

Comparison of the O(3) bootstrap σ model with lattice regularization at low energies

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(Received 6 April 1999; published 8 October 1999)

The renormalized coupling g_R defined through the connected four-point function at zero external momentum in the nonlinear O(3) sigma model in two dimensions is computed in the continuum form factor bootstrap approach with an estimated error $\sim 0.3\%$. New high precision data are presented for g_R in the lattice-regularized theory with the standard action for nearly thermodynamic lattices $L/\xi \sim 7$ and correlation lengths ξ up to ~ 122 and with the fixed point action for correlation lengths up to ~ 12 . The agreement between the form factor and lattice results is within $\sim 1\%$. We also recompute the phase shifts at low energy by measuring two-particle energies at finite volume, a task which was previously performed by Lüscher and Wolff using the standard action, but this time using the fixed point action. Excellent agreement with the Zamolodchikov S matrix is found. [S0556-2821(99)04419-7]

PACS number(s): 11.15.Ha, 11.10.Lm

I. INTRODUCTION

The only presently known practical way to define a relativistic quantum field theory nonperturbatively in four dimensions is by using lattice regularization. For example, it is hoped that one will, once sufficiently powerful computers are available, be able to answer the question as to whether QCD is the correct theory of the strong interactions by studying the continuum limit of the lattice theory.

It is, however, notoriously difficult to control the continuum limit of a lattice theory. Analyses of lattice Feynman graphs, as initially performed by Symanzik [1], show that, order by order in renormalized perturbation theory, physical quantities approach their continuum limit as integer powers in the lattice spacing (up to logarithmic corrections). However, since it is not known that such behavior controls the approach to the continuum limit in the full nonperturbatively defined theory, the invocation of such a power-law approach to extrapolate data produced in numerical simulation experiments has merely the status of a (plausible) working hypothesis. The integer nature of the powers adopted in studies of theories such as QCD is considered to be connected to the widely expected property of asymptotic freedom. Here again, the very question whether the continuum limit of the lattice

theory really describes an asymptotically free theory is highly nontrivial.¹

This work is part of an ongoing effort of the present authors to test whether the ‘‘conventional wisdom’’ is correct in a simpler model, the nonlinear O(3) sigma model in two dimensions. This model is, like QCD, perturbatively asymptotically free and also has instanton and superinstanton [2] solutions. It has, however, classically the additional, beautiful property of being integrable; in particular, there exists an infinite set of nonlocal conserved charges. Assuming that the quantum theory has a mass gap and the spectrum contains a vector multiplet of stable particles, the existence of such conserved charges in quantum theory forbid particle production in scattering and, as shown by Lüscher [3], fixes the two-particle S matrix to that previously postulated by Zamolodchikov and Zamolodchikov (ZZ) [4] [up to Castillejo-Dalitz-Dyson (CDD) ambiguities].

All these properties were obtained starting from a formal Lagrangian, where one first computes off-shell N -point functions and goes on shell via the Lehmann-Symanzik-Zimmermann (LSZ) formalism to obtain the S -matrix elements. The so-called form factor bootstrap (FFB) approach [5,6,7] proceeds in the other direction. One attempts to obtain off-shell information starting from the knowledge (postulate) of the stable particle spectrum and their S matrix. In

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¹Indeed, even the authors of this paper are divided into two subsets having different opinions on the probable answer.

the first step one constructs the form factors of (composite) operators, satisfying all physical constraints (analyticity, generalized Watson theorem, etc.) and then Green functions are obtained by saturating with a complete set of states. This is a program which is only feasible in a theory where there is no particle production (i.e., only in two dimensions). Even this program, for which there has recently been a lot of progress [8,9,10], involves mammoth effort.

Unfortunately, since lattice regularization breaks these conservation laws and the FFB relies on some nontrivial assumptions, the expectation that the continuum limit of the lattice O(3) model coincides with the FFB is not guaranteed. A first investigation of this issue was by Lüscher and Wolff [11] who computed the phase shifts on the lattice by measuring two-particle state energies in a finite volume. Their results (taking account of lattice artifacts) were completely consistent with the ZZ S matrix. In the course of a similar investigation of the nature of the continuum limit of the O(2) model [12], in order to test our programs and a slightly modified form of the analysis, we repeated the measurement of the phase shifts in the O(3) model. We also made simulations with a fixed point action [13] and found indications that the lattice artifacts are much smaller than in the case of the standard action. An account of our investigations is given in Sec. IV. Our results are again in good agreement with the ZZ S matrix [4].

An off-shell quantity of physical interest is the current-current (J - J) correlation function. It has been shown that J - J computed in the FFB approach [8,9] agrees well with conventional renormalized perturbation theory at high energies, at least up to $p/M \sim 10000$, when the analytical value of the ratio of the mass M to the Λ parameter [14] is used. Connected to this are two important interrelated properties: First, the ZZ S matrix shows an “on-shell form of asymptotic freedom (AF),” in the sense that the phase shifts fall logarithmically to zero with the energy at high energy (see Sec. IV). Second, the thermodynamic Bethe ansatz, which is used to compute M/Λ , reproduces the two-loop β -function coefficient. The agreement between the FFB and lattice computations of J - J is also within $\sim 1\%$ for the entire range of momenta up to $\sim 40M$.

Despite this wealth of circumstantial evidence for the validity of the conventional picture, there is still room for doubt. In particular, in a recent paper, two of the present authors [15], assuming a certain form of the lattice artifacts, have found statistically significant deviations between the continuum limit of the lattice J - J correlation function and the FFB at low energies.

Unfortunately, the J - J correlation function at low energies is a quantity which behaves qualitatively similarly to that in a free theory. It is plausible that a difference between two theories would manifest itself more clearly in a quantity which vanishes in the free theory, e.g., the zero-momentum coupling g_R defined through the connected four-point function. There is an enormous literature on the computation of this quantity in the two- (and higher) dimensional nonlinear sigma models; see, e.g., Ref. [16] and references therein. The main new contribution of this paper, the computation of g_R by the FFB, is outlined in Sec. II. This is the first time that

this method has been used to compute a four-point function, and it is rather surprising that one is apparently able to get such a good approximation for g_R .

In Sec. III we present results on g_R using two different lattice regularizations, the standard action (including new high precision data on thermodynamic lattices at large correlation lengths) and the fixed point (FP) action. The nature of the approach to the continuum limit is not so clear, but whatever (reasonable) extrapolation is made, it agrees with the truncated FFB result to better than $\sim 1\%$.

II. COMPUTATION OF g_R IN THE CONTINUUM THEORY

There have been various approximation schemes to compute low energy (nonperturbative) quantities in the continuum formulation of the O(n) models in two dimensions: the g expansion [17], the ϵ expansion [16], and the $1/n$ expansion [18]. In this section we will present a new approximation using the form factor bootstrap.

A. Definitions

Consider a general continuum quantum field theory in two dimensions, in infinite volume, with global O(n) symmetry. Let $\sigma^a(x)$, $a=1, \dots, n$, be a vector multiplet of (renormalized) Euclidean scalar fields with two-point function

$$S^{a_1 a_2}(x_1, x_2) = \langle \sigma^{a_1}(x_1) \sigma^{a_2}(x_2) \rangle. \quad (2.1)$$

The inverse of its Fourier transform,

$$G(k) \delta^{a_1 a_2} = \int d^2x e^{ikx} S^{a_1 a_2}(x, 0), \quad (2.2)$$

is assumed to have an expansion for small momenta:

$$G(k)^{-1} = Z_R^{-1} [M_R^2 + k^2 + O(k^4)]. \quad (2.3)$$

We denote the four-point function by

$$S^{a_1 a_2 a_3 a_4}(x_1, x_2, x_3, x_4) = \langle \sigma^{a_1}(x_1) \sigma^{a_2}(x_2) \sigma^{a_3}(x_3) \sigma^{a_4}(x_4) \rangle \quad (2.4)$$

and the connected four-point function by

$$\begin{aligned} S_c^{a_1 a_2 a_3 a_4}(x_1, x_2, x_3, x_4) &= S^{a_1 a_2 a_3 a_4}(x_1, x_2, x_3, x_4) \\ &\quad - S^{a_1 a_2}(x_1, x_2) S^{a_3 a_4}(x_3, x_4) \\ &\quad - S^{a_1 a_3}(x_1, x_3) S^{a_2 a_4}(x_2, x_4) \\ &\quad - S^{a_1 a_4}(x_1, x_4) S^{a_2 a_3}(x_2, x_3). \end{aligned} \quad (2.5)$$

Introducing the Fourier transform by

$$\begin{aligned} \widetilde{S}^{a_1 a_2 a_3 a_4}(k_1, k_2, k_3, k_4) \\ = \int \prod_{j=1}^4 [d^2 x_j e^{i k_j x_j}] S^{a_1 a_2 a_3 a_4}(x_1, x_2, x_3, x_4), \end{aligned} \quad (2.6)$$

and similarly \widetilde{S}_c for the connected part, the conventional zero-momentum (dimensionless) coupling (in two dimensions) is defined by

$$g_R = -\frac{M_R^2}{G(0)^2} \frac{1}{n^2} \sum_{a,b} G^{aabb}(0,0,0,0), \quad (2.7)$$

where

$$\begin{aligned} \widetilde{S}_c^{a_1 a_2 a_3 a_4}(k_1, k_2, k_3, k_4) &= (2\pi)^2 \delta^{(2)}(k_1 + k_2 + k_3 + k_4) \\ &\times G^{a_1 a_2 a_3 a_4}(k_1, k_2, k_3, k_4). \end{aligned} \quad (2.8)$$

We will assume that the two-point function has a spectral representation

$$G(k) = Z \int_0^\infty d\mu \frac{\rho(\mu)}{\mu^2 + k^2}, \quad (2.9)$$

where the normalization constant Z takes into account that, assuming that the spectrum of the theory contains a vector multiplet of stable particles of mass M , we normalize the spectral density ρ so that the one-particle contribution is

$$\rho^{(1)}(\mu) = \delta(\mu - M). \quad (2.10)$$

Then the coefficients appearing in the small momenta expansion above can be expressed as

$$Z_R = Z \frac{\gamma_2^2}{\delta_2}, \quad (2.11)$$

$$\frac{M_R^2}{M^2} = \frac{\gamma_2}{\delta_2}, \quad (2.12)$$

where γ_2 and δ_2 are the moments:

$$\gamma_2 = M^2 \int d\mu \frac{\rho(\mu)}{\mu^2}, \quad (2.13)$$

$$\delta_2 = M^4 \int d\mu \frac{\rho(\mu)}{\mu^4}. \quad (2.14)$$

Further, the coupling g_R can be written as

$$g_R = -\frac{n+2}{n} \frac{\gamma_4}{\gamma_2 \delta_2}, \quad (2.15)$$

where γ_4 is defined through

$$\begin{aligned} G^{a_1 a_2 a_3 a_4}(0,0,0,0) &= \frac{Z^2 \gamma_4}{M^6} (\delta^{a_1 a_2} \delta^{a_3 a_4} + \delta^{a_1 a_3} \delta^{a_2 a_4} \\ &+ \delta^{a_1 a_4} \delta^{a_2 a_3}). \end{aligned} \quad (2.16)$$

Strictly speaking, all observable physics (in a massive theory) is on shell; different interpolating fields give the same results. Off-shell amplitudes of particular composite (and ‘‘elementary’’) operators are only of physical interest if they are sources of (idealized) infinitesimal weakly interacting probes. The fields are characterized by their various quantum numbers and their dimensions, e.g., coded in the behavior of the two-point function $G(k)$. The assumption (2.9) corresponds to a limitation on the behavior of the associated spectral function $\rho(\mu)$ as $\mu \rightarrow \infty$. It is an implicit connection to the association of $\sigma^a(x)$ with a particular local field in the Lagrangian quantum field theory. In the nonlinear $O(n)$ sigma model the ‘‘elementary’’ field $\sigma^a(x)$ is characterized by its vanishing engineering dimension (in addition to being an isovector and spacetime scalar). We can therefore assume that the short distance singularities of its two-point function are sufficiently weak (only logarithmic) so that the spectral representation (2.9) holds without subtractions. Indeed, in the FFB approach, this uniquely defines (up to normalization) an operator $\hat{\sigma}^a(x)$, which has form factors that are not growing too fast at infinity so that the corresponding spectral density $\rho(\mu)$ vanishes fast enough for $\mu \rightarrow \infty$.

B. $1/n$ and ϵ expansions

The leading order computations for the spectral integrals in the $1/n$ expansion have been performed in Ref. [19].

$$\gamma_2 = 1 + 0.00671941 \frac{1}{n} + O\left(\frac{1}{n^2}\right), \quad (2.17)$$

$$\delta_2 = 1 + 0.00026836 \frac{1}{n} + O\left(\frac{1}{n^2}\right), \quad (2.18)$$

and also for the coupling [18],

$$g_R = \frac{8\pi}{n} \left[1 - 0.602033 \frac{1}{n} + O\left(\frac{1}{n^2}\right) \right], \quad (2.19)$$

which gives the approximation $g_R = 6.70$ for the case $n = 3$.

In the g expansion one obtains $g_R = 6.66(6)$ [17] and in the ϵ expansion $g_R = 6.55(8)$ [16]. Considering the rather short series in each case, it is amazing how well the estimates by the various methods agree.

C. Form factor bootstrap computation for $n = 3$

The form factor bootstrap aims at reconstructing N -point functions of local operators of integrable field theories from knowledge of the spectrum of stable particles and their S matrix. A description can be found in Smirnov’s book [5], the review of Karowski [6], a recent paper [10], and in various articles of two of the present authors [9].

TABLE I. r -particle contribution to γ_2, δ_2 .

r	$\gamma_2^{(r)}$	$\delta_2^{(r)}$
3	$1.67995(1) \times 10^{-3}$	$3.46494(1) \times 10^{-5}$
5	$6.622(1) \times 10^{-6}$	$7.114(1) \times 10^{-9}$

To our knowledge this is the first time that the method has been applied to the computation of four-point functions. The computation is rather involved, and here we will only give a very brief outline and present our results. The calculation in this and in other integrable models will be described in detail in a forthcoming paper [20].

We assume (as did the Zamolodchikov brothers in their construction of the S matrix) that there are no bound states in the $O(n)$ models. Then the spectral density ρ has an expansion over contributions from the intermediate states with an odd number of particles (due to internal parity symmetry),

$$\rho(\mu) = \sum_{k=0}^{\infty} \rho^{(2k+1)}(\mu), \quad (2.20)$$

and correspondingly the spectral integrals

$$\gamma_2 = 1 + \sum_{k=1}^{\infty} \gamma_2^{(2k+1)}, \quad (2.21)$$

$$\delta_2 = 1 + \sum_{k=1}^{\infty} \delta_2^{(2k+1)}. \quad (2.22)$$

The form factors are given by Smirnov [5] for the $O(3)$ model and have been recomputed in [9]. For example, the matrix element of the Minkowski operator $\hat{\sigma}^a(0)$ associated with the Euclidean field σ^a , connecting the vacuum to the three-particle in-state with rapidities $\theta_1 \geq \theta_2 \geq \theta_3$, is given by

$$\langle 0 | \hat{\sigma}^a(0) | a_1, \theta_1; a_2, \theta_2; a_3, \theta_3 \rangle^{\text{in}} = \sqrt{Z} \mathcal{F}_{a_1 a_2 a_3}^a(\theta_1, \theta_2, \theta_3), \quad (2.23)$$

with

$$\begin{aligned} \mathcal{F}_{a_1 a_2 a_3}^a(\theta_1, \theta_2, \theta_3) &= \pi^3 \prod_{i < j} \psi(\theta_i - \theta_j) [(\theta_3 - \theta_2) \delta_{a_1}^a \delta_{a_2 a_3} \\ &+ (\theta_1 - \theta_3 - 2\pi i) \delta_{a_2}^a \delta_{a_3 a_1} \\ &+ (\theta_2 - \theta_1) \delta_{a_3}^a \delta_{a_1 a_2}], \end{aligned} \quad (2.24)$$

where

$$\psi(\theta) = \frac{(\theta - \pi i)}{\theta(2\pi i - \theta)} \tanh^2 \frac{\theta}{2}. \quad (2.25)$$

The expression of the five-particle matrix element is also known explicitly, but it is much too long to be written here. Using these results the three- and five-particle contributions to γ_2 and δ_2 are given in Table I. It seems that the series converge extremely rapidly, and we would estimate

 TABLE II. l - m - n -particle contribution to γ_4 .

l, m, n	$\gamma_{4;lmn}$
1,2,1	$-4.16835(1)$
1,2,3	$0.05175(1)$
3,2,1	$0.05175(1)$
1,4,1	$-0.004065(1)$

$$\gamma_2 = 1.001687(1), \quad (2.26)$$

$$\delta_2 = 1.000034657(1), \quad (2.27)$$

where the estimated errors come from inspecting the pattern of relative n -particle contributions suggested by the one, three, five-particle states.

The four-point function has an expansion in terms of contributions of intermediate states with l, m, n particles, respectively,

$$\begin{aligned} &\tilde{S}^{a_1 a_2 a_3 a_4}(k_1, k_2, k_3, k_4) \\ &= (2\pi)^2 \delta^{(2)}(k_1 + k_2 + k_3 + k_4) \\ &\quad \times M^{-6} \sum_{\text{perms } P} V^{a_{P1} a_{P2} a_{P3} a_{P4}}(k_{P1}, k_{P2}, k_{P3}, k_{P4}), \end{aligned} \quad (2.28)$$

where $k_i = (k_{i1}, k_{i2})$,

$$\begin{aligned} &V^{a_1 a_2 a_3 a_4}(k_1, k_2, k_3, k_4) \\ &= (2\pi)^3 M^6 \sum_{l, m, n} \frac{\delta(P_l + k_{11})}{E_l - ik_{12}} \\ &\quad \times \frac{\delta(P_m + k_{11} + k_{21})}{E_m - ik_{12} - ik_{22}} \frac{\delta(P_n - k_{41})}{E_n + ik_{42}} \\ &\quad \times \langle 0 | \hat{\sigma}^{a_1}(0) | \underline{l} \rangle \langle \underline{l} | \hat{\sigma}^{a_2}(0) | \underline{m} \rangle \langle \underline{m} | \hat{\sigma}^{a_3}(0) | \underline{n} \rangle \langle \underline{n} | \hat{\sigma}^{a_4}(0) | 0 \rangle, \end{aligned} \quad (2.29)$$

where l, n run over all states with odd numbers l, n of particles, and m over all states with an even number $m \geq 0$. The somewhat symbolic Σ in Eq. (2.29) really means, in addition to the summation over all internal quantum numbers of the particles and integration over all particle rapidities, a sum over the integers l, m , and n . The limit of zero momenta is very delicate because each term in the sum is a distribution in the momenta where the singularities occur when certain linear combinations of the momenta are zero. In particular, the contributions from terms in the above sum with $m=0$ not only cancel the disconnected pieces $\tilde{S} - \tilde{S}_c$, but also produce extra terms proportional to $\delta(k_{11} + k_{21})$. The singularities must be canceled by other terms in the sum with $m > 0$; e.g., the singularity from the contribution 1-0-1 is canceled by that of the contribution 1-2-1. We can avoid this problem, for example, by restricting ourselves to momenta $k_{i1} = \lambda K_{i1}$, where $K_{i1} + K_{j1} \neq 0$ for any $i \neq j$, and then taking the limit $\lambda = 0$ in our analytic expressions. An additional technical

TABLE III. ξ , $\chi=3G(0)$ and g_R for the standard action.

β	L	Runs	L/ξ	ξ	χ	g_R
1.5	60	110×20k	5.469(10)	10.97(2)	173.76(31)	6.269(20)
1.5	80	344×20k	7.253(7)	11.03(1)	175.95(11)	6.553(16)
1.5	100	350×20k	9.050(8)	11.05(1)	176.51(6)	6.613(17)
1.5	140	361×20k	12.68(1)	11.04(1)	176.30(5)	6.560(18)
1.6	140	214×20k	7.361(15)	19.02(4)	447.30(6)	6.612(17)
1.7	250	367×20k	7.246(4)	34.50(2)	1267.20(57)	6.665(14)
1.8	500	361×20k	7.717(4)	64.79(3)	3839.07(1.54)	6.688(15)
1.9	910	101×20k	7.4395(6)	122.32(1)	11884.9(7.0)	6.738(24)
1.95	1230	12×20k	7.352(20)	167.30(45)	20835(57)	6.751(78)
2.0	1600	4×20k	6.949(25)	230.26(83)	36826(142)	6.981(132)
2.05	2100	5×20k	6.804(67)	308.63(3.06)	63011(731)	6.608(216)

complication comes from the fact that each term in the sum is rather involved because the matrix elements have parts with differing connectivity properties, e.g., the matrix element occurring in the 1-2-1 contribution ($\theta_1 > \theta_2$):

$$\begin{aligned}
& Z^{-1/2} \langle b, \phi | \hat{\sigma}^a(0) | a_1, \theta_1; a_2, \theta_2 \rangle^{\text{in}} \\
&= \mathcal{F}_{ba_1a_2}^a(\phi + i\pi - i\epsilon, \theta_1, \theta_2) + 4\pi \delta_{a_2}^a \delta_{ba_1} \delta(\phi - \theta_1) \\
&+ 4\pi \delta(\phi - \theta_2) S_{a_1a_2;ab}(\phi - \theta_2), \quad (2.30)
\end{aligned}$$

where the S -matrix elements $S_{a_1a_2;ab}$ are given in Sec. IV.

The practicability of the computation of the zero-momentum coupling using the form factor bootstrap approach obviously depends crucially on the question as to whether the sum over intermediate states for the four-point function,

$$\gamma_4 = \sum_{l,m,n} \gamma_{4;lmn}, \quad (2.31)$$

converges rapidly. We started to investigate this question in the Ising model, and we found that the $l+m+n=6$ contributions are much smaller than the leading 1-2-1 term [20]. Fortunately, for the O(3) model under investigation here, the situation is rather similar. The contributions of the $l-m-n$ intermediate states with $l+m+n \leq 6$ to γ_4 are given in Table II.

The leading 1-2-1 contribution is a factor ~ 42 greater in magnitude than the sum of $l-m-n$ contributions with $l+m+n=6$. It is extremely difficult to bound the rest of the contributions, especially since the signs are not known in general. Even the computation of the states with $l+m+n=8$ would be quite an undertaking.² But assuming that the pattern in Table II continues (as for the case of the two-point

²The calculation of the $l+m+n=8$ contributions in the Ising model is, however, not so difficult; the results will be presented in Ref. [20].

function) and that the sum of the remaining contributions $l+m+n \geq 8$ is $\leq 10\%$ of the sum of the $l+m+n=6$ contributions, we obtain the result

$$\gamma_4 = -4.069(10) \quad (2.32)$$

and, hence, our final result

$$g_R = 6.770(17). \quad (2.33)$$

III. LATTICE COMPUTATIONS OF g_R

In the framework of the lattice regularization, there are two methods to compute g_R in the O(n) models. The first is using high temperature (strong coupling) expansions and the second by numerical simulations.

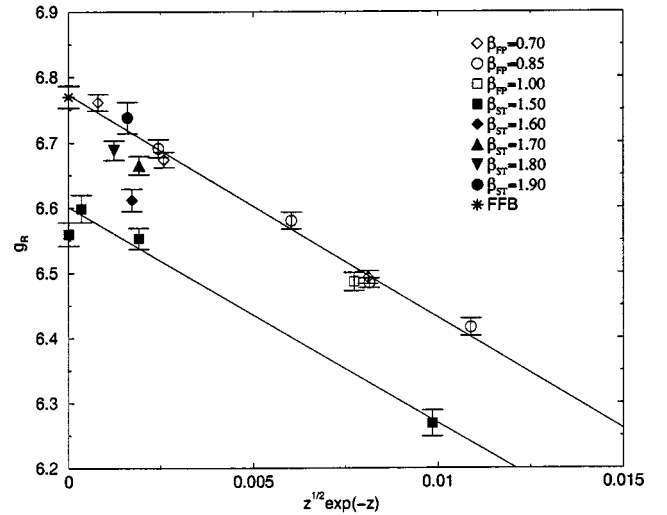


FIG. 1. The coupling $g_R(z, \beta)$ for the FP (open symbols) and standard (solid symbols) actions plotted vs $\sqrt{z} \exp(-z)$. The correlation lengths for the FP action are in the range 3.2–12.2, while for the standard action in 11–122. The theoretical value from the FFB is also shown. The linear fits are motivated by the $1/n$ prediction (3.8) and are based on the $\beta_{\text{ST}}=1.50$ and $\beta_{\text{FP}}=0.85$ data, respectively.

For numerical simulations we consider a square lattice with both the standard action

$$S = -\beta \sum_{x,\mu} \sigma(x) \cdot \sigma(x + \hat{\mu}), \quad (3.1)$$

where $\sigma(x) \cdot \sigma(x) = \sum_a \sigma^a(x) \sigma^a(x) = 1$ and the FP action of Ref. [13].

A. High temperature expansion

Concerning the high temperature (HT) expansion for the standard action, long series [21] have been obtained for the two- and four-point functions and for the second moment μ_2 defined by

$$\mu_2 \delta^{a_1 a_2} = \sum_x x^2 \langle \sigma^{a_1}(x) \sigma^{a_2}(0) \rangle \quad (3.2)$$

to obtain M_R through $M_R^2 = 4G(0)/\mu_2$, where $G(k)$ is defined analogously to Eq. (2.2), but with the integral replaced by a sum. The analyses of the HT expansion for the spectral moments give $\gamma_2 = 1.0013(2)$ [19] and $\delta_2 = 1.000029(5)$ [22]. The agreement with the FFB values Eqs. (2.26), (2.27), is acceptable; note that these are smaller than that anticipated from the leading order of the $1/n$ approximation, Eqs. (2.17), (2.18).

The coupling is defined as the continuum limit

$$g_R = \lim_{\xi \rightarrow \infty} g_R(\xi), \quad (3.3)$$

where ξ is the correlation length in lattice units. The analysis is hampered by the lack of rigorous knowledge of the position of the critical point and the exact approach to it. In particular, the conventional wisdom that the critical point is at $\beta = \infty$ is usually built into the analyses. The various Padé approximations show the coupling falling rapidly as β increases in the region of small β , then a region of rather flat behavior, after which the various approximations show diverse behavior; some analyses indicate that in fact there is a shallow minimum and that the continuum limit is actually approached from below (see, e.g., Refs. [23], [16]).

In Ref. [24] Campostrini *et al.* quote for the case $n=3$ the result $g_R = 6.6(1)$, and in a more recent publication Pelissetto and Vicari cite 6.56(4) [16]. Butera and Comi, on the

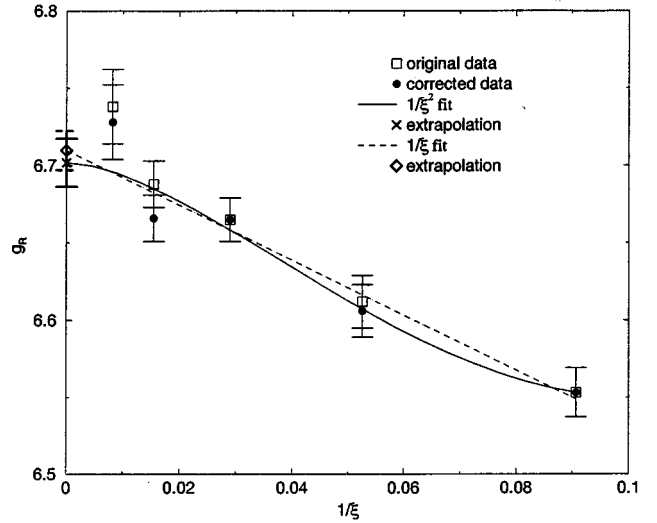


FIG. 2. The measured values for g_R together with the corrected ones at $L/\xi = 7.25$ for the standard action. The solid and dotted lines correspond to the fits (3.10) and (3.11), respectively.

other hand, are rather cautious and did not quote a value for the case $n=3$ in Ref. [21]; if pressed, they would at present cite $g_R = 6.6(2)$ [25].

B. Numerical simulations

Monte Carlo computations of g_R have a long history; see, e.g., Refs. [17], [26]. In order to attempt to match the apparent precision attained in the FFB approach outlined in Sec. II, we decided to perform even more precise measurements than were carried out previously.

We work here on a square lattice of size L in each direction and periodic boundary conditions. The coupling in finite volume is defined through Binder's cumulant

$$g_R(\xi) = \lim_{L \rightarrow \infty} g_R(\xi, L), \quad (3.4)$$

$$g_R(\xi, L) = \left(\frac{L}{\xi} \right)^2 \left[1 + \frac{2}{n} \frac{\langle (\Sigma^2)^2 \rangle}{\langle \Sigma^2 \rangle^2} \right], \quad (3.5)$$

where $\Sigma^a = \sum_x \sigma^a(x)$. In this definition we have taken (as in Ref. [17]):

TABLE IV. Data for the FP action.

β	L	Runs	L/ξ	ξ	χ	g_R
0.70	18	115×360k	5.682(3)	3.168(1)	19.501(8)	6.493(10)
0.70	22	197×360k	6.924(3)	3.177(1)	19.646(6)	6.674(12)
0.70	26	363×360k	8.176(3)	3.180(1)	19.686(4)	6.761(12)
0.85	32	31×600k	5.359(5)	5.971(5)	55.74(5)	6.417(14)
0.85	34	189×360k	5.678(2)	5.988(2)	56.03(2)	6.485(8)
0.85	36	52×360k	6.006(4)	5.994(4)	56.24(3)	6.581(13)
0.85	42	140×360k	6.986(3)	6.012(3)	56.51(2)	6.691(14)
1.00	70	691×100k	5.734(4)	12.207(8)	189.4(1)	6.487(14)

$$\xi = \frac{1}{2 \sin(\pi/L)} \sqrt{\frac{G(0)}{G(k_0)} - 1}, \quad (3.6)$$

where $k_0 = (2\pi/L, 0)$. In this paper we will use ξ to denote the second moment correlation length, to which Eq. (3.6) converges, for large L . Although conceptually different, ξ is very close to the exponential correlation length (ξ_{exp}): also using Eqs. (2.3) and (2.12) in the definition (3.6), the FFB results (2.26) and (2.27) yield

$$\frac{\xi_{\text{exp}}}{\xi} = \sqrt{\frac{\gamma_2}{\delta_2}} = 1.000826(1). \quad (3.7)$$

The standard action Monte Carlo measurements were performed using a method similar to the cluster estimator of [11]. We measured g_R at correlation lengths ranging from 11 to 122 at $L/\xi \sim 7$. These measurements were used to investigate the approach to the continuum. To study the finite volume effects, we repeated the runs at $\xi \sim 11$ on three other lattices with $L/\xi \sim 5.5$, $L/\xi \sim 9$, and $L/\xi \sim 13$. The results of all these runs (together with the preliminary results corresponding to $\xi \sim 167$, 230, and 309) are recorded in Table III.

In this table we also indicate the number of measurements. Each run consisted of 20k sweeps of the lattice with measurements after each sweep. The error was computed from this sample by using the jackknife method.

We have measured g_R with the FP action at three different values of β : 0.70, 0.85, and 1.00, corresponding to correlation lengths $\xi \approx 3.2$, 6.0, and 12.2, at the values of $z = L/\xi$ in the range 5.4–8.2.

To get a feeling of the finite volume effects, we took the expression for g_R in the leading order $1/n$ expansion from [18] and simply replaced the integral over momenta by a discrete sum. In this way we obtained

$$g_R[L] = g_R[\infty] [1 - a_1 \sqrt{z} e^{-z} [1 + O(1/z)] + \dots], \quad (3.8)$$

with $a_1 = \sqrt{8\pi} = 5.013$ for large $z = L/\xi$. Figure 1 shows these results for g_R plotted against the combination $\sqrt{z} \exp(-z)$, motivated by the $1/n$ result (3.8).

We have determined the Monte Carlo (MC) prediction of g_R both for the standard action and the FP action. Making a linear fit in $\sqrt{z} \exp(-z)$ to the four data points at $\beta = 1.50$ for the standard action (see Fig. 1), one obtains

$$g_R(z = \infty, \xi = 11.0) = 6.60(1), \quad (3.9)$$

with $a_1 = 5.0(4)$. Since the finite size dependence (at least at this correlation length) is quite well described by Eq. (3.8), we used this formula to “renormalize” our data with $z \sim 7$ in Table III to the common physical size $z = 7.25$.

Next, we extrapolated the results of our measurements to the continuum limit. In Fig. 2 we show both the measured and corrected values of g_R versus $1/\xi$ for the data with $L/\xi \sim 7$. It clearly indicates that the continuum limit of g_R is approached from below as is the case in the leading order of the $1/n$ approximation of the lattice theory [18]. The only theoretic framework for estimating lattice artifacts comes from considering Symanzik’s [1] effective action. The ab-

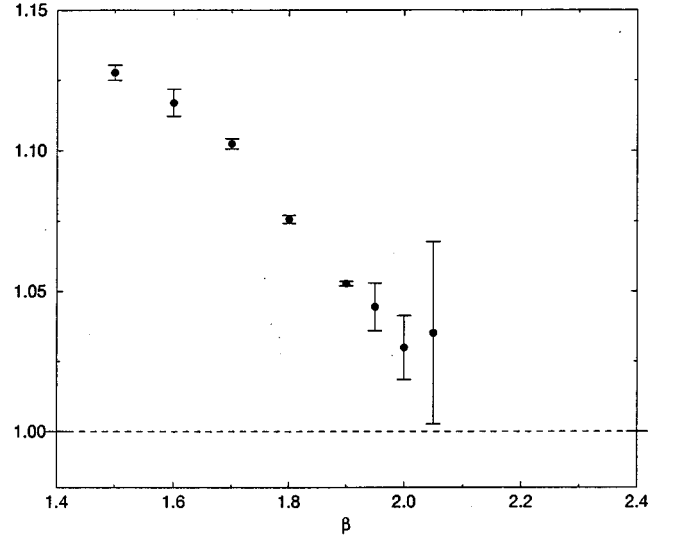


FIG. 3. The measured values of the χ^2/ξ^2 ratio divided by the four-loop approximation to the prediction (3.15).

sence of even parity O(3) invariants with odd engineering dimensions suggests an approach to the continuum limit with leading behavior $(\ln \xi)^r/\xi^2$. As stressed in the Introduction, there is no rigorous nonperturbative proof of this behavior.

Figure 2 shows two fits. The first is a quadratic fit of the form suggested by the Symanzik analysis, where we have taken $r = 1$.³

$$g_R(\xi, z = 7.25) = g_R(\infty, z = 7.25) \left[1 + \frac{b_1 \log \xi}{\xi^2} + \frac{b_2}{\xi^2} \right], \quad (3.10)$$

with $g_R(\infty, z = 7.25) = 6.702(16)$, $b_1 = -4.4(2.2)$, and $b_2 = 8(5)$. We made also a second fit in Fig. 2 of the form

$$g_R(\xi, z = 7.25) = g_R(\infty, z = 7.25) \left[1 + \frac{d_2}{\xi} \right], \quad (3.11)$$

with $g_R(\infty, z = 7.25) = 6.710(13)$, and $d_2 = -0.27(4)$. Although there is no theoretical basis for such a fit, it describes the present data as well as the first.

One sees that our data (which are the best available at present) do not allow one to discriminate between the two fits [or between any intermediate fits with leading behavior $(\ln \xi)^r/\xi^2$ with, say, large r]. The accuracy of the MC determination of the continuum value of g_R is thus unfortunately limited; nevertheless, assuming a power-law approach, we would estimate $g_R(\infty, z = 7.25) = 6.71(2)$. Needless to say, if the approach to the continuum is much slower, say, $1/(\ln \xi)^r$, the continuum value of g_R could differ considerably from this estimate.

³This is the analytic form found in the leading order $1/n$ expansion with $b_1 = -\frac{1}{4}$, $b_2 = -\frac{5}{8} \ln 2 + \frac{1}{4}$ [18].

TABLE V. Parameters of simulations in the O(3) model. On lattices *A* and *B* the standard action was used, while *D* and *E* denote simulations with the FP action.

Lattice	β	$T \times L$	m^{-1}	mL
<i>A</i>	1.54	256×128	13.632(6)	9.4
<i>B</i>	1.40	128×64	6.883(3)	9.3
<i>D</i>	0.85	128×64	6.03(1)	10.0
<i>E</i>	0.70	64×32	3.186(15)	10.6

Finally, we used Eq. (3.8) again to extrapolate the continuum result for the finite physical size $z=7.25$ to the thermodynamic limit $z=\infty$. Thus our final result based on the standard action lattice measurements (keeping in mind the cautionary remark above) is

$$g_R^{\text{ST}} = 6.77(2). \quad (3.12)$$

This error contains both the ambiguity in using the fit (3.10) or (3.11) and the error in a_1 .

The data for the FP action seem to lie on a universal curve (the slope of which roughly corresponds to the $1/n$ prediction) in spite of the extremely short correlation length. We interpret this as an indication that the lattice artifacts for the FP action are small, in any case smaller than our error bars. The measured values for the standard action show a considerable lattice artifact, but the data at $z \approx 7$ seem to converge to the FP result with increasing ξ . Extrapolating the FS effects to $z=\infty$, we get

$$g_R^{\text{FP}} = 6.77(2) \quad (3.13)$$

and $a_1=5.0(3)$. This extrapolation is based on the four $\beta_{\text{FP}}=0.85$ data points, but including all points of Table IV does not alter the extrapolation significantly.

Our results (3.12) and (3.13) are above Kim's value, 6.6(1), determined previously via finite size scaling [26], although statistically compatible within the error estimate. They are also above the central values quoted on the basis of

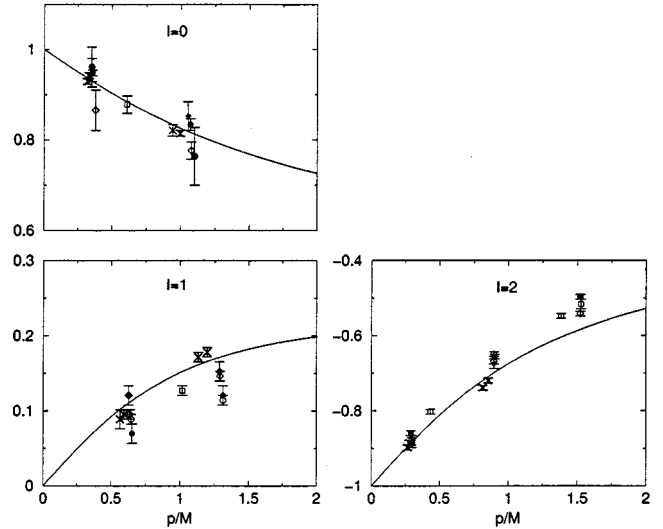


FIG. 4. The phase shifts in units of $\pi/2$ vs p/M . The open symbols are from Ref. [11]. The corresponding solid symbols are our measurements on the same lattices *A* and *B*, with the WF method discussed here. The crosses denote results using the FP action (*D* and *E*). The solid curve corresponds to the ZZ *S* matrix.

high temperature expansions discussed above, but very consistent with each other and with the result (2.33) from the form factor bootstrap.

We would like to end this section with a comparison of an analytic prediction of the ratio χ/ξ^2 with the MC data. In Ref. [9] the perturbative short distance expansion of the spin two-point function was refined to

$$S^{a_1 a_2}(x,0) = \frac{Z \delta^{a_1 a_2}}{3 \pi^3} (\ln M|x|)^2 \left\{ 1 + O\left(\frac{\ln|\ln M|x||}{\ln M|x|}\right) \right\}. \quad (3.14)$$

The new result was the exact (though nonrigorous) determination of the overall nonperturbative constant. Using this we can straightforwardly derive the relation [19]

TABLE VI. Phase shifts from lattice *A*.

<i>I</i>	<i>k</i>	δ_{exact}	δ_E	δ_{WF}	t_0	<i>M</i>	δ_{LW}
0	1	1.4595	1.36(3)	1.49(2)	1	20	1.36(7)
			1.45(5)	1.50(4)	8	8	
	2	1.2840	1.25(2)	1.30(2)	1	20	1.22(3)
			1.38(6)	1.34(5)	8	8	
1	1	0.1751	0.10(1)	0.17(3)	1	20	0.15(1)
			0.19(3)	0.19(5)	8	8	
	2	0.2692	0.15(2)	0.23(2)	1	20	0.23(1)
			0.23(4)	0.24(5)	8	8	
2	1	−1.3874	−1.51(2)	−1.37(1)	1	20	−1.39(2)
			−1.43(3)	−1.36(2)	8	8	
	2	−1.0944	−1.11(1)	−1.06(1)	1	20	−1.05(1)
			−1.04(2)	−1.06(2)	8	8	

TABLE VII. Phase shifts from lattice B .

I	k	δ_{exact}	δ_E	δ_{WF}	t_0	M	δ_{LW}
0	1	1.4584	1.41(1)	1.48(1)	1	20	1.51(7)
			1.47(1)	1.49(1)	3	10	
	2	1.2818	1.29(1)	1.29(1)	1	20	1.2(1)
			1.35(1)	1.30(1)	3	10	
1	1	0.1764	0.09(1)	0.12(1)	1	20	0.14(1)
			0.12(1)	0.12(1)	3	10	
2	1	-1.3859	-1.42(1)	-1.35(1)	1	20	-1.38(2)
			-1.36(1)	-1.35(1)	3	10	
	2	-1.0914	-1.05(1)	-1.03(1)	1	20	-1.02(1)
			-1.02(1)	-1.03(1)	3	10	
	3	-0.9102	-0.78(2)	-0.78(1)	1	20	-0.81(2)
			-0.76(1)	-0.78(1)	3	10	

$$\frac{\chi}{\xi^2} = \frac{3\pi\gamma_2^2}{4\delta_2} \frac{1}{\beta^2} \left\{ 1 + \sum_{n=1}^{\infty} \frac{c_n}{\beta^n} \right\}. \quad (3.15)$$

The first three nonuniversal perturbative coefficients are known for the standard action lattice regularization [27]:

$$c_1=0.1816, \quad c_2=0.1330, \quad c_3=0.1362. \quad (3.16)$$

Figure 3 shows the measured values of the χ/ξ^2 ratio divided by the four-loop approximation to the prediction (3.15). Note that Eq. (3.15) seems to be satisfied by our data to a better accuracy than the analogous one for ξ alone [27], but the ratios decrease rapidly and we do not know if they eventually overshoot the asymptotic value of 1. Note also that the prediction (3.15) is independent of the $M/\Lambda_{\overline{\text{MS}}}$ ratio $8/e$ of Ref. [14].

IV. PHASE SHIFT ANALYSIS FROM FOUR-SPIN CORRELATORS

The prediction for the scattering amplitude of two particles at center-of-mass momentum $p = M \sinh \frac{1}{2}\theta$ in the O(3) nonlinear sigma model by Zamolodchikov and Zamolodchikov [4] is given by

$$S_{a'b';ab}(\theta) = \sum_{I=0}^2 e^{2i\delta_I(p)} P^I_{a'b';ab}, \quad (4.1)$$

where P^I are the isospin projectors and the phase shifts δ_I are given simply by

$$e^{2i\delta_0(p)} = \frac{\theta + 2i\pi}{\theta - 2i\pi}, \quad (4.2)$$

$$e^{2i\delta_1(p)} = \frac{\theta + 2i\pi}{\theta - 2i\pi} \frac{\theta - i\pi}{\theta + i\pi}, \quad (4.3)$$

$$e^{2i\delta_2(p)} = \frac{\theta - i\pi}{\theta + i\pi}. \quad (4.4)$$

In fact, the Zamolodchikovs specified the S matrix for general $n \geq 3$ and these expressions have been verified to $O(1/n^2)$ in the $1/n$ expansion. For the particular case of O(3), Lüscher and Wolff [11] checked the expressions for low energies using MC simulations. The agreement was completely satisfactory; in particular, the data were consistent with the highly nontrivial nonperturbative property that the S matrix at zero energy is repulsive $S_{a'b';ab}(0) = -\delta_{a'b}\delta_{b'a}$, which is a crucial condition in the FFB construction. We repeated the measurements of [11] for the standard action using a modified method of analysis. In addition, we also performed measurements using the FP action. Since the S matrix is the essential ingredient in the FFB construction, we report the results here.

The method of Lüscher and Wolff [11] is based on the following idea: The momentum of one of the particles in a two-particle state with zero total momentum in a periodic box (in one dimension) takes discrete values p_n given by the periodicity condition

$$p_n L + 2\delta(p_n) = 2\pi n. \quad (4.5)$$

Accordingly, the energy of this state is given by

$$E_n = 2E^{(1)}(p_n) = 2\sqrt{p_n^2 + M^2}, \quad (4.6)$$

where $E^{(1)}(p)$ is the energy of a one-particle state with momentum p . From the measurement of the energy spectrum E_n for some low lying states, one can then calculate the momentum p_n and using Eq. (4.5) the phase shift $\delta(p_n)$. Varying L and taking different values of n , one can determine $\delta(p)$ at several values of its argument.

To determine the two-particle energies the correlation matrix has been measured:⁴

$$C_{xy}(t) = \langle \text{vac} | O(x,0) O(y,t) | \text{vac} \rangle_c, \quad (4.7)$$

⁴Actually, in Ref. [11] the measurement was done in Fourier space (i.e., in relative momenta), but this difference is not significant here. For our purpose the coordinate space representation is more convenient.

TABLE VIII. Phase shifts from lattice D .

I	k	δ_{exact}	δ_E	δ_{WF}
0	1	1.4726	1.47(3)	1.46(1)
	2	1.3107	1.29(2)	1.29(2)
1	1	0.1598	0.16(1)	0.14(2)
	2	0.2545	0.23(2)	0.27(1)
2	1	-1.4056	-1.41(2)	-1.41(1)
	2	-1.1321	-1.15(1)	-1.16(1)

where

$$O(x,t) = \frac{1}{L} \sum_{z=0}^{L-1} \sigma(z,t) \sigma(z+x,t). \quad (4.8)$$

We omit here the $O(n)$ structure and indices. The subscript c in Eq. (4.7) means that in the $I=0$ channel the vacuum contribution is subtracted.

Using the eigenvectors $|n\rangle$ of the transfer matrix as intermediate states, one has

$$C_{xy}(t) = \sum_n e^{-E_n t} \psi_n(x) \psi_n(y), \quad (4.9)$$

where

$$\psi_n(x) = \langle \text{vac} | O(x,0) | n \rangle \quad (4.10)$$

is the ‘‘wave function’’ of the corresponding state. The lowest energy states in Eq. (4.9) are the two-particle states, and they will dominate at sufficiently large values of t .

Note that the relative momentum $2p_n$ of the two-particle states is encoded not only in the energy E_n , but also in the wave function $\psi_n(x)$. For the symmetric wave functions ($I=0,2$ channels), one should have

$$\psi_n(x) = A \cos p_n(x-L/2) \quad \text{for } R < x < L-R, \quad (4.11)$$

and similarly with $\sin p_n(x-L/2)$ for the $I=1$ channel. Here R is the ‘‘interaction range.’’ For a relative distance $x > R$, the particles propagate (essentially) freely.

One expects that the additional information obtained from the wave function will provide a more precise determination of p and hence of $\delta(p)$.

A. Determination of the energy spectrum and wave functions

The rank N of the matrix $C(t)$ in Eq. (4.9) is $L/2$, $L/2 - 1$, and $L/2 + 1$ in the $I=0$, 1, and 2 channels, respectively. We assume that for $t \geq t_0$ (with some t_0) no more than N states contribute to $C_{xy}(t)$, in the sense that the total contribution of the states $n > N$ is much smaller than the statistical error $\delta C_{xy}(t)$.

TABLE IX. Phase shifts from lattice E .

I	k	δ_{exact}	δ_E	δ_{WF}
0	1	1.4664	1.49(1)	1.48(1)
	2	1.2977	1.27(1)	1.28(1)
1	1	0.1674	0.18(1)	0.15(1)
	2	0.2619	0.26(1)	0.28(1)
2	1	-1.3968	-1.35(1)	-1.39(1)
	2	-1.1138	-1.14(1)	-1.13(1)

Lüscher and Wolff [11] suggested to determine the energies of the two-particle states from the generalized eigenvalue problem⁵

$$C(t) \mathbf{v}_n = \lambda_n(t, t_0) C(t_0) \mathbf{v}_n. \quad (4.12)$$

The eigenvalues of Eq. (4.12) are given *exactly* by

$$\lambda_n(t, t_0) = e^{-E_n(t-t_0)}, \quad (4.13)$$

provided the sum in Eq. (4.9) is restricted to N terms, $1 \leq n \leq N$. It is also easy to show that (with an appropriate normalization of \mathbf{v}_n)

$$\psi_n(x) = \sum_y C_{xy}(t_0) \mathbf{v}_n(y). \quad (4.14)$$

Solving Eq. (4.12) involves an inversion of $C(t_0)$, and the distortion of its small eigenvalues by the statistical noise is enhanced. This could affect strongly the values and errors of E_n obtained. For $t_0 > 1$, taking all $N \sim L/2$ states introduces significant instability in the result.⁶ Because of this, we have introduced a modification: before considering the generalized eigenvalue problem, we truncate the correlation function to an M -dimensional subspace ($M < N$) spanned by the first M eigenvectors of $C(t_0)$ (to those with the largest M eigenvalues and still stable against the statistical fluctuations). The generalized eigenvalue problem, Eq. (4.12), is written then for the matrices $\bar{C}(t)$ in this reduced basis. The energies we used were obtained from Eqs. (4.12) and (4.13). We also determined $\mathbf{v}_n(x)$ from Eq. (4.12). One can use them as some given (nearly optimal) projectors which satisfy

$$(\mathbf{v}_m, C(t) \mathbf{v}_n) = \delta_{mn} e^{-E_n(t-t_0)}. \quad (4.15)$$

Note that as a result of statistical errors in $C_{xy}(t)$, the obtained $\mathbf{v}_n(x)$'s will differ from the true ones and hence these equations will be only approximately valid. They provide a useful consistency check and, also, a somewhat different method to determine E_n .

As an alternative way to get the phase shifts, we used the momenta p_n determined from the wave function (WF) using

⁵This equation was considered already before by Michael [28], in connection with a variational approach for evaluating the static potential in lattice gauge theory.

⁶In Ref. [11] $\sim L/4$ states were used with $t_0 \leq 1$.

Eq. (4.14). For a given t_0 and M one can also check the self-consistency of the obtained parameters by comparing $C_{xy}(t)$ built from E_n and $\psi_n(x)$ [cf. Eqs. (4.13) and (4.14)] with the MC result.

B. Results

We performed the calculations with the standard action for the same lattices (A, B) as in Ref. [11].⁷ In addition, we also repeated the calculations using the fixed point action for the O(3) model [13,29]. The parameters of our measurements are summarized in Table V (here m is the inverse of the exponential correlation length).

The phase shifts obtained from the analysis for the standard and FP actions are shown in Fig. 4 together with the results from Ref. [11]. The results for the standard action are also given in Tables VI and VII and for the FP action in

⁷Reference [11] also measured an additional lattice C with $mL \sim 5$.

Tables VIII and IX. The column δ_E gives the phase shift calculated from the energy by Eq. (4.12): WF labels the results obtained from the wave function, Eq. (4.14). The data shown correspond to $t_0=3$, $M=10$ for lattice D and $t_0=1$, $M=10$ for lattice E . However, the results—especially for δ_{WF} —are quite stable against this choice. We took $R \sim 3/m$ in Eq. (4.11). Taking into account that the correlation lengths used with the FP action were only $\xi \approx 3$ and 6, the agreement with the analytic prediction is very good. Note, however, that a similar suppression of lattice artifacts has been observed previously with this action for other observables [13,29,30].

ACKNOWLEDGMENTS

We would like to thank Michael Karowski for useful discussions and Paolo Butera, Paolo Rossi, and Ettore Vicari for informative correspondence. This investigation was supported in part by the Hungarian National Science Fund (OTKA) (under T016233 and T019917) and also by the Schweizerischer Nationalfonds. The work of M.N. was supported by NSF grant 97-22097.

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