Journal of Statistical Physics, Vol. 71, Nos. 5/6, 1993

Nonlinear Excitations in the Critical Region

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Received June 9, 1992; final January 5, 1993

The free energy transformation due to fluctuations is investigated in an exactly solvable model. This model accounts for the fluctuation interaction in a reduced manner and leads to a realistic estimation for the free energy. In particular it gives a nice critical exponent $\delta = 5$. It is shown that in spite of the monotonic character of the effective free energy in the critical region the properties of the system should be described on the basis of the φ^6 model. Localized nonlinear excitations are found to be possible with a profile rather like that known as a "bump" near the point of the first-order phase transition.

KEY WORDS: Nonlinear excitations; critical region; exactly solvable model; fluctuations.

INTRODUCTION

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.$^{(1-3)}$ Among these are qualitative effects such as the fluctuation-induced first-order phase transition (see, for example, refs. 4 and 5).

This effect manifests itself in the following process. A trial free energy functional corresponds to a second-order phase transition. A fluctuation interaction renormalizes the parameters of the free energy. This leads to transformations of the effective free energy $\mathscr{F}(\varphi)$ with temperature τ.

In anisotropic systems (at some trial parameters) the curve $\mathscr{F}(\varphi)$ undergoes transformations which are typical for the first-order phase transition.

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0022-4715/93/0600-1003$07.00/0

On the other hand, it is well known just from the mean field theory that the first-order phase transition is anticipated by nonlinear excitations which can be interpreted as nucleation centers in the para phase (for review see refs. 6 and 7). The same nucleus exists in the case of the fluctuation-induced first-order phase transition.(13)

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 this manifests itself somehow. Below it will be shown that the fluctuation interaction leads to localized nonlinear excitations at $T > T_c$.

The paper is organized as follows.

The first part presents some main relations referring to the formulation of an exactly solvable model of the phase transition(9–11) which is a generalized version of the model proposed by Schneider *et al.*(8) Use of this model accounting for the fluctuation interaction in a reduced manner allows one to calculate the free energy structure in the critical region as some realistic estimation.

As previously shown by us, the model is not trivial and one can obtain a number of fluctuation effects predicted within the more sophisticated RG approach. A new result given in this part is that the factor at φ^4 in the expansion of the effective free energy becomes zero at the critical point even for an isotropic system.

In the second part an effective free energy is calculated and applied to the study of nonlinear excitations. Both static and kinetic excitations are investigated.

1. EFFECTIVE FREE ENERGY IN THE CRITICAL REGION

The exact free energy calculation in the critical region is a very tedious problem and has not been solved. However, the essential qualitative properties of the free energy can be obtained in approximations. One way is to utilize an exactly solvable model.(8–11) Let us review this briefly.

Let us consider the Landau–Ginzburg–Wilson functional in the form

$$\mathbf{H} = \frac{1}{2} \int d\mathbf{r}\, [(\nabla\varphi)^2 + \bar{F}(\varphi)] \tag{1.1}$$

where $\bar{F}(\varphi)$ is an arbitrary function having a representation in a series form

$$\bar{F}(\varphi) = \sum_{k=1}^{\infty} u_{2k}(\varphi^2)^k \tag{1.2}$$

The model becomes exactly solvable if one replaces all integrals of the $\int d\mathbf{r}\, \varphi^{2k}(\mathbf{r})$ type by powers of the integral $a = \int d\mathbf{r}\, \varphi^2(\mathbf{r})$, i.e.,

$$\int d\mathbf{r}\, \varphi^{2k}(\mathbf{r}) \to V(a/V)^k \qquad [\bar{F}(\varphi^2) \to F(a/V)] \tag{1.3}$$

Now one can calculate the free energy of the system using the representation

$$\exp\left[-\frac{V}{2}F\left(\frac{a}{V}\right)\right] = \int_{-\infty}^{\infty} \frac{dx\, dy}{2\pi} \exp\left[-\frac{V}{2}F\left(\frac{x}{V}\right) + iy(x-a)\right] \tag{1.4}$$

The partition function of the system

$$\begin{aligned} \mathbf{Z} &= \int D\varphi \exp(-\mathbf{H}[\varphi]) \\ &\approx \int D\varphi\, dx\, dy \exp\left\{-\frac{1}{V}\sum_q (q^2 + 2iy)\, |\varphi_q|^2 + \frac{1}{2}[2ixy - VF(x/V)]\right\} \end{aligned} \tag{1.5}$$

may be directly integrated over all φ_q modes except the order parameter,

$$\mathbf{Z} \approx \int d\varphi\, dx\, dy \exp\left\{-\frac{V}{2}\left[F(x) - xy + y\varphi^2 + \frac{1}{V}\sum_{q\neq 0} \ln(y + q^2)\right]\right\} \tag{1.6}$$

Here the substitutions $x/V \to x$ and $2iy \to y$ were made for convenience. Equation (1.6) defines the effective free energy $\mathscr{F}(\varphi)$,

$$\mathscr{F}(\varphi) = -\ln \int dx\, dy \exp\left\{-\frac{V}{2}[F(x) - xy + y\varphi^2 + \Phi(y)]\right\} \tag{1.7}$$

The integrals over x and y values are exactly calculated in the thermodynamic limit $V \to \infty$ using the saddle point equations

$$\begin{aligned} y &= F_x(x) \\ \varphi^2 &= x + f(y) \end{aligned} \tag{1.8}$$

where at $d = 3$(9)

$$\begin{aligned} f(y) &= -\partial\Phi(y)/\partial y = \kappa\, \mathrm{Re}(y^{1/2}); \qquad \kappa = 1/4\pi \\ \Phi(y) &= \frac{1}{V}\sum_q [\ln(q^2 + y) - \ln q^2 - y/q^2] \equiv \frac{1}{V}\sum_q{}_R \ln(q^2 + y) \end{aligned} \tag{1.9}$$

and divergent terms in $\Phi(y)$ are eliminated by means of rescaling $F(0)$ and x, respectively. Substitution of the functions $x = x(\varphi)$ and $y = y(\varphi)$ into Eq. (1.7) gives an effective free energy $\mathscr{F} = \mathscr{F}(\varphi)$.

The above results were obtained in previous papers.(9–11) Now we will study the temperature evolution of the free energy $\mathscr{F}(\varphi)$ for an isotropic system. This evolution is defined by the temperature dependence of the first few derivatives of $\mathscr{F}(\varphi)$ at $\varphi = 0$.

To calculate them, let us note that the derivative $F_x(x)$ has the following structure:

$$F_x = \tau + \rho(x) \tag{1.10}$$

where $\tau \to 0$ at the critical point and $\rho(x)$ is an arbitrary function in the same sense as the original $F(x)$.

One can rewrite Eqs. (1.8) and (1.9) as a sole equation for $x = x(\varphi)$,

$$F_x = A(\varphi^2 - x)^2 \tag{1.11}$$

where $A = 1/\kappa^2$. Using Eqs. (1.10) and (1.11), one can easily prove that the derivative of $\mathscr{F}(\varphi)$ over φ is equal to φF_x [where $x = x(\varphi)$ is substituted]. As a result one has

$$\frac{d\mathscr{F}}{d\varphi^2} = \frac{1}{2} F_x(\varphi^2); \qquad \frac{d^2\mathscr{F}}{d(\varphi^2)^2} = \frac{1}{2} \frac{dF_x(\varphi^2)}{d\varphi^2}; \qquad \text{etc.} \tag{1.12}$$

According to Eqs. (1.8),

$$\varphi^2 = x + \kappa F_x^{1/2} \qquad (F_x > 0)$$

At $\varphi = 0$ and $\tau \to 0$ the value of F_x becomes zero, so

$$\left.\frac{d\mathscr{F}}{d\varphi^2}\right|_{\varphi=0} \xrightarrow[\tau \to 0]{} 0 \tag{1.13}$$

This fact means that $\tau = 0$ really corresponds to the physical critical point.

Direct calculation gives

$$\frac{d^2\mathscr{F}}{d(\varphi^2)^2} = (2A)^{1/2} \left(1 - \frac{dx}{d\varphi^2}\right)\left(\frac{d\mathscr{F}}{d\varphi^2}\right)^{1/2} \tag{1.14}$$

Here

$$\frac{dx}{d\varphi^2} = \frac{2F_x^{1/2}}{\kappa F_{xx} + 2F_x^{1/2}} \xrightarrow[\tau \to 0]{} 0 \qquad (F_{xx}\,|_{x=0} \not\equiv 0) \tag{1.15}$$

and the resulting coefficient at $(\varphi^2)^2$ is equal to

$$\left.\frac{d^2\mathscr{F}}{d(\varphi^2)^2}\right|_{\varphi^2=0} = \left(2A \frac{d\mathscr{F}}{d\varphi^2}\right)^{1/2} \xrightarrow[\tau \to 0]{} 0 \tag{1.16}$$

For the first moment this fact seems very surprising. It means that at least at the critical point the free energy expansion starts from the power $(\varphi^2)^k$ with $k \geqslant 3$ [it may be easily proved that at $F_{xx}|_{x=0} \neq 0$ the value of $d^3\mathscr{F}/d(\varphi^2)^3$ does not become zero when $\varphi^2 = 0$ and $\tau \to 0$, so $k = 3$]. However, this is in good accordance with the intuitively expected fluctuation effect on the free energy.

First of all it gives a nice critical exponent $\delta = 5$(9–11) in the model, which lies near the physical one ($\delta \cong 4.5$). Moreover, it reflects the right qualitative tendency to lower the factor near the term φ^4 in the free energy due to fluctuations. In anisotropic (or multicomponent) systems it may lead to a weakly first-order phase transition.(9, 11)

To obtain a self-consistant description of the phase transition the trial function $F(x)$ should be chosen in the form

$$F(x) = \tau x + g x^2 + b x^3 + \cdots \tag{1.17}$$

where at least the $b \neq 0$ term is preserved. Use of Eq. (1.11) gives after simple transformations the following $F_x(\varphi^2)$ function:

$$\begin{aligned} F_x(\varphi^2) = \frac{A}{(A-3b)^2} \{ & (g + 3b\varphi^2) \\ & - [(g+3b\varphi^2)^2 + (A-3b)(\tau + 2g\varphi^2 + 3b\varphi^4)]^{1/2}\}^2 \end{aligned} \tag{1.18}$$

It can be easily proved that the properties which were manifested in Eqs. (1.13) and (1.16) are preserved here. The resulting expansion for the effective free energy is obtained after simple but cumbersome calculations:

$$\mathscr{F}(\varphi^2) \cong A_2(\tau)\,\varphi^2 + A_4(\tau)(\varphi^2)^2 + A_6(\tau)(\varphi^2)^3 \tag{1.19}$$

where

$$\begin{aligned} A_2(\tau) &= A[v(\tau) - g]/2r^2; \qquad v(\tau) = (g^2 + r\tau)^{1/2}; \qquad r = A - 3b \\ A_4(\tau) &= -A[v(\tau) - g][3bv(\tau) - Ag]/2r^2 v(\tau) \\ A_6(\tau) &= A\{Ag[v(\tau) - g][3bv(\tau) - Ag] - v(\tau)[12Abgv(\tau) \\ &\quad - A^2(3b\tau + g^2) - 6Abg^2 + 9b^2(3b\tau - g^2)]\}/6r^2 v^3(\tau) \end{aligned} \tag{1.20}$$

All factors near the $(\varphi^2)^k$ powers are temperature functions. It simulates, in some sense, the renormalization of the free energy functional vertices in the RG approach.(1–3) The main feature of the evolution obtained is the possibility for $A_4(\tau)$ to be negative in some region near T_c [it can be proved that $A_{2,6}(\tau)$ are positive values here]. It is interesting that the

$\mathscr{F}(\varphi^2)$ remains a monotonic function even at $A_4(\tau) < 0$. This fact follows directly from Eq. (1.11):

$$\frac{d\mathscr{F}}{d\varphi^2} = \frac{1}{2} F_x(\varphi^2) = \frac{A}{2}[\varphi^2 - x(\varphi^2)]^2 > 0 \tag{1.21}$$

and may be proved for the reduced expansion (1.19) also. It means that the phase transition remains of second order, as it naturally should for isotropic systems. The effective free energy acquires only a bend, which is not essential for the equilibrium order parameter evolution; however, as will be shown in the next section, it leads to the generation of nonlinear excitations in the critical region.

2. NONLINEAR EXCITATIONS

Let us use the function $\mathscr{F}(\varphi^2)$ [instead of the trial function $F(\varphi^2)$] as an approximate local part of the nonequilibrium free energy functional $\mathbf{H}_{\text{eff}}$:

$$\mathbf{H}_{\text{eff}} = \int d\mathbf{r}\, [\tfrac{1}{2}(\nabla\varphi)^2 + \mathscr{F}(\varphi^2)] \tag{2.1}$$

The nonuniform order parameter distribution is given by the equation

$$\delta\mathbf{H}_{\text{eff}}/\delta\varphi = -[\nabla^2 - w(\varphi)]\,\varphi = 0 \tag{2.2}$$

where $w(\varphi) = \mathscr{F}_\varphi/\varphi$.

We restrict ourselves below to the one-dimensional case only: $\varphi = \varphi(r)$ and $\nabla^2 \to d^2/dr^2$. This restriction allows us to obtain exact solutions of Eq. (2.2) using standard technique:

$$d^2\varphi/dr^2 = \tfrac{1}{2} d(\varphi_r)^2/d\varphi = \mathscr{F}_\varphi \tag{2.3}$$

This equation leads to

$$(\varphi_r)^2 = 2\mathscr{F}(\varphi^2) + A_0 \tag{2.4}$$

where $A_0 = \text{const}$. Finally one obtains

$$r = \int_{\varphi_0}^{\varphi} \frac{d\varphi}{[2\mathscr{F}(\varphi^2) + A_0]^{1/2}} \tag{2.5}$$

The problem under consideration is reduced now to the calculation of the integral (2.5) for the general φ^6 model. This program was fulfilled in refs. 6 and 7 and different types of nonlinear excitations were obtained.

Here a certain peculiarity exists. Namely, when $A_4 < 0$ in the Landau theory a discontinuous transition takes place. It is accompanied by a "bump"-type excitation in the disordered phase which leads to a finite value of $\varphi_0 \neq 0$. In our situation $A_4(\tau) < 0$ at positive temperature also. But $A_4(\tau) \to 0$ when $\tau \to 0$ and $\mathcal{F}(\varphi^2)$ is a monotonic function at any $\tau > 0$. It generates an additional problem.

Let us illustrate the situation by a simple example. If $A_0 = 0$, the integral (2.5) is easily calculated in elementary functions. The substitution $\varphi^2 = 1/\eta$ transforms it to the following form:

$$\mathbf{I}(\eta) = \int_{\eta_0}^{\eta} \frac{d\eta}{(A_2\eta^2 + A_4\eta + A_6)^{1/2}} \tag{2.6}$$

The concrete formula for the resulting $\mathbf{I}(\eta)$ function is defined by the sign of the combination $\Delta = 4A_2A_6 - A_4^2$. In our case $\Delta(\tau) > 0$ at any $\tau > 0$. Taking into account also that $A_2(\tau) > 0$ at $\tau > 0$, one has the following solution:

$$\varphi(r) = \left\{ \frac{\Delta^{1/2}}{2A_2} \sinh\left[\sinh^{-1}\left(\frac{2A_2\varphi_0^{-2} + A_4}{\Delta^{1/2}} \right) \right.\right. \\ \left.\left. \pm\, 2(2A_2)^{1/2}(r - r_0) \right] - \frac{A_4}{2A_2} \right\}^{-1/2} \tag{2.7}$$

where $\varphi(r) = \varphi$. The profile of $\varphi(r)$ is presented in Fig. 1. It is clear that $\varphi_0 - \varphi(r) \propto |r - r_0|$ at $r \to r_0$ and a nonanalyticality exists at the $r = r_0$

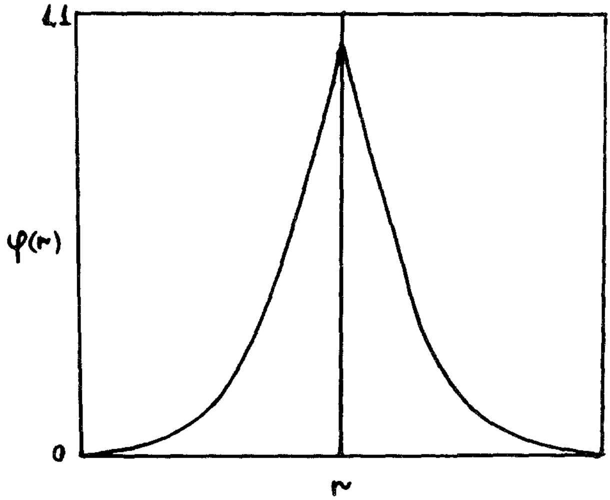

Fig. 1. Profile of $\varphi(r)$ in the stationary position.

point. This result contrasts with the analogous profile for the first-order phase transition, where a "bump" profile has an analytical form at the $r = r_0$ point.(7) Nevertheless, this does not mean that the solution obtained is an unphysical one and indicates only that the functional $\mathbf{H}_{\text{eff}}$ has a limited applicability region at small distances (or, which is the same, all integrals over momenta should be cutoff at $q \to \infty$).

Let us introduce a smooth cutoff in the usual way by using the factor $S(aq)$. Here $S(aq \to 0) \to 1$ and $\lim_{aq \to \infty} [S(aq)(aq)^m] = 0$ at arbitrary m (a is a lattice constant).(12) Instead of Eq. (2.1) one has now

$$\mathbf{H}_{\text{eff}} = \frac{1}{2} \iint d\mathbf{r}\, d\mathbf{r}'\, Q(\mathbf{r} - \mathbf{r}')\, \varphi(\mathbf{r})\, \varphi(\mathbf{r}') + \int d\mathbf{r}\, \mathscr{F}(\varphi^2(\mathbf{r})) \tag{2.8}$$

[where $Q_q = S(aq)\, q^2$]. The corresponding Euler equation takes the form

$$\int d\mathbf{r}'\, Q(\mathbf{r} - \mathbf{r}')\, \varphi(\mathbf{r}') + \partial\mathscr{F}/\partial\varphi(\mathbf{r}) = 0 \tag{2.9}$$

The concrete form of the $Q(\mathbf{r} - \mathbf{r}')$ function should be used to solve this equation. Let us rewrite Eq. (2.9) in the following way:

$$\begin{aligned} \int d\mathbf{r}'\, Q(\mathbf{r} - \mathbf{r}')\, \varphi(\mathbf{r}') &= -\nabla_r^2 \int d\mathbf{r}'\, S(\mathbf{r} - \mathbf{r}')\, \varphi(\mathbf{r}') \\ &= -\int d\mathbf{r}'\, S(\mathbf{r} - \mathbf{r}')\, \nabla_{r'}^2 \varphi(\mathbf{r}') \\ &= -\partial\mathscr{F}/\partial\varphi(\mathbf{r}) \end{aligned} \tag{2.10}$$

In the zero approximation the function $S(\mathbf{r} - \mathbf{r}')$ is the Dirac δ-function $S(\mathbf{r} - \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$. It is natural that the cutoff at large momenta leads to its slight transformation, so the difference $\delta S(\mathbf{r} - \mathbf{r}') = S(\mathbf{r} - \mathbf{r}') - \delta(\mathbf{r} - \mathbf{r}')$ is a small value everywhere except for the region $|\mathbf{r} - \mathbf{r}'| \leqslant a$. Let us rewrite Eq. (2.10) in the form

$$[\nabla_r^2 \varphi(\mathbf{r}) - d\mathscr{F}/d\varphi(\mathbf{r})] + \int d\mathbf{r}'\, \delta S(\mathbf{r} - \mathbf{r}')\, \nabla_{r'}^2 \varphi(\mathbf{r}') = 0 \tag{2.11}$$

and solve it in the perturbation theory frame. It is convenient to take that the unperturbed solution $\varphi(\mathbf{r}) = \varphi_0(\mathbf{r})$ at small distances has the form $\varphi_0(0) - \mu\, |r|$, where $\mu = \text{const}$, and utilize the relation

$$\int d\mathbf{r}'\,\delta S(\mathbf{r}'-\mathbf{r})\,\nabla_{r'}^2\varphi(\mathbf{r}')$$

$$= -\int d\mathbf{r}'\,\nabla_{r'}\,\delta S(\mathbf{r}'-\mathbf{r})\,\nabla_{r'}\varphi(\mathbf{r}')$$

$$\cong \mu \int dr'\,\mathrm{sign}(r')\,\mathrm{d}(\delta S(r-r'))/dr' = -2\mu\,\delta S(r) \tag{2.12}$$

Thus function $\varphi(r)$ satisfies the reduced equation

$$d^2\varphi/dr^2 - 2\mu\,\delta S(r) - d\mathscr{F}/d\varphi(r) = 0 \tag{2.13}$$

To obtain the solution one can concretize further the function $S(r)$ [using, for example, the form $S(r) = a/\pi(a^2 + r^2)$]. However, in any case it is quite obvious that $S(r)$ should be limited though very large at the point $r = 0$ point [while $\delta(r) \to \infty$ when $r \to 0$ and the difference $\delta S(r)$ increase at $r \to 0$, too]. On the other hand, the derivative $d\mathscr{F}/d\varphi(r)$ is limited everywhere. Thus, at small distances Eq. (2.13) can be reduced to the simple relation $d^2\varphi/dr^2 = 2\mu\,\delta S(r)$ which in turn everywhere at $|r| \leqslant a$ but $r \not\equiv 0$ can be solved using $\delta S(r) \approx S(r)$. Finally, in this region one has $\varphi(r) \approx (\mu r^2/\pi a + \text{const})$. The arbitrary constant arising here should be used for this solution together with the trial one which obviously exists as before at $|r| > a$. The resulting structure of the $\varphi(r)$ function is shown in Fig. 2.

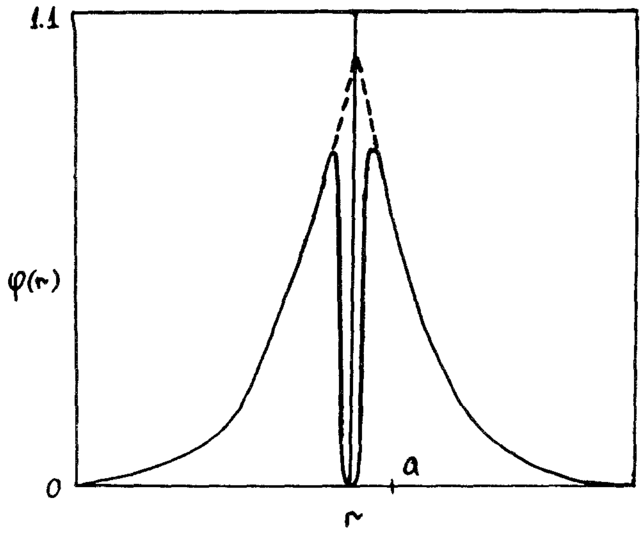

Fig. 2. Renormalized profile of $\varphi(r)$, taking account of a cutoff at small distances.

The order parameter "bump" is distributed as a usual solitary excitation and has a gap only at distances which are of the order of the lattice constant. This solution structure should be interpreted as qualitatively appropriate only. It is analytical at the zero point, but its fine structure in the region $|r| \leqslant a$ reflects only that the "order parameter language" is not adequate at very small distances.

To conclude, let us consider one kinetic property of nonlinear excitations in the critical region above T_c, namely, the kinematics of the excitations in $2n$-component systems. In this case the order parameter may be represented as a complex one and the solution for the Euler–Lagrange equation

$$-i\,\partial\varphi/\partial t = -\nabla^2\varphi + \partial\mathscr{F}/\partial\varphi \tag{2.14}$$

may be chosen in the form proposed in ref. 7,

$$\varphi(r, t) = \eta(\xi_1)\exp[i\lambda(\xi_2)] \tag{2.15}$$

Here $\xi_1 = r - v_e t$; $\xi_2 = r - v_c t$; and v_e, v_c are the velocities of "envelope" and "carrier," respectively. Substitution of this solution into Eq. (2.14) shows that for the agreement between the equations for the real and imaginary parts it is necessary to satisfy the relation $\lambda(\xi_2) = v_e\xi_2/2$. So the solution has the form

$$\varphi(r, t) = \eta(r - v_e t)\exp[iv_e(r - v_c t)/2] \tag{2.16}$$

The equation for the modulus $\eta(\xi_1)$ in this case takes the form

$$\eta_{\xi_1\xi_1} = [2\gamma + w(\eta)]\eta \tag{2.17}$$

where $\gamma = v_e(v_c - v_e/2)/4$. It is directly seen that Eq. (2.17) differs from the analogous one in the static case [see Eq. (2.2)] by the presence of the 2γ term only. This term effectively renormalizes the A_2 factor in the $w(\eta)$ expansion over η^2 powers:

$$A_{2,\text{eff}} = \gamma + A_2 \tag{2.18}$$

The difference between v_c and $v_e/2$ allows one to make the $A_{2,\text{eff}}$ value quite arbitrary. In particular, it may become zero at $v_c \leqslant v_e/2 - 4A_2/v_e$ even at $A_2 \geqslant 0$ (as it was above). So, accounting for $A_4 \leqslant 0$, one obtains the $\mathscr{F}_{\text{eff}}(\eta)$ function with all properties which are distinctive features for the first-order phase transitions.

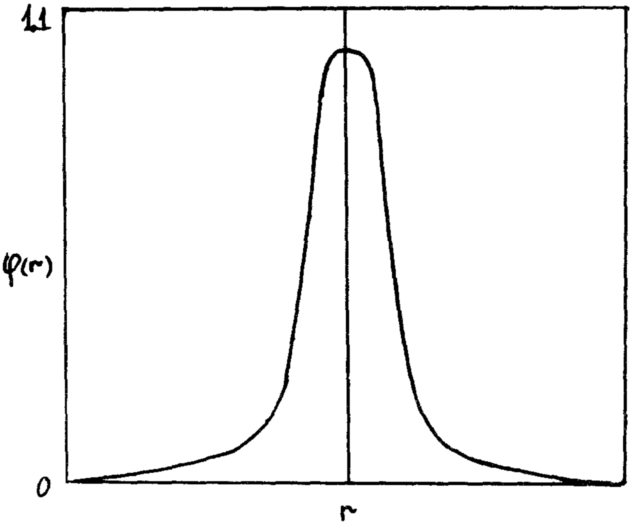

Fig. 3. Profile of moving $\varphi(r)$.

This fact makes possible the formation in the critical region of traveling nonlinear excitations with a standard profile. Their typical form is shown in Fig. 3. The analyticality of $\eta(r)$ at $r=0$ releases one from the need for a momentum cutoff which was necessary in the static case.

Summarizing, one can conclude that the fluctuation interaction leads to free energy transformations which are accompanied by localized order parameter excitations. In application to the Landau theory one can interpret the "bumps" as the critical nucleus at a discontinuous transition. It really takes place in the fluctuation region for anisotropic systems.(13)

However, a nonlinear excitation should satisfy some conditions(14) to be a real critical nucleus. It should be a special (separatrix) solution for the Euler equation and its maximum value should coincide with the equilibrium order parameter. This is not fulfilled here for a second-order transition. The solutions obtained do not satisfy the above conditions and they cannot be the critical nucleus. They are very large fluctuations only, but their presence should be pronounced in the thermodynamics.

ACKNOWLEDGMENT

One of the authors (Yu. M. I.) acknowledges support by the US Department of Energy, Office of Basic Energy Sciences, grant DE-EG02-87ER45301.

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