r}) \to V(a/V)^k \qquad [\bar{F}(\varphi^2) \to F(a/V)]$$

After this simplification the partition function and free energy of the system were calculated analytically.

It was obtained that the effective free energy in the fluctuation region remains a monotonic function, as it naturally should be for isotropic systems. However, its structure is changed and the phase transition should be described at least by the φ^6-model. It is not very essential for

equilibrium order parameter evolution, but leads to the generation of the nonlinear excitations in the critical region.

The described model is very convenient for analytical study, but it reduces the fluctuation interaction and it is impossible to control a correction which should be done to the free energy with account of the neglected fluctuations. A more correct approach may be based on the RG technique. Below this approach will be developed.

In addition, the time-space evolution of the fluctuating order parameter field will be numerically studied in the critical point. It will be shown that the fluctuating field has well-pronounced large-scale structure in spite of its scale invariance on average. This structure is similar to an analogous one recently found in the intermediate stage of the nucleation process at first-order phase transitions,[10] but it does not lead to final ordering.

1. EFFECTIVE FREE ENERGY IN CRITICAL REGION

A formally exact functional RG equation was first suggested by Wilson.[14,15] It can be written in the form

$$\begin{aligned}\hat{R}(H[\varphi]) = {} & \frac{1}{2}\int_q \eta(q)[V - G_0^{-1}(q)\,|\varphi(q)|^2] + dV\frac{\partial H}{\partial V} \\ & - \int d^d r \left[(d-2)\frac{\varphi(\mathbf{r})}{2} + \mathbf{r}\nabla_r \varphi(\mathbf{r})\right]\frac{\delta H}{\delta \varphi(\mathbf{r})} \\ & + \int_{\mathbf{r}\mathbf{r}'} \left\{ h(\mathbf{r}-\mathbf{r}')\left[\frac{\delta^2 H}{\delta\varphi(\mathbf{r})\,\delta\varphi(\mathbf{r}')} - \frac{\delta H}{\delta\varphi(\mathbf{r})}\frac{\delta H}{\delta\varphi(\mathbf{r}')}\right]\right. \\ & \left. - \frac{1}{2}\eta(\mathbf{r}-\mathbf{r}')\,\varphi(\mathbf{r})\frac{\delta H}{\delta\varphi(\mathbf{r}')}\right\} \end{aligned} \tag{3}$$

where $H = H_{\text{total}} - H_0$ and

$$H_0 = \int_q G_0^{-1}(q)\,|\varphi(q)|^2; \qquad \int_q \equiv \int d^d q/(2\pi)^d$$

$$H = \sum_{k=1}^{\infty} 2^{1-2k} \int_{\{q_i, q_{i'}\}} (2\pi)^d \delta\left(\sum_{i=1}^{k} (q_i + q_{i'})\right) \times g_k\{q_i, q_{i'}\} \prod_{i=1}^{k} \varphi_{q_i}\varphi_{q_i'}$$

d is the space dimensionality, φ is an n-component vector, $h(q) =$

$\exp(-q^2/2\Lambda^2)$ is the cutoff factor, and the function of the anomalous dimensionality is defined by the relations

$$\eta(q) = \eta(0) + \{[D(q) - D(0)] - \eta(0)\, G_0^{-1}(q)\}/[G_0^{-1}(q) + g_1]$$

$$D(q) = -g_1^2 h(q) + \tfrac{1}{2} \int_p h(p)[n g_2(\mathbf{p}, -\mathbf{p}; \mathbf{q}, -\mathbf{q}) + g_2(\mathbf{p}, -\mathbf{q}; \mathbf{q}, -\mathbf{p})]$$

The value $\eta = dD/d(q^2)|_{q=0}$ coincides with the Fisher exponent.

Recently this equation was used to formulate several variants of nonperturbative calculations of critical asymptotics.[21-25] The exact RG equation has, of course, among others the solution corresponding to the standard ε-expansion.[26-28]

The strict calculation procedure uses the essentially nonlocal Ginzburg–Landau–Wilson functional.[26-32] At the same time the expected generation of nonlocalities is small (to the extent of the smallness of the Fisher exponent $\eta \simeq 0.03$). So, in the cases when one is interested not in the calculation of the exact critical asymptotics but only in some qualitative features of the theory, one may neglect this generation limiting oneself to the local form of the exact RG equation[28,30-32]:

$$\partial f/\partial l = df - \frac{d-2}{2} \vec{\varphi}\, \vec{\nabla}_\varphi f + \nabla_\varphi^2 f - (\vec{\nabla}_\varphi f)^2 \tag{4}$$

where $\vec{\varphi}$ is the n-component fluctuating field, $F(\vec{\varphi}(r))$ is the density of the free energy functional having the form $\mathbf{H} = \int d^d r\, f(\vec{\varphi}(r))$, d is the space dimensionality, l is the renormalization group "time," and the fixed point $F^*(\vec{\varphi}; l)$ is defined by the condition $df^*/dl = 0$.

In the general case the free energy functional density $f^*(\varphi)$ should satisfy very weak restrictions. It must be defined in the whole region of φ values, be even, and be infinitely increasing at $\varphi^2 \to \infty$.

In this article we shall limit ourselves to a scalar form of $f^*(\varphi)$ (for more general study see refs. 30 and 32). It is easy to prove that at $\varphi \to \infty$ the function f^* has the asymptotics $f^* \simeq \varphi^2/2 + \cdots$. One can prove that it is the (unique) solution which has a physical sense in phase transition theory. It was found recently[30] by numerical and (partially) analytical calculation. Below we give a brief review of its properties useful for our needs.

This solution gives negative critical temperature renormalization, because the g_1 vertex in the series $f^* = \sum_k g_k(\varphi^2)^k$ is negative. Direct calculation of the spectrum leads to very good critical exponents. Both these facts are very essential for the applicability of the solution to the criticality.[33]

A local approximation for the physical free energy at the critical point can be obtained from formal renormalization of the critical temperature:

$$F(\varphi) = f(\varphi) - g_1 \varphi^2 - g_0 \tag{5}$$

Here the zeroth constant $g_0 = f(0)$, which is not essential for physical results, is subtracted also. In Fig. 1 the functions $f(\varphi)$, $F(\varphi)$ (bold line), and its derivative $F_\varphi(\varphi)$ (broken line) are shown. It is seen that near the point $\varphi = 0$ the free energy has a very wide minimum.

It is interesting to note that as a matter of the fact, at $d = 3$ one deals with φ^6-theory. The effective potential F is defined at small values of φ by a Laguerre polynomial $L_3^{(n/2-1)}(\varphi^2)$. At large φ the potential has a cross-over to the asymptotics $f \simeq \varphi^2/2 + \cdots$. This behavior is only qualitatively the same as can be expected from previous experience (for example, from the ε-expansion) in φ^4-theory. Such a structure corresponds to anomalous series of its vertices (in some analogy with the result obtained for the free energy in an exactly solvable model[19]).

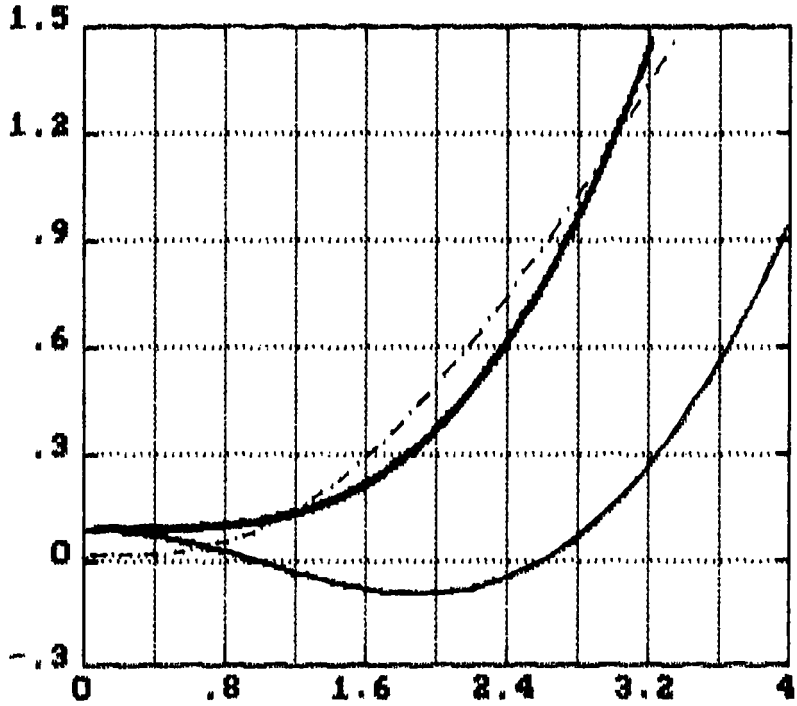

Fig. 1. Exact (local) renormalized functional $f(\varphi)$ at $d = 3$ for scalar model, local part of the effective free energy $F(\varphi)$ (bold line), and its derivative (broken line).

Table I

k	0	1	2	3	4	5	6	...
g_k	0.076	−0.456	0.373	−0.141	0.067	−0.036	0.020	...

In principle Eq. (4) can be represented as a hierarchy of equations for functional vertices $f = \sum g_k(\varphi^{2k})$. It can be shown that this set of equations may be truncated when $\varepsilon \ll 1$[25-28] to obtain the ε-expansion-like equations. However, at physical $d \leqslant 3$ such a truncation of the series leads to complex eigenvalues even for an isotropic solution. This means that large powers of φ play an essential role and one cannot cast them away. The main reason for this result is the $\varphi^2/2$ asymptotics of the physical solution branch.

The scalar equation for the vertices has a relatively simple form,

$$\bar{g}_k = [d-(d-2)k]\, g_k + (2k+1)(k+1)\, g_{k+1}/2 - \sum_{m=1}^{k+1} m(k-m+1)\, g_m\, g_{k+1-m} = 0 \tag{6}$$

and may be solved as a recursion relation which defines all vertices as functions of a given zero-point constant $f(0) = g_0$:

$$g_{k+1} = \hat{G}_{k+1}[g_k; g_{k-1}; \ldots; g_0] \tag{7}$$

$$\hat{G}_{k+1}[\cdots] = \left\{ -[d-(d-2)k]\, g_k + \sum_{m=1}^{k+1} m(k-m+1)\, g_m\, g_{k+1-m} \right\} \frac{1}{(2k+1)} \tag{8}$$

Table I gives the first vertices g_k.

It is directly seen from the table that the sequence $g_k \sim (-1)^k$ and very slowly tends to zero for large k. This effect is the result of the asymptotic behavior because it is controled by the g_k with large k values.[2]

2. LARGE-SCALE STRUCTURE OF FLUCTUATING FIELD

Let us use the function $F(\varphi^2)$ as the approximate local part of the nonequilibrium free energy functional H_{eff} renormalized due to microscopic fluctuations:

$$H_{\text{eff}} = \int d\mathbf{r}\, [\tfrac{1}{2}(\nabla\varphi)^2 + F(\varphi^2)] \tag{9}$$

[2] Recently the role of highest-order correlation functions was emphasized in a calculation of critical exponents by a renormalization of the Ornstein–Zernike equation for the liquid–vapor critical point.[34,35]

The nonuniform order parameter distribution is given by the saddle point equation $\delta H_{\text{eff}}/\delta\varphi = 0$:

$$[\nabla^2 - F_\varphi/\varphi]\,\varphi = 0 \tag{10}$$

In contrast with a previously used model approach,[19] the free energy here is known in the form of numerical data only. So an analytical solution of the equation is absolutely impossible. But one can do it numerically. Moreover, taking into account that the $F(\varphi)$ function is generated by a differential equation, numerical study here seems to be natural and convenient. Taking this in mind, one can start just from the more general form of the equation for the mesoscopic order parameter time and space distribution:

$$\gamma^{-1}\, d\varphi/dt = -\delta H/\delta\varphi + \lambda(t; \mathbf{r}) \tag{11}$$

Here and below the subscript "eff" is omitted for brevity; γ is the kinetic coefficient and the random noise $\lambda(t; \mathbf{r})$ with the properties

$$\langle \lambda(t; \mathbf{r}) \rangle = 0; \qquad \langle \lambda(t; \mathbf{r})\, \lambda(t; \mathbf{r}') \rangle = D\delta(\mathbf{r} - \mathbf{r}')$$

is introduced to account for the fact that the large-scale excitations of the order parameter field should arise not "by themselves," but as a result of an evolution of the arbitrary (small) fluctuations. The noise intensity D is defined by the temperature of the system $D = T = 1$ [following previous studies,[26-30] $T = 1$ has been chosen in Eq. (3)]. The presence of random noise $\lambda(t; \mathbf{r})$ leads to a very complicated structure of the interacting excitations with different magnitude and dispersion.

Equation (11) was studied numerically for space dimensionalities $d = 1$ and $d = 2$. In both cases similar large-scale structures were found with quite pronounced long-time excitations. Common features of the structures at $d = 1$ and $d = 2$ allow one to suppose that the same structure should occur at $d = 3$, too. The main results are presented in the figures.

Figure 2 shows a small fragment of the current order parameter φ distribution (white line) at some time $t = t_0$. Relatively large (mesoscopic) excitations of the form close to those analytically found before[19] can be observed directly. More essential is that the structure is conserved over a long time "on average." To demonstrate this fact the prehistory of the current distribution down to $t = t_0 - 2$ (in dimensionless units) is shown on the same figure by black lines. A correlation is quite obvious. The two-point correlation function

$$G(\mathbf{r} - \mathbf{r}_0) = \langle \varphi(\mathbf{r})\, \varphi(\mathbf{r}_0) \rangle \tag{12}$$

can be calculated directly from numerical data and it is shown also on the insert to Fig. 2. It has a linear behavior at small distances and an exponential one at large r. This behavior is quite the same as was obtained for solitary excitations in the model frame.[19]

Let us turn now to the two-dimensional picture. Figure 3 shows the small pattern evolution with time. The order parameter value is given by the intensity of the gray (here both signs of fluctuations $\varphi > 0$ and $\varphi < 0$ are presented, of course). Black points correspond to the maximal value of $(+\varphi) \approx 10^{-2}$.

It is easy to see some large "stable" formations. Well-pronounced noise is presented on the picture. With time, the picture will be completely changed. This reconstruction takes place in two main forms: (a) density maxima relax and disappear with time; (b) the maxima move chaotically as "small particles."

It is seen from the pictures that the excitations do not always have an isotropic structure. Moreover, taking into account that they are not equilibrium order parameter distributions, one can prove that the probability for long excitations (density folds) to arise due to random noise is larger than it is for isotropic ones. This effect is quite the same as is for a critical nucleus at a first-order phase transition[9] and the reason is that some gradient terms in the free energy functional for long fluctuations tend to

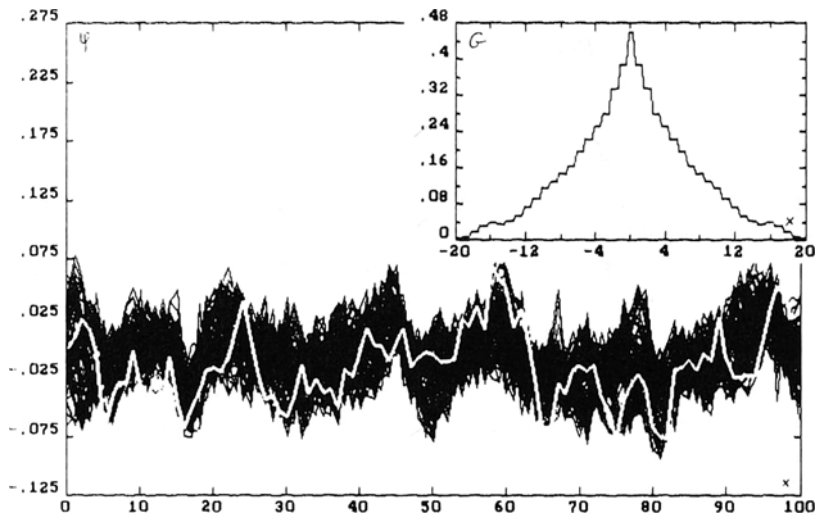

Fig. 2. Current order parameter φ distribution (white line) at some time $t = t_0$. The prehistory of this current distribution down to $t = t_0 - 2$ (in dimensionless units) is shown by black lines. The two-point correlation function is shown in the insert.

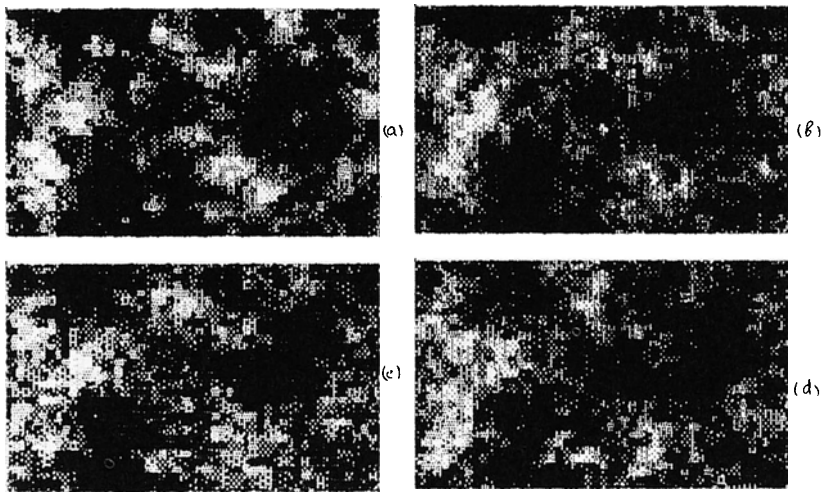

Fig. 3. Evolution of small pattern of $\varphi(t;\mathbf{r})$ with time.

zero. During its evolution a large excitation tends to an isotropic form. But in the initial steps of the evolution the probability for new excitation generation near its long "tails" is essentially larger than it is at other space points. This process leads to the formation of a specific "large-scale structure" of fluctuating field shown in Fig. 4. This picture is slightly filtered and color resolution is higher to make the structure quite obvious. It seems like the same picture arising in the intermediate stage of order parameter relaxation to a stable phase at a first-order transition recently found.[10]

Structure formed at a critical point does not lead to an ordered stable phase and exists in the kinetics only. It is transformed completely with time. Nevertheless, it should be treated as a stationary (but not static) distribution of the fluctuations. Let us calculate the averaged derivative $\langle \partial w[\varphi]/\partial t \rangle$ from the probability density functional $w[\varphi] = \exp(-H[\varphi])$:

$$\gamma^{-1}\left\langle \frac{\partial w[\varphi]}{\partial t}\right\rangle = \gamma^{-1}\left\langle \int_{\mathbf{r}} \frac{\partial \varphi(\mathbf{r})}{\partial t}\frac{\delta w[\varphi]}{\delta \varphi(\mathbf{r})}\right\rangle$$

$$= -\left\langle w[\varphi]\int_{\mathbf{r}} \frac{\delta H[\varphi]}{\delta \varphi(\mathbf{r})}\left[-\frac{\delta H[\varphi]}{\delta \varphi(\mathbf{r})}+\lambda(t;\mathbf{r})\right]\right\rangle$$

$$= -\left\langle w[\varphi]\int_{\mathbf{r}}\left[-\left(\frac{\delta H[\varphi]}{\delta \varphi(\mathbf{r})}\right)^2+\frac{\delta^2 H[\varphi]}{\delta \varphi(\mathbf{r})\,\delta \varphi(\mathbf{r})}\right]\right\rangle \quad (13)$$

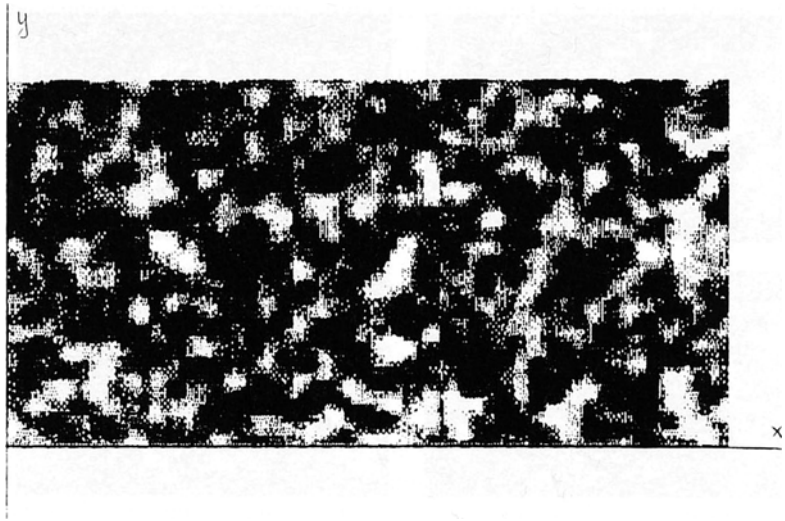

Fig. 4. Developed large-scale structure of the fluctuating field.

Here we take into account that

$$\left\langle \frac{\delta H[\varphi]}{\delta \varphi(\mathbf{r})} \lambda(t; \mathbf{r}') \right\rangle = D\delta(\mathbf{r} - \mathbf{r}') \frac{\delta^2 H[\varphi]}{\delta \varphi(\mathbf{r})\, \delta \varphi(\mathbf{r}')} \tag{14}$$

for δ-correlated random noise having only second nonzero correlator $\langle \lambda(t; \mathbf{r})\, \lambda(t; \mathbf{r}') \rangle = D\delta(\mathbf{r} - \mathbf{r}')$.

Comparing Eq. (13) with renormalization group equation (3) and taking into account that $\hat{R}(H[\varphi]) \equiv \hat{R}(H_{\text{eff}}[\varphi]) = 0$, one can conclude that at least in local approximation the evolution of the $\langle w[\varphi] \rangle$ value is equivalent to its simple scale transformation. This means that the noise will produce more large (and more small) excitations during the time, but the general structure will be conserved.

Strictly speaking, the local approximation does not correspond to the physical picture described, because it should define some special scale in the space due to a fixed factor at the gradient term. A more rigorous approach is needed in nonlocal corrections to the effective energy $H[\varphi]$ and in corrections to the kinetic coefficient $\gamma \neq \text{const}$, respectively. One can believe, however, that due to their smallness the qualitative picture obtained will be the same.

Summarizing, one can conclude that the fluctuation interaction leads to free energy transformations which are accompanied by localized order parameter excitations. These excitations form a "large-scale structure" which

is qualitatively the same as the analogous one in the intermediate stage of order parameter relaxation to the stable state at first-order phase transitions. This structure may be interpreted as a source for instabilities and nucleation at fluctuation-induced first-order phase transitions.

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