ISSN 0029 - 3865

CBPF-NF-021/86

EXPONENTS FAR FROM T_c - APPLICATION TO THE SPECIFIC HEAT OF SOME HIERARCHICAL STRUCTURES

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ABSTRACT

We claim that the utilization of a linearized version of the "static scaling hypothesis" has led to a widespread erroneous conception of the notion of "critical regime" based upon the occurrence of deviations which, in fact, reflect essentially the effect of the linearization. The discussion is illustrated here with the exact results of the specific heat of several hierarchical structures calculated in a real-space renormalization group scheme.

RESUME

Nous soutenons que l'utilisation d'une forme linéarisée de l'hypothèse du "scaling statique"a conduit à une conception erronée de la notion de "domaine critique" basée sur l'observation de déviations qui reflètent essentiellement les effets de la linéarisation. Nous illustrons notre point avec des résultats exacts de la chaleur spécifique de plusieurs structures hiérarchiques calculée dans le cadre d'un groupe de renormalisation dans l'espace réel.

Key Words : Critical exponents, phase transitions.

P.A.C.S. numbers : 75.40, 75.103, 75.104.

The utilization of a linearized version of the static scaling hypothesis (1,2) :

$$\frac{G}{T_c} = t'^{d\nu}\, g\left(\frac{\eta'}{t'^{\bar{d}\nu}}\right) \quad , \quad t' = \frac{T-T_c}{T_c} \quad , \quad \eta' = \frac{H}{T_c} \quad , \tag{1}$$

has led to the widespread belief that scaling ideas are applicable only in a restricted "critical regime" (say for $\frac{T-T_c}{T_c} \lesssim 10\ \%$) where the exponents have effective values close to their critical limits ; at higher temperatures there would be a progressive cross-over towards a situation where the effective exponents reach their mean field values. More specifically, equation 1 leads to

$$\chi = \frac{\partial^2 G}{\partial^2 \eta'} \simeq \left(\frac{T-T_c}{T_c}\right)^{-\gamma} \quad , \quad \gamma = (2\bar{d}-d)\nu \tag{2}$$

and

$$\gamma^*(T) = - \frac{\partial \ln \chi}{\partial \ln\left(\frac{T-T_c}{T_c}\right)} \tag{3}$$

has to reach one in order for the Curie law to be recovered in the high temperature limit. We propose hereafter to write the Gibbs potential near a phase transition

$$\frac{G}{T} = t^{d\nu}\left(g(\eta/t^{\bar{d}\nu}) + g_o\right) + g_1 \quad , \quad \eta = \frac{H}{T} \quad . \tag{4}$$

Following MA (1) we have introduced g_o and g_1, which are effective "constants" in the sense that they leave unchanged the singularity of the free energy at T_c ; they account for components at short wavelength which play a role in the specific heat but need not be considered in the case of the magnetization or of the correlation function G(k) which are average values of long wavelength (small k) Fourier components. The important point, though, is that we use the <u>non linear variables</u> η and t (t will be defined later) instead of the linear variables η' and t' so that for g_o and $g_1 = 0$ equation 4 generalises the static scaling hypothesis (i.e. equation 1) consistently with the original Kadanoff's construction (3) : the free energy appears as a function of $\mu_{eff}\frac{H}{T}$ extensive in the concentration of the Kadanoff's d-dimensional blocks which is ξ^{-d} by definition of the coherence length ξ; two conditions define the two exponents which are believed sufficient to describe the main features of the free energy : they state i) that the effective moment μ_{eff} of the blocks increases as $\xi^{\bar{d}}$ ($\bar{d} < d$), and ii) that ξ diverges as $t^{-\nu}$ where t cancels at T_c. On differentiating equation 4 with respect to H one obtains

$$M = \frac{\partial G}{\partial H} = t^{\beta}\mathcal{M}(\eta/t^{\gamma+\beta}) \quad , \tag{5}$$

$$\beta = (d - \bar{d})\nu$$

and

$$\chi T = \frac{\partial M}{\partial (H/T)} \simeq t^{-\gamma} . \tag{6}$$

In mean field ($\gamma = 1$) we have $\chi T \simeq t^{-1}$ which defines t for $T > T_c$:

$$t = \frac{T - T_c}{T} . \tag{7}$$

Kadanoff's argument takes advantage of a dilatation symmetry which should be exact in the "critical regime", i.e. close enough to T_c, where ξ is large and we can forget about the details of the crystalline structure which, on all Bravais lattices, obeys a translation symmetry. For this reason the "static scaling hypothesis" is in general linearized under the form of equation 1 (i.e. with the linearized variables η' and t' substituted for the <u>natural</u> variables η and t). This supposes that the difference between e.g. equation 6 and its linearized version 2 should remain negligible with respect to the physical effects which otherwise limit the validity of equation 6 and define the true critical regime. This is obviously not the case for the ranges of the order of $\frac{T-T_c}{T_c} \lesssim 10\ \%$ which have been considered by most authors. Every evidence, theoretical (4,5) and experimental (6-8), shows that this magnitude ($\sim$ 10 %) reflects essentially the artificial effect of the linearization. Thus the effective exponent

$$\hat{\gamma}(T) = -\frac{\partial \ell n \chi T}{\partial \ell n\left(\frac{T-T_c}{T}\right)} \tag{8}$$

which follows from equation 6 remains reasonably close to its critical ($t \to 0$) limit over the whole range of temperatures ($0 < t < 1$), while its linearised counterpart $\gamma^{*}(T) = \hat{\gamma} - (\hat{\gamma} - 1)t$ as given by equation 3 must attain a value of one when $T \to \infty$ (9) in order to reach the high temperature Curie limit which was naturally present in Kadanoff's assumptions and in equation 6. The latter yields $\chi(T \to \infty) \sim C/(T-T_c^{MF})$ with a prediction $T_c^{MF}/T_c = \gamma$ which works extremely well in some cases (e.g. for the Ising square lattice we have $\gamma = 1.75$ and $T_c^{MF}/T_c = -2\ell n(\sqrt{2} - 1) = 1.76275...$). The mean field limit follows from the fact that χT can be expanded in terms of $1/T$: this property is basic to the success of all high temperature expansions.

The purpose of the present paper is to show that we avoid similarly the introduction of unwanted features in the specific heat if we utilize equation 4. We have in zero field

$$S(\eta=0) = -\frac{\partial G(\eta=0)}{\partial T} \sim -(g(0)+g_0)\left(\frac{T_c}{T}(2-\alpha)t^{1-\alpha}+t^{2-\alpha}\right)-g_1 + \ldots,$$

$$\alpha = 2 - d\nu \leq 1 \tag{9}$$

and by further differentiating we obtain

$$\frac{C\ (T)}{k_B}\frac{T^2}{T_c^2} \sim At^{-\alpha} + B \tag{10}$$

instead of the usual linearized form

$$\frac{C\ (T)}{k_B} \sim A't'^{-\alpha} + B' \quad . \tag{11}$$

The "constants" B or B' follow from the additional "constants" g_0 and g_1 in equation 4. We note that with equation 10 instead of equation 11, i) we avoid the absurd implication of a specific-heat which would become infinite when $T \to \infty$ in the case of a negative α, and ii) that the simplest assumption which we can make on B, i.e. that B is actually a constant, yields the very satisfactory feature that C (T) vanishes as T^{-2} in the high temperature limit for any value of α. Equation 10 has been already used, among many other trial functions, to fit the specific heat. In reference 10, equations 10 and 6 follow from a free energy which has the form of equation 4 in the particular case of the Heisenberg model with S = 1/2 on f.c.c. lattice. The authors stress the excellent agreement obtained with both expressions over a large range of temperatures.

We hereafter present further evidence based upon the specific heat at $T > T_c$ of a number of hierarchical structures generated from the well known b-sized, planar, two-terminal self-dual clusters schematized in figure 1. We have worked with the q-state Potts model which has the following Hamiltonian :

$$H = - Jq \sum_{<i,j>} \delta\sigma_i\sigma_j \quad (\sigma_i = 1,2,\ldots,q,\ \forall\, i), \tag{12}$$

where $J \geqslant 0$ is the coupling constant and <i,j> runs over all pairs of first neighbouring sites of a given hierarchical lattice. Using the real-space renormalization scheme, which is exact on such lattices, we have computed the specific heat per bond C (T) as a function of the temperature T. The procedure is similar to that detailed in reference 11. However, in the expression of the free energy of the equation 3 of this reference we must substitute $g_\gamma(K)$ by L'_0/n_b ($\gamma = 0$) and b^{-d} by $b^{-d_i} = 1/n_b$ where $n_b = 2b^2 - 2b+1$ is the number of bonds in the basic cell. For the hierarchical lattice equation 9 becomes (12)(13)

$\alpha = 2 - d_i/y_T$ where d_i is the lattice intrinsic dimension,

$$d_i = \ln(2b^2 - 2b + 1)/\ln b \quad , \tag{13}$$

and y_T is the thermal scaling index ($\lambda_T = b^{y_T}$, where λ_T is the thermal eigenvalue of the renormalization transformation). Among other advantages, a number of quantities are known exactly :

$$T_c = qJ/k_B \ln(1 + \sqrt{q}) \qquad (\forall\, b,\ \forall\, q) \tag{14}$$

$$\alpha = 2 - \frac{\ln 5}{\ln \dfrac{8+13q^{1/2}+5q}{8+7q^{1/2}+q}} \qquad (b = 2,\ \forall\, q, \text{ see references 12 and 13}) \tag{15}$$

$$\frac{C(T)}{k_B}\left(\frac{T}{T_c}\right)^2 = \left(\frac{J}{k_B T_c}\right)^2 (q-1) + \left(\frac{J}{k_B}\right)^3 \frac{5q^2-3q-2}{5T_c^2}\frac{1}{T} + O\left(\frac{1}{T^2}\right) , \tag{16}$$

$(b = 2,\ \forall\, q)$ for $T \to \infty$.

Other quantites, like $C(T_c)$ for $\alpha < 0$, can be calculated with arbitrary accuracy (see table I). These quantities cannot be used as parameters that one is free to adjust in order to increase the performance of the fit in an appropriate temperature range as is common practice when dealing with experiments or even with high temperature expansions.

In order to test the validity of equation 10 we have represented

$$\ln \left|\frac{C(T)}{k_B}\left(\frac{T}{T_c}\right)^2 - B\right|$$ on the figure 2. More explicitely

we have shown

$$\ell n \left| \frac{C\ (T_c)}{k_B} - \frac{C_p(T)}{k_B} \left(\frac{T}{T_c}\right)^2 \right| \text{ vs. } \ell n\left(\frac{T-T_c}{T}\right) \quad , \quad \text{for } \alpha < 0$$

$$\ell n \frac{C\ (T)}{k_B} \left(\frac{T}{T_c}\right)^2 \text{ vs. } \ell n\left(\frac{T-T_c}{T}\right) \quad , \quad \text{for } \alpha > 0 \ .$$

The necessity to substract the regular part of the specific heat at T_c imposes the condition $B = C\ (T_c)\ /k_B$ in the cases where $\alpha < 0$. For $\alpha > 0$ we have arbitrarily taken $B = 0$ in the plot of figure 2 and the linearity in this plot obviously suffers from the fact that we have arbitrarily fixed this adjustable parameter that equation 10 provides. In order to adjust B, in this case (i.e. for $q = 8$, $b = 2$) we found no better way than to check which, among several attempt values, makes the fit better in the vicinity of T_c. This is done more accurately by working with the effective exponent

$$\hat{\alpha}(T) = - d\ell n \left| \frac{C\ (T)}{k_B} \frac{T^2}{T_c^2} - B \right| / d\ell n\left(\frac{T-T_c}{T}\right) \qquad (17)$$

which is represented vs. $\frac{T-T_c}{T}$ in figure 3, for different values of B. Assuming equation 10 is exact an error ΔB on B would introduce a spurious contribution $\hat{\alpha}(T) - \alpha = \alpha \frac{\Delta B}{A}\ t^{\alpha}$ capable of accounting for the initial deviation which changes sign when B is varied from -5 to -8 in figure 3. In the figure 3 we have represented $\hat{\alpha}(T)$ vs. $\frac{T-T_c}{T}$ with $B \sim -6$ for the case $q = 8$, $b = 2$ when $\alpha > 0$, and $B = C\ (T_c)/k_B$ when $\alpha < 0$. The resulting picture is very similar to that obtained in reference 4 for the effective exponent $\hat{\gamma}(T)$ deduced from the Padé approximants to the susceptibility of various model systems. In particular differences $\hat{\alpha}(T) - \alpha$ result of the same magnitude (0.1) as the differences $\hat{\gamma}(T) - \gamma$ which were determined in reference 4 (this seems reasonable if a sum rule such as $\alpha + 2\beta + \gamma = 2$ is expected to hold between the effective exponents). We note that, starting with the linearized static scaling equation 1, we obtained equation 11 from which we would have deduced an effective exponent $\alpha'(T) = (\hat{\alpha} - 2)\ \frac{T_c}{T} + 2$. If we start from equation 10 and then linearize (i.e. we change t into t') to obtain $C(T)T^2/k_B T_c^2 = At'^{-\alpha} + B$ we determine another effective exponent $\alpha^*(T) = \hat{\alpha}T_c/T$ (see figure 4). Both $\alpha'(T)$ and $\alpha^*(T)$ are compelled to reach fixed high temperature values (resp. 2 and 0) but only the latter yields the mean field result. This illustrates the precarity of the statement that mean field exponents are recovered in the high temperature regime since this limit depends on the stage in the calculations at which the linearization procedure is applied. By contrast the natural exponent $\hat{\alpha}(T)$ reaches a limit $\hat{\alpha}(t = 1)$ which is close to α (see table 1) and for which equation 16 provides an analytical expression for known B.

The general picture which emerges from this discussion can be more easily expressed within the formalism of the confluent series which introduce an additional infinite number of less divergent singularities : e.g. equation 6 is generalized as

$$\chi T = t^{-\gamma}(1 + \sum_i^{\infty} A_i t^{\omega_i \nu}) \quad .$$

The effective exponent therefore can be represented by its critical value corrected by a confluent series :

$$\hat{\gamma}(T) = \gamma - \frac{\sum_i A_i \omega_i \nu \, t^{\omega_i \nu}}{1 + \sum_i A_i t^{\omega_i \nu}} = \gamma + \sum_i a_i t^{\omega_i \nu} \tag{18}$$

On the basis of the present and former (4) evidence we claim that effective exponents deviate from their critical limit to reach an effective value which remains a good approximation to the critical one rather independently of the range in which it is determined and which differs from the mean field value. This means that $\sum_i a_i < \varepsilon_m$ where ε_m is finite and small (of the order of 0.1). If we are satisfied with values of the exponents known to that accuracy, we may claim that the critical regime extends up to the highest temperatures.

The real critical regime corresponds to the range $t < a_1^{-1}$ where the effective exponent becomes arbitrarily close to its critical value : its extension a_1^{-1} should be determined in each case and may be small if a_1 is large. The initial deviations observed in some cases (c.f. (c)(d) in figure 3) suggest that a_1 may be large in agreement with previous discussions (14). The high temperature regime, however, should not be described as a "mean field regime" but simply as a regime where exponents are determined with a limited accuracy. Indeed, as is well known, experiment usually fails to provide exponents which approach the theoretical limit to much better than $\pm$ 0.1 except when (as for example in Helium) the nature of the sample permits one to work very close to T_c.

Table 1

b	q	α	B	$\hat{\alpha}(t=1)$	Figure symbol
2	8	0.132939	~ 6 (fitted)	0.08810	(a)
2	4	-0.202032	9.827586	-0.09985	(b)
4	2	-0.542489	0.611400		(c)
2	2	-0.667034	0.525733	-0.61956	(d)

Values of the different parameters α , B and $\hat{\alpha}(t = 1)$ for the different systems studied and the corresponding symbols ((a)...(c)) in figures 2,3. For b = 2, α is given by equation 15 and $\hat{\alpha}(t = 1)$ follows from equation 16 for known B. $B = \frac{C\ (T_c)}{k_B}$ for all cases where $\alpha < 0$.

FIGURE CAPTIONS

Figure 1 : The two types of two-terminal clusters used in the present calculation : (a) $b = 2$, $q = 8$, (b) $b = 2$, $q = 4$, (c) $b = 4$, $q = 2$, (d) $b = 2$, $q = 2$ (the notations (a),(b),(c), (d) refer to the corresponding cases in figures 2 and 3 and in table 1.

Figure 2 : Plot of $\ln\left|\frac{C(T)}{k_B}\frac{T^2}{T_c^2} - B\right|$ vs. $\ln\frac{T-T_c}{T}$

with $B = 0$ for $\alpha > 0$ (curve (a))

and $B = \frac{C(T_c)}{k_B}$ for $\alpha < 0$ (curve (b)(c)(d))

Figure 3 : Upper frame : plot of $\hat{\alpha}(T)$ vs. t in the case (a)($b = 2$, $q = 8$) when $\alpha > 0$ showing the incidence of the choice of parameter B upon the behaviour of $\hat{\alpha}(T)$. For representation in the lower frame a value $B = 6$ was chosen. In the lower frame the effective exponent $\hat{\alpha}(T)$ is shown vs. $\frac{T-T_c}{T}$ for the different systems studied (•) with B, α and $\hat{\alpha}(t = 1)$ as given in table 1. For the case (c) we have also represented (curve(c')) $\alpha^*(T) = T_c\frac{\hat{\alpha}(T)}{T}$ which would be determined with the linearised variable $t' = \frac{T-T_c}{T_c}$ substituted to t (see text). The latter linearized effective exponent is compelled to reach the mean field value $\alpha = 0$ in the limit of high temperatures.

The exact values of α are indicated by horizontal arrows.

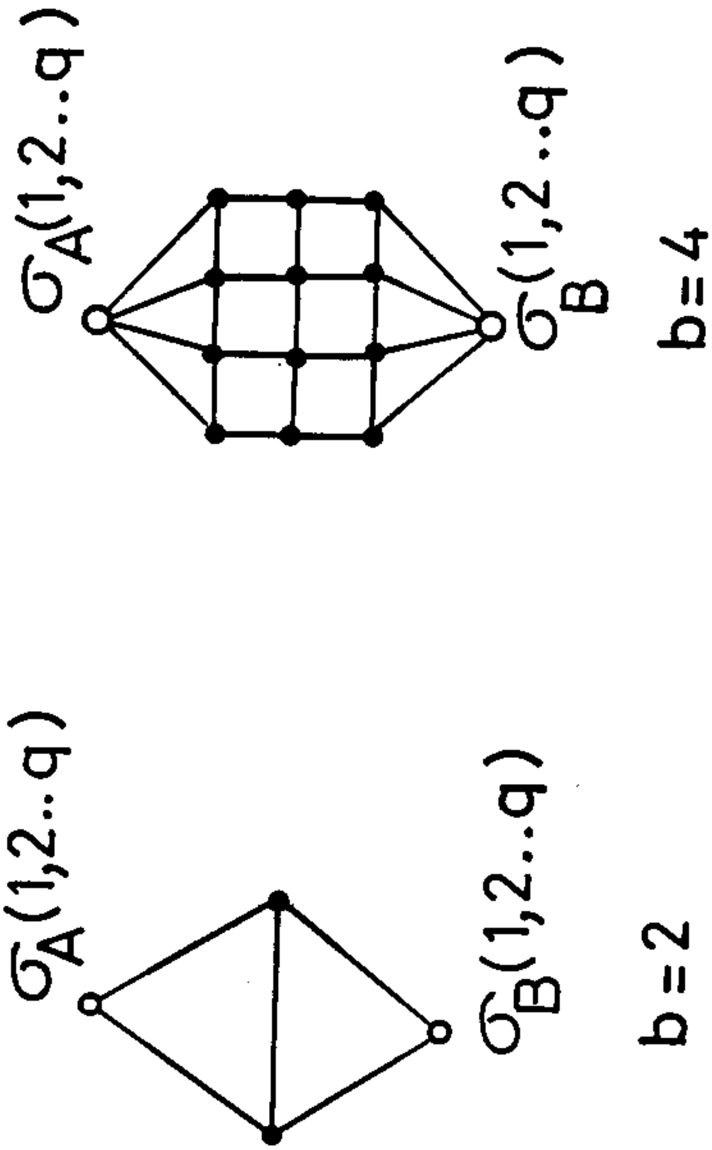

Figure 1

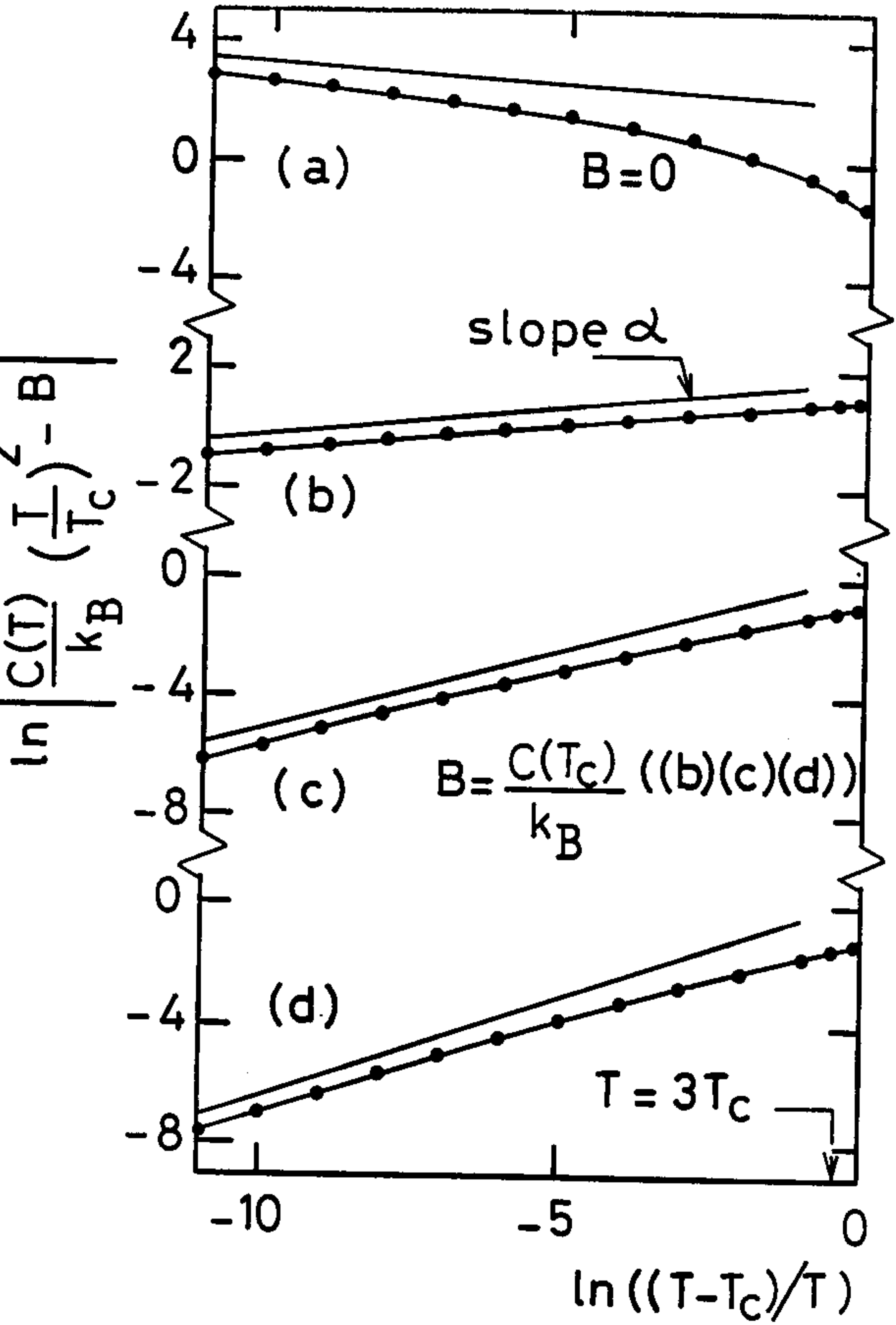
4
0
-4
2
-2
0
-4
-8
0
-4
-8
(a)
B=0
slope α
(b)
(c)
B= C(T_C)/k_B ((b)(c)(d))
(d)
T = 3T_C
-10
-5
0
ln ((T-T_C)/T)
ln |C(T)/k_B (T/T_C)^2 - B|

Figure 2

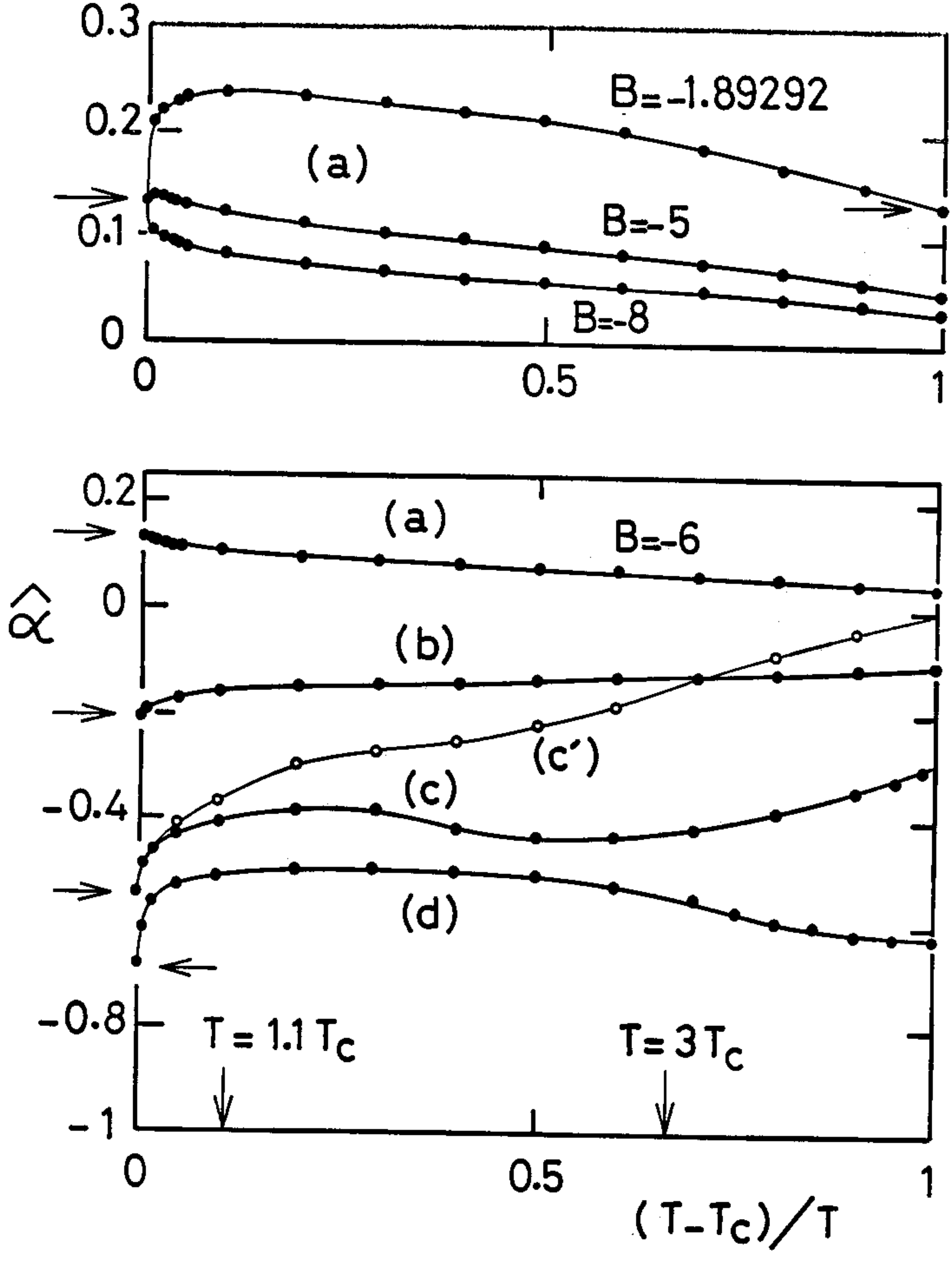
0.3
0.2
0.1
0
B=-1.89292
(a)
B=-5
B=-8
0
0.5
1
0.2
0
-0.4
-0.8
-1
$\hat{\alpha}$
(a)
B=-6
(b)
(c')
(c)
(d)
T= 1.1 T$_c$
T= 3 T$_c$
0
0.5
1
(T-T$_c$)/T

Figure 3

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+ Financially supported by CONICET, ARGENTINA.