Cutoff effects in the O(N) sigma model at large N.

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The computation of the step scaling function for the finite size mass-gap in the O(N) sigma model at large $N$ is reviewed. Practically exact nonperturbative results become available for both finite and vanishing lattice spacing. We use them as a testbed to investigate standard procedures of continuum extrapolation in lattice field theory.

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1. Introduction

Numerical simulations in lattice field theory are only possible when both the lattice spacing and the volume are finite. If the thermodynamic limit is to be taken in theories with a mass gap, it is approached exponentially fast and usually the extrapolation causes no essential problems. Often, one is even interested in the universal continuum limit at a finite volume. It remains as the main problem to extrapolate the lattice spacing $a$ to zero. Normally the use of some analytic formula for (at least) the asymptotic dependence of physical results on $a \to 0$ is unavoidable\(^1\). Often this is based on the general framework given by Symanzik [2], which for a universal dimensionless quantity $P$ in many theories, including the $\sigma$-model, amounts to setting

$$P(a) \sim P(0) + \frac{a^2}{L^2} [c_0 + c_1 \ln(a/L) + c_2 \ln^2(a/L) + \ldots] + O(a^4), \quad (1.1)$$

where the coefficients $c_i$ have a finite continuum limit. In particular, in perturbation theory they contain only renormalized couplings, the bare one is eliminated before organizing the series in powers of $\ln$. For $L$ we may take any finite renormalized length scale, an inverse mass for example. In finite volume calculations it is convenient to use the system extension. The derivation is based either on effective field theory ideas or on perturbation theory. There the power of the logarithm grows with the loop order. In applications in connection with Monte Carlo simulations one normally assumes that the function in the square bracket varies slowly over the range of accessible lattice spacings and it is often replaced by a constant. Then typically the form $A + B(a/L)^2$ is fitted to the data after discarding results for larger $a/L$ until the fit is acceptable in terms of $\chi^2$. Then the fit parameter $A$ inherits an error $\delta A$ from the data by error propagation, and in this way $P(0)$ is estimated\(^2\). Clearly this procedure inflicts some systematic error, which may not always be negligible in high precision simulations as they are hopefully becoming more and more common in QCD in the future. We hence here take the occasion to investigate this issue in a simplified model where we have access to exact but still nontrivial nonperturbative results both in the continuum and at finite lattice spacing.

In cluster simulations of the two-dimensional O(3) nonlinear $\sigma$-model [3, 1] over a rather large range of small $a$ a behavior was empirically found for some quantities, which seemed hard to describe as $a^2$ but rather looked like a linear dependence. In [4] we report additional simulations at $N = 4$ and $N = 8$ and a leading and subleading large $N$ calculation. The main conclusion is that the often neglected $\ln$ terms in (1.1) can and in fact do at large $N$ mimic a behavior of the kind found in the simulations. We extend this investigation here by performing various extrapolations with the large $N$ data and then assessing the systematic deviation from the known continuum limit. As a warning we shall demonstrate cases of significant discrepancy in combination with acceptable $\chi^2$ and a plausible extrapolation formula.

2. Step scaling function of the $\sigma$-model at large $N$

We start directly from the lattice formulation of the model where on a two-dimensional cubic

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\(^1\)See however [4] for an interesting attempt to avoid an explicit such step.

\(^2\)Sometimes more conservative criteria are invoked at this point to exclude additional coarse data or add systematic errors.
lattice of size $T \times L$ the unit length $N$-component spin field $s(x)$ with partition function

$$Z = \int \prod_x d^N s \delta(s^2 - 1) e^{-S(s)}$$

(2.1)

is governed by the euclidean action

$$S(s) = \frac{N}{2\gamma} \sum_{\mu} (\partial_\mu s)^2.$$  

(2.2)

Here $\partial_\mu$ is the forward difference operator and $\gamma$ the rescaled coupling (held fixed in the large $N$ limit).

As a physical observable that is finite in the asymptotically free (according to conventional wisdom) continuum limit we study the finite volume mass-gap $M(L)$ that can be extracted on a torus with $T \to \infty$ at finite $L$ from the decay of the fundamental spin correlation at zero spatial momentum. More precisely we study its scale dependence via the step scaling function (SSF) $\Sigma(u,N,a/L)$

$$\Sigma(u,N,a/L) = M(2L) 2L \quad \text{for} \quad M(L) L = u$$

(2.3)

under factor-two rescalings of $L$ with the continuum limit

$$\lim_{a/L \to 0} \Sigma(u,N,a/L) = \sigma(u,N).$$

(2.4)

The large $N$ evaluation of the path integral (2.3) is a standard saddle point calculation. More details on these steps can be found in [4]. At leading order gaussian fluctuations of $s(x)$ are controlled by the (euclidean) lattice Klein Gordon operator $-\Delta + m_0^2$ where the mass parameter $m_0$ is fixed dynamically in terms of $\gamma$ and $a/L$ by the gap equation for $T = \infty$

$$\frac{1}{\gamma} = \frac{1}{L} \sum_{p=\mathbb{Z}a} \frac{1}{2\omega(p)} \sqrt{1 + a^2 \omega^2(p)/4}, \quad \omega^2 = m_0^2 + \hat{p}^2, \quad \hat{p} = \frac{2}{a} \sin(ap/2).$$

(2.5)

The finite volume mass-gap is then closely related, $\sinh(aM/2) = am_0/2$.

If we expand the SSF as

$$\Sigma(u,N,a/L) = \Sigma_0(u,a/L) + \frac{1}{N} \Sigma_1(u,a/L) + O(1/N^2),$$

(2.6)

the leading term $\Sigma_0$ is obtained by twice using (2.5) – for some resolution $L/a$ and the doubled value – and by combining the two to eliminate $\gamma$. Evaluated numerically, this yields the exact SSF at finite cutoff. By an asymptotic expansion in powers of $a$ using results of [7] we obtain the continuum value $\sigma_0(u)$ and the form of the leading artefacts. The limit is determined by the transcendental equation

$$F(\sigma_0) = F(u) - \ln 2, \quad F(z) = \frac{\pi}{z} + \sum_{n=1}^{\infty} \left( \frac{1}{\sqrt{n^2 + (z/2\pi)^2}} - \frac{1}{n} \right).$$

(2.7)

This continuum equation can be expanded in powers of $u$ thus reproducing the large $N$ limit of the known orders of perturbation theory of the $\beta$-function for this renormalized coupling [5, 6, 8，253 / 3].
For large $u$ the mass-gap becomes insensitive to the volume and $\sigma_0(u)$ tends to the value $2u$ exponentially fast. The asymptotic lattice correction to $\sigma_0$ is rigorously known to be of the form (1.1) with only $c_0, c_1$ non-vanishing.

To obtain the $1/N$ correction $\Sigma_1$ we have computed the leading self-energy correction of the spin two-point function that shifts its pole by an order $1/N$ term. The diagrams could only be evaluated numerically including a numerical integration. We managed however to compute them to many digits and could extract the continuum limit shown in Fig. 1. The correction vanishes for both large and small $u$, since $\sigma$ is fixed uniformly in $N$ in these limits.

The investigation of the analytic behaviour of this correction is very hard. We know a representation of the continuum limit in terms of a numerical integral and a two-fold infinite sum which agrees with the lattice continuum extrapolation. However, it seems actually easier to perform the latter, as the sums also need an extrapolation. The small $u$ expansion of the continuum form could be shown to agree with the $1/N$ terms in the perturbative $\beta$-function up to three loop order. An extraction of the form of the asymptotic cutoff dependence has so far been beyond our capabilities. There is however strong numerical evidence [4] that it is of the same type as in the leading term, i.e. just $a^2$ and $a^2 \ln a$.

3. Sample continuum extrapolations of large $N$ data

We now use our ‘exact’ data for the nonperturbative values of $\Sigma_0, \Sigma_1$ to mimic their extrapolation based on lattices that could be simulated and with superimposed statistical noise. We test various more or less plausible fit functions. Our question is: when does this lead to significant biases beyond the error determined during the extrapolation?

We consider two sequences of lattices for our virtual simulations

$$\mathcal{L}_{\text{poor}} = \{8, 12, 16, 24\}, \quad \mathcal{L}_{\text{rich}} = \{10, 12, 16, 24, 32, 64, 96, 128\}. \quad (3.1)$$

For the lattices of either set we add artificial errors to $\Sigma_0$

$$S_i = \Sigma_0(u, L_i/a) + w \eta_i, \quad i = 1, \ldots, n, \quad (3.2)$$
where \( \{ \eta_i \} \) are gaussian random numbers of unit variance and \( w \) controls the size of the errors. We fit these numbers to a combination of \( n_f \) independent fit-functions

\[
S_i \approx F_i = F(L_i/a) = \sum_{\alpha=1}^{n_f} A_{\alpha} f_{\alpha}(L_i/a),
\]

where we always take \( f_1 = 1 \) such that \( A_1 \) is the extrapolation. It is now a simple matter of linear algebra to show that on average (over the \( \{ \eta_i \} \)) we find

\[
\chi^2_{\text{min}} \approx n - n_f = 1 + \frac{1}{w^2(n - n_f)} \sum_{ij} \Sigma_0(u, L_i/a) \bar{P}_{ij} \Sigma_0(u, L_j/a)
\]

with \( \bar{P} \) the projector to the \((n - n_f)\)-dimensional space orthogonal to the one spanned by the \( f_{\alpha}(L_i/a) \). We define that for a given set of functions a fit is accepted if \( \chi^2_{\text{min}}/(n - n_f) \leq 2 \) holds. Formula (3.4) allows now to determine a value \( w_0 \) such that this is true as long as \( w \geq w_0 \). By similar algebra we find the mean propagated extrapolation error

\[
\delta A_1 = w \sqrt{(M^{-1})_{11}}, \quad M_{\alpha\beta} = \sum_i f_{\alpha}(L_i/a) f_{\beta}(L_i/a)
\]

for the mean value of \( A_1 \) obtained by solving the linear system

\[
\sum_\beta M_{\alpha\beta} A_\beta = \sum_i f_{\alpha}(L_i/a) \Sigma_0(u, L_i/a).
\]

This in turn implies an error level, such that for \( w \geq w_1 \) the systematic error is not significant in the sense \( |A_1 - \sigma_0(u)| \leq \delta A_1 \). In other words, for \( w_0 \leq w \leq w_1 \) we typically find extrapolations that look acceptable but are intolerably biased. Of course, this is excluded, if \( w_0 \geq w_1 \) holds. We now use our data for \( \Sigma_0 \) and \( \Sigma_1 \) to determine the ‘dangerous interval’ \([w_0, w_1]\) for a number of cases. We choose the value \( u = 2 \) where the cutoff effects, which are in general rather small at large \( N \), are most noticeable for \( \Sigma_0 \). Our results are summarized in Fig. 2. The absolute errors \( w \) should be compared compared to \( \sigma_0(2) = 3.2726 \) and \( \sigma_1(2) = -0.0467 \).

### 4. Conclusions

We have sketched the computation of the step scaling function of the O(\( N \)) nonlinear \( \sigma \)-model in the large \( N \) limit including the subleading order. We focused on the approach to the continuum limit of these quantities which is reached with corrections of the form \( a^2 \) and \( a^2 \ln a \). We used these data known beyond Monte Carlo precision to investigate various extrapolation methods, for instance in terms of pure powers. It turned out that for small enough errors there are cases possible with acceptable \( \chi^2 / \text{d.g.f} \leq 2 \) and an extrapolation bias beyond the statistical error of the extrapolation. As expected this becomes less likely if the assumed form is close to the true one and/or if the range of lattice spacings measured is large (except for the fit to \( a^{1.5} \)). As a very minimal precaution, one should try also forms with logarithms beside pure powers to probe systematic errors. The whole investigation may also be interpreted as a strong case for improvement programmes since flat data are easy to extrapolate.
Cutoff effects in the O(N) sigma model at large N.

Ulli Wolff

Figure 2: Dangerous intervals for extrapolations for $\Sigma_0$ (left) and $\Sigma_1$ (right). The fit-functions employed are shown in the left of the figures, and solid and dashed lines refer to the sequences of lattices in (3.1).

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