RENORMALIZED TRAJECTORY FOR NON-LINEAR SIGMA MODEL AND IMPROVED SCALING BEHAVIOR

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We apply the block-spin renormalization group method to the O(N) Heisenberg spin model. Extending a previous work of Hirsch and Shenker, we find the renormalized trajectory for O(∞) in two dimensions. For finite N models, we choose a four-parameter action near the large-N renormalized trajectory and demonstrate a remarkable improvement in the approach to continuum limit by performing Monte Carlo simulation of O(3) and O(4) models.

1. Introduction

Critical behavior of lattice systems is of special interest since it is only in the approach to critical points that a universal behavior is recovered and contact made with the corresponding continuum field theory. The question then arises as to how to accelerate this approach to continuum behavior. This is a question of practical importance in numerical Monte Carlo simulations (MC), where one would like to observe the scaling behavior of the continuum limit already on small lattices, i.e., when the correlation length \( \xi \) cannot be much larger than the lattice spacing \( a \). In a series of papers [1], Symanzik has shown how to modify the lattice action in such a way that the \( O(a^2/\xi^2) \) corrections to scaling be cancelled and replaced by \( O(a^4/\xi^4) \). His method is of perturbative essence and seems to be effective in models where some scaling behavior is already observed before improvement. An alternative idea, based on the real space renormalization group and block-spin methods, is to determine the renormalized trajectory (RT) in coupling constant space under some block spin operation [2]. Along such an RT, there is a one-parameter renormalization group and scaling should be observed in some optimal way since points on the RT are directly connected to the euclidian invariant continuum limit (fixed point) by an exact renormalization group transformation. Also, in the vicinity of such an RT, the Monte Carlo renormalization group method should be an accurate and powerful one [3].
Although the idea of an RT is simple conceptually, it is difficult to find its location exactly. To apply this idea to an actual model one has to introduce some approximate trajectory which is supposedly not far from the RT. For example, in asymptotically free theories, the trajectory can be determined by perturbative calculation in the weak coupling region. In fact, this possibility has been recently explored by several authors [3, 4]. In this paper, we investigate the usefulness of the RT by using another approximation. Using the block-spin transformations we find the RT for the O(N) non-linear spin model in the large-N limit. Extending a previous work of Hirsch and Shenker [5], we show that these transformations are given by a simple set of equations. We determine numerically the fixed trajectory and discuss its features (sect. 2). We then propose to use this large-N RT as an approximate trajectory for finite-N models. Of course, this cannot be justified a priori but Monte Carlo results show that using this approximate trajectory O(3) and O(4) models improve considerably (sect. 3). We hope that our analysis will illustrate clearly the mechanism of improvement by the renormalized trajectory and help extend these ideas to other interesting models.

2. The renormalized trajectory for O(\infty) model

The classical O(N) symmetric Heisenberg model is described by N-component unit vectors $S_m$ defined on the sites $m$ of a $d$-dimensional lattice interacting through a translationally invariant short-ranged interaction $\rho_{mn}$. The partition function $Z$ is

$$Z = \int d\mu(S) \exp(-H),$$

$$H = -N \sum_{(m,n)} \rho_{mn}(S_m S_n - 1),$$

$$d\mu(S) = \prod_m d^{N}S_m \delta(S_m^2 - 1)$$

(1)

One convenient way of introducing block-spin variables is to divide the $d$-dimensional hypercubic lattice into cubes of $L$ sites per side and to define an average spin $t_a$ (of unit length) within a block "a" which interacts through the renormalized hamiltonian $H'(t')$ defined by

$$\exp(-H'(t)) = \int d\mu(S) \prod_a \delta(t_a - \frac{\sum_{m \in a} S_m}{\sum_{m \in a} ||S_m||}) \exp(-H(S))$$

(2)

It is, in general, difficult to find a closed expression for the renormalized hamiltonian $H'$. However, in the limit $N \to \infty$, there is considerable simplification due to the property of "factorization" [6]. This implies, for example, that the two-point correlation functions for block-spins $t$ can be related to the two-point correlation functions...
for the original spin $S$ as

$$F'_{a,b} = \langle t_a \cdot t_b \rangle_H = \frac{\sum_{i \in a} \sum_{m \in b} F_{i,m}}{\sum_{i \in a} F_{i,i}},$$

$$F_{i,j} = \langle S_i \cdot S_j \rangle_H$$

(3)

Similarly, all higher-order correlation functions factor into products of two-point correlation functions. Now, for $d = 2$, it is believed that the $O(N)$ symmetry remains unbroken which, in turn, implies that eq (3) completely defines arbitrary correlation functions of the block-spin variables in the limit $N \to \infty$. Thus, although it is difficult to get an exact expression for $H'(t)$, it is not unreasonable to assume a form bilinear in spins and determine the effective coupling constants from eq. (3) as described below.

In the limit $N \to \infty$, the Fourier transform of $F_{ij}$ is related to that of $\rho_{mn}$ in eq (1) as [5]

$$F(k) = \frac{1}{2[a - p(k)]},$$

(4)

where $\lambda$ is determined from the gap equation

$$F_{ij} = 1 = \frac{1}{2} \sum_k (\lambda - p(k))^{-1}$$

(5)

Then, eq (3) in Fourier space becomes

$$F_L(k) = \frac{1}{C_L} \sum_{l=0}^{L-1} F \left( \frac{k + 2\pi l}{L} \right) U_L^2 \left( \frac{k + 2\pi l}{L} \right),$$

$$U_L^2(k) = \prod_{\mu=1}^{d} \frac{\sin^2 \left( \frac{1}{2} L k_{\mu} \right)}{\sin^2 \left( \frac{1}{2} k_{\mu} \right)}$$

$$C_L = \int_{-\pi}^{\pi} \frac{d^d k}{(2\pi)^d} \sum_{l=0}^{L-1} F \left( \frac{k + 2\pi l}{L} \right) U_L^2 \left( \frac{k + 2\pi l}{L} \right),$$

(6)

where we have used a subscript "L" in $F_L$ to remind us that it refers to a block-spin for $L \times L$ blocks (from now on we shall be discussing the $d = 2$ case only although it applies in any dimension in an $O(N)$ symmetric phase). Now, assuming the effective block-spin Hamiltonian to be bilinear in the spin variables (i.e. $H_{L}^{\text{eff}} = -\sum_{m,n} t_m t_n \rho_{L}(m-n)$), the coupling constants can be determined from

$$\rho_L(n) = -\int_{-\pi}^{\pi} \frac{d^d k}{(2\pi)^d} \frac{\exp(i k \cdot n)}{2 F_L(k)}$$

(7)

The renormalization group (RG) transformations $\rho \to \rho_L$ embodied in eqs (4)–(7) have the merit of being explicit. One may easily verify that they form a (semi-)group; an $L \times L$ blocking followed by an $L' \times L'$ blocking amounts to an $LL' \times LL'$ blocking.
Although eq. (6), as it stands, is not fit for a continuation to non-integer $L$, one may (numerically) verify that block sizes of consecutive integers give consistent results, for example, the interaction $\rho$ resulting from a $3 \times 3$ blocking interpolates between a $2 \times 2$ and a $4 \times 4$ blocking, and so on. Also, it may be worth recalling that our block-spin transformation does not affect the long-distance behavior of the system, as wanted, from eq (6) one reads that the low-$k$ behavior of $F_L(k)$ is dominated by the $l = 0$ terms and hence
\[
F_L(k) \approx \frac{1}{C_L} F\left(\frac{k}{L}\right) L^2 \quad (k \sim 0)
\]
So the correlation length in physical units remains unchanged.

We have numerically evaluated the various block-spin couplings for blocks of size $2 \times 2$, $4 \times 4$, $8 \times 8$, etc., from eq (7) for various choices of $F(k)$. Some of the results are shown in fig 1 where we have plotted the couplings $K_2$ (interaction between spins $\sqrt{2a}$ apart), $K_3$ (for spins $2a$ apart) and $K_4$ (for spins $3a$ apart) against $K_1$ (nearest-neighbor interaction) for successive blocking. For example, starting with the point $A_0$ ($K_1 = 10$, $K_2 = 0$ for $i \neq 1$), we evaluate $K_i'$ ($i = 1, 2, \ldots$) for blocks of size $2 \times 2$ (point $A_1$), $4 \times 4$ (point $A_2$) etc. up to $128 \times 128$ (point $A_7$). This process is repeated for different choices of initial interaction $\rho(k)$. After a few blockings, all the trajectories seem to approach a limiting curve usually referred to as the renormalized trajectory (RT). Actually, what we see in fig 1 is a projection of the RT on various subspaces such as the $K_1-K_2$ plane, etc., the true RT is a one-dimensional curve in a possibly infinite-dimensional coupling constant space.

Let us now discuss some interesting features of the RT.

(i) As the ratio of correlation length to current lattice spacing decreases under the block-spin operations, one expects the couplings $K_i$ to go to smaller (higher-temperature) values and ultimately to approach the origin. Actually, what we find is that the RT is located in the region $K_1 > 0$, $K_2 < 0$, $K_3 < 0$, $K_4 > 0$, etc., but this does not exclude the possible existence of other RT's approaching the origin in different directions.

(ii) One expects the iterated block-actions to approach the RT when the correlation length becomes of the same order of magnitude as the current lattice spacing. This is what is qualitatively observed. For example, using the standard action ($K_i = 0$ for $i > 1$), point $A_0$ ($K_1 = 10$) in fig 1 corresponds to $\xi/a = 95$ and it takes about five blockings to approach the RT. In contrast, starting with Shenker–Tobocznik action (ST) ($K_1 K_2 K_3 K_4 = 1 - \frac{3}{13} - \frac{1}{13} 0$) [3], $\xi/a \approx 14$ at $K_1 = 1.5$, and one approaches the RT much faster than starting from standard action or from "tree-improved" action (TIA) ($K_1 K_2 K_3 K_4 = 0 - \frac{1}{12} 0$) [7]. For the latter cases, there is a transient regime where the couplings $K_i$ first increase (in absolute value) before receding along the RT. Such behavior has also been observed in the Migdal–Kadanoff approximate renormalization group for SU(2) lattice gauge theory, in the $\beta_1-\beta_\lambda$ plane [8], as well as in some hierarchical models [9] where an exact RG exists.
the case of SU(2) gauge theory that behavior was tacitly interpreted as a consequence of the existence of a singular (critical?) point in the upper-half plane $\beta_A > 0$. In our case, we do not know if such an explanation also applies.

(iii) It is easy to determine the shape of the RT at small and large couplings For small $K_1$’s, one assumes that $K_2, K_3 \sim O(K_1^2), K_4 \sim O(K_1^3)$, and gets for the $2 \times 2$ blocking

$$K_1' = \frac{K_1}{2} + \frac{K_2}{2} + K_3 + K_1^2 + \cdots , \quad (9a)$$

$$K_2' = \frac{K_2}{4} + \frac{K_1 K_2}{2} + \frac{K_2^2}{4} + 9K_1^3 + \cdots , \quad (9b)$$

$$K_3' = -\frac{1}{4}K_1^2 - \frac{3}{8}K_2^2 - \frac{K_1 K_2}{2} + K_3^3 + \cdots , \quad (9c)$$

$$K_4' = \frac{1}{2}K_1^3 + \cdots \quad (9d)$$

Eqs (9a, c, d) show that the RT approaches the origin along the curve $K_3 = -K_1^2$, $K_4 = K_1^3$ whereas (9a, b) are consistent with $K_2$ proportional to $K_1^2$. 

![Diagram](image-url)
For large $K$, the behavior is even simpler. In eq (4), $\lambda$ is determined by the low-$k$ behavior of $\rho(k)$ and so is exponentially small for large $K$. This means that the model is asymptotic to the gaussian model which is free of the non-linear constraint $S^2 = 1$ and whose fixed point for the previous block-spin transformation is known [10]. Then $\rho$ should approach

$$\rho (\text{gaussian model fixed point}) = -\frac{\text{const}}{\Omega^{*}(k)},$$

$$\Omega^{*}(k) = \sum_{n=1}^{\infty} \prod_{\mu=1}^{2} \frac{\frac{1}{2} \sin^2 k_{\mu}}{\left(\frac{1}{2} k_{\mu} + \pi l_{\mu}\right)^2} \frac{1}{(k^2 + 2 \pi l)^2}$$

This gaussian model projects on our four-parameter space along the line

$$K_1 \ K_2 \ K_3 \ K_4 = 1 \ -0.0948 \ -0.2187 \ 0.0492$$

We have seen that this asymptotic is indeed approached very early (down to $K \sim 0.8$) and it is only for very small $K$, that there is a crossover to the power behavior discussed above.

In the forthcoming section, we intend to use the action given by the RT for small values of the couplings. It is then convenient to take the curvature towards the origin into account and to fit the RT by

$$(K_1 - 0.5) \ (K_2 + 0.045) \ (K_3 + 0.1025) \ (K_4 - 0.021) = 1 \ 0 \ -0.1011 \ -0.2412 \ 0.056$$

These slopes differ only slightly from the gaussian values but the resulting approximation is an excellent description of the RT in the range $0.15 \leq K_1 \leq 0.8$.

Let us summarize what we have done so far. Using the block-spin technique, we have derived effective block-spin hamiltonians for any $L \times L$ blocking in the limit $N \to \infty$. The only assumption was that it is sufficient to consider hamiltonians bilinear in spins, which is plausible in the sense that in the $O(N)$ symmetric phase, any arbitrary correlation function can be obtained from two-point correlation functions by factorization, and these two-point function are in one-to-one correspondence with bilinear hamiltonians. We emphasize that there has been no truncation such as assuming that the block-spin hamiltonians have only a finite number of coupling constants.

### 3. Monte Carlo simulation of $O(3)$ and $O(4)$ models

Let us now turn to the question of how a knowledge of the RT helps in finding a model with a better continuum limit. It is well known that in the formal limit the lattice spacing $a \to 0$, the Heisenberg model reduces to an $O(N)$ non-linear sigma
model (NLSM) defined by the euclidian action

\[ H_{\text{action}} = \frac{1}{2g} \int (\partial_\mu S)^2 \, d^d x \quad (\mu = 1, 2, \ldots, d), \]  

(13)

where the continuum coupling constant \( g \) is related to the \( K_i \)'s. It is also known that NLSM is asymptotically free at space-time dimension \( d = 2 \). To verify this, one has to show that physical quantities such as correlation length \( \xi \), magnetic susceptibility \( \chi \), obey the scaling relations (see later) predicted by the renormalization group equation.

Various authors have discussed the significance of choosing a lattice action near the RT. An intuitive way of understanding this is as follows. Let us consider the points \( A_0 \) and \( A_5 \) in fig. 1. Let us denote the hamiltonians associated with these two points as \( H_0(\{ K \}, a) \) and \( H_5(\{ K \}', 2^5 a) \) respectively. Since the point \( A_5 \) is obtained from \( A_0 \) by a \( 2^5 \times 2^5 \) blocking, they describe the same physics, the important point is that simulating \( H_5(\{ K \}', 2^5 a) \) is equivalent to simulating \( H_0(\{ K \}, a) \), which has a much smaller lattice spacing. Thus, even for finite \( \{ K \}' \), we would expect \( H_5 \) to show an earlier scaling, i.e. at lower values of \( \xi / a \).

Finally, we turn to the practical aspects of an MC simulation. First, we are interested in an O(\( N \)) NLSM for finite \( N \) (such as \( N = 3, 4 \), etc.). Second, even if we knew the RT for finite \( N \), it would be difficult to work with a lattice action very near the RT as that would necessarily involve a large number of interactions. So, faced with these difficulties, we are forced to make some additional assumptions which are not obvious a priori but are only justified by the end results. These are (i) the RT for finite-\( N \) models such as O(3), O(4), etc. are in some sense close to the O(\( \infty \)) RT (with the appropriate factor of \( N \) taken out in the lattice action), and (ii) it is sensible to keep only four coupling constants (\( K_1, K_2, K_3 \) and \( K_4 \)) in the block-spin hamiltonians and neglect all longer-range interactions. This is supported by the fact that longer-range interactions such as \( K_5 \) (coupling between spins \( \sqrt{5} a \) apart) are observed to be rather small compared to \( K_1 \) for hamiltonians near the RT (for example, \( K_5 / K_1 = -0.003 \) for point \( A_5 \)). From now on we shall refer to these four-parameter actions as "renormalization group improved models" (RGIM).

So the lattice action we choose for MC simulation is

\[
S = N \left[ K_1 \sum_{n\mu} S_n \cdot S_{n+\mu} + K_2 \sum_n (S_{n+x+y} + S_{n+x-y}) \right. \\
+ \left. K_3 \sum_{n\mu} S_n \cdot S_{n+2\mu} + K_4 \sum_{n\mu} S_n \cdot S_{n+3\mu} \right],
\]  

(14)

where \( K_1, K_2, K_3 \) and \( K_4 \) lie on the approximate RT given by (12). In the continuum limit, the continuum coupling constant \( g \) given by

\[ g = \beta^{-1} = (K_1 + 2K_2 + 4K_3 + 9K_4)^{-1} \]

(15)
is small, and the mass-gap $m$ (inverse correlation length) and susceptibility $\chi$ for the $O(N)$ model scale as [12]

$$m = B_N(1 + 2 \pi \beta)^{1/(N-2)} e^{-2 \pi \beta/(N-2)} \left( 1 + O \left( \frac{1}{\beta} \right) \right),$$

$$\chi = C_N(1 + 2 \pi \beta)^{(N+1)/(N-2)} e^{4 \pi \beta/(N-2)} \left( 1 + O \left( \frac{1}{\beta} \right) \right),$$  \hspace{1cm} (16)

where we find it convenient to write the power behavior in $\beta$ in terms of $(1 + 2 \pi \beta)$.

In fig. 2, we show the result for the mass-gap of the $O(4)$ model for different values of $\lambda_4 = (1 + 2 \pi \beta)^{1/2} e^{-\pi \beta}$. We used a heat bath algorithm on a lattice of size from $20 \times 20$ to $50 \times 50$ with a periodic boundary condition. We made 3–6 runs at each temperature with different initial conditions, each run being about 3000–6000 sweeps. This was found to be better than a single long run because of the presence of metastability in low-temperature configurations. The mass-gap was obtained from zero-momentum correlation functions. The mass-gap for the standard model ($K_i \neq 0$, $K_i = 0$ for $i > 1$) are taken from ref [13]. It is clear that in our model (RGIM) scaling starts at a much smaller value of $\xi = 1.1 - 1.2$, compared to standard model where scaling seems to start at $\xi \approx 3$. The constant $B_4$ in eq (16) is estimated to be 4.98.

Of course this verification of scaling, which is sensitive to the details of the relation between the $K$'s and $g$, is not the definitive test that our improvement is operative. Computation of mass ratios or investigations of the energy-momentum dispersion.

Fig 2 Mass-gap (in units of $1/a$) for $O(4)$ models versus $\lambda_4 = \sqrt{1 + 2\pi \beta} e^{-\pi \beta}$
Encouraged by the O(4) result, we looked at O(3) model where we used lattices of size ranging from $20 \times 20$ to $70 \times 70$. The mass-gap is shown in fig. 3. Scaling starts at $\xi \approx 1.8-2.0$. The constant $B_3$ is estimated to be 10.25.

Unlike the case of O(4), there are several "improved" O(3) models (as discussed earlier). In addition to TIA and ST models, there is a one-loop improved Symanzik action (1LSA) [14] (another model has been proposed in ref. [4], but this is equivalent to an ST in the scaling region). For comparison, scaling starts at $\xi = 4$ for TIA, $\xi = 1.5-2.0$ for 1LSA, and $\xi = 3$ for ST. It is gratifying to see that our model based on the RT for $O(\infty)$ compares quite favorably to these other models even for $N = 3$.

We also evaluated magnetic susceptibility scaling defect $\delta_x = \chi(1 + 2\pi\beta)^{(N+1)/(N-2)} \exp(-4\pi\beta/(N-2))$ which should approach a constant value in the scaling region. The results for O(4) and O(3) are shown in figs. 4 and 5. They are also consistent with the observation that scaling sets in early in RGIM.

Finally, we computed the ratio of $A$-parameters (up to one-loop), and the result is:

$$\frac{A_{\text{RGIM}}}{A_{\text{STANDARD}}} = \begin{cases} 5.78 & \text{for O(3)} \\ 2.99 & \text{for O(4)} \\ 1.54 & \text{for O(\infty)} \end{cases}$$

The observed values are 8.49 for O(3) and 3.12 for O(4). The discrepancy for O(3) model may be due to one or both of two reasons:

(i) there might be a large $O(g)$ correction to the one-loop formula, and
Fig 4 Magnetic susceptibility scaling defect for \( \theta(4) \) model. Data for standard model taken from ref [13].

Scaling curve for the standard model might have a slight peculiarity as suggested in ref [16], leading to some change in the value of the ratio of \( \lambda \)-parameters.

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Fig 5 Magnetic susceptibility scaling defect for \( \theta(3) \) model. Data for standard model taken from ref [15].
$O(\infty)$ model. In refs [18], the author claims to be doing finite-$N$ models while at
the same time assuming an effective hamiltonian bilinear in spins.

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