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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 ξ 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(∞) 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 ρ_{mn} The partition function Z is

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

$$H = -N \sum_{(m,n)} \rho_{nm}(\boldsymbol{S}_m \cdot \boldsymbol{S}_n - 1) ,$$

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

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 $\boldsymbol{t}_a$ (of unit length) within a block "a" which interacts through the renormalized hamiltonian $H'(\boldsymbol{t}')$ defined by

$$\exp(-H'(\boldsymbol{t})) = \int \mathrm{d}\mu(S) \prod_a \delta\left(\boldsymbol{t}_a - \frac{\sum_{m\in a} \boldsymbol{S}_m}{\|\sum_{m\in a} \boldsymbol{S}_m\|} \right) \exp(-H(S)) \tag{2}$$

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 $\boldsymbol{t}$ can be related to the two-point correlation functions for the original spin $\boldsymbol{S}$ as

$$F'_{a,b} = \langle \boldsymbol{t}_a \cdot \boldsymbol{t}_b \rangle_{H'} = \frac{\sum_{l \in a} \sum_{m \in b} F_{l,m}}{\|\sum_{l,l' \in a} F_{l,l'}\|},$$

$$F_{i,j} = \langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle_H \tag{3}$$

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 ρ_{mn} in eq (1) as [5]

$$F(k) = \frac{1}{2[\lambda - \rho(k)]}, \tag{4}$$

where λ is determined from the gap equation

$$F_{ii} = 1 = \tfrac{1}{2} \sum_k (\lambda - \rho(k))^{-1} \tag{5}$$

Then, eq (3) in Fourier space becomes

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

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

$$C_L = \int_{-\pi}^{\pi} \frac{d^d k}{(2\pi)^d} \sum_{l=0}^{L-1} F\left(\frac{\boldsymbol{k} + 2\pi \boldsymbol{l}}{L}\right) U_L^2\left(\frac{\boldsymbol{k} + 2\pi \boldsymbol{l}}{L}\right), \tag{6}$$

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 $H_L^{\text{eff}} = -\sum_{m,n} \boldsymbol{t}_m \cdot \boldsymbol{t}_n \rho_L(\boldsymbol{m} - \boldsymbol{n})$), the coupling constants can be determined from

$$\rho_L(\boldsymbol{n}) = -\int_{-\pi}^{\pi} \frac{d^d k}{(2\pi)^d} \frac{\exp(i\boldsymbol{k} \cdot \boldsymbol{n})}{2 F_L(\boldsymbol{k})} \tag{7}$$

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 ρ resulting from a 3×3 blocking interpolates between a 2×2 and a 4×4 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 $\boldsymbol{l}=0$ terms and hence

$$F_L(k)\sim\frac{1}{C_L}F\left(\frac{\boldsymbol{k}}{L}\right)L^2 \quad (k\sim0) \tag{8}$$

So the correlation length in physical units remains unchanged

We have numerically evaluated the various block-spin couplings for blocks of size 2×2, 4×4, 8×8, 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 $\sqrt{2}a$ 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 ($K_1=1\ 0$, $K_i=0$ for $i\neq1$), we evaluate $K_i'(i=1,2\ \ .\ )$ for blocks of size 2×2 (point A_1), 4×4 (point A_2) etc up to 128×128 (point A_7) This process is repeated for different choices of initial interaction $\rho(\boldsymbol{k})$ 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 ($K_1=1\ 0$) in fig 1 corresponds to $\xi/a\simeq95$ and it takes about five blockings to approach the RT In contrast, starting with Shenker–Tobochink action (ST) ($K_1\ K_2\ K_3\ K_4=1\ \ -\frac{2}{13}.-\frac{1}{13}\ 0$) [3], $\xi/a\simeq14$ at $K_1=1.5$, and one approaches the RT much faster than starting from standard action or from "tree-improved" action (TIA) ($K_1\ K_2\ K_3.K_4=\frac{4}{3}\ 0\ -\frac{1}{12}\ 0$) [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 $\beta_f-\beta_A$ plane [8], as well as in some hierarchial models [9] where an exact RG exists In

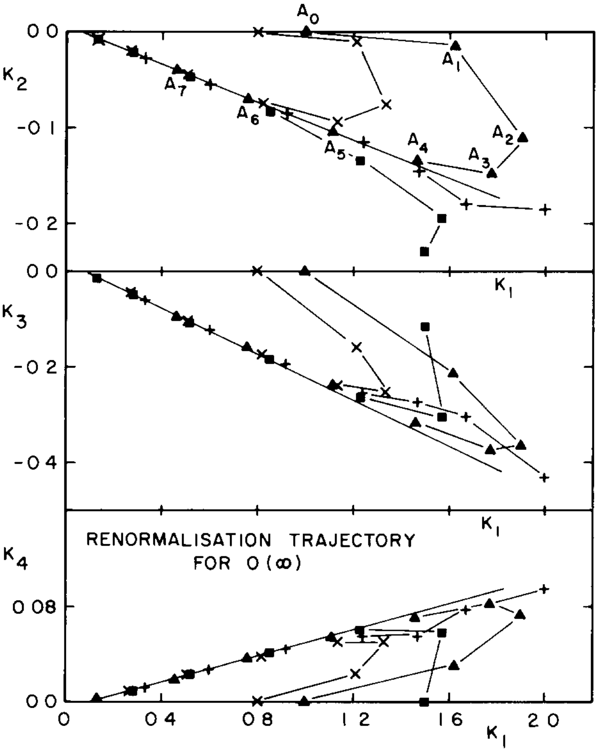

Fig 1 Trajectories starting with $K_1 = 0\ 8$, $K_i = 0$ for $i > 1$ (crosses), $K_1 = 1\ 0$, $K_i = 0$ for $i > 1$ (triangles), $K_1 = 1\ 5$, $K_2 = -0\ 2308$, $K_3 = -0\ 1154$, $K_i = 0$ for $i > 3$ (squares, corresponds to ST action), $K_1 = 2\ 0$, $K_2 = -0\ 186$, $K_3 = -0\ 430$, $K_4 = 0\ 095$ (pluses)

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_i's, one assumes that $K_2, K_3 \sim O(K_1^2)$, $K_4 \sim O(K_1^3)$, and gets for the 2×2 blocking

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

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

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

$$K_4' = \tfrac{1}{8}K_1^3 + \cdots \tag{9d}$$

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

For large K_i, the behavior is even simpler In eq (4), λ is determined by the low-k behavior of $\rho(k)$ and so is exponentially small for large K_i's 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 ρ should approach

$$\rho\ (\text{gaussian model fixed point}) = -\frac{\text{const}}{\Omega_0^*},$$

$$\Omega_0^*(k) = \sum_{l_1,l_2=-\infty}^{\infty} \left[\prod_{\mu=1}^{2} \frac{\frac{1}{2}\sin^2 k_\mu}{(\frac{1}{2}k_\mu + \pi l_\mu)^2} \right] \frac{1}{(k^2 + 2\pi l)^2} \tag{10}$$

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

$$K_1\ \ K_2\ \ K_3\ \ K_4 = 1\ \ -0\,0948\ \ -0.2187\ \ 0\,0492 \tag{11}$$

We have seen that this asymptotic is indeed approached very early (down to $K_1 \sim 0\,8$) and it is only for very small K_i 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

$$\begin{aligned}(K_1 - 0\,5)\ \ (K_2 + 0\,045)\ \ (K_3 + 0\,1025)\ \ (K_4 - 0\,021)\\ = 1\,0\ \ -0.1011\ \ -0\,2412\ \ 0.056\end{aligned} \tag{12}$$

These slopes differ only slightly from the gaussian values but the resulting approximation is an excellent description of the RT in the range $0\,15 \leqslant K_1 \leqslant 0\,8$

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

$$H \to \text{action} = \frac{1}{2g}\int (\partial_\mu \boldsymbol{S})^2\,\mathrm{d}^d x \quad (\mu = 1, 2, \ldots, d), \tag{13}$$

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 $d = 2$[11, 12]. To verify this, one has to show that physical quantities such as correlation length ξ, magnetic susceptibility χ, 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 ξ/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(∞) 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, $K_5/K_1 \simeq -0.003$ 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

$$S = N\Bigg[K_1 \sum_{n,\mu} \boldsymbol{S}_n \cdot \boldsymbol{S}_{n+\mu} + K_2 \sum_{n} \boldsymbol{S}_n \cdot (\boldsymbol{S}_{n+x+y} + \boldsymbol{S}_{n+x-y}) + K_3 \sum_{n\mu} \boldsymbol{S}_n \cdot \boldsymbol{S}_{n+2\mu} + K_4 \sum_{n\mu} \boldsymbol{S}_n \cdot \boldsymbol{S}_{n+3\mu}\Bigg], \tag{14}$$

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

$$g = \beta^{-1} = (K_1 + 2K_2 + 4K_3 + 9K_4)^{-1} \tag{15}$$

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

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

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

where we find it convenient to write the power behavior in β 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 $\lambda_4=(1+2\pi\beta)^{1/2}\exp(-\pi\beta)$. We used a heat bath algorithm on a lattice of size from 20×20 to 50×50 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 ($K_1\neq0$, $K_i=0$ for $i>1$) are taken from ref [13] It is clear that in our model (RGIM) scaling starts at a much smaller value of $\xi\simeq1.1$–1.2, compared to standard model where scaling seems to start at $\xi\simeq3$. 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

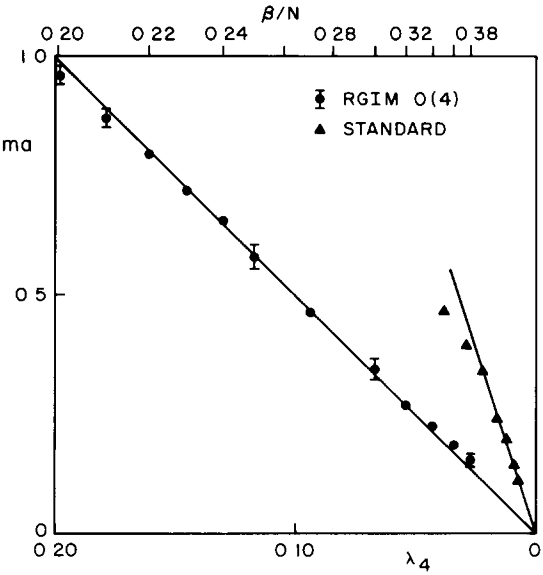

Fig 2 Mass-gap (in units of $1/a$) for O(4) models versus $\lambda_4=\sqrt{1+2\pi\beta}\, e^{-\pi\beta}$

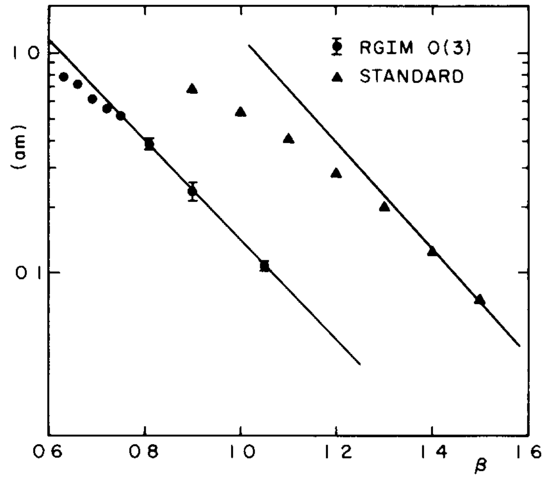

Fig 3 Mass-gap (in units of $1/a$) for O(3) models Data for standard model taken from ref [13]

relations [19] would be more canonical tests of improvement These computations are, however, time consuming, and have not been carried out in this exploratory work.

Encouraged by the O(4) result, we looked at O(3) model where we used lattices of size ranging from 20×20 to 70×70 The mass-gap is shown in fig 3 Scaling starts at $\xi \simeq 1.8$–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 $\xi \simeq 4$ for TI, $\xi \simeq 1.5$–2.0 for 1LSA, and $\xi \simeq 3$ for ST It is gratifying to see that our model based on the RT for O(∞) compares quite favorably to these other models even for $N=3$

We also evaluated magnetic susceptibility scaling defect $\delta_\chi = \chi(1+2\pi\beta)^{(N+1)/(N-2)}\exp(-4\pi\beta/(N-2))$ 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 Λ-parameters (up to one-loop), and the result is

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

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

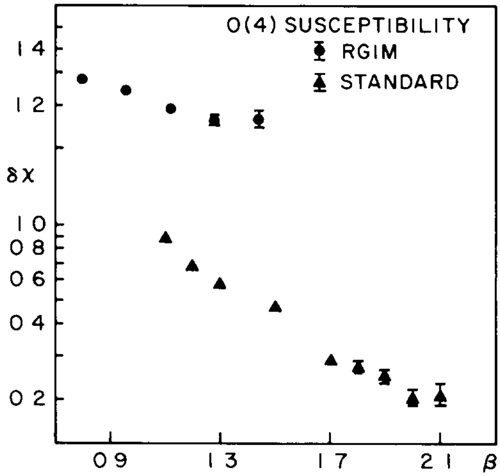

Fig 4 Magnetic susceptibility scaling defect for O(4) model Data for standard model taken from ref [13]

(ii) scaling curve for the standard model might have a slight preculiarity as suggested in ref [16] leading to some change in the value of the ratio of Λ-parameters

One of us (J B Z) was visiting Stony Brook when this work was started He wants to thank Prof Yang for his hospitality at the ITP

The numerical work was done on a VAX 11/780 at the State University of New York at Stony Brook We thank the Nuclear Theory Group for making the necessary time available After this work was completed, we received two preprints [17, 18] on related subjects In [17], a different blocking procedure is investigated for the

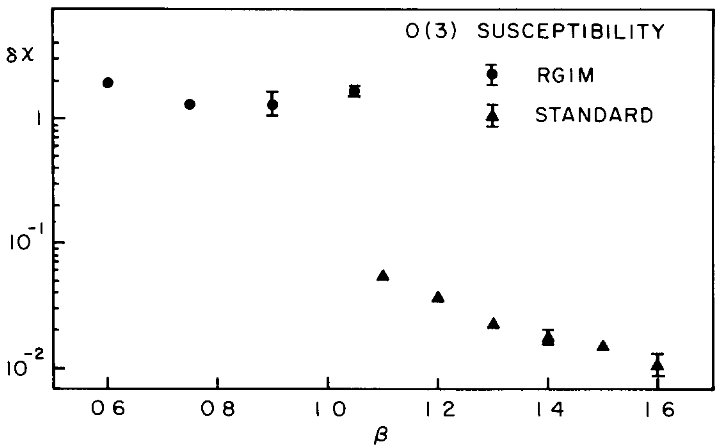

Fig 5 Magnetic susceptibility scaling defect for O(3) model Data for standard model taken from ref [15]

$O(\infty)$ 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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