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Nonasymptotic critical behaviour from field theory for Ising like systems in the homogeneous phase : theoretical framework

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Résumé. — Nous reproduisons les résultats d'un traitement non linéaire précis du modèle ϕ^4 à trois dimensions à partir du groupe de renormalisation (GR).

Nous donnons l'ensemble complet des quantités habituellement mesurables au-dessus de T_c (la longueur de corrélation ξ , la susceptibilité χ et la chaleur spécifique C) pour des systèmes de type Ising, sous forme de fonctions numériques explicites de la température.

Nous discutons la correspondance entre les hypothèses fondamentales du GR et les paramètres ajustables (seulement trois) nécessaires à une comparaison avec les expériences.

Abstract. — We report results of a precise nonlinear renormalization group (RG) treatment of the ϕ^4 model in three dimensions.

We give the complete set of usually measurable quantities above T_c (the correlation length ξ , the susceptibility χ and the specific heat C) for Ising like systems as explicit numerical functions of temperature.

We discuss the correspondence between the fundamental hypothesis of the RG and the adjustable parameters (only three) needed for a comparison with experiments.

1. Introduction.

The idea that critical phenomena are not limited to a point in a phase diagram is obviously contained in the usual expression « critical behaviour ».

The approach to the CP was first described by simple power laws [1], often in terms of the distance to the critical point (CP) — for example the reduced deviation ($\tau = (T - T_c)/T_c$) of the temperature (T) from its critical value (T_c). From the experimentalist's point of view a question arises : how close to the CP can such a power law be observed [2] ?

It was soon emphasized that corrections to scaling could be necessary in the analysis of experiments [3], and expansions such as :

$$f(\tau) = f_0^+ \tau^{-\lambda_f} (1 + a_f^{(1)} \tau^{d_1} + a_f^{(2)} \tau^{d_2} + \dots) \quad (1)$$

have been proposed to describe critical behaviour [4, 5]. $f(\tau)$ represents any singular quantity (the correlation length ξ or the susceptibility χ or the singular part of the specific heat C) as one approaches the CP along the critical isochore ($\tau \rightarrow 0^+$).

It is well known [6] that, within the various universality classes, the critical (λ_c) and subcritical (Δ_1, Δ_2) exponents, some relations among leading amplitudes (f_0^+) and ratios among the first correction amplitudes (a_1^1) have universal values which depend on the class. The Callan-Symanzik version [7] of the renormalization group (RG) approach [8] to static critical phenomena is a very efficient technique for deriving and estimating such universal features. In this scheme the leading and the first correction terms in (1) are generated within the pure ϕ^4 model (see Eq. (4)), and very precise estimates [9-12] of their universal features have been obtained from Feynman graph expansions in three dimensions ($d = 3$) [13]. The origin of the second correction term is more complex and its theoretical determination not so accurate. Besides the pure ϕ^4 model (which should give $\Delta_2 \equiv 2 \Delta_1 \simeq 1$), higher transients — especially ϕ^5 which would be relevant for fluids [14] ($0.5 \lesssim \Delta_2 \lesssim 1$) — and analytic terms ($\Delta_2 \equiv 1$) also have to be considered. As one sees, it is difficult to appreciate their relative influence in the expansion (1).

Even if it were possible to estimate very precisely the true second correction, this result would not be conclusive as long as the convergence of the expansion is not controlled. The experimentalist needs to know in which range of τ the expansion (1) is valid [15, 16]. The difficulties in going very close to the CP together with the improved accuracy in the measurements make it necessary to introduce more and more correction terms in (1). This implies an increasing number of adjustable parameters which does not allow a good determination of all of them and can even make it difficult to test the universal ratios of the first correction amplitudes.

Wegner [4] has shown that an expansion like (1) comes out clearly from the RG approach. The CP is represented by a point (a fixed point) in a multidimensional abstract space. The pure ϕ^4 model amounts to considering only one axis in this space. The fixed point is somewhere on this axis. The approach to the CP corresponds to a line in this space. Up to some distance (unknown because nonuniversal) from the CP, this line coincides with the ϕ^4 axis. The confluent correction terms in (1) come from an expansion in powers of the distance to the fixed point. The first one is proportional to the distance measured along the ϕ^4 axis. The second could be proportional to the distance to the ϕ^4 axis measured along another axis (ϕ^5 for example). This approach supposes distances sufficiently small to allow a linear treatment. However if this treatment formally gives the first terms of an expansion it does not allow either an estimation of the higher terms or the domain of validity of the truncated expansion. It is clear that calculations done in the whole abstract space are impossible. Instead one can do nonlinear calculations along one axis (the ϕ^4 axis). This presents the advantages of determining the limit of the linear treatment of the pure ϕ^4 model and of measuring the influence of the other axis in a comparison with the real critical behaviour farther from the CP.

Nonlinear treatments have already been considered by many authors in the spirit of the work of Riedel and Wegner [17]. However the calculations were limited in the best case [18] to 2nd order in the ε -expansion ($\varepsilon = 4 - d$) for static properties. This cannot give sufficient numerical accuracy to be useful in comparison with experiment.

The calculations of Nickel *et al.* [19] up to 6th order in the Feynman graph expansion at $d = 3$, contain all the information needed for a complete nonlinear RG treatment of the critical isochore above T_c . We have carried out this nonlinear analysis and obtained with great accuracy the variations of the complete set of measurable quantities (ξ , χ and C) in terms of the theoretical scaling field t which near the CP is proportional to τ [8].

We stress that the numerical accuracy obtained by Le Guillou and Zinn-Justin [10] for critical exponents is maintained throughout our study. The object of this letter is not to give the details of the calculations, which shall be presented in a forthcoming publication [20], but to discuss the implications of the results for an improved comparison with experiment.

In the following, we limit ourselves to a simple presentation of our numerical results and to a discussion of their relevance to real critical behaviour according to the fundamental hypothesis of the RG.

2. Numerical results of the nonlinear analysis.

The final results of our nonlinear RG treatment are presented in terms of three dimensionless functions (ξ^* , χ^* and C^*) depending on one dimensionless variable (t^*) defined below. This latter is the scaling field which in the RG approach is supposed to vanish linearly with τ . The other scaling field (h^*), the ordering scaling field, is not present in our results which concern only the critical isochore ($h^* = 0$), this field being supposed to vanish with the physical one (H), conjugate to the order parameter.

The nonlinear treatment accounts, in the ϕ^4 model, for a crossover between critical ($t^* \rightarrow 0$) and « classical » ($t^* \rightarrow \infty$) behaviours. The functions given in table I display these crossover behaviours.

In reading this table, one must keep in mind that our study can be seen as an extension in t^* of the sophisticated analysis of [10] at the CP. We have been led to numerically determine the crossover behaviour for discrete values of t^* . It seems to us more convenient, for a practical exploitation, to present these numerical results in terms of phenomenological continuous functions (see Eqs. (2, 3)) which reproduce within a relative error of less than 10^{-4} , the numerically calculated variations with t^* of ξ^* , χ^* and C^* . As in [10], the analysis yields error bars and we give, in table I, the results of the smoothing of the upper and lower envelopes of our calculations (min and max bounds).

Table I. — Numerical characteristics of the dimensionless functions (F^*) of t^* (defined in the text) which reproduce the classical to critical crossover behaviour of ξ^* , χ^* and C^* from the ϕ^4 model at $d = 3$. The numbers are obtained via nonlinear RG calculations in the ϕ^4 model (Ref. [20]).

$F^*(z) = Z_F z^{(-\lambda_F)} \overline{F}(z) + B$; $\overline{F}(z) = \prod_i (1 + X_i z^{D_i(z)})^{Y_i}$; $D(z) = \Delta - 1 + (S_1 \sqrt{z} + 1) / (S_2 \sqrt{z} + 1)$; $z = t^*$									
F^*	Bounds	λ_F	Z_F	B	Δ	i	X_i	Y_i	S_i
ξ^*	(v)					1	26.411	0.1496	13.430
						2	15.667	0.0752	13.314
	max (I)	0.63050	0.4706		0.4913	3	6.1350	0.0316	
						4	1.0012	0.0047	
	min (II)	0.62912	0.4781		0.5003	1	75.151	0.0117	99.989
						2	4.6333	0.0442	100.02
χ^*	(γ)					1	18.118	0.4524	10.731
	max (I)	1.24194	0.2629		0.4910	2	2.3543	0.0311	10.635
						3	0.0705	0.0004	
	min (II)	1.23949	0.2698		0.5006	1	36.047	0.0735	89.037
						2	3.1677	0.0430	89.090
						3	15.651	0.3624	
C^*	(α)					1	34.820	0.2379	17.861
	max (II)	0.11264	1.6017	-3.623	0.5003	2	10.834	-0.022	17.867
						3	12.918	0.0094	
	min (I)	0.10850	1.7341	-3.830	0.4913	1	36.456	0.2226	101.32
						2	12.331	-0.055	100.44
						3	13.931	0.0492	

Table I defines functions of t^* , whose general form we have chosen to be as follows :

$$F(t^*) = Z_F(t^*)^{-\lambda_F} \prod_i (1 + X_i t^{*D(t^*)^{y_i}} + B \quad (2)$$

$$D(t^*) = \Delta - 1 + (S_1 \sqrt{t^*} + 1)/(S_2 \sqrt{t^*} + 1). \quad (3)$$

Comparing with (1), one can easily check that in the limit $t^* \rightarrow 0$, λ_F and Δ are nothing but the critical and subcritical exponents (λ_F , Δ_1), Z_F and $\sum_i X_i Y_i$ the leading and first correction amplitudes (f_0^+ , a_ξ^1). B is the « background » term needed for C^* only.

From the values given in table I one can readily verify that all the known universal features of asymptotic critical behaviour are very precisely reproduced, namely :

- the scaling laws for critical exponents within each bound (I or II);
- the values of the critical and subcritical exponents of [10] with a similar accuracy;
- the value [11] of the universal combinations R_ξ^+ [21] between ξ and C in table I : $R_\xi^+ \equiv (\alpha Z_c)^{1/3} \times Z_\xi$;
- the values [12] of the universal ratios [22] of the first correction amplitudes.

For guidance, we point out that the phenomenological function $D(t^*)$ accounts for a crossover effect between the values $1/2$ as $t^* \rightarrow \infty$ and Δ (~ 0.5) as $t^* \rightarrow 0$ for the subcritical exponent. This gives an idea of the precision of this work.

Although the various functions (ξ^* , χ^* and C^*) contain, as $t^* \rightarrow 0$, the essential universal features of exponents, leading and correction amplitude ratios, they are not universal. From table I, it is not evident where the nonuniversality which characterizes a given system appears. One can easily realize that the dimensionless character of the quantities (F^* and t^*) involves part of this nonuniversality but another part results from the fundamental hypothesis of the RG approach.

In the following section, we discuss this point by looking at the theoretical framework of our calculations for allowing comparison with experiments and determining the validity conditions of the model used.

3. Nonuniversal parameters and two scale factor universality.

The functions that we have calculated are obtained with the ϕ^4 -Landau-Ginzburg-Wilson « Hamiltonian » which, using the usual notations, reads :

$$\mathcal{H}(\{\phi\}) = \int d^d x \left[\frac{1}{2} (\nabla \phi)^2(x) + \frac{r_0}{2} \phi^2(x) + \frac{g_0}{4!} \phi^4(x) - h \phi(x) \right] \quad (4)$$

$\phi(x)$ is the fluctuating order parameter value associated with a small volume of size L^d located at x . L is some arbitrary length greater than the range of the molecular forces a .

The quantities r_0 , g_0 and h are analytic functions of τ and H [8]. From standard fluctuation theory, the probability distribution of ϕ is proportional to $\exp(-\mathcal{H})$. As needed in the approach to the CP, the original Wilson ideas [8] allow all the fluctuations of any wavelength L between a and ξ to be taken into account by successive renormalizations of $\mathcal{H}$. The RG approach clearly breaks down when $\xi/a \sim 1$.

In the Callan-Symanzik version [7] of Wilson ideas, L (and thus a) is set, *a priori*, equal to zero and the renormalization process comes to relate the bare parameters (r_0 , g_0 , h) to renormalized ones through functions of renormalization which have been calculated within the Feynman graph expansion at $d = 3$ up to 6th order [19]. Our final results have been expressed in terms of the bare parameters which are the physical parameters.

We have defined the critical scaling field as $t = r_0 - r_{0c}$ [23], r_{0c} being the value of r_0 at which the inverse susceptibility vanishes while $h = 0$.

The nonuniversality of the model used enters through the three quantities t , h and g_0 . In other words, once they are identified for a given real system, any more explicit reference to that system disappears and only the universal features of the critical behaviour are left.

Let us detail how our functions depend on t , h and g_0 . The dependence on g_0 , the single dimensioned parameter at the CP, is simply given from dimensional analysis.

One easily verifies that $t^* = t/g_0^2$, $\xi^* = \xi/g_0$, $\chi^* = \chi/g_0^2$ and $C^* = C/g_0^3$ while $h^* = h/g_0^{5/2}$. ξ is the 2nd moment of the correlation function, χ and $(-C)$ the 2nd derivative, with respect to h and t respectively, of G defined by $\exp(-G) \propto \int \mathcal{D}\phi \exp(-\mathcal{K}\{\phi\})$. Along the critical isochore, $h = 0$, only the variable t^* remains. We are now in position to introduce the nonuniversal parameters implicitly contained in t , h and g_0 .

As noted above, these three quantities are supposed to be analytic functions of the physical critical variables τ and H . This means that near the CP :

$$\begin{aligned} t^* &= \theta\tau + 0(\tau^2, \tau H) \\ h^* &= \psi H + 0(H^2, \tau H) \\ g_0 &= \text{const.} + 0(\tau, H). \end{aligned} \quad (5)$$

While the neglected terms in these expansions lead to analytic corrections [24] it would not be consistent to consider them in the model used since other contributions have been dropped (for example ϕ^5 , ϕ^6) which could induce even greater corrections as explained in the introduction.

It seems that a contradiction could exist between the linearization of (5) and the nonlinear treatment of the ϕ^4 model. However, we stress the fact that the relations between the scaling fields t^* and h^* and the physical variables τ and H are essentially nonuniversal. Now the fundamental concept of universality in critical phenomena is closely related to the linearization of (5). Two scale factor universality [21], which states that within the same class of universality each system is characterized by only two scales (here θ and ψ) related to τ and H , is its ultimate and most general expression (including the first correction to scaling). In this context it is not clear that precise knowledge of the relations (5) in a large range of τ and H should be of some interest. Only the validity domain of the linearization of (5) seems to us of importance. This domain gives a definition of the critical domain which is not *a priori* known for a given real system (θ and ψ are not universal). Our functions which are well defined for any t^* (and for any τ through θ) could yield the opportunity to measure this critical domain. Any systematic deviation of the experimental data from our functions, as τ increases, will show that either one is out of the critical domain or higher transients have become relevant. We note that the range of τ where no systematic deviations can be observed corresponds to a domain (which belongs to the critical domain) in which two scale factor universality is automatically fulfilled including the first correction. Let us now present precisely how the nonuniversal parameters θ and ψ appear in our functions.

From the definitions of ξ , χ and C given above and (5), we have for comparison with experiment, the relations :

$$\begin{aligned} \xi_{\text{exp}}(\tau) &= \xi^*(\theta\tau)/g_0 \\ \chi_{\text{exp}}(\tau) &= g_0^{-2} \chi^*(\theta\tau)/\psi \\ C_{\text{exp}}(\tau) &= g_0^3 \theta^2 C^*(\theta\tau) + C_{\text{reg}}(\tau). \end{aligned} \quad (6)$$

Apart from dimensional factors which will be discussed in the following paper [25], the subscript « exp » indicates the experimental quantities. $C_{\text{reg}}(\tau)$ is a purely thermodynamic term which has not been accounted for in the treatment of the fluctuations. It must not be confused with the term linked with the constant B in C^* (see Table I) which is purely critical. In the simple fluids, for example, C_{reg} is adjustable. On the contrary, in the binary mixtures, this term could be inde-

pendently estimated as the sum of the specific heat of each component in the same range of T , and should no longer be adjustable.

One can easily see that the introduction of the adjustable parameters θ , ψ and g_0 do not change the universal features — listed in the previous section — of our functions.

In this letter we have set up the theoretical framework of a new kind of experimental data analysis near the CP along the critical isochore for Ising like systems based on a nonlinear treatment of the ϕ^4 model. We have shown that with a very small number of adjustable parameters, the general universal features of the critical behaviour should be globally tested according to the RG theory. In the following paper [25] we consider as an illustration the available experimental data related to ξ , χ [15] and C [26] on the simple fluid xenon.

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