

TMDPDFs and Agent for Lattice QCD

Jin-Xin Tan (SJTU)

In collaboration with:

Mu-Hua Zhang, Zhi-Chao Gong, Qi-An Zhang, Wei Wang et al.

第一届中国电子离子对撞机相关年会

2026/4/22 @ 青岛

Based on: PRD113, 054505 (2026), arXiv: 2512.19799, arXiv: 2603.22471

Outline

- **Lattice QCD Determination of TMDPDFs**
- **Autonomous AI Physicists**
From PhysMaster to LQCD Master
- **Summary**

Outline

- **Lattice QCD Determination of TMDPDFs**
 - 1. Definition**
 - 2. Method**
 - 3. Lattice Calculation**

Outline

➤ **Lattice QCD Determination of TMDPDFs**

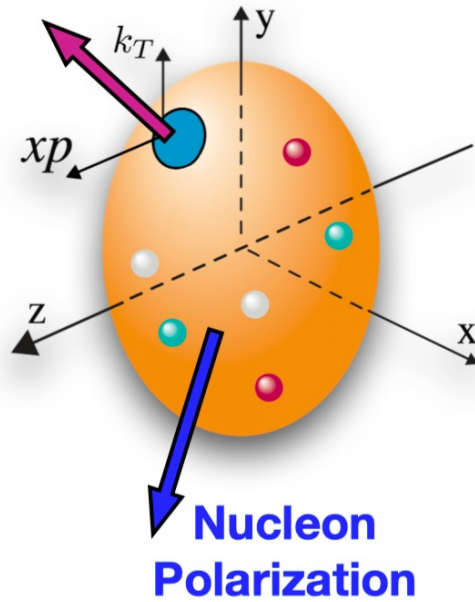
1. Definition

2. Method

3. Lattice Calculation

TMDPDFs: 3D tomography of the nucleon

Quark Polarization



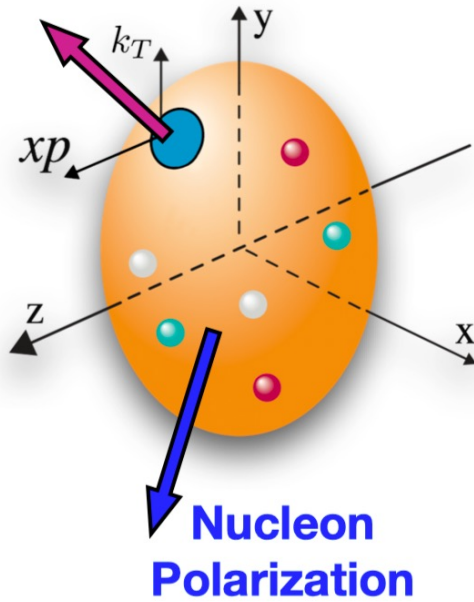
Leading Quark TMDPDFs



		Quark Polarization		
		Un-Polarized (U)	Longitudinally Polarized (L)	Transversely Polarized (T)
Nucleon Polarization	U	$f_1 = \text{○} \cdot$ Unpolarized		$h_1^\perp = \text{○} \uparrow - \text{○} \downarrow$ Boer-Mulders
	L		$g_{1L} = \text{○} \rightarrow - \text{○} \leftarrow$ Helicity	$h_{1L}^\perp = \text{○} \nearrow - \text{○} \nwarrow$ Worm-gear
	T	$f_{1T}^\perp = \text{○} \uparrow - \text{○} \downarrow$ Sivers	$g_{1T}^\perp = \text{○} \uparrow \rightarrow - \text{○} \uparrow \leftarrow$ Worm-gear	$h_1 = \text{○} \uparrow - \text{○} \downarrow$ Transversity $h_{1T}^\perp = \text{○} \nearrow - \text{○} \nwarrow$ Pretzelosity

TMDPDFs: 3D tomography of the nucleon

Quark Polarization



Leading Quark TMDPDFs



		Quark Polarization		
		Un-Polarized (U)	Longitudinally Polarized (L)	Transversely Polarized (T)
Nucleon Polarization	U	$f_1 =$ Unpolarized		$h_1^\perp =$ Boer-Mulders
	L		$g_{1L} =$ Helicity	$h_{1L}^\perp =$ Worm-gear
	T	$f_{1T}^\perp =$ Sivers	$g_{1T}^\perp =$ Worm-gear	$h_1 =$ Transversity $h_{1T}^\perp =$ Pretzelosity

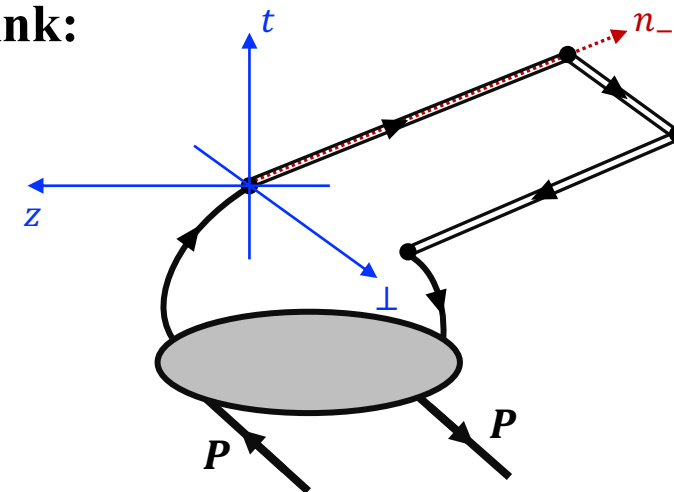


- In 2026, we will primarily concentrate on the first four distributions: f_1 , h_1^\perp , g_{1L} , and h_{1L}^\perp , while the other four will be studied in subsequent work.

- Rapidity divergence from gluons radiation collinear to lightlike gauge link:

$$I_{\text{div}} \sim \int dk^+ dk^- \frac{f(k^+ k^-)}{(k^+ k^-)^{1+\epsilon}} = \frac{1}{2} \int \frac{d(k^- / k^+)}{k^- / k^+} \int d(k^+ k^-) \frac{f(k^+ k^-)}{(k^+ k^-)^{1+\epsilon}}$$

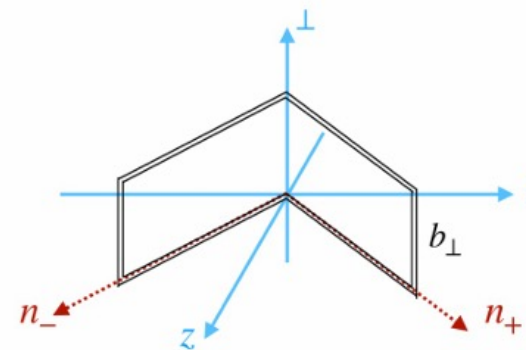
$$y_k = \frac{1}{2} \ln \frac{k^+}{k^-} \quad y_k \rightarrow \pm\infty: \text{rapidity divergence}$$



- Rapidity divergence renormalized by **soft function**:

$$S(\vec{b}_\perp, \mu, \delta^+, \delta^-) = \frac{1}{N_c} \text{Tr} \langle 0 | W_n(\vec{b}_\perp) |_{\delta^+} W_p^\dagger(\vec{b}_\perp) |_{\delta^-} | 0 \rangle$$

δ as the rapidity regulator.



➤ Physical TMDPDF is defined as: *e. g. unpolarized*

$$f(\lambda, b_{\perp}, \mu, \delta^{-} / P^{+}) = \langle P | \bar{\psi}(\lambda n / 2 + b_{\perp}) \not{n} W_n(\lambda n / 2 + b_{\perp}) |_{\delta^{-}} \psi(-\lambda n / 2) | P \rangle \Rightarrow \text{Unsubtracted TMDPDF}$$

$$f^{\text{TMD}}(x, b_{\perp}, \mu, \zeta) = \lim_{\delta^{-} \rightarrow 0} \frac{f(\lambda, b_{\perp}, \mu, \delta^{-} / P^{+})}{\sqrt{S(b_{\perp}, \mu, \delta^{-} e^{2y_n}, \delta^{-})}}$$

Rapidity regulator **cancelled** in the ratio, leaving the rapidity scale ζ dependence $\sim e^{-\frac{1}{2}K(b_{\perp}, \mu) \ln \frac{\mu^2}{\zeta^2}}$

- **Rapidity scale evolution** controlled by the Collins-Soper equation:

$$2\zeta \frac{d}{d\zeta} \ln f^{\text{TMD}}(x, b_{\perp}, \mu, \zeta) = K(b_{\perp}, \mu)$$

Collins-Soper kernel

- The **intrinsic/reduced soft function** is defined from

$$S_{\text{DY}}(b_{\perp}, \mu, Y, Y') = e^{(Y+Y')K(b_{\perp}, \mu) + \mathcal{D}(b_{\perp}, \mu)} + \dots$$

as

$$S_I(b_{\perp}, \mu) \equiv e^{\mathcal{D}(b_{\perp}, \mu)}$$

Outline


➤ **Lattice QCD Determination of TMDPDFs**

1. Definition

2. Method

3. Lattice Calculation

- Large-momentum effective theory: connecting Euclidean lattice and physical observables

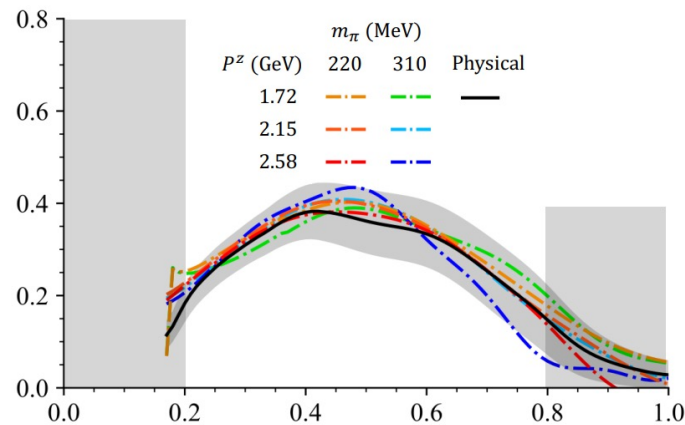
Physical TMDs 

$$\frac{f(x, b_{\perp}, \mu, \zeta)}{S_I^2(b_{\perp}, \mu)} = \exp \left[-\frac{1}{2} K(b_{\perp}, \mu) \ln \frac{-\zeta^z + i\epsilon}{\zeta} \right] H_{\Gamma}(\zeta^z, \mu) \tilde{f}_{\Gamma}(x, b_{\perp}, \mu, \zeta^z) + \mathcal{O}\left(\frac{\Lambda_{\text{QCD}}^2}{\zeta^z}, \frac{1}{b_{\perp}^2 \zeta^z}\right)$$

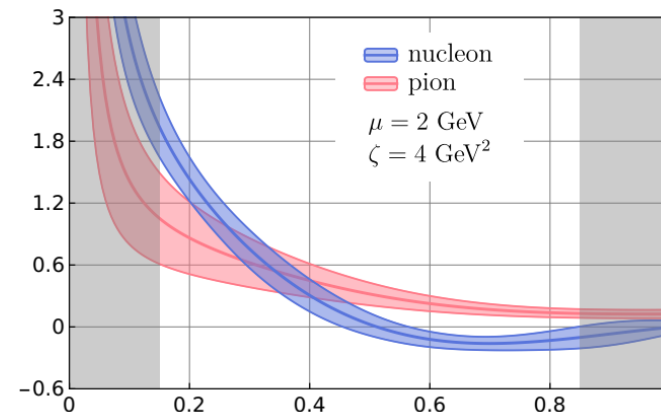
Intrinsic soft function Collins-Soper kernel Matching kernel ✓ Quasi TMDs

Lattice
Lattice
Lattice

- Achieved great success in the studies of TMDPDFs:



Unpolarized nucleon TMDPDF, PRD109 (2024)



Boer-Mulders Function, JHEP 08 (2025) 086

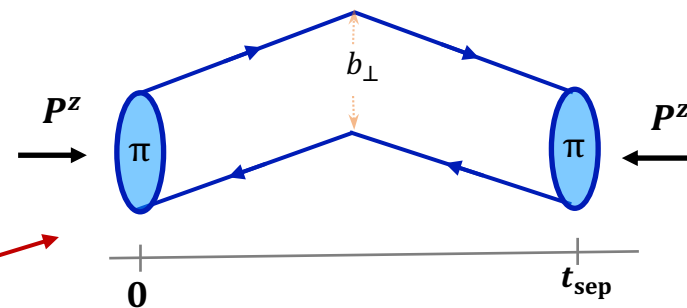
- Collins-Soper kernel from the P^z dependence of TMDs:

$$K(b_{\perp}, \mu) = \frac{1}{\ln(P_1^z/P_2^z)} \ln \left(\frac{H_{\Gamma}(\zeta_2^z, \mu) \tilde{f}_{\Gamma}(x, b_{\perp}, \zeta_1^z, \mu)}{H_{\Gamma}(\zeta_1^z, \mu) \tilde{f}_{\Gamma}(x, b_{\perp}, \zeta_2^z, \mu)} \right)$$

\tilde{f}_{Γ} could be either unsubtracted **quasi TMD wave function** or **quasi TMDPDF**.

- Intrinsic soft function from **four-quark form factors**:

$$\begin{aligned} S_I(b_{\perp}, \mu) &= \frac{S(b_{\perp}, \mu, Y, Y')}{S(b_{\perp}, \mu, Y, 0)S(b_{\perp}, \mu, 0, Y')} \\ &= \frac{F(b_{\perp}, P^z)}{\int dx dx' H(x, x', P^z) \tilde{\phi}(x, \bar{Y}, P^z, b_{\perp}) \tilde{\phi}^{\dagger}(x', \bar{Y}', P^z, b_{\perp})} \end{aligned}$$



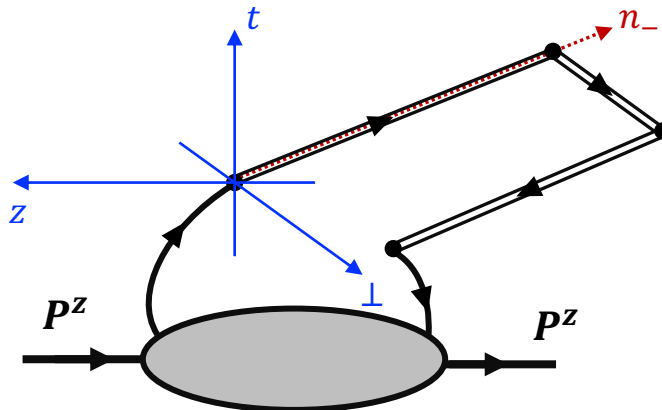
*Ji, PRL 110, 262002 (2013);
 Ji, Sci.China 57 (2014);
 Ji et al., NPB 955 (2020);
 Deng et al., JHEP 09 (2022)*

- **Hadronic matrix element from equal-time correlators:**

$$\tilde{h}_{\Gamma}^0(z, P^z, b_{\perp}) = \lim_{L \rightarrow \infty} \langle P^z, S | \bar{\psi}(b_{\perp} \hat{n}_{\perp}) \Gamma U(b_{\perp} \hat{n}_{\perp} \leftarrow b_{\perp} \hat{n}_{\perp} + L \hat{n}_z; b_{\perp} \hat{n}_{\perp} + L \hat{n}_z \leftarrow L \hat{n}_z; L \hat{n}_z \leftarrow z \hat{n}_z) \psi(z \hat{n}_z) | P^z, S \rangle$$

- **Subtracted quasi-TMDPDFs:**

$$\tilde{f}_{\Gamma}(x, P^z, b_{\perp}, \mu) = \lim_{\substack{a \rightarrow 0 \\ L \rightarrow \infty}} \int \frac{dz}{2\pi} e^{-iz(xP^z)} \frac{\tilde{h}_{\Gamma}^0(z, P^z, b_{\perp})}{\sqrt{Z_E(2L + z, b_{\perp}, a)} Z_O(1/a, \mu)}.$$



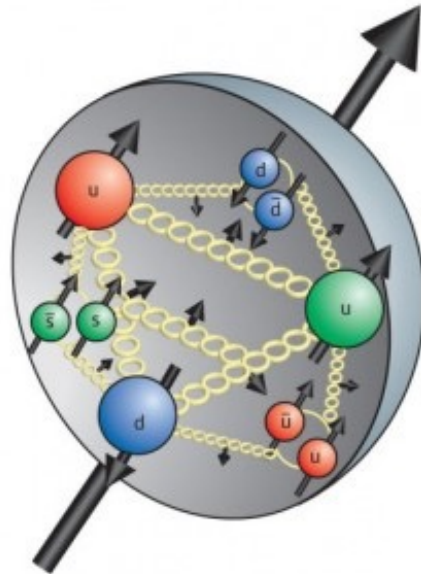
Quasi-TMD correlators with different Dirac structures and spin projectors map onto the leading-twist TMDs:

$$\int \frac{d\xi^z}{2\pi} \frac{d^2\xi_\perp}{(2\pi)^2} e^{-i x P^z \xi^z - i k_\perp \cdot \xi_\perp} \text{Tr} \langle P^z, S | \bar{\psi}(0) \Gamma U(0, \xi^z) \psi(\xi^z) | P^z, S \rangle \sim (f_1, g_{1L}, h_1, f_{1T}^\perp, h_1^\perp, \dots)$$

Quark polarization:

- Unpolarized: $\Gamma = \gamma^z$ or γ^t
- Helicity: $\Gamma = \gamma^z \gamma_5$ or $\gamma^t \gamma_5$
- Transversity: $\Gamma = i\sigma_{\perp z} \gamma_5$ or

$$i\sigma_{\perp t} \gamma_5, \sigma_{\mu\nu} = \frac{i}{2} [\gamma_\mu, \gamma_\nu]$$



Nucleon polarization:

- Unpolarized: $T_{\text{unpol}} = \frac{1+\gamma_4}{2}$
- Helicity: $T_{\text{hel}}^\pm = \frac{1+\gamma_4}{2} \frac{1\pm\gamma_5\gamma_3}{2}$
- Transversity: $T_{\text{trans}}^{(\pm,x)} = \frac{1+\gamma_4}{2} \frac{1\pm\gamma_5\gamma_1}{2}$

$$T_{\text{trans}}^{(\pm,y)} = \frac{1+\gamma_4}{2} \frac{1\pm\gamma_5\gamma_2}{2}$$

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➤ **Lattice QCD Determination of TMDPDFs**

1. Definition

2. Method

3. Lattice Calculation

Lattice Setup

	a/fm	$n_s^3 \times n_t$	m_π/MeV	$n_{cfg} \times n_{meas}$		
				CS kernel ✓	Intrinsic Soft Function ○	TMDPDFs ○
C32P29		$32^3 \times 64$	292.4	984×4	984×2 ✓	1000×4 ✓
C32P23	0.10530	$32^3 \times 64$	228.0	448×10	450×24 ✓	1000×4 ○
C48P14		$48^3 \times 96$	135.5	204×24	448×48 ○	300×12 ○
F32P30	0.07746	$32^3 \times 96$	303.2	1153×6	1100×6 ✓	1000×4 ✓
G36P30	0.06889	$36^3 \times 108$	297	—	—	1000×4 ○
H48P32	0.05187	$48^3 \times 144$	317.2	550×8	550×8 ✓	—

Outline

➤ **Lattice QCD Determination of TMDPDFs**

1. Definition

2. Method

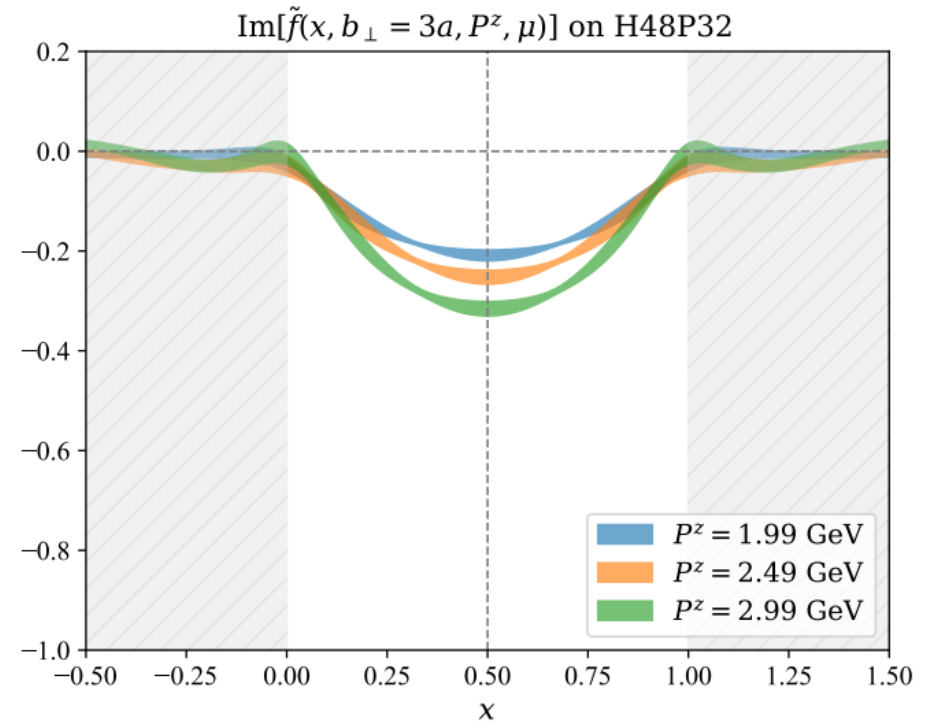
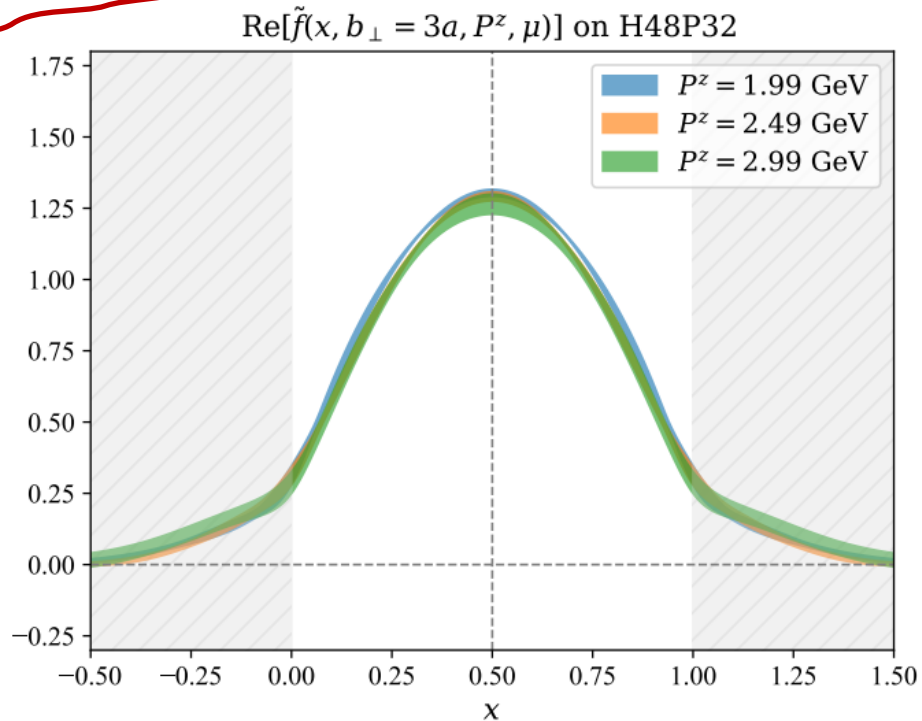
3. Lattice Calculation

a. Collins-Soper kernel

Result for Quasi-TMDWFs in Momentum Space

$$\tilde{f}(x, b_{\perp}, \mu, \zeta_z) = \lim_{L \rightarrow \infty} \int \frac{dz}{2\pi} e^{i(x - \frac{1}{2})zP^z} \frac{\tilde{\Phi}^{+0}(z, b_{\perp}, P^z, a, L)}{Z_O(\mu, a) \sqrt{Z_E(2L + z, b_{\perp}, \mu, a)}}$$

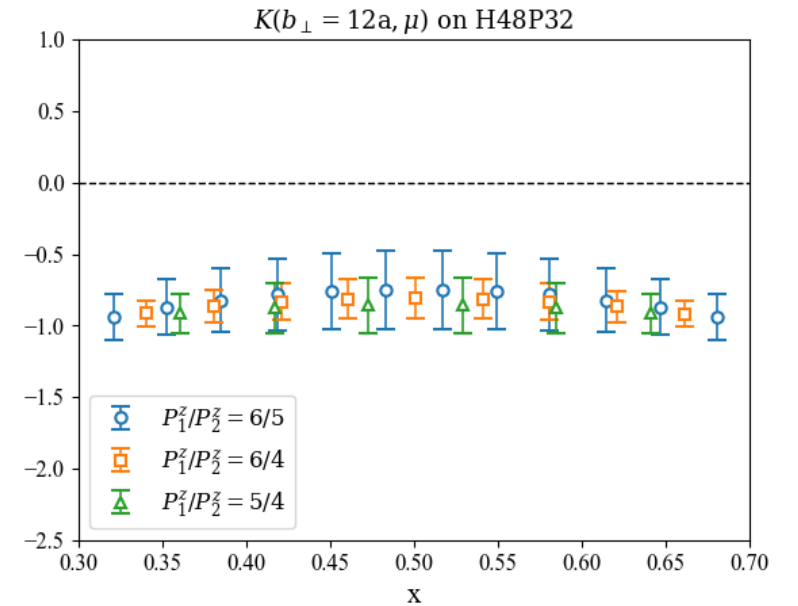
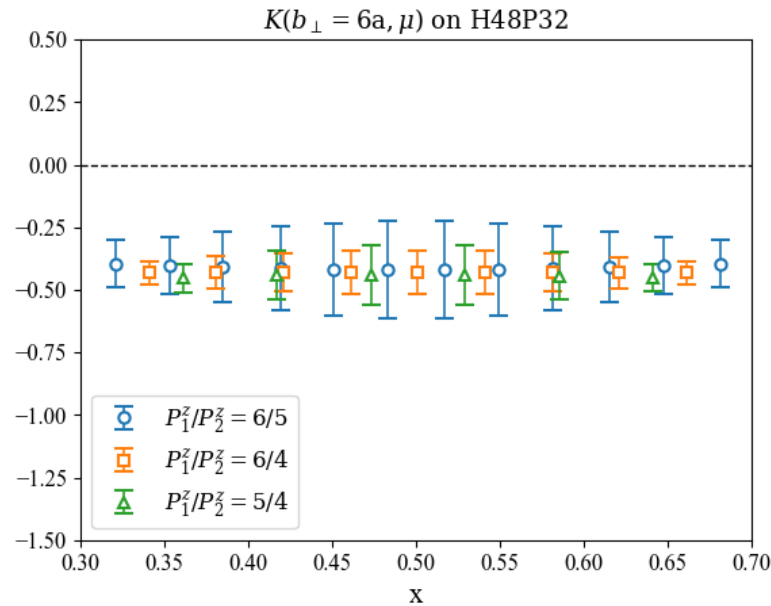
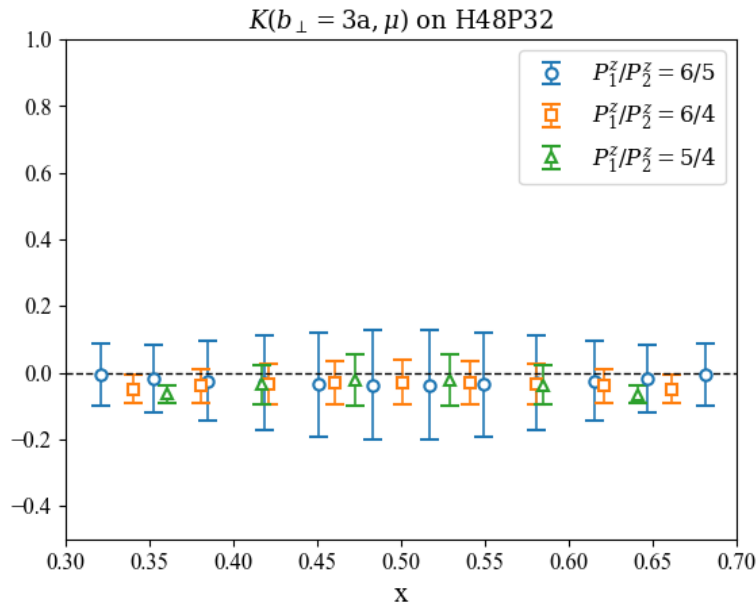
Different P^z



quasi-TMDWFs

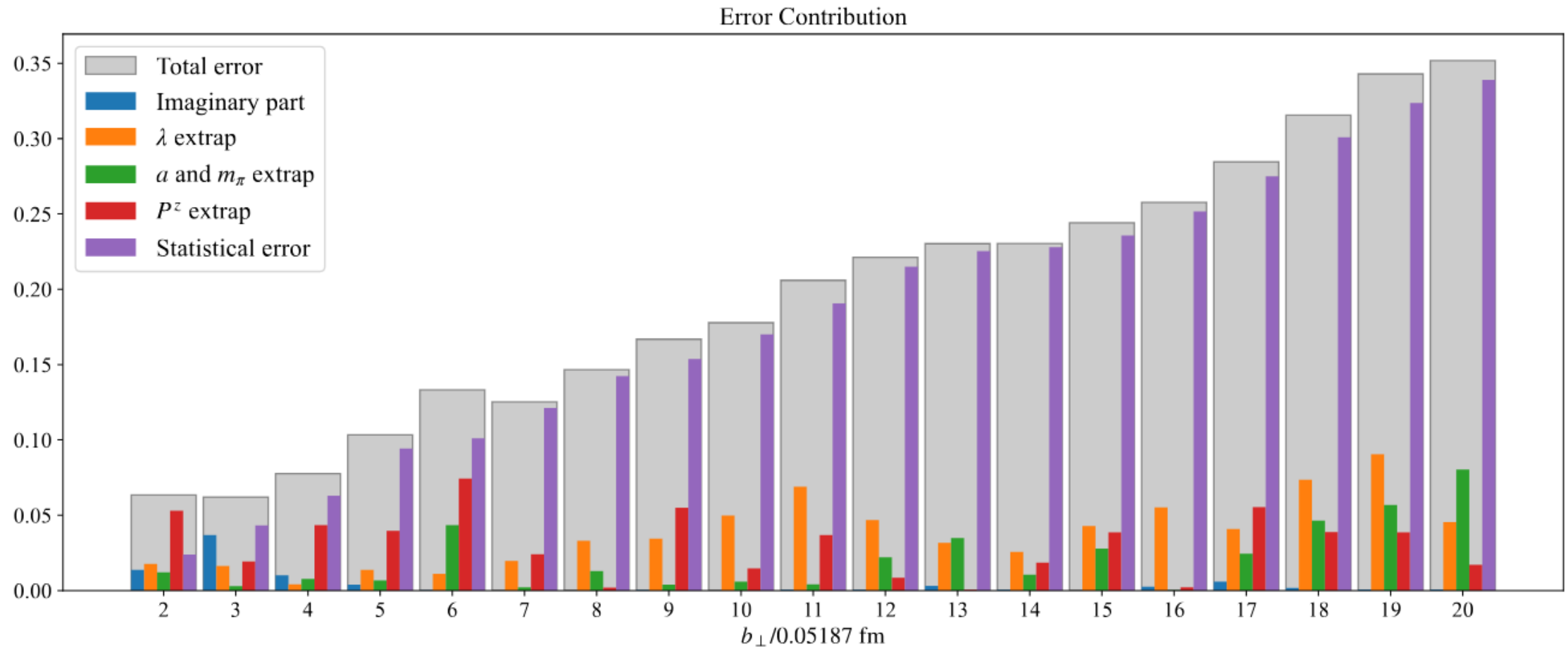
$$K(b_{\perp}, \mu, x, P_1^z, P_2^z) = \frac{1}{\ln(P_1^z / P_2^z)} \left[\ln \frac{H(\zeta_{z,2}, \bar{\zeta}_{z,2}, b_{\perp}, \mu) \tilde{f}(x, b_{\perp}, \mu, \zeta_{z,1})}{H(\zeta_{z,1}, \bar{\zeta}_{z,1}, b_{\perp}, \mu) \tilde{f}(x, b_{\perp}, \mu, \zeta_{z,2})} \right]$$

matching kernel

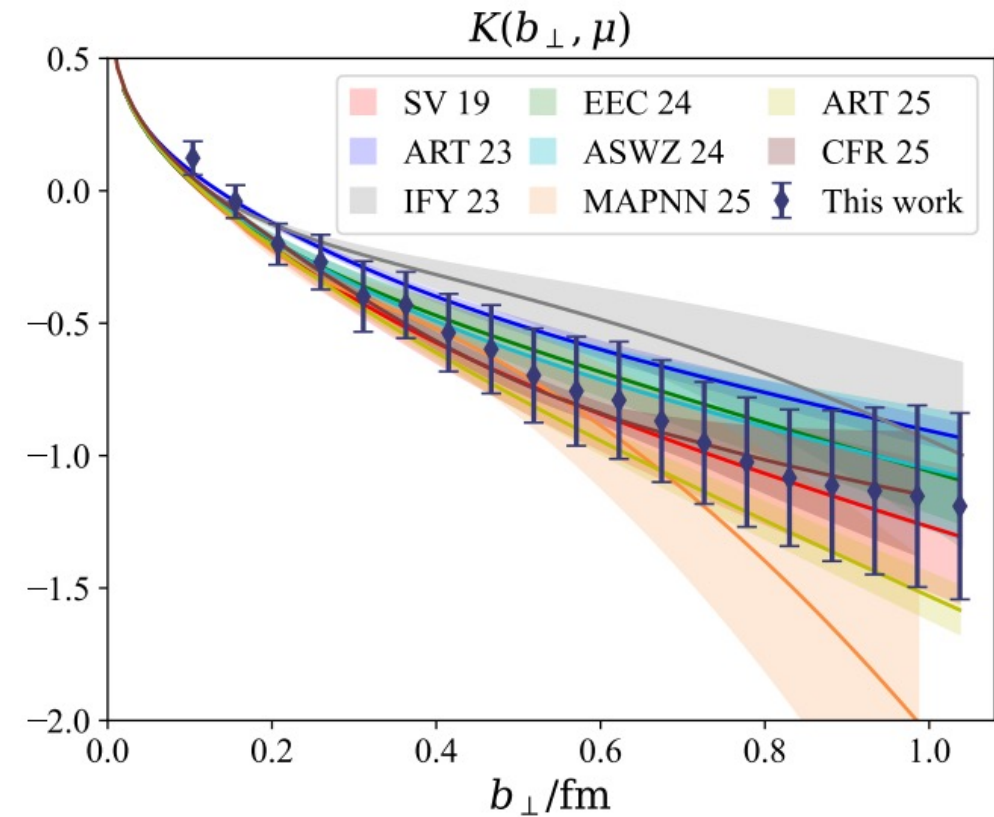
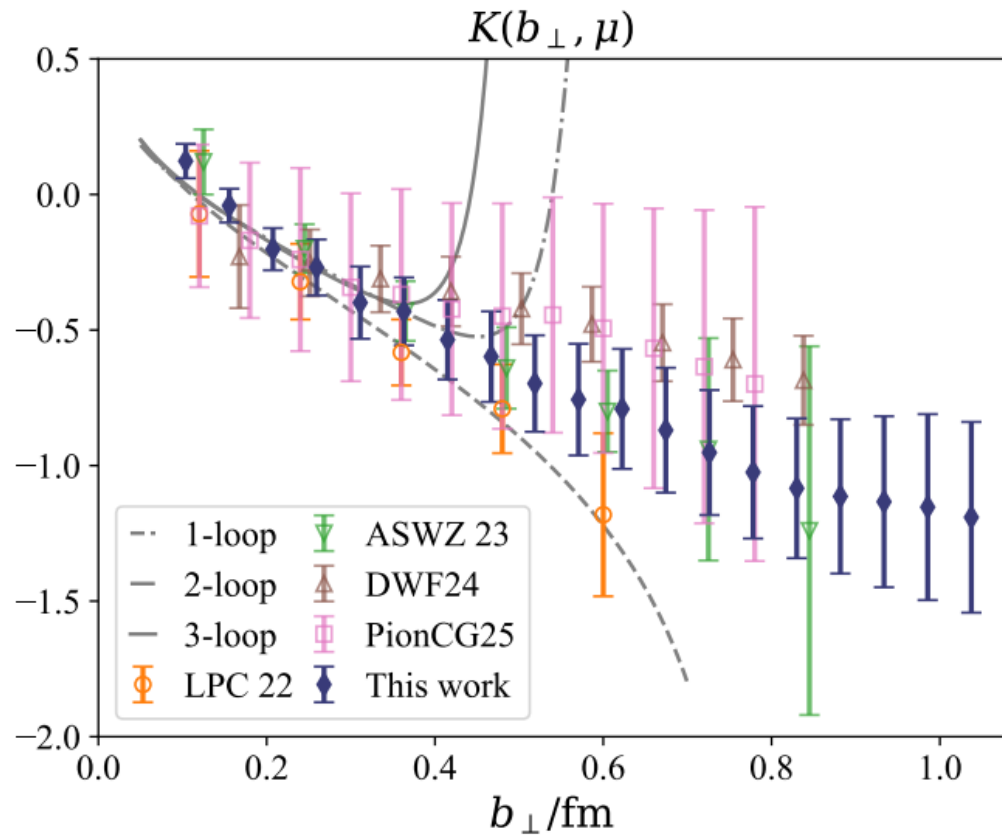


(For better visualization, we present a subset of points selected from the 200 data points in each of the 3 cases.)

➤ We have properly accounted for the systematic uncertainties.



✓ Continuum limit; ✓ Physical mass; ✓ $b_{\perp} = 1\text{fm}$.



Chu et al. (LPC), JHEP 08, 172 (2023);
Avkhadiev, et al., PRD 108, 114505 (2023);
Bollweg, et al., PRB 852, 138617 (2024);
Bollweg, et al., PRD 112, 034501(2025).

Scimemi et al., JHEP 06, 137 (2020);
Moos et al., JHEP 05, 036 (2024);
Avkhadiev et al., PRL. 132, 231901 (2024);
Isaacson et al., PRD 110, 073002 (2024);

Kang et al., arXiv:2410.21435;
Bacchetta et al., PRL. 135, 021904 (2025);
Moos et al., arXiv:2503.11201;
Camarda et al., arXiv:2508.06201.

Outline

➤ **Lattice QCD Determination of TMDPDFs**

1. Definition

2. Method

3. Lattice Calculation

a. Collins-Soper kernel

b. Intrinsic Soft Function

Previous Studies: 350~670 MeV

Li et al., PRL. 128 (2022)

Chu et al. (LPC), JHEP 08, 172 (2023)



This work:

136~320 MeV

Why?

➤ Three-Point Correlation Functions for the Extraction of Form Factors:

$$C_3(b_\perp, \Gamma, t_{seq}, t, P^z) = \sum_{\vec{z}, \vec{x}_1, \vec{x}_2} e^{-i2zP^z} \langle O_\pi(t_{seq}, \vec{x}_1, -P^z) \bar{u} \Gamma u(\vec{z} + b_\perp, t) \bar{d} \Gamma d(\vec{z}, t) O_\pi^\dagger(0, \vec{x}_2, P^z) \rangle$$

we take:

$$O_\pi^\dagger(t, \vec{x}, P^z, \Gamma_1) = \bar{u}(\vec{x}, t) \Gamma_1 d(\vec{x}, t) e^{-i\vec{x} \cdot \hat{n}_z P^z}$$

$$O_\pi(t_{seq}, \vec{x}', P^z, \Gamma_2) = \bar{d}(\vec{x}', t_{seq}) \Gamma_2 u(\vec{x}', t_{seq}) e^{i\vec{x}' \cdot \hat{n}_z P^z}$$

$$\Gamma_{1,2} = \gamma_5$$

$$\Gamma_{1,2} = \gamma_t \gamma_5 \text{ or } \gamma_z \gamma_5$$

High power: $\mathcal{O}(m^2 P_z^2)$



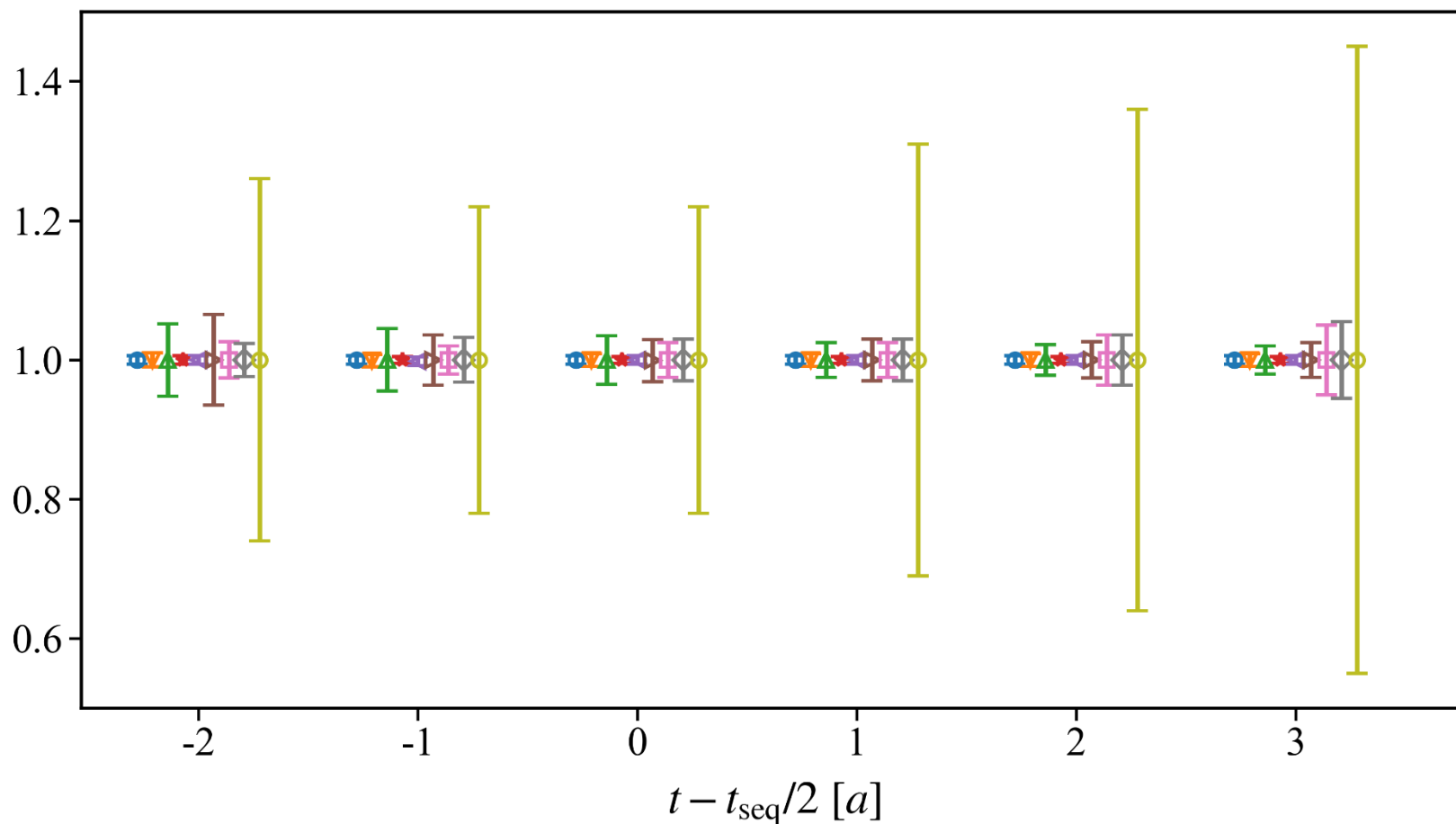
Leading power: $\mathcal{O}(P_z^4)$

Source-enhanced operators

Extraction of Form Factor near the Physical Pion Mass

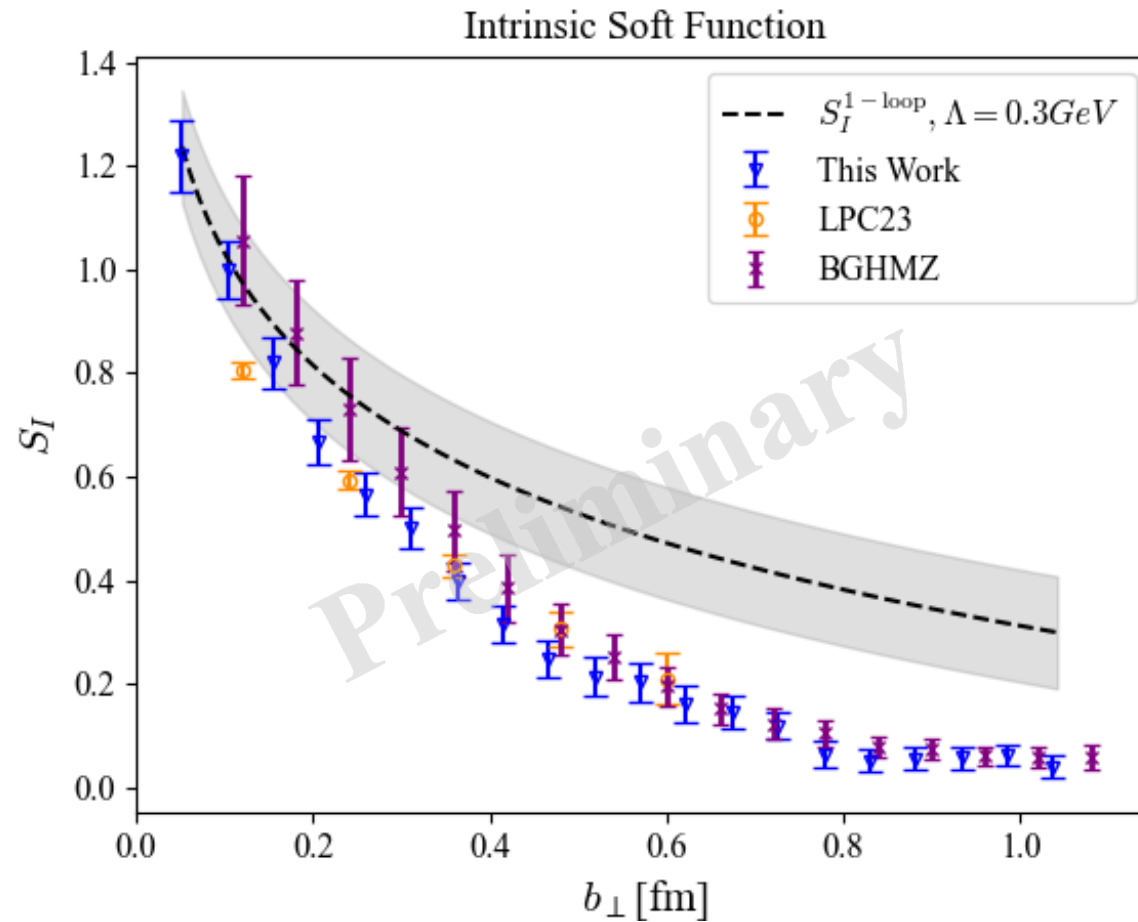
➤ Fix $m_\pi = 300\text{MeV}$ ($t_{seq} = 6a, b_\perp = 1a, P^z = 1.47\text{GeV}$)

Noise to Signal Ratio



Final Result of Intrinsic Soft Function

✓ Continuum limit; ○ Physical mass; ✓ $b_{\perp} = 1\text{fm}$.



Chu et al. (LPC), JHEP 08, 172 (2023)
Bollweg et al., Phys.Rev.D 112 (2025)

Outline

- **Lattice QCD Determination of TMDPDFs**
 1. Definition
 2. Method
 - 3. Lattice Calculation**
 - a. Collins-Soper kernel
 - b. Intrinsic Soft Function
 - c. TMDPDFs**

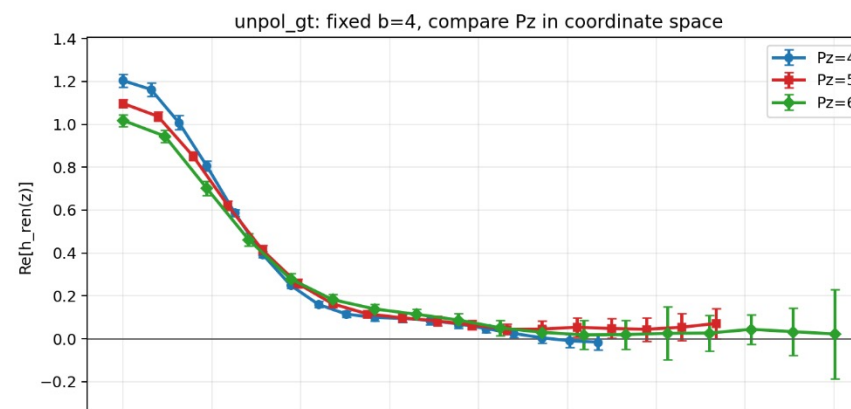
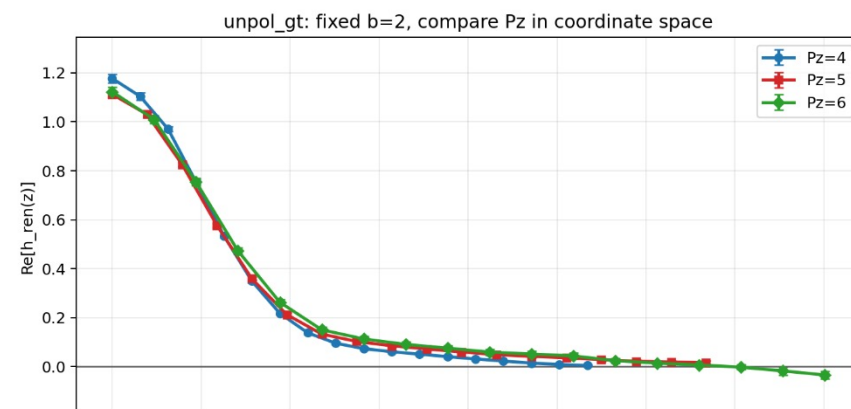
➤ unpol.

$$b_{\perp} = 2a$$

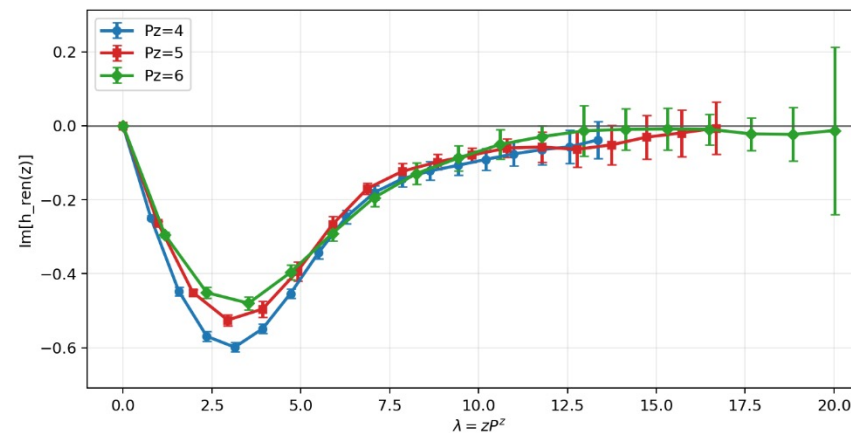
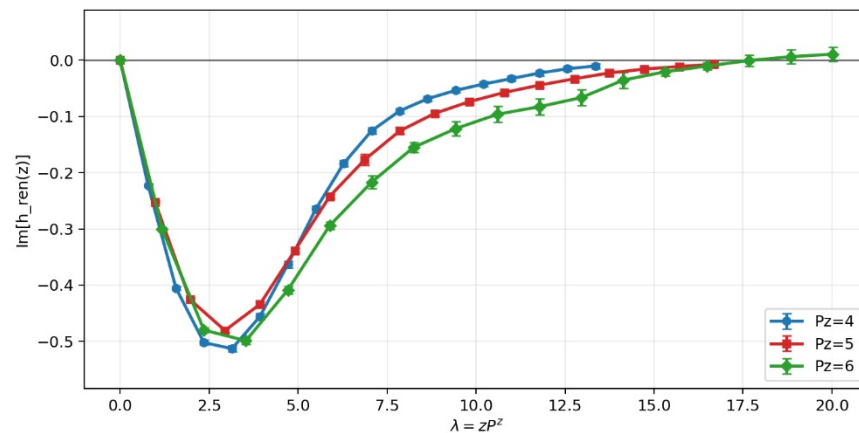
$$b_{\perp} = 4a$$

(after renormalization)

Re



Im



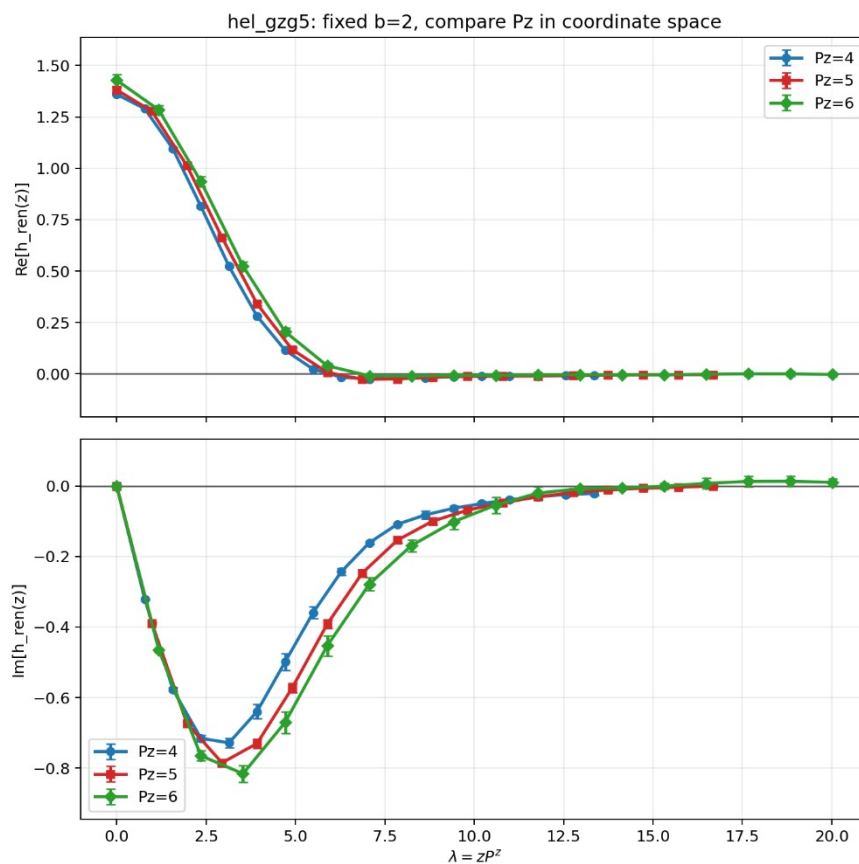
➤ helicity(+)-(-)

$$b_{\perp} = 2a$$

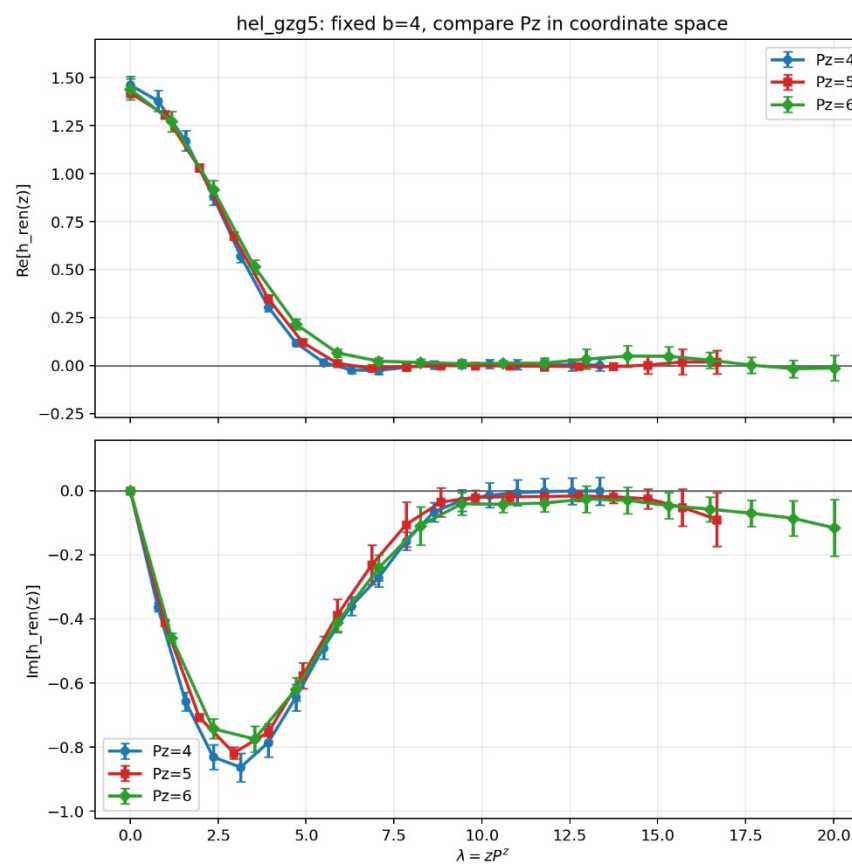
$$b_{\perp} = 4a$$

(after renormalization)

Re



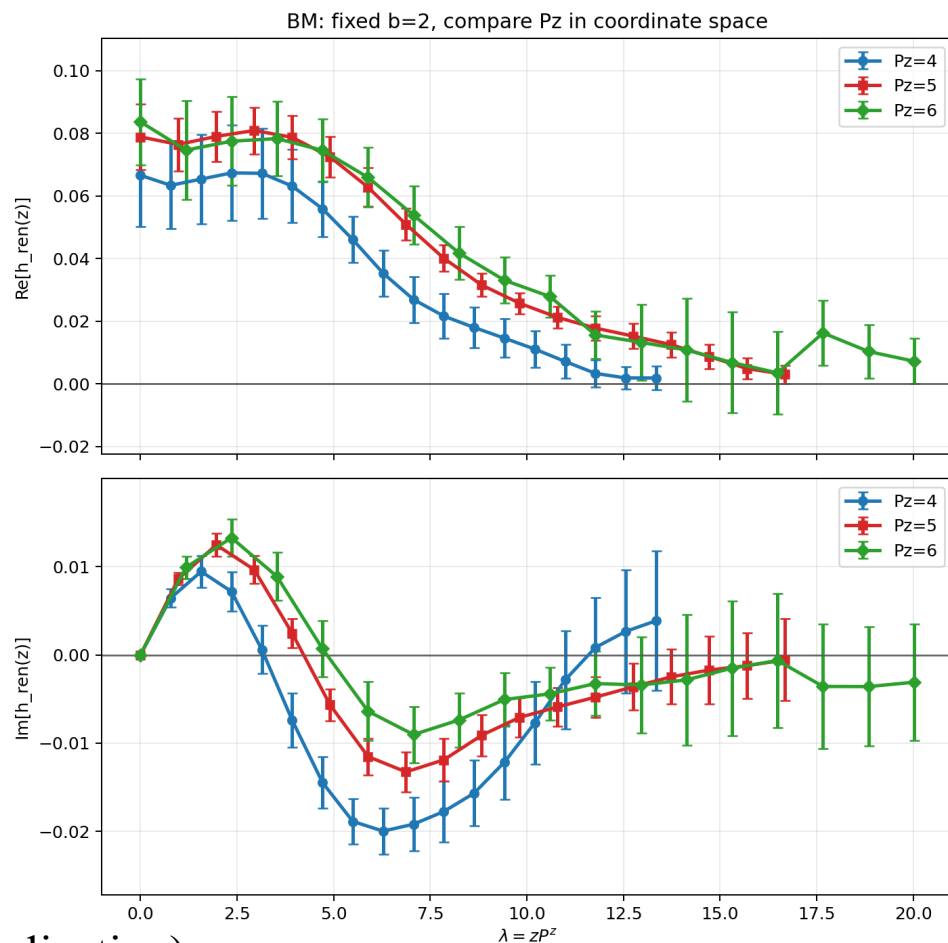
Im



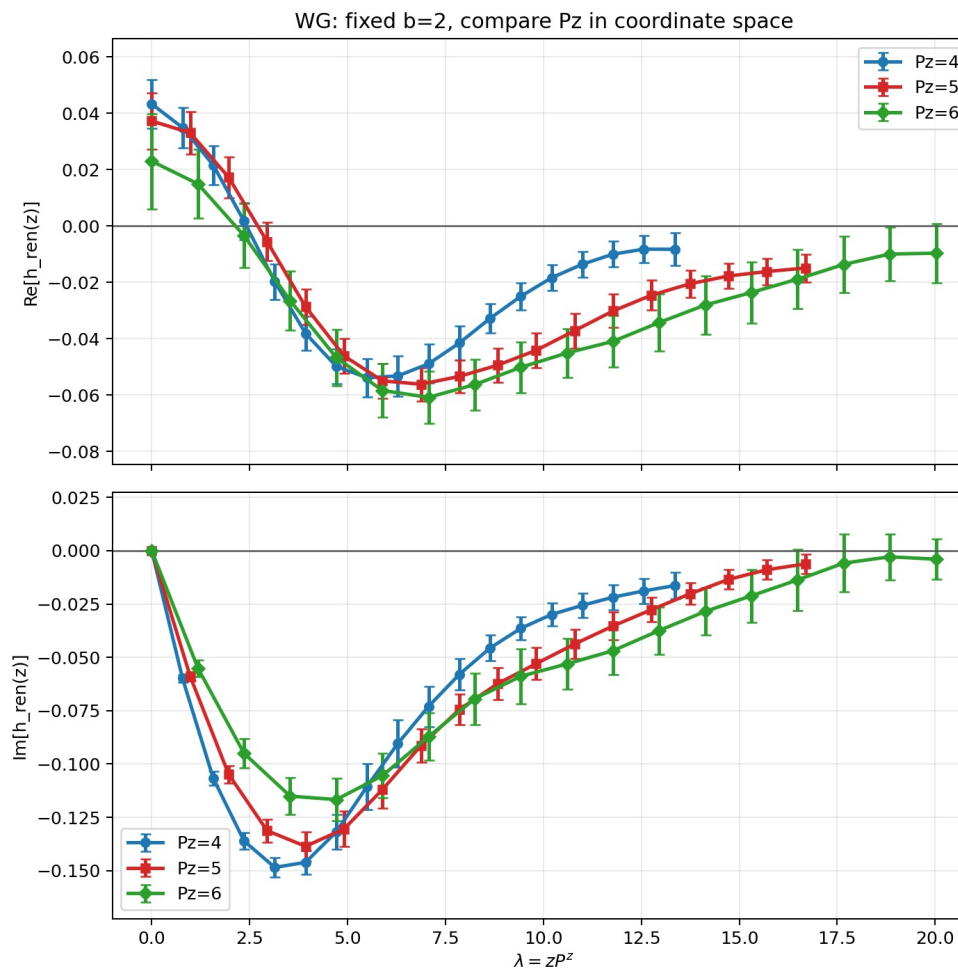
➤ Boer-Mulders, $b_{\perp} = 2a$

➤ Worm-gear(+)-(-), $b_{\perp} = 2a$

Re



Im

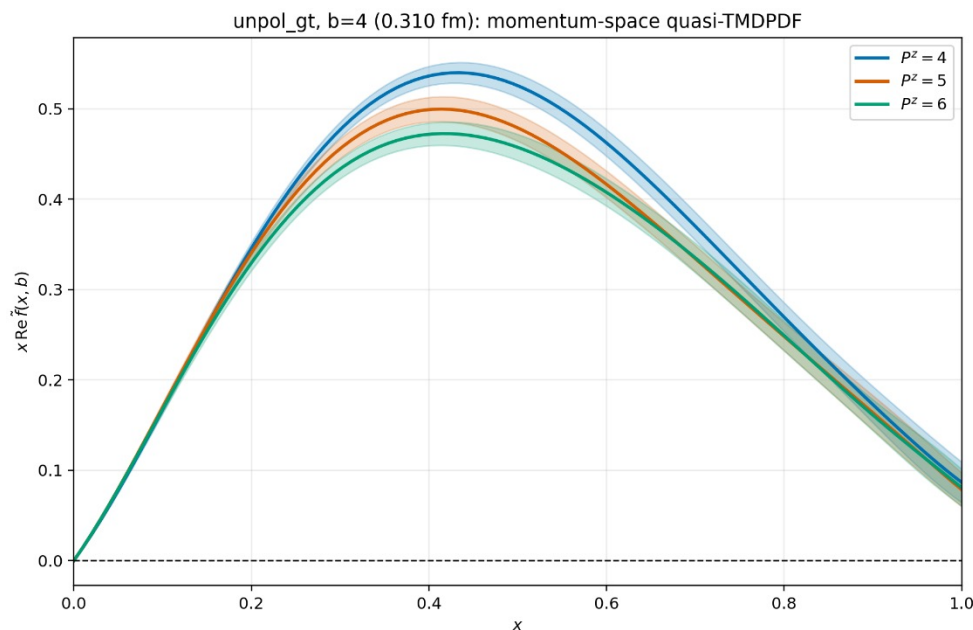


(after renormalization)

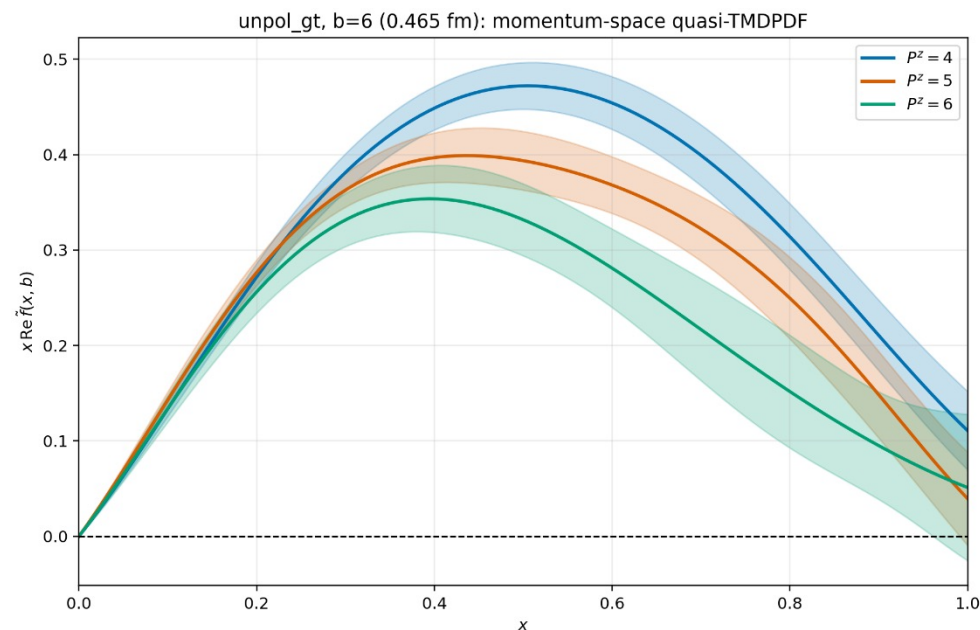
- Subtracted quasi-TMDPDFs:

$$\tilde{f}_{\Gamma}(x, P^z, b_{\perp}, \mu) = \lim_{\substack{a \rightarrow 0 \\ L \rightarrow \infty}} \int \frac{dz}{2\pi} e^{-iz(xP^z)} \frac{\tilde{h}_{\Gamma}^0(z, P^z, b_{\perp})}{\sqrt{Z_E(2L+z, b_{\perp}, a)} Z_O(1/a, \mu)}.$$


unpol. $x\tilde{f}(x, b_{\perp} = 4a, P^z)$



unpol. $x\tilde{f}(x, b_{\perp} = 6a, P^z)$



- Large-momentum effective theory: connecting Euclidean lattice and physical observables

Physical TMDs 

$$\frac{f(x, b_{\perp}, \mu, \zeta)}{S_I^2(b_{\perp}, \mu)} = \exp \left[-\frac{1}{2} K(b_{\perp}, \mu) \ln \frac{-\zeta^z + i\epsilon}{\zeta} \right] H_{\Gamma}(\zeta^z, \mu) \tilde{f}_{\Gamma}(x, b_{\perp}, \mu, \zeta^z) + \mathcal{O}\left(\frac{\Lambda_{\text{QCD}}^2}{\zeta^z}, \frac{1}{b_{\perp}^2 \zeta^z}\right)$$

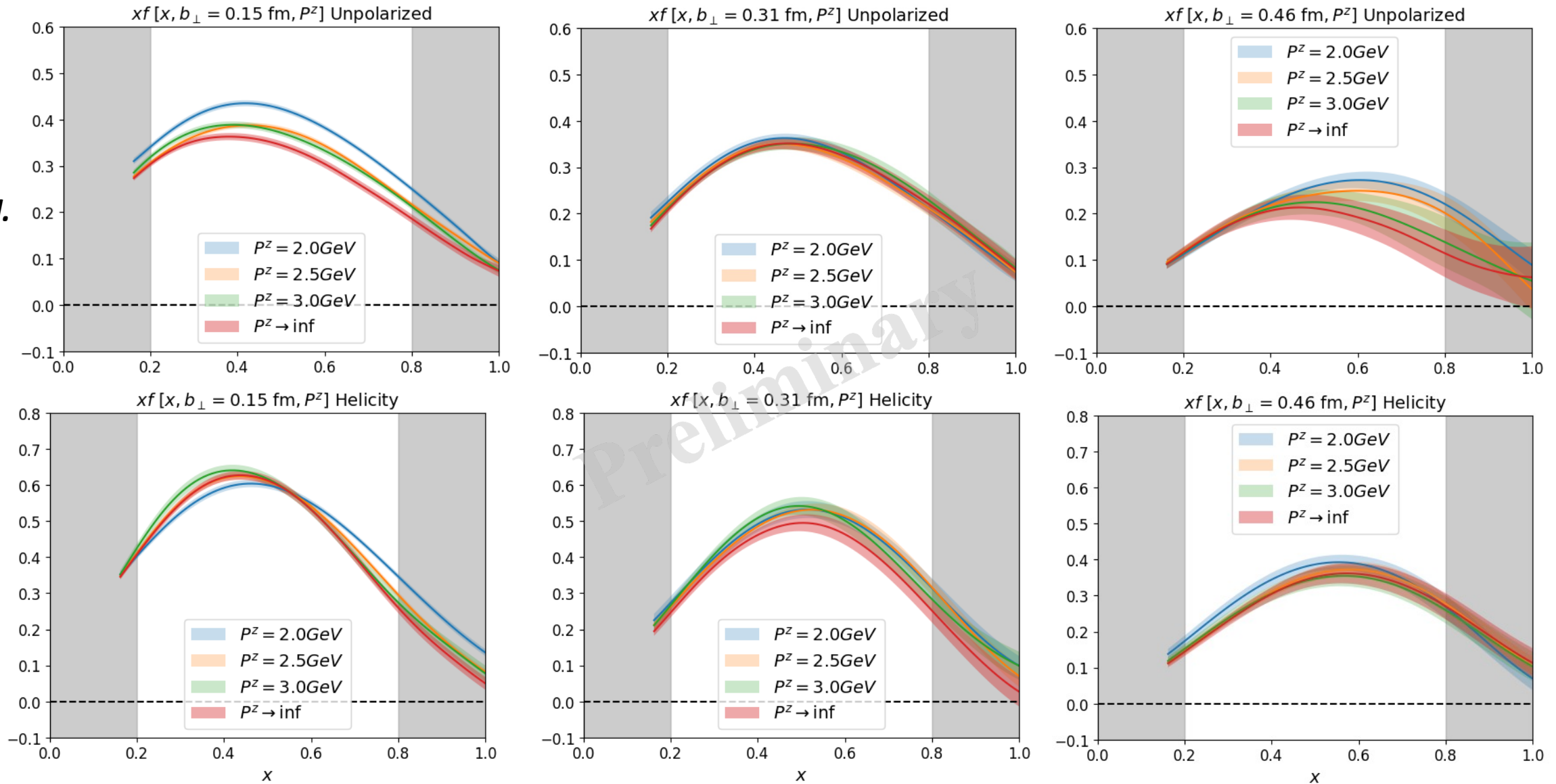
Intrinsic soft function ✓ Collins-Soper kernel ✓ Matching kernel ✓ Quasi TMDs ✓

- Large momentum limit extrapolation:

$$f(x, b_{\perp}, \mu, \zeta; P^z) = f(x, b_{\perp}, \mu, \zeta) + \frac{A(x, b_{\perp})}{(P^z)^2}$$

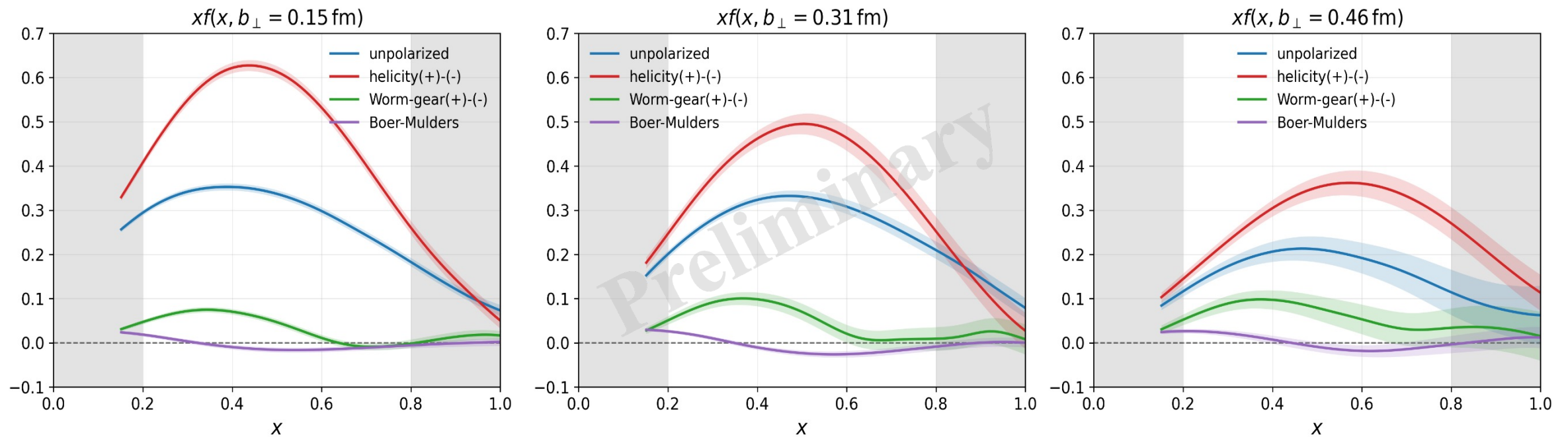
Large Momentum Limit Extrapolation

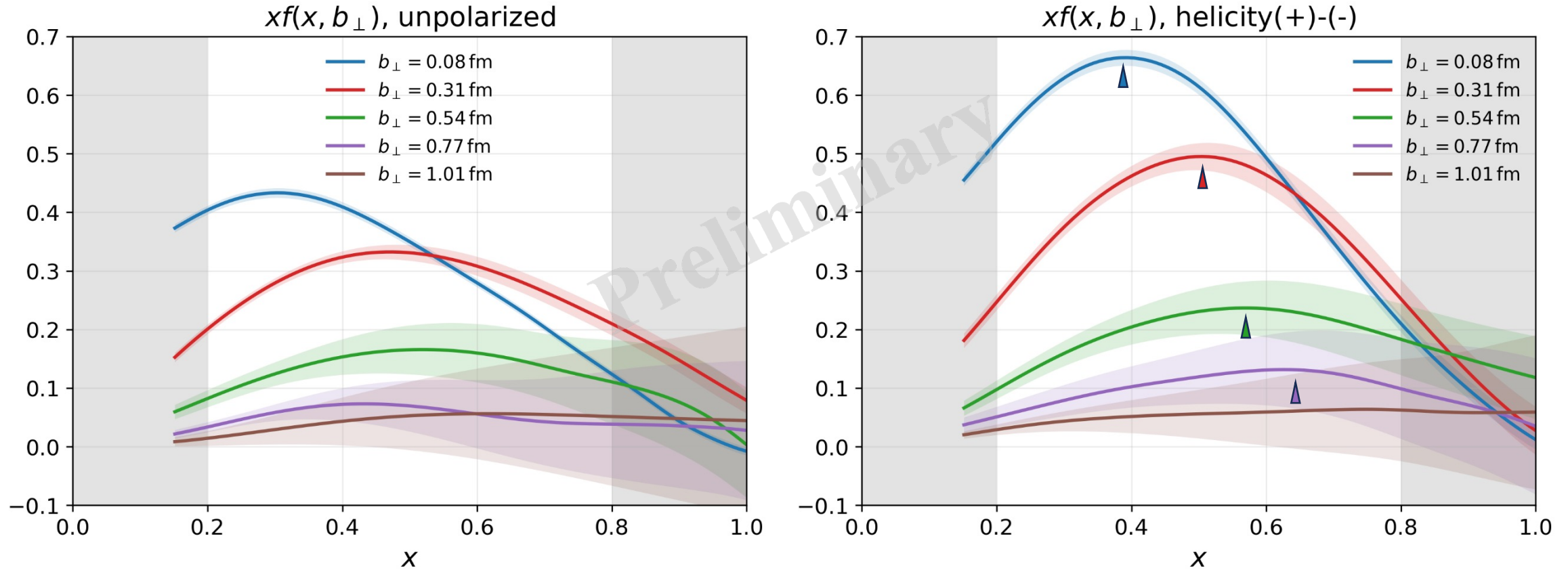
Unpol.



➤ Fix $b_{\perp} = \{0.15, 0.31, 0.46\}$ fm

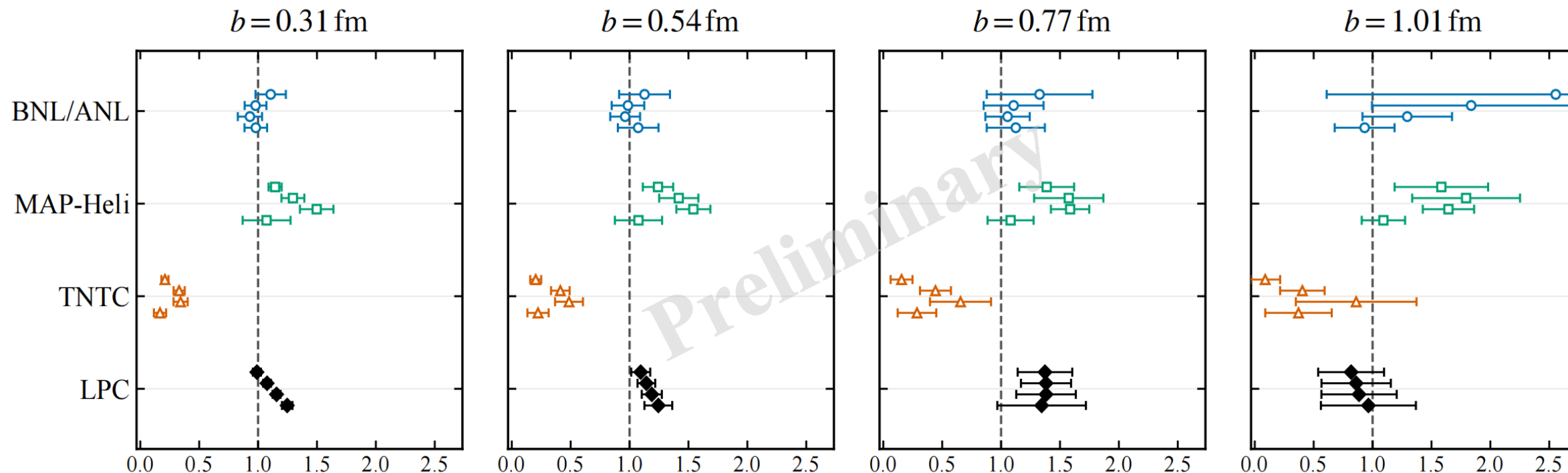
TMDPDFs for unpolarized and longitudinal polarized nucleon:





- The TMDPDFs decrease as b_{\perp} increases;
- As b_{\perp} increases, the peak of the TMDPDFs shifts to the right.

$$R_{g_{1L}/f_1}^{u-d}(x, b_T) \cdot g_A \equiv \frac{g_{1L}^{u-d}(x, b_T; \zeta, \mu)}{f_1^{u-d}(x, b_T; \zeta, \mu)} = \frac{\tilde{g}_{1L}^{u-d}(x, b_T, P_z, \mu)}{\tilde{f}_1^{u-d}(x, b_T, P_z, \mu)}.$$



Within each row, top to bottom: $x = 0.2, 0.3, 0.4, 0.6$

Bollweg et al., PRL 135 (2025)
MAP Collaboration, PRL 135(2025)
TNTC, PRL134, 121902(2025)

Outline

➤ **Autonomous AI Physicists**

1. Motivation

2. From PhysMaster to LQCD Master

Outline

➤ **Autonomous AI Physicists**

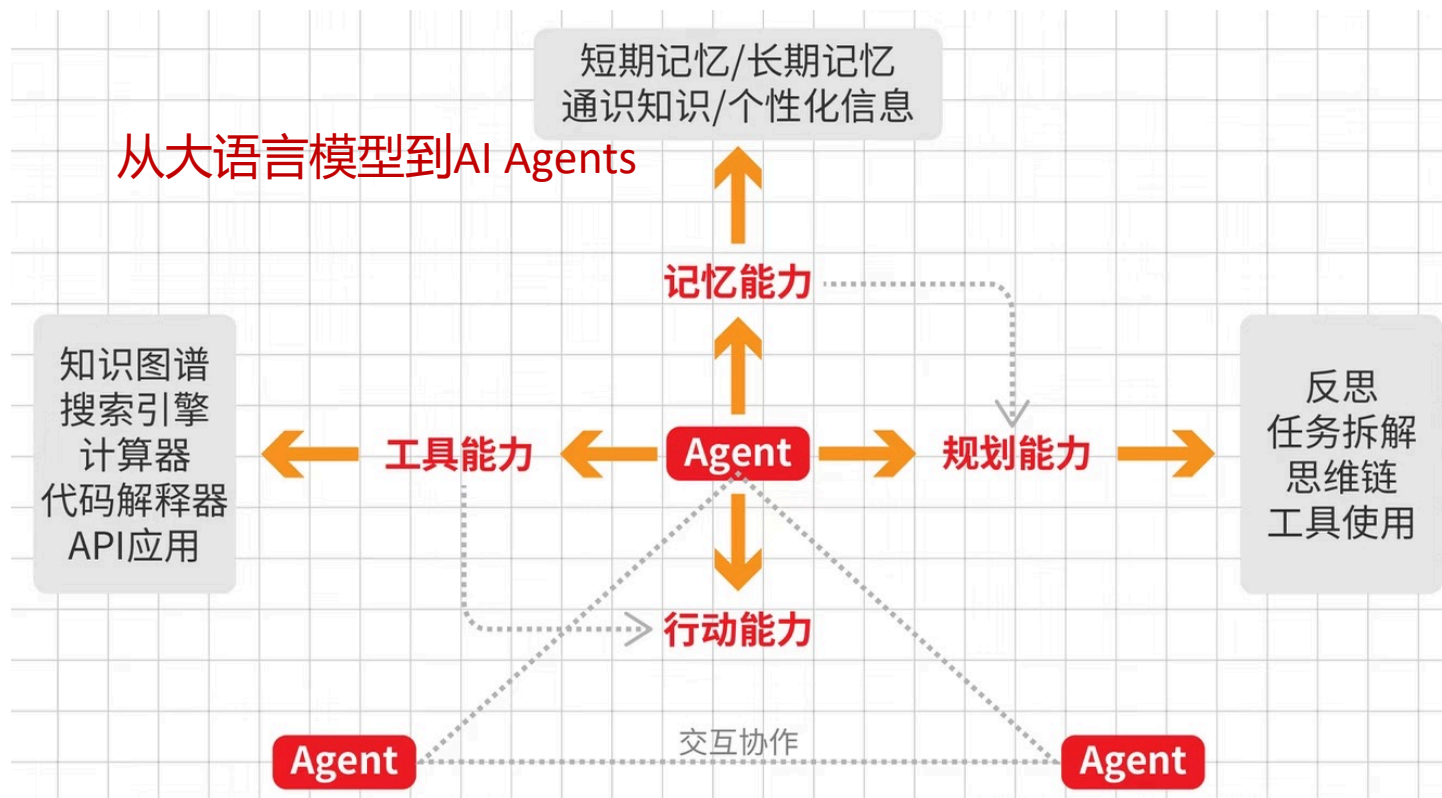
1. Motivation

2. From PhysMaster to LQCD Master

Agent (智能体)

||

LLM (大模型) + Planning (规划) + Memory (记忆) + Tools (工具)





Confinement of quarks*

Kenneth G. Wilson

Laboratory of Nuclear Studies, Cornell University, Ithaca, New York 14850

(Received 12 June 1974)

1974



~2000

**AI physicist for
Lattice QCD?**

?

Outline

➤ **Autonomous AI Physicists**

1. Motivation

2. From PhysMaster to LQCD Master

➤ **Computation: From Physics Goals to Simulation Codes**

Required physics knowledge: QFT, operator construction, correlation functions, ...

Specialized computational tools: Chroma, PyQUDA, ...

LQCD Master

➤ **Analysis: From Lattice Data to Physics Results**

Complex analyses involving long pipelines, massive datasets, and high-dimensional structures

Time-consuming and mentally exhausting

PhysMaster

➤ Three-Stage Workflow: Plan – Execute – Summarize

• Plan

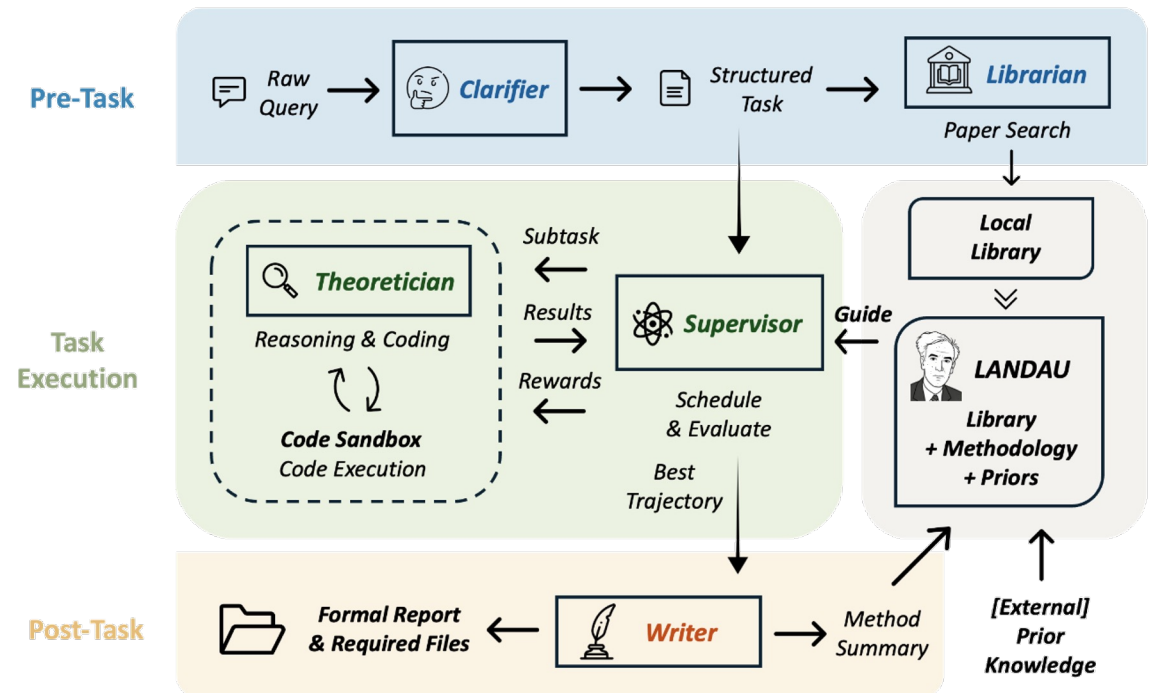
- **Clarifier:** Natural-language query → structured physics task
- **Librarian:** Build a task-specific local knowledge base

• Execute

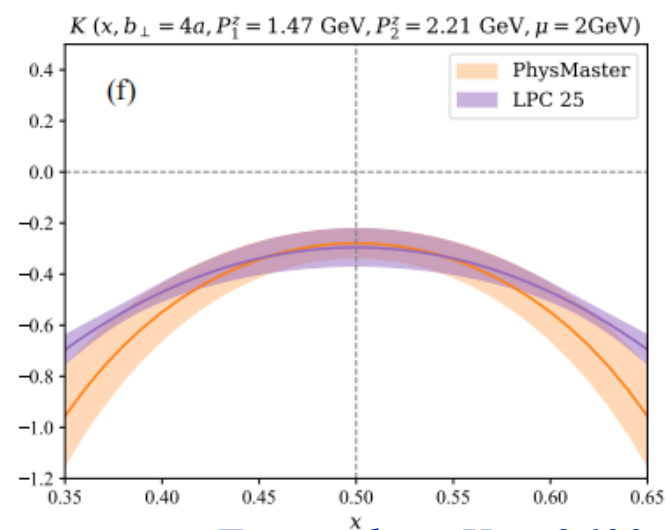
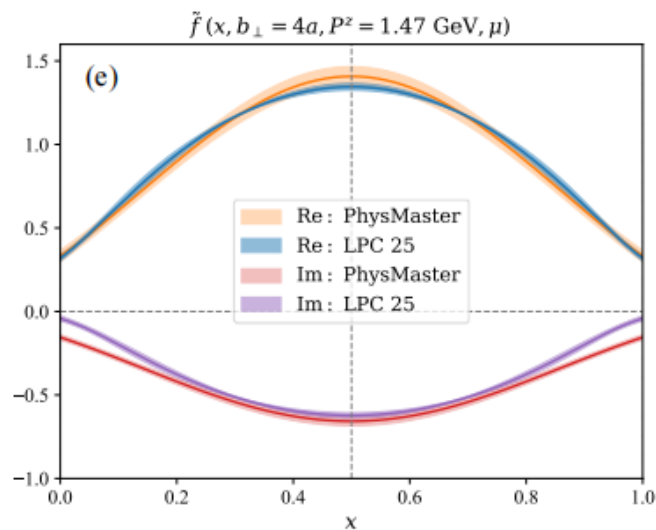
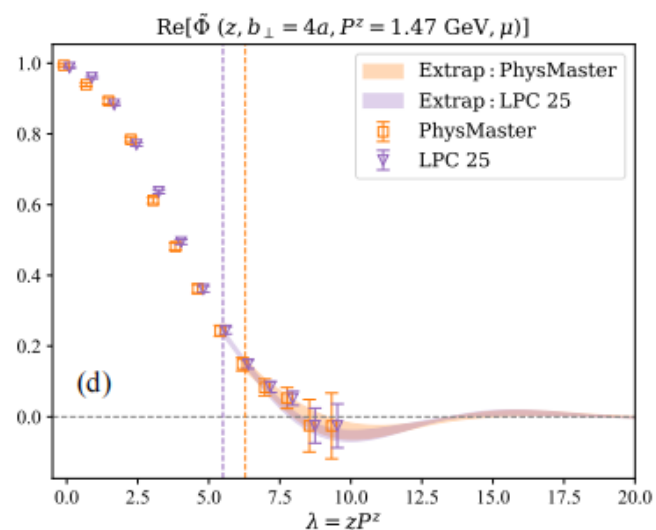
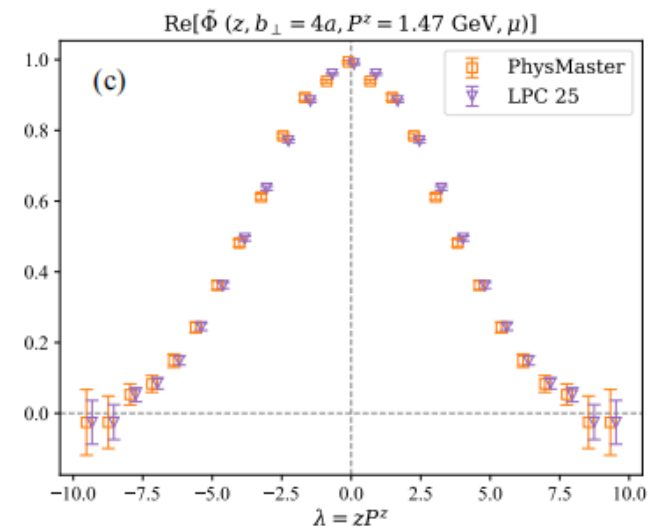
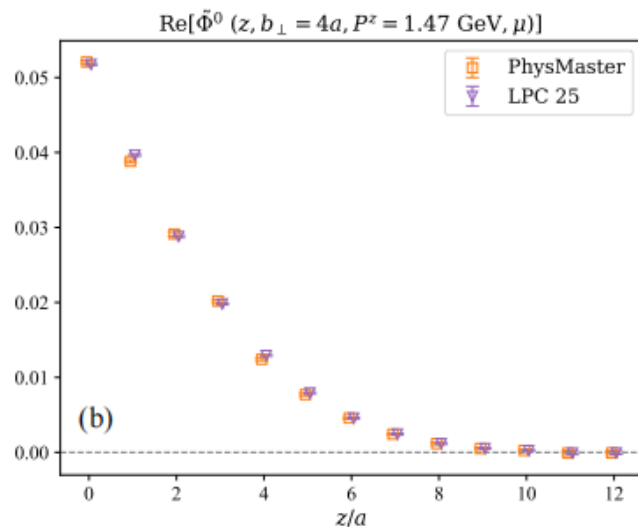
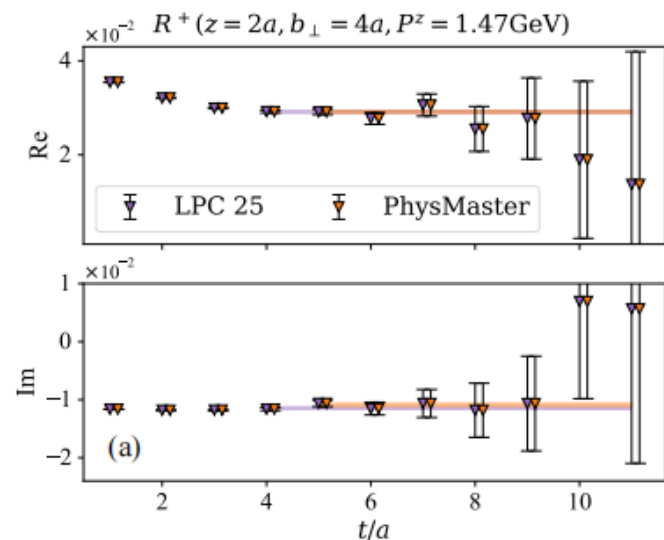
- **Monte Carlo Tree Search (MCTS)**
- **Supervisor–Theoretician hierarchical collaboration**
- **Supervisor:** manages overall progress
- **Theoretician:** performs derivations and coding

• Summarize

- Visualize exploration paths and generate reports
- Extract successful paths and expand the knowledge base



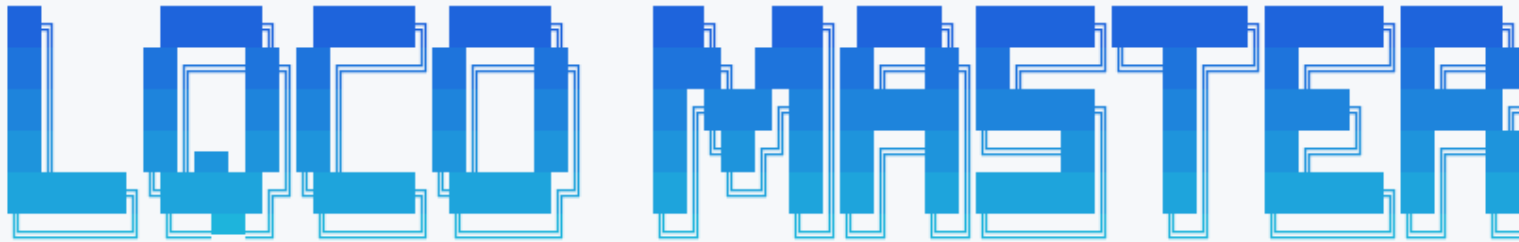
Acceleration: Extracting the CS Kernel in Lattice QCD



LQCD Master: A Specialized AI Agent for Lattice QCD

44

```
(LQCDphys) [muhuazhang@login03 QCD_Master]$ python3 run.py
```



【 An Autonomous AI Scientist for Lattice QCD 】

```
[LQCD Master] Enter task description: calculate the two-point function of pion, the point source located at [0, 0,0,0]. Inverting the propagator should use the stout smeared gauge link, with parameters 1, 0.125, 4. █
```

1、Planner

```
===== [ Planner ] =====
[Planner] [solve] stage start! 🚀
[Planner] [planner_solve] skills selected! ✅ | skills=lqcd-physics
[Planner] [solve] stage done! ✅ | tool_calls=0
[Planner] [critique] stage start! 🚀
[Planner] [planner_critique] skills selected! ✅ | skills=lqcd-physics
[Planner] [critique] stage done! ✅ | tool_calls=0
[Planner] [rewrite] stage start! 🚀
[Planner] [planner_rewrite] skills selected! ✅ | skills=lqcd-physics
[Planner] [rewrite] stage done! ✅ | tool_calls=0
```

```
=====
[Planner Checkpoint v1] Computational plan
=====
```

extras:

```
- define_operator_dagger_convention O_dagger=bar_q*Gamma_dagger*q with Gamma_dagger=gamma4*Gamma^\dagger*gamma4
- contract_connected_piPlus Ct=sum_x ReTr[S_d(x,0)gamma5 S_u(0,x)gamma5]=sum_x ReTr[S_u(x,0)^\dagger S_u(x,0)]_degenerate_ud
- enforce_gamma5_hermiticity_valid_for_Wilson_Clover_D^\dagger=gamma5*D*gamma5
- output_array_shape cfg t with t=0.71 no time folding complex stored_real expected
- save_full_propagator_disabled_default_enable_only_for_debug_cfgs
```

本计划的物理目标是：在给定的 $24^3 \times 72$ Clover 系统上，用单个点源 $(0,0,0,0)$ 计算 $\pi^+ \pi^0$ 介子两点函数并输出逐构型的 $C(t)$ ，用于后续提取 m_π （有效质量或单指数/含反向传播的拟合）。

****通道与味结构****: 明确选择带电通道 $\pi^+ = (\bar{u} d)$ 。该通道只有连通收缩，不存在 disconnected 图；因此实现上只需轻夸克传播子 (u/d) 简并时 $S_u = S_d$ ，即可构造目标相关函数。这里不计算 π^0 ，也不需要构造 $(\bar{u} u + \bar{d} d) / \sqrt{2}$ 的组合。

****算符与伴随约定****: 采用局域伪标量算符 $\Gamma = \gamma_5$ ，且在元数据中固定欧氏伴随约定 $\Gamma^\dagger = \gamma_4 \Gamma \gamma_4$ 。对应的连通两点收缩可写为 $C(t) = \sum_{\vec{x}} \text{ReTr} \{ \text{Tr} [S_d(0; \vec{x}) \gamma_5 S_u(\vec{x}; 0) \gamma_5] \}$ ，并用 Wilson/Clover 的 γ_5 -hermiticity 化为等价且数值更稳定的形式 $C(t) = \sum_{\vec{x}} \text{ReTr} [S_u(x; 0)^\dagger S_u(x; 0)]$ （在 u/d 简并下）。计划要求对结果取实部并做基本 sanity check ($C(t)$ 应为非负、随 t 衰减)。

****与系统/求解器一致性闭环****: 求解器明确绑定固定配置中的 Clover 参数 ($mass = -0.277$, $c_{SW_t} = c_{SW_r} = 1.160920226$, $\xi_0 = 1.0$, $t_{boundary} = -1$, $process_grid = [1, 1, 1, 4]$)。除给出 $tol/maxiter$ 外，要求记录并检查每次反演的最终残差范数，并将“残差定义/是否为预条件残差”等关键信息写入输出 metadata，避免“Dirac 算符用错或收敛标准不一致”导致的系统偏差。

****输出与后处理接口****: 输出为 `numpy`，按“(cfg, t)”组织 ($t=0..71$ ，不做时间折叠)，并在 metadata 中标注：格点尺寸、源位置、零动量投影方式（对每个时间片做空间求和，相位因子为 1）、通道 π^+ 、算符与伴随约定、边界条件 $t_{boundary} = -1$ 。这样可直接进入后续拟合流程（需要时再在分析端决定是否做 forward/backward 组合或时间对称化）。

****工程风险控制****: 默认不保存整份点源传播子以避免 I/O 与存储压力；如需调试，可对极少数测试构型开启保存。当前 `cfg_selection` 保持为 `test`，与本阶段“功能与一致性验证”匹配；若进入物理产出阶段，应在不改物理定义的前提下将 `cfg_selection` 扩展为 `full`/自定义范围，并在分析端进行 `binning/jackknife` 以评估误差与自相关。

Citations: []

[Planner Checkpoint] Press Enter to accept the plan, or provide revision feedback: █

2、Executor

```
===== [ Executor ] =====
[Executor] [executor:v1] stage start! 🚀
[Executor] [executor_generate] skills selected! ✅ | skills=pyquda-tool, lqcd-physics
[Executor] [executor] stage done! ✅ | tool_calls=0
[Executor] [executor_static_analysis] stage start! 🚀
[Executor] [executor_static_analysis] stage done! ✅ | errors=0
[Executor] [executor_critique] skills selected! ✅ | skills=lqcd-physics, pyquda-tool
[Executor] [executor_critique] stage done! ✅ | tool_calls=0
[Executor] [executor_critique:v1] found 1 error(s); trigger executor_rewriter static-check round 1
[Executor] [executor_rewrite] skills selected! ✅ | skills=pyquda-tool, lqcd-physics
[Executor] [executor_rewriter] stage done! ✅ | tool_calls=0
[Executor] [executor_static_analysis] stage start! 🚀
[Executor] [executor_static_analysis] stage done! ✅ | errors=0
[Executor] [executor_critique] skills selected! ✅ | skills=lqcd-physics, pyquda-tool
[Executor] [executor_critique] stage done! ✅ | tool_calls=0
[Executor] [executor_critique:v1] remaining_errors=2; pass_to_checkpoint_for_human_review
[Executor] [executor:v1] artifacts_saved=runs/20260416_213546/executor_v1

=====
[Executor Checkpoint v1] Scripts generated. Approval will trigger the test submission and queue inspection
```

PLAN SUMMARY

整体流程基本符合计划（stout 后反演、点源、零动量、MPI 规约与落盘），但当前 π 两点收缩实现对传播子指标的 dagger/颜色指标处理存在高概率错误，可能导致物理结果不对。

WARNINGS

- main.py 通过命令行读取 mpi_n 但仅用于写入 metadata，未用于校验与 core.init 的进程网格/实际 mpi run -n 一致性；当 submit 脚本或 process_grid 改动时可能出现“mpirun 进程数与 [Gx,Gy,Gz,Gt] 不匹配”的运行时错误或性能异常，建议至少做一致性检查。
- stoutSmear 为就地修改 gauge；若后续扩展脚本需要同时使用未涂抹与涂抹链接，当前写法会引入隐式状态风险（本任务单一测量尚可）。
- 输出只保存 $C(t)$ 的实部/虚部未明确约束；当前直接 np.save 可能保存复数数组（取决于 contraction 结果），后续分析链需确认能消费复数或应显式取实部并记录约定。
- submit 脚本中硬编码了大量环境模块与编译器/QUDA 路径设置；虽然不影响正确性，但可移植性较差，且不利于将“仅 mpirun 参数 + resource_path + cfg”作为薄封装范式复用到其他任务。

EXECUTOR CRITIQUE ERRORS

- π 两点函数收缩实现的指标处理不成立：S 的数据布局注明为 (... , spin_snk, spin_src, color_snk, color_src)，但代码用 swapaxes(-4,-3) 只交换了 spin_snk 与 spin_src，并未对 color_snk/color_src 做转置（也未形成完整的 (spin_src,color_src; spin_snk,color_snk) 的厄米共轭）。因此 B 并不是 S^\dagger ，对应的 $\text{Tr}[(S \gamma_5)(\gamma_5 S^\dagger)]$ 不正确，关联函数将偏离物理定义。
- einsum 指标命名与注释自相矛盾并导致颜色/自旋迹不保证正确：A 由 einsum("...jiba,ik->...jkba") 得到的尾部索引顺序为 (spin_snk, spin_src, color_snk, color_src)，但随后 corr_t = -einsum("wtzyxjab,wtzyxjiab->t", A, B) 仅假定最后两维 a,b 是需要取迹的颜色对且在 A/B 间位置一致；由于 B 的构造本身未实现颜色转置，该 contraction 不能对应规范不变的颜色迹，结果可能依赖于实现细节而错误。

3、 Sbatch & Revision

```
=====
[Executor Checkpoint] Press Enter to submit the test job, or provide revision feedback:
[Executor] [submit_test:v1] stage start! 🚀
[Executor] [submit_test] submit_script=/public/home/muhuazhang/QCD_Master/runs/20260416_213546/submit_test.sh
[Executor] [submit_test:v1] stage done! ✅ | ok=True | job_id=111752377
[Queue] Waiting for test job output...
```

```
===== [ Slurm Queue ] =====
Current state: submitted, but Job 111752377 is not yet visible in this `squeue` query

===== [ Workflow Completed ] =====
[Run dir] Path: /public/home/muhuazhang/QCD_Master/runs/20260416_213546
[Status] Completed
[Trajectory] File saved to: /public/home/muhuazhang/QCD_Master/runs/20260416_213546/trajectory.json
```

```
#SBATCH --error=/public/home/muhuazhang/QCD_Master/runs/20260408_121411/executor
#SBATCH --nodes=1
#SBATCH -n 4
#SBATCH --gres=dcu:4
#SBATCH --exclude="f17r3n00"
#SBATCH --time=00:20:00
#SBATCH --ntasks-per-node=4
#SBATCH --ntasks-per-socket=1
#SBATCH --exclusive

set -euo pipefail

module purge
module load apps/git/2.30.2
module load compiler/cmake/3.23.3
module load compiler/gnu/9.3.0
module load compiler/intel/2017.5.239
module load mpi/hpcx/2.11.0/intel-2017.5.239
module load compiler/dtk/25.04
export CUPY_INSTALL_USE_HIP=1
export HCC_AMDGPU_TARGET=gfx906
export CC=clang
export CXX=clang++
source /public/home/gzcl234/PyQUDA_configs_2604/zmh-dev-2604/bin/activate
mkdir -p /public/home/muhuazhang/QCD_Master/runs/20260408_121411/executor
cd /public/home/muhuazhang/QCD_Master/runs/20260408_121411/executor

mpirun -n 4 python3 main.py --ensemble-path /public/share/weiwang/clqcd/beta6.
tern 'beta6.20_mu-0.2770_ms-0.2400_L24x72_cfg_{cfg}.lime' --geometry 24,24,24,
ndary -1 --anisotropy 1.0 --mass -0.277 --xi0 1.0 --csw-t 1.160920226 --csw-r
,4,6]]' --output-dir outputs --task-name pion_2pt_piPlus_point_src_L24x72 --ob
```

```
(LQCDphys) [muhuazhang@login01 QCD_Master]$ sq
      JOBID PARTITION      NAME      USER      ST      TIME  NODES NODELIST(REASON)
      111130013 kshdexclu16  test_pi2pt_24x muhuazhang  PD      0:00      1 (Priority)
(LQCDphys) [muhuazhang@login01 QCD_Master]$
```

Results

C24P29_cfg10000_src0000_stout1_rho0p125_n4_clover_Cpi_t.npy ...

QCD_Master > runs > 20260416_213546 > executor_v1 > output > C24P29

```
[-1.163258200451794+2.3941403055470432e-19j,  
-0.15899417138341945+5.605321309320685e-20j,  
-0.06679277204263595+-3.4515889536339814e-21j,  
-0.043159090818385926+2.206516646212471e-21j,  
-0.03229948709785555+1.0406659695027323e-21j,  
-0.027268744041290018+1.6034973061896494e-21j,  
-0.02343857884501545+-1.4018934240633875e-22j,  
-0.01886632942633874+-1.3710837560412432e-21j,  
-0.014799854242632648+7.289682038856057e-22j,  
-0.01144286534300992+5.32031352448254e-23j,
```

LQCD Master

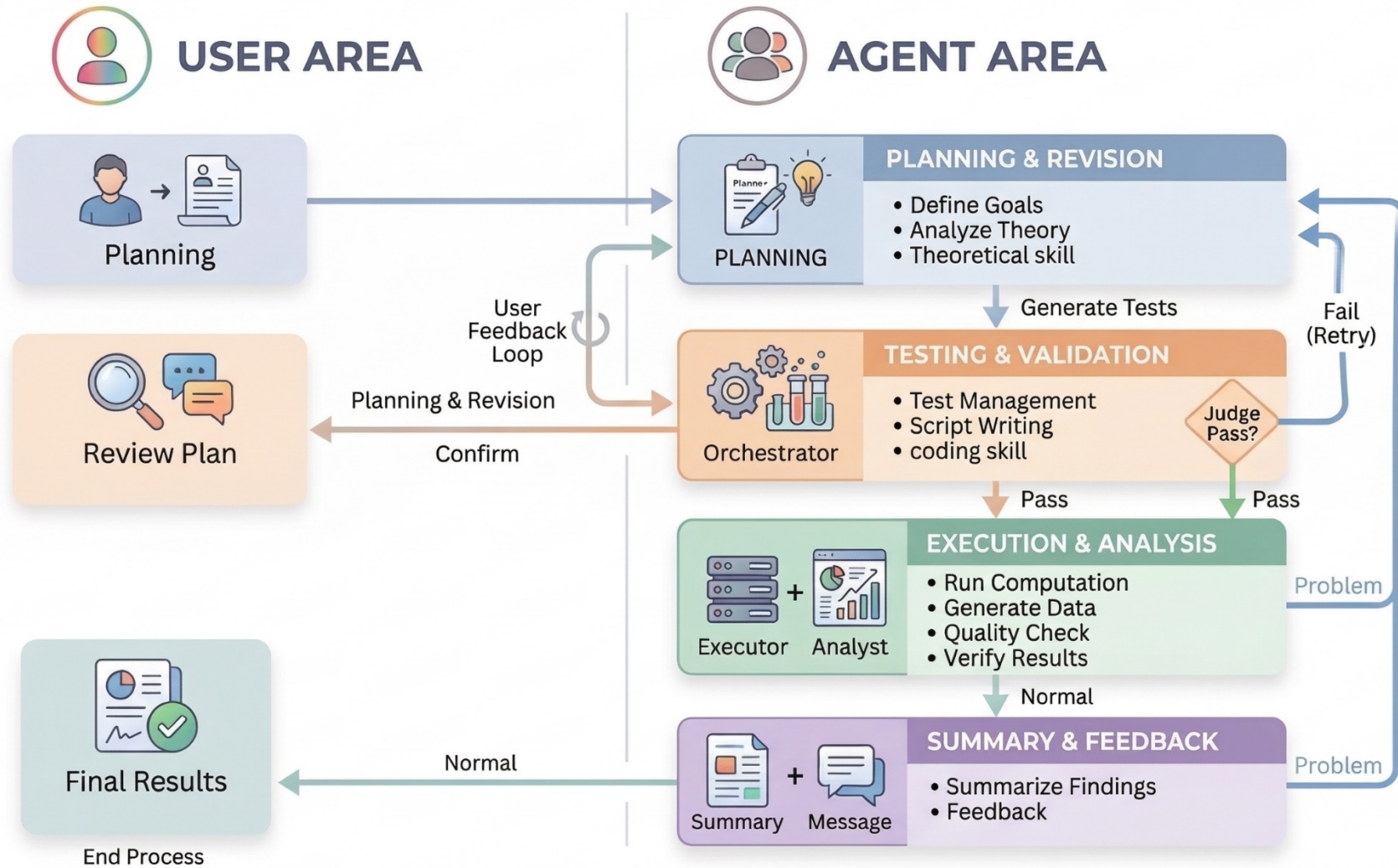
pion_2pt.npy X

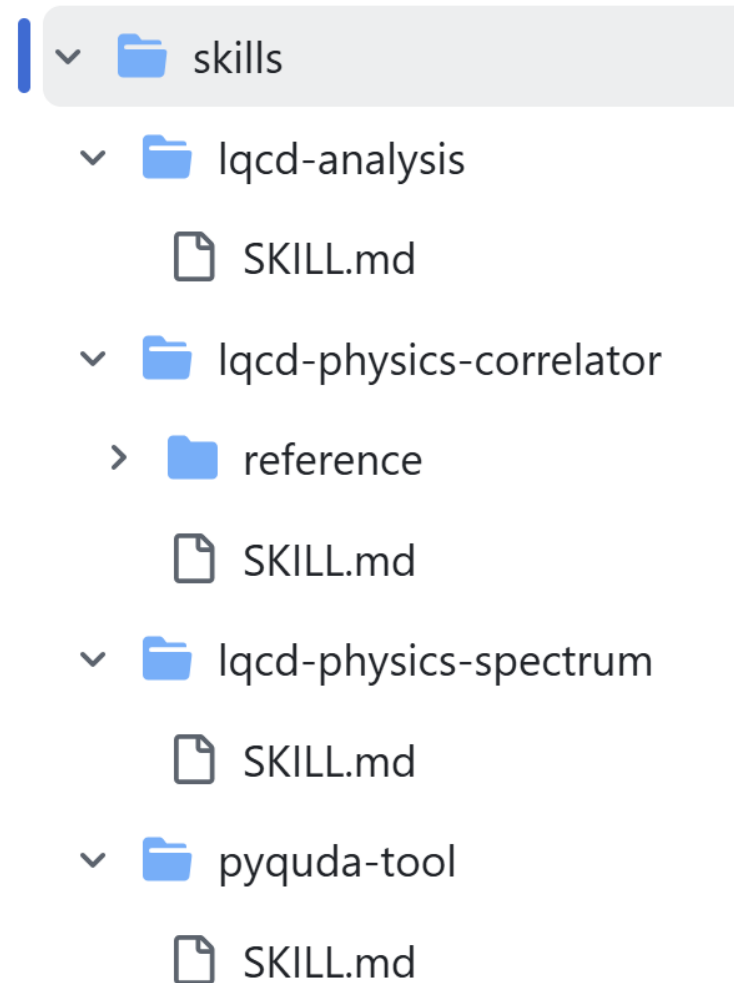
pyquda_test > pion_2pt.npy

```
[1.1632582004701688+1.5065319188174853e-19j,  
0.158994171401292+9.68714111233087e-20j,  
0.06679277206431788+1.731524998554314e-22j,  
0.04315909084677358+-7.559647829679007e-21j,  
0.03229948713362343+4.541400961643044e-22j,  
0.027268744090051197+-5.453783652210867e-22j,  
0.023438578906970074+-2.508022831936606e-21j,  
0.018866329493487002+-3.175108617532112e-22j,  
0.014799854306129321+-5.35634656470552e-24j,  
0.011442865398169976+-7.203612719902414e-22j,
```

Me

LQCD Master: A Specialized AI Agent for Lattice QCD





- skills
 - lqcd-analysis
 - SKILL.md
 - lqcd-physics-correlator
 - reference
 - SKILL.md
 - lqcd-physics-spectrum
 - SKILL.md
 - pyquda-tool
 - SKILL.md

name	lqcd-analysis
description	Lattice QCD analysis pipeline skill. Takes correlator data from lattice measurements and extracts physics results with statistical and systematic error control. Covers: source-time shifting, correlator folding, jackknife/bootstrap resampling, gvar/lsqfit integration, effective mass, multi-state correlated fits (hadron spectrum), matrix element extraction (ratio method, summation method, simultaneous C_2+C_3 two-state fit), dispersion relation and speed of light, fit diagnostics (χ^2/dof , Q-value, AIC, SVD cut), and scale conversion to physical units. Uses fit function templates from lqcd-physics-spectrum. Trigger on: "analyze correlators", "fit the data", "extract mass", "effective mass", "matrix element", "dispersion relation", "speed of light", "jackknife", "resampling", "lsqfit", or when contractions are done and results needed.

LQCD Analysis Pipeline

name	lqcd-physics-correlator
description	Lattice QCD physics reasoning skill. Derives the chain from a physics observable to a computable correlator: interpolating operator construction (mesons, baryons), correlator definition (two-point, three-point), Wick contraction with γ_5 -hermiticity and flavor symmetry, propagator requirements, and einsum expressions for contractions. Hands spectral decomposition and fit templates off to lqcd-physics-spectrum. Uses DeGrand-Rossi gamma basis (PyQUDA convention). Trigger on: hadron masses, decay constants, form factors, matrix elements, operator construction, Wick contraction, disconnected diagrams, or "what correlators/propagators do I need".

LQCD Physics Reasoning

name	pyquda-tool
description	PyQUDA tool usage skill. Generates Python code that calls PyQUDA to solve quark propagators on lattice gauge configurations. Covers: configuration loading, quark parameter setup (Wilson/clover action, mass or kappa, clover coefficient, link smearing), multigrid solver configuration, source construction (point, Gaussian smearing with APE/HYP/stout links), propagator inversion, and residual verification. Reads ensemble parameters from ensemble_registry.yaml. Trigger on: "compute propagators", "solve propagator", "run inversions", "call PyQUDA", "solve Dirac equation", or when lqcd-physics-correlator has produced a propagator requirements list.

PyQUDA Tool Usage

Outline

- Lattice QCD Determination of TMDPDFs
- Autonomous AI Physicists
From PhysMaster to LQCD Master
- **Summary**

➤ **CS kernel:**

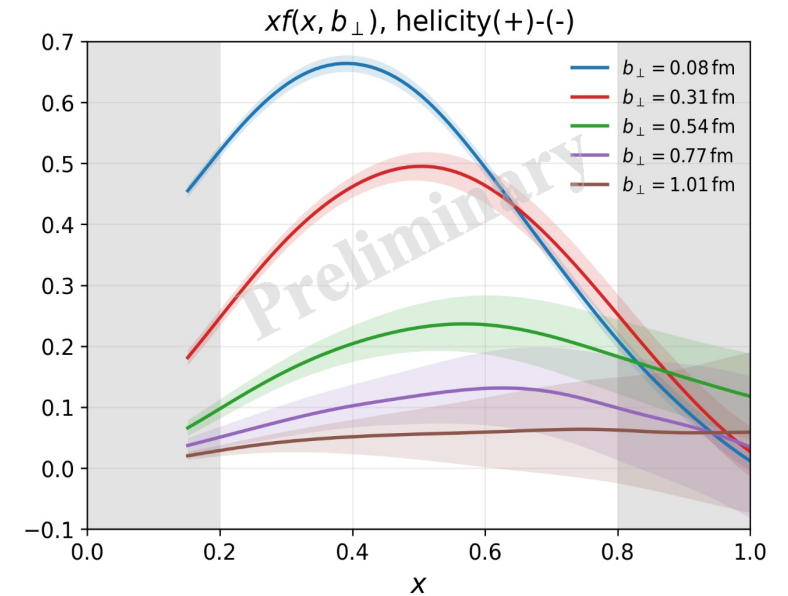
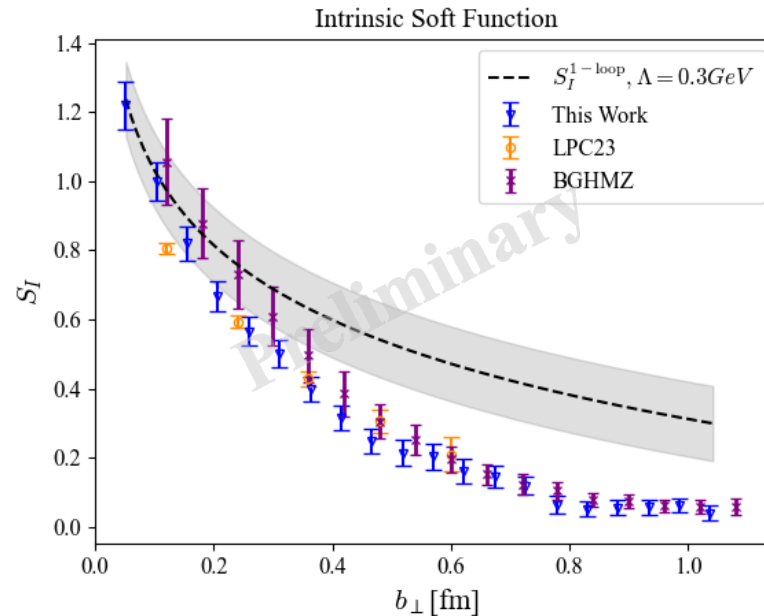
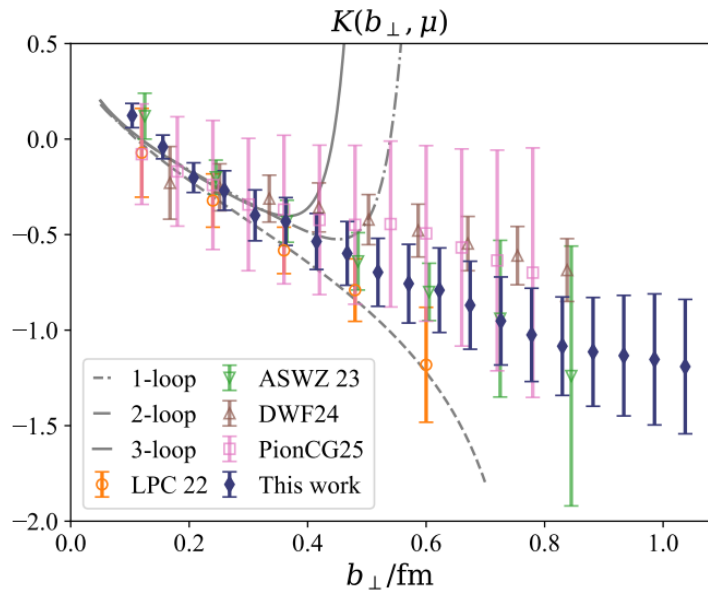
- ✓ continuum limit;
- ✓ physical mass;
- ✓ $b_{\perp} = 1$ fm;
- ✓ systematic uncertainties

➤ **Intrinsic Soft Function :**

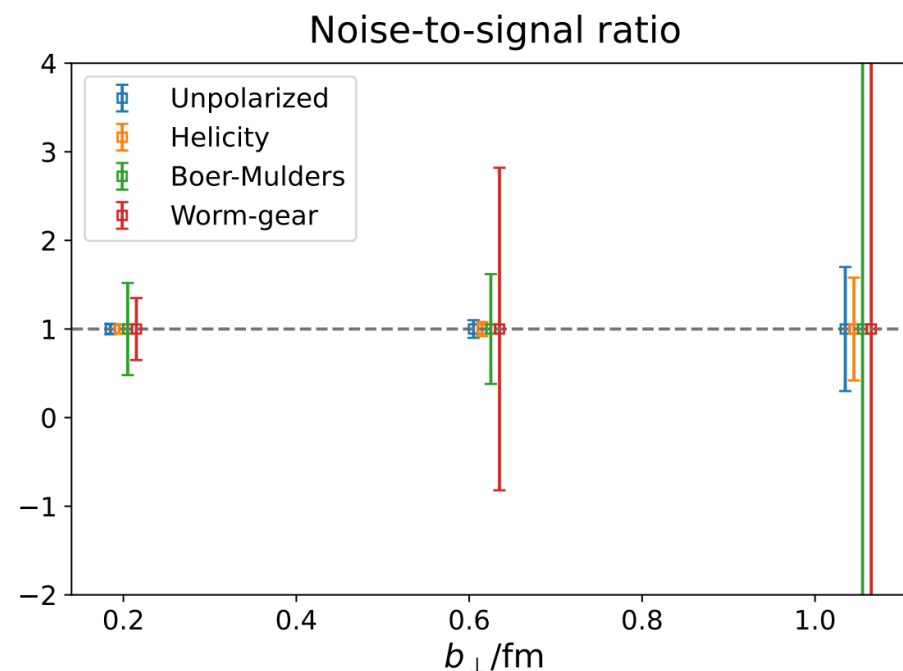
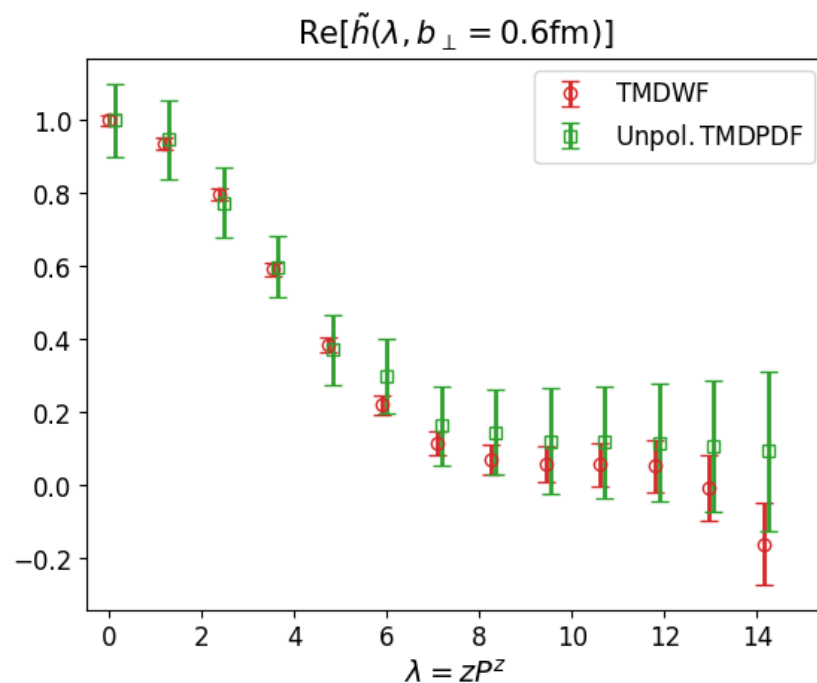
- ✓ continuum limit;
- physical mass;
- ✓ $b_{\perp} = 1$ fm;
- systematic uncertainties

➤ **TMDPDFs:**

- ✓ Polarized TMDPDFs;
- continuum limit;
- physical mass;
- ✓ $b_{\perp} = 1$ fm;
- systematic uncertainties



- Higher **statistics ($\times 10$)** and broader ensemble coverage;
- Extension to a wider class of **polarized** TMDPDFs;
- Further **phenomenological** applications and analyses;



- ✓ Broadly integrate open-source scientific tools into PhysMaster to expand its capability for solving general physics problems;
- ✓ Explore AI-agent-based solutions for domain-specific scientific problems;

Thank you for your attention!

Appendix

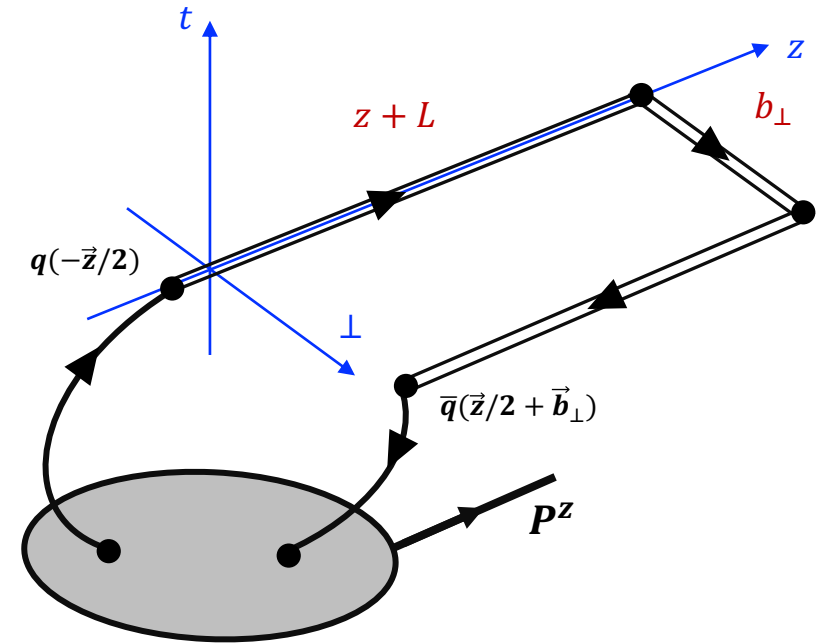
Quasi TMD Wave Function

➤ The quasi-TMD wave functions can be defined as:

$$\tilde{\Psi}^{\pm}(x, b_{\perp}, \mu, \zeta_z) = \lim_{L \rightarrow \infty} \int \frac{dz P^z}{2\pi} e^{ixzP^z} \frac{\tilde{\Phi}^{\pm 0}(z, b_{\perp}, P^z, a, L)}{Z_O(\mu, a) \sqrt{Z_E(2L + z, b_{\perp}, \mu, a)}},$$

where the bare quasi-TMD wave function can be constructed as :

$$\tilde{\Phi}^{\pm 0}(z, b_{\perp}, P^z, a, L) = \langle 0 | \bar{q}(z \hat{n}_z + b_{\perp} \hat{n}_{\perp}) \Gamma U_{\square, \pm}(L, z, b_{\perp}) q(0) | P^z \rangle.$$



*Chu et al.(LPC), PRD109(2024);
Chu et al.(LPC), PRD 106(2022);
Zhang et al., PRL125(2020).*

Self-Renormalization--a New Scheme to Extract Z_O

Subtracted matrix element

➤ **Renormalization condition:** $\tilde{h}(a, z, b_\perp) = \frac{\tilde{\Phi}^0(z, b, Pz = 0, \mu)}{\sqrt{Z_E(z + 2L, b, \mu)}} = Z_O(1/a, \mu) h_0^{\overline{MS}}(\mu, b_\perp, z) + O\left(\frac{a^2}{b^2}\right)$

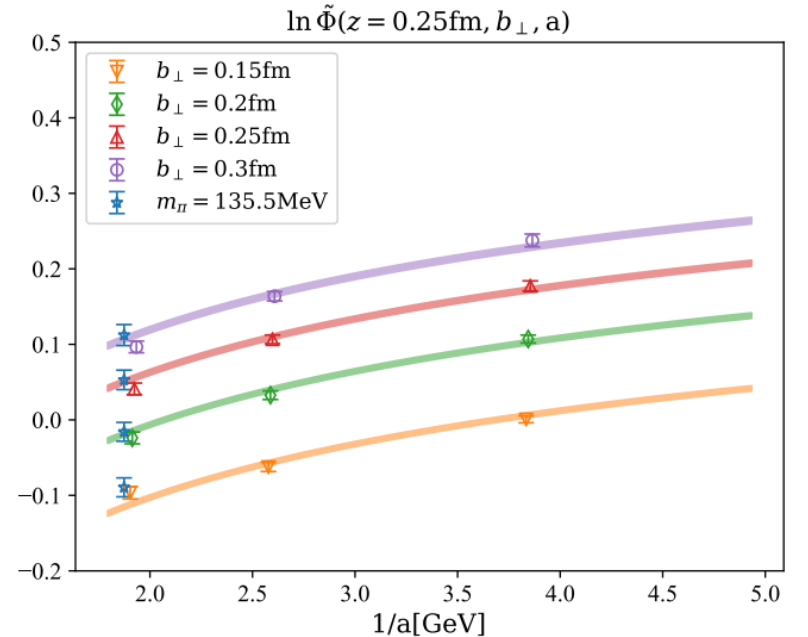
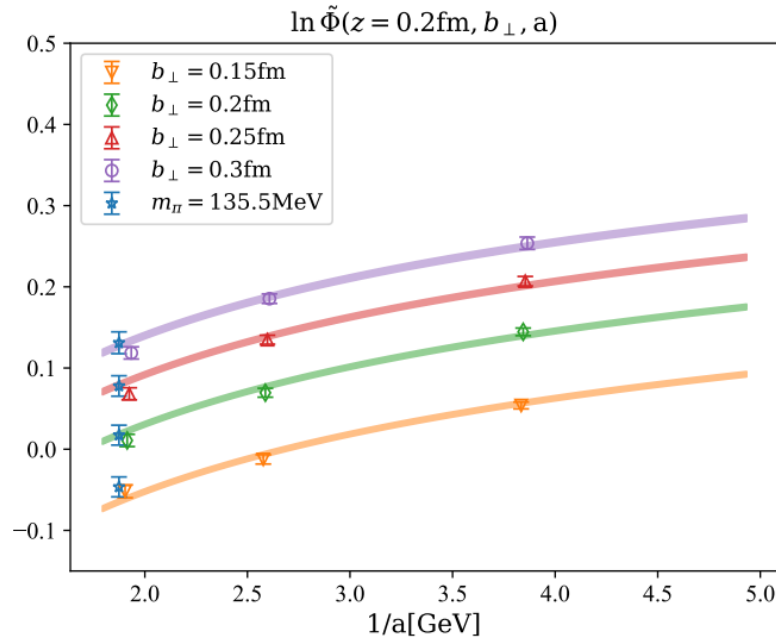
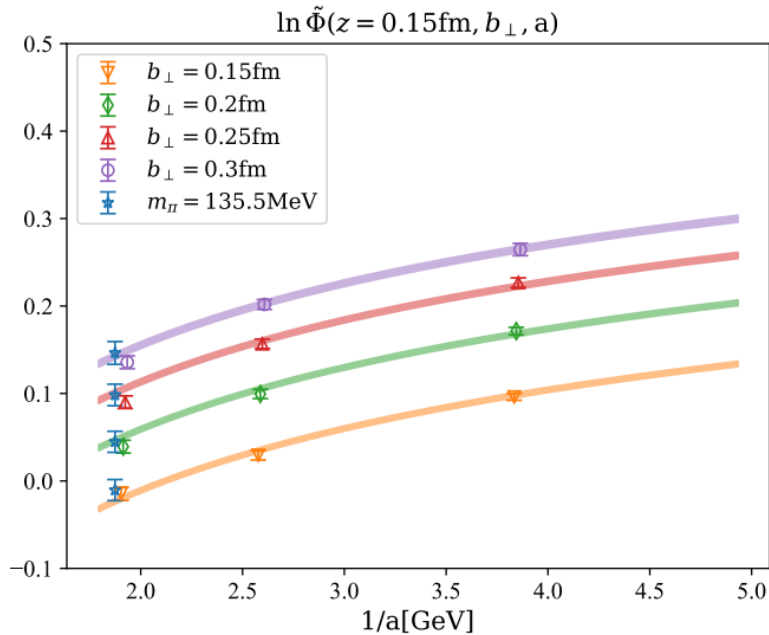
➤ **Parametrization:** $\ln \tilde{h}(a, z, b_\perp) = \frac{\gamma_0}{\beta_0} \ln \left[\ln[1/(a\Lambda_{\text{QCD}})] \right] + \frac{c_1}{\ln[1/(a\Lambda_{\text{QCD}})]} + g(z, b_\perp)$

$$\ln Z_O(a, \mu) = \frac{\gamma_0}{\beta_0} \ln \left[\ln[1/(a\Lambda_{\text{QCD}})] \right] + \frac{c_1}{\ln[1/(a\Lambda_{\text{QCD}})]} + d'(\mu)$$

Self-Renormalization--a New Scheme to Extract Z_O

Subtracted matrix element

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- Joint fit result : $c_1 = 0.020$



Self-Renormalization--a New Scheme to Extract Z_O

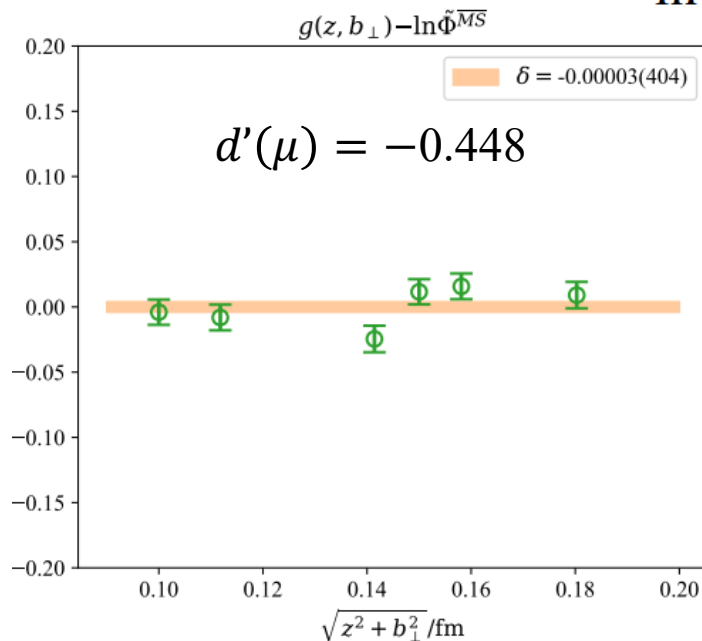
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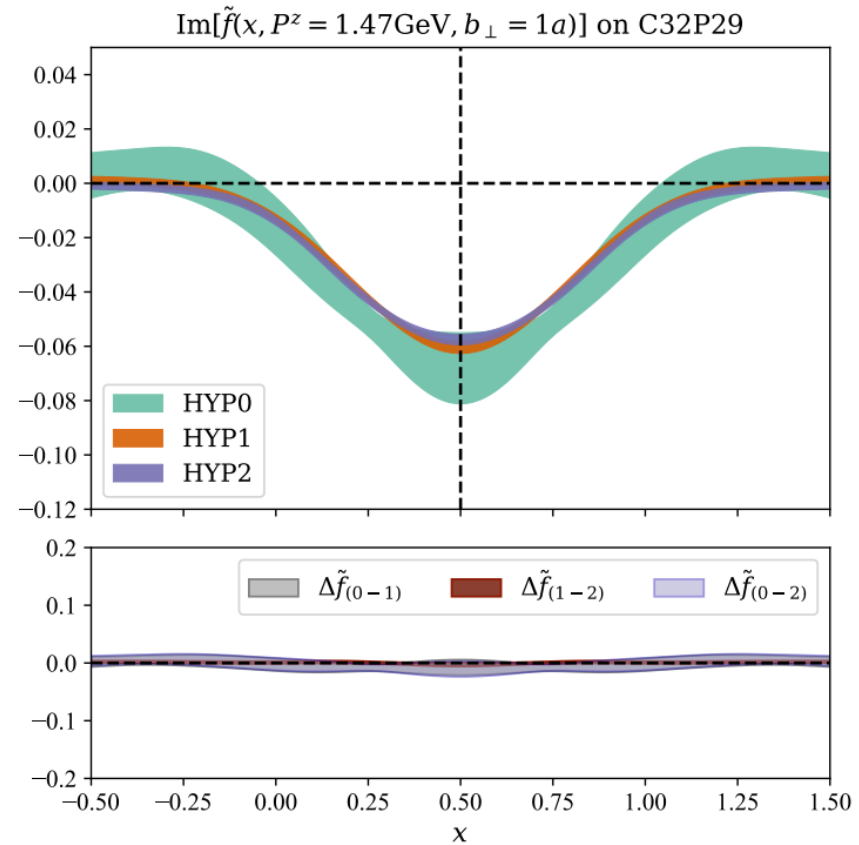
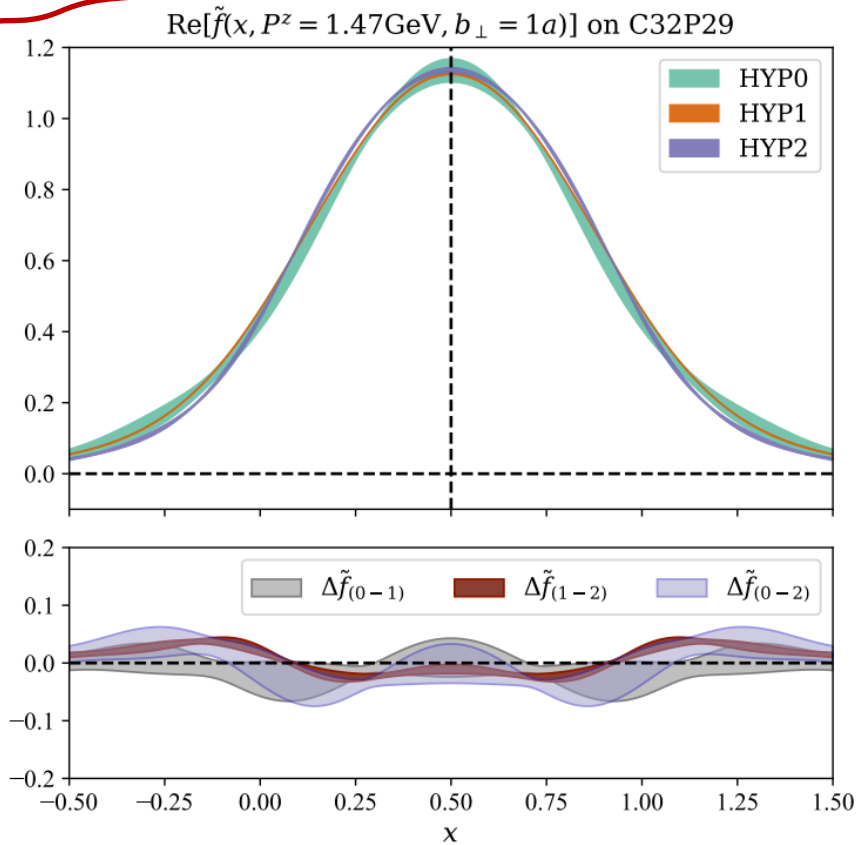
LPC, in preparation

a/fm	0.10530	0.07746	0.05187
HYP0	1.064(21)	1.145(20)	1.241(19)
HYP1	0.92208(62)	0.97526(57)	1.03969(53)

Result for Quasi-TMDWFs in Momentum Space

$$\tilde{f}(x, b_{\perp}, \mu, \zeta_z) = \lim_{L \rightarrow \infty} \int \frac{dz}{2\pi} e^{i(x - \frac{1}{2})zP^z} \frac{\tilde{\Phi}^{+0}(z, b_{\perp}, P^z, a, L)}{Z_O(\mu, a) \sqrt{Z_E(2L + z, b_{\perp}, \mu, a)}}$$

Different HYP



To suppress the fluctuation arises from the excited states, we try different Dirac structure in the interpolator, i.e. in 3pt:

$$C_3(b_\perp, \Gamma, t_{seq}, t, P^z) = \sum_{\vec{z}, \vec{x}_1, \vec{x}_2} e^{-i2zP^z} \langle O_\pi(t_{seq}, \vec{x}_1, -P^z) \bar{u} \Gamma u(\vec{z} + b_\perp, t) \bar{d} \Gamma d(\vec{z}, t) O_\pi^\dagger(0, \vec{x}_2, P^z) \rangle$$

we take:

$$O_\pi^\dagger(t, \vec{x}, P^z, \Gamma_1) = \bar{u}(\vec{x}, t) \Gamma_1 d(\vec{x}, t) e^{-i\vec{x} \cdot \hat{n}_z P^z}$$

$$O_\pi(t_{seq}, \vec{x}', P^z, \Gamma_2) = \bar{d}(\vec{x}', t_{seq}) \Gamma_2 u(\vec{x}', t_{seq}) e^{i\vec{x}' \cdot \hat{n}_z P^z}$$

Fix the current 3pt $\Gamma = \gamma_\perp$ and $\gamma_\perp \gamma_5$, at large momentum limit we have

$$F(b_\perp, P_1, P_2, \Gamma_1, \Gamma_2) \propto \text{Tr}[\Gamma_1 (\not{P}_1 - m) \Gamma (\not{P}_2 - m) \Gamma_2 (\not{P}_2 + m) \Gamma (\not{P}_1 + m)]$$

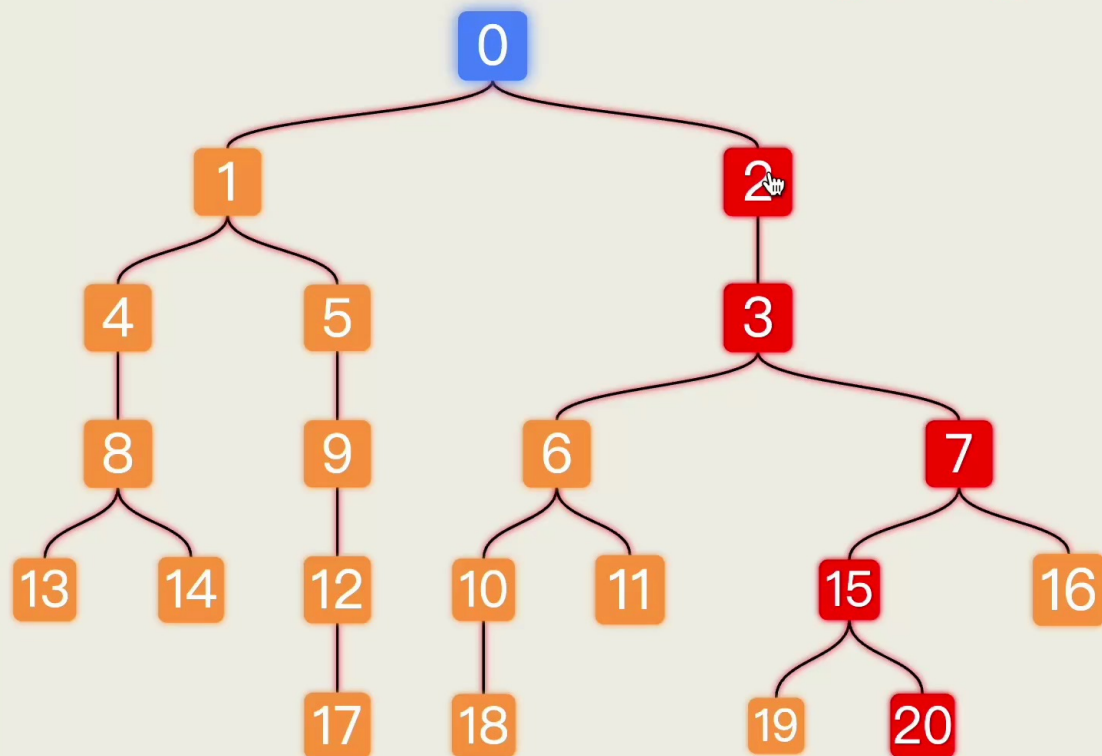
here $\Gamma_1, \Gamma_2 = \gamma^5, \gamma^z \gamma^5$ or $\gamma^t \gamma^5$. At large momentum limit:

		Γ_2		
		$\gamma_t \gamma_5$	$\gamma_z \gamma_5$	γ_5
Γ_1	$\gamma_t \gamma_5$	$O(P_z^4)$	$O(P_z^4)$	$O(mP_z^3)$
	$\gamma_z \gamma_5$	$O(P_z^4)$	$O(P_z^4)$	$O(mP_z^3)$
	γ_5	$O(mP_z^3)$	$O(mP_z^3)$	$O(m^2 P_z^2)$

Monte Carlo树搜索 (MCTS)

• 1

红色节点: 最佳轨迹 (Best Trajectory)



每个节点对应一项子任务的一次探索

NODE INFO	THEORETICIAN	CRITIC
BASIC INFO		
node_index: 0		
node_type: virtual		
status: completed		
average_reward: 0.6796296296296296		
TASK QUERY		
Virtual Root		

- **分级学术知识体系(LANDAU, Layered Academic Data Universe) :**
 - **文献库 Library** : 从精确检索文献中抽取的定量与定性知识、具体问题的专门技术
 - **方法论 Methodology** : 被验证、可以复用的成体系研究路径, 如强相关的论文
 - **先验知识 Priors** : 人工整理的高置信先验知识, 例如权威教材、奠基性经典文章

Evolving Academic Data Universe



Library \mathcal{L} : Task-specific knowledge distilled from precisely retrieved papers

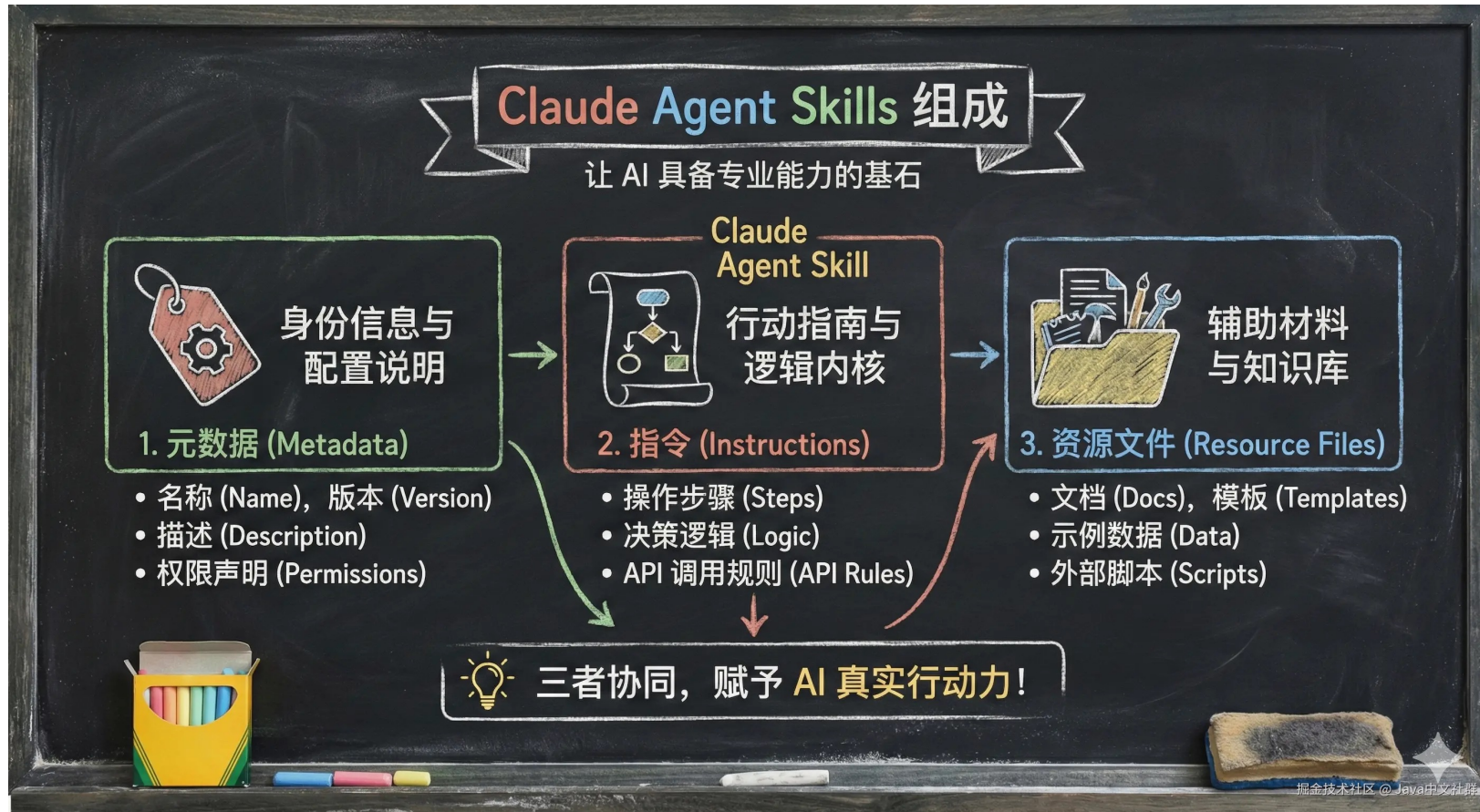


Methodology \mathcal{M} : validated reasoning paths for reuse in familiar domains



Priors \mathcal{P} : Reliable textbooks, docs and verified prior knowledge

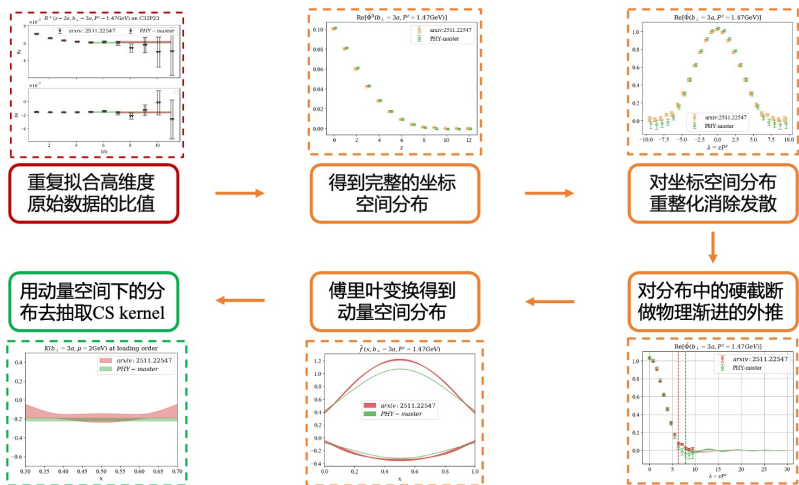
Skill



元数据 (Metadata)：对技能的简短描述。保存在全局上下文中，体积小，非常节省 **Tokens**（省钱又省心）。

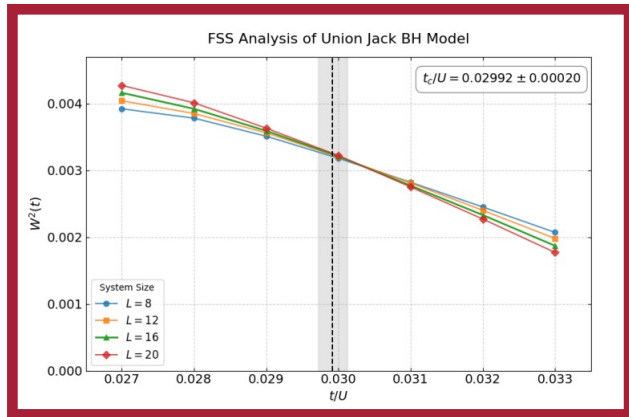
行动指南 (Action Guide)：这部分才是真正的提示词，规定了 AI 每一步该怎么做。

资源文件 (Resources)：这是最厉害的地方！它可能包含 **Python 代码** 或其他执行程序，保证程序在调用 Skill 时能完成复杂的动作。



加速：Lattice QCD数据处理

从准TMD 波函数提取 Collins-Soper 核
高复杂度流程自主实现



自动探索：

基于QMC确定Union Jack 晶格上
Bose-Hubbard 模型量子相变临界点

粲介子半轻衰变的SU(3)哈密顿量：

$$H = D^j H_i M_j^i$$

$$M_j^i = \begin{bmatrix} \frac{\pi^0 + \eta_8}{\sqrt{2} + \sqrt{6}} & \pi^+ & K^+ \\ \pi^- & -\frac{\pi^0 + \eta_8}{\sqrt{2} + \sqrt{6}} & K^0 \\ K^- & \bar{K}^0 & -\frac{2\eta_8}{\sqrt{6}} \end{bmatrix}$$

$$D^j = [D^0, D^+, D_s^+] \quad H_i = [0, V_{cd}, V_{cs}]$$

Decay channels	Amplitudes (in unit of a)
$D^0 \rightarrow \pi^- \ell \nu$	V_{cd}
$D^0 \rightarrow K^- \ell \nu$	V_{cs}
$D^+ \rightarrow \pi^0 \ell \nu$	$-\frac{1}{\sqrt{2}} V_{cd}$
$D^+ \rightarrow \eta_8 \ell \nu$	$\frac{1}{\sqrt{6}} V_{cd}$
$D^+ \rightarrow \bar{K}^0 \ell \nu$	V_{cs}
$D_s^+ \rightarrow K^0 \ell \nu$	V_{cd}
$D_s^+ \rightarrow \eta_8 \ell \nu$	$-\frac{2}{\sqrt{6}} V_{cs}$

自主发现：

基于味SU(3)对称性
构造强子味表示与衰变算符，
确定有效哈密顿量，预言衰变道振幅