ASYMPTOTICS OF CORRELATION FUNCTIONS IN THE CRITICAL REGION

PHYSICS

1969

SovietRxiv

Abstract

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UDC 530.14

PHYSICS

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ASYMPTOTICS OF CORRELATION FUNCTIONS IN THE CRITICAL REGION

(Presented by Academician N. N. Bogolyubov on 21 IV 1969)

All critical phenomena have common features associated with the growth of the correlation radius. Let us consider the asymptotic behavior of the correlation function in the critical region for the simplest physical system—a gas with short-range pair forces.

The generating functional $W(u)$ of the correlation functions has the meaning of the change in the free energy upon inclusion of an external field $\varphi(q) = -\vartheta \ln(1 + vu(q))$ and satisfies the equation (^{1})

$$\ln \frac{1}{zv} \frac{\delta W}{\delta u(1)} = W\left(u(i)(1 + f_{1i}) + \frac{1}{v} f_{1i}\right) - W(u), \tag{1}$$

where $f_{ij} = \exp(-u_{ij}/\vartheta) - 1$, and u_{ij} is the pair potential, z is the activity.

In equation (1), $\frac{1}{v}\frac{\delta W}{\delta u} = \rho$ is the density of the system in the external field. The right-hand side of (1) is a functional of ρ, expandable in an integrodifferential series for small ρ. In the case $u \equiv 0$ (the external field is absent), this functional becomes a function $K(\rho)$ of the homogeneous density ρ, expandable in a power series for small ρ. For small ρ, the condition

$$1/\rho > \partial K/\partial \rho, \tag{2}$$

is obviously satisfied, and the solution of the equation

$$\ln \rho/z - K(\rho) = 0 \tag{3}$$

is unique. Clearly, it will be unique in that range of values of ρ for which condition (2) is fulfilled.

The expression $\partial K/\partial \rho$ can be represented in the form

$$\int w_2(1,2)\,dq_2, \quad \text{where} \quad w_2(1,2) = \frac{\delta}{\delta\rho(2)} \ln \frac{\delta W}{\delta u(1)}\bigg|_{u=0} \text{ —}$$

the direct correlation function, related to the full correlation function $g_2(1,2)$ by the Ornstein-Zernike relation (^{2})

$$g_2(1,2) = w_2(1,2) + \rho \int w_2(2,3)\, g_2(1,3)\, dq_3. \tag{4}$$

By virtue of relation (4), condition (2) can be represented in the form

$$1 - \rho \int w_2(1,2)\, dq_2 = 1 \Big/ \left(1 + \rho \int g_2(1,2)\, dq_2\right) > 0. \tag{5}$$

If condition (5) is violated, the solution of equation (3) is not unique. At the stability boundary of each phase (on the spinodal), $\int g_2(r)\,dq \to \infty$. It follows from this that the spinodal is a line of singular points of the free energy, regarded as a functional of the function $g_2(r)$.

At the critical point the two branches of the spinodal merge; consequently, the critical point is also a singular point of the thermodynamic functions.

Although relation (4) is not an equation for the correlation function without bringing in one more relation between w_2 and g_2, it allows one to draw certain conclusions about the asymptotic behavior of $g_2(r)$ in a neighborhood of the critical point.

Let us define the radius of nearest correlation R_0 from the condition that, for $r > R_0$,

$$|u_{12}/\vartheta| \ll |g_2(r_{12})| \ll 1, \qquad |w_2(r)| \ll |g_2(r)|. \tag{6}$$

Assuming that in equation (4), for $r > R_0$, one may neglect $w_2(1,2)$ and the contribution of the region of integration where $r_{23} > r_{13}$, we obtain, in the coordinates of two centers,

$$\left(1 - 4\pi\rho \int_0^\infty w_2(r_1)\, r_1^2 \frac{\operatorname{sh} r_1 \partial/\partial r}{r_1 \partial/\partial r}\right) r g_2(r) = 0. \tag{7}$$

This equation has a solution of the form $g_2(r) = ae^{-\lambda r}/\lambda r$, where

$$1 - 4\pi\rho \int_0^\infty w_2(r)\, r^2 \frac{\operatorname{sh} \lambda r}{\lambda r}\, dr = 0. \tag{8}$$

More precisely, represent $g_2(r)$ in the form

$$g_2(r) = ae^{-\lambda r}/\lambda r + \varphi(r)/r, \tag{9}$$

where λ satisfies equation (8), while the function $\varphi(r)$ satisfies the equation

$$\varphi(r) - 2\pi\rho \int_0^\infty r_1 w_2(r_2)\, dr_1 \int_{|r-r_1|}^{r+r_1} \varphi(r_2)\, dr_2 =$$

$$= rw_2(r) - 4\pi\rho a \int_r^\infty w_2(r_1) \frac{\operatorname{sh} \lambda(r_1 - r)}{\lambda^2}\, r_1\, dr_1. \tag{10}$$

Integrating (10) termwise with the multiplier $\operatorname{sh} \lambda r$, we obtain

$$-\frac{\lambda^3}{2\pi\rho a} - 4\pi\rho \int_0^\infty w_2(r) \left(\operatorname{sh} \lambda r - \frac{\operatorname{sh} \lambda r}{\lambda r} \right) r^2\, dr = 0. \tag{11}$$

Equations (8) and (11) determine the asymptotics of the function g_2 at distances $r > R_1$, where $R_1 = 1/\operatorname{Re}\lambda$ is the radius of complete correlation. Obviously, in the critical region $R_1 \gg R_0$ and $\operatorname{Im}\lambda \ll \operatorname{Re}\lambda$.

Let us note that the function $e^{-\lambda r}/\lambda r$ gives a representation of the group of three-dimensional rotations, and relation (10) follows from the addition theorem for this function [3]. In the two-dimensional case, the Macdonald function $K_0(\lambda r)$ has analogous properties. Setting

$$g_2(r) = aK_0(\lambda r) + \varphi(r), \tag{12}$$

where

$$\varphi(r) - \int_0^{2\pi} d\alpha \int_0^\infty r_1 dr_1\, w_2(r_1)\, \varphi\Big(\sqrt{r_1^2 + r^2 - 2r_1 r \cos\alpha}\Big) =$$

$$= w_2(r) - 2\pi a\rho \int_r^\infty w_2(r_1)\, (K_0(\lambda r) I_0(\lambda r_1) - K_0(\lambda r_1) I_0(\lambda r))\, r_1\, dr_1, \tag{13}$$

$$1 - 2\pi\rho \int_0^\infty w_2(r) I_0(\lambda r) r\, dr, \tag{14}$$

we find that, in the two-dimensional case, g_2 behaves asymptotically as $K_0(\lambda r) \approx \sqrt{\pi/2\lambda r}\, e^{-\lambda r}$. Integrating (13) termwise with the modified

with the Bessel function $rI_0(\lambda r)$ as a weight factor, we obtain

$$\frac{\lambda}{\pi\rho a} - 3\pi\rho\int_0^{\infty} w_2(r) I_1(\lambda r)\, r^2\, dr = 0. \tag{15}$$

It is obvious that in the general case the asymptotic behavior of the correlation function coincides with the behavior of the function that realizes a representation of the symmetry group of the system and satisfies the corresponding addition theorem. The radius of complete correlation and the amplitude of the correlation function are determined from relations analogous to relations (8)–(11) or (12)–(15).

The behavior of the correlation function for $R_0 < r < R_1$ has a more complicated character. To solve equation (10) in this region, one more relation between w_2 and g_2 is required. If w_2 is expanded in g_2 for $r > R_0$, then this expansion has the form (4)

$$w_2(r) \simeq \gamma_2^2 g_2^2(r)/2 + \gamma_3^2 g_2^3(r)/3! + \dots, \tag{16}$$

where at the critical point $\gamma_2 \to 0$, $\gamma_3 > 0$. In this case the right-hand side of equation (10), and consequently also the function $\varphi(r)$, are expandable in functions $e^{-\varkappa r}$ with a continuous spectrum of correlation lengths $1/\operatorname{Re}\varkappa$. This spectrum begins with 2λ, or with 3λ in the case $\gamma_2 = 0$.

The analytic dependence of the parameters λ and a on temperature and density can be found from equations (8) and (11) through the parameters γ_2 and $1 - \rho\int w_2(r)\, dq$. However, the law according to which these parameters tend to zero at the critical point cannot be determined from general considerations. Let us note that at all points of the spinodal, except the critical point, $\gamma_2 \neq 0$. It is very important that, in solving equations (8) and (11) using an expansion of w_2 in g_2 of type (16), or of another type, it is sufficient to restrict oneself to the approximation $g_2 = ae^{-\lambda r}/\lambda r$, while the behavior of the function g_2 on the interval $R_0 < r < R_1$ is fully taken into account by the term $1 - \rho\int w_2 dq$. It is known (4,5) that the expression for the thermodynamic potential contains $\int g_2 dq$. The relations obtained make it possible to determine this integral directly through the radius of complete correlation, without resorting, as in (4,5), to an investigation of the behavior of the function g_2 on the interval $R_0 < r < R_1$.

Often the solution for the function g_2 is sought in the form of a discrete sum of terms of the form $e^{-\lambda r}/\lambda r$ (6,7). This form of the solution follows from the assumption that $w_2 = 0$ for $r > R_0$. A dependence of the form (16), as well as any other dependence between w_2 and g_2 for $r > R_0$, leads to the conclusion that there is a continuous spectrum of correlation lengths.

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Received
15 IV 1969

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