Equation of state and universal combinations of thermodynamic critical amplitudes in the Ising impurity model

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A field-theory approach is used in a study of the critical thermodynamics of a slightly disordered Ising model in a $(4-\varepsilon)$-dimensional space. The equation of state is calculated in the second-order Khmel'nitskiĭ $\sqrt{\varepsilon}$ expansion. This equation of state is then used to find universal combinations of the thermodynamic critical amplitudes. Estimates of the quantities obtained in the three-dimensional space are given.

Much attention is currently being given to studies of the influence of immobile (frozen) nonmagnetic impurities on the critical behavior of spin systems.[1] The renormalization group (RG) technique[2,3] was first used to consider this problem in Refs. 4, 5, and 6. The critical exponents of an m-vector impurity model with a frozen disorder were calculated in Refs. 4 and 5 for $m>1$ in the first and second orders of the ε expansion[3] (here, $\varepsilon = 4-d$, where d is the dimensionality of space). It was shown for the first time in Ref. 6 that in the case of a disordered Ising model ($m=1$) the parameter of the expansion in the vicinity of $d=4$ is $\sqrt{\varepsilon}$. This is due to degeneracy of the relevant RG equations considered in the single-loop approximation. Later it was pointed out in Refs. 7 and 8 that the numerical coefficients obtained in Ref. 6 for the first terms of the $\sqrt{\varepsilon}$ expansion for the critical exponents are subject to some inaccuracies, and the correct expressions were given there. The next order of the $\sqrt{\varepsilon}$ expansion for the critical exponents of the impurity Ising model was obtained[9,10] using a three-loop approximation. However, definite conclusions about the numerical values of the critical exponents for the three-dimensional space were difficult to obtain on the basis of the short $\sqrt{\varepsilon}$-expansion series given in Refs. 9 and 10.

The first attempts to calculate the critical exponents of disordered systems directly in the three-dimensional space were reported in the early eighties.[11–14] A field-theory approach to the three-dimensional problem[15] was used in Ref. 11 in the three-loop approximation to calculate the RG functions and the critical exponents for the impurity Ising model. Asymptotic series of the renormalized form of perturbation theory were not summed in Ref. 11. Moreover, it was found recently[16,17] that the expressions for RG β functions given in Ref. 11 were inaccurate. The RG functions were calculated in Ref. 13 for a slightly disordered m-vector model on the assumption that $d=3$ and $d=2$; this was done using the two-loop approximation. The expansions were summed by a simple procedure of the Padé–Borel type, which made it possible to obtain more reliable values of the critical exponents. Summation of the RG functions found in Ref. 11 was carried out in Ref. 14. In spite of the fact that the critical exponents given in Ref. 14 were calculated using incorrect expressions for the β functions, they were numerically close to the values obtained using the field-theory approach in Ref. 16 (three-loop approximation) and in Ref. 17 (four-loop approximation). The critical behavior of disordered Ising systems was investigated in Ref. 12 by the scaling field method, based on the exact RG equation obtained by Wilson and Kogut.[3] Calculations were carried out in the range of the dimensions of space $2.8 \leqslant d \leqslant 4$. The shortcoming of the approach used in Ref. 12 was a low precision of the critical exponent η of the pair correlation function.

The critical behavior of disordered spin systems at temperatures below the critical value had been investigated much less. The equation of state and the correlation functions as well as the dynamics of a "dilute" m-vector model were first investigated in Ref. 18. Some of the results given there on the static pair correlation function were reviewed and supplemented in Ref. 19. The single-loop approximation of the equation of state was used in Ref. 20 to obtain the leading terms of the $\sqrt{\varepsilon}$ expansion describing universal relationships between the critical amplitudes of the impurity Ising model.

The critical behavior of disordered systems has been the subject of many experimental investigations (for reviews see Refs. 21–23 and the literature cited there). The problem of the influence of frozen nonmagnetic impurities on a second-order phase transition in a spin system was however found to be very difficult to tackle experimentally. Over a period of years it was found that dilute magnetic materials exhibit a broadening of phase transitions. This could be related to real physical processes occurring in a given system or due to imperfections of the investigated samples. The problem was solved only in the early eighties when it became possible to grow high-quality crystals suitable for experimental investigations.[22] It is now fully accepted[22–28] that, in agreement with the theoretical predictions, dilute Ising magnetic materials exhibit a narrow (and not a broadened) second-order phase transition with critical exponents and critical amplitudes clearly different from the corresponding quantities for ordered Ising systems. One should, however, point out that the interpretation of the experimental results is in some cases ambiguous.[29–31] In particular, this applies to the determination of the correct ratio of the critical amplitudes of the magnetic specific heat A_+/A_-.

The values of the critical exponents obtained experimentally[24–28] are, in principle, in agreement with the corresponding theoretical estimates obtained for the $d=3$ case.[12–14,16,17] The values of the universal ratios of the critical amplitudes found experimentally were compared in Refs. 22, 23, 25, and 26 with the results of a theoretical calculation reported in Ref. 20. However, the calculations of Ref. 20 were carried out in the lowest order of the $\sqrt{\varepsilon}$ expansion

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and were highly unreliable.

We shall calculate the equation of state of a slightly disordered Ising system using the second order of an expansion in powers of $\sqrt{\varepsilon}$. We shall then apply the equation of state to find the universal combinations of the thermodynamic critical amplitudes in the vicinity of $d=4$. We shall propose estimates of these quantities in the three-dimensional space. In particular, we shall show that the universal ratio of the critical amplitudes of the magnetic specific heat obeys the inequality $A_+/A_- <0$.

1. EFFECTIVE HAMILTONIAN

In the presence of an external magnetic field h the impurity Ising model[1,32] is described by the Hamiltonian

$$\mathscr{H}=-\frac{1}{2}\sum_{\mathbf{r}_A,\mathbf{r}_B} J_{AB}s_As_B-h\sum_{\mathbf{r}_A} s_A. \quad (1)$$

Here, and $\mathbf{r}_B$ are the radius vectors of the sites in a d-dimensional regular lattice occupied by magnetic atoms. The total number of magnetic atoms is M and they are modeled by spins s_A, s_B,... which assume the values ± 1. If the total number of the lattice sites is N, then $N-M$ sites are occupied by nonmagnetic impurities or are vacant. In an analysis of the impurity Ising model it is assumed that the concentration of magnetic atoms $p=M/N$ is close to unity. In a system with an uncorrelated frozen disorder all the magnetic and nonmagnetic atoms are distributed at random between the lattice sites and are rigidly pinned in a certain fixed spatial configuration. The spins s_A and s_B located at the sites with the radius vectors $\mathbf{r}_A$ and $\mathbf{r}_B$ interact via a ferromagnetic translation-invariant short-range exchange integral $J_{AB}=J(|\mathbf{r}_A-\mathbf{r}_B|)>0$, where $J_{AA}\equiv 0$. It is assumed that there is no interaction between the magnetic and nonmagnetic subsystems.

In describing the thermodynamic properties of a system we must calculate first the configurational average of the free energy[1] $F=-T\langle \ln Z_c\rangle_c$, where $Z_c=\mathrm{Sp}\,\exp(-\beta\mathscr{H})$ is the partition function of a certain spatial configuration. In the expressions given above the absolute temperature is denoted by T and its reciprocal is $\beta=T^{-1}$; it is assumed that the Boltzmann constant is unity. The symbol Sp denotes the operation of summing over all the M states of the spin variables s_A, s_B,... .

The problem under discussion has been frequently tackled by the replica method,[33] which makes it possible to alter the order of the thermodynamic and configurational averaging procedures. In this method the logarithm of the configuration-dependent partition function $\ln Z_c$ is represented by a boundary $\lim_{n\to 0} n^{-1}(Z_c^n-1)$, the value of Z_c^n is averaged over the various configurations, and the free energy of the system is described by

$$F=-T\lim_{n\to 0} n^{-1}(\langle Z_c^n\rangle_c-1).$$

In the case of the model described by Eq. (1) the nth power of the partition function is

$$Z_c^n=\Big[\prod_{\alpha=1}^n \mathrm{Sp}^{(\alpha)}\Big]\exp\Big[\frac{\beta}{2}\sum_{\mathbf{r}_A,\mathbf{r}_B}J_{AB}\sum_{\alpha=1}^n s_A^{(\alpha)}s_B^{(\alpha)} +\beta h\sum_{\mathbf{r}_A}\sum_{\alpha=1}^n s_A^{(\alpha)}\Big]. \quad (2)$$

Here, $\alpha=1,\ldots,n$ is the replica index and for each value of α we have $s^{(\alpha)}=\pm 1$. Application to Eq. (2) of the Stratonovich–Hubbard version of the Gaussian transformation, summation over the spin variables, and configurational averaging of the resultant expression for Z_c^n by a cumulant expansion yield the following functional representation for the free energy in the impurity Ising model:

$$F=-T\lim_{n\to 0} n^{-1}\Big\{\mathrm{const}\int(d\phi)\exp(-\mathscr{H}[\phi])-1\Big\}, \quad (3)$$

where

$$\mathscr{H}[\phi]=\int d^d\mathbf{r}\Big\{\frac{1}{2}\sum_{\alpha=1}^n[(\nabla\phi_\alpha)^2+m_0^2\phi_\alpha^2] +\frac{u_0}{4!}\Big(\sum_{\alpha=1}^n\phi_\alpha^2\Big)^2+\frac{v_0}{4!}\sum_{\alpha=1}^n\phi_\alpha^4-H\sum_{\alpha=1}^n\phi_\alpha\Big\}. \quad (4)$$

Here, $\mathscr{H}[\phi]$ is a translation-invariant Ginzburg–Landau–Wilson effective Hamiltonian whose critical behavior in the limit $n\to 0$ is formally identical with the critical behavior of the impurity Ising model of Eq. (1) (see Ref. 7). The vector field $\vec{\phi}=\vec{\phi}(\mathbf{r})$ has n components ϕ_α, where $\alpha=1,\ldots,n$:

$$\vec{\phi}=\sum_{\alpha=1}^n \phi_\alpha \mathbf{e}_\alpha^{(0)}, \quad (5)$$

where $\{\mathbf{e}_\alpha^{(0)}\}$ are the unit vectors in the fundamental coordinate system; m_0^2 is the "free mass" which is a linear function of temperature; u_0 and v_0 are the unrenormalized (bare) coupling constants which obey $u_0<0$ and $v_0>0$ (Ref. 7). In the last term of the effective Hamiltonian (4) the external field H is related in the same manner to all the components of the field variable $\vec{\phi}$ [see Eq. (2)]. This relationship implies that in the ordered phase at temperatures $T<T_c$ (T_c is the critical temperature) all the components of the field ϕ_α, where $\alpha=1,\ldots,n$, have the average values $\bar{\phi}$ equal to one another, i.e., the "magnetization vector" $\vec{\phi}$ is then oriented along the direction $(1,\ldots,1)$. An ordered phase of this type is possible in a model with the cubic anisotropy (cubic model),[34,35] described by the effective Hamiltonian of the ϕ^4 type, which is formally identical with that given by Eq. (4).

It is convenient to rotate the system of the fundamental coordinates $\{\mathbf{e}_\alpha^{(0)}\}\to\{\mathbf{e}_\alpha\}$ in such a way that one of the old fundamental unit vectors, for example $\mathbf{e}_1^{(0)}$, becomes the unit vector $\mathbf{e}_1$ directed parallel to the magnetization vector $(\vec{1,\ldots,1})$.[35] This results in a linear transformation of the field $\vec{\phi}\to\varphi$ and the effective Hamiltonian of Eq. (4) becomes

$$\mathscr{H}[\varphi]=\frac{1}{2}\sum_{\alpha=1}^{n}[(\nabla\varphi_\alpha)^2+m_0^2\varphi_\alpha^2]$$

$$+\frac{u_0}{4!}|\varphi|^4+\frac{v_0}{4!}b_{\alpha_1\ldots\alpha_4}\varphi_{\alpha_1}\ldots\varphi_{\alpha_4}-Hn^{1/2}\varphi_1. \quad (6)$$

The symbol denoting the d-dimensional spatial integration is omitted and so is the symbol denoting summation of repeated indices. This simplified notation will be used from now on. The tensor $b_{\alpha_1\ldots\alpha_\kappa}$ is related to elements $e^\alpha_\beta=(\mathbf{e}_\beta,\mathbf{e}^{(0)}_\alpha)$ of the matrix describing rotation of the coordinate system and it is given by

$$b_{\alpha_1\ldots\alpha_k}=\sum_{\alpha=1}^{n}e_{\alpha_1}^{\alpha}\ldots e_{\alpha_k}^{\alpha}. \quad (7)$$

An external magnetic field H is now related only to one component φ_1 of the field variable φ.

The next step is the separation in the effective Hamiltonian of Eq. (6) of a longitudinal component of the field φ_1 and then determination of the average value of φ_1 (see, for example, Refs. 36–38 and the bibliography given there): φ_1 is represented by a sum $L+M_0$, where $M_0=\bar{\varphi}_1$ is the magnitude of the magnetization and L is the deviation of φ_1 from the average value M_0. After these algebraic transformations, we can now describe the effective Hamiltonian by a sum:

$$\mathscr{H}[L,\psi]=\mathscr{H}_0(M_0)+\mathscr{H}_G[L,\psi]+\mathscr{H}_{int}[L,\psi]. \quad (8)$$

The first term in Eq. (8) is the Landau free energy

$$\mathscr{H}_0(M_0)=\frac{1}{2}m_0^2M_0^2+\frac{u_0}{4!}M_0^4+\frac{v_0}{4!}n^{-1}M_0^4-Hn^{1/2}M_0. \quad (9)$$

The second term, which is the Gaussian part of the effective Hamiltonian, includes contributions which are quadratic functions of the field variables:

$$\mathscr{H}_G[L,\psi]=\frac{1}{2}[(\nabla L)^2+r_{0L}L^2]+\frac{1}{2}\sum_{i=2}^{n}[(\nabla\psi_i)^2+r_{0T}\psi_i^2]. \quad (10)$$

Here, L is the longitudinal component of the field, whereas ψ_i represents the transverse components $(i=2,\ldots,n)$; r_{0L} and r_{0T} are the unrenormalized reciprocals of the longitudinal and transverse susceptibilities:

$$r_{0L}=m_0^2+\frac{1}{2}u_0M_0^2+\frac{1}{2}v_0n^{-1}M_0^2,$$
$$r_{0T}=m_0^2+\frac{1}{6}u_0M_0^2+\frac{1}{2}v_0n^{-1}M_0^2. \quad (11)$$

The last term in Eq. (8) $\mathscr{H}_{\rm int}[L,\psi]$ contains a number of contributions which are cubic and quartic functions of the field variables and we shall deal with this term using perturbation theory:

$$\mathscr{H}_{int}[L,\psi]$$
$$=\frac{u_0}{4!}(|\psi|^2+L^2)^2+\frac{v_0}{4!}\Big(\frac{L^4}{n}+\frac{6}{n}L^2|\psi|^2+\frac{4L}{n^{1/2}}b_{ijk}\psi_i\psi_j\psi_k$$
$$+b_{i_1\ldots i_4}\psi_{i_1}\ldots\psi_{i_4}\Big)$$
$$+\frac{u_0M_0}{3!}L(|\psi|^2+L^2)+\frac{v_0M_0}{3!}\Big(\frac{L^3}{n}+\frac{3L}{n}|\psi|^2$$
$$+\frac{1}{n^{1/2}}b_{ijk}\psi_i\psi_j\psi_k\Big)$$
$$+\Big[\Big(m_0^2+\frac{u_0}{3!}M_0^2+\frac{v_0}{3!}n^{-1}M_0^2\Big)M_0-Hn^{1/2}\Big]L, \quad (12)$$

where

$$|\psi|^2=\sum_{i=2}^{n}\psi_i^2. \quad (13)$$

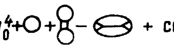
A similar expression for the effective Hamiltonian was derived in Ref. 35 using slightly different notation.

Equations (8)–(12) are the starting points in calculation of the thermodynamic potential $\Gamma(M_0)$ and of the equation of state of the impurity Ising model presented below.

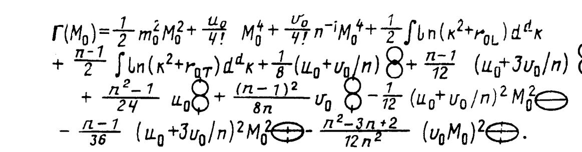
2. EQUATION OF STATE

There are two main approaches to the derivation of the equation of state starting from the effective Hamiltonian shown above. The first consists of an expansion of the equation $\bar{L}=0$ (vanishing of the average value of the field L follows directly from its definition) by the Feynman diagram technique. This approach was used in Refs. 36–38 and elsewhere to study critical thermodynamics of pure isotropic Ising and Heisenberg systems, and also in Refs. 34, 35, and 20 where the model of Eq. (4) was employed in the single-loop approximation. The second approach utilizes the methods of functional integration, developed in quantum field theory to describe spontaneous symmetry breaking. A detailed account of the method for calculating the effective potential $\Gamma(M)$ by expansion, using a number of loops in Feynman diagrams, was given in Refs. 39 and 40 together with references to earlier work on quantum field theory. This approach was used in Ref. 41 to calculate universal combinations of the critical amplitudes employing an n-component Heisenberg model accurate to within ε^2. A two-loop approximation was employed in Ref. 41 to write down, in a diagonal form, the equation of state for the Heisenberg model,[1)] which leads to familiar expressions first obtained in Refs. 42 and 37 (see also Refs. 38 and 39). A field-theory approach employed in Ref. 41 will be used below to obtain a similar representation of the equation of state for the model described by Eq. (4). An explicit expression for the equation of state describing the impurity Ising model will be obtained in a limiting case when $n\to 0$.

In the two-loop approximation the effective potential, which is a function of the magnetic moment and of the absolute temperature, can be represented diagramatically as follows:[39,40]

$$\Gamma(M_0)=\frac{1}{2}m_0^2M_0^2+\frac{u_0}{4!}M_0^4+\frac{v_0}{4!}n^{-1}M_0^4$$  + const. (14)

The ring in Eq. (14) represents the contribution of a Gaussian integral with an integrand $\exp(-\mathscr{H}_G[L,\psi])$. Vertices with three and four lines in the last two Feynman diagrams represent terms of the ϕ^3 and ϕ^4 type from $\mathscr{H}_{\text{int}}[L,\psi]$. The constant in Eq. (14) denotes the same expression, but with the minus sign when $M_0 = 0 \gg$; it is independent of M_0 and, consequently, does not influence the equation of state. We shall omit it. The results of calculations carried out using standard rules of the Feynman diagram technique can be represented as follows:



(15)

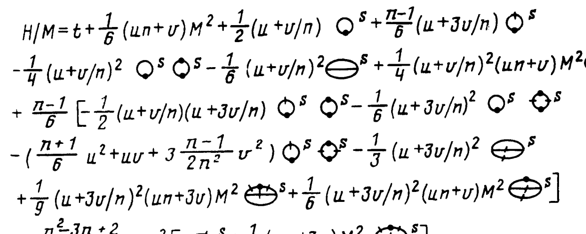
The diagrams which occur in the above expression are Feynman integrals in which the continuous lines represent propagators $(k^2 + r_{0L})^{-1}$, and the crossed lines represent $(k^2 + r_{0T})^{-1}$.

Differentiation of the thermodynamic potential $\Gamma(M_0)$ with respect to the magnetic moment yields the equation of state:

$$H = \frac{d\Gamma(M_0)}{dM_0}, \tag{16}$$

which includes unrenormalized coupling constants u_0 and v_0, the mass m_0^2, the moment M_0, as well as the Feynman integrals which are characterized by ultraviolet divergences when $d = 4$. These divergences can be removed by including counter terms that appear as a result of renormalization of the coupling constants, of the mass, and of the field. This can be achieved by substituting, in the unrenormalized equation of state, expressions for the unrenormalized quantities u_0, v_0, m_0^2, and M_0 expressed in terms of the corresponding renormalized values of the coupling constants u and v, of the reduced temperature t, and of the magnetic moment M. These relationships are derived using the normalization conditions from the mass-free field theory of Ref. 39. This renormalization method makes it possible to utilize later the values of the coordinates of a fixed point (u^*, v^*) calculated in the second order of the $\sqrt{\varepsilon}$ expansion in Refs. 9 and 10.

After subtracting the divergences which appear in the $d = 4$ case, we find that the equation of state (16) can be rewritten in the form[2)]



(17)

where $t = (T - T_c)/T_c$ is the reduced temperature. In contrast to Eq. (15), each diagram (with the index s) in the above expression represents a finite (in the $d = 4$ case) combination of diverging integrals. These combinations are presented in Fig. 1. The renormalized reciprocals of the longitudinal and transverse susceptibilities now become [compare with Eq. (11)]:

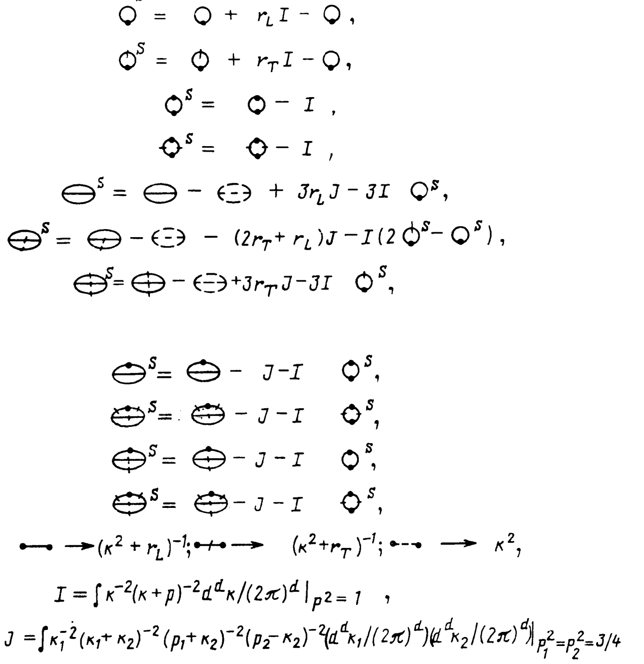


FIG. 1. Finite (for $d = 4$) combinations of Feynman integrals, which occur in the renormalized equation of state (17).

$$r_L = t + \frac{1}{2} unM^2 + \frac{1}{2} vM^2, \qquad r_T = t + \frac{1}{6} unM^2 + \frac{1}{2} vM^2. \tag{18}$$

If $v = 0$, Eq. (17) yields the equation of state for an n-component Heisenberg model (see Fig. 5 in Ref. 41), which in turn reduces to the equation of state of the Ising model if $n = 1$.

We can obtain the equation of state of the impurity Ising model explicitly by going to the limit $n \to 0$ in Eq. (17), replacing u and v by their values u^* and v^* at a fixed point, and utilizing the explicit expressions for the combinations of the integrals represented by the diagrams in Eq. (17). The procedure of going to the limit $n \to 0$ in Eq. (17) is not trivial. This equation includes contributions containing factors such as $1/n$ and $1/n^2$. It is therefore necessary to expand the coefficients in front of $1/n$ and $1/n^*$, and these coefficients are fairly cumbersome combinations of Feynman integrals; the expansion is carried out in terms of small values of n up to the first and second orders, respectively. All the negative degrees of n then cancel out. In the course of these calculations we can drop constants (nonlogarithmic terms) of the order of ε, since this simply alters the scale of the variables which can occur in the equation of state of Ref. 38.

A mixed $(u^* \neq 0, v^* \neq 0)$ fixed point, stable for $n = 0$ and for sufficiently low values of ε, has the following coordinates[9,10]

$$u^* = -3(6/53)^{1/2}\varepsilon^{1/2} + 18\varepsilon[110 + 63\zeta(3)]/(53)^2, \qquad v^* = 4(6/53)^{1/2}\varepsilon^{1/2} + 72\varepsilon[19 + 21\zeta(3)]/(53)^2, \tag{19}$$

where $\zeta(3)$ is the Riemann zeta function whose value is $\zeta(3) \approx 1.202$.

In the limit $n \to 0$ the longitudinal and transverse reciprocals of the susceptibility r_L and r_T of Eq. (18) are equal:

at the end of the calculations we obtain just one reciprocal susceptibility

$$r = t + \frac{1}{2} v^* M^2, \tag{20}$$

as expected for the Ising system. Combinations of the integrals in Fig. 1 then simplify greatly since now every line (continuous or crossed) corresponds to just one Feynman propagator $(k^2 + r)^{-1}$. The equation of state includes contributions of the following integrals obtained when

 $^{S} = \frac{1}{2} r(1+\ln r),$

 $^{S} = -1 - \frac{1}{2}\ln r,$

 $= \frac{1}{4r},$

 $^{S} = -\frac{3}{8} r \ln^2 r + \text{const},$ (21)

 $^{S} = \frac{1}{4}\ln r + \frac{1}{8}\ln^2 r + \text{const}.$

Finally, the equation of state (which is not universal) for the impurity Ising model reduces to the unexpectedly compact form

$$\frac{H}{M} = t + \frac{1}{6} y + \lambda\left[t(1+\ln r) - \frac{1}{2} y\right]$$

$$+\lambda^2 \left\{\left[(151r + 57y - 126\zeta(3)t)/53 + \frac{y^2}{4r}\right]\ln r + \frac{1}{8} t \ln^2 r\right\}. \tag{22}$$

Here, we have $y = v^* M^2$, r is given by Eq. (20), and λ is the effective parameter of the expansion proportional to $\sqrt{\varepsilon}$:

$$\lambda = \frac{1}{9}(6/53)^{1/2}\varepsilon^{1/2} \approx 0{,}168\varepsilon^{1/2}. \tag{23}$$

3. EQUATION OF STATE AND UNIVERSAL COMBINATIONS OF CRITICAL AMPLITUDES

The equation of state (22) describes correctly the behavior of various thermodynamic quantities near a critical point (at reduced temperatures ($|t| \ll 1$) in a number of special cases given below[43] (see also Ref. 38).

I. At temperatures above the critical value, when $t > 0$, in the limit $H \to 0$ the magnetic moment M also tends to zero and the ratio H/M is equal to the reciprocal of the isothermal magnetic susceptibility

$$\chi_+^{-1} = \lim_{\substack{H\to 0\\ M\to 0}} \frac{H}{M} = C_+^{-1} t^{\gamma}, \tag{24}$$

where C_+ and γ are the critical amplitude and critical power exponent in the expression for the susceptibility. In the limit $M \to 0$ the right-hand side of Eq. (22) can indeed reduce to[3)]

$$\chi_+^{-1} = (1+\lambda) t^{\gamma} + O(\varepsilon^{3/2}) \tag{25}$$

with the correct exponent γ given by[9,10]

$$\gamma = 1 + \lambda - 2\lambda^2 [63\zeta(3) - 49]/53. \tag{26}$$

II. Along the critical isotherm characterized by $t = 0$ the relationship between an external magnetic field and the magnetic moment is expressed in terms of a critical exponent δ:

$$H = DM^{\delta}. \tag{27}$$

Changes of the scales of the quantities H and M ($v^* H \to H$, $v^* M \to M$) yields the following expression, derived from Eq. (22):

$$H = \frac{1}{6}(1 - 3\lambda - 18\lambda^2 \ln 2) M^{\delta} + O(\varepsilon^{3/2}), \tag{28}$$

where

$$\delta = 3 + \frac{54}{53}\varepsilon. \tag{29}$$

The expression (29) for δ is readily obtained with the aid of the scaling relationship $\delta = (d + 2 - \eta)/(d - 2 + \eta)$ (see, for example, Ref. 39) using the values of the Fisher critical exponent η taken from Refs. 9 and 10.

III. On a coexistence curve, defined by $H = 0$ and $t < 0$, the magnetization in the vicinity of the critical point is proportional to $|t|^{\beta}$:

$$M = B(-t)^{\beta}. \tag{30}$$

This type of the $M(t)$ dependence is obtained by solving Eq. (22) with the left-hand side equated to zero, which yields M^2:

$$M^2 = 3(1 + 4\lambda + 18\lambda^2)(-2t)^{2\beta} + O(\varepsilon^{3/2}), \tag{31}$$

where

$$\beta = \frac{1}{2} + \frac{1}{2}\lambda - \lambda^2[428 + 63\zeta(3)]/53. \tag{32}$$

The expansion (32) for the critical exponent of the magnetization is readily obtained from Refs. 9 and 10 by scaling relationships.

Each of the coefficients of proportionality which occur in Eqs. (25), (28), and (31) is a nonuniversal quantity. However, a combination of the thermodynamic critical amplitudes C_+, D, and B (see Refs. 41, 44, and 45 as well as papers cited there) is universal and it is given by

$$R_\chi = C_+ D B^{\delta - 1}. \tag{33}$$

In the adopted model we have

$$R_\chi = 2^{2\beta - 1}[1 + 6\lambda^2(1 + 3\ln 3)] + O(\varepsilon^{3/2}). \tag{34}$$

The equation of state (22) can be used to calculate also a universal ratio C_+/C_- of the critical amplitudes of the magnetic susceptibility. This can be done using the relationship $\chi_-^{-1} = \partial H/\partial M$ valid in the range $t < 0$ and a nonzero magnetization M found on the coexistence curve, writing down χ_-^{-1} in the form $C_-^{-1}|t|^{\gamma}$, and dividing the resultant constant of proportionality by C_+^{-1} from Eq. (25):

$$\frac{C_+}{C_-} = 2^{\gamma}\left\{1 - \frac{3}{2}\lambda + 3\lambda^2[2507 + 252\zeta(3)]/212\right\} + O(\varepsilon^{3/2}). \tag{35}$$

A universal equation of state for slightly disordered Ising systems can be obtained by writing down in the form of a scaling law (see Ref. 46 and the papers cited there):

$$HM^{-\delta} = \mathcal{F}(t/M^{1/\beta}). \tag{36}$$

Using then the equation of state (22) to obtain the dependence of $HM^{-\delta}$ on a variable $x = t/M^{1/\beta}$, we obtain a homogeneous function $\mathscr{F}(x)$ from Eq. (36) and this function is in the form of a $\sqrt{\varepsilon}$ expansion:

$$\mathscr{F}(x)=1+x+\lambda\mathscr{F}_1(x)+\lambda^2\mathscr{F}_2(x), \tag{37}$$

where

$$\mathscr{F}_1(x)=x-3+x\ln(x+3),$$

$$\mathscr{F}_2(x)=\{x[151-126\zeta(3)]/53+15+9/(x+3)\}$$
$$\times\ln(x+3)+\frac{x}{2}\ln^2(x+3). \tag{38}$$

The equation of state (36) allows arbitrary changes in the scales of the variables H, M, and t. We can therefore go over to new thermodynamic variables whose scales are fixed by the standard normalization conditions[44,45,38,39] on the critical isotherm and on the coexistence curve [this alters the nature of the function $\mathscr{F}(x)$ so that it becomes $\mathscr{F}(x)\to f(x)$]:

(I) if $t=0$, then $h=m^\delta$, i.e., $f(0)=1$;

(II) if $h=0$, $t<0$, then $m=(-t)^\beta$, i.e., $f(-1)=0$. (39)

Transition to the relevant function

$$f(x)=1+x+\lambda f_1(x)+\lambda^2 f_2(x) \tag{40}$$

is then performed using the following relationships from Ref. 42:

$$f_1(x)=\mathscr{F}_1(x)-(1+x)\mathscr{F}_1(0)+x\mathscr{F}_1(-1),$$
$$f_2(x)=\mathscr{F}_2(x)-(1+x)\mathscr{F}_2(0)+x\mathscr{F}_2(-1)$$
$$-\mathscr{F}_1(0)f_1(x)-x\mathscr{F}_1(-1)[\mathscr{F}_1'(x)-\mathscr{F}_1'(-1)], \tag{41}$$

where $\mathscr{F}_1'$ denotes a derivative of the function $\mathscr{F}_1$ from Eq. (38).

Finally, the universal normalized equation of state for the impurity Ising model is given by the following expressions:

$$hm^{-\delta}=f(t/m^{1/\beta}),\ f(x)=1+x+\lambda f_1(x)+\lambda^2 f_2(x), \tag{42}$$

where

$$f_1(x)=x\ln\frac{x+3}{2},$$

$$f_2(x)=\frac{2}{53}[49-63\zeta(3)]x\ln\frac{x+3}{2}$$
$$+15[\ln(x+3)-(1+x)\ln 3+x\ln 2]$$
$$+\frac{x}{2}[\ln^2(x+3)-\ln^2 2]$$
$$+\frac{9}{x+3}\ln(x+3)-3(1+x)\ln 3+\frac{9}{2}x\ln 2$$
$$-x\ln 2\ln\frac{x+3}{2}-\frac{3}{2}x\frac{x+1}{x+3}\ln 2-6x\frac{x+1}{x+3}. \tag{43}$$

The first three terms of the universal function (42), $1+x+\lambda f_1(x)$, were derived in Ref. 20 by a different approach.

Exactly as in the case of the Ising model for a pure material ("pure Ising model"), the function $f(x)$ is analytic in the vicinity of $x=0$ and it can be represented by an expansion[43]

$$f(x)=\sum_{i=0}^{\infty}h_i x^i. \tag{44}$$

The universal coefficients h_i are readily calculated using Eqs. (42) and (43) for the function $f(x)$. The first three of them are

$$h_0=1,$$
$$h_1=1+\lambda\ln\frac{3}{2}+\lambda^2\left\{4-\frac{9}{53}[101+14\zeta(3)]\ln\frac{3}{2}+\frac{1}{2}\ln^2\frac{3}{2}\right\},$$
$$h_2=-\frac{1}{3}\lambda\left\{1+2\lambda\left[(49-63\zeta(3))/53+\ln\frac{3}{2}-4\right]\right\}. \tag{45}$$

As in the case of the pure Ising model, at high values of $x(x\to\infty)$ the function $f(x)$ can be described by an asymptotic expansion proposed by Griffiths:[43]

$$f(x)=\sum_{n=1}^{\infty}\eta_n x^{\beta(\delta+1-2n)}=\sum_{n=1}^{\infty}\eta_n x^{\gamma-2(n-1)\beta}. \tag{46}$$

The first three coefficients of the expansion (46) are

$$\eta_1=2^{1-2\beta}[1-6\lambda^2(1+3\ln 3)]+O(\varepsilon^{3/2}),$$
$$\eta_2=1+3\lambda+6\lambda^2\{[155-63\zeta(3)]/53-3\ln 3\}+O(\varepsilon^{3/2}),$$
$$\eta_3=-\frac{2}{9}\lambda\{1-\lambda[(61+126\zeta(3))/53-\ln 2]\}+O(\varepsilon^{3/2}). \tag{47}$$

The first of them,

$$\eta_1=\tilde{C}_+^{-1}, \tag{48}$$

is given by the following expression which follows from the definition of the universal amplitude of the magnetic susceptibility $\tilde{C}_+$ (Refs. 43–45)[4)]

$$\tilde{C}_+=\lim_{x\to\infty}[x^\gamma/f(x)]. \tag{49}$$

On the other hand, we have

$$\tilde{C}_+=R_\chi, \tag{50}$$

since—by definition [see Eq. (33)]—we have $R_\chi=\tilde{C}_+\tilde{D}\tilde{B}^{\delta-1}$, and it follows from the normalization rules of Eq. (39) that the universal critical amplitudes are $\tilde{D}=\tilde{B}=1$. The $\sqrt{\varepsilon}$ expansion for R_χ was found already above as a universal combination of the nonuniversal critical amplitudes C_+, D, and B.

The universal amplitude of the magnetic susceptibility $\tilde{C}_-$ can be calculated from the equation of state (42) using the expression[43]

$$\tilde{C}_-=\beta/f'(-1). \tag{51}$$

The explicit expressions from Eq. (43) yield

$$\tilde{C}_-=\frac{1}{2}\left\{1+\frac{3}{2}\lambda+\left[18\ln\frac{3}{2}-\frac{3}{53}(481+63\zeta(3))\right]\lambda^2\right\}. \tag{52}$$

Obviously, the ratio $\tilde{C}_+/\tilde{C}_-$ is equal to the ratio C_+/C_- in Eq. (35).

Knowing the explicit form of the universal equation of state (42), we can calculate also the universal ratio of the critical amplitudes of the magnetic specific heat using the impurity Ising model. The specific heat near a critical point is

$$c_m = (A_\pm/\alpha)|t|^{-\alpha} + C_B, \qquad (53)$$

where A_+ and A_- are the critical amplitudes corresponding to $t > 0$ and $t < 0$; α is the critical exponent of the specific heat. In the impurity Ising model we have $\alpha < 0$, and the constant in the above equation is $C_B > 0$ (Ref. 24). In the second order of expansion in $\sqrt{\varepsilon}$ (Refs. 9 and 10), we have

$$\alpha = -2\lambda + 2\lambda^2[379 + 126\zeta(3)]/53. \qquad (54)$$

In the range of variation of the critical exponent of the specific heat of interest to us, which is $-1 < \alpha < 0$, the ratio of the critical amplitudes A_+/A_- can be represented in the following form (see Ref. 47):

$$\frac{A_+}{A_-} = -\alpha^{-1}\int_0^\infty x^\alpha f''(x)\,dx \Big/ \left[f'(-1) + \alpha^{-1}f''(-1) + \alpha^{-1}\int_{-1}^{0}|x|^\alpha f'''(x)\,dx\right]. \qquad (55)$$

Here, f', f'', and f''' are the first, second, and third derivatives of the universal function $f(x)$, which occurs in the equation of state. In spite of the fact that the equation of state (42) is calculated in the second order of the $\sqrt{\varepsilon}$ expansion, the ratio A_+/A_- can be found only in the first order in $\sqrt{\varepsilon}$, since α^{-1} is of the order of $\varepsilon^{-1/2}$:

$$\frac{A_+}{A_-} = -\frac{1}{2}[1 + \lambda(3 - 2\ln 2)] = -\frac{1}{2}2^\alpha(1 + 3\lambda) + O(\varepsilon). \qquad (56)$$

The leading term of the $\sqrt{\varepsilon}$ expansion for the ratio A_+/A_-, which amounts to $-1/2$, was obtained in Ref. 20. Here, we shall simply point out that the negative value of A_+/A_- for the system under discussion is permissible, but this result will not be regarded as reliable because we have not excluded the possibility of reversal of the sign of the ratio in question in the next order of perturbation theory. It is clear from the last expression that the universal ratio A_+/A_- and the ratio obtained in the approximation following the lowest one remains negative. The structure of the expansion of A_+/A_- in terms of $\sqrt{\varepsilon}$ suggests that the ratio of the critical amplitudes remains also negative in higher orders of perturbation theory.

The last of the universal combinations of thermodynamic critical amplitudes which we shall consider here was defined in Refs. 45 and 41 as follows:

$$R_c = A_+C_+B^{-2} = \tilde{A}_+\tilde{C}_+. \qquad (57)$$

If $\alpha < 0$ (Ref. 47), then

$$\tilde{A}_+ = -\beta\int_0^\infty x^\alpha f'''(x)\,dx. \qquad (58)$$

A calculation carried out using Eq. (58) gives the following result if we use the impurity Ising model:

$$\tilde{A}_+ = \frac{\lambda}{3}2^{-2\lambda}\{1 - 2\lambda[110 + 63\zeta(3)]/53\} + O(\varepsilon^{3/2}). \qquad (59)$$

Combining the last expression with Eqs. (34) and (50), we obtain:

$$R_c = \frac{\lambda}{3}2^{-\lambda}\{1 - 2\lambda[110 + 63\zeta(3)]/53\} + O(\varepsilon^{3/2}). \qquad (60)$$

4. DISCUSSION OF RESULTS

Calculations carried out for sufficiently small deviations ε of the dimensionality of space from its upper limit are known to give a qualitatively correct description of the critical behavior of the systems of interest to us and give rise to nontrivial corrections to the classical values of the universal quantities proportional to powers of $\varepsilon \ll 1$. Series of this type diverge and the problem of finding on their basis some quantitative estimates of the physical quantities in the three-dimensional space is complex and multivalued. The simplest method used in extrapolation of the ε-expansion series to the $d = 3$ case involves derivation of various Padé approximants for these series (see, for example, Refs. 41, 45, and 48). A more complex, but a more reliable calculation method is based on the Borel summation of diverging series.[49] The application of this method to the ε expansions obtained for ordered isotropic n-vector models gives quite accurate estimates of the investigated quantities in the three-dimensional space.[50,51,48] Then, the finding of numerical estimates for combinations of critical amplitudes becomes more complex than in the case of critical power exponents.[48]

We shall now consider parts of an $\sqrt{\varepsilon}$-expansion series for the critical exponents γ [Eq. (26)], β [Eq. (32)], and α [Eq. (54)], as well as universal combinations of the thermodynamic quantities R_c [Eq. (60)], C_+/C_- [Eq. (35)], $R_\chi = \tilde{C}_+$ [Eq. (34)], $\tilde{C}_-$ [Eq. (52)], and A_+/A_- [Eq. (56)], which can generally be described by

$$f(\sqrt{\varepsilon}) = f_0 + f_1\sqrt{\varepsilon} + f_2\varepsilon. \qquad (61)$$

They obviously represent the values of these quantities in three-dimensional space. The critical exponents for $d = 3$ are calculated quite accurately in Refs. 12–14, 16, and 17. The coefficients of the expansions described by Eq. (61) in front of the powers of $\sqrt{\varepsilon}$, the absolute values of the ratios f_2/f_1, as well as the values of γ, β, and α obtained by the field-theory approach directly in the three-dimensional space (see Refs. 16 and 17) are listed in Table I.

It is clear from Table I that in the case of the critical exponents γ and α the proper sign of the correction $f_1\sqrt{\varepsilon} + f_2\varepsilon$ is identical with the sign of the coefficient in front of $\sqrt{\varepsilon}$ (this applies also to the index of the correlation length ν). The inequality $|f_2/f_1| < 2$ is then satisfied. Similar properties are exhibited by an expansion of a universal combination of the critical amplitudes R_c, which leads to

$$R_c > 0. \qquad (62)$$

However, the sign of the coefficient in front of the lowest degree of the expansion parameter $\sqrt{\varepsilon}$ does not always determine the real deviation of $f(\sqrt{\varepsilon})$ from its value f_0 in the four-dimensional space. This situation applies to the critical exponent β (and also to the Fisher exponent η). The abso-

TABLE I.

Parameter	f_0	f_1	f_2	$\lvert f_2/f_1 \rvert$	$d=3$
γ	1	0,168	−0,029	0,2	1,33
β	$^1/_2$	0,084	−0,269	3,2	0,34
α	0	−0,336	0,567	1,7	−0,01
R_c	0	0,056	−0,072	1,3	–
C_+/C_-	2	−0,272	2,166	8	–
$\tilde{C}_+$	1	0,117	0,363	3,1	–
$\tilde{C}_-$	$^1/_2$	0,126	−0,343	2,7	–
A_+/A_-	$-^1/_2$	−0,136	–	–	–

lute value of the coefficient f_2 with the opposite sign is more than three times greater than $|f_1|$, and the sign of f_2 determines the sign of the correction $f_1\sqrt{\varepsilon}+f_2\varepsilon$ to f_0. Clearly, similar properties should be exhibited also by expansions of the universal quantities C_+/C_- and $\tilde{C}_-$. It is therefore natural to draw the conclusion that in such cases the following inequalities are satisfied:

$$C_+/C_->2 \tag{63}$$

and

$$\tilde{C}_-<{}^1/_2. \tag{64}$$

Then,

$$\tilde{C}_+>1, \tag{65}$$

because this critical amplitude corresponds to a constant-sign $\sqrt{\varepsilon}$-expansion series [Eq. (61)] with positive values of f_0, f_1, and f_2. The inequality $C_+/C_->2$ is in agreement with the experimental results reported in Refs. 22–26.

A universal combination of the critical amplitudes R_c can be used to obtain a numerical estimate in the three-dimensional space. In the case of the quantity $f(\sqrt{\varepsilon}) = 1 + R_c$ the $\sqrt{\varepsilon}$ expansion is given by Eq. (61) with a nonzero value of f_0 and with the ratio $|f_2/f_1|$ less than 2. We shall apply to this expansion the simplest procedure of summation of diverging Padé–Borel series,[49] using then the Padé approximant [1/1] to obtain an analytic continuation of the Borel transform of the function $f(\sqrt{\varepsilon})$. Calculating unity from the resultant summed function and assuming that $\varepsilon = 1$, we obtain

$$R_c\approx 0{,}03. \tag{66}$$

Determination of reliable numerical values of other universal combinations of thermodynamic critical amplitudes is a more difficult task.

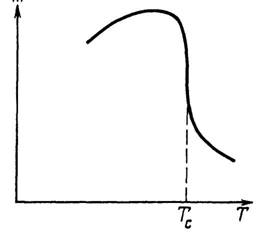


FIG. 2. Magnetic specific heat $c_m(T)$ in the case when $\alpha<0$ and $A_+/A_- <0$ [based on Fig. 6c in Ref. 30].

It is worth noting that the universal ratio of the critical amplitudes of the magnetic specific heat A_+/A_- is negative, exactly as in the principal approximation. A theoretical estimate $A_+/A_- \approx -1/2<0$ is in conflict with the results of an experimental investigation[24] where a positive value of this ratio is reported. This disagreement was already considered in Ref. 30. We point out here that this may be a consequence of the fact that the specific heat was determined experimentally outside the critical region. Another possible reason[30] may be an incorrect determination of the critical temperature: the experimental data were extrapolated in Ref. 24 on the assumption that a maximum (peak) of the magnetic specific heat corresponded to the critical temperature. We effectively excluded the possibility of obtaining a negative value of the ratio A_+/A_-. However, if the theoretically predicted inequality $A_+/A_- <0$ is satisfied, a graph of the magnetic specific heat $c_m(T)$ [see Eq. (53)] of an impurity Ising system with a small negative critical exponent α should be of the form presented schematically in Fig. 2. The critical temperature corresponds to a point of inflection $c_m(T)$, whereas the specific heat maximum occurs at a temperature different from T_c. Clearly, the problem of determination of the sign of the ratio A_+/A_- and of the profile of the maximum of the magnetic specific heat of impurity Ising systems requires precise experimental determination of the critical temperature. The critical temperature should be identified independently of measurements of the specific heat by investigation of other thermodynamic functions using the same sample. If it is found that the critical temperature is in the region of a fast fall of the specific heat, then extrapolation of the results of measurements can give a negative ratio A_+/A_- of the critical amplitudes.

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[1)] There is a misprint in Fig. 5 of Ref. 41: the factor in front of the diagram ⊖ should be $(n-1)/54$.

[2)] Simultaneously with an allowance for the counterterms, we changed the scales of the external field and of the moment: $H\to Hn^{1/2}$ and $M\to Mn^{1/2}$.

[3)] The logarithms of t are transformed here to the exponential form. A "falling" $\sqrt{\varepsilon}$ expansion can be obtained for χ_+^{-1} by expanding t^{γ} in Eq. (25) in terms of the small quantity $\sqrt{\varepsilon}$.

[4)] In contrast to the critical amplitudes, found above from the equation of state (22), the critical amplitudes deduced from the equation of state (42) are universal quantities. As is usual in the literature, these are denoted by symbols with a tilde.

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