Accessing High Momentum States In Lattice QCD

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Two measures are defined to evaluate the coupling strength of smeared interpolating operators to hadronic states at a variety of momenta. Of particular interest is the extent to which strong overlap can be obtained with individual high-momentum states. This is vital to exploring hadronic structure at high momentum transfers on the lattice and addressing interesting phenomena observed experimentally. We consider a novel idea of altering the shape of the smeared operator to match the Lorentz contraction of the probability distribution of the high-momentum state, and show a reduction in the relative error of the two-point function by employing this technique. Our most important finding is that the overlap of the states becomes very sharp in the smearing parameters at high momenta and fine tuning is required to ensure strong overlap with these states.

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I. INTRODUCTION

Lattice QCD has enjoyed great success as a tool for first-principles hadron-structure calculations. Early pion electromagnetic form factor calculations [1, 2] and nucleon form factor calculations [3, 4] established the formalism and presented first results establishing the challenges ahead for obtaining precision form factors to confront experimental data. Nucleon form factors continue to be an active area of research [6–13] and a comprehensive review of recent form factor calculations can be found in [14] and references therein.

In practice, current lattice calculations were limited to a momentum transfer of approximately $Q^2 = 3$ GeV$^2$ due to a challenge of increasing statistical errors. Recently, calculations of the nucleon and pion form factors at $Q^2 = 6$ GeV$^2$ have been performed using variational techniques [15]. In this paper we explore very high momentum states and propose that, with sufficient optimization, momentum states and near-by excited states, and show how these measures determine the optimal smeared operator for ground state isolation early in Euclidean time.

We also introduce anisotropy into the smeared operators in the direction of momentum in an effort to improve the coupling to these Lorentz-contracted high-momentum states. Our results are complementary to the variational techniques of Ref. [15] in that the optimal set of smearings for accessing a variety of momenta can be combined to create a correlation matrix providing an effective basis for eigenstate isolation.

II. TWO-POINT FUNCTIONS

The two-point function of a baryon on the lattice in momentum space is given by

$$G_2(\vec{p}, t) = \sum_x e^{-ip\cdot x} \langle \Omega | \chi_i(x) \bar{\chi}_i(0) | \Omega \rangle,$$  \hspace{1cm} (1)

where $\chi_i$ and $\bar{\chi}_i$ annihilate and create the baryon respectively at the sink point $x$ and source point 0 and the index $i$ admits various spin-flavor structures for the interpolators. In the case of the proton, the annihilation operator is

$$\chi_1 = \epsilon^{abc}(u^T_a C \gamma_5 d_b) u_c,$$  \hspace{1cm} (2)

where $u$ and $d$ represent the spinors for the up and down quarks respectively and $C$ is the charge conjugation matrix. It can be shown that, for positive parity states,

$$G_2(\vec{p}, t) = \sum_B \frac{\gamma \cdot p + m}{2E_B} \lambda_B e^{-E_B t},$$  \hspace{1cm} (3)

where the sum over $B$ represents the ground and excited states of the baryon. It is common to average the $(1,1)$
and $(2, 2)$ elements of the Dirac matrix where the signal for positive parity states is large. At zero momentum, the Dirac matrix contribution is then 1. The coefficient $\lambda_B$ provides a measure of the total overlap of $\bar{\chi}_i$ at the source and $\chi_i$ at the sink with the state $B$. It is the product of the source and sink overlaps which may be different if different smearings are used at the source and the sink. In this investigation the source will be fixed to a point source such that variation in $\lambda_B$ is proportional to the variation in the overlap of $\chi_i$ which will encounter a wide range of different sink smearings.

Each state decays at a rate proportional to the exponential of its energy. By evolving forward in Euclidean time, excited state contributions die away allowing the ground state to be isolated. This is less than ideal for the calculation of three-point functions that require effective ground state isolation close to the source to avoid large Euclidean time evolution and an associated loss of signal. It is for this reason that various techniques have been implemented for earlier Euclidean-time isolation of the ground state.

When calculating the two-point function, it is possible to choose the momentum of the baryon. On the finite lattice, momentum is quantised

$$\vec{p} = \frac{2\pi}{N_L a} (p_x, p_y, p_z)$$

(4)

where $N_L$ is the spatial extent of the lattice, $a$ is the lattice spacing and $p_x$, $p_y$, $p_z$ are integers restricted to the range

$$-\frac{N_L}{2} < p_i \leq \frac{N_L}{2}.$$  

(5)

Due to the construction of the discrete fermion propagator, momentum input into the two-point function becomes proportional to $\sin(\vec{p})$, therefore, it is only reasonable to consider momentum states where

$$|p_i| \lesssim \frac{N_L}{4},$$  

(6)

such that the dispersion relation is approximately satisfied.

### III. GAUSSIAN SMEARING

Gaussian smearing is an iterative procedure applied to the source or sink of the two-point function in order to improve the relative coupling to the ground state of the particle. Consider

$$\chi_{i+1}(x) = F(x, y)\chi_i(y).$$  

(7)

with [16]

$$F(x, y) = (1 - \alpha) \delta_{xy} + \frac{\alpha_x}{6} \left( U_1^\dagger(x - a\hat{x}) \delta_{x-\hat{x}, y} + U_1(x) \delta_{x+\hat{x}, y} \right) + \frac{\alpha}{6} \sum_{\mu = 2}^3 \left( U_\mu^\dagger(x - a\hat{\mu}) \delta_{x-\hat{\mu}, y} + U_\mu(x) \delta_{x+\hat{\mu}, y} \right)$$

(8)

where $\alpha_0 = 0.7$ and $\alpha$ and $\alpha_x$ are normalised such that

$$\frac{4\alpha + 2\alpha_x}{6} = \alpha_0.$$  

(10)

### IV. MEASURES

Gusken [16] introduced the measure

$$R = \frac{G_2(t') e^{+m_0 t'}}{G_2(0)},$$

(11)

for quantifying the ground state isolation of a hadron. By taking a point, $t'$, sufficiently late in time such that the excited state contributions become negligible, the ground state can be evolved back to the source via $e^{+m_0 t'}$ to evaluate the fraction of $G_2(0)$ it holds. However, with sufficient smearing, states can contribute negatively to the two-point function, allowing this ratio to exceed 1 and making it difficult to interpret the results.

The first measure we introduce follows from this idea by determining the deviation of $G_2(t)$ from the ideal two-point function of a single ground state. It is similar in principle to Gusken’s measure, however, it is capable of taking into account the presence of states with negative coupling to the operator. The measure, $M_1$, is defined as,

$$M_1 = \frac{1}{t_f - t_i + 1} \sum_{t = t_i}^{t_f} \frac{\left( e^{-E_0(t-t_0)} - \tilde{G}_2(t) \right)^2}{G_2^2(t)},$$

(12)

where $\tilde{G}(t) = G(t)/G(t_0)$. The factor $-1$ makes this measure maximal when $G(t)$ is a pure exponential of the ground state. The energy $E_0$ is determined from a $4 \times 4$
source-sink-smeared variational analysis \cite{23} of the zero momentum state with the correct dispersion relation applied for finite-momentum states.

Another common method of extracting coupling effectiveness is to perform a four parameter, two exponential fit on a region close to the source of the two-point function, i.e.

\[ G_{\text{fit}} = a_1 e^{-a_2 t} + b_1 e^{-b_2 t}. \]  

However, this method tends to prove unreliable with the parameters varying with the fit window. The method is limited by the fact that it cannot take into account any states with higher energy than the two considered.

The second measure we introduce works similar to this. However, the parameters of the exponentials are predetermined by a variational analysis \cite{24}. This leads to a simple linear fit of known exponentials, i.e.

\[ G_{\text{fit}} = \lambda_0 e^{-E_0 t} + \lambda_1 e^{-E_1 t} + \lambda_2 e^{-E_2 t}. \]  

We can then find the proportion of the \( i \)-th state in the two-point function with the measure

\[ M_{2,i} = \frac{|\lambda_i|}{\sum_k |\lambda_k|}. \]  

We use a 4\( \times \)4 correlation matrix to extract our excited state masses, constructed from the \( \chi_1 \) operator with 16, 35, 100 and 200 sweeps of smearing. We choose to use the larger basis in order to ensure that the first three eigenstate energies are accurately determined.

We have verified that no multi-particle states are present in the variational analysis by applying the single-particle dispersion relation to the zero momentum effective state masses to successfully predict the effective masses of the same states with non-zero momentum.

Our error analysis is performed with the second-order single-elimination jackknife method. Linear fits are performed using the normal equations with exact matrix inversion where possible and singular value decomposition otherwise.

\[ G_{\text{fit}} = a_1 e^{-a_2 t} + b_1 e^{-b_2 t}. \]  

\[ G_{\text{fit}} = \lambda_0 e^{-E_0 t} + \lambda_1 e^{-E_1 t} + \lambda_2 e^{-E_2 t}. \]  

\[ M_{2,i} = \frac{|\lambda_i|}{\sum_k |\lambda_k|}. \]  

V. LATTICE DETAILS

Our calculations are performed on configurations of size 32\( ^3 \times 64 \) with a lattice spacing of 0.0907 fm provided by the PACS-CS collaboration \cite{24}. These lattices have 2+1 sea quark flavours generated with the Iwasaki gauge action \cite{25} and the non-perturbatively improved Clover fermion action \cite{26} with the \( \kappa \) values for the light quarks and the strange quark given by 0.13754 and 0.13640 respectively, and \( C_{SW} = 1.715 \). This gives a pion mass of \( m_\pi = 389 \text{ MeV} \).

In order to eliminate any bias caused by smearing in the source, we use a single set of propagators generated with a point source. All of the smearing is then applied to the sink, making the two-point functions smearing dependent. All momentum will be in the \( x \) direction, i.e. \( p_y = 0 \) and \( p_z = 0 \) in Eq. (11).

We use a 4\( \times \)4 correlation matrix to extract our excited state masses, constructed from the \( \chi_1 \) operator with 16, 35, 100 and 200 sweeps of smearing. We choose to use the larger basis in order to ensure that the first three eigenstate energies are accurately determined.

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\[ G_{\text{fit}} = a_1 e^{-a_2 t} + b_1 e^{-b_2 t}. \]  

\[ G_{\text{fit}} = \lambda_0 e^{-E_0 t} + \lambda_1 e^{-E_1 t} + \lambda_2 e^{-E_2 t}. \]  

\[ M_{2,i} = \frac{|\lambda_i|}{\sum_k |\lambda_k|}. \]  

VI. RESULTS

A. Isotropic Smearing

We first calculate the measure from Eq. (12) where the two-point functions have been normalised 1 time slice after the source, with \( t_i = 1 \) and \( t_f = 6 \). The two-point function is calculated at every sweep of sink smearing between 1 and 480, up to an rms radius of 13.68 in lattice units. For this particular ensemble, the two-point function that shows the highest proportion of ground state has 136 sweeps of smearing at the sink, or an rms radius of 6.92 lattice units as seen in Fig. 1. Also apparent is that the effectiveness of the smearing at isolating the ground state is significantly reduced fairly close to the optimal amount of smearing. At only 30 sweeps away from the ideal number of sweeps, the deviation from the ideal two-point function has increased by a factor of 10.

When we move to \( p_x = 1 \) in Eq. (11), which gives momentum in the \( x \) direction of 427 MeV, the ideal number of smearing sweeps reduces by just one sweep to 135 (rms radius 6.90 lattice units), as shown in Fig. 2. This can be explained by considering the relativistic \( \gamma \) factor, which is given by the ratio of the relativistic energy momentum relation and the ground state mass. The fitted ground state mass for the proton is \( M_P = 1.273(21) \text{ GeV} \), giving a relativistic energy of \( E_P |_{\gamma=1} = 1.343(23) \text{ GeV} \) and \( \gamma = 1.05 \). Given that all of the excited states are more massive, and therefore exhibit less Lorentz contraction than the ground state, it is feasible that there is very little difference in the probability distribution between this state and the zero momentum state, thus the ideal amount of smearing should be very similar to the zero momentum state.

At \( p_x = 3 \) in Fig. 2 the optimal number of smearing sweeps...
FIG. 2. The measure from Eq. (12) at $p_x = 1$ (left) and $p_x = 3$ (right) in Eq. (4). There is little difference between the measure at $p_x = 0$ and $p_x = 1$, due to the fact that the probability distributions between the two momentum states are nearly identical. At $p_x = 3$, the rms radius of the optimal smearing level is smaller by a factor of 0.85 relative to the $p_x = 0$ state, whereas the relativistic $\gamma$ factor provides a Lorentz contraction factor of $\gamma^{-1} = 0.72$.

FIG. 3. The measure from Eq. (12) at $p_x = 5$ (left) and $p_x = 7$ (right) in Eq. (4). The value of the measure at the optimum number of smearing sweeps for this momentum state is approximately equal to that of the $p_x = 3$ state, indicating that good ground state isolation is possible even at higher momenta. At $p_x = 7$, the deviation from the ideal two-point function has increased by a factor of 10 only 5 sweeps from the optimal smearing level, as shown in the inset graph.

sweeps has decreased to 98. The maximum value of the measure has also decreased relative to the lower momentum states, indicating relatively more excited state contamination, though still achieving good isolation. The ratio of the rms radius of the optimal smearing for this state to the optimal smearing for the ground state is 0.89, compared to the relativistic $\gamma^{-1}$ factor of 0.72. At $p_x = 5$, corresponding to a momentum transfer of approximately 4.55 GeV$^2$, shown in Fig. 3 the optimal number of sweeps is 52 (rms radius 4.27 lattice units). However, the maximum value of the measure is close to the maximum value for the $p_x = 3$ case, indicating that very efficient isolation is possible, even at larger momentum transfers.

Moving to $p_x = 7$, equivalent to a momentum transfer of 8.93 GeV$^2$, there is significant noise far from the source in the two-point function, even for highly optimised smearing values. Hence we consider $t_f = 5$ in the measure from Eq. (12) at this value of momentum. The ideal number of sweeps decreases to 27 sweeps, or 3.08 lattice units rms radius, seen in Fig. 3. Notably, the deviation from the ideal two-point function increases by a factor of 10 only 5 sweeps from this optimal value, corresponding to a change in rms radius of less than 0.3 lattice units.

Using the measure described in Eq. (15), we first consider the three exponential fit between time slices 1 and 6 after the source with masses 1.273(21) GeV, 2.301(28) GeV and 2.786(95) GeV as determined in our correlation matrix analysis. From the results in Fig. 4, we can see that, in the region where the first measure
predicts ideal smearing levels, there is a sharp change in
the structure of the graph. In order to determine the
cause of this, we compare with the fits containing only
the ground and first excited states. Fig. 5 shows that
the optimal number of smearing sweeps lies close to the
value predicted by the first measure. The overlap at the
optimal number of sweeps, 138 in this case, is 99.31(8)%,
indicating that, in the three exponential fit, we are at-
ttempting to fit two quickly decaying exponentials using
only 0.69% of the signal available. This leads us to be-
lieve that, in the regions of ground state dominance where
we are most interested, the coefficient from the quickly
decaying third state cannot be determined accurately,
therefore dominates well beyond where it should be al-
lowed to contribute at all. For this reason, we will only
consider fits using the ground and first excited states.

The contamination due to excited states in the two ex-
ponential fit at zero momentum increases rapidly away from
the optimum smearing level. Of the smearing
sweeps used to extract the masses from the variational
analysis, the one that shows the most overlap with the
ground state is 200 sweeps, or an rms radius of 8.55 lat-
tice units, with 77.69(7)%, or 32 times more excited state
contamination than the optimal smearing level.

At the first non-zero momentum state, the results
present similarly to the first measure, the optimal amount
of smearing is 1 sweep less than that of the non-zero mo-
mentum ground state, and 2 sweeps more than the opti-
mal amount determined by the first measure. At \( p_x = 3 \)
in Eq. (4) shown in Fig. 6, the overlap is maximised at 101
sweeps of smearing, or an rms radius of 5.95 lattice units,
once again agreeing within only a few sweeps of the op-
timum level suggested by the first measure. Remarkably,
considering the use of a point source, the proportion of
ground state present at this optimal amount of smearing
is 98.87(12)\%.

At \( p_x = 5 \) and \( p_x = 7 \) in Fig. 7 there is again good
agreement between the two measures, with the optimal
smearing level being 53 and 26 sweeps respectively. Even
at a momentum transfer of 8.93 GeV\(^2\), 97.20(20)\% over-
lap is achieved with the ground state, and once again,
very few sweeps from the optimum level, the overlap
drops dramatically. At \( p_x = 7 \), far from the optimal
number of smearing sweeps, it is unlikely that any highly
Lorentz contracted state would couple to such a large
sink. The second peak in Fig. 7 can therefore be consid-
ered to signify a limit to the domain of validity of the
measure.
FIG. 7. Ground state proportion at $p_x = 5$ (left) and $p_x = 7$ (right) in Eq. (4). Even at these very high momentum transfers, good overlap with the ground state is achieved for an optimised sink. Far from the optimal number of smearing sweeps at $p_x = 7$, it is clear that the measure is no longer applicable, as there would be little, if any highly Lorentz contracted ground state present.

B. Anisotropic Smearing

As anisotropy is introduced to the smearing as described in Eq. (9), we consider the first measure from Eq. (12) at the first non-zero momentum state and find that there is no improvement to the ground state isolation, as shown in Fig. 8. There is, however, an ideal number of sweeps that increases for decreasing $\alpha_x$ that shows approximately equal ground-state proportion relative to the isotropic smearing case.

At $p_x = 3$ in Eq. (4), in spite of the clear difference in the smearing sweeps required to maximise overlap with the source, Fig. 9 shows that introducing anisotropy to the smearing does not result in improved isolation of the ground state. The structure of the curve is similar to that of the $p_x = 1$ state, where there is an optimal number of sweeps for every value of $\alpha_x$ which increases with decreasing $\alpha_x$.

Once again, there is no improvement in the ability of anisotropic smearing to isolate the ground state at the momentum of $p_x = 5$, as shown in Fig. 10. The structure revealed in the lower momentum states persists for this state and for the $p_x = 7$ state in Fig. 11. From these results, optimisation of the number of smearing sweeps alone is sufficient to achieve good isolation of the ground state of the two-point function at a range of momenta.

We now investigate how anisotropic smearing affects the signal-to-noise ratio or quality of the two-point function at high momenta. Since we have ensured that the ground state is isolated as close to the source as possible, we now determine the quality of the signal a few time slices away from the source. We consider the relative error of the two-point function four times slices after the source at the optimal number of smearing sweeps for each value of our anisotropy parameter, $\alpha_x$.

For $p_x = 3$, Fig. 12 shows the two-point function at $t = 4$. The smallest relative error occurs when the smearing is isotropic. Increasing the momentum to $p_x = 5$ lattice units shows that there is only a small improvement to the relative error for values of $\alpha_x \sim 0.48$. It is worth noting that the first of the minima visible in Fig. 13 at $\alpha_x = 0.36$ corresponds to the anisotropy expected due to Lorentz contraction as $\alpha_x/\alpha = 0.51$ equals $\gamma^{-1} = 0.51$.

The banding structure visible in Fig. 13 is a result of the optimal number of smearing sweeps increasing for decreasing values of $\alpha_x$. Each discontinuity in the graph for $\alpha_x > 0.36$ is the result of the optimal number of smearing sweeps decreasing by 1. It is an artifact resulting from the density of the points in $\alpha_x$ being much finer than the density of the points in the number of smearing sweeps. Moving to $p_x = 7$ in Fig. 13 we see a distinct improvement in the correlation-function relative error when anisotropy is introduced. Both $\alpha_x = 0.26$ and 0.32 provide a 10% reduction in the error relative to that observed at the isotropic value of 0.7. The values of $\alpha_x \simeq 0.26$ to 0.32 provide $\alpha_x/\alpha = 0.37$ to 0.46, in accord with the value of $\gamma^{-1} = 0.39$ predicted by Lorentz contraction.

VII. CONCLUSION

We have presented two new measures of the effectiveness of smeared operators in isolating the ground state of a hadron in the two-point function. Both measures show good agreement with each other. We have performed a detailed analysis of ground state isolation with each measure and have shown that optimisation of the smearing can lead to remarkable improvement to the ground state isolation. Furthermore, the ability to isolate the ground state decreases dramatically a few sweeps from the optimal number of smearing sweeps for the higher momentum states. In selecting a basis for a correlation...
matrix analysis, these optimal smearing parameters are preferred.

On the introduction of anisotropy to the smearing, we found that there was no appreciable improvement to the overlap with the ground state. The relative proportion of the ground state for an isotropic source is already high. Optimising the number of sweeps of isotropic smearing alone is sufficient to ensure maximal isolation of high-momentum ground states. The introduction of anisotropy does provide a small improvement to the correlation function of high-momentum states a few Euclidean time slices after the source.

Our results indicate that future studies of high-momentum states should adopt this relatively cheap program of tuning the smearing parameters to optimize isolation and overlap with the states of interest. We anticipate this approach will be of significant benefit in future form factor studies.

VIII. ACKNOWLEDGMENTS

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FIG. 8. The first measure from Eq. (12) (left) and the Ground State Proportion (right) with anisotropic smearing at $p_x = 1$ from Eq. (4). Introducing anisotropy to the smearing does not improve the isolation of this state. However, the Lorentz contraction is small so little improvement would be expected.

FIG. 9. The first measure from Eq. (12) (left) and the Ground State Proportion (right) with anisotropic smearing at $p_x = 3$ from Eq. (4). No improvement is seen in the isolation of the ground state, in spite of the relativistic $\gamma$ factor of 1.39 giving a length contraction factor of 0.72 in the $x$ direction.

FIG. 10. The first measure from Eq. (12) (left) and the Ground State Proportion (right) with anisotropic smearing at $p_x = 5$ from Eq. (4). The structure observed in the plots of the $p_x = 3$ state is retained, with more sweeps of smearing required as anisotropy is increased.
FIG. 11. The first measure from Eq. (12) (left) and the Ground State Proportion (right) with anisotropic smearing at $p_x = 7$ from Eq. (4). Even at a momentum of 2.99 GeV, anisotropy in the smearing does not improve isolation of the ground state.

FIG. 12. Relative error in the two-point function measured four time slices after the source for $p_x = 3$ as in Eq. (4). At this momentum, isotropic smearing provides the best relative error.
FIG. 13. Relative error in the two-point function measured four time slices after the source for $p_\perp = 5$ (left) and $p_\perp = 7$ (right) as in Eq. (4). At $p_\perp = 5$, there is a small amount of improvement for anisotropic smearing at $\alpha_x/\alpha$ in the region of $\gamma^{-1} = 0.51$. At $p_\perp = 7$, a 10% improvement in the relative error is seen for values of $\alpha_x \simeq 0.26$ to 0.32 where $\alpha_x/\alpha = 0.37$ to 0.46, in accord with the value of $\gamma^{-1} = 0.39$ predicted by Lorentz contraction. Note that the emergent banding structure reflects a change in the optimal number of smearing sweeps by one.