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Equation of state in the critical region with inclusion of non-asymptotic terms

A. T. Berestov

All-Union Research Institute for Physicotechnical and Radio-Engineering Measurements
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The leading nonasymptotic terms in the Migdal equation of state are determined by the ϵ-expansion method to order ϵ^2. The contribution of the additional terms is related to the susceptibility of the system and is proportional to $\chi^{-\Delta/\gamma}$. The equation of state is determined by the expression $H\chi^{(\beta+\gamma)/\gamma} = \varphi_0(M\chi^{\beta/\gamma}) + c\varphi_1(M\chi^{\beta/\gamma})\,\chi^{-\Delta/\gamma}$. The functions $\varphi_0(m)$ and $\varphi_1(m)$ have a simple form and are determined by formulas (3.5) and (4.4).

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1. INTRODUCTION

Substantial progress in the description of critical phenomena has recently been achieved. Using a method developed by himself, Wilson[1] has found the first terms of the ε-expansion for the critical indices to order ε^2 ($\varepsilon = 4 - d$; d is the dimensionality of space). It was found that the coefficients of ε and ε^2 are small and for $\varepsilon = 1$ give values of the indices that are close to the experimental values. This circumstance served as a stimulus for the determination of other universal quantities too. The first three terms of the ε-expansion of the equation of state of the Ising model were determined by Avdeeva and Migdal, and also by Brézin, Wallace and Wilson.[2]

However, it is essential to note that the results of[2] are applicable only in the immediate vicinity of the critical point. As we move away from it there arise additional terms,[3] a knowledge of which is important for the following reasons. First, they give the possibility of determining whether the experimental investigations are being carried out sufficiently close to the critical point, and, secondly, they give the possibility of describing the substance in a wide region about the critical point. We shall discuss these questions in more detail.

The techniques of present-day experiments in the study of critical phenomena make it possible to obtain reliable results (with error ~ 0.1–1% for the specific heat, for example) near the transition point, down to values of $t = (T - T_c)/T_c$ of the order of 10^{-4}–10^{-5},[4] where T is the temperature. On the other hand, since it is known that the theory is asymptotic in character, the fitting of the experimental data by the corresponding power laws, which define the critical indices, is usually carried out for $|t| \lesssim 10^{-2}$–10^{-1}. The best critical-index values obtained in different experiments for different substances frequently do not coincide (cf.[4]), even though current theory requires them to be universal. The principal inaccuracy in their determination is evidently associated with systematic errors—in particular, with the use of the pure-power, asymptotic laws in the whole range of the fitting. But it is completely unclear beforehand whether any particular region of measurements is asymptotic. The natural criterion for applicability of the asymptotic laws in the analysis of the experimental data is that the nonasymptotic terms be small compared with the experimental error. Strictly speaking they should be, to use the terminology of mathematical statistics, insignificant, i.e., systematic (albeit, possibly, small) deviations of the experimental points from the asymptotic dependences should be absent. Thus, taking nonasymptotic terms into account should lead to a more rigorous appraisal of the degree of universality of the experimentally obtained quantities.

The other topic in which the determination of nonasymptotic terms can play an important role is the description of the behavior of matter, e.g., a liquid and a dense gas, in a wide interval of the parameters of state. In such an approach, as was noted in[5], the universal scaling equation of state in the critical region can be used as the "zeroth" approximation. It is found that in practically the whole region $t < 1$ and $|\Delta\rho| = |(\rho - \rho_c)/\rho_c| < 1$ the discrepancies between the asymptotic dependences and the experimental data are not large and can, apparently, be described by the introduction of non-asymptotic terms. The important point here is that these turn out to be universal to the same degree as the asymptotic equation of state.[3,6]

The first results in the determination of the nonas-

ymptotic terms were obtained in[3,6]. The critical index Δ, which determines the behavior of the nonasymptotic terms, and the contribution of these terms to a number of quantities determining the behavior of the system near the critical point were calculated in[6]. In the present paper the leading nonasymptotic terms in the equation of state are determined by the Wilson method to second order inclusive in ε, for systems with a one-component order parameter.

2. METHOD OF CALCULATION

We shall discuss the calculational method used. The Hamiltonian of the problem under consideration has the form

$$\mathcal{H}=\int\left[\frac{1}{2}(\nabla\varphi')^2+\frac{1}{2}t(\varphi')^2+\frac{1}{4!}u_0(\varphi')^4\right]d^dx \qquad (2.1)$$

where d is the dimensionality of space and u_0 is an interaction constant.

The correlation functions calculated in the theory are obtained in the form of series in u_0 and ε. In order to obtain critical behavior of these functions that is independent of u_0 it is necessary to sum the entire series. However, by means of the renormalization-group equations[1] it can be shown that there exists a choice of coupling constant u_0^* such that the expected critical behavior is obtained in the first orders of perturbation theory.

For subsequent use we note the following point. Since the quantities being calculated have a universal character, i.e., do not depend on the method of cutoff, for $d=4-\varepsilon$ it is most natural to make use of the method of 't Hooft and Veltman[7] to regularize the integrals encountered. It then turns out, however, that the calculation of the coupling constant u_0^* by "matching" the power behavior of the amplitude u_R to the perturbation-theory series for it leads to $u_0^*\to\infty$. It is necessary, therefore, to go over to the renormalized theory. This implies going over from (2.1) and the unrenormalized Green functions $\Gamma'^{(N)}(t, u_0, k_i)$ to a Hamiltonian of the form

$$\mathcal{H}=\int\left[Z_3\frac{(\nabla\varphi)^2+r\varphi^2}{2}+\frac{1}{4!}u_1p^\varepsilon Z_1\varphi^4+\frac{Z_3(t-r)}{2}\right]d^dx \qquad (2.2)$$

and to the renormalized Green functions

$$\begin{aligned}\Gamma^{(N)}(r, u_1, p, k_i)&=Z_3^{N/2}(u_1)\Gamma'^{(N)}(t, u_0, k_i),\\ G^{-1}(r, u_1, p, k)&=Z_3(u_1)(G'(t, u_0, k))^{-1}.\end{aligned} \qquad (2.3)$$

Here,

$$\varphi'=Z_3^{1/2}\varphi,\quad u_0=u_1p^\varepsilon Z_1Z_3^{-2}. \qquad (2.4)$$

The momentum p has been introduced to fix the dimensions and can henceforth be put equal to unity. The constants Z_1, Z_3 and the renormalized mass can be determined from the initial conditions, e.g.,

$$\begin{aligned}&G^{-1}(k=0, p, u_1, r)=r,\quad \left.\frac{dG^{-1}(k, p, u_1, r=0)}{dk^2}\right|_{k=0}=1,\\ &u_1(k=0, u_1, r=p)=u_1p^\varepsilon.\end{aligned} \qquad (2.5)$$

Then

$$Z_1=1+\frac{3}{\varepsilon}u_1+\left(\frac{9}{\varepsilon^2}-\frac{3}{\varepsilon}\right)u_1^2,\quad Z_3=1-\frac{u_1^2}{12\varepsilon}. \qquad (2.6)$$

The connection between the unrenormalized and renormalized theories is effected by the relations (2.3), (2.4). The dependence of the bare Green functions in the renormalized theory on r and k is the same as in the unrenormalized theory, since they differ by the factor Z_3.

The specified value $u_0^*\to\infty$ corresponds to the quantity $u_1Z_1(u_1)Z_3^{-2}(u_1)$ becoming infinite at a certain value u_1^*. This value u_1^* is defined as a zero of the Gell-Mann–Low function

$$\beta(u_1)=-\varepsilon\left[\frac{\partial}{\partial u_1}\ln(u_1Z_1(u_1)Z_3^{-2}(u_1))\right]^{-1}. \qquad (2.7)$$

The function $\beta(u_1)$ has a finite limit as $\varepsilon\to0$, and can be found by perturbation theory. In our case,

$$\beta(u_1)=-\varepsilon u_1+3u_1^2-{}^{17}/_3u_1^3,\quad u_1^*={}^1/_3\varepsilon+{}^{17}/_{81}\varepsilon^2+O(\varepsilon^3). \qquad (2.8)$$

For small deviations of the coupling constant from its value at the fixed point the behavior of the system will differ from the asymptotic behavior. The most important corrections to the asymptotic laws can then be determined as a derivative with respect to the coupling constant at the fixed point[6]; this corresponds to the contribution of the "irrelevant" φ^4 operator to the quantities under consideration.

3. EQUATION OF STATE IN THE RENORMALIZED THEORY

Before proceeding directly to the calculation of the nonasymptotic terms in the equation of state we shall give a derivation of the asymptotic equation of state in the framework of the method under consideration.

In the Hamiltonian (2.1) we separate out the zeroth Fourier component

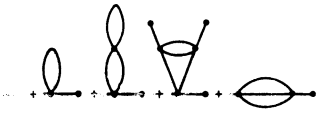
$$\varphi_0'=\frac{1}{V}\int\varphi'(x)d^dx,$$

which has the meaning of the macroscopic magnetization. Denoting the corresponding Hamiltonian as $\mathcal{H}(\varphi_0', \varphi_k')$, we obtain the equation of state in the form[8]

$$h=\langle(\partial\mathcal{H}(\varphi_0', \varphi_k')/\partial\varphi_0')_t\rangle, \qquad (3.1)$$

where h is the magnetic field. The averaging in (3.1) is performed over the distribution function $\exp\{-\mathcal{H}(\varphi_0', \varphi_k')/T\}$. Here, to the necessary accuracy $\sim\varepsilon^2$, in the expression for the field it is necessary to take into account the following diagrams:

$$h=t\varphi_0'+\frac{1}{6}u_0(\varphi_0')^3 \qquad (3.2)$$



Here a vertex corresponds to the coupling constant u_0, an external line with a blob at the end corresponds to the magnetic moment φ_0', and the internal lines corre-

spond to the bare Green functions $(G_0')^{-1} = t + \frac{1}{2} u_0(\varphi_0') + k^2$.

In the expression (3.2) we change to the renormalized quantities introduced in Sec. 2. In addition, since $u_0(\varphi_0')^2$ is of zeroth order in ε,[8] we carry out an additional renormalization of the magnetic moment and magnetic field:

$$M^2 = {}^1/_3 u_0(\varphi_0')^2, \quad H = u_0^{3/2} h. \tag{3.3}$$

As a result we arrive at the following relation between the magnetic field H, magnetic moment M and susceptibility $\chi = Z_3 r^{-1}$:

$$H = rM - M^3[1 + {}^3/_2 u_1 Z_1(u_1) I_1' + {}^3/_4 u_1^2 (I_1')^2 - u_1^2 I_2'] + {}^9/_4 u_1^2 M^5 [I_1' I_1'' + {}^1/_3 I_2''], \tag{3.4}$$

where

$I_1 =$  , $I_2 =$  ,

$$I_1 = -\left(\frac{2}{\varepsilon} + 1\right) r^{1-\varepsilon/2}, \quad I_2 = -\left(\frac{6}{\varepsilon^2} + \frac{9}{\varepsilon}\right) r^{1-\varepsilon}$$

and the prime denotes differentiation with respect to r.

Since the field H in (3.4) is a function of the magnetic moment and of the susceptibility χ, the expression obtained should correspond to the Migdal equation of state[9] defined by the function $\varphi_0(m)$ (the isocline of the family of isotherms) in the relation $H\chi^{(\beta+\gamma)/\gamma} = \varphi_0(M\chi^{\beta/\gamma})$. It follows from[9] that the coefficient of M^3 is proportional to $\chi^{-1+2\beta/\gamma}$ and that of M^5 is proportional to χ^{-1}. In the expression (3.3) the coefficient of M^3 is proportional to $\chi^{-\varepsilon/2+\varepsilon^2/54}$, which corresponds to the expression quoted, when the ε-expansions for the critical indices are substituted in the latter. The coefficient of M^5 is verified analogously. Choosing the quantity $M\chi^{\beta/\gamma}$ as the argument, we arrive at the following expression for the function $\varphi_0(m)$ in the Migdal equation:

$$\varphi_0(m) = m - m^3 + {}^1/_4 \varepsilon^2 m^5. \tag{3.5}$$

Thus, the Migdal equation has been obtained by a direct calculation.

4. NONASYMPTOTIC TERMS IN THE EQUATION OF STATE

We turn to the calculation of the nonasymptotic terms in the equation of state. We shall determine what changes occur in the isocline (3.5). As noted in Sec. 2, the contribution of the nonasymptotic terms can be determined by variation with respect to the coupling constant. In the expression (3.2), e.g., the variation is performed with respect to u_0 for constant t and φ_0'. It should be noted that, to the required accuracy, it is not necessary to take into account diagrams of higher order, since the renormalization (3.3) carried out on the magnetic moment restores the necessary order in the coupling constant. We present the expression for the magnetic field with allowance for the additional terms that arise:

$$H = rM - M^3[1 + {}^3/_2 u_1 Z_1(u_1) I_1' + {}^3/_4 u_1^2 (I_1')^2 - u_1^2 I_2'] + {}^9/_4 u_1^2 M^5 [I_1' I_1'' + {}^1/_3 I_2''] + c\{M^3[1 + 3u_1 Z_1(u_1) I_1' + {}^3/_4 u_1^2 (I_1')^2 - 3u_1^2 I_2''] - 9u_1^2 M^5 [I_1' I_1'' + {}^1/_3 I_2'']\} \tag{4.1}$$

(I_1 and I_2 are defined in (3.4)). The coefficient c is an additional scale factor that cannot be determined in the theory.

One further remark relates to the fact that the normalization coefficients in the asymptotic equation of state contain the coupling constant and, on variation with respect to the latter, mixing of the asymptotic and nonasymptotic terms occurs. Therefore, in order to determine the structure of the nonasymptotic function in the expression obtained, and the critical index Δ determining the behavior of the nonasymptotic terms, we require a knowledge of expressions proportional to the squares of logarithms (which requires an additional calculation of three-loop diagrams). It is possible, however, to make use of the fact that the index Δ is determined by the derivative of the Gell-Mann–Low function at the fixed point[6]:

$$\Delta = \nu\beta'(u_1^*) = {}^1/_2 \varepsilon - {}^{25}/_{108} \varepsilon^2, \tag{4.2}$$

which coincides with the expression obtained in[6] (here $\nu = \frac{1}{2} + \varepsilon/12 + \ldots$ is the correlation-length index). Separating out in (4.1) the terms corresponding to Δ and performing the renormalization of the coefficients, we arrive at the following expression for the equation of state:

$$H\chi^{(\beta+\gamma)/\gamma} = \varphi_0(M\chi^{\beta/\gamma}) + c\varphi_1(M\chi^{\beta/\gamma})\chi^{-\Delta/\gamma}, \tag{4.3}$$

In (4.3) the function $\varphi_0(m)$ is determined as before by the relation (3.5), and $\varphi_1(m)$ is equal to

$$\varphi_1(m) = m^3 - \varepsilon^2 m^5. \tag{4.4}$$

It should be noted that the convergence of the function $\varphi_1(m)$ in ε is worse than that of the critical indices and the asymptotic function $\varphi_0(m)$.

As can be seen from (4.3), the contribution of the nonasymptotic terms has been found to be related in a natural way to the magnitude of the susceptibility of the system. The appearance of the additional terms in the equation of state must be taken into account in comparisons with the experimental data; otherwise, splitting of the experimental points on the graph of the dependence of $H\chi^{(\beta+\gamma)/\gamma}$ on $M\chi^{\beta/\gamma}$ will occur. Inasmuch as the ε-expansion gives only approximate values of the indices, the quantity Δ must be regarded as an adjustable parameter.

From (4.3) it follows, in particular, that the susceptibility of the system in zero field is determined by an expression of the form

$$\chi(t) = D_0 t^{-\gamma}(1 + D_1 t^{\Delta}), \tag{4.5}$$

which was obtained earlier in[6]. Analogous corrections also arise in other quantities—e.g., in the dependence of the specific heat and spontaneous magnetic moment. As the transition point is approached, when these terms can be neglected, we obtain the usual asymptotic dependences and the expression (4.3) goes over into Migdal's asymptotic equation of state.

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Interference nuclear acoustic resonance in crystals with a cooperative Jahn-Teller effect

B. G. Vekhter, M. D. Kaplan, and V. A. Shutilov

Leningrad State University
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The absorption by nuclear spins of an ultrasonic wave whose direction of propagation and polarization correspond to the cooperative Jahn-Teller macrodeformation effect is investigated in crystals of the $TmVO_4$ type. A dispersion equation that describes the coupling between electron-phonon modes and nuclear spins due to the hyperfine interaction of the dipole type is obtained by the Green's function method. It is shown that resonance absorption occurs in the case $T < T_c$, with an intensity proportional to $H_x^2 H_z^2$ (H_z is the projection of the magnetic field vector on the crystallographic axis c). The resonance is of an interference type. Interference of the absorption contributions of the quasi-nuclear and quasi-phonon spectrum branches produces an asymmetry of the resonance curve.

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The method of acoustic nuclear resonance (ANR) was successfully applied to the study of the dynamic interaction of atomic nuclei with internal fields in crystals.[1–3] One of the forms of such interaction is the dipole interaction of the magnetic moment of the nucleus with the local magnetic field of a paramagnetic ion, modulated by lattice vibrations. In crystals with the cooperative Jahn–Teller effect (CJTE),[4,5] the indicated hyperfine interaction, together with the electron–phonon interaction, leads to the coupling of the subsystem of nuclear spins with the electron and phonon subsystems. Since the interaction of the electron states with the lattice is appreciable in Jahn–Teller crystals as a consequence of orbital degeneracy of the ground state of the ions, the nuclear spin–phonon coupling caused by the electrons can be very effective. For this reason, it turns out to be possible to obtain information on the dynamic electron–phonon coupling by ultrasonic studies of the subsystem of nuclear spins in crystals with CJTE, as well as by changes in the state of the electron subsystem due to structural phase transitions that are characteristic of Jahn–Teller crystals. Moreover, crystals with a fundamental non-Kramers doublet of Jahn–Teller ions are characterized by a peculiar combination of elastic and magnetic properties, as a consequence of the mutual suppression of distortion of the crystal lattice and the magnetic moment, caused by the external (or internal) magnetic field.[6,7] The mutual suppression of the structural and magnetic orderings leads to singularities of the temperature and field dependence of the nuclear absorption of ultrasound, caused by the hyperfine interaction.

So far, CJTE has been most widely investigated in the rare-earth vanadates, arsenates and phosphates.[5] In the present paper we consider sound absorption by nuclei in crystals of the $TmVO_4$ type (local symmetry D_{4h}, the ground state of the Tm^{3+} ion is a non-Kramers doublet, and the nuclear spin of Tm^{169} is $I = \frac{1}{2}$).

1. The interaction operator of the electrons with the lattice vibrations in such crystals is of the form

$$\mathcal{H}' = \sum_{mx} V_{mx}(b_x^+ + b_x)\sigma_z^m,$$

where σ_z^m is the electron operator on functions of the fundamental doublet, b is the operator of the phonon field, m enumerates the sites, and x is the wave vector and branch of phonons. Since only the z component of the orbital momentum is conserved in systems with symmetry D_{4h}, the hyperfine dipole interaction of the magnetic moments of electrons and nuclei at a single site can be written in the form

$$\mathcal{H}'' = -B\sum_m I_z^m \sigma_y^m.$$