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FINITE SIZE EFFECTS IN PHASE TRANSITIONS

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We develop a systematic approach to the calculations of finite size effects in phase transitions. The method consists of constructing an effective hamiltonian for the homogeneous modes, obtained by tracing out all other degrees of freedom. These modes are obtained by averaging the order parameter over the finite dimensions of the system. These techniques, together with the renormalization group, lead to explicit calculations of universal finite size scaling functions, under the form of $(2+\varepsilon)$ or singular $(4-\varepsilon)$ expansions. Some simple universal results above the upper critical dimension are presented. Simple and universal properties of the rounding of first order transitions are derived.

1. Introduction

Formulated for the first time in 1971 by Fisher [1], the finite size scaling (FSS) properties in the vicinity of a critical point, or at first order transitions, are more and more studied and used for practical purposes. It is almost invariably used as an efficient extrapolation procedure for numerical simulations of Monte Carlo type limited in general to rather small samples. It is also the basis of the powerful phenomenological renormalization group method [2]. A recent review article on FSS by Barber [3] describes many other aspects of the subject.

In this work we consider some new aspects of FSS; in particular we discuss analytical means of calculating the size-dependent universal scaling functions through ε-expansions, a problem left unanswered by previous renormalization group attempts to understand FSS [4-6]. Indeed in ref. [4] it was shown that, above the upper critical dimension, four for our purposes here, since the lattice spacing cannot be removed from the problem - there is a trivial critical point, but no scaling limit - this additional length scale must be included in the finite size formulation. This fact, equivalent to Fisher's dangerous irrelevant variables [7] description, had the more serious consequence that an attempt to expand below four dimensions in ε yielded a singularity, a power $\varepsilon^{1/3}$ in the case considered in ref. [4], and it was not at all clear that any expansion could be envisaged. In this work we describe a systematic method applicable below the upper critical dimension. We have focused our attention on two different geometrical shapes though the method could easily be extended to different boundary conditions, different shapes etc.... The first case corresponds to a periodic cube of volume L^d (it would be trivial to modify it for a large rectangular box with sizes going to infinity simultaneously); this case is encountered in numerical simulations. The second case corresponds to a cylindrical geometry: a tube of "square" basis (or L^{d-1} in general dimension) infinite along one direction, called "time" in this work since it corresponds to a hamiltonian (or transfer matrix) formulation of the problem; periodic boundary conditions are imposed on the "square". In the first case we use discrete Fourier analysis along the d dimensions and the leading long-distance singularities correspond to the zero-momentum component $\varphi \equiv \Phi(\boldsymbol{q}=0)^{\star}$. All non-zero modes may be treated perturbatively (within the ε-expansion) and we compute an effective action for this mode φ by tracing out all the $\boldsymbol{q}$ non-zero modes

$$\exp\left(-S_{\mathrm{eff}}[\varphi]\right) = \sum_{\{\Phi_q\}}{}' \exp\left(-S[\Phi]\right).$$

The averages are finally performed with the Boltzmann weight $\exp(-S_{\mathrm{eff}}[\varphi])$. This turns out to lead to a systematic expansion in powers of $\varepsilon^{1/2}$.

In the cylindrical case, after Fourier analysis over the $(d-1)$ finite dimensions, we can isolate the leading long-distance modes $\varphi(\tau) = \Phi(\tau, \boldsymbol{q}_{\perp}=0)$, which depend upon the position τ, along the axis of the cylinder. The same procedure, namely tracing out all modes except $\varphi(\tau)$, yield an effective action $S_{\mathrm{eff}}[\varphi(\tau)]$ which may be written, for large L, as the integral over a local "lagrangian" density:

$$S_{\mathrm{eff}}[\varphi(\tau)] = \int_0^{\infty} \mathrm{d}\tau\, L_{\mathrm{eff}}(\varphi, \dot{\varphi}).$$

The remaining sum over the $\varphi(\tau)$ modes corresponds to an (imaginary time) Feynman path integral and may be conveniently replaced by a Schrödinger equation, in the usual way. The spectrum of this Schrödinger operator provides the FSS functions that we are looking for. The results take the form of an expansion in powers of $\varepsilon^{1/3}$. The calculations can be performed for an arbitrary number n of components of the order parameter. In the large-n limit one recovers the $\varepsilon^{1/3}$ singularity discussed in ref. [4], but with now a systematic handle on the corrections.

As a byproduct we have also considered the situation above the upper critical dimension, in which some very simple results, which do not seem to have been noticed up to now, are derived. They are based upon the same technique, which simplifies considerably since corrections to the tree-level approximation for the effective action of the φ or $\varphi(\tau)$ modes respectively, are irrelevant. As a result we have obtained some universal answers above dimension four. For instance we have considered in the cubic geometry the ratio M_4/M_2^2 (in which $M = (1/N)\sum_1^N S_i$, and $M_n = \langle M^n \rangle$), which is related at T_c to the renormalized coupling constant. Above four dimensions, for an Ising-like system for instance, one obtains at T_c

$$\frac{M_4}{M_2^2} = \frac{1}{8\pi^2}[\Gamma(\tfrac{1}{4})]^4 \simeq 2.188440.$$

* Other boundary conditions would lead to different calculations and different results, even if translation invariance is not broken (twisted periodic conditions for instance).

We also considered in this work some aspects of FSS for broken continuous symmetries below T_c, which has recently been extensively studied by Fisher and Privman [8]. In these problems the quasi-Goldstone modes dominate the long distance properties in the infinite volume limit, at fixed temperature below T_c. The FSS analysis of the spin wave fluctuations (i.e. the non-linear σ model) leads to a zero-temperature fixed point. The properties may thus be related to a low temperature expansion and studied in a $(2+\varepsilon)$ expansion.

We have considered FSS properties at Ising-like first-order transitions [9] within the same technique of isolating the non-perturbative long-distance modes. Although the correlation length of the infinite system remains finite at and below the first order transition, simple and universal results for the rounding of these transitions may be obtained. This universality results from the divergence of the finite size correlation length with the size of the system.

Finally some additional results about rounding in n-vector models below T_c are discussed.

The paper is organized as follows. In sect. 2 we review briefly the renormalization group set-up and its consequence in the presence of boundaries. In sect. 3 we discuss FSS in a cubic geometry; results for dimensions larger than four are derived, and afterwards we discuss the principles - and compute the first terms - of the $\varepsilon^{1/2}$ expansion. Sect. 4 deals with the cylinder $L^{d-1}\times\infty$ and the $\varepsilon^{1/3}$ expansion. Sect. 5 is devoted to spin waves and the corresponding $(2+\varepsilon)$ expansion. Finally in sect. 6 we discuss some properties of FSS for first-order transitions.

2. Renormalization group and FSS

Let us briefly recall here the renormalization group formalism in the presence of (periodic) boundaries and its application to FSS [4]. It is well-known that there are many ways of writing renormalization group transformations (though, naturally, the physics is independent of this arbitrariness) and it is convenient in order to describe FSS to use a continuum description. In this scaling limit (or renormalized theory), all the renormalizations, namely of the magnitude of the order parameter, of the coupling constant, the shift of the critical temperature, are defined in the infinite volume bulk theory. This scaling limit exists only below the upper critical dimension. In this continuum theory or scaling limit, the lattice spacing has completely disappeared; the integrations over the wave vectors of the fluctuations are performed without cut-off and they are convergent. If some of the dimensions of the sample are finite the integrations over the corresponding momenta are replaced by discrete sums. These sums still extend to infinity, since we have taken a zero lattice spacing, but they converge exactly as the infinite volume integrals. The sides of the sample are finite if expressed in units of the dimensional scale of the renormalized theory, which is infinite in lattice spacing units. We therefore limit ourselves to a regime in which L/a and ξ/a go simultaneously to infinity, however their ratio L/ξ is finite and remains at our disposal. This is precisely the regime in which FSS is expected to hold. Since there is no need for any new renormalization in this scheme (if we use periodic boundary conditions) we obtain the usual renormalization group equations, without any renormalization of L. (The situation is very similar to that of a field theory, such as QED, at finite temperature. The integrals over frequencies are replaced by discrete sums but the renormalizations are temperature independent [10]).

In a ϕ^4, Landau-Ginzburg-Wilson formalism [11], the observables depend upon the temperature $t=(T-T_c)/T_c$, the dimensionless coupling constant g, a length l in order to fix up the renormalization procedure, and the finite size parameter L. For an observable X of (length) dimension p_x, we conclude from the previous analysis [12] that, for a dilatation ρ

$$X[t, g; l; L]=\zeta(\rho)X[t(\rho), g(\rho), l\rho; L], \tag{2.1}$$

which summarizes the renormalization group transformation and the non-renormalization of L. From the bulk problem one knows that for large dilatations $g(\rho)$ approaches the infrared stable fixed point g^*,

$$t(\rho)\approx t\rho^{(1/\nu)-2} \qquad \text{and} \qquad \zeta(\rho)\approx\rho^{(\gamma_x/\nu)-p_x},$$

in which γ_x is the bulk exponent of $X: X \underset{t\to 0}{\approx} t^{-\gamma_x}$. Using now dimensional analysis, together with eq. (1), one obtains

$$X[t, g; l; L]=(\rho l)^{p_x}\zeta(\rho)X[t(\rho)(l\rho)^2, g(\rho), 1; L/l\rho]. \tag{2.2}$$

Choosing $\rho=L/l$, which is a large parameter, we obtain the well-known FSS result

$$X[t, g; l; L]=t^{-\gamma_x}f[tL^{1/\nu}], \tag{2.3}$$

in which the function f is universal (up to scales fixing).

Let us next consider the FSS renormalization group for an n-vector model below T_c. The long-distance properties of the bulk system are governed by massless spin wave excitations, whose fluctuation properties are reproduced by the non-linear σ-model [13, 14]. Observables are now functions of a coupling constant t, equal to kT divided by the (renormalized) spin stiffness constant, of a renormalization scale l, and of the sizes L. Instead of eq. (2), one obtains in a similar way,

$$X[t; l; L]=(\rho l)^{p_x}\tilde{\zeta}(\rho)X[t(\rho); 1; L/l\rho]. \tag{2.4}$$

With the same choice for ρ, we have to consider the behaviour of $t[L/l]$. From the β-function we know that there is an ultraviolet stable fixed point at the critical temperature, and an infra-red stable fixed point at $t=0$ (zero temperature). In the large-ρ limit $t(\rho)$ is thus governed by the zero-temperature fixed point. The large-ρ behavior of $t(\rho)$ is given by the lowest term of the β-function [14] and

$$t(\rho) \underset{\rho\to\infty}{\sim} \rho^{-(d-2)}. \tag{2.5}$$

For large L, $\tilde{\zeta}(L/l)$ has a limit which is a function of t, and in the spin wave regime (fixed temperature below T_c) one recovers from (2.4) the FSS property

$$X[t;l;L]=X_\infty[t]\left(\frac{L}{\xi(t)}\right)^{p_x} f\left(\frac{\xi(t)}{L}\right), \tag{2.6}$$

in which $f(u)$ is calculable in a low-temperature perturbation theory.

The correlation length $\xi(t)$ is equal to [14]

$$\xi(t)=lt^{1/(d-2)}\exp\left\{\int_0^t \mathrm{d}t'\left[\frac{1}{\beta(t')}-\frac{1}{(d-2)t'}\right]\right\} \tag{2.7}$$

with, at one-loop order,

$$\beta(t)=(d-2)t-\frac{n-2}{2\pi}t^2+\mathrm{O}(t^3)\,. \tag{2.8}$$

Near the critical point $\xi(t)$ diverges as $(t_c-t)^{-\nu}$ (with $\nu=-\beta'(t_c)$); at low temperature (t small),

$$\left(\frac{\xi(t)}{l}\right)^{d-2}=t\left[1+\frac{n-2}{d-2}\frac{t}{2\pi}+\mathrm{O}(t^2)\right]. \tag{2.9}$$

This implies that the low-temperature scaling variable is proportional to

$$tL^{-(d-2)}\left[1+\frac{n-2}{d-2}\frac{t}{2\pi}+\mathrm{O}(t^2)\right].$$

In a magnetic field similar arguments lead to

$$X[t,H;l;L]=L^{p_x}f\left[\frac{\xi(t)}{L},\frac{H\sigma(t)\xi^d(t)}{t}\right], \tag{2.10}$$

in which $\sigma(t)$ is the spontaneous magnetization [14]

$$\sigma(t)=\exp\left\{-\frac{1}{2}\int_0^t \mathrm{d}t'\frac{\zeta(t')}{\beta(t')}\right\} \tag{2.11}$$

with, at one-loop order,

$$\zeta(t)=(n-1)\frac{t}{2\pi}+\mathrm{O}(t^2)\,. \tag{2.12}$$

The magnetization vanishes with a power β at T_c and may be expanded at low temperature as

$$\sigma(t)=\left[1-\frac{1}{2}\frac{n-1}{d-2}\frac{t}{2\pi}+\mathrm{O}(t^2)\right]. \tag{2.13}$$

In sect. 5 we compute in the $(d-2)$ expansion the correlation length ξ_L in zero field, for a cylinder geometry.

3. FSS for a periodic cube

In the critical domain we can replace the spin hamiltonian, by a Landau-Ginzburg-Wilson [11] model, for an n-component order parameter

$$S[\Phi]=\int_v \mathrm{d}^d x\left\{\tfrac{1}{2}(\nabla\boldsymbol{\phi})^2+\tfrac{1}{2}r_0\boldsymbol{\phi}^2+\frac{1}{4!}u_0(\boldsymbol{\phi}^2)^2\right\} \tag{3.1}$$

with some ultra-violet cut-off $\Lambda\approx a^{-1}$ (a is the lattice spacing). In a finite periodic box we expand Φ in Fourier modes

$$\boldsymbol{\Phi}(\boldsymbol{x})=\sum_q \mathrm{e}^{i\boldsymbol{q}\cdot\boldsymbol{x}}\boldsymbol{\varphi}_q \tag{3.2}$$

in which each component of $\boldsymbol{q}$ runs over discrete values, multiples of $2\pi/L$, and is still cut-off at a^{-1}. As long as L is finite, the oscillations in the q non-zero modes will be damped, even at bulk T_c, by the q^2 restoring force of the kinetic energy. However there is nothing to prevent the mode

$$\boldsymbol{\varphi}\equiv\boldsymbol{\varphi}(\boldsymbol{q}=0) \tag{3.3}$$

from growing at bulk T_c, and therefore it cannot be treated perturbatively. In other words the propagator of Φ has an isolated pole at $q=0$, and diagrams involving a φ-loop would be divergent. The method consists of computing the effective action for φ defined by tracing out all modes except φ in perturbation theory (or rather in the loop expansion). Physical observables are then calculated, without any further approximation, since φ is certainly not small, with the averaging weight $\exp[-S_{\mathrm{eff}}(\varphi)]$. Finally the renormalization group equations of sect. 2 are used. Let us first illustrate this program in the simple case of dimensions larger than four.

3.1. $d\geqslant 4$

Splitting as usual r_0 into t, which vanishes at T_c, and a counterterm (r_0-t), we obtain the effective action at the tree level, by ignoring the $\Phi_{q\neq 0}$ modes and the mass counterterm since they would both contribute only to loops. This procedure will be justified below. At the tree level we thus obtain

$$S_{\mathrm{eff}}(\varphi)=L^d\left\{\frac{1}{2}t\boldsymbol{\varphi}^2+\frac{1}{4!}u_0(\boldsymbol{\varphi}^2)^2\right\}. \tag{3.4}$$

Let us note that $\boldsymbol{\varphi}$ is nothing but the total spin per unit volume

$$\boldsymbol{\varphi} = \frac{1}{v} \int_v \mathrm{d}^d x \, \boldsymbol{\Phi}(x) . \tag{3.5}$$

We have kept only one collective mode, a stochastic uniform magnetization of the system, and this explains why one finds a factor of the volume in front of the action (3.4). This collective mode is treated exactly whereas the others may be eliminated by a perturbative scheme.

We now compute averages of $\boldsymbol{\varphi}$, such as

$$M_{2p} = \langle (\boldsymbol{\varphi}^2)^p \rangle = \frac{\int \mathrm{d}^n \boldsymbol{\varphi} (\boldsymbol{\varphi}^2)^p \exp(-S_{\text{eff}})}{\int \mathrm{d}^n \boldsymbol{\varphi} \exp(-S_{\text{eff}})} . \tag{3.6}$$

A simple rescaling of $\boldsymbol{\varphi}$

$$\boldsymbol{\varphi} \to (u_0 L^d)^{-1/4} \boldsymbol{\varphi} \tag{3.7}$$

leads to the scaling relation

$$M_{2p} = (u_0 L^d)^{-p/2} f_{2p}[t L^{d/2} u_0^{-1/2}] , \tag{3.8}$$

in which f_{2p} is given by the ratio of two single integrals:

$$g_{2p}(x) = \int_0^\infty \mathrm{d}\varphi \, \varphi^{2p+n-1} \exp\left(-\left(\tfrac{1}{2} x \varphi^2 + \tfrac{1}{24} \varphi^4\right)\right) \tag{3.9}$$

with

$$f_{2p}(x) = \frac{g_{2p}(x)}{g_0(x)} . \tag{3.10}$$

Eq. (3.8) shows that, above dimension four, the usual FSS does not hold. Consider for instance the magnetic susceptibility

$$\chi = \frac{1}{r} \int \mathrm{d}^d x \langle \boldsymbol{\phi}(x) \cdot \boldsymbol{\phi}(0) \rangle = \frac{L^d}{n} M_2 . \tag{3.11}$$

From (3.8) one obtains

$$\chi(r, L) = L^{d/2} f(t L^{d/2}) \tag{3.12}$$

and since t vanishes linearly with the temperature we can write (3.12) as

$$\chi(t, L) = t^{-1} \tilde{f}(L^{(d-4)/4} \times L/\xi) \tag{3.12'}$$

which exhibits the classical exponent $\gamma = 1$, together with the breakdown of FSS, identical to that found in ref. [4] in the large-n limit and suggested for finite n in ref. [9].

The universal character of the result (3.8) above dimension four is even more explicit if we work at bulk T_c ($t=0$) and consider dimensionless ratios which eliminate any dependence upon u_0. For instance the ratios

$$r_p(T) = \frac{M_{2p}}{(M_2)^p} \tag{3.13}$$

are given in terms of the scaling variable $x = rL^{d/2}u_0^{-1/2}$ as

$$r_p(T) = \frac{g_{2p}(x) g_0^{p-1}(x)}{(g_2(x))^p} \tag{3.13'}$$

in which $g(x)$ is defined in eq. (3.9).

At T_c ($x=0$) an elementary calculation gives for an n-vector model,

$$r_p(T_c) = \frac{\Gamma(\frac{1}{4}(2p+n))[\Gamma(\frac{1}{4}n)]^{p-1}}{[\Gamma(\frac{1}{4}(n+2))]^p}\,. \tag{3.14}$$

The renormalized coupling constant is related to

$$r_2(T_c) = \frac{M_4}{M_2^2} = \frac{\langle(\boldsymbol{\varphi}^2)^2\rangle}{\langle\boldsymbol{\varphi}^2\rangle^2} = \frac{n+2}{3n}\,\frac{\langle\varphi_1^4\rangle}{\langle\varphi_1^2\rangle^2}$$

and from (3.14) we obtain

$$r_2(T_c) = \frac{n}{4}\,\frac{\Gamma^2(\frac{1}{4}n)}{\Gamma^2(\frac{1}{4}n+\frac{1}{2})}\,. \tag{3.15}$$

For Ising-like models in particular, we predict from (3.15) that for any $d \geqslant 4$

$$r_2(T_c) = \frac{\Gamma^4(\frac{1}{4})}{8\pi^2} \simeq 2.1884396\,. \tag{3.16}$$

Recent Monte Carlo measurements by Binder et al. [15, 16] on a five-dimensional Ising system, for lattices of linear sizes up to $L=7$, give an estimate $r_2(T_c) = 2.0$.

What is the effect of loop corrections that we have neglected in (3.4)? Apart from a shift of the critical temperature they yield a series of diagrams, which are not singular for large L, according to the well-known power counting arguments. Two kinds of terms are generated by these loop corrections. The first type corresponds to operators which would contribute to the infinite volume limit: they lead to a finite renormalization of u_0 and to higher powers of $\boldsymbol{\varphi}^2$:

$$\delta S^{(1)} = L^d(\delta u_0(\boldsymbol{\varphi}^2)^2 + v(\boldsymbol{\varphi}^2)^3 + \cdots)\,. \tag{3.17a}$$

Performing again the rescaling (3.7) of φ one finds immediately that higher operators such as φ^6 are down at least by powers of $(a/L)^{d/2}$.

In addition there are small corrections, vanishing for $d=4$ in the infinite volume limit, which come from the sum over the lowest discrete modes. As an example let us compute the one-loop corrections to $S_{\text{eff}}(\varphi)$ coming from the gaussian integration over the $\phi_{q\neq 0}$ modes:

$$\sum_{q\neq 0} \ln\left(1+\frac{u_0}{2(q^2+t)}\varphi^2\right);$$

(for simplicity we have restricted ourselves to $n=1$). This leads to operators of the form considered in (3.17a) and to corrections coming from the lowest non-zero momenta:

$$\delta S^{(2)} = c_1 L^2 \varphi^2 + c_2(L^2\varphi^2) + \cdots . \tag{3.17b}$$

The same rescaling shows that these terms contribute to corrections proportional to $(a/L)^{(d-4)/2}$. Consequently, as was said earlier, the tree level approximation which led to the scaling relations (3.8) is exact for large L. In addition there are correction terms multiplied by the small factor $(a/L)^{(d-4)/2}$ which are of the same scaling form (3.8). In particular the coefficient of φ^2 in (3.17b) can be absorbed into a shift of the temperature at which the total coefficient of φ^2 vanishes. This defines, as in ref. [15], an effective critical temperature $T_c(L)$ which differs from the bulk T_c by an amount proportional to $L^{-(d-2)}$ (this conflicts with ref. [16], in which this shift was assumed to be proportional to $L^{-d/2}$).

3.2. $d=4-\varepsilon$

At the tree level (or lowest order in ε) the same effective action (3.4) will govern the long distance limit and at this order we recover the same form (3.8) for the result. Furthermore, in less than four dimensions, loop corrections are responsible of strong long-distance singularities, that are dealt with through the renormalization group formalism and the ε-expansion. Using eq. (2.2), we know that the dimensionless ratios r_p of eq. (3.13) satisfy

$$r_p(t, u_0, L) \underset{L\,\text{large}}{\sim} r_p(t(L)L^2, u_0^*);\tag{3.18}$$

the fixed point u_0^* being of order ε, one notes already from (3.18) and (3.8) the presence of an $\varepsilon^{-1/2}$ singularity (analogous to the $\varepsilon^{-1/3}$ singularity discussed in ref. [4]). However this singularity is explicit in terms of the integrals (3.9) and we can still perform loop corrections by integrating perturbatively on the non-zero q modes. At one-loop this integration generates a shift of T_c, a change of u_0, and new operators involving powers of φ larger than four. We first consider the shift of t, and the renormalization of u_0 and argue afterwards that the other terms lead to (calculable) higher order corrections.

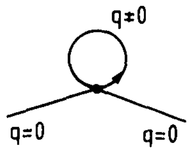
From now on we will work within the renormalized theory. The renormalized coupling constant u_R is expressed in terms of the dimensionless coupling constant

$$g = l^{\varepsilon} u_R ,\tag{3.19}$$

in which l is an arbitrary length scale. The minimal subtraction scheme [13] is used throughout all these calculations. In this scheme, the counterterms of the massless theory including the φ^2 insertion counterterm are introduced; the one-loop counterterm for the coupling constant and the φ^2 insertion will be the only one relevant in the lowest corrections.

3.3. SHIFT OF T_c

The simple diagram



$$= gl^{-\varepsilon}\frac{n+2}{6}\sum_q{}' \frac{1}{(q^2+t)}, \tag{3.20}$$

combined with the one-loop φ^2 counterterm yields a finite shift of t (we now use the system of units in which $l=1$):

$$t \to \tilde{t} = t + \tfrac{1}{12}(n+2)\hat{g}t \ln t + \tfrac{1}{3}(n+2)\hat{g}L^{-2}\int_0^\infty \mathrm{d}u\, \mathrm{e}^{-utL^2/4\pi^2}[A^4(u) - 1 - \pi^2/u^2] + \mathrm{O}(\hat{g}^2), \tag{3.21}$$

in which

$$\hat{g} = g\frac{2\pi^{d/2}}{\Gamma(\frac{1}{2}d)(2\pi)^d} = \frac{g}{8\pi^2}[1 - \tfrac{1}{2}\varepsilon(C - 1 - \ln 4\pi) + \mathrm{O}(\varepsilon^2)], \tag{3.22}$$

$$A(u) \equiv \sum_{-\infty}^{+\infty} \mathrm{e}^{-un^2}. \tag{3.23}$$

For large u, $A(u)-1$ decreases exponentially and the integral (3.21) converges at infinity, even at T_c ($t=0$). For small u, the Poisson transformation of (3.23)

$$A(u) = \left(\frac{\pi}{u}\right)^{1/2} \sum_{-\infty}^{+\infty} \mathrm{e}^{-n^2\pi^2/u} = \left(\frac{\pi}{u}\right)^{1/2} A(\pi^2/u), \tag{3.23'}$$

shows that (3.21) converges.

Let us show in more detail how one goes from (3.20) to (3.21). We first write the integral representation

$$\begin{aligned}\frac{1}{L^d}\sum_q{}' \frac{1}{q^2+t} &= \frac{1}{L^d}\sum_q{}' \int_0^\infty \mathrm{d}u\, \mathrm{e}^{-u(t+q^2)} \\ &= L^{-d}\int_0^\infty \mathrm{d}u\, \mathrm{e}^{-ut}\left[\left(\sum_{-\infty}^{+\infty} \mathrm{e}^{-u(4\pi^2n^2/L^2)}\right)^d - 1\right].\end{aligned} \tag{3.24}$$

An analytic continuation in d is required to give a meaning to the integral (3.24) which diverges at small u (i.e. in the ultraviolet) for $\mathrm{Re}\, d > 2$. Subtracting and adding the asymptotic behaviour at small u, given by (3.23′), one obtains

$$L^{-d}\sum_q{}'\frac{1}{q^2+t}=\frac{L^{2-d}}{4\pi^2}\int_0^\infty \mathrm{d}u\,\mathrm{e}^{-u(tL^2/4\pi^2)}\left[A^d(u)-1-(\pi/u)^{d/2}\right]$$
$$+\frac{L^{2-d}}{4\pi^2}\pi^{d/2}\Gamma(1-\tfrac{1}{2}d)\left(\frac{tL^2}{4\pi^2}\right)^{d/2-1}. \tag{3.25}$$

The second term of (3.25) is continued analytically above Re $d=2$; it has a pole at $\varepsilon=0$. Therefore keeping the pole and the finite part one obtains

$$\frac{1}{L^d}\sum{}'\frac{1}{q^2+t}=-\frac{t}{8\pi^2\varepsilon}+\frac{t}{16\pi^2}[\ln t-(\ln 4\pi-C+1)]$$
$$+\frac{1}{4\pi^2L^2}\int_0^\infty \mathrm{d}u\,\mathrm{e}^{-utL^2/4\pi^2}\left[A^4(u)-1-\pi^2/u^2\right]+\mathrm{O}(\varepsilon). \tag{3.26}$$

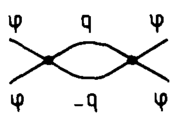
The φ^2 insertion counterterm replaces t by tZ_{φ^2} [12]; at one-loop order, in the minimal scheme, it leads to the replacement $t\to t\,[1+\hat{g}(n+2)/6\varepsilon]$. Therefore the one-loop corrections lead to

$$t\to\tilde{t}=t[1+\hat{g}\tfrac{1}{6}(n+2)]+\frac{g}{L^d}\frac{n+2}{6\varepsilon}\sum{}'\frac{1}{(q^2+t)}. \tag{3.27}$$

Using (3.26) one first verifies that, as renormalization theory implies, the $1/\varepsilon$ pole of the counterterm cancels the pole of the diagram. The finite terms add up to give the eq. (3.21).

3.4. RENORMALIZATION OF THE COUPLING CONSTANT

In a similar way, we add the one-loop counterterm for the coupling constant to the one-loop diagram



$$=\frac{1}{L^d}\sum_q{}'\frac{1}{(q^2+t)^2}$$

and replace, as in (3.27), g by

$$\tilde{g}=g\left[1+\hat{g}\frac{n+8}{6\varepsilon}\right]-g^2\frac{n+8}{6}\frac{1}{L^d}\sum_q{}'\frac{1}{(q^2+t)^2}. \tag{3.28}$$

Similar algebraic transformations lead, after cancellation of the $1/\varepsilon$ poles, to

$$\tilde{g}=g\Bigg[1+\hat{g}\tfrac{1}{12}(n+8)(\tfrac{1}{2}+\ln t)-\tfrac{1}{12}(n+8)\hat{g}\int_0^\infty \mathrm{d}u\,u^{-utL^2/4\pi^2}$$
$$\times[A^4(u)-1-\pi^2/u^2]+\mathrm{O}(\hat{g}^2)\Bigg]. \tag{3.29}$$

Finally, since no higher-order operator contributes at this order, we can use the eq. (3.8), with the same function $f_{2p}(x)$ provided $tL^{d/2}g^{-1/2}$ is replaced by $\tilde{t}L^{d/2}\tilde{g}^{-1/2}$ with $\tilde{t}$ and $\tilde{g}$ given by eqs. (3.21) and (3.29). At the fixed point

$$\hat{g}^* = \frac{6\varepsilon}{n+8} + \mathrm{O}(\varepsilon^2)\,, \tag{3.30}$$

one verifies the FSS, namely all the logarithms do exponentiate provided one introduces the scaling variable

$$y = tL^{1/\nu}\,. \tag{3.31}$$

A few lines of algebra lead indeed to,

$$\begin{aligned}\tilde{t}L^{d/2}\tilde{g}^{-1/2}|_{\text{fixed-point}} = (g^*)^{-1/2}\Big\{ & y - \tfrac{1}{8}\varepsilon y + \frac{n-4}{2(n+8)}\varepsilon y \ln y \\ & + \frac{1}{4}\varepsilon y \int_0^\infty \mathrm{d}u\, u\, \mathrm{e}^{-uy/4\pi^2}\,[A^4(u) - 1 - \pi^2/u^2] \\ & + \varepsilon \frac{2(n+2)}{(n+8)} \int_0^\infty \mathrm{d}u\, \mathrm{e}^{-uy/4\pi^2}\,[A^4(u) - 1 - \pi^2/u^2] + \mathrm{O}(\varepsilon^2)\Big\}\,.\end{aligned} \tag{3.32}$$

Finally the moments M_{2p}, and the ratios r_p, are given by the same formulae (3.8), (3.13') in which one substitutes to $tL^{d/2}u_0^{-1/2}$ the expression (3.32). In particular at T_c ($t=0$, hence $y=0$) we obtain for the ratios $r_p(T_c)$ the result (3.13') in which we substitute for x the value of (3.32) at T_c ($y=0$)

$$\begin{aligned} x_0 &= (g^*)^{-1/2}\left[\frac{2\varepsilon(n+2)}{n+8}\int_0^\infty \mathrm{d}u(A^4(u) - 1 - \pi^2/u^2) + \mathrm{O}(\varepsilon^2)\right] \\ &= \varepsilon^{1/2}\left\{\frac{1}{2}\frac{n+2}{\sqrt{3(n+8)}}\frac{I}{\pi} + \mathrm{O}(\varepsilon)\right\}, \end{aligned} \tag{3.33}$$

in which

$$\frac{I}{\pi} = \frac{1}{\pi}\int_0^\infty \mathrm{d}u(A^4(u) - 1 - \pi^2/u^2) = -1.7650848012\ldots. \tag{3.34}$$

Therefore at this order we obtain for $r_2(T_c)$ for instance instead of (3.14)

$$r_2(T_c) = \frac{g_4(x_0)g_0(x_0)}{(g_2(x_0))^2}\,. \tag{3.35}$$

Expanding in ε (x_0 small) one finds

$$r_2(T_c)=\frac{n}{4}\frac{\Gamma^2(\frac{1}{4}n)}{\Gamma^2(\frac{1}{4}(n+2))}\left\{1-x_0\sqrt{6}\left[\frac{\Gamma(\frac{1}{4}(n+6))}{\Gamma(\frac{1}{4}(n+4))}+\frac{\Gamma(\frac{1}{4}(n+2))}{\Gamma(\frac{1}{4}n)}-2\frac{\Gamma(\frac{1}{4}(n+4))}{\Gamma(\frac{1}{4}(n+2))}\right]\right.$$
$$\left.+6x_0^2\left[\frac{\Gamma(\frac{1}{4}(n+6))\Gamma(\frac{1}{4}(n+2))}{\Gamma(\frac{1}{4}(n+4))\Gamma(\frac{1}{4}n)}+\frac{3\Gamma^2(\frac{1}{4}(n+4))}{\Gamma^2(\frac{1}{4}(n+2))}-n-1\right]+\mathrm{O}(\varepsilon^{3/2})\right\}, \tag{3.36}$$

in which x_0 is given by (3.33).

Setting $\varepsilon=1$ in (3.35) or (3.36) we obtain three-dimensional estimates for an ($n=1$) Ising-like system which are

$$r_2(T_c)=1.800 \quad \text{and} \quad 1.786, \quad \text{respectively}.$$

(instead of (2.19) at order zero). This ε-expansion estimate is not very far from the Monte Carlo measurement of Pearson et al. [18] which gives $g_{\mathrm{Ren}}=-1.4$, i.e. $r_2(T_c)=1.6$.

3.5. HIGHER-ORDER CORRECTIONS

In this calculation we have neglected higher loops, which would lead to corrections of order $\varepsilon^{k+1/2}$ with $k\geqslant 1$, and higher operators such as φ^6, coming from the determinant of gaussian fluctuations, $\sum_q' \log(1+g\varphi^2/(q^2+t))$ (for simplicity written only for $n=1$), expanded in powers of φ. Such higher operators do contribute to the FSS functions, but they are multiplied by higher powers of g (g^3 for φ^6, etc...) and are negligible at this order of the ε-expansion.

4. FSS for a cylinder

In the transfer matrix (or hamiltonian) formulation of the problem, one deals with the geometry of a cylinder (or ribbon, or tube, according to the dimension) infinite along one dimension called time, and finite and periodic in the $(d-1)$ other dimensions. We assume for simplicity that the transverse sizes are all equal to the same length L. The fields are expanded in Fourier modes of fluctuations in the $(d-1)$ directions perpendicular to the axis of the cylinder

$$\Phi(\boldsymbol{x}_\perp,\tau)=\sum_{\boldsymbol{q}_\perp} \mathrm{e}^{i\boldsymbol{q}_\perp\cdot\boldsymbol{x}_\perp}\varphi_{q_\perp}(\tau) \tag{4.1}$$

in which again the components of $q_\perp$ are quantized, in units of $2\pi/L$. The discussion of the sect. 3, may be repeated here: the dangerous modes, which cannot be treated perturbatively, correspond to $\boldsymbol{q}_\perp=0$; however now instead of one single mode, arbitrary functions of τ have to be considered, since nothing prevents

$$\boldsymbol{\varphi}(\tau)\equiv\boldsymbol{\varphi}_{q_\perp=0}(\tau) \tag{4.2}$$

from taking arbitrary large values (at T_c).

The effective action $S_{\text{eff}}[\boldsymbol{\varphi}(\tau)]$, defined by tracing out all the $q_\perp \neq 0$ modes, can be written as the time integral of a local density

$$S_{\text{eff}}[\varphi(\tau)] = \int \mathrm{d}\tau\, L_{\text{eff}}[\varphi(\tau), \dot{\varphi}(\tau)] \,; \tag{4.3}$$

L_{eff}, the euclidean lagrangian of field theory is nothing but the matrix element of the transfer matrix between two infinitesimally close "times". Again let us begin the discussion with the simpler case of a spin system above its upper critical dimension.

4.1. $d \geqslant 4$

Neglecting again loop contributions, one reads immediately the effective action from the LGW formalism (3.1)

$$S_{\text{eff}}[\varphi] = L^{d-1} \int \mathrm{d}\tau \left\{ \tfrac{1}{2}(\dot{\varphi})^2 + \tfrac{1}{2} t \varphi^2 + \frac{u_0}{4!}(\varphi^2)^2 \right\}. \tag{4.4}$$

Averages are now performed with the weight $\exp[-S_{\text{eff}}(\varphi)]$ by summing over all possible trajectories $\boldsymbol{\varphi}(t)$. This is nothing but a Feynman path integral corresponding to an n-dimensional, imaginary time, quantum mechanical problem. Indeed let us recall that Feynman's formulation for the hamiltonian

$$H = \frac{1}{2m}\boldsymbol{p}^2 + V(\boldsymbol{q}) \tag{4.5}$$

gives the evolution operator

$$\langle \boldsymbol{q}_2 | \mathrm{e}^{-TH} | \boldsymbol{q}_1 \rangle = \int_{q(0)=q_1}^{q(T)=q_2} \mathrm{D}q(\tau) \exp\left(- \int_0^T \mathrm{d}\tau [\tfrac{1}{2} m (\dot{\boldsymbol{q}})^2 + V(q)] \right). \tag{4.5$'$}$$

Consequently identifying $\boldsymbol{\varphi}(\tau)$ of (4.4) with $\boldsymbol{q}(\tau)$ of (4.5′) we can associate to the action (4.4) an hamiltonian in n dimensions (note that the mass parameter of (4.5′) is L^{d-1}):

$$H(p, q) = \frac{\boldsymbol{p}^2}{2L^{d-1}} + L^{d-1}\left[\frac{t}{2}\boldsymbol{q}^2 + \frac{u_0}{24}(\boldsymbol{q}^2)^2 \right]. \tag{4.6}$$

The association of a quantum mechanical hamiltonian in $(d-1)$ dimensions to a classical statistical mechanics problem in d dimensions is well-known. Here in addition we have kept only the zero-momentum mode of this $(d-1)$-dimensional hamiltonian. The spectrum of the low-lying states of the hamiltonian (4.6) will govern the exponential decay of correlations along the axis of the cylinder. In particular the gap $(E_1 - E_0)$ between the lowest two levels gives the correlation length

$$\xi_L = (E_1 - E_0)^{-1}, \tag{4.7}$$

according to standard transfer matrix arguments (correlations along the axis of the cylinder correspond to large time separations). The spectrum of this n-dimensional anharmonic hamiltonian (4.6) has to be found by solving a Schrödinger equation. The lowest states being $0(n)$ rotationally invariant, one has to solve a radial one-dimensional problem. However the scaling properties of the eigenlevels may be obtained very simply without any numerical work. Indeed the dilatation

$$\begin{aligned} q &\to L^{-1/3(d-1)} u_0^{-1/6} q , \\ p &\to L^{1/3(d-1)} u_0^{1/6} p \end{aligned} \tag{4.8}$$

shows that the hamiltonian (4.6) may be written as

$$H(p, q) = u_0^{1/3} L^{-(d-1)/3} [\tfrac{1}{2} \boldsymbol{p}^2 + \tfrac{1}{24} (\boldsymbol{q}^2)^2 + \tfrac{1}{2} t u_0^{-2/3} L^{2/3(d-1)} \boldsymbol{q}^2] . \tag{4.9}$$

Therefore any eigenvalue of (4.6) satisfies the scaling property

$$E_\alpha(t, L, u_0) = u_0^{1/3} L^{-(d-1)/3} f_\alpha [t L^{2/3(d-1)} u_0^{-2/3}] . \tag{4.10}$$

Consequently the correlation length ξ_L scales as

$$\xi_L(t, L, u_0) = u_0^{-1/3} L^{(d-1)/3} f [t L^{2/3(d-1)} u_0^{-2/3}] \tag{4.11}$$

in which $f(x)$ is the inverse of the gap of the hamiltonian

$$h = \tfrac{1}{2} \boldsymbol{p}^2 + \tfrac{1}{2} x \boldsymbol{q}^2 + \tfrac{1}{24} (\boldsymbol{q}^2)^2 . \tag{4.12}$$

Let us stress again the breakdown of FSS exhibited by (4.11) which may be written as

$$\xi_L = \xi_\infty(t) g \left[\frac{L}{\xi_\infty(t)} L^{(d-4)/3} \right] \tag{4.13}$$

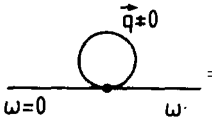
(with $\xi_\infty(t)$ given by the mean-field result $\xi_\infty \propto t^{-1/2}$), in agreement with the large-n result of ref. [4]. Note also the "dangerous irrelevant character" of u_0, manifest in (4.11).

Let us finally show that loop corrections are truly irrelevant. The discussion is completely parallel to the one of sect. 3. Higher-order operators, such as φ^6, will add terms proportional to $L^{d-1}(\boldsymbol{q}^2)^3$ to the hamiltonian (4.6). The rescaling (4.7) shows that such terms provide corrections of relative order $(a/L)^{-2/3(d-1)}$ to the eigenvalues (4.10).

Finally, as in (3.17b), we have to consider the corrections due to the discrete nature of the sums involved in the loop expansion. In order to avoid redundancy in the presentation, this question will be answered after the discussion of the expansion in $\varepsilon = 4 - d$.

4.2. $d=4-\varepsilon$

The discussion follows closely the lines of sect. 3. The shift of T_c given by the diagram



$$= \int \frac{d\omega}{2\pi} \sum_{q_\perp}' \frac{1}{q^2+\omega^2+t},$$

together with the φ^2 insertion counterterm leads, through similar steps to

$$t \to \tilde{t} = t + \hat{g}\tfrac{1}{12}(n+2) t \ln t + \hat{g}\tfrac{1}{3}(n+2)\frac{\sqrt{\pi}}{L^2}$$
$$\times \int_0^\infty \frac{du}{\sqrt{u}} e^{-utL^2/4\pi^2}[A^3(u) - 1 - (\pi/u)^{3/2}] + O(\hat{g}^2). \qquad (4.14)$$

The modification of the coupling constant, together with the one-loop counterterm leads to

$$g \to \tilde{g} = g[1 + \tfrac{1}{12}(n+8)\hat{g}(1+\ln t) - \tfrac{1}{12}(n+8)\hat{g}\frac{1}{\pi^{3/2}}$$
$$\times \int_0^\infty du\sqrt{u}\, e^{-utL^2/4\pi^2}(A^3(u) - 1 - (\pi/u)^{3/2}) + O(\hat{g}^2)\Big]. \qquad (4.15)$$

Neglecting, for the same reasons, irrelevant operators (which are required at higher orders in ε), we substitute in eq. (4.11) $\tilde{t}$ and $\tilde{g}$ to t and u_0 respectively. This gives a scaling variable

$$x = \tilde{t}(\tilde{g})^{-2/3} L^{2/3(d-1)}, \qquad (4.16)$$

which, at the fixed point $\hat{g}^*$, taking into account (4.14) and (4.15), takes the expected scaling form in terms of

$$y = tL^{1/\nu},$$

$$x = (g^*)^{-2/3}\Big\{ y(1-\tfrac{1}{3}\varepsilon) + \frac{\varepsilon}{6}\frac{n-10}{n+8} y \ln y$$
$$+ y\frac{1}{3\pi^{3/2}} \int_0^\infty du\,\sqrt{u}\, e^{-uy/4\pi^2}[A^3(u) - 1 - (\pi/u)^{3/2}]$$
$$+ \varepsilon\frac{2(n+2)}{n+8}\sqrt{\pi} \int_0^\infty \frac{du}{\sqrt{u}} e^{-uy/4\pi^2}[A^3(u) - 1 - (\pi/u)^{3/2}] + O(\varepsilon^2)\Big\}. \qquad (4.17)$$

Consequently we obtain for ξ_L the scaling result

$$\frac{\xi_L}{L} = (g^*)^{-1/3} f[x](1+O(\varepsilon)), \qquad (4.18)$$

in which $f(x)$ is the (inverse) gap of the hamiltonian (4.12) for the variables x given in (4.17).

In particular at T_c $(y=0)$, one obtains

$$\frac{\xi_L}{L}=\left(\frac{48\pi^2}{n+8}\varepsilon\right)^{-1/3} f\left[\left(\frac{6\varepsilon}{n+8}\right)^{1/3}\frac{n+2}{12}\pi^{-5/6}I\right](1+\mathrm{O}(\varepsilon)) \tag{4.19}$$

with

$$I=\int_0^\infty \frac{\mathrm{d}u}{\sqrt{u}}[A^3(u)-1-(\pi/u)^{3/2}]=-5.0289788 \tag{4.20}$$

(in which $A(u)$ was defined in (3.23)).

In the large-n limit the result (4.19) agrees with the ε-expansion of the equation for ξ_L/L given in ref. [4].

Finally let us consider corrections to this result. The effective action (4.4) is modified by the inclusion of loop corrections given by integrating out the $q_\perp$ non-zero modes; at one-loop order (for simplicity we deal with the $n=1$ case)

$$\begin{aligned} S^{(1)}_{\mathrm{eff}}[\varphi] = L^{d-1}\int \mathrm{d}\tau\left\{\tfrac{1}{2}\dot{\varphi}^2+\tfrac{1}{2}t\varphi^2+\frac{u_0}{4!}\varphi^4\right\} \\ +\tfrac{1}{2}\sum_{q_\perp}\mathrm{tr}\ln\left[-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}+t+\tfrac{1}{2}u_0\varphi^2+q_\perp^2\right]. \end{aligned} \tag{4.21}$$

A rescaling of φ and τ:

$$\begin{aligned} \varphi &\to L^{-1/3(d-1)}u_0^{-1/6}\varphi\,, \\ \tau &\to L^{1/3(d-1)}\,u_0^{-1/3}\tau\,, \end{aligned} \tag{4.22}$$

yields (at T_c, for instance)

$$\begin{aligned} S^{(1)}_{\mathrm{eff}}(\varphi) = \int \mathrm{d}\tau\{\tfrac{1}{2}\dot{\varphi}^2+\tfrac{1}{24}\varphi^4\} \\ +\tfrac{1}{2}\sum_{n_\perp}\mathrm{tr}\ln\left[-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}+\tfrac{1}{2}\varphi^2+L^{2/3(d-4)}\,4\pi^2u_0^{-2/3}n_\perp^2\right]. \end{aligned} \tag{4.23}$$

Expanding the second term of (4.23) in powers of φ^2 we have to consider the propagator

$$\langle\tau_1|\left(-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2}+4\pi^2L^{2/3(d-4)}\,u_0^{-2/3}n_\perp^2\right)^{-1}|\tau_2\rangle\,. \tag{4.24}$$

Above four dimensions, for large L, the propagator is proportional to $L^{-2/3(d-4)}$ $\delta(\tau_1-\tau_2)$; this gives a negligible modification of u_0 proportional to $L^{-4/3(d-4)}$, a small φ^6 correction, etc... Below four dimensions we have to use the renormalization group equations, which relate the theory at L with coupling u_0, to the theory at

$L=1$ with coupling $u_0(L) \simeq u_0^*$, which is proportional to ε. Therefore again the "mass" of the propagator (4.24) is large, for small ε, and this propagator is proportional to $\varepsilon^{2/3}\delta(\tau_1-\tau_2)$: this gives (calculable) $\varepsilon^{4/3}$ correction to u_0, a φ^6 operator proportional to ε^2 etc.... Therefore the results (4.18)-(4.19) are correct up to order $\varepsilon^{2/3}$.

5. Low-temperature expansion of FSS

When a continuous transition is spontaneously broken, below the critical temperature (or the transition temperature of a first-order transition) massless Goldstone modes give singularities at large distances for any value of the temperature. The thermodynamics of these "spin waves" modes is described by the non-linear σ-model [13, 14], which is nothing but a model for an order parameter with a fixed magnitude varying over a sphere (for the single O(n) case). In a finite volume these modes have a small mass and we consider the corresponding non-linear σ-model in a low-temperature expansion, which is valid up to T_c in a $(d-2)$ expansion. Note that the renormalization group analysis of sect. 2 revealed that for $T<T_c$ the large-L properties are related to the zero-temperature fixed point.

Several authors, in particular Lüscher [20] and Floratos and Petcher [21] have already considered the two-dimensional case ($n>2$), in order to deduce the mass gap from a low-temperature expansion. The method that we have followed here for $T<T_c$, $d>2$ has many features in common with the work of Floratos and Petcher [21].

In the cubic geometry the final integration over the $q=0$ mode projects out O(n)-invariant observables. (All the other ones vanish, as expected since for L finite the symmetry is unbroken.) The invariant observables can be calculated from perturbation theory with a finite zize propagator $[(2\pi \boldsymbol{m}/L)^2]^{-1}$ in which the zero mode $\boldsymbol{m}=0$ is omitted. As long as L is finite there is an infrared cut-off, but even in the infinite-L limit, the low-temperature expansion of the invariant observables remains finite [19] (whereas non-invariant observables are infrared singular in the large-L limit).

In the cylindrical geometry, let us consider this problem in more details. The general method of sect. 4, which leads to an effective Schrödinger equation for a quantum rotor, may be applied. However, without going to this hamiltonian formulation, it is also possible to calculate directly with the path integral. The model in the geometry $L^{d-1}xT$ is described by

$$S[\phi]=\frac{1}{2t}\int_{L^{d-1}} \mathrm{d}^{d-1}x \int_0^T \mathrm{d}\tau[(\nabla_\perp \boldsymbol{\phi})^2+(\dot{\boldsymbol{\phi}})^2] \tag{5.1a}$$

with the constraints

$$\phi_1^2(x)+\cdots+\phi_n^2(x)=1\,. \tag{5.1b}$$

An ultraviolet regularization is meant; the dimensional regularization, which does not break the $O(n)$ symmetry, is particularly convenient. The parameter t is proportional to the temperature divided by the spin-wave stiffness constant.

Let us consider a situation with periodic boundary conditions over the L^{d-1} sides of the cylinder and

$$\begin{aligned} \boldsymbol{\phi}(\tau=0, \boldsymbol{x}_\perp) &= \boldsymbol{u}_1 , \\ \boldsymbol{\phi}(\tau=T, \mathbf{x}_\perp) &= \boldsymbol{u}_2 , \end{aligned} \tag{5.2}$$

in which $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$ are two given unit vectors with

$$\boldsymbol{u}_1 \cdot \boldsymbol{u}_2 = \cos\theta . \tag{5.3}$$

The corresponding partition function takes the form

$$\begin{aligned} Z(T,\theta) &= \langle \boldsymbol{u}_2 | \, e^{-TH} | \boldsymbol{u}_1 \rangle \\ &= \sum_l \delta_l p_l(\cos\theta) \, e^{-T\varepsilon_l} , \end{aligned} \tag{5.4}$$

in which the ε_l are the eigenvalues of the hamiltonian, and $p_l(\cos\theta)$ are orthogonal polynomials with the measure $\sin^{n-2}\theta$ and δ_l is the degeneracy of the lth level. One can project any eigenvalue ε_l, by multiplying Z by the appropriate polynomial p_l and integrating over θ.

Let us parametrize the fields $\boldsymbol{\Phi}$ in a frame in which

$$\begin{aligned} \boldsymbol{u}_1 &= [1, 0; \boldsymbol{0}] , \\ \boldsymbol{u}_2 &= [\cos\theta, \sin\theta; \boldsymbol{0}] , \end{aligned} \tag{5.5}$$

$$\begin{aligned} \Phi_1 &= \varphi_1 \cos(\theta\tau/T) + \varphi_2 \sin(\theta\tau/T), \\ \Phi_2 &= -\varphi_1 \sin(\theta\tau/T) + \varphi_2 \cos(\theta\tau/T), \end{aligned} \tag{5.6}$$

and $(n-2)$ components $\boldsymbol{\Phi}_\perp$, in which φ_1, φ_2 and $\boldsymbol{\Phi}_\perp$ are functions of $\boldsymbol{x}$, and τ, satisfying the boundary conditions

$$\Phi_\perp = \varphi_2 = 0 , \qquad \varphi_1 = 1 \tag{5.7}$$

at $\tau = 0$ and $\tau = T$ together with the constraint

$$\varphi_1^2 + \varphi_2^2 + \boldsymbol{\Phi}_\perp^2 = 1 . \tag{5.8}$$

Note that $(\varphi_1 - 1)$, φ_2 and $\boldsymbol{\Phi}_\perp$ are the deviations from the minimum energy configuration with interpolates between $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$. With this parametrization

$$\dot{\boldsymbol{\phi}}^2 = \frac{\theta^2}{T^2}(\varphi_1^2 + \varphi_2^2) + \dot{\varphi}_1^2 + \dot{\varphi}_2^2 + (\dot{\boldsymbol{\phi}}_\perp)^2 \tag{5.9}$$

and with the constraint (5.8)

$$\dot{\boldsymbol{\phi}}^2 = \frac{\theta^2}{T^2}(1 - \boldsymbol{\phi}_\perp^2) + \dot{\varphi}_1^2 + \dot{\varphi}_2^2 + \dot{\boldsymbol{\phi}}_\perp^2 . \tag{5.10}$$

The low-temperature expansion is obtained as usual, by solving for φ_1

$$\varphi_1=(1-\varphi_2^2-\Phi_\perp^2)^{1/2} \tag{5.11}$$

and expanding in powers of φ_2 and $\mathbf{\Phi}_\perp$. At leading order we keep the quadratic terms in φ_2 and $\mathbf{\Phi}_\perp$ and

$$S(\varphi_2,\mathbf{\Phi}_\perp)=\frac{\theta^2}{2tT^2}L^{d-1}+\frac{1}{2t}\int \mathrm{d}^{d-1}x\,\mathrm{d}\tau \times\left[-\frac{\theta^2}{T^2}\mathbf{\Phi}_\perp^2+\dot{\mathbf{\Phi}}_\perp^2+(\nabla\mathbf{\Phi}_\perp)^2+\dot{\varphi}_2^2+(\nabla\varphi_2)^2\right]+S_{\text{int}}(\varphi_2,\mathbf{\Phi}_\perp)\,, \tag{5.12}$$

in which S_{int} contains terms of degree higher than two in the $(n-1)$ fields φ_2, $\mathbf{\Phi}_\perp$. The integral over φ_2 is independent of θ, and gives a normalization constant in front of Z. The integral over $\mathbf{\Phi}_\perp$ gives the $-\frac{1}{2}(n-2)$-th power of the determinant of the quadratic form. Hence, at one-loop order of the low-t expansion

$$\ln\frac{Z(T,\theta)}{Z(T,0)}=-\frac{\theta^2}{2tT}L^{d-1}-\tfrac{1}{2}(n-2)\left[\operatorname{tr}\ln\left(-\frac{\theta^2}{T^2}-\nabla_\perp^2-\frac{\mathrm{d}^2}{\mathrm{d}\tau}\right)-\operatorname{tr}\ln\left(-\nabla_\perp^2-\frac{\mathrm{d}^2}{\mathrm{d}t^2}\right)\right]. \tag{5.13}$$

The eigenmodes of the operator $-\nabla_\perp^2-\mathrm{d}^2/\mathrm{d}t^2$, given the boundary conditions (5, 7) at $\tau=0$ and T and periodic boundary conditions on $\boldsymbol{x}$, are

$$\left(\frac{2\pi}{L}\boldsymbol{p}\right)^2+\frac{m^2\pi^2}{T^2} \tag{5.14}$$

in which $p_1,\dots,p_{n-2}$ are algebraic integers and m is a positive integer:

$$\ln\frac{Z(T,\theta)}{Z(T,0)}=\theta^2\left\{-\frac{L^{d-1}}{2tT}+\frac{n-2}{2T^2}\sum_{\boldsymbol{p}}\sum_{m=1}^{\infty}\frac{1}{(4\pi^2/L^2)\boldsymbol{p}^2+\pi^2m^2/T^2}\right\}+\mathrm{O}(\theta^4)\,, \tag{5.15}$$

in which we have expanded (5.13) around $\theta=0$, since the relevant values of θ needed to project out the eigenvalues ε_l are peaked around $\theta=0$ in the small-t domain. In order to evaluate the rhs of (5.15), in the large-T limit it is necessary to separate the $\boldsymbol{p}=0$ contribution

$$\sum_{\boldsymbol{p}}\sum_{m}\frac{1}{(4\pi^2/L^2)\boldsymbol{p}^2+\pi^2m^2/T^2}\underset{T\to\infty}{\simeq}\frac{T^2}{6}+\sum_{\boldsymbol{p}}{}'\frac{TL}{4\pi|\boldsymbol{p}|}\,. \tag{5.16}$$

The sum over $\boldsymbol{p}$ in the r.h.s. of (5.16) is dimensionally regularized

$$\begin{aligned}\sum_{\boldsymbol{p}}\frac{1}{|\boldsymbol{p}|}&=\frac{1}{\sqrt{\pi}}\int_0^\infty \mathrm{d}u\,u^{-1/2}\sum{}'\,\mathrm{e}^{-u\boldsymbol{p}^2}\\&=\frac{1}{\sqrt{\pi}}\int_0^\infty \mathrm{d}u\,u^{-1/2}\{[A(u)]^{d-1}-1\}\,,\end{aligned} \tag{5.17}$$

in which $A(u)$ is the function defined in (3.23). The integral (5.17) converges for $d<2$; an expansion in powers of $\varepsilon=(d-2)$ gives, after some labour,

$$\sum_p \frac{1}{|p|}=-\frac{2}{\varepsilon}+C-\ln 4\pi+\mathrm{O}(\varepsilon)\,, \tag{5.18}$$

in which C is Euler's constant ($C=-\Gamma'(1)$). Consequently

$$\ln\frac{Z(T,\theta)}{Z(T,0)}=\theta^2\left\{\frac{n-2}{12}-\frac{L^{d-1}}{2tT}+\frac{n-2}{4T}\frac{L}{2\pi}\left(-\frac{2}{\varepsilon}+C-\ln 4\pi\right)+\mathrm{O}(\varepsilon)\right\}+\mathrm{O}(\theta^4;t,1/T^2)\,. \tag{5.19}$$

In order to project out the lowest eigenvalues ε_0 and ε_1 defined in (5.4), we multiply successively Z by one and $\cos\theta$ and integrate (with the $\sin^{n-2}\theta$ measure). This gives the correlation length

$$\frac{1}{\xi_L}=\varepsilon_0-\varepsilon_1=\frac{n-1}{2}\frac{t}{L^{d-1}}\left\{1+\frac{t(n-2)}{4\pi}L^{-\varepsilon}\left(-\frac{2}{\varepsilon}+C-\ln 4\pi+\mathrm{O}(\varepsilon)\right)+\mathrm{O}(\varepsilon^2)\right\}. \tag{5.20}$$

The $1/\varepsilon$ poles disappear, as they should, when one introduces the renormalized temperature t_{R}, with

$$t=t_{\mathrm{R}}+\frac{n-2}{2\pi\varepsilon}t_{\mathrm{R}}^2+\mathrm{O}(t_{\mathrm{R}}^3) \tag{5.21}$$

taken from ref. [14].

The result satisfies the expected scaling relation

$$\xi_L[t_{\mathrm{R}},L]=L\xi_L[t_{\mathrm{R}}(L),1] \tag{5.22}$$

with, at this order,

$$\frac{1}{t_{\mathrm{R}}}=\frac{1}{t_{\mathrm{R}}^*}+L^{-\varepsilon}\left(\frac{1}{t_{\mathrm{R}}(L)}-\frac{1}{t_{\mathrm{R}}^*}\right), \tag{5.23}$$

$$t_{\mathrm{R}}^*=\frac{2\pi\varepsilon}{n-2}+\mathrm{O}(\varepsilon^2)\,. \tag{5.24}$$

This allows one finally to write (5.20) under the scaling form

$$\frac{\xi_L}{L}=\frac{2}{(n-1)t_{\mathrm{R}}(L)}\left[1-(C-\ln 4\pi)\frac{n-2}{4\pi}t_{\mathrm{R}}(L)+\mathrm{O}(t_{\mathrm{R}}^2)\right]. \tag{5.25}$$

For large L and $T<T_c$, $t_{\mathrm{R}}(L)$ vanishes (eq. (2.5)) and from (2.7) one obtains

$$t_{\mathrm{R}}(L)=\left(\frac{\xi(t_{\mathrm{R}})}{L}\right)^{d-2}\left[1-\frac{1}{2\pi}\frac{n-2}{d-2}\left(\frac{\xi(t_{\mathrm{R}})}{L}\right)^{d-2}+\mathrm{O}\left(\frac{1}{L^{2(d-2)}}\right)\right]. \tag{5.26}$$

Thus from (5.25) one has

$$\frac{\xi_L}{L}=\frac{2}{n-1}\left(\frac{L}{\xi}\right)^{d-2}\left[1+\frac{n-2}{2\pi}\left(\frac{\xi}{L}\right)^{d-2}\left(\frac{1}{d-2}+\tfrac{1}{2}\ln(4\pi)-\tfrac{1}{2}C\right)+\mathrm{O}\left(\frac{1}{L^{2(d-2)}}\right)\right]. \tag{5.27}$$

Irrelevant operators of the non-linear σ-model generate additional $1/L^2$ corrections to (5.27).

For large L and at low temperature (since from (2.9) $\xi(t)\propto t^{1/(d-2)}$) one recovers a result of Fisher and Privman [8].

In dimension two, this result has been already derived by a different method by M. Lüscher [20], and by Floratos and Petcher [21] up to two-loop.

5.1. MAGNETIZATION IN A BOX

For an n-vector model below T_c the spontaneous magnetization in a finite box vanishes. In a field a magnetization $M[H, t, L]$ is induced, which vanishes if H goes to zero first but not if L goes first to infinity. This cross-over is contained in the same renormalization group equations, which for large L reads

$$M[H,t,L]=\sigma(t)M\left[\frac{H\sigma(t)}{t}\xi^{d-2}(t)L^2,\left(\frac{\xi(t)}{L}\right)^{d-2},1\right], \tag{5.28}$$

in which $\sigma(t)$ and $\xi(t)$ are the infinite system spontaneous magnetization (per unit volume) and correlation length given by eqs. (2.11) and (2.7). For large L, fixed t, since the effective temperature $t(L)\simeq(\xi(t)/L)^{d-2}$ is small, the magnetization of the r.h.s. of (6.7) can again be calculated in a low-t expansion. At lowest order in t, one keeps only the uniform mode and the partition function is

$$Z(H,t,L=1)=\int \mathrm{d}^n\hat{\varphi}\exp\left(\frac{H\varphi}{t}\right)=C\int_0^{\pi}\mathrm{d}\theta\sin^{n-2}\theta\exp\left(\frac{H\cos\theta}{t}\right) \tag{5.29}$$

(a modified Bessel function). Therefore the magnetization of the r.h.s. is given by a logarithmic derivative of Z and one substitutes for H/t the variable

$$x=\frac{H(L)}{t(L)}=\frac{H\sigma(t)}{t}\xi^{d-2}(t)L^2\Big/\left(\frac{\xi(t)}{L}\right)^{d-2}=\frac{H\sigma(t)L^d}{t}. \tag{5.30}$$

The final formula is

$$M[H,t,L]=\sigma(t)\frac{\partial}{\partial x}\ln\int_0^{\pi}\mathrm{d}\theta\sin^{n-2}\theta\,\mathrm{e}^{x\cos\theta} \tag{5.31}$$

with x given by (5.30), in agreement with the formula given by Fisher and Privman [8]. The technique of this section is also useful in the context of lattice gauge theories [22].

6. First-order transitions and FSS

In this section we shall study *uniform* first-order transitions in which the order parameter jumps from a constant value to another constant value throughout the sample, excluding thereby transitions such as crystallization. The FSS properties at first-order transitions have been considered from a transfer matrix formalism by Privman and Fisher [9]. We want now to show that the method that we have applied to continuous transitions explains also the rounding of first-order transitions and leads to a simple derivation of some universal properties. Thus many of the formulae that we shall derive are already given in ref. [9]. Again we can introduce one single $\boldsymbol{q}=0$ mode to describe the system. In the case of a cubic L^d geometry, one defines

$$\varphi=\frac{1}{L^d}\int_v \Phi(x)\,\mathrm{d}^d x\,, \tag{6.1a}$$

and for a cylinder $L^{d-1}\times\infty$

$$\varphi(\tau)=\frac{1}{L^{d-1}}\int \Phi(x_\perp,\tau)\,\mathrm{d}^{d-1}x_\perp\,; \tag{6.1b}$$

periodic boundary conditions are used in all this section. Tracing out the $q\neq 0$ modes, one obtains

$$S_{\text{eff}}(\varphi, L)=L^d s(\varphi) \tag{6.2a}$$

or

$$S_{\text{eff}}(\varphi, L)=L^{d-1}\int \mathrm{d}\tau\, s(\varphi(\tau))\,. \tag{6.2b}$$

for the two geometries respectively.

At a first-order transition the correlation length remains finite, the integrations over the $q\neq 0$ modes are non-singular, therefore the coefficients of $s(\varphi)$ are regular functions of the physical parameters, such as the temperature, the chemical potentials etc. . . .

The physical observables will be defined through an integration over φ (or $\varphi(\tau)$). The Boltzmann weight $(\exp(-S_{\text{eff}}))$ is governed by the L^d (or L^{d-1}) factor in front of s, and these last integrations can be performed, exactly in the large-L limit, by a saddle-point approximation. This yields some universal formulae for the rounding of first-order jumps independent of all the details of the actual interaction. Let us distinguish now several cases.

6.1. CUBIC GEOMETRY, ISING-LIKE SYSTEMS

In the first case the zero-field action (6.2) is symmetric under $\varphi\to-\varphi$. We consider, specifically an Ising-like system below T_c in a small external field H. When H changes from plus zero to minus zero the infinite volume magnetization jumps from $+M_0$ to $-M_0$. This jump is rounded at finite L, since M now vanishes with L. In the presence of a field

$$S_{\text{eff}}(\varphi, H, L) = L^d[s(\varphi) - \beta H\varphi] \tag{6.3}$$

and $s(\varphi)$ is an even function of φ, with two minima at $+M_0$ and $-M_0$. For small H (finite HL^d) the minima of (6.3) are close to M_0 and $-M_0$ and we can expand the Boltzmann weight near these two points [9, 23]:

$$\begin{aligned} e^{-S_{\text{eff}}(\varphi)} \propto & \exp\left(-L^d[\tfrac{1}{2}s''(M_0)(\varphi - M_0)^2 - \beta H\varphi]\right) \\ & + \exp\left(-L^d[\tfrac{1}{2}s''(M_0)(\varphi + M_0)^2 - \beta H\varphi]\right). \end{aligned} \tag{6.4}$$

With the weight (6.4) one can calculate any average; for instance the magnetization is given by

$$M = \langle\varphi\rangle = M_0 \tanh(\beta HL^d M_0) + \frac{\beta H}{s''(M_0)}, \tag{6.5}$$

$$\chi = \frac{\beta}{s''(M_0)} \tag{6.6}$$

is the bulk zero-field magnetic susceptibility.

For H small, HL^d finite, the second term is negligible and the rounded magnetization is given by the well-known [9], but indeed universal formula

$$M = M_0 \tanh(\beta HL^d M_0). \tag{6.7}$$

6.2. CUBIC GEOMETRY, NO SYMMETRY

A first-order transition often takes place for an effective action, which has no symmetry (such as $\varphi \to -\varphi$) but simply a minimum at $\varphi = M$ which becomes lower (for $T < T_c$) than the minimum at $\varphi = M_0$. Let us define the "driving parameter"

$$t = s(M_1) - s(M_0), \tag{6.8}$$

which is proportional to $T - T_c$. The statistical weight or the order parameter, becomes proportional to

$$\exp(-S_{\text{eff}}) \propto \{\exp(-\tfrac{1}{2}L^d s''(M_1)(\varphi - M_1)^2) + \exp(+tL^d - \tfrac{1}{2}L^d s''(M_0)(\varphi - M_0)^2)\} \tag{6.9}$$

and averages such as the magnetization $M = \langle\varphi\rangle$ are easily calculated. One finds

$$M = M_0 + \frac{M_1 - M_0}{1 + e^{+tL^d}\sqrt{s''(M_1)/s''(M_0)}} \tag{6.10}$$

which describes the rounding of the jump of M for t small, L large, finite tL^d; $s''(M_1)/s''(M_0) = \chi(M_0)/\chi(M_1)$ is the ratio of bulk susceptibilities in the two phases.*

* We thank Dr. M.E. Fisher for pointing out to us that this normalization depends on the definition (6.8) of the parameter t and is therefore non-universal.

6.3. CYLINDER, ISING-LIKE SYSTEMS

The effective action (6.2b) is the (euclidean) weight of a Feynman path integral for a quantum mechanical problem. Below T_c, the zero-field action has two (degenerate) minima. The quantum mechanical problem has an exponentially small splitting between the symmetric and antisymmetric lowest states. This splitting is exponentially small in $\hbar$, which is replaced here by $1/L^{d-1}$. A semi-classical computation of this splitting, valid for small $\hbar$ i.e. large L, may be done easily by a saddle-point expansion (instanton calculus [24]). The saddle-point itself corresponds to trajectories which interpolate between the two minima, a simple picture of a dilute gas of domain walls. The result takes the form for the correlation length (the inverse of the energy splitting) at finite T below T_c

$$\xi_L = A(T) L^{-(d-3)/2} \exp\left(\beta L^{d-1} \sigma(T)\right) . \tag{6.11}$$

This result is valid below the transition temperature for Ising-like systems, namely symmetric under $\varphi \to -\varphi$, whether the transition is first order or continuous. The exponential factor in (6.11) is typical of a WKB behaviour; the coefficient $\beta\sigma(T)$ of L^{d-1} is the value of the effective action for the kink solution and coincides with the surface tension [25]. The power of L in the prefactor of (6.11) is in fact a delicate problem. We believe that it is correctly given by (6.11) for arguments exposed below, but we have not made a systematic investigation of higher order corrections. The first contribution to this prefactor is nothing but the WKB normalization $L^{-(d-1)/2}$. In the semi-classical language it comes from an integration over the location of the center of the kink. An extra-factor L^{-1} comes from one loop fluctuations [26], a contribution from the modes $q_\perp \neq 0$, or in physical terms a result of the fuziness of the interface, i.e. of the capillary modes of the interface. It is worth noting that the result (6.11) is in agreement with exact results on the two-dimensional Ising model in a strip [27], which lead after some calculations to

$$\xi_L = \sqrt{\frac{\pi L}{2 \sinh m}}\, e^{Lm} \tag{6.12a}$$

with

$$m = -2(\beta J) - \ln \operatorname{th}(\beta J) , \tag{6.12b}$$

in units in which the lattice spacing is equal to one. In the vicinity of a second-order transition temperature T_c, $A(T)$ and $\sigma(T)$ may be expanded in powers of ε along the lines of sect. 4 [28].

7. Conclusion

We have presented a general approach to FSS for a phase transition. To illustrate the method we have presented some calculations, but it is clear that it would not be difficult to compute many other physical quantities of interest. It would also be feasible to calculate higher orders in the ε-expansions for the quantities considered in this article, such as the correlation length or the renormalized coupling constant.

Similarly one may consider different geometrical shapes, or new situations in which for instance two dimensions are infinite and $(d-2)$ remain finite. This would be relevant to the study of the dimensional cross-over between a 3D and a 2D critical behaviour. Indeed it would involve the solution of a two-dimensional field theory, but in a non-critical region accessible to numerical methods.

Another extension of this approach would be the study of the dynamics of a finite system. Technically this is similar to the cylindrical geometries considered in this work, but the real time and the space propagations are now anisotropic. This would be relevant to the study of the critical slowing down in Monte Carlo measurements.

Finally, another possible use of this approach would be the study of three-dimensional systems at their critical point. In the infinite volume limit, perturbation theory at T_c breaks down at finite order because of infrared singularities but L provides an infrared cut-off. This could lead to calculations, similar in their spirit, although quite different in practice, to those proposed by Parisi [29] and extended in refs. [30].

It seems clear that, in spite of the extensive literature on the subject, there is still a lot to say about finite size effects.

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