Hadron Masses From Novel Fat-Link Fermion Actions

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Abstract

The hadron mass spectrum is calculated in lattice QCD using a novel fat-link clover fermion action in which only the irrelevant operators in the fermion action are constructed using smeared links. The simulations are performed on a $16^3 \times 32$ lattice with a lattice spacing of $a = 0.125$ fm. We compare actions with $n = 4$ and 12 smearing sweeps with a smearing fraction of 0.7. The $n = 4$ Fat-Link Irrelevant Clover (FLIC) action provides scaling which is superior to mean-field improvement, and offers advantages over nonperturbative $O(a)$ improvement, including a reduced exceptional configuration problem.

PACS number(s): 11.15.Ha, 12.38.Gc, 12.38.Aw
I. INTRODUCTION

The origin of the masses of light hadrons represents one of the most fundamental challenges to the theory of strong interactions, Quantum Chromodynamics (QCD). Despite the universal acceptance of QCD as the basis from which to derive hadronic properties, there has been slow progress in understanding the generation of hadron mass from first principles. Solving the problem of the hadronic mass spectrum would allow considerable improvement in our understanding of the nonperturbative nature of QCD. The only available method at present to derive hadron masses directly from QCD is a numerical calculation on the lattice. In the last few years impressive progress has been made both in computer hardware and in developing more efficient algorithms, bringing realistic simulations of hadronic observables with sufficiently large volumes, small quark masses and fine enough lattices within reach.

The high computational cost required to perform accurate lattice calculations at small lattice spacings, however, has led to increased interest in quark action improvement. In order to avoid the famous doubling problem, Wilson originally introduced an irrelevant (energy) dimension-five operator (the “Wilson term”) to the standard “naive” lattice fermion action, which explicitly breaks chiral symmetry at \( O(a) \). To extrapolate reliably to the continuum, simulations must be performed on fine lattices, which are therefore very computationally expensive. The scaling properties of the Wilson action at finite \( a \) can be improved by introducing any number of irrelevant operators of increasing dimension which vanish in the continuum limit.

The Sheikholeslami-Wohlert (clover) action introduces an additional irrelevant dimension-five operator to the standard Wilson quark action,

\[
S_{SW} = S_W - \frac{iaC_{SW}}{4} \bar{\psi}(x)\sigma_{\mu\nu}F_{\mu\nu}\psi(x),
\]

where \( S_W \) is the standard Wilson action,

\[
S_W = \bar{\psi}(x) \left[ \sum_\mu \left( \gamma_\mu \nabla_\mu - \frac{1}{2}ra\Delta_\mu \right) + m \right] \psi(x),
\]

\( \nabla_\mu \) and \( \Delta_\mu \) are the standard covariant first and second order lattice derivatives,

\[
\nabla_\mu \psi(x) = \frac{1}{2a} \left[ U_\mu(x)\psi(x + \mu) - U_\mu^\dagger(x - \mu)\psi(x - \mu) \right],
\]

\[
\Delta_\mu \psi(x) = \frac{1}{a^2} \left[ U_\mu(x)\psi(x + \mu) + U_\mu^\dagger(x - \mu)\psi(x - \mu) - 2\psi(x) \right],
\]

and \( C_{SW} \) is the clover coefficient which can be tuned to remove \( O(a) \) artifacts,

\[
C_{SW} = \begin{cases} 
1 & \text{at tree-level,} \\
1/u_0^3 & \text{mean-field improved,}
\end{cases}
\]

with \( u_0 \) the tadpole improvement factor which corrects for the quantum renormalization of the operators. Nonperturbative (NP) \( O(a) \) improvement tunes \( C_{SW} \) to all powers in \( g^2 \) and displays excellent scaling, as shown by Edwards et al., who studied the scaling
properties of the nucleon and vector meson masses for various lattice spacings (see also Section IV below). In particular, the linear behavior of the NP-improved clover actions, when plotted against $a^2$, demonstrates that $O(a)$ errors are removed. It was also found in Ref. 4 that a linear extrapolation of the mean-field improved data fails, indicating that $O(a)$ errors are still present.

A drawback to the clover action, however, is the associated problem of exceptional configurations, where the quark propagator encounters singular behavior as the quark mass becomes small. In practice, this prevents the use of coarse lattices ($\beta > 5.7 \sim a < 0.18$ fm) 5-7. Furthermore, the plaquette version of $F_{\mu\nu}$, which is commonly used in Eq. (1), has large $O(a^2)$ errors, which can lead to errors of the order of 10% in the topological charge even on very smooth configurations 7.

The idea of using fat links in fermion actions was first explored by the MIT group 8 and more recently has been studied by DeGrand et al. 6,9,10, who showed that the exceptional configuration problem can be overcome by using a fat-link (FL) clover action. Moreover, the renormalization of the coefficients of action improvement terms is small. In principle it is acceptable to smear the links of the relevant operators. The symmetry of the APE smearing process ensures that effects are $O(a^2)$. The factors multiplying the link and staple ensure the leading order term is $e^{i a g A_\mu}$, an element of SU(3). Issues of projecting the smeared links to SU(3) are $O(a^2)$ effects and therefore correspond to irrelevant operators 11. However, the net effect of APE smearing the links of the relevant operators is to remove gluon interactions at the scale of the cutoff. While this has some tremendous benefits, the short-distance quark interactions are lost. As a result decay constants, which are sensitive to the wave function at the origin, are suppressed.

A possible solution to this is to work with two sets of links in the fermion action. In the relevant dimension-four operators, one works with the untouched links generated via Monte Carlo methods, while the smeared fat links are introduced only in the higher dimension irrelevant operators. The effect this has on decay constants is under investigation and will be reported elsewhere.

In this paper we present the first results of simulations of the spectrum of light mesons and baryons using this variation on the clover action. In particular, we will start with the standard clover action and replace the links in the irrelevant operators with APE smeared 12, or fat links. We shall refer to this action as the Fat-Link Irrelevant Clover (FLIC) action. Although the idea of using fat links only in the irrelevant operators of the fermion action was developed here independently, suggestions have appeared previously 13. To the best of our knowledge, this is the first report of lattice QCD calculations using this novel fermion action.

In Section II we describe the gauge action used in our lattice simulations, while Section III contains the procedure for creating the FLIC fermion action. Our results are presented in Section IV and finally in Section V we draw some conclusions and discuss future work.

II. THE GAUGE ACTION

The simulations are performed using a mean-field improved, plaquette plus rectangle, gauge action on a $16^3 \times 32$ lattice at $\beta = 6/g^2 = 4.60$, providing a lattice spacing $a =$
0.125(2) fm determined from the string tension with $\sqrt{\sigma} = 440$ MeV. The tree-level $\mathcal{O}(a^2)$–Symanzik-improved gauge action \[14\] is defined as

$$S_G = \frac{5\beta}{3} \sum_{sq} \Re \text{ tr}(1 - U_{sq}(x)) - \frac{\beta}{12u_0^2} \sum_{\text{rect}} \Re \text{ tr}(1 - U_{\text{rect}}(x)) ,$$

where the operators $U_{sq}(x)$ and $U_{\text{rect}}(x)$ are defined as

$$U_{sq}(x) = U_{\mu}(x)U_{\nu}(x + \hat{\mu})U_{\mu}^\dagger(x + \hat{\nu})U_{\nu}^\dagger(x) ,$$

$$U_{\text{rect}}(x) = \left[ U_{\nu}(x)U_{\mu}(x + \hat{\mu})U_{\nu}(x + 2\hat{\nu}) \right. + \left. U_{\mu}(x)U_{\mu}(x + \hat{\nu})U_{\nu}(x + 2\hat{\mu}) \right. 
+ \left. U_{\mu}^\dagger(x + \hat{\mu} + \hat{\nu})U_{\mu}(x + \hat{\nu})U_{\nu}^\dagger(x) .$$

The link product $U_{\text{rect}}(x)$ denotes the rectangular $1 \times 2$ and $2 \times 1$ plaquettes, and for the tadpole improvement factor we employ the plaquette measure

$$u_0 = \left( \frac{1}{3} \Re \text{ tr}(U_{sq}) \right)^{1/4} .$$

Gauge configurations are generated using the Cabibbo-Marinari pseudoheat-bath algorithm with three diagonal SU(2) subgroups looped over twice. Simulations are performed using a parallel algorithm with appropriate link partitioning \[15\]. A total of 50 configurations are used in this analysis, and the error analysis is performed by a third-order, single-elimination jackknife, with the $\chi^2$ per degree of freedom ($N_{DF}$) obtained via covariance matrix fits.

### III. F A T-LINK I RRELEVANT FERMION A C TION

Fat links \[6,9\] are created by averaging or smearing links on the lattice with their nearest neighbours in a gauge covariant manner (APE smearing). The smearing procedure \[12\] replaces a link, $U_{\mu}(x)$, with a sum of the link and $\alpha$ times its staples

$$U_{\mu}(x) \rightarrow U'_{\mu}(x) = (1 - \alpha)U_{\mu}(x) + \frac{\alpha}{6} \sum_{\nu=1}^{4} \sum_{\nu \neq \mu} \left[ U_{\nu}(x)U_{\mu}(x + \nu a)U_{\nu}^\dagger(x + \mu a) 
+ U_{\nu}^\dagger(x - \nu a)U_{\mu}(x - \nu a)U_{\nu}(x - \nu a + \mu a) \right] ,$$

followed by projection back to SU(3). We select the unitary matrix $U^{FL}_{\mu}$ which maximizes

$$\Re \text{ tr}(U^{FL}_{\mu}U'^{\dagger}_{\mu}) ,$$

by iterating over the three diagonal SU(2) subgroups of SU(3). We repeat the combined procedure of smearing and projection $n$ times. We create our fat links by setting $\alpha = 0.7$ and comparing $n = 4$ and 12 smearing sweeps. The mean-field improved FLIC action now becomes
\[ S_{SW}^{FL} = S_{W}^{FL} - \frac{iC_{SW} F_{\mu \nu}}{2(u_0^{FL})^4} \bar{\psi}(x) \sigma_{\mu \nu} F_{\mu \nu} \psi(x), \tag{8} \]

where \( F_{\mu \nu} \) is constructed using fat links, \( u_0^{FL} \) is calculated in an analogous way to Eq. (6), and where the mean-field improved Fat-Link Irrelevant Wilson action is

\[ S_{SW}^{FL} = \sum_x \bar{\psi}(x) \psi(x) + \kappa \sum_{x, \mu} \bar{\psi}(x) \left[ \gamma_{\mu} \left( \frac{U_{\mu}(x)}{u_0} \psi(x + \hat{\mu}) - \frac{U_{\mu}^\dagger(x - \hat{\mu})}{u_0} \psi(x - \hat{\mu}) \right) \right. \]
\[ - r \left( \frac{U_{\mu}(x)}{u_0^{FL}} \psi(x + \hat{\mu}) + \frac{U_{\mu}^\dagger(x - \hat{\mu})}{u_0^{FL}} \psi(x - \hat{\mu}) \right), \tag{9} \]

with \( \kappa = \frac{1}{2m + 8r} \). We take the standard value \( r = 1 \). Our notation uses the Pauli representation of the Dirac \( \gamma \)-matrices defined in Appendix B of Sakurai [16]. In particular, the \( \gamma \)-matrices are hermitian and \( \sigma_{\mu \nu} = \frac{1}{2} [\gamma_{\mu}, \gamma_{\nu}] \).

As reported in Table 1, the mean-field improvement parameter for the fat links is very close to 1. Hence, the mean-field improved coefficient for \( C_{SW} \) is expected to be adequate. In addition, actions with many irrelevant operators (e.g. the \( D_{234} \) action) can now be handled with confidence as tree-level knowledge of the improvement coefficients should be sufficient. Another advantage is that one can now use highly improved definitions of \( F_{\mu \nu} \) (involving terms up to \( u_0^{12} \)), which give impressive near-integer results for the topological charge [17].

In particular, we employ an \( O(a^4) \) improved definition of \( F_{\mu \nu} \) in which the standard clover-sum of four \( 1 \times 1 \) Wilson loops lying in the \( \mu, \nu \) plane is combined with \( 2 \times 2 \) and \( 3 \times 3 \) Wilson loop clovers. Bilson-Thompson et al. [17] find

\[ F_{\mu \nu} = -\frac{i}{8} \left[ \left( \frac{3}{2} W^{1 \times 1} - \frac{3}{20} u_0^2 W^{2 \times 2} + \frac{1}{90} u_0^3 W^{3 \times 3} \right) \right]_{\text{Traceless}} \tag{10} \]

where \( W^{n \times n} \) is the clover-sum of four \( n \times n \) Wilson loops and \( F_{\mu \nu} \) is made traceless by subtracting \( 1/3 \) of the trace from each diagonal element of the \( 3 \times 3 \) color matrix. This definition reproduces the continuum limit with \( O(a^6) \) errors. On approximately self-dual configurations, this operator produces integer topological charge to better than 4 parts in 10^4.

Work by DeForcrand et al. [18] suggests that 7 cooling sweeps are required to approach topological charge within 1% of integer value. This is approximately 16 APE smearing sweeps at \( \alpha = 0.7 \) [19]. However, achieving integer topological charge is not necessary for the purposes of studying hadron masses, as has been well established. To reach integer topological charge, even with improved definitions of the topological charge operator, requires significant smoothing and associated loss of short-distance information. Instead, we regard this as an upper limit on the number of smearing sweeps.

Using unimproved gauge fields and an unimproved topological charge operator, Bonnet et al. [4] found that the topological charge settles down after about 10 sweeps of APE smearing.

\(^1\)Our experience with topological charge operators suggests that it is advantageous to include \( u_0 \) factors, even as they approach 1.
at $\alpha = 0.7$. Consequently, we create fat links with APE smearing parameters $n = 12$ and $\alpha = 0.7$. This corresponds to $\sim 2.5$ times the smearing used in Refs. [6,9]. Further investigation reveals that improved gauge fields with a small lattice spacing ($a = 0.125$ fm) are smooth after only 4 sweeps. Hence, we perform calculations with 4 sweeps of smearing at $\alpha = 0.7$ and consider $n = 12$ as a second reference. Table I lists the values of $u_0^{FL}$ for $n = 0, 4$ and 12 smearing sweeps.

We also compare our results with the standard Mean-Field Improved Clover (MFIC) action. We mean-field improve as defined in Eqs. 8 and 9 but with thin links throughout. The standard Wilson-loop definition of $F_{\mu\nu}$ is used.

A fixed boundary condition is used for the fermions by setting

$$U_t(\vec{x}, nt) = 0 \quad \text{and} \quad U_t^{FL}(\vec{x}, nt) = 0 \quad \forall \, \vec{x} \quad (11)$$

in the hopping terms of the fermion action. The fermion source is centered at the space-time location $(x, y, z, t) = (1, 1, 1, 3)$, which allows for two steps backward in time without loss of signal. Gauge-invariant gaussian smearing in the spatial dimensions is applied at the source to increase the overlap of the interpolating operators with the ground states.

### TABLE I. The value of the mean link for different numbers of APE smearing sweeps, $n$, at $\alpha = 0.7$.

| $n$  | $u_0^{FL}$          | $(u_0^{FL})^4$          |
|------|---------------------|-------------------------|
| 0    | 0.88894473          | 0.62445197              |
| 4    | 0.99658530          | 0.98641100              |
| 12   | 0.99927343          | 0.99709689              |

**IV. RESULTS**

Hadron masses are extracted from the Euclidean time dependence of the calculated two-point correlation functions. For baryons, the correlation functions are given by

$$\langle G(t; \vec{p}, \Gamma) \rangle = \sum_x e^{-i \vec{p} \cdot \vec{x}} \Gamma^{\beta \alpha} \langle \Omega | T [ \chi^\alpha(x) \bar{\chi}^\beta(0) ] | \Omega \rangle ,$$

where $\chi$ are standard baryon interpolating fields, $\Omega$ represents the QCD vacuum, $\Gamma$ is a $4 \times 4$ matrix in Dirac space, and $\alpha, \beta$ are Dirac indices. At large Euclidean times one has

$$\langle G(t; \vec{p}, \Gamma) \rangle \simeq \frac{Z^2}{2E_p} e^{-E_p t} \text{tr} \left[ \Gamma (-i\gamma \cdot p + M) \right] ,$$

where $Z$ represents the coupling strength of $\chi(0)$ to the baryon, and $E_p = (\vec{p}^2 + M^2)^{1/2}$ is the energy. Selecting $\vec{p} = 0$ and $\Gamma = (1 + \gamma_4)/4$, the effective baryon mass is then given by
FIG. 1. Effective mass plot for the nucleon for the FLIC action with 4 sweeps of smearing at $\alpha = 0.7$ from 200 configurations. The five sets of points correspond to the $\kappa$ values listed in Table II, with $\kappa$ increasing from top down.

\[ M(t + 1/2) = \log[G(t)] - \log[G(t + 1)] \, . \]  

(14)

Meson masses are determined via analogous standard procedures. The critical value of $\kappa$, $\kappa_c$, is determined by linearly extrapolating $m_\pi^2$ as a function of $m_q$ to zero. The quark masses are defined by $m_q = (1/\kappa - 1/\kappa_c)/(2a)$, and the strange quark mass was taken to be the second heaviest quark mass in each case.

Figure 1 shows the nucleon effective mass plot for the FLIC action when 4 APE smearing sweeps at $\alpha = 0.7$ are performed on the fat links (“FLIC4”). The effective mass plots for the other hadrons are similar, and all display acceptable plateau behavior. Good values of $\chi^2/N_{DF}$ are obtained for many different time-fitting intervals as long as one fits after time slice 8. All fits for this action are therefore performed on time slices 9 through 14. For the Wilson action and the FLIC action with $n = 12$ (“FLIC12”) the fitting regimes used are 9-13 and 9-14, respectively.

The values of $\kappa$ used in the simulations for all quark actions are given in Table III. We have also provided the values of $\kappa_{cr}$ for these fermion actions when using our mean-field improved, plaquette plus rectangle, gauge action at $\beta = 4.60$. We have mean-field improved our fermion actions so we expect the values for $\kappa_{cr}$ to be close to the tree-level value of 0.125. Improved chiral properties are seen for the FLIC and MFIC actions, with FLIC4 performing better than FLIC12.

The behavior of the $\rho$, nucleon and $\Delta$ masses as a function of squared pion mass is shown in Fig. 2 for the various actions. The first feature to note is the excellent agreement between the FLIC4 and FLIC12 actions. On the other hand, the Wilson action appears to lie somewhat low in comparison. It is also reassuring that all actions give the correct
TABLE II. Values of $\kappa$ and the corresponding $\pi, \rho, N$ and $\Delta$ masses for the FLIC action with 4 sweeps of smearing at $\alpha = 0.7$. The value for $\kappa_{cr}$ is provided in Table III. A string tension analysis provides $a = 0.125(2)$ fm for $\sqrt{\sigma} = 440$ MeV.

| $\kappa$  | $m_{\pi}a$     | $m_{\rho}a$    | $m_{N}a$       | $m_{\Delta}a$  |
|----------|----------------|----------------|----------------|----------------|
| 0.1260   | 0.5797(23)     | 0.7278(39)     | 1.0995(58)     | 1.1869(104)    |
| 0.1266   | 0.5331(24)     | 0.6951(45)     | 1.0419(64)     | 1.1387(121)    |
| 0.1273   | 0.4744(27)     | 0.6565(54)     | 0.9709(72)     | 1.0816(152)    |
| 0.1279   | 0.4185(30)     | 0.6299(65)     | 0.9055(82)     | 1.0310(194)    |
| 0.1286   | 0.3429(37)     | 0.5843(97)     | 0.8220(102)    | 0.9703(286)    |

TABLE III. Values of $\kappa$ and $\kappa_{cr}$ for the four different actions.

|          | Wilson | FLIC12 | FLIC4 | MFIC |
|----------|--------|--------|-------|------|
| $\kappa_1$ | 0.1346 | 0.1286 | 0.1260 | 0.1196 |
| $\kappa_2$ | 0.1353 | 0.1292 | 0.1266 | 0.1201 |
| $\kappa_3$ | 0.1360 | 0.1299 | 0.1273 | 0.1206 |
| $\kappa_4$ | 0.1367 | 0.1305 | 0.1279 | 0.1211 |
| $\kappa_5$ | 0.1374 | 0.1312 | 0.1286 | 0.1216 |
| $\kappa_{cr}$ | 0.1390 | 0.1328 | 0.1300 | 0.1226 |

mass ordering in the spectrum. The value of the squared pion mass at $m_{\pi}/m_{\rho} = 0.7$ is plotted on the abscissa for the three actions as a reference point. This point is chosen in order to allow comparison of different results by interpolating them to a common value of $m_{\pi}/m_{\rho} = 0.7$, rather than extrapolating them to smaller quark masses, which is subject to larger systematic and statistical uncertainties.

The scaling behavior of the different actions is illustrated in Fig. 3. The present results for the Wilson action agree with those of Ref. [4]. The first feature to observe in Fig. 3 is that actions with fat-link irrelevant operators perform extremely well. For both the vector meson and the nucleon, the FLIC actions perform significantly better than the mean-field improved clover action. It is also clear that the FLIC4 action performs systematically better than the FLIC12. This suggests that 12 smearing sweeps removes too much short-distance information from the gauge-field configurations. On the other hand, 4 sweeps of smearing combined with our $\mathcal{O}(a^4)$ improved $F_{\mu\nu}$ provides excellent results, without the fine tuning of $C_{SW}$ in the NP improvement program.

Notice that for the $\rho$ meson, a linear extrapolation of previous mean-field improved clover results in Fig. 3 passes through our mean-field improved clover result at $a^2\sigma \sim 0.08$ which
lies systematically low relative to the FLIC actions. However, a linear extrapolation does not pass through the continuum limit result, thus confirming the presence of significant $O(a)$ errors in the mean-field improved clover fermion action. While there are no NP-improved clover plus improved glue simulation results at $a^2\sigma \sim 0.08$, the simulation results that are available indicate that the fat-link results also compete well with those obtained with a NP-improved clover fermion action.

Having determined FLIC4 is the preferred action, we have increased the number of configurations to 200 for this action. As expected, the error bars are halved and the central values for the FLIC4 points move to the upper end of the error bars on the 50 configuration result, further supporting the promise of excellent scaling.

Finally, in Fig. 4 we compare the convergence rates of the different actions by plotting the number of stabilized biconjugate gradient [20] iterations required to invert the fermion matrix as a function of $m_\pi/m_\rho$. For any particular value of $m_\pi/m_\rho$, the FLIC actions converge faster than both the Wilson and mean-field improved clover fermion actions. Also, the slopes of the FLIC lines are smaller in magnitude than those for Wilson and mean-field improved clover actions, which provides great promise for performing cost effective simulations at quark masses closer to the physical values. Problems with exceptional configurations have prevented such simulations in the past.
FIG. 3. Nucleon and vector meson masses for the Wilson, NP-improved, mean-field clover and FLIC actions. Results from the present simulations, indicated by the solid points, are obtained by interpolating the results of Fig. 2 to $m_\pi/m_\rho = 0.7$. The fat links are constructed with $n = 4$ (solid squares) and $n = 12$ (stars) smearing sweeps at $\alpha = 0.7$. The solid triangles are results for the FLIC4 action when 200 configurations are used in the analysis. The FLIC results are offset from the central value for clarity. Our MF clover result at $a^2\sigma \sim 0.08$ lies systematically low relative to the FLIC actions.

V. CONCLUSIONS

We have examined the hadron mass spectrum using a novel Fat-Link Irrelevant Clover (FLIC) fermion action, in which only the irrelevant, higher-dimension operators involve smeared links. One of the main conclusions of this work is that the use of fat links in the irrelevant operators provides excellent results. Fat links promise improved scaling behavior over mean-field improvement. This technique also solves a significant problem with $O(a)$ nonperturbative improvement on mean field-improved gluon configurations. Simulations are possible and the results are competitive with nonperturbative-improved clover results on plaquette-action gluon configurations. We have found that minimal smearing holds the promise of better scaling behavior. Our results suggest that too much smearing removes relevant information from the gauge fields, leading to a poorer performance. Fermion matrix inversion for FLIC actions is more efficient and results show no sign of exceptional
configuration problems.

This work paves the way for promising future studies. It will be of great interest to consider different lattice spacings to further test the scaling of the fat-link actions. Furthermore, the exceptional configuration issue can be explored by pushing the quark mass down to lower values. We are currently performing simulations at $m_\pi/m_\rho = 0.36$ and these results will available soon. A study of the spectrum of excited hadrons using the FLIC actions is also currently in progress [21].

ACKNOWLEDGMENTS

This work was supported by the Australian Research Council. We are grateful to Herbert Neuberger for helpful discussions regarding the gauge invariance of APE smearing. We have also benefited from discussions with Robert Edwards and Urs Heller during the Lattice Hadron Physics workshop held in Cairns, Australia. We would also like to thank the Australian National Computing Facility for Lattice Gauge Theories for the use of the Orion Supercomputer. W.M. and F.X.L. were partially supported by the U.S. Department of Energy contract DE-AC05-84ER40150, under which the Southeastern Universities Research Association (SURA) operates the Thomas Jefferson National Accelerator Facility (Jefferson Lab).
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