“Lattice QCD Calculation of Nucleon Structure” Final Technical Report*

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1 Research Progress

It is emphasized in the 2015 NSAC Long Range Plan [1] that "understanding the structure of hadrons in terms of QCD's quarks and gluons is one of the central goals of modern nuclear physics." Over the last three decades, lattice QCD has developed into a powerful tool for *ab initio* calculations of strong-interaction physics. Up until now, it is the only theoretical approach to solving QCD with controlled statistical and systematic errors.

Since 1985, we have proposed and carried out first-principles calculations of nucleon structure and hadron spectroscopy using lattice QCD which entails both algorithmic development and large scale computer simulation. We started out by calculating the nucleon form factors – electromagnetic [2], axial-vector [3], πNN [4], and scalar [5] form factors, the quark spin contribution [6] to the proton spin, the strangeness magnetic moment [7], the quark orbital angular momentum [8], the quark momentum fraction [9], and the quark and glue decomposition of the proton momentum and angular momentum [10]. These first round of calculations were done with Wilson fermions in the 'quenched' approximation where the dynamical effects of the quarks in the sea are not taken into account in the Monte Carlo simulation to generate the background gauge configurations.

Beginning in 2000, we have started implementing the overlap fermion formulation into the spectroscopy and structure calculations [11, 12]. This is mainly because the overlap fermion honors chiral symmetry as in the continuum. It is going to be more and more important to take the symmetry into account as the simulations move closer to the physical point where the u and d quark masses are as light as a few MeV only. We began with lattices which have quark masses in the sea corresponding to a pion mass at $\sim$ 300 MeV and obtained the strange form factors [13], charm and strange quark masses, the charmonium spectrum and the D_s meson decay constant f_{D_s} [14], the strangeness and charmness [15], the meson mass decomposition [16] and the strange quark spin from the anomalous Ward identity [17]. Recently, we have started to include multiple lattices with different lattice spacings and different volumes including large lattices at the physical pion mass point. We are getting quite close to being able to calculate the hadron structure at the physical point and to do the continuum and large volume extrapolations which is our ultimate aim. We have now finished several projects which have included these systematic corrections. They include the leptonic decay width of the ρ [18], the πN sigma and strange sigma terms [19], and the strange quark magnetic moment [20].

Over the years, we have also studied hadron spectroscopy with lattice calculations and in phenomenology. These include Roper resonance [21, 22], pentaquark state [23], charmonium spectrum [24, 14], glueballs [25, 26, 27, 28], scalar mesons $a_0(1450)$ and $\sigma(600)$ [29] and other scalar mesons [30], and the 1^{-+} meson [31].

In addition, we have employed the canonical approach to explore the first order phase transition and the critical point at finite density and finite temperature [32, 33]. We have also discovered a new parton degree of freedom – the connected sea partons, from the path-integral formulation of the hadronic tensor [34, 35] which explains the experimentally observed Gottfried sum rule violation [34]. Combining experimental result on the strange parton distribution, the CT10 global fitting results of the total u and d anti-partons and the lattice result of the ratio of the momentum fraction of the strange vs that of u or d in the disconnected insertion, we have shown that the connected sea partons can be isolated [36].

In this final technical report, we shall present a few representative highlights that have been achieved in the project.

2 Highlights

2.1 πN and strangeness sigma terms

As measures of explicit and spontaneous chiral symmetry breaking in the baryon sector, $\sigma_{\pi N}$, defined as

$$\sigma_{\pi N} \equiv \hat{m}\langle N|\bar{u}u + \bar{d}d|N\rangle, \tag{1}$$

where $\hat{m} = (m_u + m_d)/2$ is the averaged light quark mass, and f_s^N defined as the strangeness σ term as a fraction of the nucleon mass

$$\sigma_{sN} \equiv m_s\langle N|\bar{s}s|N\rangle, \qquad f_s^N = \frac{\sigma_{sN}}{m_N}, \tag{2}$$

are fundamental quantities which pertain to a wide range of issues in hadron physics. They include the quark mass contribution in the baryon which is related to the Higgs contribution to the observable matter [37, 38], the pattern of SU(3) breaking [37], πN and KN scatterings [39, 40], and kaon condensate in dense matter [41]. Using the sum rule of the nucleon mass, the heavy quark mass contribution can be deduced by that from the light flavors, in the heavy quark limit and also in the leading order of the coupling [42, 15, 38]. At the same time, precise values of the quark mass term for various flavors, from light to heavy, are of high interest for dark matter searches [43, 44, 45], where the popular candidate of dark matter (like the weakly interacting mass particle) interacts with the observable world throughout the Higgs couplings, so that the precise determination of the $\sigma_{\pi N}$ and σ_{sN} can provide constraints on the dark matter candidates.

Phenomenologically, the $\sigma_{\pi N}$ term is typically extracted from the πN scattering amplitude. To lowest order in m_π^2, the unphysical on-shell isospin-even πN scattering amplitude at the Cheng-Dashen point corresponds to $\sigma(q^2 = 2m_\pi^2)$ [39, 40] which can be determined from πN scattering via fixed-q^2 dispersion relation [40]. $\sigma_{\pi N}$ at $q^2 = 0$ can be extracted through a soft correlated two-pion form factor [46, 47, 48]. Analysis of the πN scattering amplitude to obtain $\sigma_{\pi N}(0)$ from the Lorentz covariant baryon chiral perturbation and the Cheng-Dashen low-energy theorem are also developed [49, 50, 51]. They give $\sigma_{\pi N}$ values in the range $\sim 45 - 64$ MeV, while the most recent analysis [51] gives 59.1(3.5) MeV.

Lattice calculation should be a good tool in giving reliable results to these quantities. Again, there is an issue about chiral symmetry. It was pointed out [52, 53] that due to explicit chiral symmetry breaking, the quark mass in the Wilson type fermions has an additive renormalization and the flavor-singlet and non-singlet quark masses renormalize differently. In this case, the renormalized strange scalar matrix element $\langle N|\bar{s}s|N\rangle^R$ can be written as

$$\langle N|\bar{s}s|N\rangle^R = \frac{1}{3}\Big[(Z_0 + 2Z_8)\langle N|\bar{s}s|N\rangle + (Z_0 - Z_8)\langle N|\bar{u}u + \bar{d}d|N\rangle\Big], \tag{3}$$

where Z_0 and Z_8 are the flavor-singlet and flavor-octet renormalization constants respectively. Z_0 differs from Z_8 by a disconnected diagram which involves a quark loop. In the massless renormalization scheme, one can calculate these renormalization constants perturbatively. For the massless case where $\bar{\psi}\psi = \bar{\psi}_L\psi_R + \bar{\psi}_R\psi_L$, a quark loop for the scalar density vanishes no matter how many gluon insertions there are on the loop, since the coupling involving γ_μ does not change helicity. Thus, the massless scalar quark loop is zero and $Z_0 = Z_8$. There is no mixing of the scalar matrix element with that of u and d. This is the same with the overlap fermion, since the overlap has

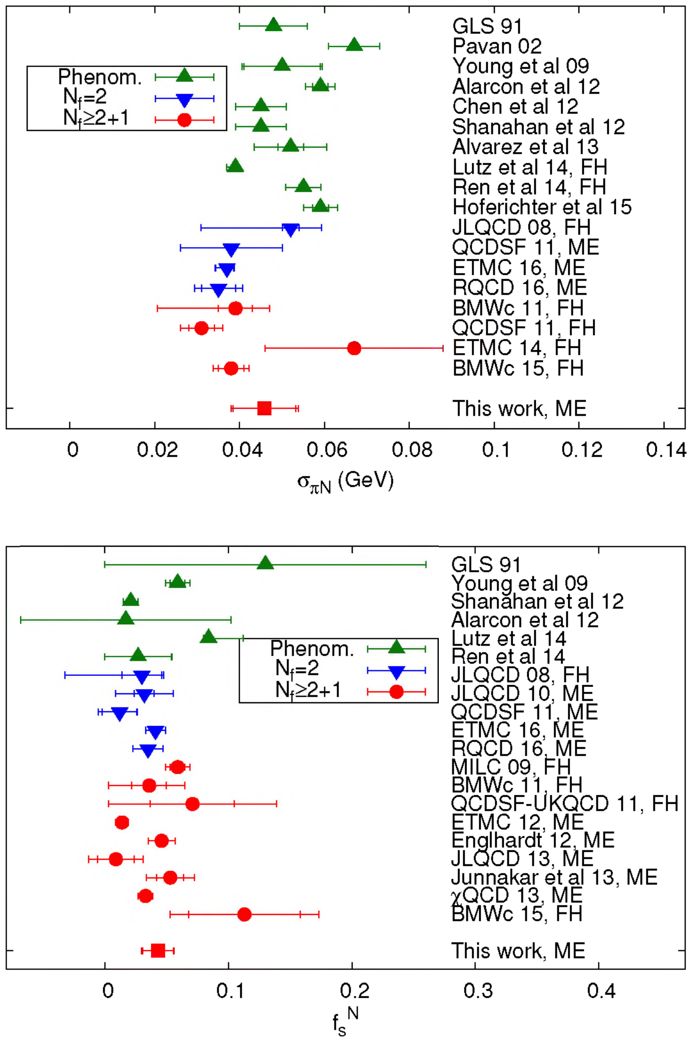


Figure 1: The results of $\sigma_{\pi N}$ (upper panel) and f_s^N (lower panel) from both phenomenology and lattice simulations. The narrow error bar for each data point is the statistical, and the broad one is that for the total uncertainty. The physical proton mass 938MeV is used to obtain f_s^N in this work. They are color-coded in phenomenological and indirect approaches (green), $N_f = 2$ lattice calculations (blue), and $N_f = 2 + 1$ lattice calculations (red). Detailed references are given in Ref. [19].

chiral symmetry and the inverse of its massless quark propagator D_c anti-commutes with γ_5, i.e. $\{D_c, \gamma_5\} = 0$ as in the continuum.

This is not so for Wilson type fermion where its free quark propagator contains a term proportional to the Wilson r term which violates chiral symmetry and will give a non-zero contribution to the scalar matrix element at the massless limit, leading to $Z_0 \neq Z_8$. Since the u and d matrix elements in the nucleon are not small, there can be a substantial flavor mixing at finite a. This lattice artifact due to non-chiral fermions can be removed by calculating Z_0 and Z_8 [54]. Furthermore, the direct calculation of the matrix element with Wilson type fermions faces the complication that the sigma term with bare quark mass is not renormalization group invariant. This can also be corrected with the introduction of various renormalization constants to satisfy the Ward identities [54]. All of these involve additional work and will introduce additional errors. On the contrary, there is no flavor mixing in the overlap fermion and the sigma terms are renormalization group invariant with bare mass and bare matrix element, since the renormalization constants of quark mass and scalar operator cancel, i.e. $Z_m Z_s = 1$ due to chiral symmetry. For the latest calculation with overlap fermion on $2+1$ flavor domain wall fermion gauge configurations for several ensembles with different lattice spacings, volume, and sea masses including one at the physical pion mass, the global fit gives the prediction of $\sigma_{\pi N} = 45.9(7.4)(2.8)$ MeV and $\sigma_{sN} = 40.2(11.7)(3.5)$ MeV. This value of $\sigma_{\pi N}$ has a two-sigma tension with the recent results based on Roy-Steiner equations [51] which gives $\sigma_{\pi N} = 59.1(3.5)$ MeV.

To conclude, we believe that to calculate $\sigma_{\pi N}$ and σ_{sN} which are fundamental quantities reflecting both the explicit and spontaneous chiral symmetry, it is theoretically clean and straightforward procedure-wise to calculate them with chiral fermions on the lattice in order to obtain reliable results without the complication of renormalization and flavor-mixing as compared to non-chiral fermions.

2.2 Quark spin and orbital angular momentum

The quark spin content of the nucleon was found to be much smaller than that expected from the quark model by the polarized deep inelastic lepton-nucleon scattering experiments and the recent global analysis reveals that the total quark spin contributes only $\sim 25\%$ to the proton spin [55]. This is dubbed 'proton spin crisis' since no model seems to be able to explain it convincingly and, moreover, quantitatively.

Once again, first principle lattice calculation should be able to address this issue. The ideal calculation would be to use the conserved axial-vector current of the chiral fermions which satisfies the anomalous Ward identity (AWI) on lattice at finite lattice spacing. However, it is somewhat involved to construct the current itself for the overlap fermion [56]. Before it is implemented, one can use the AWI as the normalization condition for the simpler local axial-vector current

$$\partial_\mu \kappa_A A_\mu^1 = 2mP - 2iN_f q, \tag{4}$$

where $A_\mu^1 = \sum_{i=u,d,s} \overline{\psi}_i i\gamma_\mu\gamma_5(1 - \frac{1}{2}D_{ov})\psi_i$ is the local singlet axial-vector current and $mP = \sum_{i=u,d,s} m_i\overline{\psi}_i i\gamma_5(1 - \frac{1}{2}D_{ov})\psi_i$ is the pseudoscalar density with D_{ov} being the massless overlap operator and q the local topological charge as derived in the Jacobian factor from the fermion determinant under the chiral transformation whose local version is equal to $\frac{1}{16\pi^2} tr_c G_{\mu\nu}\tilde{G}_{\mu\nu}(x)$ in the continuum [57], i.e.

$$q(x) = \mathrm{Tr}\,\gamma_5(\frac{1}{2}D_{ov}(x,x) - 1) \underset{a\to 0}{\longrightarrow} \frac{1}{16\pi^2} tr_c\, G_{\mu\nu}\tilde{G}_{\mu\nu}(x). \tag{5}$$

κ_A in Eq. (4) is the finite lattice renormalization factor (often referred to as Z_A in the literature for the flavor non-singlet case) needed for the local axial-vector current to satisfy the AWI on the lattice with finite lattice spacing, much like the finite renormalization for the vector and non-singlet axial-vector currents. We shall call it lattice normalization. On the other hand, the mP and q defined with the overlap operators do not have multiplicative renormalization. There is a two-loop renormalization of the singlet A^1_μ and the topological charge q mixes with $\partial_\mu A^1_\mu$. It turns out that they are the same. Thus, the renormalized AWI is the same as the unrenormalized AWI (but normalized) to the α_s^2 order. To utilize the AWI, one needs to calculate the matrix elements of $2mP$ and $2q$ on the r.h.s. of the AWI and extrapolate to $q^2 = 0$. However, the smallest $|q^2|$ is larger than the pion mass squared on the lattices that we work on, the extrapolation to q^2 is not reliable. Instead, we shall match the form factors at finite $|q^2|$ from both sides, i.e.

$$2m_N\kappa_A g^1_A(q^2) + q^2\kappa_A h^1_A(q^2) = 2mg_P(q^2) + N_f g_G(q^2). \tag{6}$$

where the singlet $g^1_A(q^2)$ and the induced pseudoscalar $h^1_A(q^2)$ are the bare form factors. $2mg_P(q^2)$ and $g_G(q)$ are the form factors for the pseudoscalar current and topology respectively. From this normalization condition one can determine κ_A and the normalized g^1_A is $\kappa_A g^1_A(0)$. This has been employed in the calculation of the strange quark spin to find $\Delta s + \Delta\bar{s} = -0.0403(44)(61)$ [17]. This is more negative than the other lattice calculations with and axial-vector current, mainly because $\kappa_A = 1.36(4)$ is found to be larger than that of the flavor-octet axial-vector current. The lesson here is that, unless the conserved current is used to carry out the calculation, it is essential to adopt the AWI to obtain the normalization of the local axial-vector current. This is possible with the overlap fermion.

While the final numbers on the u and d spin fraction which include the connected insertion are still being worked out, the initial results indicate that it is the larger negative $2mP$ matrix elements that cancel the positive topological charge term in the triangle anomaly in the disconnected insertions that lead to a small g^1_A.

There are various ways to decompose the proton spin into quark and glue spins and orbital angular momenta [58, 59]. From the symmetrized energy-momentum tensor of QCD (the Belinfante form), it is shown [60] that the proton spin can be decomposed as

$$\vec{J}_{\rm QCD} = \vec{J}_q + \vec{J}_g = \frac{1}{2}\vec{\Sigma}_q + \vec{L}_q + \vec{J}_g, \tag{7}$$

where the quark angular momentum $\vec{J}_q$ is the sum of quark spin and orbital angular momentum,

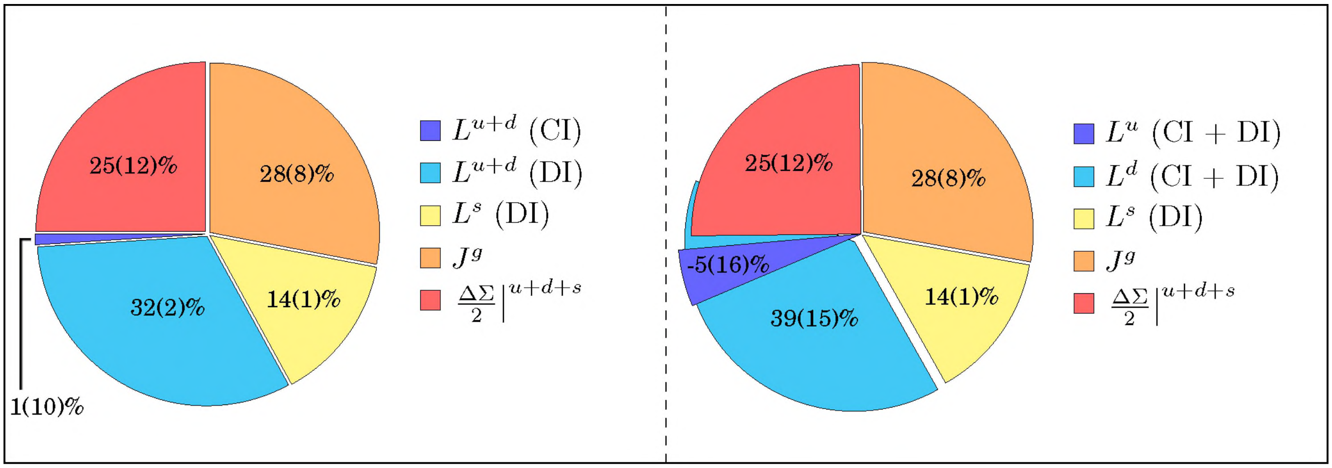
$$\vec{J}_q = \frac{1}{2}\vec{\Sigma}_q + \vec{L}_q = \int d^3x \left[\frac{1}{2}\,\overline{\psi}\,\vec{\gamma}\,\gamma^5\,\psi + \psi^\dagger\left\{\vec{x}\times(i\vec{D})\right\}\psi\right], \tag{8}$$

and each of which is gauge invariant. The glue angular momentum operator

$$\vec{J}_g = \int d^3x \left[\vec{x}\times(\vec{E}\times\vec{B})\right], \tag{9}$$

is also gauge invariant. However, it cannot be further divided into the glue spin and orbital angular momentum gauge invariantly with the Belinfante tensor.

Since it has a large finite volume effect to calculate the operator with a spatial $\vec{r}$ on the lattice with periodic boundary condition, one can instead calculate the quark and glue momentum and angular momentum from their form factors $T_1(q^2)$ and $T_2(q^2)$ and obtain the momentum and angular momentum fractions from their forward limits, i.e. $\langle x\rangle = T_1(0)$ and $J = \frac{1}{2}(T_1(0) + T_2(0))$, much like the electric charge and magnetic moment from the forward Dirac and Pauli form factors $F_1(0)$ and $F_2(0)$. After determining the quark angular momentum, the quark orbital angular momentum is obtained by subtracting the quark spin from it. This has been carried out in a quenched approximation [10]. The OAM fractions $2\langle L^q_{\rm kin}\rangle$ for the u and d quarks in the CI have different signs and add up to 0.01(10), *i.e.* essentially zero. This is the same pattern which has been seen with dynamical fermion configurations and light quarks, as pointed out earlier. The large OAM fractions $2\langle L^q_{\rm kin}\rangle$ for the u/d and s quarks in the DI is due to the fact that g^1_A in the DI is large and negative, about $-0.12(1)$ for each of the three flavors. All together, the quark OAM constitutes a fraction of 0.47(13) of the nucleon spin. The majority of it comes from the DI.



(a)

Figure 2: Pie charts for the quark spin, quark orbital angular momentum and gluon angular momentum contributions to the proton spin. The left panel show the quark contributions separately for CI and DI, and the right panel shows the quark contributions for each flavor with CI and DI summed together for u and d quarks.

As far as the spin decomposition is concerned, it is found that the quark spin constitutes 25(12)% of the proton spin, the gluon total AM takes 28(8)% and the rest is due to the quark kinetic OAM which is 47(13)%.

Since this calculation is based on a quenched approximation which is known to contain uncontrolled systematic errors, it is essential to repeat this calculation with dynamical fermions of light quarks and large physical volume. However, we expect that the quark OAM fraction may still be large in the dynamical calculation.

In the naive constituent quark model, the proton spin comes entirely from the quark spin. On the other hand, in the Skyrme model [61] the proton spin originates solely from the OAM of the collective rotational motion of the pion field [62]. What is found in the present lattice calculation suggests that the QCD picture, aside from the gluon contribution, is somewhere in between these two models, indicating a large contribution of the quark OAM due to the meson cloud ($q\bar{q}$ pairs in the higher Fock space) in the nucleon.

2.3 Strange Quark Magnetic Moment in the Nucleon

The determination of the strange (s) quark contribution to nucleon electromagnetic (EM) form factors is of immense importance since this is a pure sea quark effect. A nonzero value of Sachs strange electric form factor G_E^s at any $Q^2 \neq 0$ would mean that the spatial distribution of s and $\bar{s}$ quarks are not the same in the nucleon. Since the extraction of the vector strange matrix elements $\langle \bar{s}\gamma_\mu s \rangle$ was proposed in [63, 64, 65] via parity-violating $e - N$ scattering for which the dominant contribution arises from interference between photon (γ) and weak boson (Z^0) exchanges. A considerable number of experimental efforts by the SAMPLE, HAPPEX, G0, and A4 experiments have been going on for the last two decades. The world data constrains that $G_M^s(0)$ contributes less than 6% and $\langle r_s^2 \rangle_E$ contributes less than 5% to the magnetic moment and the mean-square charge radius of the proton respectively [66]. However, all these experimental results are limited by rather sizable error bars. The two recent global analyses give $G_M^s(Q^2 = 0.1\,(\mathrm{GeV/c})^2) = 0.29 \pm 0.21$ [67] and -0.26 ± 0.26 [68] which are consistent with zero and differ in sign in their central values.

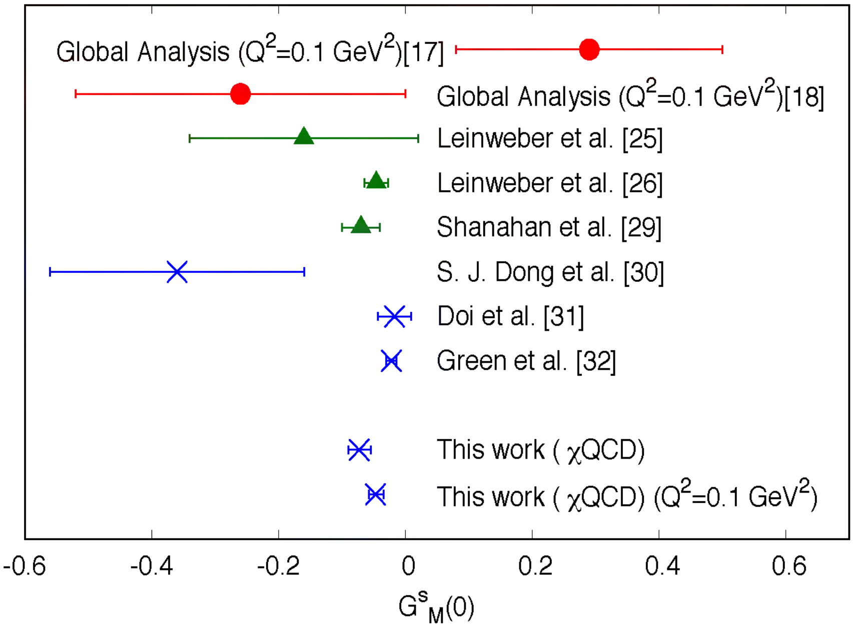


Figure 3: Comparison of some of the many determinations of strange magnetic moment. Results in the *red* are from global analysis of world data, results in the *green* are from indirect calculations, and results in the *blue* are from lattice QCD calculations.

Despite tremendous theoretical efforts, a detailed convincing understanding about the sign and magnitude of strange EM form factors is still lacking. In view of the experimental and theoretical uncertainties on the strange quark magnetic moment, we we have performed a robust first-principles lattice QCD calculation [20] using three different $2 + 1$ flavor dynamical fermion lattice ensembles including, for the first time, the physical pion mass with chiral fermion to explore the quark mass dependence and with finite lattice spacing and volume corrections to determine the strange quark matrix elements in the vector channel. We have performed a two-state fit where we combined both the ratio method and the summed-ratio method to control excited-state contamination. The statistical error is greatly reduced by improving the nucleon propagator with low-mode substitution and quark loop with low-mode average. To explore the strange vector form factors at different momentum transfers, we implemented model-independent $z-$expansion fits. Given our precise lattice prediction for the strange quark magnetic moment of $G_M^s(0) = -0.073(19)\mu_N$ and strange charge radius $\langle r_s^2\rangle_E = -0.0046(24)\,\mathrm{fm}^2$ at the physical point with systematic errors included, we anticipate these results will be verified by experiments in the future and, together with experimental inputs, can lead to more precise determination of various weak form factors. We present Fig. 3 to compare our result of $G_M^s(0)$ and $G_M^s(Q^2 = 0.1\,\mathrm{GeV}^2) = -0.047(11)(06)$ with some other measurements of $G_M^s(0)$ and a global fit of G_M^s at $Q^2 = 0.1\,\mathrm{GeV}^2$.

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