Lattice QCD determination of the Collins-Soper kernel from chiral quarks at physical masses

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Proton structure

- Protons composed of point-like constituents called partons (gluons or quarks).
- Partons are not directly observed as individual particles (confinement) but only inferred from interactions with probing particle in scattering experiments.
- Proton structure encoded in distribution functions:
  - parton distribution functions (PDFs) $f_i(x) \sim$ probability amplitude of finding parton $i$ inside hadron with longitudinal momentum fraction $x$.
  - transverse momentum distributions (TMDs) $f_i(x, k_{\perp}) \sim$ probability amplitude of finding parton $i$ with $x$ and transverse momentum $k_{\perp}$.
  - Generalized parton distributions (GPDs), ...
- Proton transverse structure subject of many current and future experiments: JLab 12GeV, EIC, RHIC, COMPASS, etc.
Goal: Tomography of hadrons in 3D momentum space
This talk: Computing Collins-Soper kernel (scale evolution) of TMDs via lattice QCD.
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How can we perform QCD calculations when analytical methods fail?

- Discretize the theory.
- Solve it numerically at different “resolutions”.
- Extrapolate towards continuum theory.

Starting point: Continuum partition function, wick rotation:

$$ Z_{\text{cont.}} = \int \mathcal{D}A \prod_{f=u,d,s,...} \mathcal{D}\psi_f \mathcal{D}\bar{\psi}_f e^{-S_E}, $$

$S_E$: Euclidean QCD Action.
Discretization of the physical 4-volume $V$ with lattice spacing $a$: $V = a^3 N^3_{\sigma} \times aN_T$:

\[ D\nu \psi(x) \rightarrow \frac{U\nu(x)\psi(x + \hat{\nu}) - U_{-\nu}(x)\psi(x - \hat{\nu})}{2a} \]

\[ \int d^4x \rightarrow a^4 \sum_{x \in \Lambda} \]

Partition function:

\[ Z_{\text{cont.}} = \int DA \prod_{f=u,d,s,...} D\psi_f D\bar{\psi}_f e^{-S_E} \rightarrow Z_{\text{lat.}} = \int \prod_{x,\nu} dU_{x,\nu} \prod_f \det M_f e^{-S_g} \]

\[ M_f = \gamma^\mu D_\mu + m_f: \text{ large } (\mathcal{O}(10^7) \times \mathcal{O}(10^7)) \text{ sparse matrix} \]
Fermion discretization has to be done very carefully. Naive prescription results in **doubler problem**: 16 fermions instead of 1.

No-go theorem: No local, doubler free fermion discretization without breaking chiral symmetry.

Domain-wall fermion discretization solves chiral symmetry problem at the cost of introducing additional 5th dimension $L_s \rightarrow$ our discretization of choice for this work.
Lattice QCD overview

Lattice QCD workflow in a nutshell:
To compute observables $\mathcal{O}$, we need to solve lattice path integrals of the form

$$\frac{1}{Z} \int \prod_{x,\mu} dU_{x,\mu} d\phi d\bar{\phi} \, \mathcal{O}[U_{x,\mu}, \phi, \bar{\phi}] \, e^{-S_{\text{eff}}[U_{x,\mu}, \phi, \bar{\phi}]}$$

These are calculated via Markov-Chain Monte-Carlo:

1. Generate $\{U_{x,\nu}\}$-ensembles via HMC-type algorithm with $\exp(-S_{\text{eff}}[U,\phi,\bar{\phi}])$ acting as weight factor.
2. Evaluate $\mathcal{O}[U_{x,\mu}, \phi, \bar{\phi}]$ on $\{U_{x,\nu}\}$-ensembles. For fermionic observables this potentially requires $\mathcal{O}(1000)$ inversions of $M_f^\dagger M_f$ per $\{U_{x,\nu}\}$ configuration.
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Lattice QCD needs Euclidean formulation due to sign problem.

Parton physics defined on light-cone, not directly accessible via lattice QCD.

Large-momentum effective theory\(^1\) offers a solution: linking euclidean correlation functions to light-cone correlation functions via Lorentz boost + perturbative matching.

\[^1\text{X. Ji, PRL 110 (2013)}\]
quasi-TMD beam function $\tilde{\phi}_\Gamma(x, b_\perp, P_z, \mu)$ can be related to light-cone TMD beam function via LaMET:

$$\frac{\tilde{\phi}_\Gamma(x, b_\perp, P_z, \mu)}{\sqrt{S_r(b_\perp, \mu)}} = H(x, \bar{x}, P_z, \mu) \phi(x, b_\perp, \zeta, \mu) \times \exp \left[ \frac{1}{4} \left( \ln \left( \frac{(2xP_z)^2}{\zeta} \right) + \ln \left( \frac{(2\bar{x}P_z)^2}{\zeta} \right) \right) \gamma^{\text{MS}}(b_\perp, \mu) \right] + \text{p.c.}$$

$\sqrt{S_r(b_\perp, \mu)}$: soft function, $H(x, \bar{x}, P_z, \mu)$: pert. matching kernel, $\gamma^{\text{MS}}(b_\perp, \mu)$: Collins-Soper Kernel. Collins-Soper kernel $\gamma^{\text{MS}}(b_\perp, \mu)$ governs rapidity scale evolution from $\zeta$ to $(2xP_z)^2$ (or $(2\bar{x}P_z)^2$).
CS kernel can be extracted from ratio of quasi-TMD beam functions at different momenta $P_1$ and $P_2$:

$$\gamma_{\overline{\text{MS}}}^{\text{MS}}(b_\perp, \mu) = \frac{1}{\ln(P_2/P_1)} \ln \left[ \frac{\tilde{\phi}(x, b_\perp, P_2, \mu)}{\tilde{\phi}(x, b_\perp, P_1, \mu)} \right] + \delta \gamma_{\overline{\text{MS}}}^{\text{MS}}(x, \mu, P_1, P_2) + \text{p.c.}$$

Soft functions cancel, $\delta \gamma_{\overline{\text{MS}}}^{\text{MS}}(x, \mu, P_1, P_2)$ computable from matching kernel $H(x, \bar{x}, P_z, \mu)$. 

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Simplest choice for quasi-TMD beam function: pion TMD wave function

\[ \tilde{\phi}_\Gamma(b_\perp, b_z, P_z, \mu) = \langle \Omega | \bar{\psi}(\frac{b}{2}) \Gamma W_{\parallel}(\frac{b}{2}, -\frac{b}{2}, \eta) \psi(-\frac{b}{2}) | \pi^+; P_z \rangle, \]

with \( \mathbf{b} = (b_\perp, b_z) \) and \( W_{\parallel} \): staple-shaped Wilson line of length \( 2\eta + b_\perp \).
quasi-TMD wave function

quasi-TMDs involve matrix elements of equal-time gauge-invariant (GI) operators:

\[ \mathcal{O}_{\Gamma}^{GI}(\mathbf{b}; \eta) = \bar{\psi}(\frac{\mathbf{b}}{2}) \Gamma W_{\parallel}(\frac{\mathbf{b}}{2}, -\frac{\mathbf{b}}{2}, \eta) \psi(-\frac{\mathbf{b}}{2}), \]

with \( \mathbf{b} = (b_{\perp}, b_{z}) \) and \( W_{\parallel} \): staple-shaped Wilson line of length \( 2\eta + b_{\perp} \).

- Bad signal-to-noise ratio: exponential decay with total length of Wilson line! Difficult to investigate large \( b_{\perp} \) region which would complement phenomenological studies.
- Complicated renormalization of the Wilson line.
- New approach to compute parton physics in Coulomb gauge\(^2\) eliminates need for Wilson-lines!
- In large momentum limit, CG quasi-PDF, quasi-TMD fall into same universality class as the GI case.

Coulomb gauge fixed quasi-TMD matrix elements:

\[ \mathcal{O}_{\Gamma}^{CG}(\mathbf{b}) = \bar{\psi}(\frac{\mathbf{b}}{2}) \Gamma \psi(-\frac{\mathbf{b}}{2}) |\nabla \cdot A = 0\).

\(^2\)Gao et al.: 2306.14960, Zhao: 2311.01391
To obtain bare matrix elements of the pion quasi-TMD wave function, we compute

\[ C_{\pi^G0}(t_s; b_\perp, b_z, P_z) = \left< O_{\Gamma}^{CG}(b, P, t_s) \pi^\dagger(y_0, 0) \right>, \]

with

\[ O_{\Gamma}^{CG}(b, P, t_s) = \sum_y e^{-iP \cdot (y-y_0)} \bar{d}(y + \frac{b}{2}, t_s) \Gamma u(y - \frac{b}{2}, t_s) | \nabla \cdot A = 0, \]

\[ y_0 : \text{source position, } t_s: \text{time separation}. \]

To improve signal-to-noise, we use extended pion sources through boosted Gaussian smearing and also compute the smeared-smeared pion two point function

\[ C_{\pi\pi}(t_s, P_z) = \left< \pi(P, t_s) \pi^\dagger(y_0, 0) \right>, \]

to extract the energy spectrum created by \( \pi^\dagger \) and overlap amplitudes.
Spectral decomposition:

\[
C_{\pi\pi}(t_s; P_z) = \sum_{n=0}^{N_{st}-1} \frac{|Z_n|^2}{2E_n} \left( e^{-E_nt_s} + e^{-E_n(L_t-t_s)} \right),
\]

\[
C_{\pi CG}(t_s; b_\perp, b_z, P_z) = \sum_{n=0}^{N_{st}-1} \frac{Z_n}{2E_n} \langle \Omega | O^{CG}_{\gamma_\perp \gamma_5} | n \rangle \left( e^{-E_nt_s} + e^{-E_n(L_t-t_s)} \right).
\]

\(E_n(P_z):\) energy level, \(Z_n = \langle n | \pi^\dagger(P_z) | \Omega \rangle\) overlap amplitude.

We construct the ratio

\[
R(t_s; b_\perp, b_z, P_z) = \frac{-iC_{\pi CG}(t_s; b_\perp, b_z, P_z)}{C_{\pi\pi}(t_s; P_z)},
\]

and fit the above spectral decomposition with a two-state fit \(N_{st} = 2\).
2+1-flavor Domain Wall fermions with $N_s^3 \times N_t \times L_s = 64^3 \times 128 \times 12$.

$a^{-1} = 2.3549(49) GeV \rightarrow a = 0.0836 fm$.

Boosted Gaussian smeared sources with $r_G = 0.58 fm$.

64 gauge-configurations in total.

All mode averaging technique with 128 sloppy sources, 2 exact sources for $n_z \in [4, 8] \rightarrow$ max. $P_z = \frac{2\pi n_z}{N_s} = 1.85$ GeV.

32 sloppy sources, 1 exact for $n_z \in [0, 3]$.

Accelerate matrix inversions with EV deflation with 2000 lowest EV’s and mixed precision solver.
Figure: $R(t_s; b_\perp, b_z, P_z)$ as a function of $t_s$ for $n_z = 8$ and $b_\perp = 10a$. The bands are results from the two-state fits.
- CG quasi-TMD operator renormalization: overall multiplicative factor.
- GI quasi-TMD operator renormalization: multiplicative renormalization and cusp divergences, linear divergences and pinch pole singularities from Wilson line.
- Renormalization is proportional to total Wilson line length: $2\eta + b_\perp$
- Form RG invariant ratios without affecting $x$- and $P_z$-dependence of quasi-TMDWF:

$$\tilde{\Phi}(b_\perp, b_z, P_z) = \frac{\tilde{\phi}^B(b_\perp, b_z, P_z, \eta, a)}{\tilde{\phi}^B(b_\perp, 0, 0, \eta, a)}.$$
Figure: The real (left) and imaginary (right) parts of the renormalized quasi-TMDWF matrix elements at $n_z = 8$ with $b_\perp = 2a, 6a, 8a$ for the CG (filled squared symbols) and GI cases (open circled symbols).
Fourier transform

- Matrix elements decrease as function of $b_z$, reaching zero within errors for $b_z > 1$ fm.
- Apply first order spline interpolation to smooth data points.
- Truncate maximum $b_z$ value in numerical fourier transform to $x$-space:

$$\tilde{\Phi}(x, b_\perp, P_z) = \frac{P_z}{\pi} \int_{0}^{b_{\max}} e^{i(x-\frac{1}{2})P_z b_z} \tilde{\Phi}(b_\perp, b_z, P_z).$$
Figure: CG quasi-TMDWFs at momentum $n_z \in [4, 8]$ and $b_\perp = 2a, 10a$. 
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We define CS kernel estimators:

\[
\hat{\gamma}_{\text{MS}}(x, b_\perp, P_1, P_2, \mu) = \frac{1}{\ln(P_2/P_1)} \ln \left[ \frac{\Phi(x, b_\perp, P_2)}{\Phi(x, b_\perp, P_1)} \right] + \delta \gamma_{\text{MS}}(x, \mu, P_1, P_2).
\]

**Figure:** CS kernel estimators $\hat{\gamma}_{\text{MS}}(x, b_\perp, P_1, P_2, \mu)$ derived from the ratio of quasi-TMDWFs.
Figure: The Collins-Soper kernel from CG quasi-TMDWFs (black points), GI quasi-TMDWFs (blue points), PT (black line) and phenomenological parameterizations.
LaMET opens the way for lattice QCD calculations of parton physics.

We have calculated the Collins-Soper Kernel via ratios of pion quasi-TMD wavefunctions with new Coulomb gauge-fixed method.

CG method offers much better signal-to-noise ratio, easier renormalization, allowing us to reach large $b_\perp$.

Results agree with recent phenomenological parameterizations of experimental data.