Published by Institute of Physics Publishing for SISSA

Received: *May 25, 2007*
Revised: *July 6, 2007*
Accepted: *August 16, 2007*
Published: *September 3, 2007*

On the reduction of hypercubic lattice artifacts

Feliciano de Soto

Dpto. de Sistemas Físicos, Químicos y Naturales,
Universidad Pablo de Olavide, Ctra. Utrera Km 1, 41013 Sevilla, Spain, and
Laboratoire de Physique Subatomique et Cosmologie, IN2P3,
53 av. des Martyrs, 38026 Grenoble, France
E-mail: fcsotbor@upo.es

Claude Roiesnel

Centre de Physique Théorique, Ecole Polytechnique,
CNRS, 91128 Palaiseau, France
E-mail: roiesnel@cpht.polytechnique.fr

Abstract: This note presents a comparative study of various options to reduce the errors coming from the discretization of a Quantum Field Theory in a lattice with hypercubic symmetry. We show that it is possible to perform an extrapolation towards the continuum which is able to eliminate systematically the artifacts which break the $O(4)$ symmetry.

Keywords: Lattice Quantum Field Theory, Lattice QCD, Lattice Gauge Field Theories.

JHEP09(2007)007

Contents

1. Introduction

The problem of restoration of rotational invariance was the focus of much work in the early days of numerical simulations of lattice gauge theories, which were performed on very small lattices. Most noteworthy were the attempts to find alternative discretizations which would approach the continuum limit more rapidly than the simple hypercubic lattice. One line of attack [1] was to discretize gauge theories on the most symmetric of all four-dimensional lattices, the four-dimensional body-centered hypercubic lattice, whose point symmetry group is three times as large as the hypercubic group. Another angle of investigation worth mentioning was to formulate gauge theories on random lattices [2]. The interest in these alternate formulations faded away in subsequent years, first because of their inherent complications, but mainly when it was realized that rotational invariance was in fact restored within statistical errors at larger distances on the hypercubic lattice.

However, the treatment of discretization errors in numerical simulations of a lattice gauge theory can remain a vexing problem in some data analyses. Indeed, the signal of some lattice observables, such as the two-point Green functions in momentum space, has become so good that the systematic errors become very much larger than the statistical errors. A general method, which we call the H4 method, has been devised quite some time ago [3, 4] to eliminate hypercubic artifacts from the gluon two-point functions and extrapolate the lattice data towards the continuum. This extrapolation is crucial to succeed in a quantitative description, at least in the ultraviolet regime. Such a method, despite its success in describing other two-point functions as well, as the fermion [5] or the ghost [6] propagators, has not been widely adopted. Indeed, most other studies of the lattice two-point functions are still using phenomenological recipes [7] which only allow for a qualitative description of the data, since it is usually not possible to make quantitative fits with a reasonable chisquare.

The purpose of this note is threefold. First we want to gather some pieces about the H4 technique which are scattered in various sections of previous publications and which may have been overlooked. Our second objective is to stress, on a simple controllable model, that the H4 method can be systematically improved, contrarily to the empirical methods, when the statistical errors decrease. Our last goal is to point out the general applicability of the method, not only to those scalar form factors in momentum space which depend on a single invariant, but also to various other lattice observables.

The plan of the paper is as follows. In the next section we recall the general technique of hypercubic extrapolations towards the continuum of any lattice scalar form factor depending upon a single momentum. In the following section we show that a simple model, a free real scalar field in four dimensions, can be used as a testbed for the hypercubic extrapolations. Then we make a detailed comparison of the different strategies to eliminate the hypercubic lattice artifacts. The concluding section is devoted to recommendations about the best usage of the H4 extrapolation method. We also outline some straightforward generalizations.

2. Hypercubic artifacts

Any form factor $F_L(p)$ which is a scalar invariant on the lattice, is invariant along the orbit $O(p)$ generated by the action of the isometry group $H(4)$ of hypercubic lattices on the discrete momentum $p \equiv \frac{2\pi}{La} \times (n_1, n_2, n_3, n_4)$ where the n_μ's are integers, L is the lattice size and a the lattice spacing. The general structure of polynomial invariants under a finite group is known from group-invariant theory [8]. In particular, it can be shown that any polynomial function of p which is invariant under the action of $H(4)$ is a polynomial function of the 4 invariants

$$p^{[n]} \equiv \sum_\mu p_\mu^n, \quad n = 2, 4, 6, 8 \tag{2.1}$$

which index the set of orbits. The appendix contains an elementary derivation.

It is thus possible to use these 4 invariants to average the form factor over the orbits of $H(4)$ to increase the statistical accuracy:

$$F_L(p) \equiv F_L(p^{[2]}, p^{[4]}, p^{[6]}, p^{[8]}) = \frac{1}{\|O(p)\|} \sum_{p \in O(p)} F_L(p) \tag{2.2}$$

where $\|O(p)\|$ is the cardinal number of the orbit $O(p)$.

The orbits of the continuum isometry group $O(4)$ are of course labeled by the single invariant $p^{[2]} \equiv p^2$, and lattice momenta which belong to the same orbit of $O(4)$ do not belong in general to the same orbit of $H(4)$. For instance, as soon as $n^2 \equiv \sum_{\mu=1}^4 n_\mu^2 = 4$ in integer lattice units, the $O(4)$ orbit splits into two distinct H(4) orbits, those of the vectors $(2, 0, 0, 0)$ and $(1, 1, 1, 1)$ respectively. Therefore we can distinguish two kinds of lattice artifacts, those which depend only upon the invariant p^2, and which produce the scaling violations, and those which depend also upon the higher-order invariants $p^{[n]}$ $(n = 4, 6, 8)$ and which we call hypercubic artifacts. When the difference between the values of $F_L(p)$

along one orbit of $O(4)$ become larger than the statistical errors, one needs at least to reduce the hypercubic artifacts from the lattice data before attempting any quantitative analysis.

The treatment of these discretization artifacts can be inferred from lattice perturbation theory, as Green functions will depend on some lattice momentum[1]

$$\widehat{p}_\mu \equiv \frac{2}{a}\sin\left(\frac{ap_\mu}{2}\right) \tag{2.3}$$

instead of the continuum one, $p_\mu = \frac{2\pi}{La}n_\mu$. By developing the lattice momentum $\widehat{p}^2 \equiv \sum_\mu \widehat{p}_\mu^2$ in terms of the lattice spacing a, one gets:

$$\widehat{p}^2 \approx\ p^2 - \frac{a^2}{12}p^{[4]} + \frac{a^4}{360}p^{[6]} - \frac{a^6}{20160}p^{[8]} + \cdots \tag{2.4}$$

and thus, the lattice momentum differs from the "continuum" one by discretization artifacts that are proportional to the invariants $p^{[4]}$ (of order a^2), $p^{[6]}$ (order a^4), etc.

The strategies to minimize the hypercubic artifacts are based on the fact these artifacts depend on the non O(4) invariants, $p^{[4]}$, $p^{[6]}$, etc. and thus reducing $p^{[4]}$ would also reduce the artifacts. For example, the improved restoration of the rotational symmetry on the four-dimensional body-centered hypercubic lattice can be analyzed in terms of the primitive invariant $p^{[4]}$ [9] [2]. These strategies fall into three general groups:

- The simplest one is just to keep only the H(4) orbits which minimizes $p^{[4]}$ along each O(4) orbit. As they lay near the diagonal, a more efficient prescription [7] is to impose a "cylindrical" cut on the values of p, keeping only those that are within a prescribed distance of the diagonal. This completely empirical recipe has been widely adopted in the literature and we shall refer to it in the sequel as the "democratic" method. The main drawbacks are that the information for most of the momenta is lost (for moderate lattices only a small fraction of the momenta is kept) and that although $p^{[4]}$ is small for the orbits kept, it is not null, and therefore the systematic errors are still present.

- The other methods try to fully eliminate the contribution of $p^{[4]}$, etc. and we will generically refer to them as the H4 methods. By analogy with the free lattice propagators, it is natural to make the hypothesis that the lattice form factor is a smooth function of the discrete invariants $p^{[n]}$, $n \geq 4$, near the continuum limit,

$$F_L(p^2, p^{[4]}, p^{[6]}, p^{[8]}) \approx F_L(p^2,0,0,0) + p^{[4]}\frac{\partial F_L}{\partial p^{[4]}}(p^2,0,0,0) + \tag{2.5}$$
$$p^{[6]}\frac{\partial F_L}{\partial p^{[6]}}(p^2,0,0,0) + (p^{[4]})^2\frac{\partial^2 F_L}{\partial^2 p^{[4]}}(p^2,0,0,0) + \cdots$$

  and $F_L(p^2,0,0,0)$ is nothing but the form factor of the continuum in a finite volume, up to lattice artifacts which do not break $O(4)$ invariance and which are true scaling

[1] Depending on the discretization scheme, it will be $\widehat{p}_\mu$ or $\overline{p}_\mu = \frac{1}{a}\sin ap_\mu$, etc.

[2] We thank Ph. de Forcrand for pointing out this reference to us.

violations. We emphasize that we are merely conjecturing that the restoration of rotational invariance is smooth when taking the continuum limit at fixed p^2. When several orbits exist with the same p^2, the simplest method [3] to reduce the hypercubic artifacts is to extrapolate the lattice data towards $F_L(p^2,0,0,0)$ by making a linear regression at fixed p^2 with respect to the invariant $p^{[4]}$ (note that the contributions of other invariants are of higher order in the lattice spacing).

Obviously this method only applies to the O(4) orbits with more than one H(4) orbit. If one wants to include in the data analysis the values of p^2 with a single H(4) orbit, one must interpolate the slopes extracted from (2.5). This interpolation can be done either numerically or by assuming a functional dependence of the slope with respect to p^2 based, for example, on dimensional arguments [4]. For instance, for a massive scalar lattice two-point function, the simplest ansatz would be to assume that the slope has the same leading behavior as for a free lattice propagator:

$$\frac{\partial F_L}{\partial p^{[4]}}(p^2,0,0,0) = \frac{a^2}{\left(p^2+m^2\right)^2}\left(c_1 + c_2 a^2 p^2\right) \tag{2.6}$$

The range of validity of the method can be checked a posteriori from the smoothness of the extrapolated data with respect to p^2. The quality of the two-parameter fit to the slopes, and the extension of the fitting window in p^2, supplies still another independent check of the validity of the extrapolations, although the inclusion of $O(4)$-invariant lattice spacing corrections is usually required to get fits with a reasonable χ^2.

This strategy based on independent extrapolations for each value of p^2 will be referred to as the local H4 method.

- The number of distinct orbits at each p^2 –in physical units– increases with the lattice size and, eventually, a linear extrapolation limited to the single invariant $p^{[4]}$ breaks down. But, by the same token, it becomes possible to improve the local H4 method by performing a linear regression at fixed p^2 in the higher-order invariants as well. Therefore, when the lattice size increases, the H4 technique provides a systematic way to include higher-order invariants and to extend the range of validity of the extrapolation towards the continuum. For those p^2 which do not have enough orbits to perform the extrapolation, it is still possible to make use of all available physical information in the modelling of the functional derivatives appearing in (2.5) and to perform an interpolation.

  An alternative strategy is based on the fact that the functional derivatives which appear in (2.5) are functions of p^2 only. These functions can be represented by a Taylor development in their domain of analyticity, or, more conveniently, by a Laurent series, as it does not assume analyticity and makes appear all the terms allowed by dimensional arguments. Moreover, it is always possible to use polynomial approximation theory and expand the functional derivatives in terms of, e.g., Chebyshev polynomials or in a fourier series, etc.

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In any case, these linear expansions allow to perform the continuum extrapolation through a global linear fit of the parameters for all values of p^2 inside a window at once. Such a strategy has been developed for the analysis of the quark propagator [5] and we shall refer to it as the global H4 method. The global H4 extrapolation is simple to implement since the numerical task amounts to solving a linear system. It provides a systematic way to extend the range of validity of the extrapolation towards the continuum, not only for large lattices (where the inclusion of $O(a^4)$ and even $O(a^6)$ discretization errors becomes possible) but also for small lattices (where the local H4 method for $O(a^2)$ errors is inefficient due to the small number of orbits), by using in the fit all available lattice data points.

3. The free scalar field

In order to analyze a model simple enough to provide a complete control of the hypercubic errors in four dimensions, we have chosen a free real scalar field, whose dynamics is given by the lagrangian:

$$\mathcal{L} \;=\; \frac{1}{2}m^2\phi(x)\phi(x) + \frac{1}{2}\partial_\mu\phi(x)\partial^\mu\phi(x) \tag{3.1}$$

The naive discretization of (3.1) leads to the lattice action:

$$S \;=\; \frac{a^4}{2}\sum_x \left\{ m^2\phi_x^2 + \sum_{\mu=1}^{4}(\nabla_\mu\phi_x)^2 \right\} \tag{3.2}$$

where ∇_μ is the forward lattice derivative, or in momentum space,

$$S \;=\; \frac{a^4}{2}\sum_p \left(m^2 + \widehat{p}^2\right)|\widetilde{\phi}_p|^2 \tag{3.3}$$

where p is the discrete lattice momentum. Therefore, the field $\widetilde{\phi}_p$ can be produced by means of a gaussian sampling with standard deviation $\sqrt{m^2+\widehat{p}^2}$. As this is a cheap lattice calculation, we can go to rather big volumes, up to 64^4 in this work, and we can generate a high number of fully decorrelated configurations. In order to study the effect of statistics over the results, averages will be made over ensembles of 100 till 1000 configurations.

This lattice model is of course solvable, and the propagator reads:

$$\Delta_L(p) \;=\; \frac{1}{\widehat{p}^2 + m^2} \tag{3.4}$$

The lattice artifacts are exactly computable by expanding $\widehat{p}^2$ in terms of the $H(4)$ invariants introduced in the previous section and plugging the development (2.4) into (3.4),

$$\begin{aligned}\Delta_L(p^2, p^{[4]}, p^{[6]}, p^{[8]}) \approx \frac{1}{p^2+m^2} \;+\; a^2\left\{\frac{1}{12}\frac{p^{[4]}}{(p^2+m^2)^2}\right\} \\ +a^4\left\{\frac{1}{72}\frac{{p^{[4]}}^2}{(p^2+m^2)^3} - \frac{2}{8!}\frac{p^{[6]}}{(p^2+m^2)^2}\right\} + \cdots\end{aligned} \tag{3.5}$$

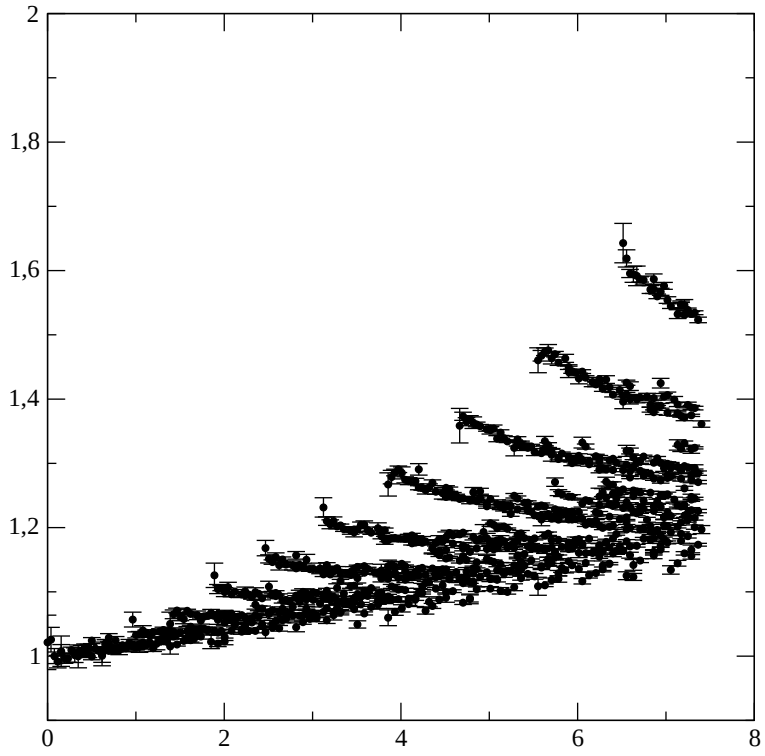

Figure 1: Raw dressing function $\Delta_L(p)/\Delta_0(p)$ as a function of p^2/m^2 for a 32^4 lattice and $am = 1$ from a sample size of 1000 configurations.

and the continuum propagator $\Delta_0(p)$ is indeed recovered *smoothly* in the limit $a \to 0$. But as long as we are working at finite lattice spacing, there will be corrections in a^2, a^4, etc. that are not at all negligible, as can be appreciated in figure 1 which plots the ratio $\Delta_L(p)/\Delta_0(p)$ for a 32^4 lattice.

One could wonder whether such a model is really useful since the lattice artifacts are exactly known. For instance one can recover the continuum propagator from the lattice propagator by merely plotting the lattice data as a function of $\widehat{p}^2$ rather than p^2! However this simple recipe is no longer applicable to an interacting theory where the lattice two-point functions *do depend* upon the independent variables $\widehat{p}^{[n]} = \sum_\mu (\widehat{p}_\mu)^n,\ n = 4, 6, 8$ (as illustrated in figure 1 of reference [3]). And there is no systematic way to separate out cleanly the effect of these additional variables because $\widehat{p}^2$ is not an $O(4)$ invariant. Indeed, because $\widehat{p}^2$ takes on different values on every $H(4)$ orbit, there is only one data point per value of $\widehat{p}^2$ and the H4 method, either local or global, is not appropriate for the choice of momentum variable $\widehat{p}$.

However one should exercise special attention at using this model without the information provided by expression (3.5) (except of course the smoothness assumption in the $H(4)$ invariants $p^{[n]}$). Under this proviso, the model can serve as a bench test of the different approaches to eliminate hypercubic artifacts. In particular *we will not use* eq. (2.6).

The model has one mass parameter m which fixes the scale. We will study the worst-

case scenario where m cannot be neglected with respect to p when the lattice artifacts are large.[3]

The case of QCD is, in fact, simpler, as long as $\Lambda_{\rm QCD}$ and quark masses are negligible in comparison to the momentum scale, which would correspond to the case $am \ll 1$. Then, by dimensional arguments, the artifacts can be modeled at least in the ultraviolet regime, as proposed in [4] and [5].

4. Comparative study of H4 extrapolations

We will now use a free scalar field with $am = 1$ to compare the different strategies to extract the continuum behavior from the lattice data. We will use lattice units and set $a \equiv 1$ throughout this section. We restrict ourselves to one or two representative methods within each strategy:

- The democratic method with a cylindrical cut selecting out the orbits that are within a distance of 2 lattice units from the diagonal $(1, 1, 1, 1)$.

- The local H4 method with independent extrapolations up to $\mathcal{O}(a^2)$ artifacts for every p^2 with several orbits within the window $n^2 > 5$ ($p = \frac{2\pi}{L} n$) up to some $n^2_{\rm max}$:

$$\Delta_L(p^2, p^{[4]}, p^{[6]}, p^{[8]}) = \Delta_L(p^2, 0, 0, 0, 0) + c(p^2) p^{[4]}$$

  The slopes $c(p^2)$ are then fitted with the following functional form

$$c(p^2) = \frac{c_{-1}}{p^2} + c_0 + c_1 p^2 \tag{4.1}$$

  which is used to extrapolate the points with only one orbit inside the window $]5, n^2_{\rm max}]$.

- The global H4 methods with the coefficients of the artifacts up to $\mathcal{O}(a^2)$ or up to $\mathcal{O}(a^4)$ chosen as a Laurent series:

$$\begin{aligned} \Delta_L(p^2, p^{[4]}, p^{[6]}, p^{[8]}) &= \Delta_L(p^2, 0, 0, 0, 0) + f_1(p^2) p^{[4]} + f_2(p^2) p^{[6]} + f_3(p^2) (p^{[4]})^2 \\ f_n(p^2) &= \sum_{i=-1}^{1} c_{i,n} (p^2)^{-i}, \quad n = 1, 2, 3 \end{aligned} \tag{4.2}$$

  With such a choice, a global fit within the window $]5, n^2_{\rm max}]$ amounts to solving a linear system of respectively $n^2_{\rm max} - 2$ and $n^2_{\rm max} + 4$ equations.[4]

Notice that we do not use the knowledge of the mass, $m = 1$, in both the local H4 method and the global H4 method, neither directly nor indirectly (by introducing a mass scale as a parameter). Our purpose is to stress the H4 extrapolation methods to their limits. In practice, of course, all the physical information can be used in order to improve the elimination of the discretization artifacts.

[3] As $p = \frac{2\pi}{La} n$, with $n = 0, \cdots, L/2$, a suitable value is $am = 1$.

[4] Those variables correspond respectively to the extrapolated propagators, $\Delta_L(p^2, 0, 0, 0, 0)$, and the 3 coefficients of each Laurent series.

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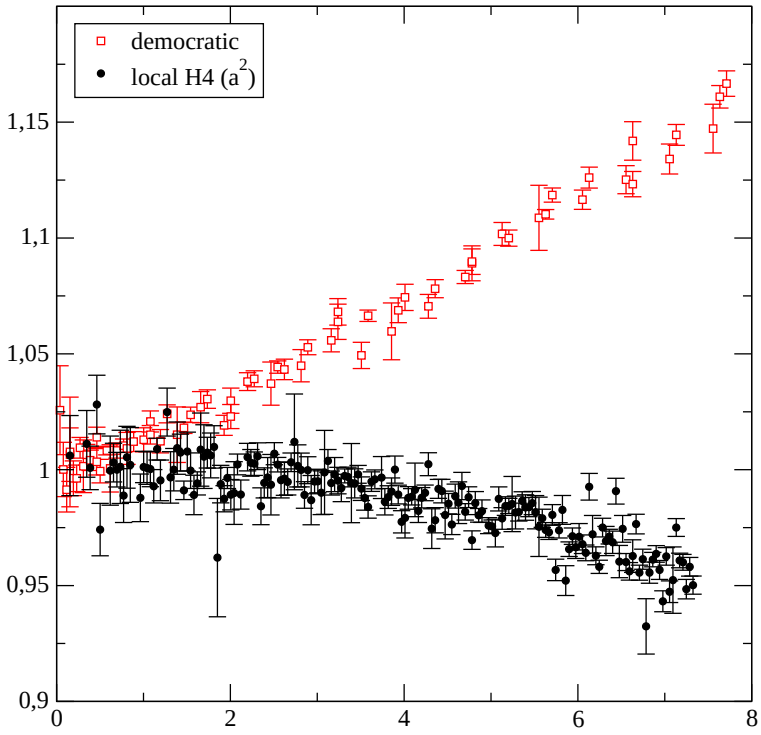

Figure 2: Comparison of the extrapolated dressing function $\Delta_E(p^2)/\Delta_0(p^2)$ as a function of p^2 on a 32^4 lattice ($a = m = 1$), between the democratic method (open squares) and the local H4 method (black circles) - **1000 configurations**.

In figure 2 the extrapolated dressing functions $\Delta_E(p^2)/\Delta_0(p^2)$, with the notation $\Delta_E(p^2) \equiv \Delta_L(p^2, 0, 0, 0)$, of the democratic method and of the local H4 method (with $p^2_{\text{max}} = 3\pi^2/4$), are compared for 1000 configurations generated on a 32^4 lattice. It can be seen that the dressing function of the democratic method deviates very early from unity whereas the dressing function of the local H4 method is pretty consistent with unity within statistical errors for p^2 up to $\approx \pi^2/4$.

Figure 3 compares the extrapolated dressing functions of the global H4 methods, with respectively up to $\mathcal{O}(a^2)$ and up to $\mathcal{O}(a^4)$ artifacts (again with $p^2_{\text{max}} = 3\pi^2/4$), for 1000 configurations generated on a 64^4 lattice. The global H4 method up to $\mathcal{O}(a^2)$ performs roughly as the local H4 method. The global H4 method which takes into account $\mathcal{O}(a^4)$ artifacts is able to reproduce the continuum dressing function within statistical errors for p^2 up to $\approx \pi^2/2$.

It is possible to put these qualitative observations on a more quantitative basis, and show precisely the effect of both the lattice size and the sample size on each extrapolation method. Since all components of a free scalar field in momentum space are independent gaussian variables, the statistical distribution of the quantity

$$\chi^2 = \sum_{p^2=1}^{p^2_{\text{max}}} \left(\frac{\Delta_E(p^2) - \Delta_0(p^2)}{\delta\Delta_E(p^2)} \right)^2 \tag{4.3}$$

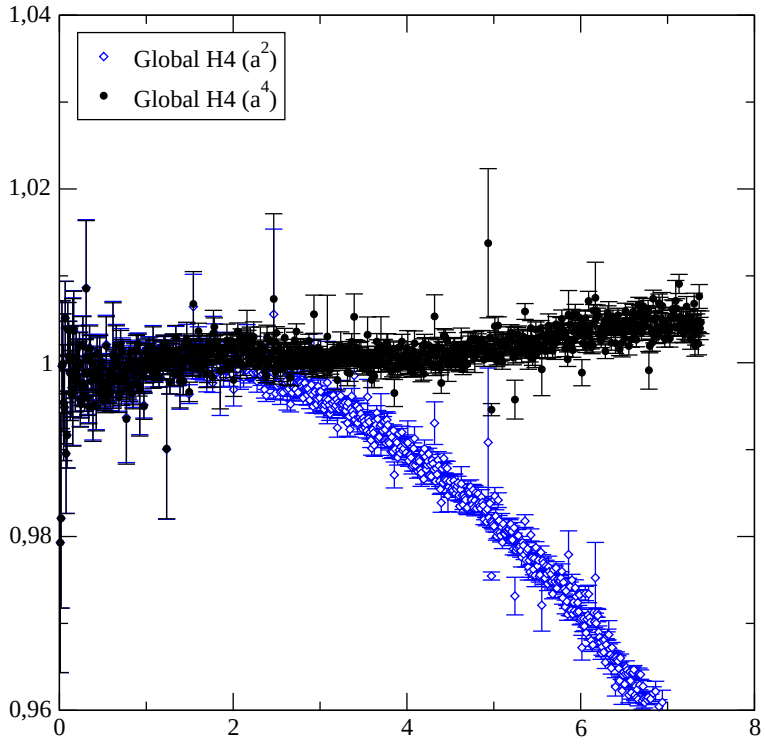

Figure 3: Comparison of the extrapolated dressing function $\Delta_E(p^2)/\Delta_0(p^2)$ as a function of p^2 on a 64^4 lattice ($a = m = 1$), between the global methods with $\mathcal{O}(a^2)$ artifacts (open losanges) and $\mathcal{O}(a^4)$ (black circles) - **1000 configurations**.

should follow exactly the chisquare law for $n^2_{\max}$ independent variables, if the systematic errors of an extrapolation method are indeed smaller than the statistical errors. The criterion is exact for the democratic and local H4 methods which produce independent extrapolated values. Extrapolations by the global H4 method are correlated and one must include the full covariance matrix of the fit in the definition of the chisquare:

$$\chi^2 = \sum_{p^2=1}^{p^2_{\max}} \sum_{q^2=1}^{p^2_{\max}} (\Delta_E(p^2) - \Delta_0(p^2)) M(p^2, q^2) (\Delta_E(q^2) - \Delta_0(q^2)) \,, \tag{4.4}$$

and $M(p^2, q^2) = p^2_{\max}(C^{-1})(p^2, q^2)$ is related to the covariance matrix $C(p^2, q^2)$.

With these considerations, we compute the $\chi^2/d.o.f.$ of a zero-parameter fit of the extrapolated form factor to its known value $\Delta_0(p^2) = 1$ for all p^2. Figure 4 displays the evolution of the chisquare per degree of freedom as a function of the fitting window $]5, n^2_{\max}]$ on a 32^4 lattice, for each extrapolation method. The local and global H4 methods which cure just $\mathcal{O}(a^2)$ artifacts are indeed safe up to $p^2_{\max} \approx \pi^2/4$.

For the range of lattice sizes and sample sizes considered in this work, the global H4 method which takes into account $\mathcal{O}(a^4)$ artifacts performs best. With such a method it is possible to extend the range of validity of the extrapolation towards the continuum up

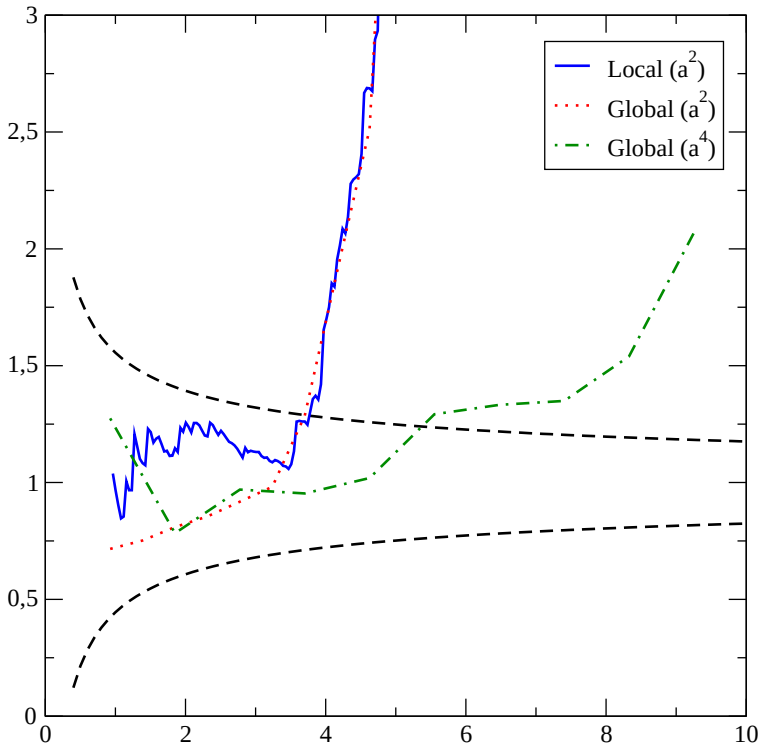

Figure 4: Evolution of the $\chi^2/d.o.f$ as a function of $p^2_{\rm max}$ on a 32^4 lattice ($a = m = 1$), for the local a^2 method (blue solid line), the global a^2 method (red dotted line) and the global a^4 method (green dash-dotted line). The smooth curves are the 95% confidence levels lines - **1000 configurations**.

Lattice size	32	32	64	64
Sample size	100	1000	100	1000
Democratic method	1.4 (2%)	0.54 (0.9%)	1.8 (1.9%)	1.1 (0.6%)
Local a^2 method	6.3 (2%)	4.2 (0.8%)	4.4 (1.4%)	3.4 (0.5%)
Global a^2 method	6.3 (0.7%)	4.3 (0.3%)	4.0 (0.46%)	3.1 (0.15%)
Global a^4 method	π^2 (0.9%)	9.2 (0.4%)	π^2 (0.35%)	6.7 (0.12%)

Table 1: $p^2_{\rm max}$ as a function of the lattice size and the sample size for which $\chi^2/d.o.f. = 2$. The statistical error on the extrapolated dressing function is shown between parentheses.

to $p^2 \approx 5 - 6$, according to the lattice size and at least down to the levels of statistical accuracy studied here.

5. Conclusion

Table 1 summarizes our findings. For each lattice size, sample size and extrapolation method studied in this work, the table displays the upper bound $p^2_{\rm max}$ of the momentum window $]0, a^2 p^2_{\rm max}]$ ($am = 1$), inside which the extrapolated dressing function $\Delta_E(p^2)/\Delta_0(p^2)$ is consistent with 1 at a $\chi^2/d.o.f. = 2$ level.

The limits established in table 1 have been obtained as described in section 4. They could be improved by adding more terms to the Laurent's development, or taking into account their perturbative form in the parametrization of the artifacts.

Table 1 is all what is needed to set up an H4 extrapolation towards the continuum. Our recommendations are the following. If it is not required to push the extrapolation in a^2p^2 above $\approx \pi^2/4$, then it is sufficient to use an H4 method, either local or global, up to $\mathcal{O}(a^2)$ artifacts. On larger windows, the global H4 method at least up to $\mathcal{O}(a^4)$ artifacts should be used. The precise tuning of $p^2_{\rm max}$ can be read off the table in each case.

The sample sizes used in this study are what is typically achieved in lattice studies of two-point functions with $\mathcal{O}(1-10)$ GFlops computers. With sufficient time allocated on $\mathcal{O}(1)$ Tflops computers, it would become possible to increase the statistics by one or two orders of magnitude. Then table 1 would no longer be accurate enough and the analysis of this work would need to be repeated, including the global H4 method up to $\mathcal{O}(a^6)$ artifacts in order to keep the extrapolation windows as large. Let us emphasize that such an analysis is straightforward to implement. With adequate statistics, the global H4 extrapolation method can be systematically improved.

A one or two order of magnitude increase of statistics would also allow to apply the H4 extrapolation techniques to three-point functions as well. Indeed, with a sample size around 1000 configurations, the discretization errors in such lattice observables, although noticeable, are not large enough to be separated from the statistical errors. Three-point functions depend on two momenta. It can be shown that there are now 14 *algebraically* independent symmetric invariants $\phi(p,q)$ under the action of the hypercubic group H(4), and among them, we have the three $O(4)$ invariants

$$\sum_\mu p_\mu^2\,, \quad \sum_\mu q_\mu^2\,, \quad \sum_\mu p_\mu q_\mu$$

and 5 algebraically, and functionnally, independent invariants of order a^2 which can be chosen as

$$\sum_\mu p_\mu^4\,, \quad \sum_\mu q_\mu^4\,, \quad \sum_\mu p_\mu^2 q_\mu^2\,, \quad \sum_\mu p_\mu^3 q_\mu\,, \quad \sum_\mu p_\mu q_\mu^3$$

Three-point form factors are usually measured only at special kinematical configurations. Assuming again smoothness of the lattice form factor with respect to these $\mathcal{O}(a^2)$ invariants, the global H4 extrapolation method could still be attempted provided that enough lattice momenta and enough H4 orbits are included in the analysis.

A more straightforward application of the (hyper)cubic extrapolation method is to asymmetric lattices $L^3\times T$ with spatial cubic symmetry. Lattices with $T \gg L$ are produced in large scale simulations of QCD with dynamical quarks at zero temperature, whereas simulations of QCD at finite temperature require lattices with $T \ll L$. For such lattices, the continuum limit can still be obtained within each time slice by applying the techniques described in this note to the cubic group O_h.

We want to end by pointing out that (hyper)cubic extrapolations methods are not restricted to momentum space but can also be used directly in spacetime. We will sketch one example for illustration, the static potential.

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Lattice artifacts show up in the static potential at short distances and the standard recipe [10] to correct the artifacts is to add to the functional form which fits the static potential a term proportional to the difference $\delta G(R)$ between the lattice one-gluon exchange expression and the continuum expression $1/R$. The technique we advocate is rather to eliminate the cubic artifacts from the raw data measured on the lattice.

Indeed the lattice potential extracted from the measurements of an "off-axis" Wilson loop connecting the origin to a point at distance $R = \sqrt{x^2+y^2+z^2}$ can be expressed,[5] after averaging over the orbits of the cubic group O_h, as a function of three invariants:

$$V_L(x,y,z) \equiv V_L(R^2, R^{[4]}, R^{[6]}) \,, \quad R^{[n]} = x^n + y^n + z^n$$

An extrapolation towards the continuum can be performed with the methods described in section 2 by making the smoothness assumption with respect to the invariants $R^{[4]}$, $R^{[6]}$.

Acknowledgments

We wish to thank our colleagues, Ph. Boucaud, J.P. Leroy, A. Le Yaouanc, J. Micheli, O. Pène, J. Rodríguez-Quintero, who have collaborated to the development of the H4 extrapolation method. These calculations were performed at the IN2P3 computing center in Lyon. F.S. is specially indebted to J. Carbonell and LPSC for their warm hospitality.

A. $H(4)$ invariants

A general polynomial of degree N in the four components of the momentum p reads:

$$P_N(p_1,p_2,p_3,p_4) = \sum_{n=0}^{N} \sum_{n_1+n_2+n_3+n_4=n} c_{n_1 n_2 n_3 n_4}\, p_1^{n_1} p_2^{n_2} p_3^{n_3} p_4^{n_4} \,.$$

But any polynomial function of p which is invariant under the action of $H(4)$ must be invariant under every permutation of the components of p and every reflection $p_\mu \to -p_\mu$. In particular such a polynomial must be an even function of each component p_μ and contain only symmetric combinations of the components. As there are 4 components, we can construct 4 symmetric combinations that are independent. They are usually chosen as the elementary symmetric polynomials:

$$\begin{aligned}
\sigma_1 &= p_1^2 + p_2^2 + p_3^2 + p_4^2 \\
\sigma_2 &= p_1^2 p_2^2 + p_1^2 p_3^2 + p_1^2 p_4^2 + p_2^2 p_3^2 + p_2^2 p_4^2 + p_3^2 p_4^2 \\
\sigma_3 &= p_1^2 p_2^2 p_3^2 + p_1^2 p_2^2 p_4^2 + p_1^2 p_3^2 p_4^2 + p_2^2 p_3^2 p_4^2 \\
\sigma_4 &= p_1^2 p_2^2 p_3^2 p_4^2
\end{aligned}$$

Noticing that the variables p_μ^2 are the roots of the polynomial

$$Q(t) = t^4 - \sigma_1 t^3 + \sigma_2 t^2 - \sigma_3 t + \sigma_4$$

[5] At least for L-shaped loops.

the invariant polynomial P_N can be written, after recursive substitution of all fourth powers of the p_μ^2's, as a polynomial $\widetilde{P}_N$ in the four symmetric invariants:

$$P_N(p_1, p_2, p_3, p_4) = \widetilde{P}_N(\sigma_1, \sigma_2, \sigma_3, \sigma_4) \ .$$

We could have chosen other invariants to represent the polynomial, as the power sums $p^{[n]} \equiv p_1^n + p_2^n + p_3^n + p_4^n$. They can be indeed recovered from the symmetric invariants σ_n via the recursive formulas:

$$\begin{aligned} \sigma_1 &= p^2 \\ 2\sigma_2 &= \sigma_1 p^2 - p^{[4]} \\ 3\sigma_3 &= \sigma_2 p^2 - \sigma_1 p^{[4]} + p^{[6]} \\ 4\sigma_4 &= \sigma_3 p^2 - \sigma_2 p^{[4]} + \sigma_1 p^{[6]} - p^{[8]} \ . \end{aligned}$$

Thus, any polynomial on the four components of p invariant under the action of H(4) can be written as a polynomial in terms of the power sums $p^{[n]}$. A complete, elegant proof can be found in [8].

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