Variance Reduction and Cluster Decomposition

Keh-Fei Liu\textsuperscript{1}, Jian Liang\textsuperscript{1}, and Yi-Bo Yang\textsuperscript{2}
\textsuperscript{1}Department of Physics and Astronomy, University of Kentucky, Lexington, KY 40506, USA
\textsuperscript{2}Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA

It is a common problem in lattice QCD calculation of the mass of the hadron with an annihilation channel that the signal falls off in time while the noise remains constant. In addition, the disconnected insertion calculation of the three-point function and the calculation of the neutron electric dipole moment with the \( \theta \) term suffer from a noise problem due to the \( \sqrt{V} \) fluctuation. We identify these problems to have the same origin and the \( \sqrt{V} \) problem can be overcome by utilizing the cluster decomposition principle. We demonstrate this by considering the calculations of the glueball mass, the strangeness content in the nucleon, and the CP violation angle in the nucleon due to the \( \theta \) term. It is found that for lattices with physical sizes of 4.5 - 5.5 fm, the errors of these quantities can be reduced by a factor of 3 to 4.

As the physical pion mass is accessible in lattice QCD simulations nowadays with larger physical volumes and several lattice spacings with different lattice actions to estimate the associated systematic errors, lattice QCD calculation is getting mature, particularly for flavor physics where the quark masses, heavy-light decay constants, CKM matrices, and strong coupling constant are reviewed and averaged by FLAG \textsuperscript{1}. On the other hand, the baryon physics is not as settled as that of mesons. Part of the reasons is illustrated in the Parisi-Lepage consideration of the signal-to-noise ratio of the nucleon two-point function. Since the variance of the nucleon propagator has three-pions as the lowest state in the correlator, the signal to noise (S/N) ratio is proportional to \( e^{-\left(m_N-\frac{3}{2}m_s\right)t} \) \textsuperscript{2} and noticeably grows exponentially with \( t \) when the pion mass is close to the physical one in lattice calculations. This is why baryon physics is more noisy than that of mesons. Furthermore, the S/N ratio for the pseudoscalar meson is independent of time so the pseudoscalar meson properties have the smallest statistical errors in lattice calculations.

While the systematic errors, such as the excited state contamination and \( O(a) \) errors with the local currents \textsuperscript{4}, are being addressed in addition to the usual large volume and continuum limits in the isovector nucleon matrix elements which involve only the connected insertion (CI) calculations, calculations of matrix elements in the disconnected insertion (DI) pose much larger a challenge. First of all, the calculation of the quark loop is numerically intensive. Despite various improvements with a better noise \textsuperscript{5}, noise reduction with hopping expansion \textsuperscript{6}, space-time dilution \textsuperscript{7}, and hierarchical probing \textsuperscript{8}, low-mode average to take into the large low-mode contribution to the quark loop exactly \textsuperscript{7, 9, 10}, and \( Z_3 \) grid noise with low-mode substitution for the nucleon propagator \textsuperscript{9, 11, 12}, the statistical errors of the DI are still in the 20 - 30% range which are an order of magnitude larger than those of the CI.

One special problem associated with the correlators of mesons involving annihilation channels or glueballs is that the signal falls off exponential with time, but the noise remains constant. Thus, after certain time separation, the signal falls below the noise and succumbs to the sign problem. Another aspect of the DI is observed in the DI three-point function involving a quark loop or the topological charge in the neutron electric dipole moment (nEDM) calculation from the \( \theta \) term, the fluctuations of the quark loop and the topological charge are proportional to \( \sqrt{V} \) which pose a challenge for calculations large volumes lattices. In this work, we shall show that the constant error and \( \sqrt{V} \) fluctuation in the DI have the same origin and they can be ameliorated with the help of the property of the cluster decomposition principle so that the S/N ratio can be improved by a factor of \( \sqrt{V/V_{R_e}} \) where \( V_{R_e} \) is the volume with radius \( R_e \) which is the effective correlation length between the operators.

One often invokes the locality argument to justify that experiments conducted on Earth is not affected by events on the Moon. This is a consequence of the cluster decomposition principle (CDP) in that if color-singlet operators in a correlator are separated by a large enough space-like distance, the correlator will be zero. In other words, the operators are not correlated in this circumstance. To be specific, it is shown \textsuperscript{13} that under the assumptions of translation invariance, stability of the vacuum, existence of a lowest non-zero mass and local commutativity, one has

\[
|\langle 0|B_1(x_1)B_2(x_2)|0\rangle|_4 \leq Ar^{-\frac{4}{3}}e^{-Mr} \tag{1}
\]

for a large enough space-like distance \( r = |x_1 - x_2| \), where \( \langle 0|B_1(x_1)B_2(x_2)|0\rangle \) is the vacuum-subtracted correlation function. \( B_1(x_1) \) and \( B_2(x_2) \) are two color-singlet operator clusters whose centers are at \( x_1 \) and \( x_2 \) respectively, \( M \) is the smallest non-zero mass for the correlator, and \( A \) is a constant. This is the asymptotic behavior of
a boson propagator $K_1(r)/r$. This means the correlation between two operator clusters far apart with large enough space-like distance $r$ tends to be zero at least as fast as $r^{-3}e^{-Mr}$. Given that the longest correlation length in QCD is $1/m_π$, one has $M \geq m_π$. Since the Euclidean separation is always 'space-like', the cluster decomposition principle (CDP) is applicable to the Euclidean correlators. Some of the recent attempts to reduce variences in the muon $g−2$ calculation [15], factorization of fermion determinant [16], and reweighting of nEDM calculation with topological charge density [17] have applied concepts similar to that of CDP. In this work, we prove that, applying the CDP explicitly, the error of an DI correlator can be improved by a factor of $\sqrt{V/V_{R_s}}$.

In evaluating the correlators, one often takes a volume sum over the three-dimensional coordinates. To estimate at what distance the large distance behavior saturates, we integrate the fall-off to a cut off distance $R$,

$$A(R,M) = \int_0^R d^3r \, r^{-\frac{3}{2}} e^{-Mr}$$
$$= 4\pi \left( \frac{\sqrt{\pi} erf(\sqrt{MR})}{2M^{\frac{3}{2}}} - \frac{\sqrt{\pi} erf(\sqrt{MR})}{2M^{\frac{3}{2}}} \right). \quad (2)$$

Here erf is the error function. Since the kernel of the integral decays very quickly, the integral has already gained more than 99.5% of its total value for $R = 8/M$. Assuming the fall-off behavior dominates the volume-integrated correlator, we consider $R_s \sim \frac{8}{M}$ as an effective cutoff and the correlation with separation $r > R_s$ has negligible contribution.

To test the principle of cluster decomposition with lattice data, we consider the two-point correlator for a fixed $t$ with a cutoff of $R$ in the relative coordinate between the two color-singlet operators $O_1$ and $O_2$

$$C(R,t) = \frac{1}{V^2} \left( \sum_{r < R} O_1(\vec{x} + r^2, t) \sum_{\vec{x}} O_2(\vec{x}, 0) \right), \quad (3)$$

where $r = \sqrt{[r^2]^2 + t^2}$. The correlation functions in the present work are calculated using valence overlap fermions on the RBC-UKQCD 2 + 1 flavor domain-wall configurations. More detailed definitions and numerical implementations can be found in previous works [10, 11, 18, 19].

We examine the nucleon two-point function first on the $48^3 \times 644$ lattice (48f) with the physical sea quark mass [20]. We use 3 valence quark masses corresponding to pion masses 70 MeV, 149 MeV and 260 MeV respectively.

The results for the nucleon correlators at $t = 9$ for three different valence quark masses are plotted in Fig. 1 as a function of $R$ which is the cutoff of the Euclidean distance $r$ between the point source and the sink. We see that the nucleon correlator basically saturates after $R \sim 15 = 1.71$ fm with $a = 0.114$ fm for the three cases. This agrees well with our earlier estimate of a saturation radius $R_s = 8/M$ which corresponds to $\sim 1.66$ fm. This shows that the CDP works and Eq. (2) gives a good estimate of $R_s$.

Since the signal of the correlators falls off exponentially with $r$, summing over $r$ beyond the saturating radius $R_s$ does not change the signal and will only gather noise. Let’s consider the disconnected insertion first and see how the $S/N$ ratio can be improved with this observation. In the case of the DI, the variance of the correlator in Eq. (3) $\frac{1}{V^2} \left( \langle \sum_{r < R} O_1(\vec{x} + r^2, t) \sum_{\vec{x}} O_2(\vec{x}, 0) \rangle^2 \right)$ can have a vacuum insertion in addition to the exponential fall off in $t$ due to the $O^1O$ operator. Incorporating translational invariance

$$\text{Var}(R,t) = \frac{1}{V^2} \sum_{\vec{x}} \left( \langle \sum_{r_1 < R} O_1(\vec{r}_1^2, t) \sum_{r_2 < R} O_2(\vec{r}_2, 0) \rangle \right)$$
$$+ \langle O_1(0,0)O_2^\dagger(\vec{x},0) \rangle + \ldots, \quad (4)$$

where $r_1 = \sqrt{|r_1|^2 + t^2}$ and $r_2 = \sqrt{|r_2|^2 + t^2}$ respectively. For the case where the $r_1^2$ and $r_2^2$ are integrated over the whole lattice volume, the leading vacuum insertion is proportional to unity and is independent of $t$. This is the reason why the noise remains constant over $t$ in DI. It is interesting to note that, in this case, the sum over $x$ and $r_2$ can be carried out separately. Consequently, $O_1$ and $O_2$ in DI fluctuate independently which leads to a variance which is the product of their respective variances. On the other hand, the constant variance is reduced to $V_{R_s}/V$ when $r$ is integrated to $R_s$, while the signal is not compromised. The sub-leading contribution (denoted by ...) in Eq. (4) has an exponential decay in $t$ with a mass in the scalar channel. It is clear that to leading order, the ratio of the cutoff $S/N$ at $R_s$ to that without cutoff is

$$\frac{S/N(R_s)}{S/N(L)} \sim \sqrt{\frac{V}{V_{R_s}}}. \quad (5)$$
We shall consider several DI examples involving volume summations over two or more coordinates. Since the convoluted sum with a relative coordinate in Eq. (3) can be expensive, we shall invoke the standard convolution theorem by calculating the product of two functions

\[
\tilde{K}(\vec{p},t) = \tilde{O}_1(-\vec{p})\tilde{O}_2(\vec{p}),
\]

where \( \tilde{O}_1(-\vec{p})/\tilde{O}_2(\vec{p}) \) is the Fourier transforms of \( O_1(\vec{x})/O_2(\vec{x}) \) in each configuration on their respective time slices. Then

\[
C(R,t) = \langle \int_{r<R} d^3\vec{r} K(\vec{r},t) \rangle.
\]

where \( K(\vec{r},t) \) is the Fourier transform of \( \tilde{K}(\vec{p},t) \). In this way, the cost of the double-summation, which is order \( V^2 \), is reduced to that of the fast Fourier transform (FFT) which is in the order of \( V \log V \).

The first example is the disconnected insertion for the nucleon matrix element with a scalar loop which involves a three-point function and can be expressed as

\[
C_3(R,\tau,t) = \sum_{\vec{x}} \sum_{r<R} O_N(\vec{x},t)S(\vec{x} + \vec{r},\tau)\tilde{O}_N(\vec{G},0),
\]

where \( S \) is the vacuum-subtracted scalar loop, \( \vec{G} \) denotes the source grid for increasing statistics [11]. Note here \( r = \sqrt{r_x^2 + (t-\tau)^2} \) is the 4-D distance and \( r_x \) is the spatial separation between the loop and the sink. Since the low-modes dominate the strangeness in the nucleon [9], we calculate the strange quark loop with low-modes only to illustrate the CDP effect. The sum over the spatial relative coordinate between the scalar quark loop \( S \) and the sink interpolation operator \( O_N(\vec{x},t) \) is carried out through the convolution in Eqs. (6-7). This calculation is done on the domain-wall \( 32^3 \times 64 \) (32ID) lattice [20] with pion mass \( \sim 170 \) MeV and the lattice size is \( 4.6 \) fm.

The upper panel of Fig. 2 gives the value and the error of \( C_3(R,\tau,t) \) in Eq. (8) as a function of \( R \) at \( \tau = 4 \) and \( t = 9 \). The The nucleon source-sink separation is 1.29 fm in this case. We see the error grows with \( R \) greater than \( \sim 12 \) while the central value remains constant within errors. This behavior reflects the fact that the signal without summing over \( |\vec{r}| \) falls off exponentially with \( \vec{r} \), while the error remains constant as shown in the lower panel.

Fig. 3 shows DI (scalar)—the disconnected three-point to two-point function ratio to obtain the scalar matrix element for the strange quark in the nucleon as a function of \( \tau - t/2 \) for two source-sink separations at 1.00 fm (upper panel) and 1.57 fm (lower panel). Two results with cutoffs of \( R_c = 27 \) and \( R_c = 12 \) are plotted. \( R_c \) is the cutoff radius for the relative coordinate between the sink and the quark loop in the spatial sum. It can be seen that the central values of the two cutoffs are all consistent within errors, while the errors with cutoff \( R_c = 12 \) are smaller than the ones with cutoff 27 by a factor of 4 or so. Thus, cutting off the spatial sum at the saturation distance can gain \( \sim 16 \) times more statistics.

Next, we consider the glueball correlators in Eq. (3) on the 48I lattice with \( La = 5.5 \) fm. The correlators from the scalar \( E^2 \) and \( B^2 \) operators and the pseudoscalar \( E \cdot B \) operator are presented in Fig. 4, where they are plotted as a function of \( R \) in Eq. (3) at \( t = 4 \). We note the scalar correlators saturate after \( R \sim 9 \) and the pseudo scalar one saturates after \( \sim 12 \), which can be understood in terms of the different ground state masses in these two channels. Again, comparing the error at \( R = 9 \) to that at \( R = 25 \) for the scalar case, the error is reduced by a factor of \( \sim 4 \) which is in reasonable agreement with the prediction of \( \sim (\frac{12}{16})^2 = 4.6 \) from Eq. (5). For the pseudoscalar case, the improvement is around 3 times and is consistent with the estimate of \( \sim (\frac{12}{16})^2 = 3.0 \).

Finally, we examine the CP-violation phase \( \alpha^1 \) on the
same 48I lattice which is needed for calculating the neutron electric dipole moment (nEDM). The phase is defined as

\[ \alpha^1 = \frac{\text{Tr}[C_3 Q(t) \gamma_5]}{\text{Tr}[C_2(t) \Gamma_c]} \]  

(9)

for large enough \( t \), where \( C_2(t) \) is the common nucleon two-point function, \( \Gamma_c = \frac{1 + \gamma_4}{2} \) is the parity projector, \( C_3 Q(t) \) is the nucleon propagator weighted with the total topological charge \( Q \)

\[ C_3 Q(t) = \sum_{\vec{x}} O_N(\vec{x}, t) \overline{O}_N(\vec{G}, 0) Q. \]  

(10)

We can turn the total topological charge into the summation of its density, i.e. \( Q = \sum_{x} q(x) \) where we use the plaquette definition for \( q(x) \). Then the expression of \( C_3 Q(t) \) with a cutoff \( R \) can be cast in the same form as in Eq. (8), except the scalar quark quark loop \( S \) is replaced with the local topological charge \( q(x) \) and the sum of the topological charge density is over the four sphere with a radius \( R \).

The result of \( \alpha^1 \) as a function of \( R \) in Fig. 5 shows that the signal saturates after \( R \sim 16 \). Cutting off the sum of \( q(x) \) at this \( R \) leads to a factor of \( \sim 3.6 \) times reduction in error compared to the case of reweighting with the total topological charge as in Eq. (10). This example indicates that for four-dimensional sums, our new method employing the CDP can also improve the S/N. As we illustrated in the introduction, the nEDM from the \( \theta \) term suffers from a \( \sqrt{N} \) problem. It is shown here it is related to the vacuum insertion in the variance. This problem is resolved by turning the topological charge into a 4-D sum of the local charge density and applying the CDP by cutting off the relative 4-D distance in the sum.

Regarding the nucleon correlator in Fig. 1, we notice that there is no conspicuous increase of the error as a function of \( R \). This is because, unlike the DI, the variance does not have an vacuum insertion for the CI. The leading contribution to the variance is expected to be \( e^{-3m_\pi r} \). This has a longer range than that of the signal which falls off with the nucleon mass. Therefore, in principle, one would expect some gain in the S/N when \( R \) is cut off at \( R_s \). Therefore, the corresponding ratio of S/N in Eq. (5) is

\[ \frac{S/N(R_s)}{S/N(L)} \sim \sqrt{\frac{A(L/2, 3m_\pi)}{A(R_s, 3m_\pi)}}. \]  

(11)

For the 48I lattice in Fig. 1, this ratio is 1.13 for the physical pion mass with the cutoff \( R_s = 8/M \). This is not nearly as much a gain as in the DI where the variance is dominated by the vacuum insertion. In the CI case, the noise saturates at \( \sim 8/(3m_\pi) = 3.5 \) fm. There is no gain for a lattice with a size larger than this.

To summarize, we have shown that the exponential fall off of the Cluster Decomposition Principle (CDP) seems to hold numerically for the several correlators that we examined. For the disconnected insertions (DI), we find that the vacuum insertion dominates the variance so that the relevant operators fluctuate independently and is independent of the time separation. This explains why the signal fall off exponentially, while the error remains constant in the DI. To employ the CDP, one can restrict the volume sum of the relative coordinate between the operators to the saturation radius \( R_S \) so as to gain a factor of \( V/V_s \) in statistics without compromising the signal. This applies to all DI cases. For the cases we have considered, namely the glueball mass, the strangeness content in the nucleon, and the CP violation angle in the nucleon due to the \( \theta \) term, we found that for lattices with a physical sizes of 4.5 - 5.5 fm, the errors of these quantities can be reduced a factor of 3 to 4. For the connected insertions, there is no vacuum insertion in the variance, the gain in statistics is limited.
[1] S. Aoki et al., Eur. Phys. J. C77, 112 (2017), arXiv:1607.00299 [hep-lat].
[2] G. Parisi, COMMON TRENDS IN PARTICLE AND CONDENSED MATTER PHYSICS. PROCEEDINGS, WINTER ADVANCED STUDY INSTITUTE, LES HOUCHES, FRANCE, FEBRUARY 23 - MARCH 11, 1983, Phys. Rept. 103, 203 (1984).
[3] G. P. Lepage, in Boulder ASI 1989:97-120 (1989) pp. 97–120.
[4] J. Liang, Y.-B. Yang, K.-F. Liu, A. Alexandru, T. Draper, and R. S. Sufian, (2016), arXiv:1612.04388 [hep-lat].
[5] S.-J. Dong and K.-F. Liu, Phys. Lett. B328, 130 (1994), arXiv:hep-lat/9308015 [hep-lat].
[6] C. Thron, S. J. Dong, K. F. Liu, and H. P. Ying, Phys. Rev. D57, 1642 (1998), arXiv:hep-lat/9707001 [hep-lat].
[7] M. Gong, Y.-B. Yang, A. Alexandru, T. Draper, and K.-F. Liu, (2015), arXiv:1511.03671 [hep-ph].
[8] A. Stathopoulos, J. Laeuchli, and K. Orginos, (2013), arXiv:1302.4018 [hep-lat].
[9] Y.-B. Yang, A. Alexandru, T. Draper, J. Liang, and K.-F. Liu (xQCD), Phys. Rev. D94, 054503 (2016), arXiv:1511.09089 [hep-lat].
[10] R. S. Sufian, Y.-B. Yang, A. Alexandru, T. Draper, J. Liang, and K.-F. Liu, Phys. Rev. Lett. 118, 042001 (2017), arXiv:1606.07075 [hep-ph].
[11] A. Li et al. (xQCD), Phys. Rev. D82, 114501 (2010), arXiv:1005.5424 [hep-lat].
[12] Y.-B. Yang, R. S. Sufian, A. Alexandru, T. Draper, M. J. Glatzmaier, K.-F. Liu, and Y. Zhao, Phys. Rev. Lett. 118, 102001 (2017), arXiv:1609.05937 [hep-ph].
[13] H. Araki, K. Hepp, and D. Ruelle, Helv. Phys. Acta 35, 164 (1962).
[14] Y. Chen, A. Alexandru, T. Draper, K.-F. Liu, Z. Liu, and Y.-B. Yang, (2015), arXiv:1507.02541 [hep-ph].
[15] T. Blum, N. Christ, M. Hayakawa, T. Izubuchi, L. Jin, and C. Lehner, Phys. Rev. D93, 014503 (2016), arXiv:1510.07100 [hep-lat].
[16] M. Cé, L. Giusti, and S. Schaefer, Phys. Rev. D95, 034503 (2017), arXiv:1609.02419 [hep-lat].
[17] E. Shintani, T. Blum, T. Izubuchi, and A. Soni, Phys. Rev. D93, 094503 (2016), arXiv:1512.00566 [hep-lat].
[18] M. Gong et al. (XQCD), Phys. Rev. D88, 014503 (2013), arXiv:1304.1194 [hep-ph].
[19] Y.-B. Yang, A. Alexandru, T. Draper, M. Gong, and K.-F. Liu, Phys. Rev. D93, 094503 (2016), arXiv:1509.04616 [hep-lat].
[20] T. Blum et al. (RBC, UKQCD), Phys. Rev. D93, 074505 (2016), arXiv:1411.7017 [hep-lat].