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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 firstprinciples, hadron-structure calculations. Early pion electromagnetic form-factor calculations [1,2] and nucleon form-factor calculations [3–5] 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 Ref. [14] and references therein.

In practice, current lattice calculations were limited to a momentum transfer of approximately $Q^2 = 3 \text{ GeV}^2$ due to a challenge of increasing statistical errors. Recently, calculations of the nucleon and pion form factors at $Q^2 = 6 \text{ GeV}^2$ have been performed using variational techniques [15]. In this paper we explore very high momentum states and propose that, with sufficient optimization of the smearing parameters alone, momentum transfers of the order $Q^2 = 10 \text{ GeV}^2$ can be accomplished in lattice hadron-structure calculations.

Smearing techniques have seen widespread use in many applications in lattice QCD since first being applied to fermion operators [16]. The most notable impacts can be found in spectroscopy calculations using variational methods [17–22]. In spite of these successes, there has been little in the way of the optimization of smearing parameters for high-momenta states. For low-momenta states there is no real need for optimization as the overlap of states is typically slowly varying with the smearing parameters. In the following we reveal that this is not the case for highmomenta states, and finely tuned optimization is very beneficial in accessing these states on the lattice.

Isolation of the ground state at high momentum is essential to removing otherwise large and problematic excited state contaminations. However, suppression of excited states through Euclidean evolution alone encounters a rapid onset of statistical noise. We introduce two different measures to quantify the coupling of a smeared operator to the ground state of a proton relative to the nearby 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

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

where χ_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

$$\chi_1 = \epsilon^{abc} (u_a^T C \gamma_5 d_b) u_c, \qquad (2)$$

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,

$$G_2(\vec{p},t) = \sum_B \frac{\gamma \cdot p + m}{2E_B} \lambda_B e^{-E_B t},$$
(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 λ_B provides a measure of the total overlap of $\bar{\chi}_i$ at the source and χ_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 λ_B is proportional to the variation in the overlap of χ_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 quantized

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

$$-\frac{N_L}{2} < p_i \le \frac{N_L}{2}.$$
(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

$$|p_i| \lesssim \frac{N_L}{4},\tag{6}$$

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

$$\chi_{i+1}(x) = F(x, y)\chi_i(y) \tag{7}$$

with [16]

$$F(x, y) = (1 - \alpha)\delta_{xy} + \frac{\alpha}{6}\sum_{\mu=1}^{3} (U^{\dagger}_{\mu}(x - a\hat{\mu})\delta_{x - a\hat{\mu}, y} + U_{\mu}(x)\delta_{x + a\hat{\mu}, y}),$$
(8)

where α is a constant, which we set to 0.7. We can introduce anisotropy to the smearing by introducing a

new constant α_x , which will act only in the x direction; the expression for the smearing then becomes,

$$F(x, y) = (1 - \alpha_o)\delta_{xy} + \frac{\alpha_x}{6}(U_1^{\dagger}(x - a\hat{x})\delta_{x - a\hat{x}, y} + U_1(x)\delta_{x + a\hat{x}, y}) + \frac{\alpha}{6}\sum_{\mu=2}^3(U_{\mu}^{\dagger}(x - a\hat{\mu})\delta_{x - a\hat{\mu}, y} + U_{\mu}(x)\delta_{x + a\hat{\mu}, y}),$$
(9)

where $\alpha_o = 0.7$ and α and α_x are normalized such that

$$\frac{4\alpha + 2\alpha_x}{6} = \alpha_o. \tag{10}$$

IV. MEASURES

In order to show improvement in the two-point function due to operator choice, quantitative measures must be introduced. Following the original motivation for introducing smeared sources, we consider measures that are capable of determining the deviation from the ideal scenario where the two-point function contains only the ground state.

Gusken [16] introduced the measure

$$R = \frac{G_2(t')e^{+m_0t'}}{G_2(0)},\tag{11}$$

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 $e^{+m_0t'}$ 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

$$M_1 = \frac{-1}{t_f - t_i + 1} \sum_{t=t_i}^{t_f} \frac{(e^{-E_0(t-t_0)} - \tilde{G}_2(t))^2}{\tilde{G}_2^2(t)},$$
 (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 4×4 source-sink-smeared variational analysis [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., ACCESSING HIGH MOMENTUM STATES IN LATTICE QCD

$$G_{\rm fit} = a_1 e^{-a_2 t} + b_1 e^{-b_2 t}.$$
 (13)

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 account for any states with higher energy than the two considered, as the energy of the second state, and thus the residue of the pole, becomes a superposition of all higher-energy states.

The second measure we introduce works similarly to this. However, the parameters of the exponentials are predetermined by a variational analysis [23]. This leads to a simple linear fit of known exponentials, i.e.,

$$G_{\rm fit} = \lambda_0 e^{-E_0 t} + \lambda_1 e^{-E_1 t} + \lambda_2 e^{-E_2 t}.$$
 (14)

We can then find the proportion of the *i*th state in the twopoint function with the measure

$$M_{2,i} = \frac{|\lambda_i|}{\sum_k |\lambda_k|}.$$
(15)

This measure is more ideal than directly fitting the six parameters of a three-exponential fit as having fewer parameters to fit allows the use of a smaller window, where only the lightest three states are contributing. Furthermore, the energy of the heaviest state has already been determined by the variational analysis, and therefore the χ^2 per degree of freedom is constrained well and can be used to find the appropriate fit window.

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 [24]. These lattices have 2 + 1 sea quark flavors generated with the Iwasaki gauge action [25] and the nonperturbatively improved Clover fermion action [26] with the κ values for the light quarks and the strange quark given by 0.13 754 and 0.13 640, respectively, and $C_{SW} = 1.715$. This gives a pion mass of $m_{\pi} = 389$ 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. (4).

We use a 4×4 correlation matrix to extract our excited state masses, constructed from the χ_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 multiparticle 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 nonzero 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.

VI. RESULTS

A. Isotropic smearing

We first calculate the measure from Eq. (12), where the two-point functions have been normalized 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. (4), 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 γ 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 $M_p = 1.273(21)$ GeV, giving a relativistic energy of $E_p|_{p=1} = 1.343(23)$ 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



FIG. 1. The measure from Eq. (12) at $p_x = 0$ in Eq. (4). Deviation from the ideal two-point function increases by a factor of 10 less than 30 sweeps from the ideal smearing level, as shown in the inset graph.



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 γ factor provides a Lorentz contraction factor of $\gamma^{-1} = 0.72$.

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 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 0.85, compared to the relativistic γ^{-1} factor of 0.72. At $p_x = 5$, corresponding to a momentum transfer of approximately 4.55 GeV², 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 GeV², there is significant noise far from the source in the two-point function, even for highly optimized 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), 2.301(28) 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. Figure 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 attempting to fit two quickly decaying exponentials using only 0.69% of the signal available. This leads us to believe that, in the regions of ground-state dominance where we are most interested, the coefficient



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.



FIG. 4. Ground-state proportion from the three exponential fit at $p_x = 0$ in Eq. (4). There is insufficient information on the second excited state close to the optimal amount of smearing, thus requiring use of the two exponential fit to determine the optimal amount of smearing with this measure.

from the quickly decaying third state cannot be determined accurately and, therefore, dominates well beyond where it should be allowed 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 exponential 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 lattice units, with 77.69(7)%, or 32 times more excited-state contamination than the optimal smearing level.



FIG. 5. Ground-state proportion at $p_x = 0$ in Eq. (4). Contamination due to excited states increases rapidly away from the optimal smearing level. There is good agreement between the two exponential fit here and the three exponential fit in Fig. 4 away from the optimum smearing levels.



FIG. 6. Ground state proportion at $p_x = 3$ in Eq. (4). As momentum increases, the contamination due to excited states increases more rapidly away from the ideal smearing level.

At the first nonzero-momentum state, the results present similarly to the first measure, the optimal amount of smearing is 1 sweep less than that of the nonzero-momentum ground state and 2 sweeps more than the optimal amount determined by the first measure. At $p_x = 3$ in Eq. (4) shown in Fig. 6, the overlap is maximized at 101 sweeps of smearing, or an rms radius of 5.95 lattice units, once again agreeing within only a few sweeps of the optimum 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 GeV², 97.20(20)% overlap 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 considered to signify a limit to the domain of validity of the measure.

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 nonzero-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 α_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 maximize overlap with the source, Fig. 9 shows that introducing anisotropy to the smearing does not result in improved isolation of the



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 optimized 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.



FIG. 8 (color online). 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 (color online). 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 γ factor of 1.39 giving a length contraction factor of 0.72 in the x direction.



FIG. 10 (color online). 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 (color online). 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.

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 α_x , which increases with decreasing α_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, optimization 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.

It is perhaps worth noting that a different conclusion would be drawn if one was to consider a single smearing level beyond the peak at the isotropic limit. For example, consider Fig. 10 with $p_x = 5$, with the number of smearing sweeps fixed at 80, the introduction of anisotropy has a favorable effect, restoring ground-state isolation at $\alpha_x = 0.12$.



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 $p_x = 5$ (left) and $p_x = 7$ (right) as in Eq. (4). At $p_x = 5$, there is a small amount of improvement for anisotropic smearing at α_x/α in the region of $\gamma^{-1} = 0.51$. At $p_x = 7$, 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.

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 time slices after the source at the optimal number of smearing sweeps for each value of our anisotropy parameter, α_r .

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 $\alpha_x/\alpha = 0.51 = \gamma^{-1}$.

The banding structure visible in Fig. 13 is a result of the optimal number of smearing sweeps increasing for decreasing values of α_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 α_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 optimization of the smearing can lead to remarkable improvement to the groundstate 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. 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. Optimizing the number of sweeps of isotropic smearing is sufficient to ensure maximal isolation of high-momentum ground states and ameliorates the need for considering anisotropic operators. We note that a subsequent study considering the effect of anisotropic operators on mesons [27] has already appeared.

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

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