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Kosterlitz–Thouless theory and lattice artifacts

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Abstract

The massive continuum limit of the (1+1)-dimensional $O(2)$ nonlinear σ -model (XY -model) is studied using its equivalence to the sine–Gordon model at its asymptotically free point. It is shown that leading lattice artifacts are universal but they vanish only as inverse powers of the logarithm of the correlation length. Such leading artifacts are calculated for the case of the scattering phase shifts and the correlation function of the Noether current using the bootstrap S -matrix and perturbation theory respectively.

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1. Introduction

In this paper we study the properties of the two-dimensional $O(2)$ nonlinear σ -model, better known as the XY -model. This model has been the subject of extensive theoretical and numerical analysis, starting with the seminal papers of Kosterlitz and Thouless (KT) [1]. For a review of KT theory, see [2].

Analytical work is usually based on a series of mappings that starts from the original (lattice) XY -model and arrives at the sine–Gordon (SG) model or its fermionic equivalent, a (deformed) version of the chiral Gross–Neveu (CGN) model. This latter formulation is most useful if one wants to study questions related to the dynamically generated $SU(2)$ symmetry of the model.

Most papers on the XY -model study its properties of interest for statistical physics, in particular the peculiarities of the KT phase transition, which is of infinite order. In this paper we look at the XY -model as an example of (1 + 1)-dimensional relativistic quantum field theory. More precisely, we study the massive continuum limit of the lattice theory, which, in the language of statistical physics, means that we approach the KT phase transition point from the high-temperature phase.

Treating the XY -model as the $n = 2$ member of the family of $O(n)$ nonlinear σ -models gives additional insights, since a lot is known about the $n \geq 3$ models [3]. More importantly,

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using the SG language, we show that the approach to the continuum limit in this model is much slower than in most other lattice models. Lattice artifacts vanish in this model, instead of the usual Symanzik-type behaviour [4] (i.e. integer powers of the lattice spacing), as inverse powers of the logarithm of the lattice spacing only. Of course, as in all other $O(n)$ lattice models with $n \geq 3$, there are usual lattice artifacts corresponding to higher-order derivative couplings also in the XY -model. They are expected to have Symanzik-type behaviour. What makes this model different is that in an MC study even after these usual lattice artifacts disappeared (became smaller than statistical fluctuation), there remained a very slowly decreasing component.

On the other hand, we can show that these leading artifacts are universal and calculable. Our main result is equations (79) and (81) in section 4, which allow us to calculate leading lattice artifacts in terms of SG data. We use the continuum regularization scheme of [5]. Because of universality, our results are valid for the leading corrections in any regularization scheme, thus also for the one corresponding to the standard lattice action (8).

We can make use of the fact that the SG model is exactly solvable and its bootstrap S -matrix is exactly known. We calculate the leading artifacts for the scattering phase shifts using the bootstrap results. An alternative method is perturbation theory (PT). Since the SG model is asymptotically free if we use suitable expansion parameters [5], the methods of renormalization-group- (RG-) improved PT are thus available.

In section 2 we review the chain of mappings leading from the XY -model to the SG model and its equivalent fermionic formulation.

In section 3 we recall the analysis of the phase diagram of the model in the vicinity of the KT phase transition point. This is described in the SG language.

In section 4 we explain how to calculate the lattice artifacts and apply this to the case of the scattering phase shifts.

Finally in section 5 we calculate the lattice artifacts for the two-point correlation function of the Noether current corresponding to the $O(2)$ symmetry. Here we use the method of RG-improved PT. To calculate the value of a non-perturbative constant needed here, we also consider the system in the presence of an external field coupled to the Noether charge. (This calculation is analogous to that used previously to determine the M/Λ ratio for the $O(n)$ models [6].) We give here a parameter-free two-loop formula for the lattice artifacts.

A precision MC study of the massive continuum limit of the $O(2)$ model will be described in a forthcoming paper [7].

2. From the XY -model to the sine–Gordon model and beyond

In this section we describe in some detail the chain of mappings starting with the XY -model and ending at the SG model and its fermionic equivalent.

We can treat the XY -model as the $n = 2$ member of the family of $O(n)$ nonlinear σ -models with Lagrangian

$$\mathcal{L}^{O(n)} = \frac{1}{2g^2} \partial_\mu S^a \partial_\mu S^a \quad S^a S^a = 1 \quad a = 1, 2, \dots, n. \quad (1)$$

Much is known about the integrable, non-Abelian $n \geq 3$ models [3, 8, 9]. It is natural to assume that the Abelian $O(2)$ model is also integrable and that its spectrum consists of a single $O(2)$ doublet of massive particles. As we will see, this conclusion follows indeed from the KT theory [1] of the XY -model.

Before turning to the KT theory we make a small digression to discuss the two-dimensional SG model. Its Lagrangian can be written as

$$\mathcal{L}^{\text{SG}} = \frac{1}{2} \partial_\mu \phi \partial_\mu \phi + \frac{\alpha}{\beta^2 a^2} [1 - \cos(\beta\phi)] \quad (2)$$

where α is the dimensionless mass parameter, a is a constant of dimension mass^{-1} and β is the SG coupling. It is also integrable and its spectrum and S -matrix were found in [3]. The spectrum depends on β in a complicated way but it becomes simple for the range $8\pi > \beta^2 > 4\pi$, when it is free of any bound states and consists of a single $O(2)$ vector of massive particles whose S -matrix can be written as

$$S_{ab;cd}(\theta) = \sigma_1(\theta) \delta_{ab} \delta_{cd} + \sigma_2(\theta) \delta_{ac} \delta_{bd} + \sigma_3(\theta) \delta_{ad} \delta_{bc} \quad (3)$$

where

$$\begin{aligned} \sigma_1(\theta) &= \cosh \frac{i\pi\nu}{2} \sinh \frac{\theta\nu}{2} \frac{s^{(2)}(\theta)}{\sinh \frac{(i\pi-\theta)\nu}{2}} \\ \sigma_2(\theta) &= -\sinh \frac{i\pi\nu}{2} \sinh \frac{\theta\nu}{2} \frac{s^{(2)}(\theta)}{\cosh \frac{(i\pi-\theta)\nu}{2}} \\ \sigma_3(\theta) &= \cosh \frac{i\pi\nu}{2} \cosh \frac{\theta\nu}{2} \frac{s^{(2)}(\theta)}{\cosh \frac{(i\pi-\theta)\nu}{2}}. \end{aligned} \quad (4)$$

We have introduced the parametrization

$$\nu = \frac{8\pi}{\beta^2} - 1. \quad (5)$$

The ‘isospin 2’ phase shift for the SG model is

$$s^{(2)}(\theta) = -\exp \left\{ 2i \int_0^\infty \frac{d\omega}{\omega} \sin \omega\theta \tilde{k}(\omega) \right\} \quad (6)$$

with

$$\tilde{k}(\omega) = \frac{\sinh \frac{\pi\omega(1-\nu)}{2\nu}}{2 \cosh \frac{\pi\omega}{2} \sinh \frac{\pi\omega}{2\nu}}. \quad (7)$$

The XY -model can be identified with the $\nu \rightarrow 0$ limit of the SG model. This is surprising since in this limit the bootstrap S -matrix (4) becomes $SU(2)$ symmetric, coinciding with the S -matrix of the $SU(2)$ CGN model [10]. It is not obvious where this enlarged symmetry comes from. The existence of a nontrivial XY -model is even more surprising in the light of the fact that the beta-function of the coupling g^2 in (1) vanishes for $n = 2$ and by making the substitution $S^1 = \cos \varphi$, $S^2 = \sin \varphi$ the Lagrangian (1) naively becomes free.

Kosterlitz and Thouless [1] argued that the fact that φ is a periodic (angular) variable plays an important role and therefore the model has nontrivial dynamics. They have shown that topologically nontrivial objects, vortices, are present in typical spin configurations and their interaction makes the theory nontrivial.

The standard lattice action of the XY -model is

$$S_{XY} = K \sum_{x,\mu} [1 - \cos(\varphi(x) - \varphi(x + \hat{\mu}))]. \quad (8)$$

We denote by K the inverse of the XY -model coupling to avoid confusion with the SG coupling β . Assuming universality, not only the cosine function but any other 2π -periodic

function $W(\varphi)$ which has a local minimum at $\varphi = 0$ defines a possible XY -model lattice action. The Villain model action [11] is characterized by

$$W(\varphi) = -\frac{1}{K_V} \ln \left[\sum_m \exp \left\{ -\frac{K_V}{2} (\varphi - 2\pi m)^2 \right\} \right]. \quad (9)$$

Kosterlitz and Thouless showed that typical spin configurations can be represented as a mixture of smooth, topologically trivial configurations (spin waves) and a gas of vortices (of integer topological charge). The KT vortices are not interacting with the spin waves, but there is a logarithmic interaction potential between the vortices, which are therefore identical to a two-dimensional Coulomb gas. This spin wave + Coulomb gas (SWCG) picture is only approximate if we start from the standard action (8) but it is an exact duality transformation [12] for the Villain action corresponding to (9). That the XY -model with standard action is in the same universality class as the Villain model was demonstrated using Monte Carlo RG techniques [13]. On the other hand, it has been shown rigorously [14] that the Coulomb gas has a phase transition point at some finite critical coupling K_c . KT interpreted this phase transition as one of vortex condensation and by a (heuristic) energy–entropy consideration showed that in the vicinity of K_c vortices of topological charge ± 1 only are important; higher vortices can be neglected. It is easy to see that this system (SWCG with unit charge vortices only) is exactly equivalent to the SG model. In [5] it was shown that the extremal SG fixed point $\beta^* = \sqrt{8\pi}$, $\alpha^* = 0$ is appropriate to describe the KT phase transition. The renormalizability of the SG model around this point was explicitly demonstrated up to two-loop order in a simultaneous perturbative expansion in α and $\delta = \frac{\beta^2 - 8\pi}{8\pi}$.

Finally, there is a further transformation that explains the dynamical $SU(2)$ symmetry of the XY -model. The SG model can be exactly mapped [15] to a fermionic model formulated in terms of a two-component Dirac fermion ψ . The transformation is similar to the well known one that relates the SG model to the massive Thirring model [16]. Here the fermionic model is a deformation of the CGN model with four-fermion interaction:

$$\mathcal{L}_F = i(\bar{\psi}\gamma_\mu\partial_\mu\psi) - g_0(J_\mu^1)^2 - g_0(J_\mu^2)^2 - (g_0 + f_0)(J_\mu^3)^2 \quad (10)$$

where

$$J_\mu^a = \frac{1}{2} \bar{\psi}\gamma_\mu\sigma^a\psi \quad (11)$$

is the fermionic $SU(2)$ current. The relation between the SG couplings δ , α and the fermion couplings g_0 , f_0 is

$$\alpha = \frac{8}{\pi}g_0 + \dots \quad \delta = -\frac{1}{\pi}(g_0 + f_0) + \dots \quad (12)$$

where the dots indicate that the relations (12) receive higher-order corrections in PT. In the fermionic formulation the KT fixed point is the Gaussian one and for vanishing deformation parameter, $f_0 = 0$, the model is manifestly $SU(2)$ symmetric. The corresponding relation in the SG language is $\alpha + 8\delta = 0$ at lowest order.

To summarize, the XY -model in the vicinity of the KT transition point is believed to be described by the SG model with extremal coupling $\beta = \sqrt{8\pi}$. This is further equivalent to the two-component CGN model around its Gaussian point. We will use the SG language throughout this paper.

3. The SG description of the O(2) model

In this section we review the SG description of the KT theory, closely following the approach of Amit *et al* [5]. Without loss of generality we can adopt the somewhat unusual regularization

scheme of the authors, since, as we will see, all important results are universal, i.e. independent of the regularization scheme. Nevertheless, it would be interesting to repeat all the calculations below using some of the more customary regularizations such as the lattice or dimensional regularization.

Our starting point is the Euclidean Lagrangian [5]

$$\mathcal{L} = \frac{1}{2} \partial_\mu \phi \partial_\mu \phi + \frac{m_0^2}{2} \phi^2 + \frac{\alpha_0}{\beta_0^2 a^2} [1 - \cos(\beta_0 \phi)] \quad (13)$$

where m_0 is an IR regulator mass and a is the UV cutoff (of dimension length). We have denoted the dimensionless SG couplings by β_0 and α_0 to emphasize that they are bare (unrenormalized). UV regularized correlation functions are calculated by using

$$G_0(x) = \frac{1}{2\pi} K_0 \left(m_0 \sqrt{x^2 + a^2} \right) \quad (14)$$

where K_0 is the modified Bessel function, as the ϕ propagator. Our strategy is slightly different from [5], who really considered the renormalization of the massive SG model (13) of mass m_0 . We treat m_0 as an IR regulator mass and consider IR-stable physical quantities for which we can take the limit $m_0 \rightarrow 0$ already at the UV regularized level (before UV renormalization). All renormalization constants are, for example, IR stable and independent of m_0 .

The SG coupling β_0 is close to its special value $\sqrt{8\pi}$ and a simultaneous perturbative expansion in the mass parameter α_0 and the deviation δ_0 is defined, where

$$\beta_0^2 = 8\pi(1 + \delta_0) \quad (15)$$

and the parameters are renormalized according to

$$\alpha_0 = Z_\alpha \alpha \quad (16)$$

$$\beta_0^2 = Z_\phi^{-1} \beta^2. \quad (17)$$

Here the Z -factors are functions of the renormalized couplings α and δ and the combination

$$l = \ln \mu a \quad (18)$$

where μ is an arbitrary mass parameter (basically the normalization point). Similarly, a renormalization constant Z is necessary to make \mathcal{G} , the spin–spin two-point function, finite:

$$\mathcal{G}_R = Z\mathcal{G}. \quad (19)$$

For vanishing mass parameter α the Lagrangian (13) is trivial and $Z_\phi = 1$ since there is no need to renormalize the SG coupling. The spin–spin correlation function (which is an exponential of the basic field ϕ) is renormalized even at this point, but in this case its renormalization constant is simply

$$Z = (\mu a)^{-\frac{1}{4(1+\delta)}}. \quad (20)$$

In addition, there is a symmetry $\alpha \leftrightarrow -\alpha$ (which corresponds to a $\frac{\pi}{\beta_0}$ shift in the basic field).

Taking into account the above constraints, the perturbative expansion of the Z -factors must be of the form

$$Z_\phi = 1 + f_1 \alpha^2 l + \alpha^2 \delta (\bar{f}_2 l^2 + f_2 l) + \dots \quad (21)$$

$$Z_\alpha = 1 + g_1 \delta l + \alpha^2 (\bar{g}_2 l^2 + g_2 l) + \delta^2 (\bar{g}_3 l^2 + g_3 l) + \dots \quad (22)$$

$$Z = e^{-\frac{l}{4(1+\delta)}} \{ 1 + \alpha^2 (\bar{h}_1 l^2 + h_1 l) + \dots \}. \quad (23)$$

Amit *et al* [5] found the following results:

$$\begin{aligned} f_1 &= \frac{1}{32} & \bar{f}_2 &= -\frac{1}{16} & f_2 &= -\frac{3}{32} \\ g_1 &= -2 & \bar{g}_2 &= \frac{1}{32} & g_2 &= -\frac{5}{64} \\ \bar{g}_3 &= 2 & g_3 &= 0. \end{aligned} \quad (24)$$

Furthermore $\bar{h}_1 = -1/256$, but the number h_1 is not known at present. The above two-loop beta-function coefficients were calculated also by other methods. The original calculation has recently been reconsidered and the results (24) have been confirmed [17].

The spin-spin correlation function satisfies the equation

$$\mathcal{D}\mathcal{G} = \gamma\mathcal{G} \quad (25)$$

where \mathcal{D} is the RG operator

$$\mathcal{D} = -a \frac{\partial}{\partial a} + D = -a \frac{\partial}{\partial a} + \beta_\alpha(\alpha_0, \delta_0) \frac{\partial}{\partial \alpha_0} + \beta_\delta(\alpha_0, \delta_0) \frac{\partial}{\partial \delta_0} \quad (26)$$

and the β - and γ -functions are given by

$$\beta_\alpha(\alpha_0, \delta_0) = -g_1\alpha_0\delta_0 - g_2\alpha_0^3 - g_3\alpha_0\delta_0^2 + \dots \quad (27)$$

$$\beta_\delta(\alpha_0, \delta_0) = f_1\alpha_0^2 + (f_1 + f_2)\alpha_0^2\delta_0 + \dots \quad (28)$$

$$\gamma(\alpha_0, \delta_0) = -\frac{1}{4} + \frac{1}{4}\delta_0 - \frac{1}{4}\delta_0^2 + h_1\alpha_0^2 + \dots \quad (29)$$

Now, as is well known, not all β -function coefficients are universal. For example, under a redefinition

$$\tilde{\alpha}_0 = \alpha_0 + L\alpha_0\delta_0 + \dots \quad (30)$$

$$\tilde{\delta}_0 = \delta_0 + K\alpha_0^2 + \dots \quad (31)$$

the coefficients change as

$$\begin{aligned} \tilde{g}_1 &= g_1 & \tilde{f}_1 &= f_1 \\ \tilde{g}_2 &= g_2 - Kg_1 - Lf_1 & \tilde{f}_2 &= f_2 - 2Kg_1 - 2Lf_1 \\ \tilde{g}_3 &= g_3. \end{aligned} \quad (32)$$

(Equations (30) and (31) are the most general perturbative redefinition respecting the $\alpha_0 \leftrightarrow -\alpha_0$ symmetry together with the requirement that for $\alpha_0 = 0$ δ_0 is not redefined.) From (32) we see that in addition to the one-loop coefficients g_1 and f_1 there exist also two-loop invariants. They are g_3 and the combination

$$J = 2g_2 - f_2. \quad (33)$$

Two important physical quantities are the correlation length

$$\xi = \frac{1}{Ma} = e^{\Psi(\alpha_0, \delta_0)} \quad (34)$$

where M is the mass of the physical particle and the dimensionless susceptibility

$$\chi = \frac{1}{a^2} \int d^2x \mathcal{G}(x) = e^{\Phi(\alpha_0, \delta_0)}. \quad (35)$$

From (25) it follows that the exponents satisfy

$$D\Psi = 1 \quad (36)$$

$$D\Phi = 2 + \gamma. \quad (37)$$

It is useful to introduce the RG-invariant quantity $Q(\alpha_0, \delta_0)$, which satisfies $DQ = 0$. Introducing the inverse function $k(\delta_0, Q)$, that satisfies

$$\alpha_0 = k(\delta_0, Q(\alpha_0, \delta_0)) \quad (38)$$

we can define new β - and γ -functions:

$$b(\delta_0, Q) = \beta_\delta(k(\delta_0, Q), \delta_0) \quad (39)$$

$$\Gamma(\delta_0, Q) = \gamma_\delta(k(\delta_0, Q), \delta_0). \quad (40)$$

The advantage of using the variables δ_0 and Q is that the RG invariant Q can be treated in many respects as if it were a numerical constant and δ_0 were a single coupling constant. For example, if we write

$$\Psi(\alpha_0, \delta_0) = \Psi_1(\delta_0, Q(\alpha_0, \delta_0)) \quad (41)$$

and

$$\Phi(\alpha_0, \delta_0) = \Phi_1(\delta_0, Q(\alpha_0, \delta_0)) \quad (42)$$

then the functions Ψ_1 and Φ_1 can be determined from

$$\frac{\partial}{\partial \delta_0} \Psi_1(\delta_0, Q) = \frac{1}{b(\delta_0, Q)} \quad (43)$$

and

$$\frac{\partial}{\partial \delta_0} \Phi_1(\delta_0, Q) = \frac{2 + \Gamma(\delta_0, Q)}{b(\delta_0, Q)} \quad (44)$$

respectively.

Using (27) and (28) Q can be determined:

$$Q(\alpha_0, \delta_0) = \frac{1}{32}\alpha_0^2 - 2\delta_0^2 + 2g_2\alpha_0^2\delta_0 + F_2\delta_0^3 + \dots \quad (45)$$

and using this in (39) we find

$$b(\delta_0, Q) = Q + 2\delta_0^2 + AQ\delta_0 + B\delta_0^3 + \dots \quad (46)$$

while the Γ function to this order is

$$\Gamma(\delta_0, Q) = -\frac{1}{4} + \frac{1}{4}\delta_0 + \dots \quad (47)$$

Here

$$A = 1 - \frac{J}{f_1} \quad B = -\frac{2}{3}g_3 + \frac{2}{3}A \quad F_2 = \frac{2}{3}g_3 + \frac{4}{3}A \quad (48)$$

or numerically

$$A = 3 \quad B = 2 \quad F_2 = 4 \quad (49)$$

but we will keep these constants in the following to explicitly demonstrate that all our results are universal.

We know that a one-parameter renormalizable subspace in the δ_0 – α_0 plane is equivalent to the $SU(2)$ CGN model. (This is most evident in the fermionic formulation.) This subspace must correspond to the $Q = 0$ RG trajectory because we know that it goes through the point $\alpha_0 = \delta_0 = 0$. Moreover, it must be the $\delta_0 < 0$ branch of the $Q = 0$ trajectory, since it is the one that is asymptotically free in PT.

Following [5] the phase diagram of our model is represented in figure 1. The CGN model corresponds to the separatrix S_2 on this plot, which will be referred to as PD for short. Region III corresponds to $Q > 0$, whereas regions I and II correspond to $Q < 0$, $\delta_0 > 0$ and $Q < 0$, $\delta_0 < 0$, respectively.

In the neighbourhood of S_2 , i.e. close to the CGN case, we have

$$b(\delta_0, Q) = b_0(\delta_0) + Qb_1(\delta_0) + \dots \quad (50)$$

where

$$b_0(\delta_0) = 2\delta_0^2 + B\delta_0^3 + \dots \quad (51)$$

$$b_1(\delta_0) = 1 + A\delta_0 + \dots \quad (52)$$

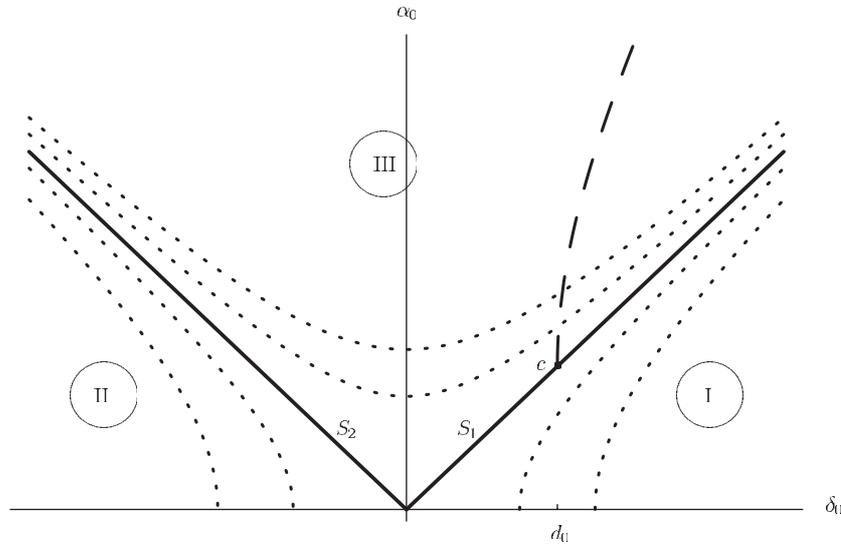


Figure 1. Phase diagram of the KT theory. The entire region I is critical. The model is massive in region III ($Q > 0$) and region II ($Q < 0$). The dotted curves are RG trajectories. The full lines S_1 and S_2 correspond to the critical surface of the XY-model and the (bare) CGN model respectively. The dashed curve is the XY-model hitting the critical surface at c .

It is a crucial observation that near the CGN line the correlation length exponent Ψ_1 is a smooth analytic function of Q :

$$\Psi_1(\delta_0, Q) = H_0(\delta_0) + QH_1(\delta_0) + \dots \quad (53)$$

where

$$H_0(\delta_0) = -\frac{1}{2\delta_0} - \frac{B}{4} \ln |2\delta_0| + \Psi_0 + \dots \quad (54)$$

$$H_1(\delta_0) = \frac{1}{12\delta_0^3} + \frac{A-B}{8\delta_0^2} + \dots \quad (55)$$

We will calculate the value of the nonperturbative constant Ψ_0 in section 5.

Now we can integrate (43) using the perturbative expansion (46) and for $Q > 0$ we obtain

$$\Psi_1(\delta_0, Q) = \frac{1}{\sqrt{2Q}} \left(\frac{\pi}{2} + \operatorname{arctg} \frac{\sqrt{2}\delta_0}{\sqrt{Q}} \right) - \frac{B}{8} \ln 2(Q + 2\delta_0^2) + \frac{2A-B}{8} \frac{Q}{Q + 2\delta_0^2} + \Psi_0 + \dots \quad (56)$$

Here the dots represent higher-order terms in the perturbative expansion (these are, in principle, calculable) and also for an unknown (nonperturbative) function of Q only. For small Q (56) becomes

$$\Psi_1(\delta_0, Q) = \frac{\pi}{\sqrt{2Q}} \Theta(\delta_0) + H_0(\delta_0) + QH_1(\delta_0) + \dots \quad (57)$$

where the dots represent terms of higher order in Q . They come from the higher perturbative terms of (56) and also from the nonperturbative function mentioned above. The point is that there are no terms, singular in Q , from any of these two sources. This is obvious for the perturbative terms, but must also be true for the nonperturbative contributions, since otherwise Ψ_1 would be singular on the S_2 line. Requiring it to be nonsingular on S_2 , we force Ψ_1 to

diverge on S_1 , which is therefore part of the critical surface of the phase diagram PD. Another line, on which we know the correlation length must diverge, is the δ_0 axis $\alpha_0 = 0$, because this corresponds to a free, massless model.

For $Q < 0$, it is convenient to parametrize Q in terms of the δ_0 value at which the RG trajectory intersects this axis. In other words, we have to express Q in terms of d , that solves

$$b(d, Q) = 0. \quad (58)$$

(Note that in this parametrization $|\delta_0| \geq |d|$, because $\alpha_0^2 \geq 0$.) The perturbative solution of (58) is

$$Q = -2d^2 + (2A - B)d^3 + \dots. \quad (59)$$

Using this parametrization the perturbative solution for $Q < 0$ is

$$\begin{aligned} \Psi_1(\delta_0, Q) = & -\frac{1}{4d} \ln \left(\frac{\delta_0 + d}{\delta_0 - d} \right) \left[1 + \frac{2A - 3B}{4} d \right] + \frac{2A - B}{8} \frac{d}{\delta_0 + d} \\ & - \frac{B}{4} \ln 2|\delta_0 + d| + y(d) + \dots \end{aligned} \quad (60)$$

where

$$\text{for } d < 0 \quad y(d) = \Psi_0 + \dots \quad (61)$$

$$\text{for } d > 0 \quad y(d) = \infty. \quad (62)$$

Equation (61) is obtained by matching (60) to (53) for small Q , while (62) is formally true since this is the only way to ensure that the correlation length diverges on the positive half of the δ_0 axis. (Without the infinite constant ξ actually *vanishes* there.)

Now we can discuss the phase diagram of our model. The entire region I is critical. The massive phase is regions II and III and the critical surface bordering them is S_1 plus the negative part of the δ_0 axis. They are smoothly connected across S_2 , which is the (bare) CGN model. The O(2) NLS model corresponds to the dashed curve of PD. In an MC experiment we are approaching the critical point c from the massive phase (region III). We will denote the δ_0 coordinate of c by d_0 . Because the RG trajectories are running basically parallel to S_1 , it is physically irrelevant at which point the critical surface is reached and therefore the parameter d_0 is irrelevant. The continuum model will be the same for all points on S_1 , including the origin. However, the origin is the point where (coming along S_2) the continuum CGN model is defined! So our continuum theory is inevitably identical to the (massive part of the) $SU(2)$ -invariant CGN model.

If we start from somewhere in the middle of region II, we can define a massive continuum limit by approaching the negative half of the δ_0 axis. The intercept d is then relevant. The continuum theory is the SG model with

$$\beta^2 = 8\pi(1 + d). \quad (63)$$

Returning to the O(2) model, the dashed trajectory can be parametrized as

$$\delta_0 = d_0 + d_1 \tau + \dots \quad (64)$$

$$\alpha_0 = k(d_0, 0) + \alpha_1 \tau + \dots \quad (65)$$

where

$$\tau = K_c - K \quad (66)$$

is the reduced coupling and we have assumed that physical quantities are analytic in K . ($K_c = 1.1197(5)$ [13].) Then also Q is analytic in τ :

$$Q \sim \tau. \quad (67)$$

From (57) we see that along the $O(2)$ curve

$$\ln \xi = \frac{\pi}{\sqrt{2Q}} + H_0(d_0) + \dots \quad (68)$$

where the dots represent terms analytic in Q (and vanishing for $Q = 0$). In other words, for the $O(2)$ model [1]

$$\xi = C \exp \left\{ \frac{b}{\sqrt{\tau}} \right\} (1 + \mathcal{O}(\sqrt{\tau})) \quad (69)$$

where the constants C and b are not universal. This is the famous KT formula showing that the phase transition is of infinite order in the reduced temperature.

It is more important for us that (68) can be rewritten as

$$Q = \frac{\pi^2}{2(\ln \xi + u)^2} + \mathcal{O}((\ln \xi)^{-5}) \quad (70)$$

where

$$u = -H_0(d_0) \quad (71)$$

which is given (if d_0 is sufficiently small) perturbatively by

$$u \approx \frac{1}{2d_0} + \frac{B}{4} \ln(2d_0) - \Psi_0. \quad (72)$$

Note that the leading $1/(\log \xi)^2$ term in (70) is universal and only the subleading terms (depending on the value of the parameter u) are model dependent.

The susceptibility exponent Φ_1 can be studied similarly. It can be written as

$$\Phi_1 = \frac{7}{4} \Psi_1 + \tilde{\Phi}_1 = \frac{7}{4} \Psi_1 + \frac{1}{16} \ln(2\delta_0^2 + Q) + \dots \quad (73)$$

where $\tilde{\Phi}_1$ satisfies

$$\frac{\partial \tilde{\Phi}_1}{\partial \delta_0} = \frac{\Gamma(\delta_0, Q) + \frac{1}{4}}{b(\delta_0, Q)}. \quad (74)$$

Now the crucial observation is again that, for small Q ,

$$\Phi_1 = \frac{7}{4} \Psi_1 + c_1 + c_2 Q + \dots \quad (75)$$

because the (calculable) perturbative terms are analytic in Q , while the (not calculable) purely Q -dependent terms in $\tilde{\Phi}_1$ must also be analytic in Q otherwise these latter singularities would also turn up for the CGN line S_2 , where they must not.

From (75) we have

$$\chi = \xi^{\frac{7}{4}} e^{c_1} (1 + c_2 Q + \dots) \quad (76)$$

i.e. there are no (multiplicative) log corrections in the scaling relation for the susceptibility. The possibility of such multiplicative logarithmic corrections is discussed in [18].

4. Determination of the lattice artifacts

Recall that the RG invariant Q has a completely different meaning for region III (which contains the massive phase of the XY -model) and for region II (where the usual massive SG model with $\beta^2 < 8\pi$ can be defined). Indeed, in the positive δ_0 part of region III, close to S_1 , the (positive) parameter Q merely measures the distance from the XY critical surface on which it vanishes, whereas in region II Q is a relevant (negative) parameter related to the SG coupling β by (58) and (63). Our main assumption is that in spite of this difference physical quantities

are smoothly dependent on Q in the vicinity of the separatrix S_2 connecting the two regions. More precisely, we will assume that close to S_2 any physical quantity U has the form

$$U(Q) = U_0 + U_1 Q + \mathcal{O}(Q^2). \quad (77)$$

Here $U_0 = U(0)$ is its value for the CGN model (and thus also in the continuum limit of the XY -model). The first correction coefficient U_1 can be calculated from the SG model as follows. Using the identification (58) and its perturbative solution (59) together with (63) and (5) we have

$$Q = -2v^2 + \mathcal{O}(v^4). \quad (78)$$

This means that if in the SG model, close to the CGN point $v = 0$, we have

$$U(v) = u_0 + u_1 v^2 + \mathcal{O}(v^4) \quad (79)$$

then

$$U_0 = u_0 \quad \text{and} \quad U_1 = -u_1/2. \quad (80)$$

Translated to the language of lattice artifacts by (70) we thus have

$$U(\xi) = u_0 - \frac{u_1 \pi^2}{4(\ln \xi + u)^2} + \mathcal{O}((\ln \xi)^{-4}). \quad (81)$$

This means that lattice artifacts typically disappear very slowly, only as $1/(\log \xi)^2$. On the other hand the leading artifacts are universal and calculable.

We apply this method first to the scattering phase shifts. Recall the SG model S -matrix (3) with (4). The three distinct S -matrix eigenvalues are

$$s^{(0)}(\theta) = 2\sigma_1(\theta) + \sigma_2(\theta) + \sigma_3(\theta) = \frac{\sinh \frac{v}{2}(i\pi + \theta)}{\sinh \frac{v}{2}(i\pi - \theta)} s^{(2)}(\theta) \quad (82)$$

$$s^{(1)}(\theta) = \sigma_2(\theta) - \sigma_3(\theta) = -\frac{\cosh \frac{v}{2}(i\pi + \theta)}{\cosh \frac{v}{2}(i\pi - \theta)} s^{(2)}(\theta) \quad (83)$$

and

$$s^{(2)}(\theta) = \sigma_2(\theta) + \sigma_3(\theta) = -\exp \left\{ 2i \int_0^\infty \frac{d\omega}{\omega} \sin(\theta\omega) \tilde{k}(\omega) \right\} \quad (84)$$

where $\tilde{k}(\omega)$ is given by (7).

We now write

$$s^{(i)}(\theta) = \exp \{ 2i\delta_0^{(i)}(\theta) + 2iv^2\delta_1^{(i)}(\theta) + \mathcal{O}(v^4) \} \quad (85)$$

for $i = 0, 1$ and 2 . Here $\delta_0^{(i)}$ are the CGN phase shifts. The first correction coefficients can be obtained by a simple calculation. The result is

$$\delta_1^{(0)}(\theta) = 0 \quad \delta_1^{(1)}(\theta) = \frac{\pi\theta}{6} \quad \delta_1^{(2)}(\theta) = -\frac{\pi\theta}{12}. \quad (86)$$

This can be used to obtain the leading lattice artifacts in the XY -model by the relation (81).

5. Current–current two-point function and free energy

Consider the two-point function of the Noether current

$$J_\mu = i \frac{\beta_0}{2\pi} \epsilon_{\mu\nu} \partial_\nu \phi. \quad (87)$$

Its Fourier transform $I(p)$ is defined by

$$\langle J_\mu(x) J_\nu(y) \rangle = \int \frac{d^2 p}{(2\pi)^2} e^{-ip(x-y)} \frac{p_\mu p_\nu - p^2 \delta_{\mu\nu}}{p^2} I(p). \quad (88)$$

It is easy to calculate $I(p)$ to second order:

$$I(p) = \frac{2}{\pi} \{1 + \delta_0 + \alpha_0^2 [\Omega(p, a) + \dots]\} \quad (89)$$

where

$$\Omega(p, a) = f_1(\ln pa + \Omega_0) \quad (90)$$

and

$$\Omega_0 = C - \frac{1}{2} - \ln 2 \quad (91)$$

C being Euler's constant.

Standard RG considerations give

$$I(p, \delta_0, Q, a) = I(p_0, \bar{\lambda}, Q, a) = \tilde{I}(p/M, Q) \quad (92)$$

where the running coupling is the solution of

$$\Psi_1(\bar{\lambda}, Q) = \ln \frac{p}{M} - \ln p_0 a. \quad (93)$$

Let us consider the $Q < 0$, $\delta_0 < 0$ case (region II) first. For $p \rightarrow \infty$ also $\Psi_1 \rightarrow \infty$ and therefore $\bar{\lambda} \rightarrow d$, where d is defined by

$$b(d, Q) = 0 \quad \text{or equivalently} \quad \alpha_0 = k(d, Q) = 0. \quad (94)$$

This gives

$$\tilde{I}(\infty, Q) = \frac{2}{\pi} (1 + d) \quad (95)$$

where d parametrizes Q according to (59). (95) is consistent with the identification in (63).

Next we study the case of small Q , because this is relevant if we are interested in the approach to the continuum limit along the $O(2)$ curve. We assume that \tilde{I} is analytic in Q :

$$\tilde{I}(z, Q) = \tilde{I}_0(z) + Q \tilde{I}_1(z) + \dots \quad (96)$$

It is a standard exercise to obtain the asymptotic expansion of the coefficients \tilde{I}_0 and \tilde{I}_1 in PT. One obtains

$$\tilde{I}_0(p/M) = \frac{2}{\pi} \{1 - \lambda + 2\kappa\lambda^2 + \dots\} \quad (97)$$

$$\tilde{I}_1(p/M) = \frac{2}{3\pi} \left\{ \frac{1}{2\lambda} + \kappa + \frac{2B - 3A}{4} + \dots \right\} \quad (98)$$

where

$$\kappa = \Omega_0 - \Psi_0 \quad (99)$$

and the coupling λ is the solution of

$$\frac{1}{2\lambda} - \frac{B}{4} \ln(2\lambda) = \ln \frac{p}{M}. \quad (100)$$

The asymptotic expansions (97) and (98) are valid for $\lambda \ll 1$, i.e. for $p \rightarrow \infty$ but also Q must satisfy

$$Q \ll 6\lambda^2 \quad (101)$$

so that the expansion (96) makes sense.

It is by now standard how the nonperturbative constant κ can be calculated. For this it is necessary to consider the free energy in an external field and we now turn to this calculation. We follow here [19] and start from the modified Lagrangian

$$\mathcal{L}_h = \frac{1}{2}(\partial_\mu \phi)^2 - \frac{\alpha_0}{\beta_0^2 a^2} \cos(\beta_0 \phi) + \frac{\beta_0 h}{2\pi} \partial_1 \phi \quad (102)$$

which corresponds to adding a term ihJ_2 to the Lagrangian density. The modified ground state energy must be of the form

$$\mathcal{E}(h) = -\frac{h^2}{\pi} \mathcal{F}(h) \quad (103)$$

where $\mathcal{F}(h)$ is dimensionless.

In PT we obtain

$$\mathcal{F}(h) = 1 + \delta_0 + \alpha_0^2 [\tilde{\Omega}(h, a) + \dots] \quad (104)$$

where

$$\tilde{\Omega}(h, a) = f_1(\ln ha + \tilde{\Omega}_0) \quad (105)$$

and

$$\tilde{\Omega}_0 = C - \frac{1}{2} + \ln 2. \quad (106)$$

For $Q = 0$ therefore $\mathcal{F}(h)$ has the following asymptotic expansion:

$$\mathcal{F}(h) = 1 - \frac{1}{2 \ln \frac{h}{M}} - \frac{B \ln \ln \frac{h}{M}}{8 \ln^2 \frac{h}{M}} + \frac{\kappa + \ln 4}{2 \ln^2 \frac{h}{M}} + \mathcal{O}\left(\frac{(\ln \ln \frac{h}{M})^2}{\ln^3 \frac{h}{M}}\right). \quad (107)$$

This is to be compared to the exact result [20]

$$\mathcal{F}(h) = 1 - \frac{1}{2 \ln \frac{h}{M}} - \frac{\ln \ln \frac{h}{M}}{4 \ln^2 \frac{h}{M}} + \frac{\frac{3}{2} \ln 2 - \frac{1}{4} - \frac{1}{2} \ln \pi}{2 \ln^2 \frac{h}{M}} + \mathcal{O}\left(\frac{(\ln \ln \frac{h}{M})^2}{\ln^3 \frac{h}{M}}\right). \quad (108)$$

It is a nontrivial check on the overall consistency of our considerations that using (49) for the numerical value of our universal constant B the third term in (107) matches the corresponding one in (108). Comparing (107) to (108) we also obtain

$$\kappa = -\frac{1}{4} - \ln \sqrt{2\pi}. \quad (109)$$

Using the exact value (109) we obtain the asymptotic expansion of the first correction in Q :

$$\tilde{I}_1(p/M) = \frac{2}{3\pi} \left\{ \frac{1}{2\lambda} - \frac{3}{2} - \ln \sqrt{2\pi} \right\} = \frac{2}{3\pi} \left\{ \frac{1}{2\lambda} - 2.419 \right\}. \quad (110)$$

Note that the leading correction term (110) does not contain any free parameter.

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