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Renormalization-group analysis of heat-capacity critical amplitudes

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Critical amplitudes $A_\pm$ associated with the temperature (t) variation of the heat capacity $(C \sim A_\pm |t|^{-\alpha})$ are analyzed by means of renormalization-group techniques in both position and momentum spaces. We describe a mechanism according to which the amplitudes $A_\pm$ diverge as the critical exponent α approaches a nonpositive integer. In between two consecutive divergences at least one amplitude vanishes at least once. The coefficient P in the expansion $A_+/A_- \approx 1 - P\alpha + O(\alpha^2)$ is computed by means of ϵ expansion and Migdal-Kadanoff renormalization-group technique. Systems for which the critical exponent α is negative but larger than -1 exhibit either a cusped heat capacity if $A_+/A_- > 0$ or a smooth maximum in the heat capacity at a temperature other than the critical one $(T \neq T_c)$ and an infinite slope at T_c if $A_+/A_- < 0$. Implications of this observation for the interpretation of experiments on random-bond systems such as $Fe_{1-x}Zn_xF_2$ are discussed.

I. INTRODUCTION

Critical amplitudes are as important as critical exponents for the identification of the universality class of a given physical system and for the interpretation of experimental data. Unlike exponents, however, amplitudes have been studied almost entirely by means of the renormalization group in the momentum space. Only recently have studies of amplitudes by means of renormalization-group techniques in the position space been published.[1-3] This study continues and generalizes the work of Ref. 1 by considering systems with a nonsymmetric specific heat.

By continuously changing appropriate parameters such as the dimension of the order parameter or the number of states in the q-state Potts model, the critical exponent α and the critical amplitudes $A_\pm$ (the free energy $f \sim A_\pm |t|^{2-\alpha}$) can be continuously varied. In Sec. II it is shown that, quite generally, the amplitudes $A_\pm$ ($+$ and $-$ refer to above, $t>0$, and below, $t<0$, the critical temperature) diverge whenever $-\alpha$ approaches an integer, and that they diverge with the same sign if the integer is even and with opposite signs if the integer is odd. Hence, on the interval determined by two consecutive integers, one of the amplitudes expressed as a function of α will have opposite signs at the ends of this interval. Therefore, there will be (at least) one value in this interval where (at least) one amplitude is zero. The occurrence of zeros is therefore intimately linked to the occurrence of divergences of $A_\pm$. The universal ratio A_+/A_- approaches $(-1)^n$ linearly in $\alpha+n$ as α approaches $-n$, $n=0,1,2,\ldots$ We find the coefficient $P \sim 4.6$ on the expansion

$$A_+/A_- = 1 - P\alpha + O(\alpha^2)$$

for systems with α small, by considering the N-vector model in $4-\epsilon$ dimensions and varying the critical parameters by changing N at fixed ϵ. This coefficient is also determined in Sec. III, $P \sim 5$, by applying the Migdal-Kadanoff renormalization-group[4] technique to the three-dimensional q-state Potts model.

In Sec. III we also explain a *numerical* procedure for computing amplitudes after pointing out that the *analytical* "linear" approximation[3] violates the convexity of the free energy, and thus it is inadequate. The amplitudes $A_\pm$ computed with the Migdal-Kadanoff renormalization group are plotted against the exponent α which is changed by continuously varying the number of states q at fixed dimension d. We note that the divergences and zeros of $A_\pm(\alpha)$ are produced by the mechanism described in Sec. II and explain the singularity of f in these cases.

Section IV contains computations of the heat-capacity dependence on temperature for systems with $\alpha>0$, i.e., divergent heat capacity, and $-1<\alpha<0$. In the latter case we distinguish two generic situations: if $A_+/A_- > 0$, a cusped heat capacity which achieves its maximum value at the critical temperature; (ii) if $A_+/A_- < 0$, a smooth maximum in the heat capacity C occurring at a temperature other than the critical one and an infinite slope dC/dT at the critical temperature. We also note that random exchange systems such as iron fluoride with impurities of zinc probably fall into this latter class. Difficulties with the interpretation[5] of heat-capacity data which were pointed out in Ref. 6 could conceivably originate in the erroneous identification of the critical temperature as the temperature where the maximum in C occurs.

II. GENERAL MECHANISM FOR PRODUCING DIVERGENCES AND ZEROS OF CRITICAL AMPLITUDES

When, by varying an appropriate parameter such as the spatial dimension or the dimension of the order parameter, the exponent α approaches a nonpositive integer $-n$, $n=0,1,2,\ldots$, the amplitudes $A_\pm$ diverge inversely proportional to $\alpha+n$. When n is even the two amplitudes have the same sign, while when n is odd they have opposite signs. As $-\alpha$ varies between two consecutive integers there will be at least one special value where at least one amplitude is zero.

Close to a critical point the free energy f expressed as a function of a temperaturelike scaling field t is the sum of a regular part which is a Taylor expansion in powers of t and a singular part proportional to $|t|^{2-\alpha}$ with the exponent α, in general, equal to a noninteger:

$$f=\sum_{m=0}^{\infty} f_m t^m + A_{\pm}|t|^{2-\alpha} . \quad (1)$$

$A_{\pm}$ is the critical amplitude, and the subscripts + and − refer to above ($t>0$) and below ($t<0$) the critical temperature, respectively. As α approaches $-n$, the right-hand side of Eq. (1) can be approximated by

$$f=\sum_{\substack{m=0\\ m\neq 2+n}}^{\infty} f_m t^m + t^{2+n}[f_{2+n}+A_{\pm}(\mathrm{sgn}t)^n - (\alpha+n)A_{\pm}(\mathrm{sgn}t)^n \ln|t|] , \quad (2)$$

where $\mathrm{sgn}t=1$ if $t>0$ and -1 if $t<0$. To preempt the vanishing of the amplitude of $t^{2+n}\ln|t|$ and the divergence of the amplitude of t^{2+n} as $\alpha+n$ approaches zero, $A_{\pm}(\mathrm{sgn}t)^n$ and f_{2+n} have to diverge as

$$A_{\pm}(\mathrm{sgn}t)^n = -\frac{a}{\alpha+n}+c_{\pm}-c_0 ,$$
$$f_{2+n}=\frac{a}{\alpha+n}+c_0 , \quad (3)$$

where a, $c_{\pm}$, and c_0 are finite.

Then, for $\alpha=-n$,

$$f=\sum_{\substack{m=0\\ m\neq 2+n}}^{\infty} f_m t^m + a t^{2+n}\ln|t| + c_{\pm}t^{2+n} . \quad (4)$$

Equation (3) also provides information on the universal ratio A_+/A_-:

$$\frac{A_+}{A_-}=(-1)^n[1-P(\alpha+n)+O(\alpha+n)^2] , \quad (5)$$

where $P=(c_+-c_-)/a$. Hence, for n even $A_+/A_-\to 1$, meaning that both amplitudes have the same sign as they diverge, while for n odd $A_+/A_-\to -1$, meaning that one amplitude diverges to $+\infty$ while the other diverges to $-\infty$. It follows that as α varies between two consecutive integers at least one of the amplitudes will cross the zero line (at least once) as it varies between $-\infty$ and $+\infty$.

Equation (5) is particularly useful for estimating amplitude ratio since many realistic systems exhibit a small exponent α [i.e., $n=0$ in Eq. (3)]. We computed the coefficient P for the N-vector model in $4-\epsilon$ dimensions by using[7,8]

$$\alpha=\frac{4-N}{2(N+8)}\epsilon-\frac{(N+2)^2(N+28)}{4(N+8)^3}\epsilon^2+O(\epsilon^3) , \quad (6)$$

$$\frac{A_+}{A_-}=2^{\alpha}\frac{N}{4}(1+\epsilon)+O(\epsilon^2) . \quad (7)$$

At fixed ϵ the exponent α, Eq. (6), vanishes at

$$N=4(1-\epsilon)+O(\epsilon^2) . \quad (8)$$

The coefficient P is then given by

$$P=\left.\frac{1-A_+/A_-}{\alpha}\right|_{N=4(1-\epsilon)} = \frac{6}{\epsilon}\left[1-\left[\frac{1}{8}+\frac{\ln 2}{6}\right]\epsilon+O(\epsilon^2)\right] . \quad (9)$$

By setting $\epsilon=1$, i.e., $d=3$, in Eq. (9) we find $P\cong 4.6$, which is in the range of experimental and other theoretical estimates[9] of P.

III. COMPUTATION OF AMPLITUDES IN THE POSITION-SPACE RENORMALIZATION GROUP

Unlike critical exponents, there is no trustworthy *analytical* scheme to calculate critical amplitudes in the position-space renormalization group. Indeed, the linear approximation[3,10] in which the *nonlinear* recursion equation for the coupling is replaced by a linear approximation (valid only close to the critical point) violates the convexity of the free energy as a function of linear couplings on the Hamiltonian by producing a negative heat capacity.[11] As a consequence of this unphysical feature, the sign of the critical amplitude (within the *linear approximation* of Ref. 3) is incorrect. Since the linear approximation does not give reliable estimates of amplitudes, we are using a computational scheme, which is exact (within the numerical accuracy).

The free energy per degree of freedom $f=+\ln Z/N$, as a function of a linear coupling J appearing in the Hamiltonian, is given, within a position-space renormalization group (PSRG), by an infinite sum:

$$f(J)=g(J)+b^{-d}f(J_1)=\sum_{n=0}^{\infty} b^{-nd}g(J_n) , \quad (10)$$

where the coupling J renormalizes according to

$$J_{n+1}=R(J_n), \quad n=0,1,2,\ldots \quad (11)$$

where g and R are analytical functions, d is the spatial dimension, and b is the linear change in scale. Close to the critical coupling $J_{n+1}=J_n\equiv J_c$, the free energy f is the sum of a regular part f_{reg}, i.e., a Taylor expansion in powers of $J-J_c$, and a singular part f_{sing}:

$$f=f_{\mathrm{reg}}+f_{\mathrm{sing}} , \quad (12)$$

$$f_{\mathrm{reg}}=\sum_{n=0}^{\infty} f_n(J-J_c)^n , \quad (13)$$

$$f_{\mathrm{sing}}=A_{\pm}|J-J_c|^{2-\alpha} , \quad (14)$$

where + holds for $J_c-J>0$ and − for $J_c-J<0$, and

$$2-\alpha=d\ln b/\ln\left[\left.\frac{dR}{dJ}\right|_{J=J_c}\right] .$$

The coefficients f_n in Eq. (13) are determined by comparing the two sides of

$$f_{\text{reg}}(J)=g(J)+b^{-d}f_{\text{reg}}[R(J)] ,$$

after expanding f_{reg}, g, and R in powers of $J-J_c$. We compute numerically f and f_{reg} at small values of $J-J_c$ and then find the amplitudes $A_\pm$ from

$$A_\pm=[f(J)-f_{\text{reg}}(J)]\,|J-J_c|^{\alpha-2} . \tag{15}$$

We apply this scheme to the Migdal-Kadanoff renormalization-group solution of the d-dimensional q-state Potts model. At each site i of a d-dimensional lattice there is a spin $\sigma_i=1,2,\ldots q$, and we associate with each edge (ij) an energy

$$-H_{ij}/k_BT=2J\delta(\sigma_i,\sigma_j) .$$

We consider a change in scale $b=2$, and in this case the functions g and R are

$$g(J)=\tfrac{1}{2}\ln(2e^{2J}+q-2) , \tag{16}$$

$$R(J)=2^{d-2}\ln\left[\frac{e^{4J}+q-1}{2e^{2J}+q-2}\right] . \tag{17}$$

As first noted by Berker and Ostlund,[12] this scheme provides the exact solution of the Potts model on a hierarchical lattice[12,13] constructed by repeatedly replacing one bond by a cluster as shown in Fig. 1.

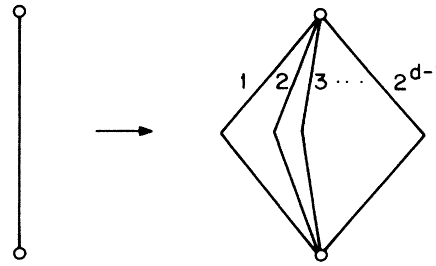

FIG. 1. Hierarchical lattice associated with the Migdal-Kadanoff scheme, $b=2$.

The amplitudes' dependence on α is shown for a few different dimensions, $d=1.5,2,2.5,3$, in Fig. 2. The case of two dimensions studied first in Ref. 1 is special due to the duality symmetry which forces[2] the equality of amplitudes $A_+=A_-$. It also follows[2] that when $-\alpha$ is equal to an odd integer, $a=0$ [see Eqs. (3) and (4)], and thus there are no divergences of $A_\pm$ as $-\alpha$ approaches 1,3,5,. . . in two dimensions.

For $d\neq2$ the amplitudes diverge as $-\alpha$ approaches any integer. Due to the positivity of the heat capacity the amplitudes $A_\pm$ are positive for $\alpha>0$. For α slightly negative both amplitudes are negative, while for $\alpha\to-1$ they diverge with opposite signs [cf. Eq. (3)]. Hence, at least a zero for either amplitude is expected in the interval $-1<\alpha<0$. Indeed, for $d=3$, $A_-=0$ at $\alpha\cong-0.2$.

For any dimension d both amplitudes $A_\pm$ vanish for the case $q=1$. Indeed, the 1-state Potts free energy (per bond) is $f=2J$, and therefore no singularity is exhibited $(A_\pm=0)$.[1] The free energy f of the Potts model with

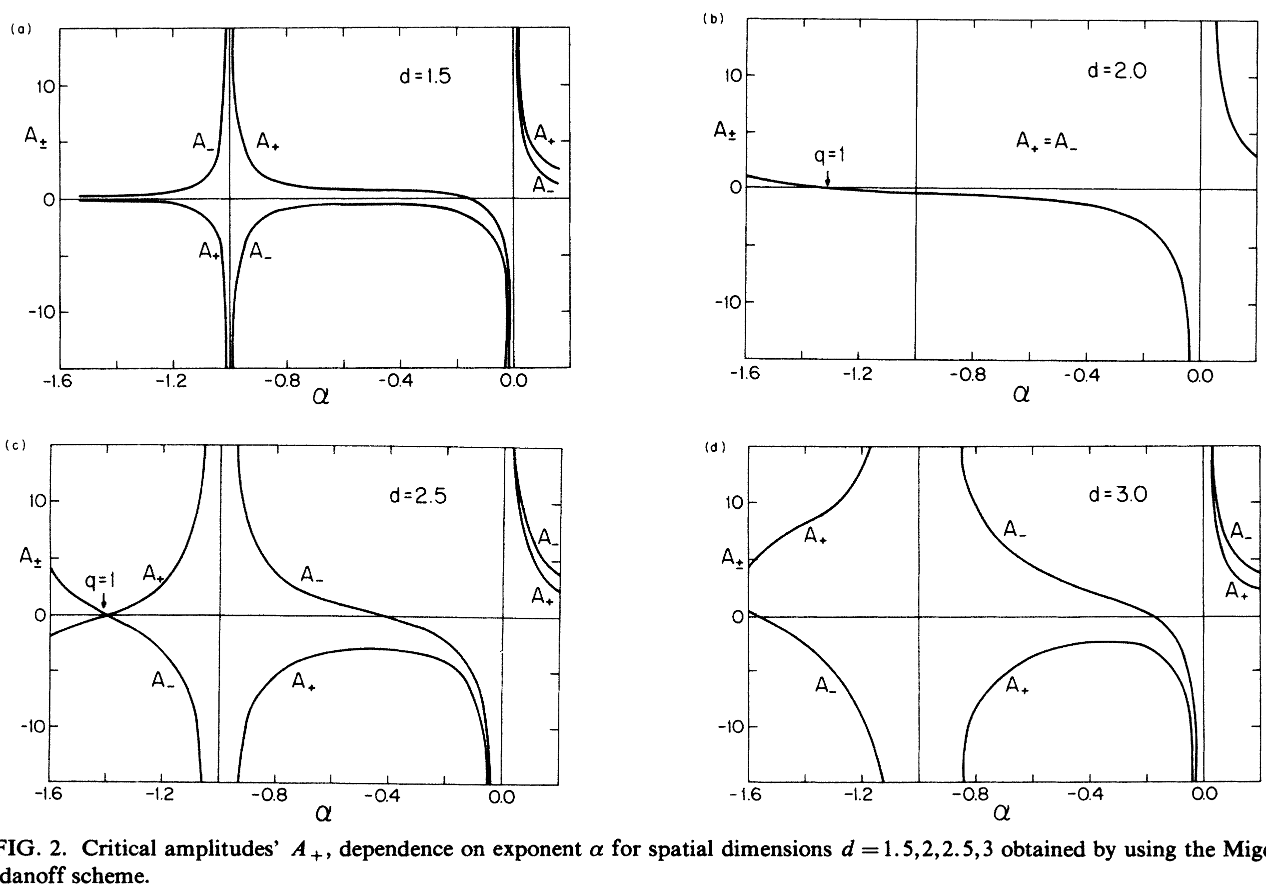

FIG. 2. Critical amplitudes' A_+, dependence on exponent α for spatial dimensions $d=1.5,2,2.5,3$ obtained by using the Migdal-Kadanoff scheme.

$q \to 1$ is related[14] to the bond-percolation mean number of clusters G:

$$G = \left.\frac{\partial f}{\partial q}\right|_{q=1} .$$

Then

$$G_{\text{sing}} = \frac{\partial}{\partial q}(A_{\pm} |t|^{2-\alpha})|_{q=1} ,$$

and since $A(q=1)=0$ it follows that

$$G_{\text{sing}} = \left[\left.\frac{dA_{\pm}}{dq}\right|_{q=1} \right] |t|^{2-\alpha} ,$$

i.e., the bond-percolation exponent α is the exponent of the 1-state Potts model, while the bond-percolation amplitudes $\hat{A}_{\pm}$ are $dA_{\pm}/dq\,|_{q=1}$. ϵ expansion[15] for bond percolation suggest that the exponent α is negative but larger than -1 and, of course, in this case, $q=1$, $A_{\pm}=0$. On the other hand, the $3d$ Ising model, $q=2$, has a divergent heat capacity, $\alpha \cong 0.11$, $A_{\pm}>0$. As α approaches 0 and -1, by varying q at $d=3$, the amplitudes diverge with the same sign and with opposite sign, respectively [cf. Sec. II]. The simplest qualitative dependence $A_{\pm}(\alpha)$, $d=3$, and α is varied by changing q, which incorporates these pieces of information is shown in Fig. 3. Two consequences of Fig. 3 are the following:

(i) Since the bond-percolation amplitudes

$$\hat{A}_{\pm} = \left.\frac{dA_{\pm}}{dq}\right|_{q=1} = \left[\frac{d\alpha}{dq}\right] \left[\frac{dA_{\pm}}{d\alpha}\right]_{q=1} ,$$

it follows that the $\hat{A}_{\pm}$ have opposite signs, which is in agreement with the ϵ-expansion prediction[16] that $\hat{A}_{+}/\hat{A}_{-}<0$. In fact, the agreement is more detailed as we predict $\hat{A}_{+}<0$ and $\hat{A}_{-}>0$ (assuming $d\alpha/dq>0$), and this can also be deduced from Eqs. (2.14), (3.23), (3.24), and (B4) of Ref. 16.

(ii) There is a value of q in the interval [1,2], where $A_{-}=0$ while $A_{+}<0$.

Another interesting quantity, useful for the interpretation of experiments, is the universal ratio of the critical amplitudes A_{+} and A_{-}. Since for $d=3$ A_{-} vanishes at certain values of α, it is more convenient to plot A_{-}/A_{+}, rather than the more familiar A_{+}/A_{-}, against α, Fig. 4. For α close to zero we note that A_{-}/A_{+} increases linearly with α:

$$A_{-}/A_{+} \cong 1+P\alpha+O(\alpha^2) ,$$

and $P \cong 5$ is to be compared with $P \cong 4.6$ derived in Sec. II for the N-vector model in $4-\epsilon$ dimensions.

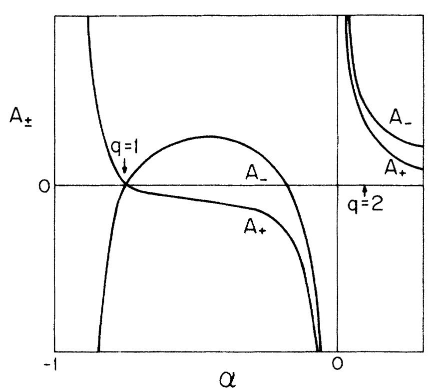

FIG. 3. The likely dependence of critical amplitudes $A_{\pm}$ on exponent α for three-dimensional systems.

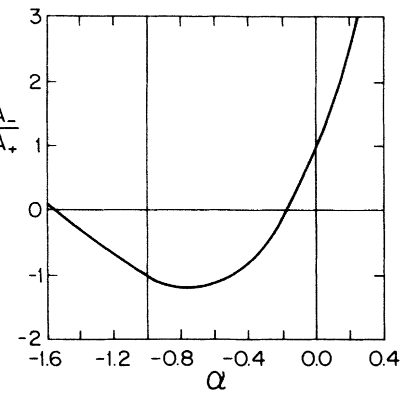

FIG. 4. Ratio of amplitudes, A_{+}/A_{-}, dependence on exponent α for $d=3$ obtained by using the Migdal-Kadanoff scheme.

IV. HEAT-CAPACITY COMPUTATION

Numerical computations of the temperature dependence of the heat capacity are presented in this section. We emphasize that systems exhibiting a critical exponent α negative but larger than -1 do not necessarily show a cusp in the heat capacity. The other possibility is a heat capacity with a smooth maximum occurring at a temperature other than the critical temperature, and an infinite slope at the critical temperature. We also suggest that three-dimensional random-bond systems such as $Fe_{1-x}Zn_xF_2$ exhibit this behavior.

Equation (10) and two other equations obtained by differentiating once and twice, respectively, both sides of Eq. (10) can be written in the following matricial form:[17]

$$\tilde{f}(J)=\tilde{g}(J)+\mathbf{R}(J)\tilde{f}(J_1) , \tag{18}$$

where

$$\tilde{f} = \begin{bmatrix} f \\ df/dJ \\ d^2g/dJ^2 \end{bmatrix} ,$$

$$\tilde{g} = \begin{bmatrix} g \\ dg/dJ \\ d^2g/dJ^2 \end{bmatrix} ,$$

$$\mathbf{R} = b^{-d} \begin{bmatrix} 1 & 0 & 0 \\ 0 & dR/dJ & 0 \\ 0 & d^2R/dJ^2 & (dR/dJ)^2 \end{bmatrix} ,$$

and $J_1=R(J)$.

Our computation of the heat capacity $C/k_B = J^2(d^2f/dJ^2)$ is based on a repeated iteration of Eq. (18):

$$\tilde{f}(J)=\tilde{g}(J)+\mathbf{R}(J)\tilde{g}(J_1)+\mathbf{R}(J)\mathbf{R}(J_1)\tilde{g}(J_2)+\cdots . \quad (19)$$

In Fig. 5 we show two heat-capacity curves corresponding to $\alpha>0$, i.e., divergent heat capacity: The curve in Fig. 5(a) belongs to a two-dimensional system, and thus it is symmetric about the critical temperature $A_+=A_-$; the curve in Fig. 5(b) corresponds to a three-dimensional system and it is not symmetric, $A_+\neq A_-$.

In Fig. 6 we show the two generic types of heat-capacity curves for systems with $-1<\alpha<0$. In Fig. 6(a), A_+/A_- is positive, and the heat capacity has a cusp (maximum) at the critical temperature T_c. In Fig. 6(b), $A_+/A_-<0$ and the maximum in the heat capacity occurs at a temperature other than the critical one,[18] while at T_c the heat capacity shows an abrupt change with temperature (infinite slope).

Random-bond systems are predicted[19,20] to exhibit $\alpha\approx-0.09$ and $A_+/A_-\approx-0.5$, and thus the heat-capacity dependence on temperature should be of the type illustrated in Fig. 6(b): the maximum in C occurs at $T\neq T_c$. A particular experimental realization of this model is iron fluoride, which is an Ising antiferromagnet, with nonmagnetic impurities of zinc. Heat-capacity data from this system have been, however, analyzed[5] on the assumption that the maximum in the heat capacity occurs at T_c. It is conceivable that some of the difficulties pointed out in Ref. 6, such as an overly large correction-to-scaling term on the heat-capacity fitting form, compared to no correction-to-scaling in the fitting of the susceptibility data, are rooted in this erroneous identification of the critical temperature. An alternative explanation[6] of the data invokes the Ginzburg criterion:[21] close to the critical point, but not in its immediate vicinity, mean-field criticality, i.e., discontinuous heat capacity, could be observed. We finally note that it could be quite difficult, in an experiment, to distinguish between a discontinuous (mean-field) heat capacity and a heat capacity of the type illustrated in Fig. 6(b) ($-1<\alpha<0, A_+/A_-<0$), which exhibits an abrupt but continuous variation at the critical temperature.

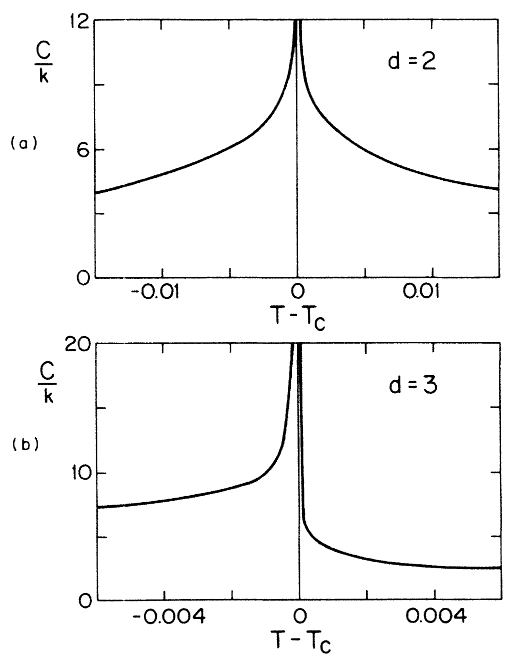

FIG. 5. Heat-capacity dependence on temperature for systems with $\alpha>0$: (a) symmetric case $A_+=A_-$, $d=2$; (b) asymmetric case $A_+\neq A_-$, $d\neq 2$. We used the Migdal-Kadanoff scheme for (a) $d=2, q=21$ and (b) $d=3, q=30$.

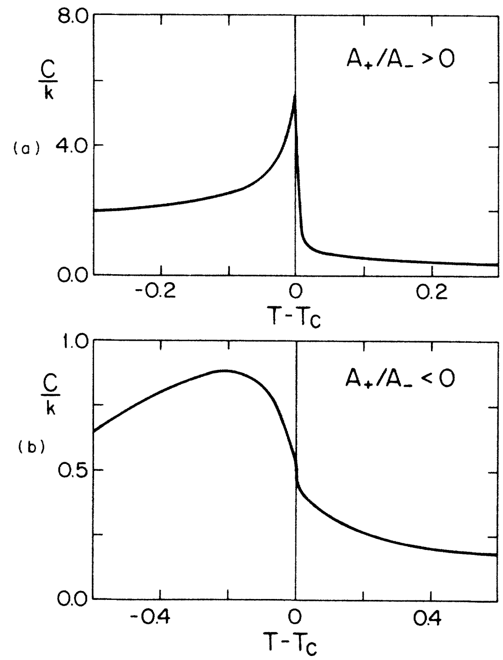

FIG. 6. Heat-capacity dependence on temperature for systems with $-1<\alpha<0$: (a) cusp if $A_+/A_->0$; (b) smooth maximum at $T\neq T_c$ and abrupt variation (infinite slope) at T_c if $A_+/A_-<0$. We used the Migdal-Kadanoff scheme for (a) $d=3, q=15$ and (b) $d=3, q=5$.

V. DISCUSSION

Critical amplitudes associated with the temperature dependence of the heat capacity were analyzed by means of renormalization-group techniques. In particular, we predict that the three-dimensional q-state Potts model will exhibit a vanishing amplitude $A_-=0$, while $A_+\neq 0$, for some q between 1 (bond percolation) and 2 (Ising model). The occurrence of zeros of $A_\pm$ as a function of α is linked to the divergence of amplitudes as $-\alpha$ approaches integers. We also estimated the coefficient P on the expansion $A_+/A_-\cong 1-P\alpha+O(\alpha^2)$ by means of both momentum-space and position-space renormalization-group techniques and found P to be close to 5. When $-1<\alpha<0$, the heat capacity exhibits a cusp if $A_+/A_->0$ or a smooth maximum at a temperature other than the critical temperature (T_c) and an abrupt variation at T_c if $A_+/A_-<0$. We suggest that the latter situation occurs in random-exchange systems such as $Fe_xZn_{1-x}F_2$.

The only available *analytical* procedure to compute amplitudes within the position-space renormalization-group formalism is inadequate, e.g., produces a negative heat capacity. It will be interesting to see whether this scheme can be improved upon systematically to eliminate such an unphysical feature.

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