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CRPC-TR90078
December, 1990

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C^3P-943
COLO-HEP-231
CRPC-TR90078

Investigation of the 2d O(3) model using the overrelaxation algorithm.

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ABSTRACT

We investigate the 2d O(3) model with the standard action by Monte Carlo simulation at couplings β up to 2.05 . We measure the energy density, mass gap and susceptibility of the model, and gather high statistics on lattices of size $L \leq 1024$ using the FPS T-series vector hypercube. Asymptotic scaling does not appear to set in for this action, even at $\beta = 2.05$, where the correlation length is 304. We observe a 20% difference between our estimate $m/\Lambda_{\overline{MS}} = 3.52(6)$ at this β and the recent exact analytical result. We use the overrelaxation algorithm interleaved with Metropolis updates and show that decorrelation time scales with the correlation length and the number of overrelaxation steps per sweep. We determine its effective dynamical critical exponent to be $z' = 1.079(10)$; thus critical slowing down is reduced significantly for this local algorithm that is vectorizable and parallelizable.

PACS Numbers: 05.70.Fh, 64.60.Fr, 75.10.Hk, 75.40.Cx

12/12/90

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1. Introduction

Monte Carlo studies of the two-dimensional O(3) spin model, which is the discretized $1+1$-dimensional O(3) non-linear sigma model, have been pursued extensively for about ten years. An important reason for this is that in $1+1$ dimensions O(N) models with $N \geq 3$ are asymptotically free [1] [2] , just as gauge theories like QCD are in $3+1$ dimensions. Thus by investigating the simpler O(3) model one hopes to understand critical behavior similar to that of QCD. Moreover, the O(3) model also possesses instanton solutions – another feature in common with QCD.

A consequence of asymptotic freedom is that, at weak enough coupling, all physical quantities will scale according to the two-loop β function; this is called asymptotic scaling. It is the main goal of the Monte Carlo simulations of the O(3) model to seek to test and hopefully demonstrate asymptotic scaling. This however has proven to be an elusive goal. Early studies of the standard, nearest neighbor, action (SA) [3] [4] [5] [6] [7] [8] using standard Monte Carlo techniques on small lattices ($L \leq 100$), and Monte Carlo Renormalization Group (MCRG) methods, failed to demonstrate asymptotic scaling. Using a tree-level improved action (TIA), which includes next-nearest neighbor interactions, and a 1-loop improved action Ref. [8] observed behavior closer to the asymptotic behavior, but did not provide conclusive evidence.

Analysis of high temperature expansions [9] [10] have also addressed the problem. Ref. [9] explains the lack of asymptotic scaling for the susceptibility in terms of a pair of complex singularities in $\chi(\beta)$ near the real axis. Knowledge of this behavior is used by [10] to design a better fitting procedure. They used the 14 term high temperature series of [11] to obtain an expansion for the susceptibility. The result is a good fit to Monte Carlo data of [5] for $\beta \leq 1.7$, providing a better fit to the deviation from asymptotic scaling.

Recently, using his cluster algorithm, Wolff [12] has investigated the O(3) model up to $\beta = 1.9$, where the large correlation length is 121. He finds that, even at this large β, asymptotic scaling does not hold for the SA. Finally, Hasenfratz and Niedermayer [13] using different MCRG methods in the region $1.9 \leq \beta \leq 2.26$ see agreement in the discrete β function $\Delta\beta$ with the 2-loop results at $\beta = 2.26$. They also show that asymptotic scaling holds for the TIA starting at a correlation length of ≈ 40 with $m/\Lambda_{\overline{MS}} = 3.4(1)$, and the value for $m/\Lambda_{\overline{MS}}$ agrees with that for the SA : $m/\Lambda_{\overline{MS}} = 3.3(1)$ (at $\beta = 2.26$).

In a very exciting development a new analytical calculation [14] has determined the exact value of $m/\Lambda_{\overline{MS}} = 8/e \simeq 2.943$ for the O(3) non-linear σ-model. Thus there exists a significant gap between this prediction and the Monte Carlo results. In another comparison, of the direct Monte Carlo results of [12] with the exact result, Ref. [15] shows that using a redefined inverse temperature β_E, behavior much closer to asymptotic scaling is seen.

Another non-perturbative method that has been extensively developed recently is the

1/N expansion [16] . The three leading orders of the expansion have been obtained and evaluated for small lattices [17] . The comparison to the above Monte Carlo results shows differences that are not more than those expected from the estimated size of neglected terms. These results have been extended to infinite lattices by finite size scaling [18] giving behavior that tends slowly towards the exact value for $\xi > 170$ from about 10% away.

Our calculation was done using what was the best available alternative to the cluster algorithms – the over-relaxed algorithm, which we had previously used to investigate the XY model [19] . Combined with a fast parallel vector computer, the FPS T-series hypercube, this algorithm allowed us to simulate lattices up to 1024^2 at β up to 2.05, corresponding to a correlation length of about 300. We attained performance of 1.5 MFlops per node on the 128 node machine. This algorithm is optimal for this machine because it vectorizes and parallelizes trivially and obtains very high efficiency. Although cluster algorithms are intrinsically faster algorithms, they require significant effort to achieve adequate efficiency on parallel machines [20] and do not vectorize well.

Our results are in good agreement with Refs. [12] and [13]. In fact they provide one of only two known computationally feasible methods by which the cluster algorithm results can be confirmed (in this region of large correlation lengths). The other method is multigrid Monte Carlo, which has used for $\beta \leq 1.7$ [21] . We see that there is no dramatic change in the behavior of the mass gap and susceptibility in the range $1.9 < \beta \leq 2.05$. We also see that the behavior in the rescaled temperature β_E remains closer to the exact value, but the agreement does not get better with increasing correlation length. Finally we show that overrelaxation can be used in a manner in which the effective dynamical critical exponent is close to 1.

2. The Model

The classical Heisenberg model in two dimensions is described by the Hamiltonian and partition function

$$H = -\sum_{<i,j>} \vec{s_i} \cdot \vec{s_j} \tag{1}$$

$$Z = \int \prod_i d\mu(\vec{s_i}) e^{-\beta H} \tag{2}$$

where $\vec{s_i}$ are unit 3-d vectors and $<\ ,\ >$ denotes the inclusion of nearest neighbor sites only in the sum. $d\mu()$ denotes the measure on the sphere and $\beta = 1/T$ where T is a dimensionless temperature.

Its continuum limit is the O(3) non-linear sigma model in one space and one (imaginary) time dimension. Of interest is the behavior of this model in the low temperature, weak coupling limit. This was shown [1] to be a continuation of the high temperature

phase of exponential correlation functions. The model is asymptotically free, and a renormalization group calculation has given the beta function of the theory to two loops [2]:

$$\beta(T) = -\frac{dT}{d(lna)} = -\frac{1}{2\pi}T^2 - \frac{1}{(2\pi)^2}T^3 + O(T^4) \tag{3}$$

where a is the lattice spacing. These terms are universal - i.e. the same for any regularization. Using this and the anomalous dimension we obtain the mass gap m and susceptibility χ of the theory:

$$m = C(2\pi\beta)\exp(-2\pi\beta)\ \{1 + a_1/\beta + O(1/\beta^2)\} \tag{4}$$

$$\chi = C'\beta^{-4}\exp(4\pi\beta)\ \left\{1 + b_1/\beta + O(1/\beta^2)\right\} \tag{5}$$

where C and C' are constants that cannot be calculated in perturbation theory.

The terms with coefficients a_1 and b_1 are the first non-universal terms and arise for three loop diagrams. Falcioni and Treves [22] calculated these by computing of the third loop contribution to the beta and gamma functions for the standard action. Their values are $a_1 = 0.575/2\pi$ and $b_1 = 0.0$; these have been confirmed by independent calculation [23]

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3. The Simulation.

To produce the sample configurations of our Monte Carlo simulation we use a hybrid of microcanonical overrelaxation [24] , and the Metropolis algorithm. For an O(N) spin-model, the rule used to obtain a new spin by microcanonical overrelaxation (μOR) is to reflect the old spin $\vec{s}_{old}$ through the direction of the sum $\vec{\Sigma}$ of its neighboring spins. If $\hat{\Sigma} = |\vec{\Sigma}|^{-1}\vec{\Sigma}$, then

$$\vec{s}_{new} = 2(\hat{\Sigma}\cdot\vec{s}_{old})\hat{\Sigma} - \vec{s}_{old} \tag{6}$$

This provides the largest possible step while preserving the energy. To provide ergodicity OR updates are interleaved with Metropolis updates. In a simulation of the XY model [19] this combination drastically improved critical slowing down, giving $z = 1.48$ and 1.2 for number of overrelaxation steps $N_{or} = 8$ and 15 respectively. The number of Metropolis steps was kept constant at $N_{met} = 2$.

In each Metropolis step we construct a new trial spin by adding to the old spin a random vector of fixed length α. The resulting vector is normalized and then accepted or rejected using the usual Metropolis criterion [25] . α is an adjustable parameter, chosen so as to give acceptances between 50 and 55 per cent. The random vectors are constructed to sample a uniform distribution on an S^2 sphere.

A 'sweep' is made up of a number of overrelaxation sweeps (N_{or}) , and a number of Metropolis sweeps (N_{met}). Measurements are made every 'sweep'. The errors in all quantities except the correlation length have been computed by binning the data in groups

of 500 for 256^2 lattices, 200 for 512^2, and 100 for larger. We also calculate the 'sweep' to 'sweep' correlation by measuring the autocorrelation time of the magnetization $\tau_{\vec{M}} \equiv \tau$. Table 1 summarizes our results.

4. Results

A comparison with [12] of the energy per site $E = < \vec{s_i} \cdot (\vec{s}_{i+\hat{x}} + \vec{s}_{i+\hat{y}}) >$, susceptibility χ and correlation length ξ shows good agreement on nearly all the values. There are two estimates which disagree to any significant degree, χ at $\beta = 1.6$ by 2.6σ and the energy at $\beta = 1.7$ by 2.8σ. Our value for the latter is in good agreement with a the result of a simulation using MultiGrid Monte Carlo [21]. Our results are consistent between a number of independent runs in each case, 3 and 2 respectively . The agreement to the high accuracy of these results, e.g. $\frac{\delta\chi}{\chi}$ about 0.3% for most points, provides confirmation that all these new methods work.

4.1. Mass-gap

To obtain the correlation length ξ or mass-gap $m = 1/\xi$ we fit the zero-momentum correlation function (CF) [6] to $A \cdot (e^{-mx} + e^{-m(L-x)})$. A fit is done in the interval ξ to 3ξ, where ξ is determined self-consistently. To estimate the statistical error of ξ we split the data into 10 parts and averaged the values obtained from the individual fits. For $\beta \geq 1.9$ we have used the jacknife method to obtain estimates of the statistical error, because the increasing autocorrelation times make the statistics gathered less significant. The two error estimates agree for $\beta = 1.9$. (In Table 1 we quote these values.)

To check the stability and significance of these fits, further fits were also done in the intervals $\frac{1}{2}\xi$ to $\frac{3}{2}\xi$, ξ to 2ξ, $\frac{3}{2}\xi$ to $\frac{5}{2}\xi$, up to as large a distance as a fit as can be obtained. In all cases we saw that the values obtained for all subintervals were consistent. We note that the statistical errors increase in this progression. This was expected since the relative error of the correlation function increases with distance - because the variance of the measurements of the CF is roughly constant, while the CF itself falls exponentially. Also for $\beta < 1.9$ the value of the effective mass $\log(C(n)/C(n+1))$ was plotted and in all cases showed a plateau at least between 10 and 3ξ. This allows us to extract a mass-gap with confidence that finite size effects are not significant for $\beta \leq 1.9$.

For our largest values of β the finite lattice size will affect our measurements. To obtain an estimate of the effect on the mass-gap we used the results of [26] , which were tested and used extensively in conjunction with Monte Carlo results in [27] . For all runs with $\beta \leq 1.95$ except that at $\beta = 1.90$ with $L = 512$ and $T = 1024$, the ratio of the lattice length and the correlation length, $z = \frac{L}{\xi}$, is larger than 6 . Thus the correction to the correlation length is very small, i.e. $\theta(\zeta) < 2 \cdot 10^{-3}$ where $\theta(\zeta)$ is defined from

the ratio of masses measured on a lattice of finite length L to that on an infinite lattice: $m(L)/m(\infty) = 1+\theta(\zeta)$, where $\zeta = L \cdot m(\infty)$. Only for the cases $\beta \geq 2.0$ and the one singled out above is the correction appreciable. With $3.46 \leq z \leq 4.56$ we use the result quoted by [27] to obtain an estimate of the correction $\theta(z)$. This is a valid estimate only if the length in one direction is very much larger than the correlation length, but the numerical results of [27] lead us to believe that for all these cases they provide a good estimate of the correction. The correction is only appreciable for $\beta = 2.05$, where $\theta_0(z) = 2.9\%$; even for $\beta = 2.00$ it is only $\theta_0(z) = 0.77\%$. The corrected values are $\xi(\beta = 2.00) = 226.0 \pm 4.2$ and $\xi(\beta = 2.05) = 304.1 \pm 5.3$.

To compare the behavior of the correlation length with asymptotic scaling predictions we use the correlation length defect δ_ξ. This is obtained by dividing the correlation length by the 2-loop result, i.e. equation (4):

$$\delta_\xi = \beta \, e^{-2\pi\beta} \, \xi \tag{7}$$

Obviously asymptotic scaling is seen if δ_ξ goes to a constant as $\beta \to \infty$. Figure 1 shows that asymptotic scaling does not set in for $\beta < 2.00$, but it is not possible to draw a clear conclusion for $\beta \geq 2.00$. The trends of the last two points towards a constant behavior is only a $\frac{1}{4}\sigma$ effect, i.e. a $\frac{1}{4}\sigma$ fluctuation would change it. We note that the finite size correction affected our evaluation of δ_ξ, so we must expect it to be important in the case of the susceptibility.

In order to compare with the analytical result [14] we calculate the value of $m/\Lambda_{\overline{MS}}$. In our case it is given by $m/\Lambda_{\overline{MS}} = 1/(2\pi\delta_\xi)\ (\Lambda_L/\Lambda_{\overline{MS}})^{-1}$ where $\Lambda_L/\Lambda_{\overline{MS}} = 27.31$ is the ratio of the lattice and minimal subtraction scheme Λ parameters [28] . As figure 2 shows, using the 3-loop correction term moves our results towards the analytical result, but by a small amount compared to the distance from it. Thus at $\beta = 2.05$ our estimate $m/\Lambda_{\overline{MS}} = 3.52(6)$ is 20% higher than the analytical result.

We can also compare with the results of Ref. [13] which uses Monte Carlo Renormalization Group methods to obtain estimates of the discrete beta function. The values are consistent with asymptotic scaling for $\beta \geq 2.14$, giving $m/\Lambda_{\overline{MS}} = 3.35(9)$. To compare directly with our results we used their data and the 3 loop correction to obtain $m/\Lambda_{\overline{MS}}(\beta = 2.02) = 3.47(8)$. An interpolation of our results at the two neighboring points, yields $m/\Lambda_{\overline{MS}}(\beta = 2.02) = 3.55(5)$; we see that the two estimates differ by about one standard deviation. Our results are thus consistent with those of Ref. [13] , although they tend favor a slower fall of $m/\Lambda_{\overline{MS}}$ towards the exact result.

A comparison to the results of the third order 1/N expansion (see the figure in [18]) shows that for increasing β their estimate of $m/\Lambda_{\overline{MS}}$ and our measurements are tending closer.

Another approach to the problem of asymptotic scaling, proposed by [29] and tried recently in [15], uses a redefined inverse temperature derived from the energy. This is an

alternative bare coupling, and effectively performs an infinite order resummation; there are arguments that asymptotic scaling in β_E should be observed earlier [29]. β_E is defined from the $O(1/\beta)$ perturbation expansion of the energy . For our definition of the energy ($E_{ours} = 2E_{Wolff}$) it is $\beta_E = (2 - E)^{-1}$. As Figure 2 shows, our results agree with [15] that asymptotic scaling in β_E (i.e. the 2-loop curve) is better and much closer to the exact value predicted by Ref. [14]. However the effect of the 3rd loop correction (for which $a_1 = 0.575/(2\pi) + 1/8 - 499\pi/4000$) moves the result away from the analytical result and towards the results scaled by β. We note that the statistical error of our estimates of the energy are much smaller than those of [12], e.g. for $\beta > 1.6$ it is more than an order of magnitude smaller. This makes the contribution of the statistical error of β_E to the error of our estimates of $m/\Lambda_{\overline{MS}}(\beta_E)$ negligible, which is not the case for [15].

4.2. Susceptibility

We measured the susceptibility on lattices of different size for $\beta = 1.70$ to 1.80 and at 1.90. The agreement , within errors, seen for $1.70 \leq \beta \leq 1.80$ shows that the finite size effects are very small, so that, effectively, the infinite volume limit has been reached. The disagreement at $\beta = 1.90$ shows that there is a finite size effect for this point on the smaller lattice, but the data for the other βs lead us to believe that the larger lattice gives us an estimate with very small finite size error. We would expect that for $\beta \geq 2.0$ the finite size effect would be significant ; a rough estimate would be something of the same order as that for the mass gap, i.e. a fraction of a percentage point and a few percent for $\beta = 2.00$ and $\beta = 2.05$ respectively.

To compare with the expected behavior, from equation 5, we divide this behavior out and get a 'scaled susceptibility' or susceptibility defect δ_χ [5]:

$$\delta_\chi = 2 \cdot 10^5 \, \beta^4 \, e^{-4\pi\beta} \, \chi \tag{8}$$

This should behave as a power series in $T = \frac{1}{\beta}$, and approach a constant for $T \to 0$. From Figure 3 it is obvious that we have not reached the region of β where a constant can be extracted, and that the susceptibility for $\beta = 2.05$ at least suffers from finite size effects. We note that for the standard action the third loop term for the susceptibility is 0 to the accuracy calculated [22], and thus doesn't affect this result.

We also compare the behavior of the susceptibility with predictions based on the assumption of complex singularities in $\chi(\beta)$. Table 2 shows another susceptibility defect G_3 for our data and the values obtained by a sophisticated Pade approximant of the 14 term high temperature series. This shows that this approximant is unable to adequately describe the defect in this region of β, although it does a good job of coarsely describing the significant deviations from asymptotic scaling at smaller values of β.

4.3. *Dynamical Critical Exponent of Overrelaxation*

The decorrelation time τ is used to measure the speed with which new, i.e. statistically independent, configurations are generated. Its dependence on the correlation length is parametrized by the dynamical critical exponent z :

$$\tau = c \cdot \xi^z \tag{9}$$

Most local algorithms, like Metropolis and heat-bath, have $z \geq 2$. For a free field overrelaxation gives $z = 1$ [30] . Neuberger [31] argues that for an interacting field, z should not change substantially from this. Previous work with the same algorithm as we use for the O(2) or XY model [19] measured τ_{exp} (defined e.g. in [32]) and gave $z = 1.48$ for $N_{or} = 8$ and $z = 1.2$ for $N_{or} = 15$ where $N_{met} = 2$. For the $O(4)$ model [33] used another variation of overrelaxation and showed that in 1 dimension $z = 1$, but could not determine it for 2 dimensions.

We obtain the decorrelation time by measuring the auto-correlation function of the magnetization. We will use $c(n)$ to denote this, where n is a distance in number of MC sweeps. To obtain the integrated decorrelation time τ_{int} [34] we use the definition of [34] for its estimator $\widehat{\tau}_{int}$:

$$\tau_{int} = \sum_{n=-\infty}^{\infty} \frac{c(n)}{c(0)} \quad , \qquad \widehat{\tau}_{int} = \sum_{n=-M}^{M} \frac{c(n)}{c(0)} \tag{10}$$

with M a multiple of τ, in our case $M = 4\tau$, defined self-consistently. Using these measurements and fitting to the equation (9) for $N_{or} = 12$ gives $z = 1.33(1)$.

However we discovered that it is possible to improve on this substantially. We note that when ξ increases and more work is required to produce a decorrelated configuration, it is natural to increase N_{or}. This allows us to perform measurements only on configurations that are less correlated. What we observed was that the performance of the algorithm improves. To compare the speed of decorrelation between runs with different N_{or} we define a new quantity which we call 'effort' $e = N_{or} \times \tau$. It is roughly proportional to the computational effort expended to obtain a configuration 1 τ away.

We found that we can define a new exponent z' from $e \sim \xi^{z'}$ when N_{or} is tuned to keep τ constant. This choice was made because we observed that the effort has a plateau at almost the same value of τ for every ξ. We also found that the behavior of the decorrelation time can be approximated over a good range by

$$\tau = C'' \cdot \xi^z \cdot N_{or}^{-z/z'} \tag{11}$$

A fit to $\log \tau = c'' + z \log \xi - \frac{z}{z'} \log N_{or}$ gives $z' = 1.1(1)$, for τ in the ranges $1.1 \rightarrow 1.8$, $2.1 \rightarrow 2.4$ and $3.0 \rightarrow 3.6$. This indicates we have achieved a considerable improvement .

A fit to the set of points (N_{or}, ξ , $\tau > 1.0$) gives $z = 1.301 \pm 0.012$, $z' = 1.079 \pm 0.010$ and has a $\chi^2/dof = 1.86$ for 32 degrees of freedom. Of course, the values for z and z' we measure are only effective values because in the limited range of τ and ξ we worked in, logarithmic corrections can mask the true (limit) values. Figure 4 shows the decorrelation time τ vs. the number of overrelaxation sweeps for the different coupling constants. The solid lines show the fit to the above equation. We note that the points for $\tau < 1.0$ were not included in these fits because do not follow equation (11).

We also try to fit to a general scaling function by plotting τ/ξ^d vs. N_{or}/ξ^f [35] . A plot for $f = 1.0$ and $d = 0.0$ shows that this is close to the correct behavior. Using our knowledge from (11) we constrained the values of d and f to one free parameter with $d = 1.33 - fz/z'$. We saw that for $1.06 < f < 1.14$ the plots are good, but the best fit is for $f = 1.1$. Figure 5 shows the data in this case. Only the points for $\beta > 1.9$ do not lie on a universal curve; such a deviation is expected for those points with L/ξ that is small. Another way of seeing this is shown in figure 6. This shows a scaled effort e/ξ^{f+d} (instead of a scaled τ) versus N_{or}/ξ^f for all values of β. The tightness of the points in these plots around a single curve demonstrates conclusively that, for τ roughly constant, the effort $e \propto \xi^{1.1}$.

We can attempt to understand the lower value of z' in the following way: the overrelaxation algorithm has a tendency to decorrelate much faster than other local algorithms, i.e. with an exponent close to the free field value of 1 . The addition of the Metropolis steps destructively interferes with it . The μOR algorithm moves on a deterministic path through phase space. But when ξ is increased the distance in phase space that a set number of overrelaxation steps travels decreases. Thus the addition of Metropolis steps can cause a larger disruption.

This explanation indicates that the effort should flatten out for increasing N_{or}. Our data clearly shows that after a broad plateau the effort slowly increases. This can be seen in figure 6, which is a log-log plot. (This effect is also the one that causes the deviation of points with $\tau < 1.0$ from our fit to equation 11 .) We can understand the minimum in e vs. N_{or} if we assume that a certain set of (N_{or}, N_{met}) corresponds to overrelaxation with a parameter $\omega \neq 2$, a non-microcanonical variation [33] . It is obvious that as $\frac{N_{met}}{N_{or}} \rightarrow 0$ that $\omega \rightarrow 2$. What is seen in the case of O(4) in 1 dimension is that the function $\tau(\omega)$ has a minimum close to $\omega = 2$.

5. Conclusions and discussion

Our results confirm those obtained using the Wolff cluster algorithm and extend them to larger lattices and correlation lengths. However asymptotic scaling is not reached with the standard action even at $\beta = 2.05$ and $\xi = 300$ and our results give a value of $m/\Lambda_{\overline{MS}}$ that is 20% higher than the exact result. We also showed that overrelaxation can be

used in a manner in which the effective decorrelation exponent is close to 1, confirming the prediction of [31]. By comparison, cluster algorithms do require fewer arithmetic operations at large correlation lengths because they have a smaller dynamical critical exponent; however not all problems are suitable to their use, and vector and parallel computers, which are necessary for large problems, are currently not used very efficiently by cluster methods. Overrelaxation remains a simple, vectorizable and efficient algorithm well suited to vector and parallel machines and competitive for many problems.

Since the perturbative 3-loop terms are small, it is likely that higher order terms are small (the next term is of the order of 2%) and cannot provide an explanation for the behavior of the mass-gap or susceptibility in the region $1.5 \leq \beta \leq 2.05$. It seems that deviations from the perturbative β-function are caused by non-perturbative effects, which contribute significantly to the β function in this region. It is not clear what the effects result from, if not the singularities in the complex β plane [9], which are hard to quantify. One can speculate that another possibility is that they are connected to instantons, which are a property of this model unique amongst O(N) models. A first calculation of the effect of instantons [36] , however, does not provide an answer. The correction to the beta function calculated has the wrong sign to explain the deviations from asymptotic scaling observed by us. It would thus be very interesting to use the new efficient algorithms in a large scale investigation of the effects of instantons in the O(3) model.

Acknowledgements

This project would not have been possible without the hardware and software support from FPS and C-Division at Los Alamos. We are especially grateful to Jerry DeLapp for his continuous help with the T-series. We would also like to thank Rajan Gupta for directing our attention to this problem and help during the initial stages of this work. JA thanks H.Q. Ding for helpful discussions. This work was partially supported by DOE Grants DE-FG03-85ER25009 and DE-AC03-81ER40050 and the NSF through the Center for Research on Parallel Computation under Cooperative Agreement No.CR-8809615 .

References

[1] A.M. Polyakov, *Phys. Lett.* **59B** (1975) 79.
[2] E. Brezin and J. Zinn-Justin, *Phys. Rev.* **B14** (1976) 3110.
[3] S. H. Shenker and J. Tobochnik, *Phys. Rev.* **B22** (1980) 4462.
[4] G. Martinelli, G. Parisi and R. Petronzio, *Phys. Lett.* **100B** (1981) 485.
[5] B.Berg and M.Luscher, *Nucl. Phys.* **B190** [FS3] (1981) 412 .
[6] G. Fox, R. Gupta, O. Martin and S. Otto, *Nucl. Phys.* **B205** (1982) 188.
[7] A. Hasenfratz and A. Margaritis, *Phys. Lett.* **133B** (1983) 211; *ibid* **148B** (1984) 129.

[8] B. Berg, S. Meyer and I. Montvay, *Nucl. Phys.* **B235** [FS11] (1984) 149.
[9] P. Butera, M.Comi and G.Marchesini, *Nucl. Phys.* **B300**(1988) 1 .
[10] B.Bonnier and M.Hontebeyrie, *Phys. Lett.* **226B** (1989) 361 .
[11] M.Luscher and P.Weiss, *Nucl. Phys.* **B300** (1988) 325 .
[12] U. Wolff, *Phys. Lett.* **222B** (1989) 473 and *Nucl. Phys.* **B334** (1990) 581 .
[13] P. Hasenfratz and F. Niedermayer, *Nucl. Phys.* **B337** (1990) 233.
[14] P. Hasenfratz, M. Maggiore and F. Niedermayer, *Phys. Lett.* **245B** (1990) 522 ; P. Hasenfratz and F. Niedermayer, *Phys. Lett.* **245B** (1990) 529 .
[15] U.Wolff, DESY Report DESY-90-070 .
[16] J-M Drouffe and H. Flyvbjerg, *Phys. Lett.* **206B** (1988) 285 and *Nucl. Phys.* **B332** (1990) 687 ; H. Flyvbjerg, *Phys. Lett.* **219B** (1989) 323 .
[17] H. Flyvbjerg, Proc. of the Int. Conf. 'Lattice 89', Nucl. Phys. B (Proc. Suppl.) **17** (1990) 343 and *Nucl. Phys.* **B344** (1990) 646.
[18] H. Flyvbjerg, Proc. of the Int. Conf. 'Lattice 90', Tallahasee 8-12 October 1990, *Nucl. Phys. B (Proc. Suppl.)*, to appear .
[19] R. Gupta, J. DeLapp, G. G. Batrouni, G. C. Fox, C. F. Baillie and J. Apostolakis, *Phys. Rev. Lett.* **61** (1988) 1996.
[20] C.F. Baillie and P.D. Coddington, "Cluster Identification Algorithms for Spin Models — Sequential and Parallel", Caltech preprint C^3P-855 (June 1990) .
[21] S.Meyer, private communication.
[22] M.Falcioni and A.Treves, *Phys. Lett.* **159B** (1985) 140 ; *Nucl. Phys.* **B265** (1986) 671.
[23] M.Luscher and P.Weiss, unpublished.
[24] S.L.Adler, *Phys. Rev.* **D23** (1981) 2901 ; M.Creutz, *Phys. Rev.* **D36** (1987) 515 ; F.R.Brown and T.W.Woch, *Phys. Rev. Lett.* **58** (1987) 2394 .
[25] N. Metropolis *et al.*, *J. Chem. Phys.* **21** (1953) 1087.
[26] M. Luscher, Cargese lectures 1983.
[27] I.Bender, W.Wetzel and B.Berg, *Nucl. Phys.* **B269** (1986) 389 .
[28] G. Parisi, *Phys. Lett.* **92B**(1980) 133.
[29] S.Samuel, O.Martin and K.Moriarty, *Phys. Lett.* **153B** (1985) 87 .
[30] S.L.Adler, *Phys. Rev.* **D37**, (1988) 458 ; H.Neuberger, *Phys. Rev. Lett.* **59**, (1987) 1877 .
[31] H.Neuberger, *Phys. Lett.* **B207**, (1988) 461 .
[32] A.D.Sokal, Proc. of the Int. Conf. 'Lattice 90', *Nucl. Phys. B (Proc. Suppl.)*, to appear.
[33] U.Heller and H.Neuberger, *Phys. Rev.* **D39**, (1989) 616.
[34] N.Madras and A.D.Sokal, *J. of Stat. Phys.* **50**, (1988) 179.
[35] This was pointed out to us by A.D. Sokal.
[36] M. Evans, *Nucl. Phys.* **B208** (1982) 122 .

Table Captions

1. Data from Monte Carlo runs: β, lattice length in each direction , total number of OR sweeps in thousands, number of OR steps per full sweep, average effort (i.e. decorrelation time in terms of OR sweeps) , energy per lattice site, susceptibility and correlation length.
2. Comparison of results for another susceptibility scaling defect $G_3 \propto \delta_\chi^{1/4}$. Our Monte Carlo estimates are labeled MC, the Pade Approximant of [9] is Pade and the numbers of [5] are BL.

Figure Captions

1. Correlation length defect δ_ξ , i.e. correlation length scaled by the 2-loop form. The solid squares are corrected for the expected finite size effect. Note that the errors on these are the same as those for the uncorrected points.
2. The estimates of the ratio $m/\Lambda_{\overline{MS}}$ to 2- and 3-loops in terms of β and $\beta_E = 1/(2-E)$ vs. the inverse temperature β.
3. Susceptibility defect δ_χ , i.e. susceptibility scaled by the 2-loop form. Note that the 3-loop correction is zero.
4. Decorrelation time τ vs. number of overrelaxation steps N_{or} for different values of β. Solid lines are the fit to equation (11), i.e. $\tau \propto \xi^z N_{or}^{-z/z'}$.
5. Plot for test of scaling of decorrelation time τ, number of overrelaxation steps N_{or} and correlation length ξ according to $\tau/\xi^d = f(N_{or}/\xi^f)$ including data from all the different couplings β. This plot is for the values $f = 1.1$ and $d = -0.017$.
6. Plot similar to fig. 5 for test of scaling of the effort e by e/ξ^{d+f} vs. N_{or}/ξ^f , with $f = 1.1$ and $d = -0.017$. The error in N_{or}/ξ^f is smaller than the width of the points. The labels are the same as in figure 5.

Table 1.

Beta	L,T	#or(K)	Eff.	N_{or}	Energy	χ	ξ
1.50	256	12600	18	8,12	1.20324(7)	176.4 ± 0.2	11.05(1)
1.60	256	12400	38	12,15	1.27141(7)	448.4 ± 0.7	19.00(2)
1.70	256	9100	85	12	1.32843(7)	1263.4 ± 2.9	34.39(6)
1.70	512	11400	85	20,30,35	1.32848(4)	1263.7 ± 3.3	34.44(6)
1.75	512	7700	66	40,60,120	1.35329(5)	2208.1 ± 6.8	47.4(2)
1.75	768	8000	98	50	1.35322(6)	2197 ± 15	47.2(2)
1.80	512	10100	143	40,45	1.37599(4)	3845 ± 11	64.7(3)
1.80	768	3100	141	40	1.37587(6)	3823 ± 21	64.5(5)
1.85	768	11200	185	60,80	1.39667(3)	6732 ± 25	88.7(5)
1.90	1024,512	6000	184		1.41583(4)	11602 ± 59	121.5(1.1)
1.90	1024	5900	263	100,120	1.41582(2)	11867 ± 62	122.7(1.1)
1.95	1024	700	330	200	1.43363(10)	20640 ± 310	164.8(5.3)
2.00	1024	2700	420	250,300	1.45022(6)	35100 ± 400	224.3(4.2)
2.05	1024	1800	510	300	1.46578(7)	56220 ± 550	295.6(5.2)

Table 2.

β	G_3 MC	σ	Pade	BL
1.50	1028.5	0.3	1015	1048
1.60	1011.8	0.4	983	962
1.70	1017.4	0.7	964	927
1.75	1027.8	1.8		
1.80	1039.2	0.8		
1.85	1050.0	1.0		
1.90	1055.0	1.7		
1.95	1069.6	4.0		
2.00	1070.7	3.1		
2.05	1055.0	2.6		
∞			944	

Figure 1

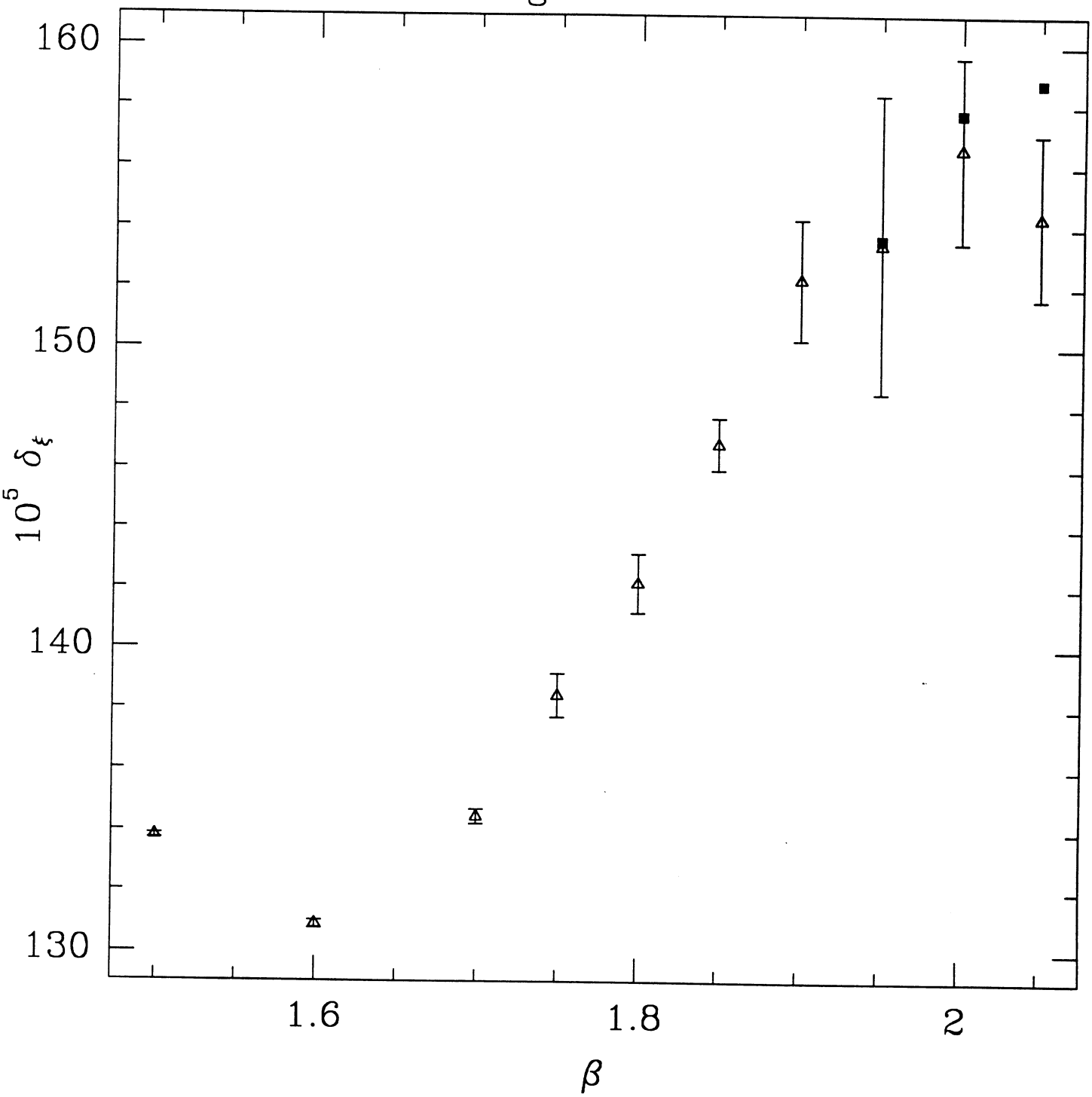

Figure 2

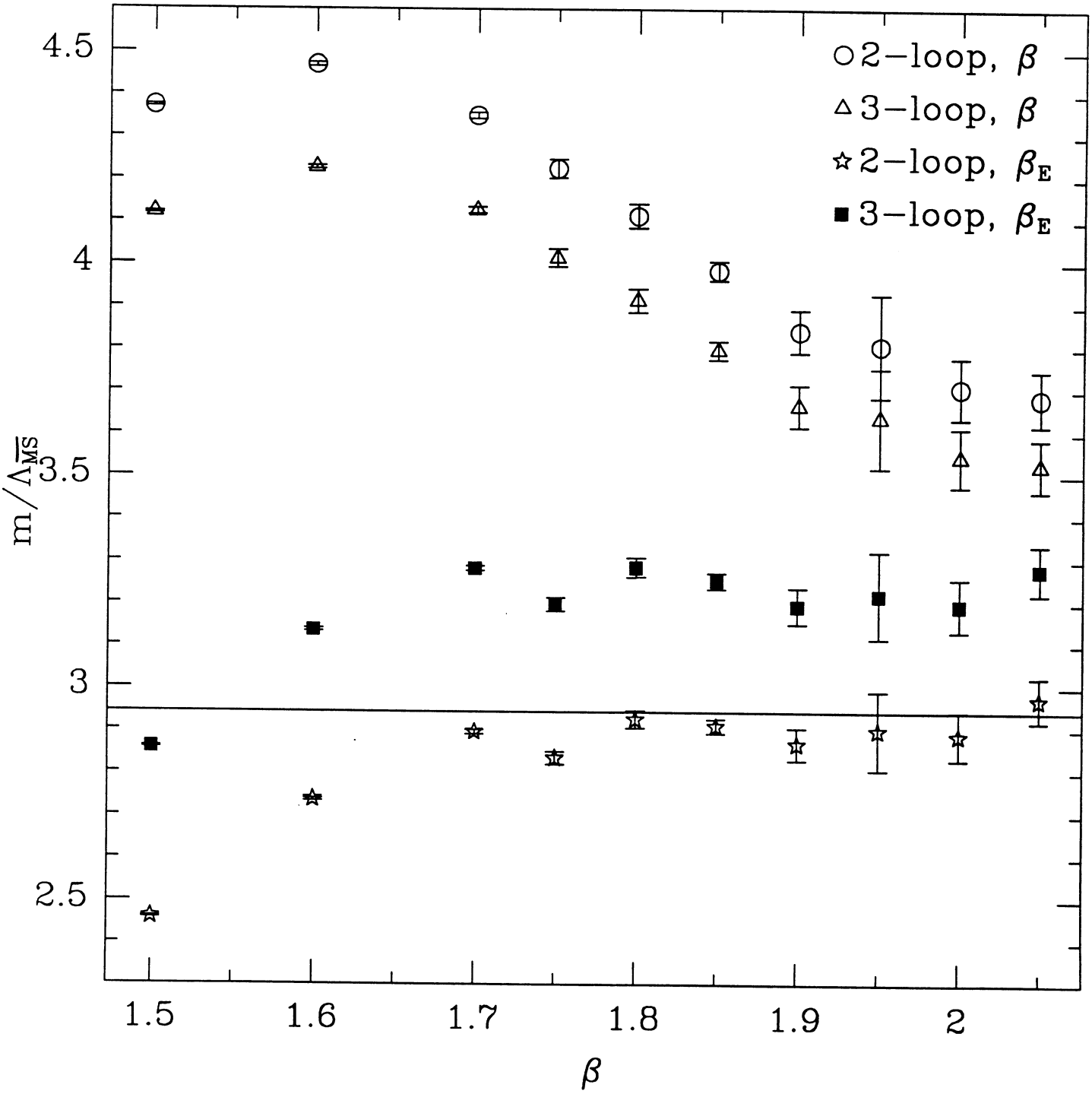
4.5
4
3.5
3
2.5
$m/\Lambda_{\overline{MS}}$
1.5
1.6
1.7
1.8
1.9
2
β
○ 2−loop, β
△ 3−loop, β
☆ 2−loop, β_E
■ 3−loop, β_E

Figure 3

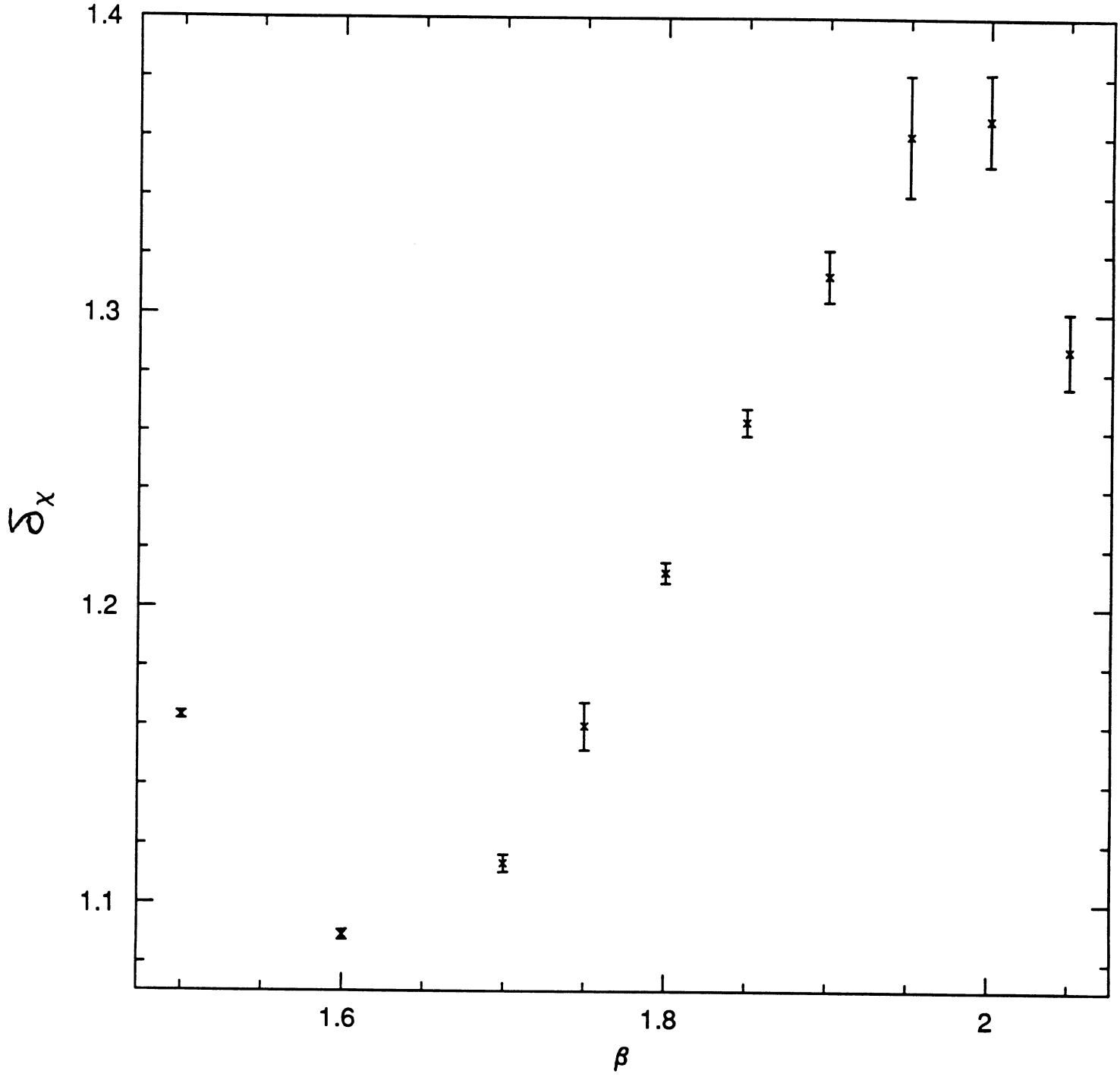

Figure 4

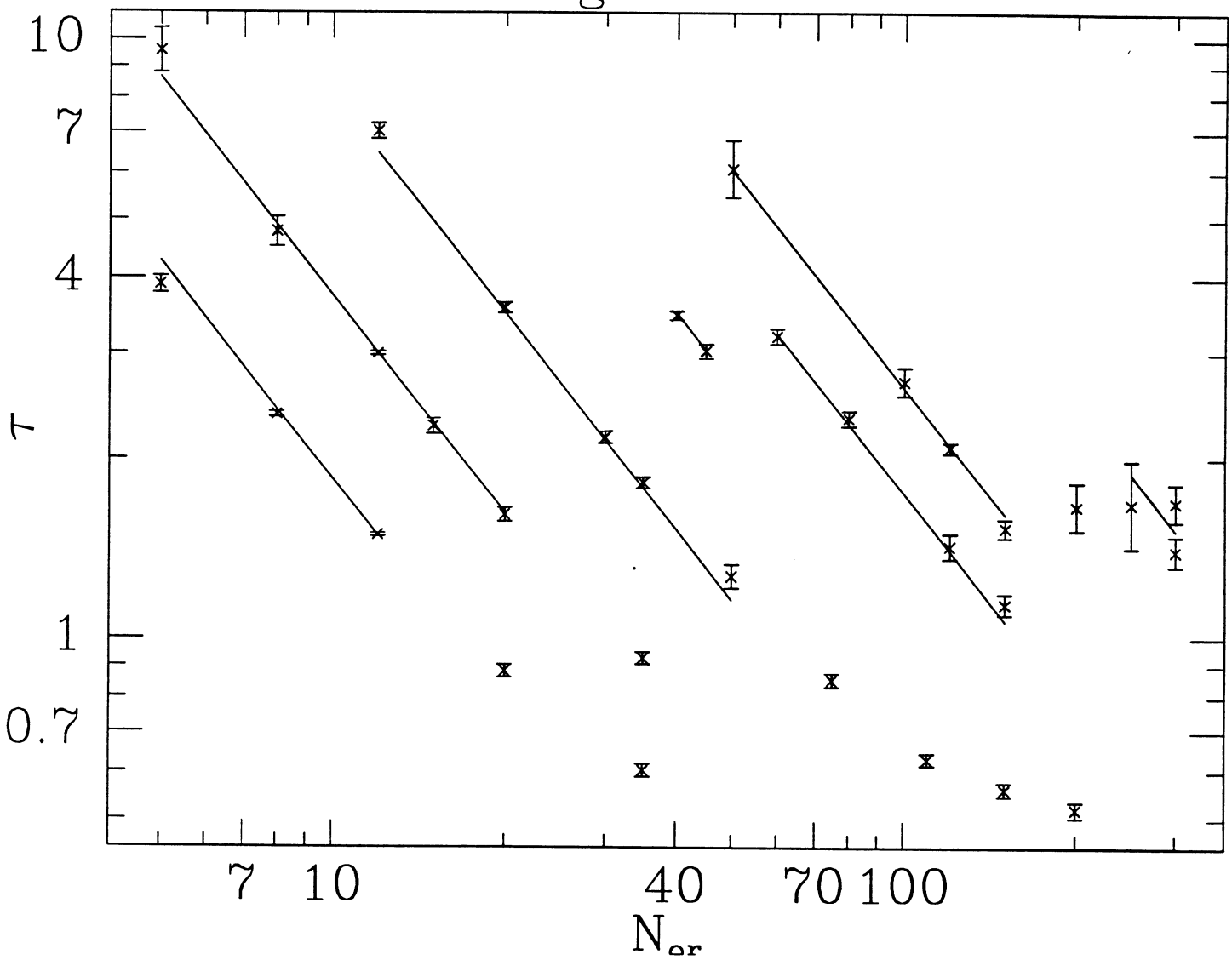

Figure 5

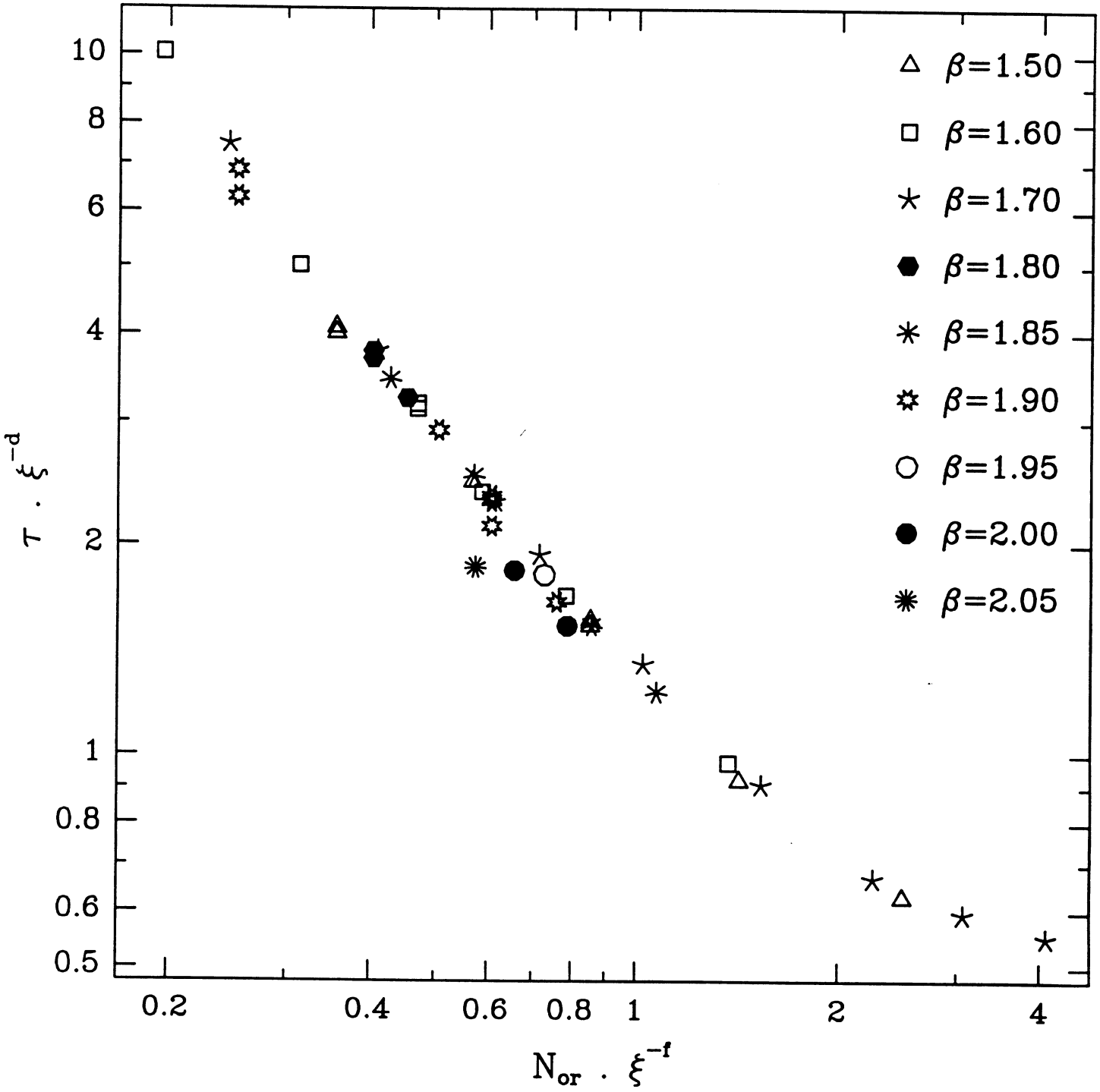
10
8
6
4
2
1
0.8
0.6
0.5
0.2
0.4
0.6
0.8
1
2
4
$\tau \cdot \xi_p^{-d}$
$N_{or} \cdot \xi^{-f}$
β=1.50
β=1.60
β=1.70
β=1.80
β=1.85
β=1.90
β=1.95
β=2.00
β=2.05

Figure 6