Systematic study of transverse-momentum dependent soft function from lattice QCD

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In this work, we perform a systematic lattice QCD study of the intrinsic, rapidity-independent soft function within the framework of large momentum effective theory. The computation is carried out using a gauge ensemble of $N_f = 2 + 1 + 1$ clover-improved twisted mass fermions. After applying an appropriate renormalization procedure and the removal of significant higher-twist contamination, we obtain the intrinsic soft function that is comparable to the one-loop perturbative result at large external momentum. The determination of the non-perturbative soft function from first principles is crucial to sharpen our understanding of the processes with small transverse momentum such as the Drell-Yan production and the semi-inclusive deep inelastic scattering. Additionally, we calculate the Collins-Soper evolution kernel using the quasi-transverse-momentum-dependent wave function as input.

Introduction – Understanding the structure of matter within the framework of Quantum Chromodynamics is one of the central goals of hadron and nuclear physics. The main physical observables used in this quest are form factors and parton distribution functions (PDFs), unified in the concept of generalized PDFs. In contrast to the collinear PDFs, which depend essentially on the fraction of the longitudinal momentum of the parent hadron carried by quarks and gluons at a given hard scale $Q^2$, the transverse momentum PDFs (TMDPDFs) are also dependent on the transverse momentum $Q_⊥$ carried by its constituents. Although the study of partonic transverse momentum phenomena started few years after QCD was proposed [1], our knowledge of them is limited, both experimentally and theoretically (see, e.g., [2,3]) since, until recently, a systematic ab initio computation of TMDPDFs was out of reach.

Knowledge of TMDPDFs would open a new window in our understanding of the structure of hadrons, arising, for instance, from probing the coupling of $k_⊥$ of a given quark with its spin [4]. However, these functions cannot be obtained from totally inclusive processes, as we need an observable in the final state carrying information on $k_⊥$, obtained, for example, by measuring the transverse momentum $Q_⊥$ of a lepton pair produced in a Drell-Yan (DY) process. Consequently, they are intrinsically harder to measure. Nevertheless, the future Electron-Ion Collider in US (EIC) [5] and that in China (EicC) [6] have as one of their goals to make precise measurements of TMDPDFs, aiming to reconstruct a 3-dimensional picture of hadrons in momentum space. As in the case of collinear PDFs, the extraction of TMDPDFs from the measured DY or semi-inclusive deep inelastic cross sections is possible, thanks to factorization theorems, which isolate the non-perturbative physics into suitable definitions of TMDPDFs [7,11]. Unfortunately, for distributions dependent on $k_⊥$ there appears an extra divergence associated with the emission of gluons carrying small momenta, which is not canceled by the real and virtual perturbative corrections. These divergences are encoded into functions called soft functions. At large transverse momentum $Q_⊥ \gg \Lambda_{QCD}$, the soft function can be calculated using perturbation theory [12,13]. However, when the soft function captures the soft-gluon effects at small $Q_⊥$, it is generically non-perturbative.

Recently, using the framework of large momentum effective theory (LaMET) [14,16], a novel method has been proposed to extract the soft function from pion matrix elements [17] that can be calculated in lattice QCD, enabling a solution of the difficult problem of non-perturbatively determining the soft function. A first exploratory lattice QCD calculation was carried out by the LPC collaboration [18]. However, a better understanding of the new method with a deeper examination of the various systematic aspects involved in a lattice calculation is important in order to further establish the validity of the approach.

In this work, we perform a calculation of the soft function using a different fermion discretization scheme, namely the twisted mass fermion formulation. We demonstrate the validity of the methodology proposed by Ref. [17] and determine the soft function, showing that to
obtain the final results requires highly non-trivial steps that we develop here. These steps include the following:
i) We apply an appropriate renormalization procedure to remove the power and logarithmic divergences in the non-local operator; ii) we examine various pion matrix elements and find that some of the so-called higher-twist contaminations are substantial and can even flip the sign of the matrix elements. By designing improved pion matrix elements to cancel the higher-twist effects, we show that we can reliably obtain the soft function; iii) we perform the calculation at four different pion masses in order to confirm the process-independence of the soft function; iv) we perform a detailed investigation of excited states; and v) we examine its convergence when the external momentum increases.

An important additional component of this work is the calculation of the Collins-Soper evolution kernel, where we find results that are in qualitative agreement with other lattice QCD calculations [18-20].

Theoretical framework – As proposed in Ref. [17], the intrinsic, rapidity-independent soft function $S(b_{1}, \mu)$ depends on the transverse separation $b_{1}$ and the renormalization scale $\mu$. Using LaMET, it can be extracted from the pion matrix element $F_{T}(b_{1}, P^{z})$, which is defined in Euclidean spacetime as [17]

$$F_{T}(b_{1}, P^{z}) = \langle \pi(-P^{z})|u\Gamma u(b_{1})\frac{d}{d\tau}d(0)|\pi(P^{z})\rangle. \quad (1)$$

Here, $P^{z}$ is a large momentum in the $z$-direction carried by the pion. Two current operators $\bar{u}\Gamma u$ and $d\Gamma d'$ are inserted at the same timeslice, but with a spatial separation $b_{1}$ that is perpendicular to the momentum direction. To extract the leading-twist contribution, one can choose the Dirac matrices as $\Gamma = \gamma_{t}, \gamma_{y}$ or $\gamma_{t}\gamma_{y}$. $F_{T}(b_{1}, P^{z})$ can be factorized into the quasi-TMD wave function (quasi-TMDWF) $\Phi$ and the intrinsic soft function $S(b_{1}, \mu)$ [14,17] in the large momentum limit through

$$F_{T}(b_{1}, P^{z}) \xrightarrow{P^{z} \to \infty} S(b_{1}, \mu) \int_{0}^{1} dx \, dz' \, H_{T}(x, x', P^{z}, \mu) \times \Phi^{\dagger}(x', b_{1}, -P^{z}) \Phi(x, b_{1}, P^{z}), \quad (2)$$

where $H_{T}(x, x', P^{z}, \mu)$ is the perturbative hard kernel. The quasi-TMDWF $\Phi$ is defined as

$$\Phi(x, b_{1}, \pm P^{z}) = \lim_{l \to 0} \int \frac{d\xi}{2\pi} e^{i2\pi \xi} \phi(z, b_{1}, \pm l, P^{z}) \quad (3)$$

with $\xi = zP^{z}$. The wave function $\phi$ is given by

$$\phi(z, b_{1}, l, P^{z}) = \langle 0|O_{\phi}(t, z, b_{1}, l)|\pi(P^{z})\rangle e^{-E_{\pi}t} \quad (4)$$

with $E_{\pi} = \sqrt{m_{\pi}^{2} + P^{z^{2}}}$. The operator $O_{\phi}$ is defined as

$$O_{\phi}(t, z, b_{1}, l) \equiv \bar{u}(t, z/2, b_{1})\Gamma_{\phi}W(z, b_{1}, l)d(t, -z/2, 0). \quad (5)$$

The quark fields $\bar{u}, d$ and Wilson link $W$ entering $O_{\phi}$ are all located at the same timeslice $t$. $W$ has a staple shape and goes through the spatial sites $(-z/2, 0) \to (-l, 0) \to (z/2, 0)$. The Dirac matrix $\Gamma_{\phi}$ can be chosen as $\gamma_{5}\gamma_{0}$ or $\gamma_{5}\gamma_{3}$ so that $\Phi$ contains the leading-twist contribution. (Here $\gamma_{i}$ with $i = 0, 1, 2, 3$ indicate the polarization direction $t, x, y, z$, respectively.)

Up to $O(\alpha_{s})$ corrections, the hard kernel takes a simple form, denoted here as $H_{0}^{T}$. It can be obtained from a Fierz identity that $H_{T}^{T} = 1/(2N_{c})$ for $\Gamma = \gamma_{t}, \gamma_{y}$ or $-1/(2N_{c})$ for $\Gamma = \gamma_{t} \gamma_{y}$ with $N_{c} = 3$ the number of colors. Using $H_{0}^{T}$ as an input, one can further simplify the expression (2) as

$$F_{T}(b_{1}, P^{z}) \xrightarrow{P^{z} \to \infty} S(b_{1}, \mu) \int_{0}^{1} dx \, dz' \, H_{T}(x, x', P^{z}, \mu) \frac{d}{d\tau}\phi(z = 0, b_{1}, l = \infty, P^{z})^{2}. \quad (6)$$

The soft function can be extracted by taking a ratio between $F_{T}$ and $H_{0}^{T}|\phi|^{2}$. When using Eq. (6), one always fixes $z = 0$. Thus, in the following context, the variable $z$ is left out for simplicity.

Lattice setup – The ensemble of gauge field configurations used in this work was generated by the Extended Twisted Mass Collaboration [21]. We use the clover-improved twisted mass fermions and Iwasaki gauge action. In Eqs. (2) and (6), both $F_{T}$ and $\Phi$ contain the structure information of the pion, which is expected to be cancelled out at sufficiently large $P^{z}$, leaving the intrinsic soft function independent of either the structure or the mass of the pion. To check such independence, we use four valence quark masses, which correspond to pion masses ranging from 827 MeV to 350 MeV. These valence quark masses together with other ensemble information are listed in Table I.

The three-point correlation function for the pion matrix element

$$C_{T}^{pt}(b_{1}, P^{z}, t_{s}, t) = \frac{1}{L^{3}} \sum_{\bar{z}} e^{-2iP^{z}\cdot\bar{z}} Z_{1}^{2} O_{\pi}(t_{s}, -P^{z}) \bar{u}\Gamma u(t, \bar{x} + b_{1}) \frac{d}{d\tau}d(t, \bar{x}) O_{\pi}(0, P^{z}) \quad (7)$$

where $t_{s}$ is the source-sink separation. The operators $\bar{u}\Gamma u$ and $d\Gamma d'$ are inserted at timeslice $t$ and constructed using the Coulomb-gauge-fixed-wall-source operators

$$O_{\pi}(t, \bar{P}) = \sum_{\bar{x}, \bar{y}} \bar{u}(t, \bar{x})\gamma_{5}d(t, \bar{y})e^{-i\bar{P} \cdot \bar{y}}, \quad (8)$$

| $(L/a)^{3} \times T/a$ | $a$ (fm) | $a_{\mu,sea}$ | $m_{sea}$ | $N_{conf}$ |
|-----------------------|--------|-------------|----------|----------|
| 24$^{3} \times 48$    | 0.093  | 0.0053      | 350      | 126      |
|                       | $a_{\mu,sea}$ | $m_{0}$ | $m_{1}$ | $m_{2}$ | $m_{3}$ |
|                       | 0.0053 | 350        | 545      | 640      | 827      |
which are known to have a good overlap with the pion ground state. \( Z_\Gamma \) is the renormalization factor to convert the bare lattice operator \( q \bar{q} \) to the renormalized one in the \( \overline{\text{MS}} \) scheme. The pion matrix element can be obtained from the three-point function at sufficiently large \( t_\pi \) through

\[
C_{\Gamma}^{3pt}(b_1, P^z, t, \frac{t_\pi}{2}) = \frac{|A_w(P^\pi)|^2}{(2E)^2} e^{-E_\pi t_\pi} \Gamma_\pi(b_1, P^z),
\]

where \( A_w(P^\pi) = L^{-\frac{1}{2}} (\pi(P^\pi)|O^\perp_{\pi}(0, P^z)|0) \) is the overlap amplitude for the pion operator. According to parity, we have \( A_w(P^\pi) = A_w(-P^\pi) \).

The correlation function for the quasi-TMDWF is constructed as

\[
C_{\Gamma_\phi}^{w_f}(b_1, l, P^z, t) = \frac{Z_\phi}{L^3} \sum_x e^{-ilP^x_z} (O_\phi(t, b_1, l) O^\perp_{\phi}(0, P^z)),
\]

where \( Z_\phi \) is the renormalization factor for the staple-shaped operator, which is found to be multiplicative [24, 23]. We use \( \Gamma_\phi = \gamma_0 \gamma_0 \) to avoid operator mixing for Wilson-type fermions in the renormalization procedure [23]. When constructing the operator \( O_\phi(t, b_1, l) \), we apply 5 steps of stout smearing [24] to the gauge links that enter in the Wilson line of the operator. This enables us to reduce significantly both the power divergence and the statistical noise in the correlator \( C_{\Gamma_\phi}^{w_f}(b_1, l, P^z, t) \). At large time separation \( t \), one can extract the wave function \( \phi \) via

\[
C_{\Gamma_\phi}^{w_f}(b_1, l, P^z, t) = \frac{A_w(P^\pi)}{2E} e^{-E_\pi t} \phi(b_1, l, P^z).
\]

Combining Eqs. (9) and (11), the intrinsic soft function defined in Eq. (6) can be obtained through

\[
S(b_1) = \lim_{t \to \infty} \lim_{l \to \infty} \frac{C_{\Gamma}^{3pt}(b_1, P^z, t, \frac{t_\pi}{2})}{H^2 \left[ C_{\Gamma_\phi}^{w_f}(b_1, l, P^z, t, \frac{t_\pi}{2}) \right]^2}.
\]

The lattice data show that \( C_{\Gamma_\phi}^{w_f} \) carries a small but non-vanishing imaginary part. In the determination of \( S(b_1) \), we take into account the contributions from both the real and imaginary part of the wave function.

To examine the convergence of the lattice results at large momentum, we utilize 8 momenta with \( P^z = \pm n(2\pi/L) \) for \( n = 3, 4, 5, 6 \), which correspond to a range from \( \pm 1.7 \text{ GeV} \) to \( \pm 3.3 \text{ GeV} \). Given each \( P^z \), we average the transition modes \( \pi(P^z) \to \pi(-P^z) \) and \( \pi(-P^z) \to \pi(P^z) \) and obtain a 15%-20% reduction in the statistical error. For each momentum, we place the wall-source operator at every two timeslices, which allows us to perform a time translation average for both \( C_{\Gamma}^{3pt} \) and \( C_{\Gamma_\phi}^{w_f} \). This helps to reduce the uncertainty of the soft function by nearly a factor of \( \sqrt{F/2} \).

**Renormalization** – In our past calculation of the nucleon and Delta quasi-parton distribution functions (quasi-PDFs) [25, 26], we have utilized the regularization-independent momentum-subtraction (RI-MOM) scheme [27] developed for non-local operators [24, 28]. The RI-MOM renormalized correlator is defined as

\[
C_{\Gamma_\phi}^{w_f,R}(b_1, l, P^z, t) = C_{\Gamma_\phi}^{w_f}(b_1, l, P^z, t) Z_{\phi}^{R}(b_1, l, P^z, t),
\]

where the bare correlators \( C_{\Gamma_\phi}^{w_f,R}(b_1, l, P^z, t) \) and \( C_{\Gamma_\phi}^{w_f,R}(b_1, l, 0, t) \) contain the same operator \( O_\phi(b_1, l, l) \) and only differ by the external momentum. Thus, one can expect that a clean cancellation of power and logarithmic divergences and other systematics can be achieved using the ratio scheme, without the introduction of an renormalization function. The coefficient \( C_{\Gamma_\phi}^{w_f,\overline{\text{MS}}}(0, 0, 0, t) \) is introduced to restore the correct normalization condition when \( b_1 \to 0 \). As \( C_{\Gamma_\phi}^{w_f,\overline{\text{MS}}}(0, 0, 0, t) \) contain only local operators, it can be determined using the standard renormalization procedure as described below.

The renormalization for the local current operator \( \bar{u}_\Gamma \) or \( \Gamma \bar{d}d \) in \( C_{\Gamma}^{3pt} \) is straightforward. We find \( Z_{S^{\overline{\text{MS}}}}(2 \text{ GeV}) = 0.641(3) \), \( Z_{P^{\overline{\text{MS}}}}(2 \text{ GeV}) = 0.475(4) \) and \( Z_{V} = 0.712(2) \), \( Z_A = 0.753(3) \). Note that \( Z_V \) and \( Z_A \) are scheme- and scale-independent. These are calculated on dedicated \( N_f = 4 \) ensembles with the same lattice action and lattice spacing as the \( N_f = 2 + 1 + 1 \) ensemble used for the matrix elements. The definitions of \( Z_V, Z_A, Z_S \) and \( Z_P \) follow the convention given in Ref. [31]. Note that when the two operators \( \bar{u}_\Gamma \) and \( \Gamma \bar{d}d(0) \) approach each other, a contact term appears and additional renormalization is required to match two bilinear quark operators to a local four-quark operator. For more details of such renormalization procedure, we refer to Refs. [32, 31]. In this work, we target the soft function at \( b_1 \neq 0 \) and, thus, avoid the complication of the above mentioned renormalization.

**Systematic effects** – In Eq. (3), the quasi-TMDWF is defined at an infinitely-large length of the Wilson line \( l \). In a realistic lattice calculation, \( l \) is truncated by a finite lattice size. At sufficiently large \( l \), we find that the lattice results of \( C_{\Gamma_\phi}^{w_f} \) converge and yield a plateau for the region of \( l \gtrsim 0.8 \text{ fm} \). Thus, fits to a constant lead to
LO perturbation theory and find at finite $P^z$
\[ F_T(b_1, P^z) = S(b_1) H^0_{\Gamma_0} |\phi(b_1, l, P^z)|^2 \]
\[ + \sum_{\Gamma' \neq \gamma_5 \gamma_7 \gamma_7} S_{\Gamma'}(b_1) H^0_{\Gamma \Gamma'} |\phi_{\Gamma'}(b_1, l, P^z)|^2, \]
where the factor $H^0_{\Gamma \Gamma'}$ arises from Fierz rearrangement through
\[ \bar{u} \Gamma \gamma_0(b_1) d \Gamma 0 = \sum_{\Gamma'} H^0_{\Gamma \Gamma'} \bar{u}(b_1) \Gamma' 0 d 0 \Gamma' \gamma_0(u_0). \]

With $H^0_{\Gamma \Gamma'} = \frac{1}{16 N_c} \text{Tr}(\Gamma' \Gamma' \Gamma')$. The leading-twist contribution carries a factor of $H^0_{\Gamma_0}$, which is the summation of $H^0_{\Gamma \Gamma'}$ with $\Gamma' = \gamma_5 \gamma_7 \gamma_7$. The higher-twist contributions enter in the second term of Eq. (14) with the wave function $\phi_{\Gamma'}(b_1, l, P^z) = (0|\bar{u}(b_1) \Gamma' W(b_1, l)|P^z)$.

Although the higher-twist contributions are expected to be much smaller than the leading-twist one at sufficiently large momentum, in a realistic lattice calculation, where the typical size of $P^z$ is a few GeV, the contamination from higher-twist may be significant. We find that the lattice result of $\phi_{\Gamma'}$ for $\Gamma' = \gamma_5 \gamma_7 \gamma_7$ is about twice larger than the leading-twist $\phi$. Such large higher-twist contamination explains why some $F_T(b_1, P^z)$ carry the opposite sign, as observed in Fig. 1.

Note that in Fig. 1 results at the largest momentum $P^z = 6.27 \text{ fm}^2 \approx 3.3 \text{ GeV}$ are presented. When $P^z$ decreases, the situation becomes even worse. This is not surprising, as the leading-twist contributions are enhanced at large $P^z$. Considering the fact that the values of $P^z$ accessible in the lattice calculation are quite limited, we draw the conclusion that it is essential to remove the higher-twist effects in the calculation of the soft function. Here we take two steps.

- Firstly, we calculate $\phi_{\Gamma'}$ with various $\Gamma'$ and then pick up all the $\phi_{\Gamma'}$ with relatively large size. It leads to four $\phi_{\Gamma'}$ with $\Gamma' = \gamma_5, \sigma_{02}, \sigma_{12}, \sigma_{23}$. The other higher-twist $\phi_{\Gamma'}$ vanish in the LO perturbation theory and have only small sizes, as found in the lattice calculation.

- Secondly, we define improved pion matrix elements as $\sum_{\Gamma} c_\Gamma F_{\Gamma}(b_1, l)$, where the coefficients $c_\Gamma$ (with $\Gamma = I, \gamma_5 \gamma_7, \gamma_7 \gamma_7$) are chosen appropriately to cancel the contributions from $\phi_{\Gamma'}$ (with $\Gamma' = \gamma_5, \sigma_{02}, \sigma_{12}, \sigma_{23}$).

Following the above two steps, we finally obtain five improved pion matrix elements as a simple combination of two $F_T(b_1)$, namely
\[ \frac{1}{2}(F_{\gamma_5 \gamma_7} + F_{\gamma_7}), \quad \frac{1}{2}(F_{\gamma_5 \gamma_7} + F_{\gamma_7}), \quad \frac{1}{2}(-F_{\gamma_5} + F_{\gamma_7 \gamma_7}), \]
\[ \frac{1}{2}(-F_{\gamma_5} + F_{\gamma_7}), \quad \frac{1}{2}(F_{\gamma_5} + F_{\gamma_7}). \]

The right panel of Fig. 1 shows the soft function compiled using the five improved pion matrix elements. By

Figure 1. The intrinsic soft function $S(b_1)$ as a function of transverse separation $b_1$ at $P^z = 6.27 \approx 3.3 \text{ GeV}$. On the left panel, $S(b_1)$ are compiled using the pion matrix elements $F_T$ as inputs, with $\Gamma = I, \gamma_5, \gamma_7, \gamma_5 \gamma_7$. For $\gamma_5$, there are two choices: $\gamma_5$ parallel to $b_1$ and $\gamma_7$ perpendicular to $b_1$. On the right panel, $S(b_1)$ are compiled using the improved pion matrix elements, where the high transverse separation contamination has been cancelled significantly and the results show much better consistency.

Good $\chi^2$/dof and provide the results of $|C_{\Gamma_0}^{\text{soft}, f}|$ at $l \to \infty$.

To extract reliably the pion matrix element from $|C_{\Gamma_0}^{\text{soft}, f}|$, the excited-state contamination is another systematic effect to be controlled. Using the most precise lattice results at $P^z = 3(2\pi/L) \approx 1.7 \text{ GeV}$, we find that there is a $2\%-3\%$ deviation between the soft functions obtained at $t_s/a = 8$ and 10. Therefore, we use the setup of $t_s/a = 10$ to determine the soft function at $P^z \approx 1.7 \text{ GeV}$. For larger momenta, due to the rapid increase of the noise, the excited-state effects are within the reported statistical uncertainties of $t_s/a = 8$.

After taking the extrapolation of $l \to \infty$ and examining the ground-state saturation at sufficiently large $l$, we use the simplified notation $C_{\Gamma_0}^{\text{soft}, f}(b_1, P^z)$ to replace $C_{\Gamma_0}^{\text{soft}, f}(b_1, l, P^z, t)$ in the following context. To reveal the systematic effects more clearly, all the figures presented in this work are compiled using the most precise lattice data at $m_\pi = 827 \text{ MeV}$, unless specified otherwise.

**Extraction of leading-twist contribution** — According to the proposal of Ref. [17], in the large momentum limit, the same intrinsic soft function can be extracted from various pion matrix elements $F_T$ as far as $F_T$ contain the leading-twist contribution. In this work, we make a complete investigation of the $\Gamma$ dependence of the soft function. The left panel of Fig. 1 illustrates that the results of the soft function are significantly different when using various $F_T$ as inputs. Some results even carry the opposite sign.

To resolve this puzzle, we check the factorization in the
cancelling the dominant higher-twist effects, the results become much more consistent. The residual deviations serve as measure of important systematic effects to be controlled in future studies.

**Results of the soft function** – After checking the consistency among the various improved pion matrix elements, we use the choice of $\frac{1}{2}(F_{\gamma_1} + F_{\gamma_1})$ as an example to present the results of $S(b_1)$ for various momenta $P^z$ and pion masses $m_\pi$.

In Fig. 2 $S(b_1,P^z)$ is shown together with the one-loop perturbative curve [35],

$$S_{\text{MS}}(b_1, \mu) = 1 - \frac{\alpha_s C_F}{\pi} \ln \frac{\mu^2 b_1^2}{4 e^{-2\gamma_E}} + O(\alpha_s^2),$$

where one-loop and four-loop values of $\alpha_s$ are used at the physically most relevant scale of $S(b_1)$, i.e. $1/b_1$. The scale $\mu$ is set as $\mu = 2$ GeV. We note that the lattice results agree qualitatively with the perturbative function at around $b_1 \sim 0.2$ fm, particularly at the largest boost and when the higher-order effects are partially included via $\alpha_s$. At larger $b_1$, non-perturbative features start to set in and the decay of $S(b_1)$ is slower than the perturbative prediction. It is also noteworthy that the convergence of the lattice results in $P^z$ clearly increases with $b_1$ – the results from the two largest $P^z$ are compatible for $b_1 \geq 0.2$ fm, while smaller transverse separations will need yet larger boosts to establish convergence.

In Fig. 3 we examine the pion mass dependence of the soft function. Although $S(b_1)$ is extracted from pion matrix elements which depend on the detailed process of $\pi(P^z) \to \pi(-P^z)$, the factorization allows us to cancel this process dependence. Performing the calculation at four pion masses, we find that the lattice results are generally consistent within statistical errors, although a small systematic increase is found when decreasing $m_\pi$.

This observation supports the statement from the factorization [17] that the soft function does not depend on the detailed hadronic information from the initial/final state.

**Results for the Collins-Soper kernel** – The Collins-Soper kernel $K(b_1, \mu)$ governs the rapidity evolution of the TMDPDFs. In LaMET, the quasi-TMDPDF is factorized into the light-cone TMDPDF and a $K(b_1, \mu)$ factor, where $\zeta^2 = 2(x P^z)^2$, with $P^z$ playing the role of the rapidity, while $\zeta$ is the light-cone counterpart of $\zeta^2$ [30]. Thus, by taking the ratio of quasi-TMDPDFs at different values of $P^z$, one can extract $K(b_1, \mu)$. This ratio can also be expressed in terms of the quasi-TMDWFs [18] as

$$K(b_1, \mu) = \frac{1}{\ln(P_1^z/P_2^z)} \left| \frac{\phi(b_1, l, P_1^z)/E_1}{\phi(b_1, l, P_2^z)/E_2} \right|,$$

where $\phi(b_1, l, P^z)$ is the light-cone factor, with $100 \%$.

Figure 4. The lattice results for the Collins-Soper kernel $K(b_1, \mu)$ from various calculations, described by the color of yellow [20], blue [19], green [13] and red. The results from a same calculation are shifted horizontally to make an easier comparison.
are shown together with data from other calculations. The results exhibit similar dependence on $b_t$ with some discrepancies, which indicate unquantified systematic uncertainties. Both the LPC results and ours are calculated using the quasi-TMDWFs as inputs. Thus, it is not surprising that these results are in better agreement.

**Conclusion** – Within the framework of the lattice formulation we calculate the intrinsic soft function introducing a number of crucial steps that enable its reliable extraction. Our work adds evidence that the methodology proposed in Ref. [17] is indeed suitable for the determination of these quantities. There is room for further improvements. For example, only the LO perturbative hard kernel is used in this calculation and future work needs to examine higher-order corrections. On the lattice side, several sources of systematics need to be addressed, including e.g. cutoff effects and further investigation of quark mass dependence towards the physical one. Nevertheless, this methodology coupled with the improvements introduced in his work, requiring synergy of perturbative and lattice QCD, is shown to be very promising and can provide important first-principle insights into transverse-momentum-dependent hadron structure.

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SUPPLEMENTARY MATERIAL

In this section, we expand on a selection of technical details and add results to facilitate cross-checks of different calculations of the soft function.

Extrapolation of $l \to \infty$ – Although in the lattice QCD calculation the length of the Wilson link $l$ is not allowed to be larger than half of the lattice size $L/2$, it is straightforward to explore the limit of $l \to \infty$ if the renormalized correlation function $|C_{\Gamma_o}^{wf,r}|$ has a plateau at large $l$. In Fig. 5, we show two examples with the external momentum $P^z = 3\frac{2\pi}{T}$ and $5\frac{2\pi}{T}$. In both cases, the plateau appears when $l \geq 0.84$ fm. Using a correlated fit to the constant and extrapolating to the $l \to \infty$ limit, we finally obtain the results of $|C_{\Gamma_o}^{wf,r}|$ at $l = \infty$.

![Figure 5](image)

Figure 5. The $l$ dependence of the renormalized correlation function $|C_{\Gamma_o}^{wf,r}|$ at $P^z = 3\frac{2\pi}{T}$ (top) and $5\frac{2\pi}{T}$ (bottom). Results at four different $b_1$ are shown. The $\chi^2$/dof, which describes the quality of the correlated fit, is listed as $\{1.1, 0.3, 0.4, 0.6\}$ for the case of $P^z = 3\frac{2\pi}{T}$ and $\{0.8, 1.4, 0.4, 0.3\}$ for $5\frac{2\pi}{T}$.

Examination of the excited-state effects – We examined the excited-state contamination of the soft function for various momenta $P^z$. Here, we show the case of $P^z = 3\frac{2\pi}{T}$ and $5\frac{2\pi}{T}$ as an example. In Fig. 6, we compare the soft function at the source-sink separation $t_s/a = 8$ and 10. At the smallest momentum $P^z = 3\frac{2\pi}{T}$, where the lattice results are most precise, the comparison shows about 2%-3% deviation for $S(b_1)$ at $b_1/a = 0, 1, 2, 3$. These deviations are small compared to other systematic effects. To be conservative, we use $t_s/a = 10$ to determine the $S(b_1)$ at $P^z = 3\frac{2\pi}{T}$. When $P^z$ increases, the statistical uncertainties increase significantly. At $P^z = 5\frac{2\pi}{T}$, the results of $S(b_1)$ are fully consistent between the cases of $t_s/a = 8$ and 10. By using $t_s/a = 10$ for $P^z = 3\frac{2\pi}{T}$ and $t_s/a = 8$ for the other momenta, we expect that the excited-state effects are under control in our analysis.

![Figure 6](image)

Figure 6. A comparison is made for the soft function $S(b_1)$ determined using the source-sink separation $t_s/a = 8$ and 10. At momentum $P^z = 3\frac{2\pi}{T}$, 2%-3% deviations are found at $b_1/a = 0, 1, 2, 3$. For the larger momentum $P^z = 5\frac{2\pi}{T}$, the results for $t_s/a = 8$ and 10 are all consistent.

Removal of the higher-twist contamination – In Fig. 7, we show the bare correlators $|C_{\Gamma}^{wf}(b_1, l, P^z, t)|$ as a function of $b_1$ for various $\Gamma'$. Only the correlation functions $|C_{\gamma_5}^{wf}|$ and $|C_{\gamma_5\gamma_3}^{wf}|$ contain the leading-twist contribution, while all the others also contain a higher-twist contribution. We obtain from the figure that some higher-twist correlators have comparable size to the leading-twist ones. We, thus, identify the four largest higher-twist correlators with $\Gamma' = \gamma_5, \sigma_{02}, \sigma_{12}, \sigma_{23}$. The next step to remove the large higher-twist effects is to form appropriate combinations of $F_{\Gamma}$ with $\Gamma = I, \gamma_5, \gamma_1, \gamma_5\gamma_4$.

![Table S I](image)

Table S I. Leading-order hard kernel $H_{\Gamma'}^{0}$ using the Euclidean gamma matrices as input. All values from the table should be multiplied by a factor of $1/N_c$.

In Table S I, the values of the LO hard kernel $H_{\Gamma'}^{0}$ for $\Gamma = I, \gamma_5, \gamma_1, \gamma_5\gamma_4$ are shown for $\Gamma' = \gamma_5, \gamma_1, \gamma_5\gamma_4$ associated with $\Gamma' = \gamma_5, \gamma_1, \gamma_5\gamma_4$.
Figure 7. The bare correlators $|C_{\nu f}(b_\perp, l, P^z, t)|$ as a function of $b_\perp$ for various $\Gamma'$.

Figure 8. Examination of the convergence of the soft function when $P^z$ increases. For a comparison, we show the results using the $F_\Gamma$ with $\Gamma = I, \gamma_5, \gamma_\perp, \gamma_5\gamma_\perp$ in the upper panel and the results using the improved pion matrix elements in the lower panel. From left to right, the momentum $P^z$ increases from $3\frac{2\pi}{L}$ to $6\frac{2\pi}{L}$ and better convergence is observed at larger momentum. Unfortunately, due to the large higher-twist contamination, even at $P^z = 6\frac{2\pi}{L}$ $F_\Gamma$ with various $\Gamma$ still show a strong variation. On the other hand, the improved pion matrix elements show much better convergence, demonstrating that the higher-twist effects are reduced significantly.