Coupled-cluster expansions for the lattice O(3) σ model

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The coupled-cluster method with the eigenvalue equations truncated according to the continuum limit is applied to the Hamiltonian lattice O(3) σ model. The long wavelength approximation of the vacuum wave function and mass gaps are calculated up to order 8. The results show general scaling behavior according to the full β function. [S0556-2821(96)06720-3]

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I. INTRODUCTION

The nonlinear O(3) σ model in 1+1 dimensions is similar to (3+1)-dimensional non-Abelian gauge theories in many respects, such as, asymptotic freedom and the existence of instanton solutions. In addition, this model seems simple for testing theoretical ideas on asymptotic freedom. Many different lattice methods have been applied to the lattice version of this model, but the conclusions differ widely.

In Refs. [1–3], the Monte Carlo (MC) and MC renormalization group (MCRG) measurements on the standard (i.e., nearest-neighbor) action,

$$A = -\beta \sum_{n,\mu} S_n S_{n+\mu}, \qquad (1.1)$$

observed asymptotic scaling at $\beta > 1.6$ ($\beta \sim 1.6$ in Ref. [1], and $\beta > 1.6$ in Refs. [2,3]) and predicted a mass gap

$$m_T a = C_T \Lambda_{\text{latt}} a, \tag{1.2}$$

with $C_T = (110 \pm 10)$ [2,3], where a is the lattice spacing and

$$\Lambda_{\text{latt}} a = 2\pi\beta e^{-2\pi\beta} \left[1 + \frac{\delta}{2\pi\beta} + O\left(\frac{1}{\beta^2}\right) \right]$$
 (1.3)

is the asymptotic scaling parameter with δ =0.570 resulting from the three-loop approximation. In Ref. [4], the same model was studied by a collective MC method, and no asymptotic scaling was observed up to β =1.9. Reference [5] also reported the absence of asymptotic scaling to β =2.05 in MC simulations. In Ref. [6], the model was investigated in the region β \in (1.4,2.26) with direct mass measurements and using different MCRG methods. The results were

$$C_T = 91 \pm 3 \pm 1,$$
 (1.4)

and the asymptotic scaling emerged in the region $\beta \in (2.14,2.26)$. A high precision MC simulation in which a powerful method is used to extrapolate finite volume MC data to infinite volume was carried out by Caracciolo *et al.* [7]. The results support asymptotic scaling, but with still about 4% deviation from it even at such a large correlation length as $\xi=10^5$ ($\beta=3.0$).

As for the analytical calculation, in Ref. [8], the exact mass gap of the model was obtained; that is,

$$C_T = 80.08638 \dots,$$
 (1.5)

but, the range of β , for which the lattice model exhibits the asymptotic scaling, remains unknown. In Ref. [9], a variational method was used; the results were similar to those in Ref. [1].

In Ref. [10], scaling other than asymptotic scaling in the O(N) model was studied by 1/N expansion in a continuous version. Because the scaling was obtained not by perturbation theory, it was assumed that this scaling is correct for all β . In the lattice case, similar work was done and the mass gap was evaluated numerically up to 400×400 sites [11]. Reference [3] also studied scaling according to the full β function using the MCRG method, and indicated that there probably is some scaling before β goes into the weak coupling region.

In this paper, we use the coupled-cluster method (CCM) to study the model. Our purposes are to test the idea of scaling according to the full β function [3], and, at the same time, to test the effectiveness of the method. In the CCM, an essential problem is how to truncate the coupled-cluster equations. Various schemes have been proposed [12–14]. Here we use the scheme in Ref. [12], that is, to truncate the eigenvalue equations according to the continuum limit. In this scheme, the continuum limit of terms in the eigenvalue equations are preserved [12]. We expect this may soften the cutoff and result in rapid convergence.

This paper is organized as follows. In Sec. II, we introduce the Hamiltonian formalism of the model and the truncated equations. Section III is devoted to the concrete calculations. In Sec. IV, our conclusions and discussion are presented.

II. THE TRUNCATED EIGENVALUE EQUATIONS

According to Eq. (1.1), the Hamiltonian is

$$H = \frac{g^2}{2a_{n,c}} \sum_{b} L_{n,cb}^2 + \frac{1}{2ag^2} \sum_{n} (S_{n+1} - S_n)^2, \quad (2.1)$$

where *n* denotes the lattice space sites, c,b=1,2,3 are the indices of group O(3), $g^2=1/\beta$ is the lattice coupling constant, and S_n is the lattice field satisfying

$$S_n \cdot S_n = 1. \tag{2.1a}$$

Let

$$E_n^b = \frac{1}{2} \epsilon^{bcd} L_{n,cd}.$$

Then the commutators are

$$[E_n^b, S_m^c] = i \epsilon^{bcd} S_n^d \delta_{mn}, \quad [S_n^b, S_m^c] = 0.$$
 (2.2)

 E_n^b are the generators of the group, i.e., the rotation operators in three-dimensional group space. Defining

$$W \equiv \frac{2a}{g^2}H,$$

we have, ignoring irrelevant constants,

$$W = \frac{2a}{g^2}H = \sum_{n} E_n^2 - \frac{2}{g^4} \sum_{n} S_n \cdot S_{n+1}.$$
 (2.3)

The form Eq. (2.3) is very similar to the lattice form of SU(N) gauge theories, with $S_n \cdot S_{n+1}$ replacing the "plaquette" variable $trU_p(n)$. As we mentioned above, the model possesses many properties similar to SU(N) gauge theory, especially, it has instanton solutions, so we suppose the same form of the vacuum state as in Refs. [12,14,15]; that is

$$|\phi_0\rangle = e^R|0\rangle, \tag{2.4}$$

where the state $|0\rangle$ is defined by $E_n^b|0\rangle = 0$, and R is a function of coupled clusters.

From $W|\phi_0\rangle = w_0|\phi_0\rangle$, we get

$$\sum_{n} ([E_{n}^{b}, [E_{n}^{b}, R]] + [E_{n}^{b}, R][E_{n}^{b}, R])$$

$$-\frac{2}{g^{4}} \sum_{n} S_{n} \cdot S_{n+1} = w_{0}.$$
(2.5)

We expand R as a series of clusters which are the various combinations of lattice field S_n , and with the same symmetry as the ground state. Defining the order of clusters in the same way as in Ref. [15], we have

$$R = R_1 + R_2 + R_3 + \cdots,$$
 (2.6)

and choose

$$R_1 = c_{1,1} \sum_{n} S_n \cdot S_{n+1} \equiv c_{1,1} G_{1,1},$$
 (2.7a)

where $c_{1,1}$ is a coefficient to be determined. We call $S_n \cdot S_{n+1}$ a link connecting site n and site n+1. The first order cluster $G_{1,1}$, which is composed of the sum of one link over lattice sites, is the simplest cluster with the same symmetry as the vacuum. The term $[E_n^b, G_{1,1}][E_n^b, G_{1,1}]$ produces new clusters

$$\begin{split} [E_n^b, G_{1,1}][E_n^b, G_{1,1}] &= -2 + 2 \sum_n \left[(S_n \cdot S_{n+1})^2 - S_n \cdot S_{n+2} \right. \\ &+ S_n \cdot S_{n+1} S_{n+1} \cdot S_{n+2} \right] \\ &= -2 + 2 (G_{2,1} - G_{2,2} + G_{2,3}). \end{split}$$

We define these three new clusters as the second order clusters. The order of a cluster is defined in this way by iteration of this operation. So R_2 can be written as

$$R_2 = \sum_{s=1}^{3} c_{2,s} G_{2,s}, \qquad (2.7b)$$

where $c_{2,s}(s=1,2,3)$ are coefficients to be determined. The terms $[E_n^b,G_{1,1}][E_n^b,G_{2,s}]$ (s=1,2,3) will produce six new clusters which are different from those in R_1 and R_2 . They are defined as third order clusters. Higher order clusters can be produced and defined similarly. As H is invariant under space rotation and reflection, the clusters generated in this way automatically preserve the symmetries of $G_{1,1}$. Therefore, they will be in the same sector with definite quantum numbers in the Hilbert space.

Now, suppose we expand R up to Mth order,

$$R \approx R_1 + R_2 + \dots + R_M \,. \tag{2.8}$$

Substituting it into Eq. (2.5), we have

$$\sum_{i=1}^{M} \left[E_{n}^{b}, \left[E_{n}^{b}, R_{i} \right] \right] + \sum_{i,j} \left[E_{n}^{b}, R_{i} \right] \left[E_{n}^{b}, R_{j} \right] - \frac{2}{g^{4}} \sum_{i=1}^{M} S_{n} \cdot S_{n+1} = w_{0}.$$
(2.9)

From the above discussion, we know that generally

$$[E_n^b, R_i][E_n^b, R_j] \in (i+j)$$
th clusters + lower order clusters,

so terms with an order higher than M will be generated in $[E_n^b, \sum_{i=1}^M R_i][E_n^b, \sum_{j=1}^M R_j]$. We have to truncate it. There are many truncation schemes. One of them is to calculate $[E_n^b, R_i][E_n^b, R_j]$ for all $i, j \leq M$ and discard those clusters with an order higher than M [14]. Another scheme is to compute $[E_n^b, R_i][E_n^b, R_j]$ only for $i+j \leq M$, so that no clusters with an order higher than M are produced. Therefore, terms in $[E_n^b, R_i][E_n^b, R_j]$ are wholly preserved $(i+j \leq M)$ or discarded $(i+j \geq M)$, while in the former scheme, clusters are partly preserved for $i+j \geq M$. In Ref. [12], it was proved that

$$[E_n^b, R_i][E_n^b, R_j] \sim$$
 order $a^3 +$ higher orders. (2.10a)

However, if we discard some terms in $[E_n^b, R_i][E_n^b, R_j]$, then

$$part([E_n^b, R_i][E_n^b, R_j]) \sim \underset{a \to 0}{\text{order } a + \text{order } a^3}$$

$$+$$
 higher orders, $(2.10b)$

where $part([E_n^b, R_i][E_n^b, R_j])$ denotes the remainder after discarding. Because lattice calculation should recover the

continuum limit by taking $a \rightarrow 0$, we think the latter scheme, where the truncation preserves the continuum limit, may lead to a more effective approach to scaling. In this scheme, the truncated eigenvalue equation of the vacuum state is

$$\sum_{i=1}^{M} \left[E_{n}^{b}, \left[E_{n}^{b}, R_{i} \right] \right] + \sum_{i+j=2}^{M} \left[E_{n}^{b}, R_{i} \right] \left[E_{n}^{b}, R_{j} \right]$$

$$- \frac{2}{g^{4}} \sum_{i=1}^{M} S_{n} \cdot S_{n+1} = w_{0}. \tag{2.11}$$

Because clusters are independent from each other, the coefficients of each cluster on both sides of Eq. (2.11) should be equal. This leads to a set of nonlinear equations for $\{c_{i,s}, i=1,\ldots,M\}$. $\{c_{i,s}\}$ can be determined by solving these equations.

Now, we return to the mass gap. In the CCM, the excited states are assumed to be

$$|\phi\rangle = F(S_n)|\phi_0\rangle,\tag{2.12}$$

where $F(S_n)$ is a function of $\{S_n\}$ with appropriate symmetry so as to make $|\phi\rangle$ possessing the required quantum numbers. Expanding F as a series of coupled clusters up to Mth order

$$F=F_1+F_2+\cdots+F_M$$
,

we obtain the eigenvalue equation truncated in the scheme preserving the continuum limit

$$\sum_{i=1}^{M} \left[E_{n}^{b}, \left[E_{n}^{b}, F_{i} \right] \right] + \sum_{i+j=2}^{M} \left[E_{n}^{b}, F_{i} \right] \left[E_{n}^{b}, R_{j} \right] = \Delta w \sum_{i=1}^{M} F_{i},$$
(2.13)

where $\Delta w = w - w_0$, and w is defined by $W|\phi\rangle = w|\phi\rangle$.

III. THE CALCULATION OF THE VACUUM WAVE FUNCTION AND MASS GAPS

In this section, we will discuss the detail of calculation. From Eq. (2.7), any vacuum cluster can be written as

$$G_{i,s} = \sum_{l,l} S_{l}^{b} S_{l+k_{s}}^{b} f_{s}(S_{l}), \tag{3.1}$$

where f_s is an arbitrary scalar function of lattice field. Then, the calculation of $[E_n^b, G_{i,s}][E_n^b, G_{j,r}]$ is reduced to calculate such a quantity with its form as $[E_n^b, \Sigma_l S_l \cdot S_{l+k_s}] f_s(S_l) [E_n^b, \Sigma_m S_m \cdot S_{m+k_r}] f_r(S_m)$. Using Eq. (2.2), we have

$$\sum_{b,n,l,m} \left[E_{n}^{b}, S_{l} \cdot S_{l+k_{s}} \right] f_{s}(S_{l}) \left[E_{n}^{b}, S_{m} \cdot S_{m+k_{r}} \right] f_{r}(S_{m}) = -\sum_{n} \left\{ (S_{n+k_{s}} \cdot S_{n+k_{r}} - S_{n} \cdot S_{n+k_{s}} S_{n} \cdot S_{n+k_{r}}) f_{s}(S_{n}) f_{r}(S_{n}) + (S_{n-k_{r}} \cdot S_{n+k_{s}} - S_{n-k_{r}} \cdot S_{n} S_{n} \cdot S_{n+k_{s}}) f_{s}(S_{n}) f_{r}(S_{n-k_{r}}) + (S_{n-k_{s}} \cdot S_{n-k_{r}} - S_{n-k_{r}} \cdot S_{n} S_{n} \cdot S_{n-k_{s}}) f_{s}(S_{n-k_{s}}) f_{r}(S_{n-k_{r}}) + (S_{n-k_{s}} \cdot S_{n+k_{s}} - S_{n-k_{s}} \cdot S_{n} \cdot S_{n+k_{s}}) f_{s}(S_{n-k_{s}}) f_{r}(S_{n}) \right\}.$$
 (3.2)

The calculation of terms $[E_n^b, [E_n^b, G_{i,s}]]$ is similar. We have encoded it in C language.

Evaluating the continuum limit of each cluster $G_{i,s}$, we get the long wavelength expansion of the vacuum wave function. Let the lattice spacing $a \rightarrow 0$, then

$$S_{n+k} = S_n + ka\Delta S_n + \frac{k^2}{2!}a^2\Delta^2 S_n + \cdots$$
 (3.3)

Using this, we obtain

$$R \underset{a \to 0}{\sim} A + \sum_{n} (\mu_0 a^2 (\Delta S)^2 + \mu_{2,1} (\Delta^2 S)^2 a^4 + \mu_{2,2} (\Delta S)^2 (\Delta S)^2 a^4 + \cdots)$$

$$\to A + \int dx (\mu'_0 (\partial S)^2 + \mu'_{2,1} (\partial^2 S)^2 + \mu'_{2,2} (\partial S)^2 (\partial S)^2 + \cdots), \tag{3.4}$$

where the constant A can be absorbed in the normalization constant of the vacuum wave function, and

$$\mu_0' = \mu_0 a, \quad \mu_{2,1}' = \mu_{2,1} a^3, \quad \mu_{2,2}' = \mu_{2,2} a^3, \quad (3.5)$$

with

$$\mu_0 = -\sum_{i,s} c_{i,s} \sum_{k=1}^N \frac{(k-k')^2}{2},$$

$$\mu_{2,1} = \sum_{i,s} c_{i,s} \sum_{k=1}^{N} \frac{(k-k')^4}{4!},$$
 (3.6)

$$\mu_{2,2} = \sum_{i,s} c_{i,s} \sum_{k_1 > k_2 = 1}^{N} \frac{(k_1 - k_1')^2 (k_2 - k_2')^2}{4}.$$

Here, N is the number of links in $G_{i,s}$, and k,k' the two end

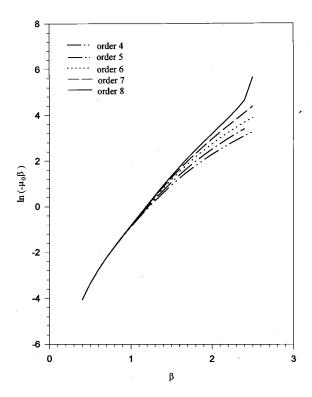


FIG. 1. The coefficients $\ln(-\mu_0\beta)$ of vacuum wave function versus $\beta = 1/g^2$.

point coordinates of a link. Equation (3.4) gives the long wavelength vacuum wave function. The coefficients μ'_0 , $\mu'_{2,1}$, and $\mu'_{2,2}$ describe the long wavelength behavior. They are physical, while μ_0 , $\mu_{2,1}$, and $\mu_{2,2}$ are lattice dimensionless quantities, computed by Eq. (3.6). From Eq. (1.2) and Eq. (1.3), we have, in the asymptotic scaling region,

$$a = \frac{C_T}{m_T} 2\pi\beta e^{-2\pi\beta} \equiv C_0 2\pi\beta e^{-2\pi\beta},$$

where we have neglected the three or more loop corrections. Hence,

$$\mu_{0}\beta \to \frac{\mu'_{0}}{C_{0}2\pi}e^{2\pi\beta},$$

$$\mu_{2,1}\beta^{3} \to \frac{\mu_{2,1}}{C_{0}^{3}8\pi^{3}}e^{6\pi\beta}, \text{ as } a \to 0,$$

$$\mu_{2,2}\beta^{3} \to \frac{\mu_{2,2}}{C_{0}^{3}8\pi^{3}}e^{6\pi\beta}.$$
(3.7)

For order M=4,5,6,7,8, we solve Eq. (2.11). The numbers of clusters in these cases are 31,86,276,866,2886. For simplicity, we present only the results of μ_0 . Figure 1 shows the results. The various order curves show obviously the trend of convergency, particularly in the region $\beta \le 1.4$, Although asymptotic scaling is not reached in this region, the eighth order curve for $\ln(-\mu_0\beta)$ should exhibit the scaling sccording to the full β function as described in Ref. [3]. We will return to this point later.

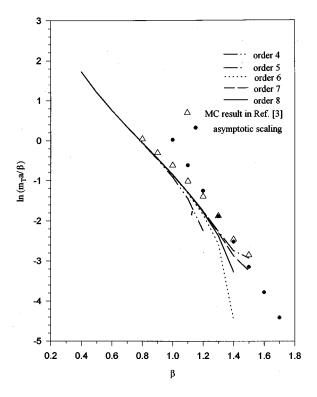


FIG. 2. Calculated values of triplet $\ln(m_T a/\beta)$ versus $\beta = 1/g^2$. We also plot the Monte Carlo results in Ref. [3] and the three loop approximation for asymptotic scaling.

Let us turn to the mass gap. It is expected that the above mentioned full β scaling emerges in the results if the scaling actually exists. Considering the singlet mass m_s and triplet mass m_T , the first order cluster approximations are chosen to be

$$F_1^s = \sum_n S_n \cdot S_{n+1} \text{ for } m_s, F_1^T = \sum_n S_n^b \text{ for } m_T,$$
(3.8)

where b=1,2,3 is the index of the group. m_T is degenerate for b. Higher order clusters are generated by recursion. Solving Eq. (2.13), we get the lattice dimensionless quantities $\Delta w_s(\beta)$ and $\Delta w_T(\beta)$. Equation (1.2) leads to

$$\ln \frac{m_T a}{\beta} = \ln \frac{\Delta w_T}{2 \beta^2} \rightarrow \ln C_T + \ln \frac{\Delta a}{\beta},$$
 as $a \rightarrow 0$, (3.9)

$$\ln \frac{m_s a}{\beta} = \ln \frac{\Delta w_s}{2\beta^2} \rightarrow \ln C_s + \ln \frac{\Lambda a}{\beta}.$$

The curves of $\ln(m_T a/\beta)$ and $\ln(m_S a/\beta)$ against β are plotted in Figs. 2 and 3 respectively. Strong evidence of convergence is shown in Fig. 2 for the triplet mass. We also plot the MC result taken from Ref. [3]. Our result is reasonably consistent with this MC result in the region $\beta \le 1.4$, confirming the existence of scaling according to the full β function. (The MC result is for the Lagrangian formulation, the Hamiltonian result is slightly lower than the MC result as discussed in Ref. [16].)

For comparison, we also plot the three loop approximation for asymptotic scaling

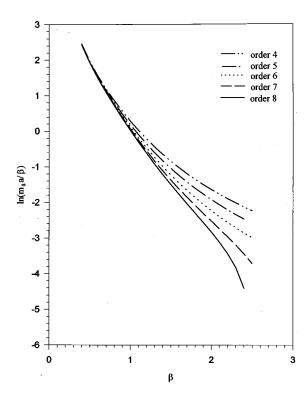


FIG. 3. The mass gap $\ln(m_s a/\beta)$ versus $\beta = 1/g^2$.

$$\ln\left(\frac{m_T a}{\beta}\right) = \ln\left[2\pi C_T \left(1 + \frac{\delta}{2\pi\beta}\right)\right] - 2\pi\beta,$$

with the exact value C_T = 80.08638 taken from Ref. [8]. In spite of not reaching the asymptotic scaling region, our results in Fig. 2 are not inconsistent with it.

The convergence of the curves in Fig. 3 for the scalar mass is not as rapid as that for the triplet mass. This can be accounted for by the higher singlet mass, which requires higher order calculations to attain good convergence. Since good convergence for m_s has not been reached in our calculations, we cannot give a reliable estimate of the parameter C_s for the singlet mass.

To give more direct evidence to support the idea of full β scaling, let us calculate $m_T \mu'_0$. The full β scaling is

$$\Lambda_{\text{latt}} a = 2\pi\beta e^{-2\pi\beta} f(\beta)$$
with $f(\beta) \underset{\beta \to \infty}{\sim} + \frac{0.57}{2\pi\beta} + O\left(\frac{1}{\beta^2}\right)$. (3.10)

From Eq. (1.2) and Eq. (3.5), we know $m_T \mu_0'$ is independent of β and should be a constant in the full scaling region. In Fig. 4, the eighth order plot of $-m_T \mu_0'$ against β is presented. The results show nice scaling in the region $\beta \in (0.8,1.2)$ and we obtain

$$-m_T \mu_0' = -\mu_0 \frac{\Delta w_T}{2\beta} = 0.18. \tag{3.11}$$

For comparison, we also plot the eighth order result of $-m_s\mu_0'$ against β in Fig. 4. No scaling is exhibited in the curve as we expected.

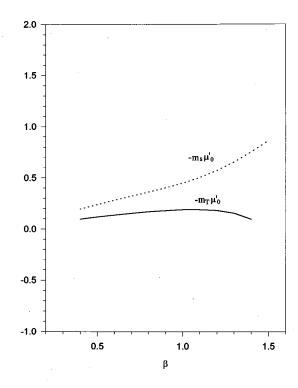


FIG. 4. The eighth order results of $-m_T \mu_0'$ versus $\beta = 1/g^2$ and $-m_s \mu_0'$ versus $\beta = 1/g^2$.

IV. CONCLUSIONS AND DISCUSSION

Despite the apparent simplicity of the O(3) σ model, it is rather hard to obtain asymptotic scaling because it emerges only in a deep weak coupling region. This is in contrast with (2+1)-dimensional U(1) lattice theory for which asymptotic scaling occurs at a much earlier stage [15]. These results are consistent with conclusions from Monte Carlo calculations. Our results, though not showing the asymptotic scaling, give strong evidence for the convergence of the truncation method. All the quantities we calculate show the trend of convergence, especially for $\ln(m_T a/\beta)$ in Fig. 2 and μ_0' in Fig. 1.

Our results also show some trace of asymptotic scaling. In Fig. 2, the seventh and eighth order curves bend downward for $\beta \ge 1.4$ to make the slope tending to -2π , and in Fig. 1, the slope of the eighth order curve begins to increase obviously when $\beta > 2$.

Perhaps the most important conclusion is that our results verify the idea of "full β scaling" [3]. In the region $\beta \in (0.8, 1.2)$, the results of μ'_0 and m_T show this scaling behavior (see Figs. 1, 2, and 4). We obtain

$$m_T \mu_0' = -0.18.$$

This scaling is not obvious in Fig. 3. We think the reason is that m_s is larger than m_T . It is expected that higher order calculations will exhibit the full β scaling and eventually the asymptotic scaling.

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