Improving meson two-point functions in lattice QCD

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Abstract

We describe and test a method to compute Euclidean meson two-point functions in lattice QCD. The contribution from the low-lying eigenmodes of the Dirac operator is averaged over all positions of the quark sources. The contribution from the higher modes is estimated in the traditional way with one or a few source points per lattice. In some channels, we observe a significant improvement in the two-point functions for small quark masses.
FIG. 1: Pseudoscalar-scalar difference correlator at $am_q = 0.020$, from the $a = 0.13$ fm $12^3 \times 36$ data set used in this study, showing the contribution of the lowest 20 eigenmodes of $D^\dagger D$, the contribution of the high modes, and the full correlator.

I. INTRODUCTION

In current lattice QCD computations a significant amount of effort is put into the simulation at small quark masses. Unfortunately, the noise in the meson correlators increases with decreasing quark mass. The purpose of this paper is to examine a method to reduce this noise. We are motivated by observations that for lighter quarks the low-lying eigenmodes of the Dirac operator make an important contribution to hadron correlators in some channels. Traditionally one restricts oneself to the computation of propagators using a single position of the quark source. However, by computing the low-lying eigenmodes, one can average their contribution over all possible positions of the source and hope that this improves the signal. The contribution from the high modes can be estimated in the standard way.

The saturation of the correlators has, for example, been studied in Refs [1, 2]. Refs [1, 3] have shown that for actions similar to the one used in this study, the long distance part of many meson correlators is dominated by the low eigenmode contribution to the quark propagator. Fig. 1 shows an example of this behavior. This is the pseudoscalar-scalar difference correlator evaluated at a quark mass which is about $0.3m_{\text{strange}}$, with a Gaussian source and a point sink.

We wish to calculate a correlator

$$C(t) = \frac{1}{L^3 T} \sum_{x',x'',t''} \langle O_1(x', t'' + t)O_2(x'', t'') \rangle.$$  \hfill (1)

Inserting a complete set of relativistically normalized states this becomes up to boundary
effects,
\[ C(t) = \sum_n \frac{\langle 0 | O_1 | n \rangle \langle n | O_2 | 0 \rangle}{2m_n} e^{-m_n t}, \]  
(2)

from which a fit allows us to read off masses and matrix elements. For bilinear operators,
\[ O_i = \bar{\psi} \Gamma_i \psi, \]
\[ C(t) = \frac{1}{L^3 T} \sum_{x',x'',t''} \langle \text{Tr} \Gamma_1 G(x', t'' + t; x'', t'') \Gamma_2 G(x'', t''; x', t') \rangle \]  
(3)

where \( G(x', t'; x, t) \) is the quark propagator, \((D + m)G(x', t'; x, t) = \delta_{x,x'} \delta_{t,t'}\). Evaluating \( G \) in a way that it can be usefully combined in Eq. 3 requires a separate inversion of \((D + m)\) for every source point \((x, t)\). Usually, lattice calculations replace the \(1/(L^3 T) \sum_{x'', t''}\) of Eq. 1 by one or a few points per lattice,
\[ C_1(t) = \sum_{x',x'',t''} \langle O_1(x', t'' + t)O_2(x'', t'') \rangle. \]  
(4)

Obviously, \( C_1(t) \) is an approximation to \( C(t) \) on a single background configuration, so in an average over an ensemble of gauge configurations \( \langle C_1(t) \rangle = \langle C(t) \rangle + O(1/\sqrt{L^3 T}) \).

If preparation of lattices for use in a data set were expensive (for example, in a dynamical fermion simulation) it would be a more efficient use of them to compute correlators like \( C(t) \) rather than \( C_1(t) \). If it were possible to do part of the calculation cheaply, it might also be advantageous to break up the calculation
\[ C(t) = C_A(t) + C_B(t) + \ldots \]  
(5)

and approximate only some parts of the correlator (only \( C_A(t) \), say) by a \( C_1 \). This can be done easily if one has constructed \( n \) eigenmodes of the massless Dirac operator \( D|j\rangle = i\lambda_j |j\rangle \). Then the quark propagator can be broken into two pieces, \( G = G_L + G_H \), where \( G_L \) is given by an explicit mode sum
\[ G_L(x, t; x', t') = \sum_{j=1}^n \frac{\langle x, t | j \rangle \langle j | x' t' \rangle}{i\lambda_j + m}. \]  
(6)

and \( G_H \) is the remainder. Then the meson correlator becomes
\[ C(t) = C_{LL}(t) + C_{HL}(t) + C_{LH}(t) + C_{HH}(t). \]  
(7)

\( C_{LL} \) would be calculated from all source points on the lattice, while \( C_{HL}, C_{HL}, \) and \( C_{HH} \) would come from only a few source points, or a single point. Note that as long as one does
not include all eigenmodes into the sum, either directly or indirectly through Eq. 7, one is only approximating the two point function. \( C(t) \) does not equal \( C_{LL}(t) \) alone.

Does this trick gain anything in statistics? One might suspect that it would, for several reasons. First, there is just more sampling per lattice. If we could do a full “all-to-all” calculation (with no mode truncation) we might expect some gain due to the larger data sample. It would not be a complete reduction by \( 1/\sqrt{L^3T} \), because correlators from nearby sources on the lattice are highly correlated, but some gain might result. Second, it is reasonably well-known that at low quark masses, hadron propagators from a single source do not show a regular exponentially-falling behavior. Some averaging over position is needed to smooth the signal. This can be done by using several propagators for several source points, at a cost which increases linearly per source point. However, most of the irregularity comes from the low eigenmode part of the propagator. Computing “all to all”propagators from the low mode part of the quark propagator is essentially free once the low modes are computed.

Using Eq. 7 at larger quark mass is not likely to improve the signal, simply because low modes do not make a significant contribution to any meson correlator. At larger quark mass, \( C_{LL}(t) \) remains very “flat” while \( C(t) \) falls steeply. There is a considerable cancellation between \( C_{LL}(t) \), \( C_{HH}(t) \), and the interference terms. The noise in this cancellation is not reduced by averaging \( C_{LL}(t) \) alone.

The method has an obvious additional cost, compared to a usual spectroscopy simulation: the eigenmodes must be computed. This may or may not be a significant overhead. For the data set of our tests, computing the lowest twenty eigenmodes of the squared massless Dirac operator takes about 8 time units, while the complete set of quark propagators from the lightest mass studied to the heaviest takes about 16 time units times two (for two sets of propagators) per lattice. These eigenmodes were used to precondition the inversion of the Dirac operator, and this appeared to reduce the number of Conjugate Gradient steps needed at the lowest quark mass by about forty per cent. Even doing one source point of propagators is accelerated by projecting out low modes.

We are not aware of previous applications of this rather simple idea. It is common to use low eigenmodes of the Dirac operator directly in overlap fermion calculations. (Compare the recent work by Giusti, Hernandez, Laine, Weisz, and Wittig.) DeGrand and Heller used a similar “hybrid” method to compute disconnected diagrams, summing the low mode contribution exactly and using a stochastic estimator for the high mode part of the correla-
tor. “All-to-all” quark propagators have been computed using rather different (stochastic) methods by Duncan, Eichten and Yoo \[6\]. We believe that C. Michael and S. Wright \[7\] are doing similar work.

II. NUMERICAL TESTS

In order to test these statements we used quark propagators and eigenmodes used in a previous measurement of the $B_K$ parameter \[8\]. They were computed on 80 quenched gauge configurations of size $36 \times 12^3$ generated with the Wilson gauge action at $\beta = 5.9$. The fermion action is an overlap \[9\] Dirac operator with a kernel action which uses first and second nearest neighbor interactions \[10\] which are themselves composed of HYP blocked \[12\] gauge links. The lowest twenty eigenmodes of the massless overlap Dirac operator $D(0)$ are constructed from eigenmodes of the squared Hermitian Dirac operator $H(0)^2 = D(0)^\dagger D(0)$ with $H(0) = \gamma_5 D(0)$, using an adaptation of a Conjugate Gradient algorithm of Bunk et al. and Kalkreuter and Simma \[11\]. We consider spectroscopy with four quark masses $m_q = 0.015, 0.020, 0.025$ and 0.035, which correspond to pseudoscalar to vector meson mass ratios $m_{PS}/m_V$ ranging between about 0.4 to 0.64. The correlators used Gaussian sources $\Phi = \exp(-r/r_0)^2$ with a size $r_0/a = 3$. All the data shown will use point sinks projected onto zero momentum by summing over each time slice. On each of the configurations the inversion of the Dirac operator was done on two sources, one located on time-slice $t = 0$, the other on $t = 16$. We average over these two positions. The $\Gamma$ matrices depend on the meson in question and we shall use the following abbreviations:

\[
\begin{array}{cccc}
P & S & A_\mu & V_\mu & B_{\mu\nu} \\
\gamma_5 & 1 & \gamma_5\gamma_\mu & \gamma_\mu & \gamma_\mu\gamma_\nu
\end{array}
\]

In order to remove the zero modes from the pion correlator we consider primarily the difference of the pseudo-scalar and the scalar correlator ($PP - SS$).

To begin our study of the effect of keeping all source points for the low eigenmodes, we show the ratio of the error bars for $C(t)$ at fixed time-slice $t = 5$ for $n = 20$ eigenmodes included as “all-to-all” propagators and $n = 0$ in Fig.\[5\]. We observe a gain of up to 30%. The gain is also larger if one does not average over the two sources for each configuration.
FIG. 2: Ratio of the error bars for $n = 20$ compared $n = 0$ at time-slice $t = 5$ for the different meson correlators. Data uses two source points for the high eigenmode part of the correlator.

For correlators which are well behaved for $t$ closer to $T/2$, the gain in this region is also larger as the low-lying modes become more important there.

Next, we turn to spectroscopy. In Fig. 3 we show the effective mass plots for the $PP−SS$ correlator and the vector meson. $n = 0$ is the correlator computed with the conventional method, whereas $n = 20$ labels the one which the average over the sources taken over the 20 lowest eigenmodes. We observe a significant improvement in the error bars of the two-point functions. The jackknife error bars for both methods are consistent.

In Figs. 4 and 5 we show the effective mass plots for the vector meson extracted from the $VV$ and the $B_{0i}B_{0i}$ correlators. In both channels large fluctuations at large $t$ due to the small box size are visible. The improvement in the two-point function due to the eigenmodes is small in the $VV$ channel. In the $B_{0i}B_{0i}$ however the signal improves significantly. (This channel has a contribution when both the quark and antiquark propagate through zero modes, as opposed to the $VV$ channel, which has only zero mode-nonzero mode interference terms.) The masses extracted from the two correlators are consistent.

The question arises, how many eigenmodes are sufficient to achieve the desired improve-
FIG. 3: Effective mass of the $PP - SS$ correlator for different quark masses.

FIG. 4: Effective mass of the $B_0i$ (vector) correlator for different quark masses.
ment in the error bar. (Obviously, the answer will depend on quark mass, simulation volume, and also probably on lattice spacing and choice lattice fermion discretization.) In Fig. 6 we show the dependence of the extracted mass from the $PP - SS$ and $B_{0i}$ correlator on the number of eigenmodes included. For the $PP - SS$ the gain in the error bar is negligible when only 4 eigenmodes are included. This is understandable as we have typically 3 to 4 zero modes per configuration, and these channels do not couple to zero modes. The gain is 23% for 12 and 30% for 16 and 20 modes included. For the vector meson mass from the $B_{0i}$ correlator, the gain is almost linear in from 0 to 12 included eigenmodes and constant at 40% thereafter. In this case we gain because the correlator has contributions from zero modes.

Let us finally look at the interplay between the inclusion of a second source and the eigenmodes. In Fig. 7 we plot the uncertainty for the masses divided by the uncertainty for the mass extracted from the correlator with two sources and 20 eigenmodes. We see that the uncertainty of $m_{PP-SS}$ ($m_V$) decreases by about 12% (30%) by including the second source. However, by including a sufficiently large number of eigenmodes, the effect of the second source becomes smaller, i.e. a 6% and 14% gain, respectively.
FIG. 6: Dependence of the extracted $PP - SS$ and $B_{0i}$ mass on the number of eigenmodes included at $am_q = 0.025$.

FIG. 7: The error of the $PP - SS$ and $B_{0i}$ mass for one and two source points normalized to the error for the mass extracted from the correlator with two source points and 20 eigenmodes included. Again, $am_q = 0.025$ and the fit range was from $t = 8$ to $18$.

III. SUMMARY

To summarize, replacing the contribution of low eigenmodes to hadron propagators by an “all to all” contribution significantly improves the quality of the signal in some channels. This is especially the case for the pseudoscalar-scalar difference and the $B_{0i}$ vector meson correlator. We demonstrated that for these channels this gain translates into a smaller uncertainty in the meson masses.

We studied the dependence of their error bars on the number of eigenmodes included and found that for our simulation parameters it is sufficient to include about 12 eigenmodes. This number is presumably simulation volume dependent. If one had a set of eigenmodes
in hand, it would be easy to test how many eigenmodes would be needed, and over what quark mass range the method would reduce fluctuations enough to be worth pursuing. This could be done with low statistics investigations, basically by making pictures like Fig. [10].

During most of the work we combined the data from two sources on \( t = 0 \) and \( t = 16 \). This stabilizes the extraction of the masses significantly for \( n = 0 \). However, as we include more eigenmodes in the sum over source positions, this gain decreases and becomes almost negligible for \( n = 20 \). At light quark masses an “all to all” calculation restricted to low eigenmodes is competitive in cost of reducing fit uncertainty with the use of full propagators from several source points per lattice.

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