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$O(N)$ Vector Model with Twisted Boundary Conditions

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Prompted by a recent article of Chakravarty, we reexamine the $O(N)$ vector model with twisted boundary conditions in d dimensions in the various frameworks of the $\varepsilon = d - 2$ expansion, the $\varepsilon = 4 - d$ expansion, and the large-N expansion. These continuum models describe the physics below the critical temperature T_c and near T_c of a lattice $O(N)$ spin model. We determine the effect of the twisting on finite-size scaling functions, for various geometries.

KEY WORDS: Finite-size scaling; nonlinear σ-model; ε-expansion; large-N expansion.

1. INTRODUCTION

In a recent article Chakravarty[1] studied the effect of twisted boundary conditions on the spin stiffness constant of an N-vector model in two dimensions. In this article we discuss the effect of the twisting on finite size-scaling functions, for various geometries, and for all dimensions d, $2 \leqslant d \leqslant 4$.

The calculation can be performed within various schemes. In Section 2 we first study the $O(N)$ vector model from the point of view of the low-temperature expansion. In the continuum, large-distance, limit this leads to the nonlinear σ-model. If we want to be able to characterize the whole range of ratios L/ξ, L being the size of the system and ξ the correlation length, we need to interpolate between the critical fixed point and the zero-temperature IR fixed point. This can be achieved only near two dimensions because T_c is then small. In higher dimensions only the situation $L \gg \xi$,

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which, according to RG arguments, is governed by the zero-temperature IR fixed point, can be described.

In Section 3 the large-N limit is discussed. Two types of boundary conditions have then to be distinguished: macroscopic boundary conditions, where the average magnetization is fixed, which are easy to handle, and microscopic boundary conditions, where the microscopic spin variables are given, which lead to much more complicated calculations.

The same problem appears in the framework of the ϕ^4 field theory, which provides a natural framework to discuss the N-vector model near four dimensions, as is shown in Section 4. We prove, however, that both types of boundary conditions yield identical results for any fixed temperature below T_c.

2. THE NONLINEAR σ-MODEL

Let us first consider the action of the nonlinear σ-model[2] (for notations and methods see, e.g., ref. 3)

$$S(\phi) = \frac{\Lambda^{d-2}}{2t} \int d^d x \, [\partial_\mu \phi(x)]^2 \tag{1}$$

with a spin of length 1:

$$\phi^2(x) = 1 \tag{2}$$

Λ is a mass scale, for instance, the UV cutoff which regularizes the theory, introduced to make t dimensionless. This model is known to describe the N-vector model in the low-temperature, long-distance limit. We discuss here the model in the following geometry: one dimension is distinguished which has a size L and corresponds to *twisted* boundary conditions

$$\phi(\tau = 0) = \phi_1, \qquad \phi(\tau = L) = \phi_2, \qquad \phi_1 \cdot \phi_2 = \cos\theta \tag{3}$$

In the other $d-1$ dimensions of size $L_\perp$ we assume periodic boundary conditions. We consider here only the situations $L_\perp \gg L$ (lamellar geometry) or $L_\perp \sim L$ (hypercubic geometry). The case $L \gg L_\perp$ has been already extensively studied and requires a different technique.[4]

With the boundary conditions (3) all momenta are quantized and the eigenmodes p^2 of the operator $-\partial_\mu^2$ are

$$p^2(m, \mathbf{k}) = \frac{m^2\pi^2}{L^2} + \left(\frac{2\pi\mathbf{k}}{L_\perp}\right)^2, \qquad \mathbf{k} \in \mathbb{Z}^{d-1} \tag{4}$$

and m is a positive integer. To avoid potential IR problems due to a degeneracy of the classical minimum we impose $|\theta| < \pi$.

Renormalization Group. In the case of a geometry characterized by two finite-size parameters L, $L_\perp$, the free energy per unit volume F defined for convenience by

$$F = -\frac{1}{LL_\perp^{d-1}} \ln\left(\frac{Z(\theta)}{Z(0)}\right)$$

is an RG invariant. Thus it satisfies, as a consequence of the renormalization group equations,

$$F = L^{-d} f(L/\xi, L/L_\perp) \tag{5}$$

with

$$\xi(t) = \Lambda^{-1} t^{1/(d-2)} \exp\left[\int_0^t \left(\frac{1}{\beta(t')} - \frac{1}{(d-2)\,t'}\right) dt'\right] \tag{6}$$

Below the critical temperature the length ξ is not a correlation length, since the phase is massless, but a length which characterizes the crossover scale between the low-temperature IR behavior, governed by free Goldstone modes, and the critical behavior governed by the UV fixed point at T_c (the large-momentum behavior of the corresponding field theory). As an RG invariant this length satisfies the RG equation

$$\left(\Lambda \frac{\partial}{\partial \Lambda} + \beta(t) \frac{\partial}{\partial t}\right) \xi = 0$$

from which (6) follows.

Remark. For an Ising-like system (or more generally a system with only discrete symmetries) F characterizes the surface tension between two different phases. For large L it vanishes as $1/L$ with a coefficient proportional to the surface tension. The RG equation (5) is consistent with this behavior provided the surface tension vanishes at T_c like $(T_c - T)^{\nu(d-1)}$, which is Widom's scaling law.

In a model with continuous symmetry, due to the Goldstone modes, F vanishes like $1/L^2$ instead, and the coefficient of $1/L^2$ (the equivalent of the surface tension for continuous symmetries) is constrained by the RG equation (5) to vanish like $(T_c - T)^{\nu(d-2)}$, Josephson's scaling law.[5]

The β-function in $d = 2 + \varepsilon$ dimensions at two-loop order is

$$\begin{aligned} \beta(t) &= \varepsilon t - N_d(N-2)\, t^2 - N_d^2(N-2)\, t^3 + O(t^4, \varepsilon t^3) \\ N_d &= \frac{2\pi^{d/2}}{\Gamma(d/2)(2\pi)^d} = \frac{1}{2\pi} + O(d-2) \end{aligned} \tag{7}$$

We shall see that with the boundary conditions (3) and for $d>2$ and $L/L_\perp$ finite the function $f(x, L/L_\perp)$ is regular near the critical temperature $x=0$ ($|\theta|<\pi$). For $x \to \infty$ the behavior of the function $f(x, L/L_\perp)$ is governed by the IR fixed point $t=0$ and thus is given by perturbation theory.

It is useful to introduce a size-dependent coupling constant defined by

$$\frac{dt(\lambda)}{d\ln\lambda} = \beta(t(\lambda)), \qquad t(1)=t \tag{8}$$

For λ small, $t(\lambda)$ approaches the IR fixed point at $t=0$. At one-loop order for ε small

$$t(\lambda) = t\lambda^{\varepsilon}[1-(N-2)\,N_d t \ln\lambda] \tag{9}$$

and thus, choosing $\lambda = 1/(\Lambda L)$,

$$t_L \equiv t[1/(\Lambda L)] = [t/(\Lambda L)^{\varepsilon}][1+(N-2)\,N_d t \ln(\Lambda L)] \tag{10}$$

2.1. The Cylindrical Geometry at One-Loop Order

For convenience we call space dimensions the $d-1$ dimensions of size $L_\perp$, and "time" the dimension of size L. We mainly discuss the two situations $L \ll L_\perp$ and $L = L_\perp$. We do not study the case $L \gg L_\perp$, which requires a separate analysis. In the time direction we impose twisted boundary conditions [conditions (3)]:

$$\phi(\tau=0, \mathbf{x}) = \phi_1, \qquad \phi(\tau=L, \mathbf{x}) = \phi_2, \qquad \mathbf{x} \in \mathbb{R}^{d-1} \tag{11}$$

in which ϕ_1 and ϕ_2 are two constant vectors such that

$$\phi_1 \cdot \phi_2 = \cos\theta, \qquad 0 \leqslant \theta < \pi \tag{12}$$

To calculate the one-loop corrections we extend the method explained in ref. 3. The corresponding partition function is given by

$$Z(L_\perp, L, \theta) = \langle \phi_2 |\, e^{-LH} \,| \phi_1 \rangle \tag{13}$$

By projecting $Z(L_\perp, L, \theta)$ over the hyperspherical polynomials $P_l^N(\cos\theta)$ it is possible to calculate the eigenvalues of the Hamiltonian H. Let us now choose a frame such that

$$\phi_1 = [1, 0; \mathbf{0}], \qquad \phi_2 = [\cos\theta, \sin\theta; \mathbf{0}] \tag{14}$$

We parametrize then the field $\phi(\tau, x)$ by

$$\phi(\tau, x) = \begin{cases} \cos(\theta\tau/L)\,\sigma_1(\tau, x) - \sin(\theta\tau/L)\,\sigma_2(\tau, x) \\ \sin(\theta\tau/L)\,\sigma_1(\tau, x) + \cos(\theta\tau/L)\,\sigma_2(\tau, x) \\ \boldsymbol{\pi}(\tau, x) \end{cases} \tag{15}$$

in which the field $\boldsymbol{\pi}(\tau, x)$ has here only $N-2$ components. With this parametrization the boundary conditions (11) take the simple form

$$\sigma_1 = 1, \qquad \sigma_2 = 0, \qquad \boldsymbol{\pi} = \mathbf{0} \qquad \text{for} \quad \tau = 0 \quad \text{and} \quad \tau = L \tag{16}$$

and the solution to the classical field equation satisfying (16) is then $\sigma_1 = 1$, $\sigma_2 = 0$, $\boldsymbol{\pi} = \mathbf{0}$. Finally the transformation (15) is a rotation. Therefore the three fields σ_1, σ_2, $\boldsymbol{\pi}$ satisfy the constraint

$$\sigma_1^2 + \sigma_2^2 + \boldsymbol{\pi}^2 = 1 \tag{17}$$

and the integration measure in the functional integral is left invariant.

The action $S(\phi)$ in the new fields reads

$$S(\sigma_1, \sigma_2, \boldsymbol{\pi}) = \frac{\Lambda^{d-2}}{2t} \int d\tau\, d^{d-1}x \left[\frac{\theta^2}{L^2}(\sigma_1^2 + \sigma_2^2) + \dot\sigma_1^2 + \dot\sigma_2^2 + \dot{\boldsymbol{\pi}}^2 \right.$$
$$\left. + 2\frac{\theta}{L}(\dot\sigma_2\sigma_1 - \dot\sigma_1\sigma_2) + (\partial_i\sigma_1)^2 + (\partial_i\sigma_2)^2 + (\partial_i\boldsymbol{\pi})^2 \right] \tag{18}$$

Remark. It is easy to see that the partition function is a regular even function of θ near $\theta = 0$. If we expand up to order θ^2, we find the average of the quantity

$$-\frac{\Lambda^{d-2}}{2t} \int d\tau\, d^{d-1}x \frac{1}{L^2}(\sigma_1^2 + \sigma_2^2) + \frac{\Lambda^{2d-4}}{2t^2L^2} \left[\int d\tau\, d^{d-1}x (\dot\sigma_2\sigma_1 - \dot\sigma_1\sigma_2) \right]^2 \tag{19}$$

Due to the second term the coefficient of θ^4 is not the average of the square of the coefficient of θ^2. However, at one-loop order the second term does not contribute and thus the fluctuations of the quantity (19) can indeed be inferred from the coefficient of θ^4. The θ^2 coefficient has been called the spin stiffness or the helicity modulus.[6] Previous studies have proposed a vanishing near T_c of the helicity modulus as $|T - T_c|^{\nu(d-2)}$,[7] which is the so-called Josephson relation.

One-Loop Calculation. To calculate the effects of small fluctuations around the classical minimum $\sigma_1 = 1$, $\sigma_2 = 0$, $\boldsymbol{\pi} = \mathbf{0}$, we eliminate the field σ_1 using Eq. (17):

$$\sigma_1 = (1 - \sigma_2^2 - \boldsymbol{\pi}^2)^{1/2} \tag{20}$$

and expand the action in powers of σ_2 and π. The quadratic part of the action $S_2(\sigma_2, \pi)$ needed for the one-loop calculation is then

$$S_2(\sigma_2, \pi) = \frac{\theta^2 \Lambda^{d-2}}{2tL} L_\perp^{d-1} + \frac{\Lambda^{d-2}}{2t} \int d\tau\, d^{d-1}x \times \left[-\frac{\theta^2}{L^2} \pi^2 + \dot{\sigma}_2^2 + \dot{\pi}^2 + (\partial_i \sigma_2)^2 + (\partial_i \pi)^2 \right] \tag{21}$$

At this order the integration over σ_2 gives a factor independent of θ which can be absorbed in the normalization of the functional integral. The integral over π gives a determinant to the power $(N-2)/2$. Hence the result at this order is

$$-\ln \frac{Z(L_\perp, L, \theta)}{Z(L_\perp, L, 0)} = \frac{\theta^2}{2tL} \Lambda^{d-2} L_\perp^{d-1} + \frac{1}{2}(N-2) \operatorname{tr} \ln \left[\left(-\frac{\theta^2}{L^2} - \partial_\tau^2 - \partial_i^2 \right) (-\partial_\tau^2 - \partial_i^2)^{-1} \right] \tag{22}$$

Taking into account the boundary conditions (16), we have to sum over quantized momenta and thus obtain from (4)

$$-\ln \frac{Z(L_\perp, L, \theta)}{Z(L_\perp, L, 0)} = \theta^2 \frac{L_\perp^{d-1}}{2tL} \Lambda^{d-2} + \frac{N-2}{2} \sum_{\mathbf{k}} \sum_{m=1}^{\infty} \ln \left[1 - \frac{\theta^2}{L^2 p^2(m, \mathbf{k})} \right] + O(t) \tag{23}$$

We then use the representation

$$\ln(p^2 - \theta^2 L^{-2}) - \ln p^2 = \int_0^{+\infty} \frac{ds}{s} \left[e^{-sp^2} - e^{-s(p^2 - \theta^2/L^2)} \right] = \int_0^{+\infty} \frac{ds}{s} (1 - e^{s\theta^2/L^2})\, e^{-sp^2}$$

The sum over m and $\mathbf{k}$ can be expressed in terms of the function $A(s)$ (which is a Jacobi theta function):

$$A(s) = \sum_{n=-\infty}^{+\infty} e^{-sn^2} \tag{24}$$

From the Poisson formula one proves that $A(s)$ satisfies

$$A(s) = \left(\frac{\pi}{s} \right)^{1/2} A\left(\frac{\pi^2}{s} \right) \tag{25}$$

One then finds

$$-\ln\frac{Z(L_\perp, L, \theta)}{Z(L_\perp, L, 0)} = \theta^2 \frac{L_\perp^{d-1}}{2tL} \Lambda^{d-2} + \frac{N-2}{4}\int_0^{+\infty}\frac{ds}{s}\,(1-e^{s\theta^2/L^2})\left[A\left(\frac{\pi^2 s}{L^2}\right)-1\right] \times A^{d-1}\left(\frac{4\pi^2 s}{L_\perp^2}\right) \tag{26}$$

The expression is IR finite but UV divergent (at small s) for $d \geqslant 2$. In order to regularize the theory, we first go to $d<2$, renormalize the temperature, and continue back to $d \geqslant 2$. More specifically we note that

$$(1-e^{s\theta^2})[A(\pi^2 s)-1]\,A^{d-1}(4\pi^2 sL^2/L_\perp^2) \underset{s\to 0}{\simeq} -\theta^2(L_\perp/L)^{d-1}\,N_d\Gamma(d/2)\,e^{-s}s^{1-d/2}$$

and thus

$$-\ln\frac{Z(L_\perp, L, \theta)}{Z(L_\perp, L, 0)} = \theta^2 \frac{L_\perp^{d-1}}{2L}\Lambda^{d-2}\left(\frac{1}{t}+\frac{(N-2)\,N_d\pi}{2\sin(\pi d/2)}(\Lambda L)^{2-d}\right) + \frac{N-2}{4}\int_0^{+\infty}\frac{ds}{s}\left[(1-e^{s\theta^2})[A(\pi^2 s)-1] \times A^{d-1}\left(\frac{4\pi^2 sL^2}{L_\perp^2}\right)+\theta^2\left(\frac{L_\perp}{L}\right)^{d-1} N_d\Gamma\left(\frac{d}{2}\right)e^{-s}s^{1-d/2}\right] \tag{27}$$

2.2. Dimension $d=2+\epsilon$

We now perform a double expansion in t and $d-2$ which is valid in the whole range of temperature from 0 to T_c and thus for an arbitrary value of the ratio L/ξ. Renormalizing the temperature at a scale $\Lambda = 1/L$, i.e., defining the renormalized temperature

$$\frac{1}{t_L}=\frac{1}{t}+\frac{N-2}{2\pi\varepsilon}$$

we obtain

$$F=\frac{\theta^2}{2t_L L^d}+\frac{1}{L^d}\varphi\left(\frac{L}{L_\perp},\theta\right)$$

with

$$\varphi\left(\frac{L}{L_\perp},\theta\right)=\frac{N-2}{4}\int_0^\infty ds$$
$$\times\left\{\frac{1-e^{s\theta^2}}{s}\left[A(\pi^2 s)-1\right]\left[\frac{L}{L_\perp}A\left(\frac{4\pi^2 sL^2}{L_\perp^2}\right)\right]+\theta^2\frac{e^{-s}}{2\pi s}\right\} \tag{28}$$

This is in agreement with finite-size scaling provided we express t_L as a function of L/ξ. This follows immediately from the renormalization group since

$$\left(\frac{\xi}{L}\right)^\varepsilon = t_L \exp\left[\varepsilon\int_0^{t_L} dt'\left(\frac{1}{\beta(t')}-\frac{1}{\varepsilon t'}\right)\right]$$

At one-loop order this leads to

$$\frac{1}{t_L}=\frac{1}{t_c}+\left(\frac{\xi}{L}\right)^{-\varepsilon}$$

Therefore for ξ/L large, t_L flows as expected to the UV fixed point t_c, and thus F vanishes at t_c as L^{-d} as expected from finite-size scaling. For large L, fixed ξ, t_L vanishes as $(\xi/L)^\varepsilon$ and we recover the $1/L^2$ behavior of the free energy which is characteristic of spin waves below t_c.

Dimension $d>2$. In dimension $2<d<4$ we can still use the low-temperature expansion in the regime in which $L \gg \xi$, since zero temperature is an IR fixed point. We now define a renormalized temperature

$$\frac{1}{t_L}=\frac{1}{t}-\frac{(N-2)\,N_d\pi}{2\sin(\pi d/2)}+O(t)$$

From the RG equations we find that t_L vanishes in that limit as $(\xi/L)^{d-2}$. Therefore we end up at first order with

$$F=\theta^2\frac{\xi^{2-d}}{2L^2}+\frac{1}{L^d}\varphi\left(\theta,\frac{L}{L_\perp}\right) \tag{29}$$

with

$$\varphi=\frac{N-2}{4}\int_0^\infty ds\left\{\frac{1-e^{s\theta^2}}{s}\left[A(\pi^2 s)-1\right]\left[\frac{L}{L_\perp}A\left(\frac{4\pi^2 sL^2}{L_\perp^2}\right)\right]^{d-1}\right.$$
$$\left.+\,\theta^2 N_d\Gamma\left(\frac{d}{2}\right)e^{-s}s^{1-d/2}\right\} \tag{30}$$

This result is consistent with Josephon's relation.[5]

Dimension Two. Expression (27) also determines the form of F at $d=2$. The renormalization group tells us that the free energy per unit volume has the form

$$F=L^{-2}f(L/\xi,\, L/L_{\perp})$$

For $d=2$ we may now reach from the loop expansion the opposite limit $\xi \gg L$ since the origin is now a UV fixed point; we have

$$f=\theta^2/(2t_L)+\varphi(\theta,\, L/L_{\perp})+O(t_L) \tag{31}$$

where φ is given by (30) and where t_L has the expansion

$$\frac{1}{t_L}=\frac{N-2}{2\pi}\ln\left(\frac{\xi}{L}\right)+\frac{1}{2\pi}\ln\ln\left(\frac{\xi}{L}\right)+O(1)$$

Note that it is justified to take this two-loop expression for t_L although we only computed F at one-loop order. Indeed we are neglecting $1/\ln(\xi/L)$ but not $\ln\ln(\xi/L)/\ln(\xi/L)$. Let us also note that the correction terms in $\ln\ln(\xi/L)$ have important practical consequences. It is in principle feasible to compute the helicity modulus in a Monte Carlo simulation. As a function of $\ln L$, one can hope to see the leading-order slope $(N-2)/2\pi$.[8] However, we expect the logarithmic behavior to be quite difficult to observe due to the very slow decay of subleading terms.

2.3. The Lamellar Geometry

Let us now take the limit $L_{\perp}\to\infty$. The expressions simplify; the function φ defined by Eq. (30), valid for $d>2$, becomes

$$\varphi=\frac{N-2}{4}\int_0^\infty ds\left\{\frac{1-e^{s\theta^2}}{s}\left[A(\pi^2 s)-1\right]\left(\frac{1}{4\pi s}\right)^{(d-1)/2}\right.$$
$$\left.+\;\theta^2 N_d\Gamma\left(\frac{d}{2}\right)e^{-s}s^{1-d/2}\right\} \tag{32}$$

For $d=2+\varepsilon$ the scaling function (27) becomes

$$f=\frac{\theta^2}{2t_L}+\varphi(\theta) \tag{33}$$

with

$$\varphi=\frac{N-2}{4}\int_0^\infty ds\left\{\frac{1-e^{s\theta^2}}{(4\pi)^{1/2}s^{3/2}}\left[A(\pi^2 s)-1\right]+\theta^2\frac{e^{-s}}{2\pi s}\right\} \tag{34}$$

2.4. The Hypercubic Geometry

This geometry should be the most convenient for numerical studies. The function φ relevant for $2+\varepsilon$ dimension [Eq. (28)] is now given by the following expression:

$$\varphi = \frac{N-2}{4} \int_0^\infty ds \left\{ \frac{1-e^{s\theta^2}}{s} \left[A(\pi^2 s) - 1 \right] A(4\pi^2 s) + \theta^2 \frac{e^{-s}}{2\pi s} \right\} \tag{35}$$

3. THE LARGE-N LIMIT

Let us solve now the σ-model in the large-N limit. Using the linear formalism, we rewrite the partition function:

$$Z = \int [d\phi(x)\, d\lambda(x)] \exp[-S(\phi, \lambda)] \tag{36}$$

with

$$S(\phi, \lambda) = \frac{1}{2T} \int d^d x \left[(\partial_\mu \phi)^2 + \lambda(\phi^2 - 1) \right] \tag{37}$$

It is convenient for our problem to integrate only over $N-2$ components of ϕ. Calling $\boldsymbol{\sigma}$ the remaining two components, we obtain

$$Z = \int [d\boldsymbol{\sigma}(x)\, d\lambda(x)] \exp[-S_{\text{eff}}(\boldsymbol{\sigma}, \lambda)] \tag{38}$$

with

$$S_{\text{eff}}(\boldsymbol{\sigma}, \lambda) = \frac{1}{2T} \int \{ (\partial_\mu \boldsymbol{\sigma})^2 + [\boldsymbol{\sigma}^2(x) - 1]\, \lambda(x) \}\, d^d x + \frac{1}{2}(N-2) \operatorname{tr} \ln[-\Delta + \lambda(x)] \tag{39}$$

The large-N limit is taken at TN fixed. The saddle point equations, in the infinite-volume limit, are

$$\lambda \sigma = 0 \tag{40}$$

$$\sigma^2 = 1 - \frac{(N-2)T}{(2\pi)^d} \int^\Lambda \frac{d^d p}{p^2 + \lambda} \tag{41}$$

At low temperature σ is different from zero and thus λ, which is the square of the mass of the π-field, vanishes. Equation (41) gives the spontaneous magnetization:

$$\sigma^2 = 1 - \frac{(N-2)T}{(2\pi)^d} \int^{\Lambda} \frac{d^d p}{p^2} \tag{42}$$

At T_c, σ vanishes:

$$\frac{1}{T_c} = \frac{N-2}{(2\pi)^d} \int^{\Lambda} \frac{d^d p}{p^2} \tag{43}$$

Therefore Eq. (42) can be rewritten:

$$\sigma^2 = 1 - T/T_c \tag{44}$$

Above T_c, σ instead vanishes and λ, which is now the square of the common mass of the π- and σ-field, is given for $2 < d < 4$ by

$$\frac{1}{T_c} - \frac{1}{T} = \lambda^{d/2-1} \frac{N-2}{(2\pi)^d} \int \frac{d^d p}{p^2(p^2+1)} + O(\lambda \Lambda^{d-4}) \tag{45}$$

3.1. Finite-Size Calculations

The action now takes the form

$$S_{\text{eff}}(\boldsymbol{\sigma}, \lambda) = \frac{1}{2T} \int d\tau \, d^{d-1}x \left[\frac{\theta^2}{L^2} \boldsymbol{\sigma}^2 + \dot{\boldsymbol{\sigma}}^2 + 2\frac{\theta}{L}(\dot{\sigma}_2 \sigma_1 - \dot{\sigma}_1 \sigma_2) \right.$$
$$\left. + (\partial_i \boldsymbol{\sigma})^2 + \lambda(\boldsymbol{\sigma}^2 - 1) \right] + \frac{1}{2}(N-2) \operatorname{tr} \ln[-\Delta + \lambda(x)] \tag{46}$$

The main problem is now that two types of boundary conditions, which are hardly distinguishable in the low-temperature expansion, are possible. We can look for constant saddle points in λ, σ, and the calculations are then simple. However, this corresponds to imposing the direction of the magnetization, rather than the values of the microscopic spin variables. We can instead impose the values of the microscopic variables, but then the saddle point fields are τ dependent and the saddle point equations become integral equations. A guess is that for T fixed below T_c the difference between both procedures is negligible while it is essential near T_c. We examine the simple case first.

Macroscopic Boundary Conditions. The saddle point equations are then

$$\sigma\left(\lambda+\frac{\theta^2}{L^2}\right)=0 \tag{47}$$

$$1-\sigma^2=\frac{(N-2)T}{LL_\perp^{d-1}}\sum_{k}\sum_{m=1}^{\infty}\left[\frac{m^2\pi^2}{L^2}+\left(\frac{2\pi\mathbf{k}}{L_\perp}\right)^2+\lambda\right]^{-1} \tag{48}$$

In the second equation a cutoff is of course implied.

In the low-temperature phase we thus find

$$\lambda=-\theta^2/L^2 \tag{49}$$

Note that the free energy depends only on the value of λ. The equation (48) for σ, however, even at leading order, contains an important information. Because of the condition that the lhs is smaller than 1, Eq. (49) is only valid up to $T(\theta)<T_c$. We have

$$1-\frac{T}{T_c}-\sigma^2=\frac{1}{2}(N-2)\frac{TL}{L_\perp^{d-1}}\int_0^\infty ds\left\{e^{s\theta^2}[A(\pi^2 s)-1]\,A^{d-1}\right.$$
$$\left.\times\left(\frac{4\pi^2 sL^2}{L_\perp^2}\right)-2\left(\frac{L_\perp}{L}\right)^{d-1}\frac{1}{(4\pi s)^{d/2}}\right\}$$

The free energy for $d>2$ is then

$$F=\left(\frac{1}{T}-\frac{1}{T_c}\right)\frac{\theta^2}{2L^2}+\frac{1}{L^d}\varphi(\theta)$$

with $\varphi(\theta)$ given by Eq. (30).

The saddle point equation in the case of microscopic boundary conditions is much more complicated because it involves the calculation of time-dependent operators and has not been studied.

4. THE $(\phi^2)^2$ FIELD THEORY

We consider now the action suited for a study near four dimensions,

$$S[\phi]=\int d^dx\left[\frac{1}{2}(\partial_\mu\phi)^2+\frac{1}{2}r\phi^2+\frac{1}{4!}g(\phi^2)^2\right] \tag{50}$$

At leading order we need only the action for the two σ-components. Again the simple calculation corresponds to macroscopic boundary conditions.

Macroscopic Boundary Conditions. The mean field free energy in the low-temperature phase becomes

$$F = \frac{\theta^2}{2L^2}\sigma^2 + \frac{1}{2}r\sigma^2 + \frac{1}{4!}g\sigma^4 - \text{value at } \theta = 0$$

with the equation

$$\frac{\theta^2}{L^2} + r + \frac{1}{6}g\sigma^2 = 0$$

This last equation implies the condition

$$\theta^2 \leqslant -rL^2 \Leftrightarrow \theta \leqslant L/\xi$$

At the saddle point,

$$F = -3r\frac{\theta^2}{gL^2} - \frac{3}{2}\frac{\theta^4}{gL^4}$$

an expression which is consistent with the low-temperature and large-N calculation.

Microscopic Boundary Conditions. The calculations are lengthy and delicate even at the simple mean field level, and we shall not go beyond this tree level. Then $N-2$ components of the field ϕ are set to zero and we keep the two components σ_1 and σ_2, parametrized as

$$\sigma_1 = \sigma\cos\varphi, \qquad \sigma_2 = \sigma\sin\varphi$$

The boundary conditions are $\varphi(0) = 0$, $\varphi(L) = \theta$ for the angle. For σ we impose on the boundary a magnetization of order $\Lambda^{(d-2)/2}$, in which Λ is an inverse length which is large compared to $(r)^{1/2}$ (r vanishes linearly at T_c). Therefore we will later take the limit in which $\sigma(0)$ and $\sigma(L)$ go to infinity. The mean field action reduces to

$$S(\sigma,\varphi) = L_\perp^{d-1}\int_0^L d\tau\left[\frac{1}{2}(\dot{\sigma})^2 + \frac{1}{2}\sigma^2(\dot{\varphi})^2 + \frac{1}{2}r\sigma^2 + \frac{1}{4!}g\sigma^4\right] \tag{51}$$

and we minimize it with respect to σ and φ. This is a simple mechanical motion in a plane, and with the two constants of motion, the angular momentum b and the energy E, the trajectories $\sigma(\tau)$ are given by

$$b\int_0^L \frac{d\tau}{\sigma(\tau)^2} = \theta \tag{52}$$

and

$$\int^{\sigma} \frac{d\sigma'}{p(\sigma')} = \tau \tag{53}$$

in which $p(\sigma)$ is the velocity defined as

$$p(\sigma) = (b^2/\sigma^2 + r\sigma^2 + g\sigma^4/12 - 2E)^{1/2} \tag{54}$$

The motion $\sigma(\tau)$ takes place between a large initial value, which will be taken later as infinite, bounces on the potential wall at a value $\sigma_{\min}(b)$ at which the velocity $p(\sigma)$ vanishes, and returns to infinity. Therefore the two constants of motion E and b are determined by the equations

$$2\int_{\sigma_{\min}}^{\infty} \frac{d\sigma}{p(\sigma)} = L \tag{55}$$

$$2b\int_{\sigma_{\min}}^{\infty} \frac{d\sigma}{\sigma^2 p(\sigma)} = \theta \tag{56}$$

The constants of motion E and b both depend on θ. When $\theta = 0$, b vanishes, E takes the value E_0, and the velocity $p(\sigma)$ becomes

$$p_0(\sigma) = (r\sigma^2 + g\sigma^4/12 - 2E_0)^{1/2}$$

The free energy per unit volume is finally given by

$$F = \frac{2}{L}\int_{\sigma_{\min}(b)}^{\infty} d\sigma\, [p(\sigma) - p_0(\sigma)] - \frac{2}{L}\int_{\sigma_{\min}(0)}^{\sigma_{\min}(b)} d\sigma\, p_0(\sigma) + E(\theta) - E_0 \tag{57}$$

For small θ, F vanishes as θ^2 and we neglect from now on all higher powers of θ. After a tedious and long calculation, we end up with

$$F = \frac{\theta b}{2L} + O(\theta^4) \tag{58}$$

with

$$2b\int_{\sigma_{\min}(0)}^{\infty} \frac{d\sigma}{\sigma^2 p_0(\sigma)} = \theta \qquad \text{and} \qquad 2\int_{\sigma_{\min}(0)}^{\infty} \frac{d\sigma}{p_0(\sigma)} = L$$

These complete elliptic integrals are easy to analyze in the various limits of interest, but first a simple rescaling will reveal the expected finite-size scaling property of F:

$$\sigma \to \sigma/L, \qquad b \to b/L^3, \qquad E_0 = g\omega/24L^4$$

$$p_0(\sigma) = (g/12)^{1/2}\, L^{-2} q(\sigma)$$

with

$$q(\sigma) = (\sigma^4 + \rho\sigma^2 - \omega)^{1/2} \tag{59}$$

and

$$\rho = 12rL^2/g \tag{60}$$

which is proportional to $(L/\xi)^2$ in mean field theory. The expression for the free energy is thus

$$FL^4 = \frac{\theta b}{2} + O(\theta^4) \tag{61}$$

with the conditions

$$b = \frac{1}{2}\theta\left(\frac{g}{12}\right)^{1/2}\left[\int_a^\infty \frac{dx}{x^2(x^4+\rho x^2-\omega)^{1/2}}\right]^{-1} \tag{62}$$

and

$$1 = 2\left(\frac{12}{g}\right)^{1/2}\int_a^\infty \frac{dx}{(x^4+\rho x^2-\omega)^{1/2}} \tag{63}$$

in which a is the zero of $q(\sigma)$ given by $a = [-\rho/2 + (\rho^2/4+\omega^2)^{1/2}]^{1/2}$.

Equations (62) and (63) define ω and b as functions of ρ, i.e., of L/ξ, and Eq. (61) shows that indeed $F = L^{-d}f(L/\xi, \theta)$ (with $d=4$ for mean field theory), as expected from the previous scaling theory. It is now easy to study the resulting properties of F in the various limits:

(i) $L \gg \xi$ (for $T > T_c$), ρ goes to plus infinity. One finds that ω vanishes exponentially, and the final result is

$$FL^4 = 48(L/\xi)^3\,\theta^2/ge^{-L/\xi} + O(\theta^4) \tag{64}$$

in which $\xi = (r)^{-1/2}$. As expected, above the critical temperature the dependence in the twist angle θ vanishes exponentially.

(ii) $\xi \gg L$ (i.e., T near T_c), ρ goes to zero, and we find

$$FL^4 = [3\Gamma^8(1/4)/(32g\pi^3)]\,\theta^2 + O(\theta^4) \tag{65}$$

Since L is finite, we did expect, as exhibited on (65), that the function $f(L/\xi, \theta)$ is regular in the limit in which L/ξ goes to zero.

(iii) $L \gg \xi$ (for $T < T_c$), ρ goes to minus infinity, and ω is negative. The integrals in Eqs. (62) and (63) behave both logarithmically for large ρ, and one finds that $\omega=\rho^2/4-16\rho^2(\exp -L/\xi)$, with now $\xi=(-2r)^{-1/2}$. Neglecting the exponentially small corrections, we obtain finally

$$FL^4 = -3rL^2\theta^2/g + O(\theta^4, \exp -L/\xi) \tag{66}$$

in agreement with the mean field calculation with macroscopic boundary conditions. Below the critical temperature we recover the characteristic $1/L^2$ behavior of the free energy due to spin waves.

5. CONCLUDING REMARKS

Finite-size scaling functions for twisted boundary conditions have been computed for an arbitrary ratio L/ξ in a $2+\varepsilon$ expansion and for $L \gg \xi$ for any dimension between two and four, owing to the property that the size-dependent effective temperature t_L goes to zero in this limit.

Similarly, $4-\varepsilon$ and $1/N$ expansions have been applied to this problem. Calculations are simple at fixed temperature below T_c because microscopic boundary conditions, i.e., fixed spin on the boundary, and macroscopic boundary conditions, i.e., fixed magnetization, are equivalent. However, near T_c these boundary conditions lead to different physics, and microscopic boundary conditions are not easy to handle. In all these calculations we see no evidence for an alleged breakdown of the nonlinear σ model. Indeed if this phenomenon exists, it cannot manifest itself in a perturbative calculation.

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