Effectiveness of Nonperturbative $O(a)$ Improvement in Lattice QCD

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The ALPHA Collaboration has determined the $O(a)$ improved Wilson quark action for lattice spacings $a \leq 0.1$ fm, in the quenched approximation. We extend this result to coarser lattices, $a \leq 0.17$ fm, and calculate the hadron spectrum on them. The large range of lattice spacings obtained by combining our results with earlier ones on finer lattices allows us to present a convincing demonstration of the efficiency of nonperturbative $O(a)$ improvement. We find that scaling violations of the hadron masses studied drop from 30%–40% for the unimproved Wilson action on the coarsest lattice to only 2%–3%. [S0031-9007(98)05874-8]

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To measure standard model parameters, like Cabibbo-Kobayashi-Maskawa (CKM) matrix elements and quark masses, and to find signatures of new physics, accurate knowledge of weak matrix elements between hadronic states is required. Lattice QCD is the only systematically improvable method of obtaining this information. The high cost of lattice QCD simulations has lead to a renewed appreciation of the fact that progress in this field depends to a large extent on the successful use of "improvement" ideas (see the proceedings of the last few lattice field theory conferences, e.g., [1] for the last one). The reason is the following: To avoid doublers, the Wilson-type quark actions most commonly used in simulations must break chiral symmetry at some level. On the quantum level, at least, this violation will generically occur at leading order in the lattice spacing, $O(a)$. These errors therefore decrease only slowly with the lattice spacing and their absolute value is large, as experience has shown. To perform accurate and reliable continuum extrapolations would require the use of very fine lattices, for which simulations are very expensive.

A much better approach [2] is to correct the discretization errors of a lattice action by adding higher-dimensional (irrelevant) operators to the action which reproduce the effects of the UV modes omitted on the lattice. Trying to do so perturbatively did initially not appear to be a significant improvement. It was then realized [3] that large perturbative corrections arise due to lattice-specific "tadpole" graphs, and can be corrected by a mean-field type method. Nevertheless, as a resummation of certain graphs in perturbation theory, this approach can basically only reduce quark errors from $O(a)$ to order $g^2 a$ or $g^4 a$. This is only a logarithmic suppression compared to $O(a)$ and would still require the inclusion of at least $g^4 a$ (say) and a^2 terms in an honest continuum extrapolation of the discretization errors. This leads to large errors and potentially unstable fits.

To eliminate the $O(a)$ errors of spectral quantities there is only one term that has to be added to the Wilson QCD action [4]. The gauge action retains the standard plaquette form, and the quark action (density) becomes

$$\overline{\psi}(x)\left[\sum_\mu(\gamma_\mu\nabla_\mu - \frac{1}{2}\,a\Delta_\mu) - \frac{1}{4}\,a\omega\sum_{\mu\nu}\sigma_{\mu\nu}F_{\mu\nu}\right]\psi(x)\,. \tag{1}$$

Here ∇_μ and Δ_μ are the standard covariant first, respectively, second order lattice derivatives. The new $\sigma \cdot F$ term involves the σ matrices $\sigma_{\mu\nu} = -\frac{i}{2}[\gamma_\mu, \gamma_\nu]$ and a discretization of the field strength $F_{\mu\nu}$. Inspired by the form of its most popular discretization, this term is also known as the "clover" term, and the coefficient ω as the clover coefficient. To eliminate $O(a)$ errors, ω has to be determined as a function of the gauge coupling g.

A great step forward was recently taken by the ALPHA Collaboration [5], which used the chiral Ward identity as an improvement condition to determine the nonperturbative value of ω. This was accomplished in the context of the Schrödinger functional [6], where one imposes fixed boundary conditions on the gauge and fermion fields in the time direction, and can then work at zero, or at least small, quark masses. The ALPHA Collaboration determined improvement coefficients for lattice spacings of about $a \leq 0.1$ fm (more precisely, $\beta \equiv 6/g^2 \geq 6.0$ in standard notation).

Since one needs a minimum of three or four reasonably separated lattice spacings to perform accurate and reliable continuum extrapolations, this goal will not easily be accomplished, even in the "quenched" approximation (where quark loops are ignored, and to which the above results refer), if only lattices of spacing 0.1 fm and less are considered. We will explicitly see this below. We have therefore attempted to extend the results of the ALPHA Collaboration to coarser lattices.

Chiral symmetry restoration at $O(a)$.—Consider QCD with (at least) two flavors of mass-degenerate quarks. The idea [5] for determining the clover coefficient is that chiral symmetry will hold only if its Ward identity is satisfied as a *local operator equation*. In Euclidean space this means that the PCAC relation between the isovector axial current and the pseudoscalar density,

$$\langle \partial_\mu A_\mu^b(x)\, \mathcal{O}\rangle = 2m\,\langle P^b(x)\, \mathcal{O}\rangle\,, \tag{2}$$

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should hold for all operators $\mathcal{O}$, boundary conditions, x (as long as x is not in the support of $\mathcal{O}$), and also for volumes that are not necessarily large in physical units. More precisely, it should hold *with the same mass* m up to a^2 errors. This will only be the case for the correct value of the clover coefficient.

Several issues have to be addressed before this idea can be implemented in practice. First of all, even though here we can ignore the multiplicative renormalization of A_μ^b and P^b, there is an additive correction to A_μ^b at $O(a)$,

$$P^b(x) \propto \overline{\psi}(x)\gamma_5 \frac{1}{2}\tau^b\psi(x)\,,$$

$$A_\mu^b(x) \propto \overline{\psi}(x)\gamma_\mu\gamma_5\frac{1}{2}\tau^b\psi(x) + a\,c_A\,\partial_\mu P^b(x)\,. \quad (3)$$

The determination of ω is therefore tied in with that of the axial current improvement coefficient c_A. Since, in principle, (2) provides infinitely many conditions, this is not a fundamental difficulty. How to solve it in practice is discussed in [5,7].

Note that ω and c_A have an $O(a)$ ambiguity; different improvement conditions will give somewhat different values for ω and c_A. Instead of assigning a systematic error to ω and c_A one should choose a specific, "reasonable" improvement condition—the difference in observables from this versus some other choice is guaranteed to extrapolate away like $O(a^2)$ in the continuum limit.

For various reasons it is preferable to impose the PCAC relation at zero quark mass. Because of zero modes this is not possible with periodic boundary conditions; the quark propagator would diverge. Another reason to abandon periodic boundary conditions is that to be sensitive to the value of ω it would be highly advantageous to have a background field present; it couples directly to the clover term.

The Schrödinger functional provides a natural setting to implement these goals. By choosing suitable boundary conditions at the "top" ($x_0 = T$) and "bottom" ($x_0 = 0$) of the lattice world, one induces a chromoelectric classical background field, and, at least at weak coupling, the quark operator has no zero modes at vanishing quark mass (the lowest eigenvalue being of order $1/T$).

We must now choose a specific improvement condition for ω. The idea is that by averaging Eq. (2) over spatial volume, each choice of $\mathcal{O}$ defines an estimate $m_{\mathcal{O}}(x_0)$ of the current quark mass. Requiring the *difference* $\Delta m(x_0) \equiv m_{\mathcal{O}_1}(x_0) - m_{\mathcal{O}_2}(x_0)$ for two specific $\mathcal{O}_1$ and $\mathcal{O}_2$ to vanish for suitable x_0, provides a nonperturbative condition to fix ω. In practice, one calculates all required correlation functions in a Monte Carlo simulation for several trial values of ω and finds the zero crossing of $\Delta m(x_0)$ (more precisely, one should equate it to its small, order a^2 tree-level value). This determines the nonperturbative ω, with some statistical error, for the chosen value of the gauge coupling.

A natural choice of $\mathcal{O}_1$ and $\mathcal{O}_2$ is provided by *boundary fields* [5] associated to the lower and upper boundaries of the lattice. We will not elaborate on these and other choices one makes in the calculation of ω; the details have been discussed in the literature [5,7] and the specifics of the simulations described here can be found in [8].

We have to mention, however, one important point. The above simulations at different trial values of ω should be performed at a fixed value of the quark mass [defined by, say, $m \equiv m_{\mathcal{O}_1}(z_0)$ for suitable z_0], preferably zero. It turns out that in the quenched approximation this is not possible on coarse lattices: Despite the nonperiodic boundary conditions one finds in practice that for roughly $\beta \leq 6.0$ one occasionally hits configurations, known as "exceptional configurations," with an accidental (near-) zero mode, leading to a (near-)divergence of the quark propagator. (With periodic boundary conditions configurations with near-zero modes at small quark mass exist for *any* finite β in the quenched approximation; however, their frequency rapidly decreases at weak coupling.) They can be avoided by using a larger quark mass, but the question is to what extent this affects the value of ω. Fortunately, it turns out that the mass dependence of ω is extremely weak, so that one can reliably determine ω at larger masses. This is illustrated in Figs. 1 and 2 for coarse lattices (cf. also [8]).

For use of the nonperturbatively improved action in later simulations it is advisable to present the results for ω in terms of a smooth function of the gauge coupling. Combining the results of the ALPHA Collaboration [9] with our measurements for $\beta = 5.7, 5.85, 6.0$, and 6.2, we find that they can be represented by

$$\omega(g^2) = \frac{1 - 0.6084\,g^2 - 0.2015\,g^4 + 0.03075\,g^6}{1 - 0.8743\,g^2} \quad (4)$$

for $\beta \equiv 6/g^2 \geq 5.7$. This curve incorporates the one-loop perturbative result [10]. It never deviates by more than

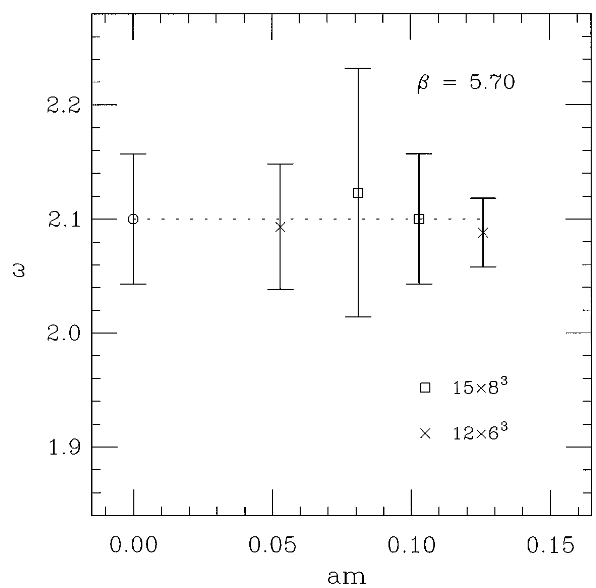

FIG. 1. The nonperturbative clover coefficient as function of quark mass and volume for $\beta = 5.7$. We also show our choice of the $m = 0$ value.

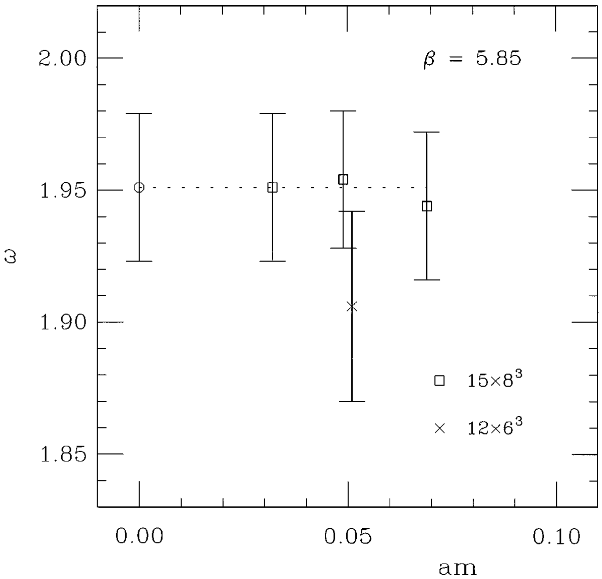

FIG. 2. As in Fig. 1 for $\beta = 5.85$.

1.0% from the curve presented in [5] for $\beta \geq 6.0$. This is illustrated in Fig. 3, where we used the parametrization of the string tension from [11] to present the clover coefficient as a function of lattice spacing.

Hadron spectrum.—To check how small scaling violations of spectral quantities are after nonperturbative improvement of the action, we have calculated the hadron spectrum using Eq. (4) for $\beta = 5.7$ and 5.85. For a scaling check it is not necessary to consider light hadrons. To avoid the uncertainties of the chiral extrapolation we will instead consider hadrons at a pseudoscalar to vector meson mass ratio of $m_P/m_V = 0.7$, corresponding roughly to the strange quark. This also avoids problems with exceptional configurations, which afflict simulations at smaller masses on our coarsest lattice. We regard them as an essentially technical problem of Wilson-type quarks in the quenched approximation (it does not occur for full QCD or staggered fermions), orthogonal to the issue of improvement.

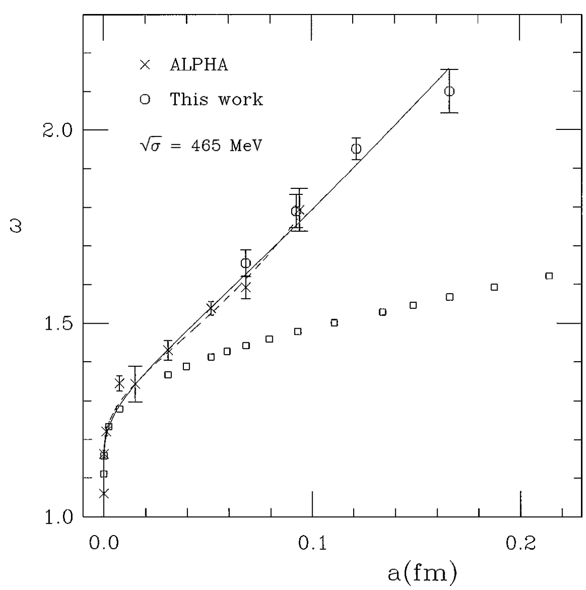

FIG. 3. The measured nonperturbative clover coefficient and its parametrization for $\beta \geq 5.7$ (solid line). The dashed line denotes the curve from [5]. The tree-level tadpole estimate from the plaquette is also shown (□). (Using the mean link in Landau gauge gives an estimate closer to the nonperturbative determination, cf. [12].)

Masses were obtained through two-exponential fits of correlators from one under- and one over-smeared source. We used 400 configurations, statistically enhanced through the use of sources constructed by superimposing different origins with random $\mathbb{Z}_3$ phases [13]. Our results are given in Table I. We also show data from other groups on finer lattices, which we interpolated to $m_P/m_V = 0.7$. Since we cannot do correlated fits of their data, we multiplied the naive error from interpolating fits with a factor of 1.5. This gives values close to the actually measured errors for neighboring mass values. We hope that in the future it will become customary to quote hadron masses interpolated to $m_P/m_V = 0.7$ and perhaps a few other benchmark values (like 0.6 and 0.5). The results in [14,15] were obtained using the parametrization of ω from [5], instead of Eq. (4). We estimate that this changes the masses by less than 0.4%, which is negligible compared to the current statistical errors. The string tensions were taken from our interpolation formula [11], which is based on recent precise measurements by us and others. We assign [11] these string tensions a 1% (or smaller) error, that can be added at the end. We find that excellent fits to a $\mathrm{const} + a^2$ *Ansatz* are possible, yielding $m_V/\sqrt{\sigma} = 2.351(20)$ and $m_N/\sqrt{\sigma} = 3.466(36)$.

We have also considered joint fits with data for the standard quenched Wilson QCD action ($\omega = 0$). Results from different groups for seven couplings in the range $\beta = 5.7$–6.3 have been conveniently collected in [14] (errors are treated similarly as above). In a joint fit we demand that the *Ansätze* for the improved and standard Wilson data intercept at the same point in the continuum limit. The results are shown in Table II and Fig. 4. The joint fits agree perfectly with fits using only the improved action data. For the Wilson data it is necessary to have $O(a)$ and $O(a^2)$ terms in the *Ansatz* to get a reasonable Q in fits where $\beta = 5.7$ is included. Fitting the Wilson data alone yields fits that have either bad Q's or large errors; they are also not very stable under leaving out

TABLE I. Simulation parameters, string tensions [11], and results for the vector meson and "nucleon" (octet) masses at $m_P/m_V = 0.7$ for the nonperturbatively improved action.

β	$a\sqrt{\sigma}$	Volume	N_{confgs}	$m_V/\sqrt{\sigma}$	$m_N/\sqrt{\sigma}$
5.7	0.3917	$16^3 \times 32$	400	2.427(10)	3.532(17)
5.85	0.2863	$16^3 \times 32$	400	2.392(16)	3.515(28)
6.0[a]	0.2196	$(16,24)^3 \times 32$	200–1000	2.380(17)	3.488(34)
6.2[a]	0.1610	$24^3 \times 48$	300	2.319(53)	3.315(93)
6.2[b]	0.1610	$24^3 \times 48$	104	2.425(91)	3.55(10)

[a]Ref. [14].
[b]Ref. [15].

TABLE II. Fit parameters and confidence level Q for joint and separate fits of the improved and Wilson hadron mass data (at $m_P/m_V = 0.7$) to *Ansätze* of the form $m_V/\sqrt{\sigma} = V_0 + V_1\, a\sqrt{\sigma} + V_2\, a^2\sigma$ (for the vector meson; similarly for the nucleon).

		Improved		Wilson		
$\beta_{\min}$	V_0	V_1	V_2	V_1	V_2	Q
5.7	2.356(20)	0	0.46(16)	−2.2(2)	1.1(5)	0.29
5.7	2.332(17)	0	0.64(14)	−1.82(8)	0	0.09
5.85	2.357(34)	0	0.43(52)	−2.0(2)	0	0.26
5.7	2.351(20)	0	0.50(16)			0.74
5.85	2.343(40)	0	0.63(60)			0.55
5.7	2.59(13)			−3.9(10)	4.1(17)	0.27
5.7	2.286(32)			−1.6(1)	0	0.05
5.85	2.392(65)			−2.1(3)	0	0.12
	N_0	N_1	N_2	N_1	N_2	
5.7	3.478(35)	0	0.35(28)	−3.1(3)	2.2(6)	0.38
5.7	3.393(26)	0	0.98(22)	−2.1(1)	0	0.01
5.85	3.472(57)	0	0.46(87)	−2.6(3)	0	0.56
5.7	3.466(36)	0	0.44(28)			0.52
5.85	3.425(69)	0	1.1(10)			0.41
5.7	3.97(22)			−6.7(16)	8.2(27)	0.87
5.7	3.312(38)			−1.8(1)	0	0.07
5.85	3.58(10)			−3.1(5)	0	0.65

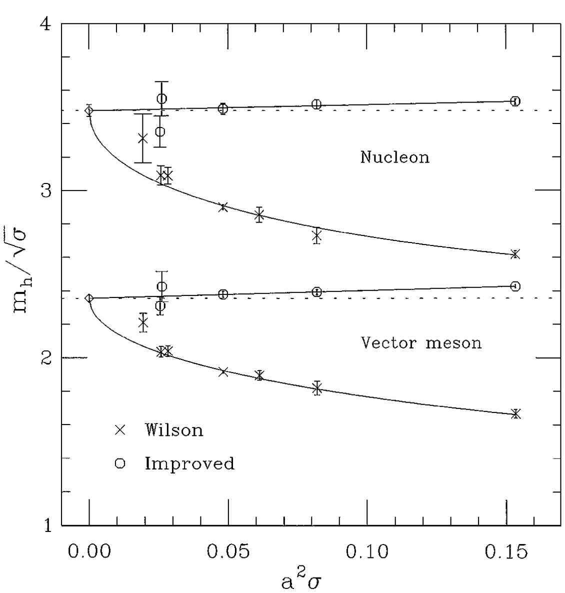

FIG. 4. The hadron spectrum from Wilson and improved actions at $m_P/m_V = 0.7$. Also shown are joint fits of both data sets (the first vector meson, respectively, nucleon fit from Table II).

small (or large) β points. This illustrates how difficult it is to perform reliable continuum extrapolations with the Wilson action. Figure 4 also demonstrates that continuum extrapolations using only lattices with $\beta \geq 6.0$ ($a^2\sigma < 0.05$ or about $a \leq 0.1$ fm) would be quite expensive.

In conclusion, Fig. 4 is impressive proof for the effectiveness of nonperturbative $O(a)$ improvement: The scaling violations at $\beta = 5.7$ are reduced from 41% to 3% for the vector meson mass, and from 33% to 2% for the "nucleon" mass. Even more important, the scaling in Fig. 4 indicates that $O(a)$ errors really have been eliminated from the improved action to high precision. We should remark that without the accurate string tension measurements from [11] it would have been impossible to reach this conclusion.

An analysis of the above data and some toy examples shows that it is a factor of 100 or so cheaper to achieve a 1% (say) error in the hadron masses using the improved instead of the standard Wilson action. Since there is no fundamental difference in the improvement program between quenched and full QCD, we expect very large improvements also in more realistic situations like full QCD with lighter quark masses.

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