Quantum simulations of non-perturbative quantities in hadron scattering

Speaker: Tianyin Li (李天胤), form RIKEN iTHEMS

Collaborate with: Xingyu Guo, Wai Kin Lai, Xiaohui Liu, Enke Wang, Hongxi Xing, Dan-Bo Zhang and Shi-Liang Zhu (QuNu Collaboration)

26th International Symposium on Spin Physics

Outline

I. Background

II. Quantum simulations of hadron scattering based on QCD factorization

III. Scattering amplitude from quantum computing with the reduction formula

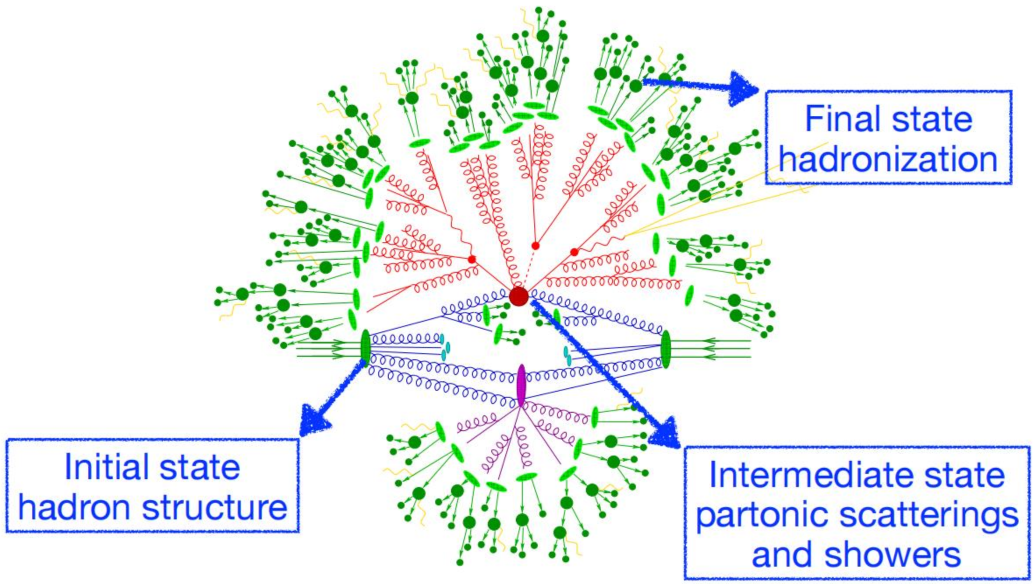
IV. Discussions of mapping gauge fields to qubits

V. Summary

Part I: Background

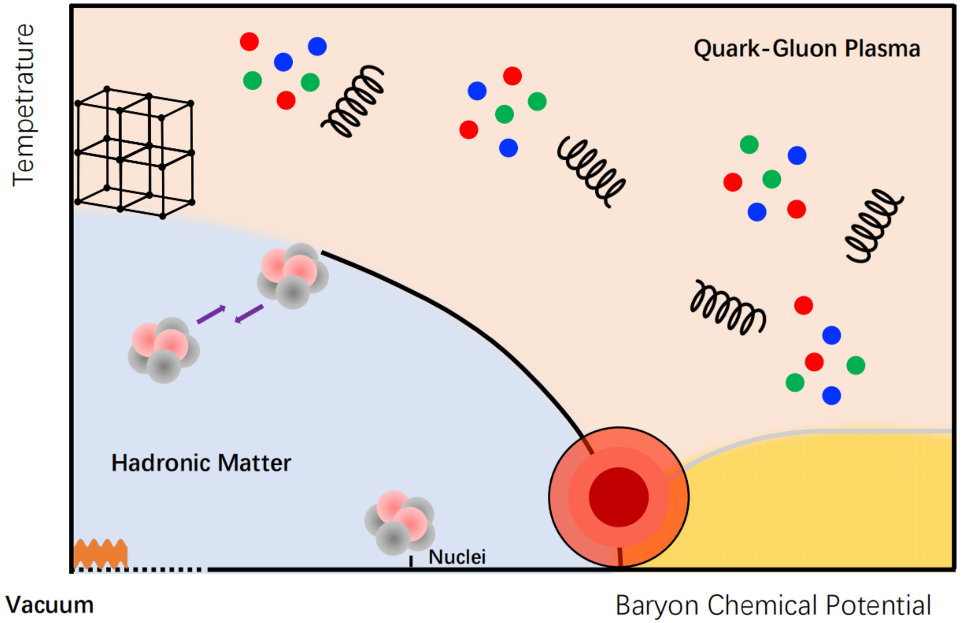
Non-perturbative problems with sign problem

- Time-dependent problem:
  Cross sections of hadron scattering



From H. Xing's slides

- Finite chemical potential problem:
  QCD phase diagram



From L. Wang's slides

They are the primary goals of RHIC, LHC, and other similar experiments. But it is a big challenge to simulate those quantities on a classical computer due to the limitation of computational resources.

Quantum computing: A new computing paradigm

What is a quantum computer?

- A quantum computer is a computer that uses the physical rules of quantum mechanics to perform calculations.

Advantages of the Quantum computing method:

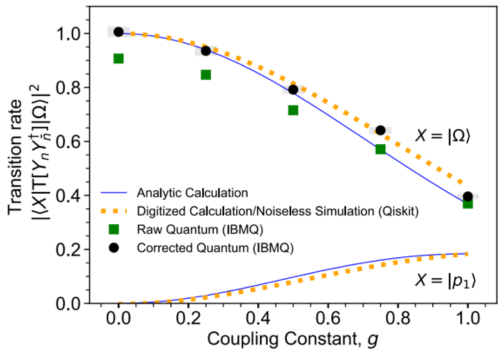
- It is Controllable.
- It can store quantum states efficiently.
- Compared to classical computers, quantum computers can achieve exponential acceleration when simulating time-dependent systems. (No sign problem.)

“... and if you want to make a simulation of nature, you’d better make it quantum mechanical, ...” – R. Feynman

Quantum simulations of scattering on a collider: An overview

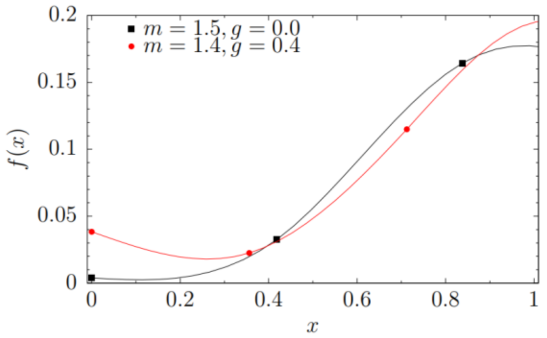
Red technical route:
- ➢ Based on QCD factorization.
- ➢ Suitable for near-term quantum computers.

Simulating Collider Physics on Quantum Computers Using Effective Field Theories:



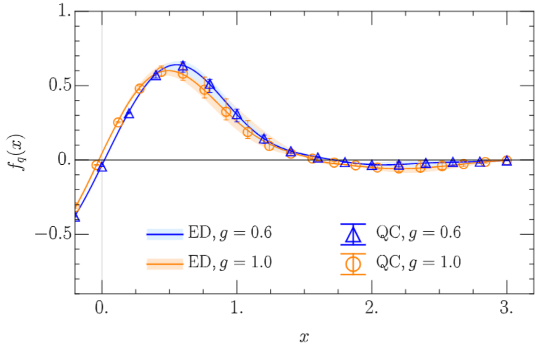
C. W. Bauer, and B. Nachman, PRL, (2021)

Parton distribution functions (PDFs) form hadron tensor by quantum computing:



H. Lamm, S. Lawrence, and Y. Yamauchi, PRR, (2020)

PDFs from light-cone correlation functions



TL et al (QuNu), PRD (letter, 2022)

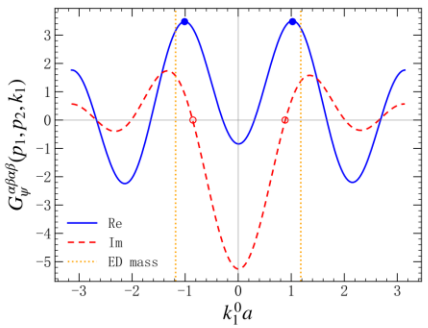
Orange technical route:
- ➢ Catch all information of scattering process
- ➢ Suitable for future fault-tolerant quantum computers.

First attempt to simulate scattering amplitude on quantum computers:

$$G_{\rm weak} \sim \begin{cases} \left(\frac{1}{\varepsilon}\right)^{1.5+o(1)}, & d=1 \\ \left(\frac{1}{\varepsilon}\right)^{2.376+o(1)}, & d=2 \\ \left(\frac{1}{\varepsilon}\right)^{5.5+o(1)}, & d=3 \end{cases}$$

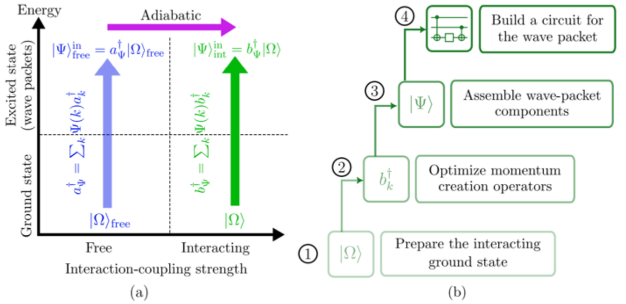
S. Jordan, K. S. M. Lee, and J. Preskill, Science, (2012).

Scattering amplitude from quantum computing with reduction formula:



TL et al (QuNu), PRD, (2024)

Bound state scattering of the scalar field and gauge theories



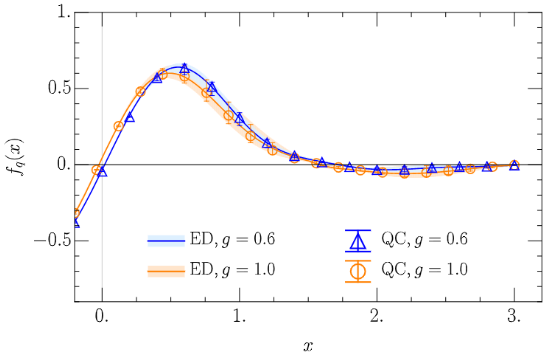
M. Turco et al, PRX Quantum, (2024). Z. Davouid et al, Quantum (2024).

Part II: Quantum simulations of hadron scattering based on QCD factorization

Red technical route:

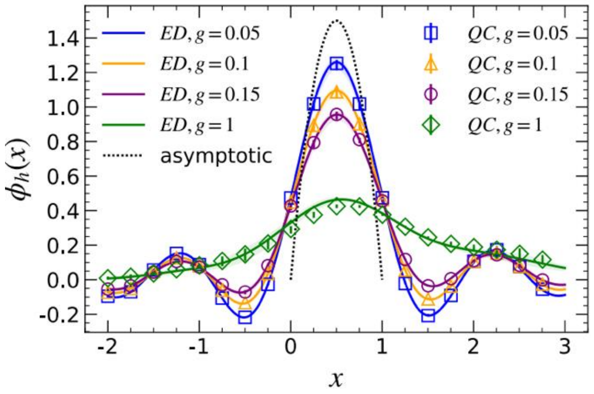
- Based on QCD factorization.
- Suitable for near-term quantum computers.

PDFs from light-cone correlation functions



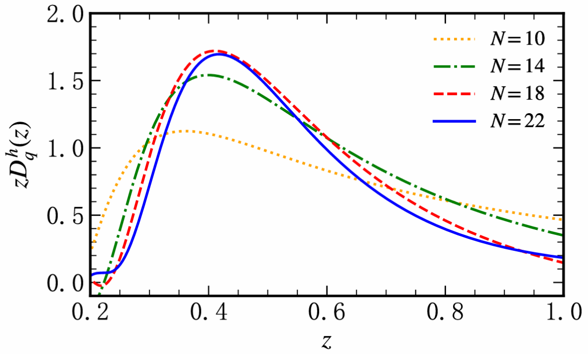
TL et al (QuNu), PRD (letter, 2022)

Quantum simulation of light-cone distribution amplitudes (LCDAs)



TL et al (QuNu), SCPMA (2023)

Quantum simulation of fragmentation functions (FFs)



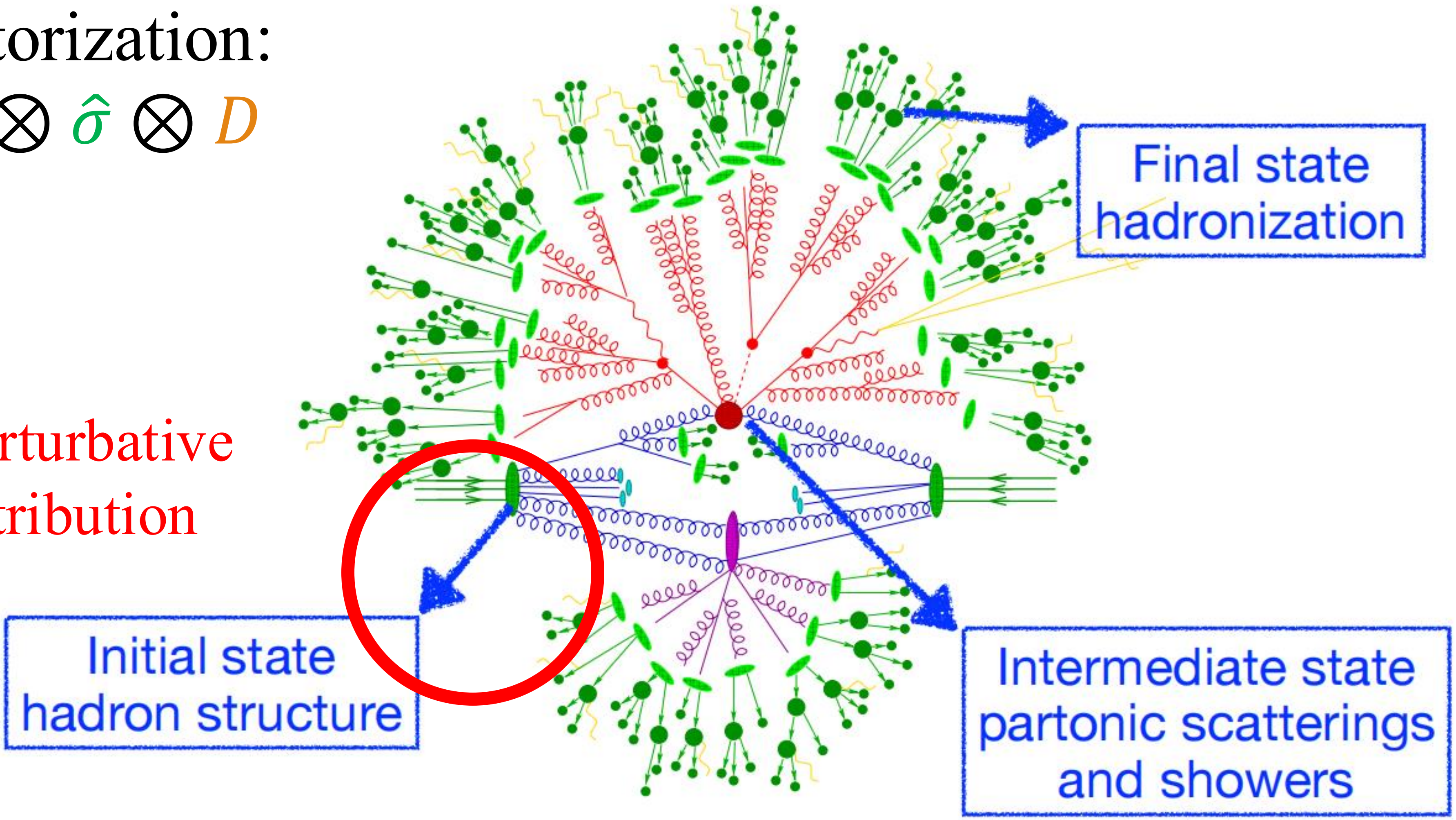
TL, H. Xing and D.B. Zhang, arXiv:2406.05683.

QCD factorization in high-energy scattering

QCD factorization:

$$\sigma = f \otimes \hat{\sigma} \otimes D$$

f: Non-perturbative parton distribution function



Quantum simulations of PDFs in NJL model

Hamiltonian of NJL model: $H = \int dx\, [\bar{\psi}(-i\gamma^1\partial_1 + m)\psi - g(\bar{\psi}\psi)^2]$

The operator definition of PDFs, with $n^\mu = (1, -1)$:

$$f_{q/h}(x) = \int \frac{dz}{4\pi} e^{-ixm_h z} \langle h(\vec{p}=0) | e^{iHz} \bar{\psi}(0, -z) e^{-iHz} \gamma^+ \psi(0) | h(\vec{p}=0) \rangle$$

$$\equiv \int \frac{dz}{4\pi} e^{-ixm_h z} \tilde{f}_{q/h}(z)$$

→ Need to be simulated on quantum computers

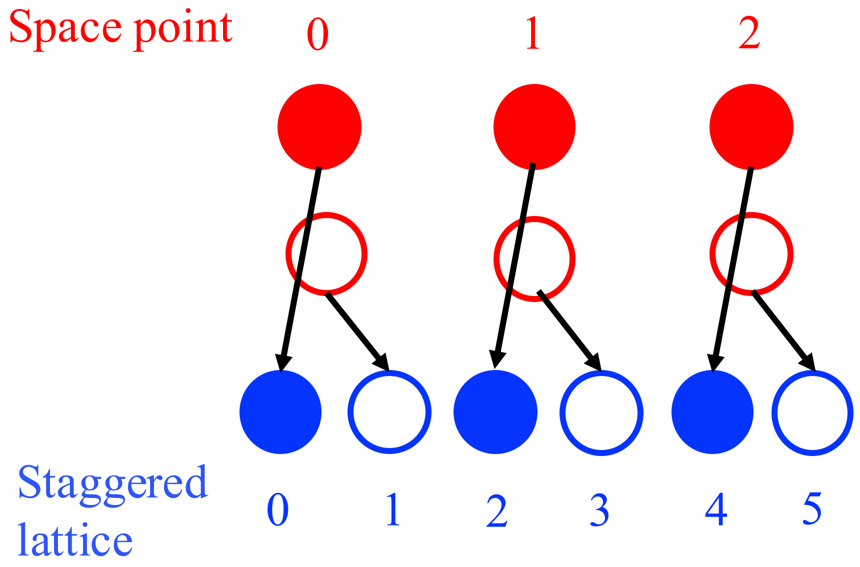
Four steps to simulate PDFs on a quantum computer:

- Discretize and map fields to qubits.
- Preparation of the hadron state $|h\rangle$.
- Evaluate the light-cone correlation function.

Discretization and mapping of fermion fields to qubits

Discretization: staggered fermion

$$\begin{pmatrix}\psi_1(N)\\ \psi_2(N)\end{pmatrix} = \begin{pmatrix}\phi(2N)\\ \phi(2N+1)\end{pmatrix} \equiv \begin{pmatrix}\phi(n)\\ \phi(n+1)\end{pmatrix}$$



Mapping to qubits by Jordan-Wigner transformation:

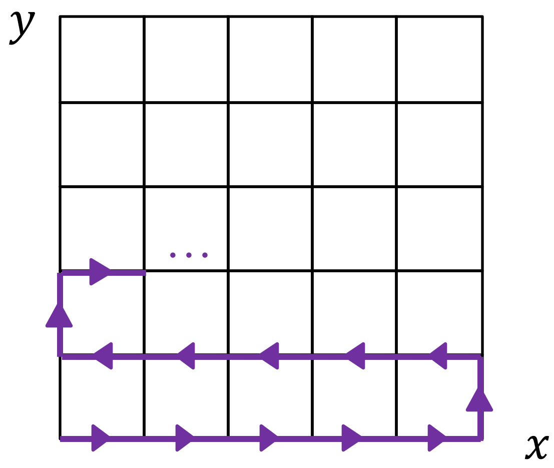
$$\phi(n) = \prod_{i<n} \sigma_i^z (\sigma_n^x + i\sigma_n^y).$$

(σ_n^x, σ_n^y and σ_n^z are Pauli operators)

- This transformation preserves the anti-commutator

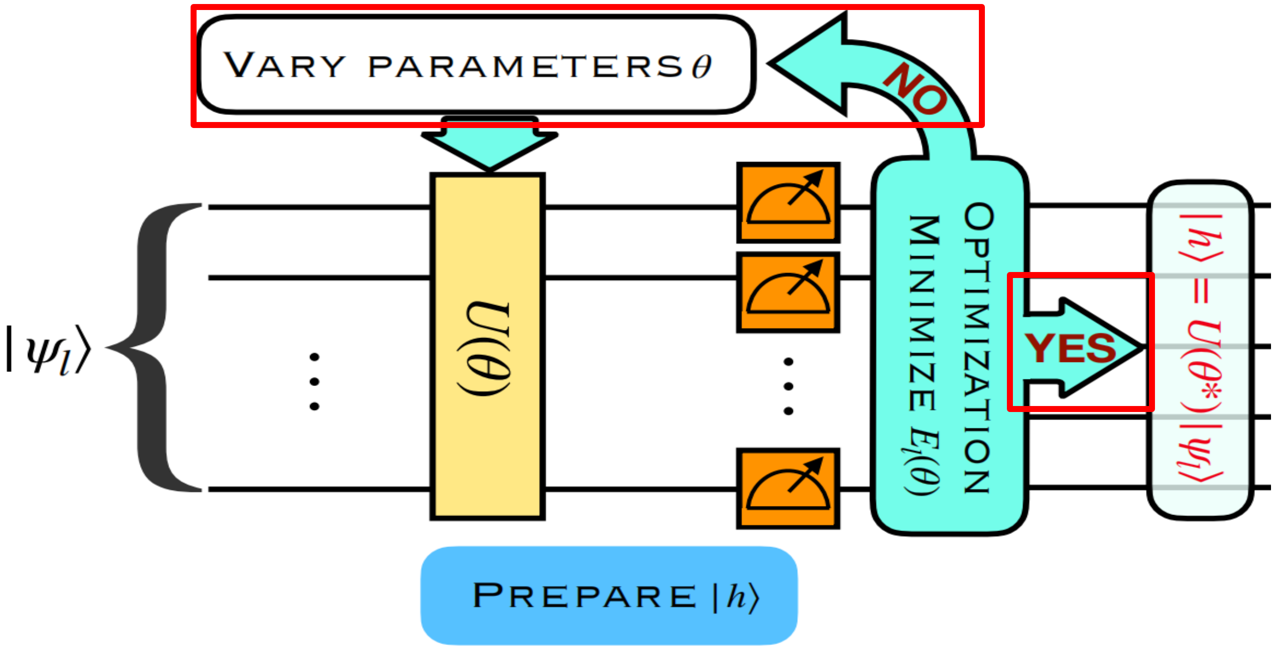
$$\{\phi(n), \phi^\dagger(m)\} = \delta_{nm}$$

- A path is needed in more than (1+1)-D:



Variational quantum eigensolver (VQE) to prepare the hadron state

TL et al (QuNu), PRD (letter, 2022)



- For given quantum numbers l, we use k reference states to obtain the first k excited states.
- Divide $H = H_1 + H_2 + \cdots + H_n$:
  - $[H_i, H_{i+1}] \neq 0$.
  - Every H_i preserve all symmetry of the full Hamiltonian H.
  - $U(\theta) = \prod_{i=1}^{p}(\prod_{j=1}^{n} \exp(i\theta_{ij}H_j))$.
- Trial wave function: $|\psi_{li}(\theta)\rangle = U(\theta)|\psi_{li}\rangle_{ref}$
- Measure the loss function $E_l(\theta) = \sum_i^k w_{li}\langle\psi_{li}(\theta)|H|\psi_{li}(\theta)\rangle$ on quantum computers.
- Optimize loss function on classical computers

Details of this quantum algorithm will be given in Dairui's presentation.

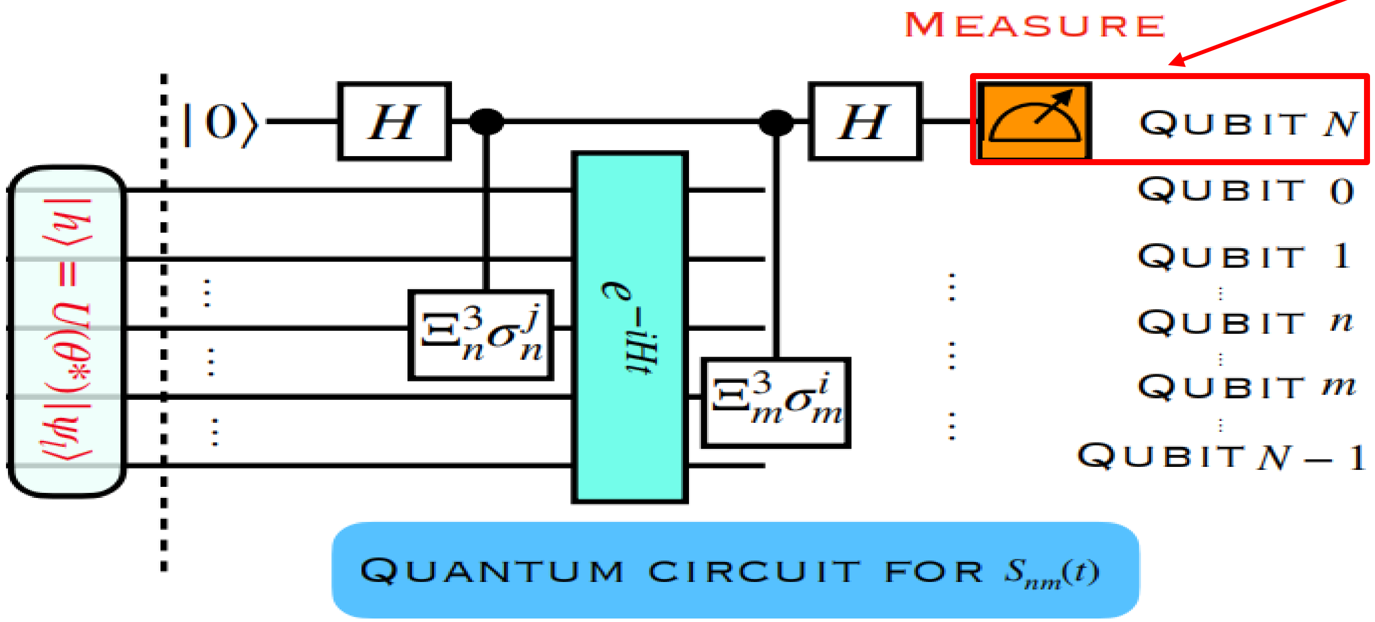
Evaluate the dynamical correlation function

- Evaluate the dynamical two-point correlation function

$$S_{mn}(t) = \langle h | e^{iHt} \Xi_m^3 \sigma_m^i e^{-iHt} \Xi_n^3 \sigma_n^j | h \rangle.$$

Qubit PDFs can be written as sum of such correlation functions.

Re(Im)[$S_{mn}(t)$] can be obtained by measuring σ_N^x (σ_N^y).

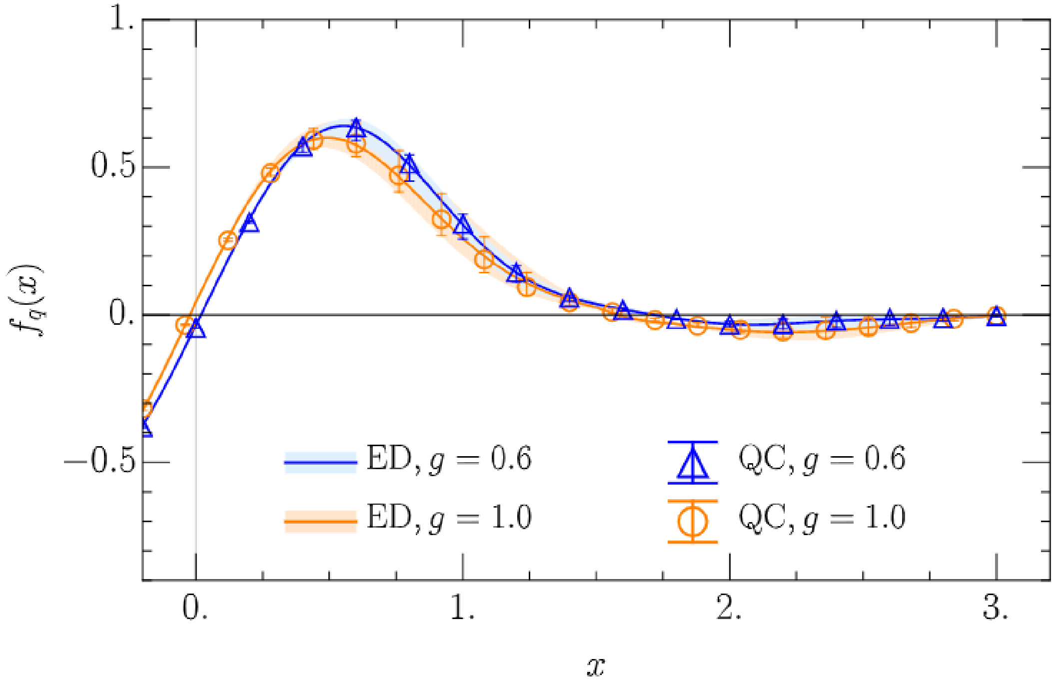


Details of this quantum algorithm will be given in Dairui's presentation.

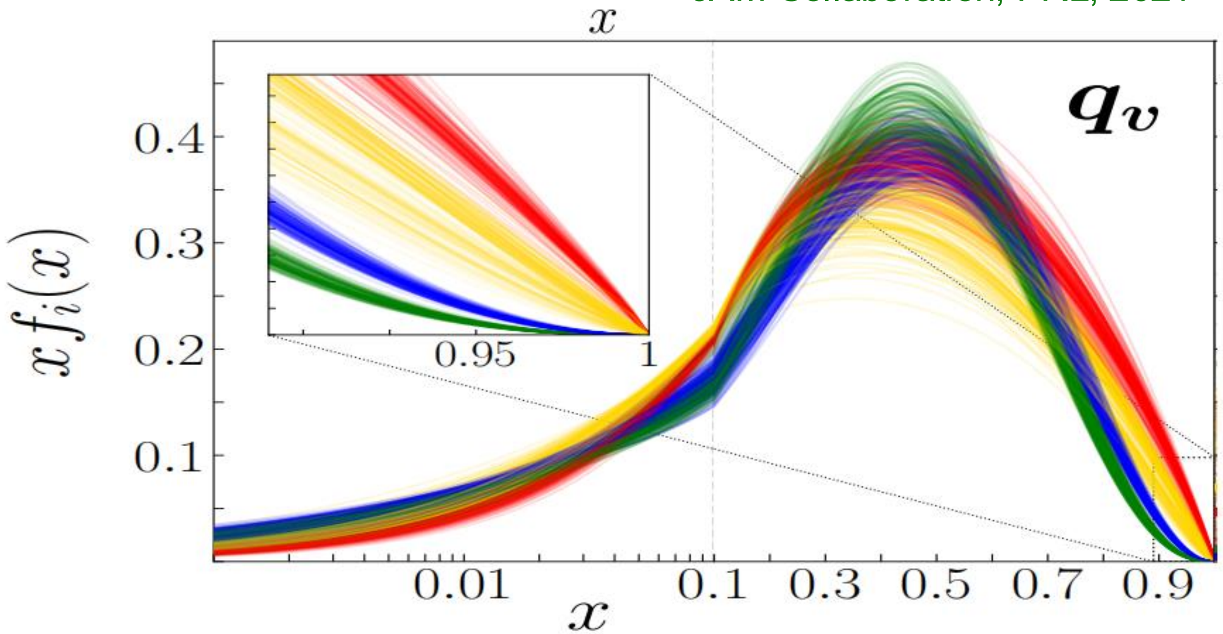
Pedernales et al, PRL, (2014)

Results of lowest $q\bar{q}$ bound state quark PDF in NJL model

TL et al (QuNu), PRD (letter, 2022)



JAM Collaboration, PRL, 2021

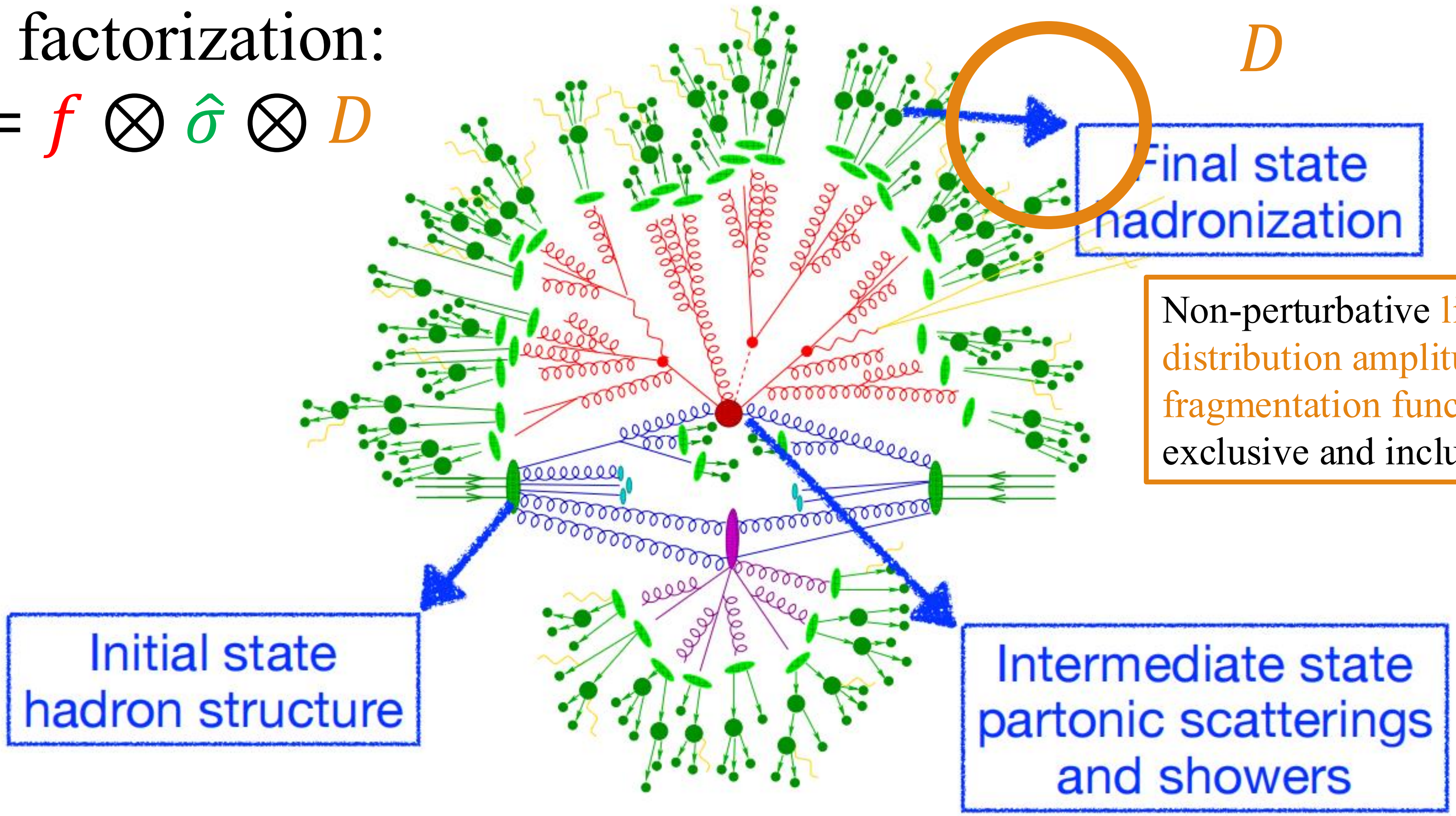


- Our result is obtained from a classical simulator.
- Good agreement between quantum computing (QC) and numerical exact diagonalization (ED) results.
- The non-vanishing contribution in the $x > 1$ is partly due to the finite volume effect.
- Our result has an expected peak around $x = 0.5$, it is also in qualitative agreement with pion PDFs.

Simulating hadronization on quantum computers

QCD factorization:

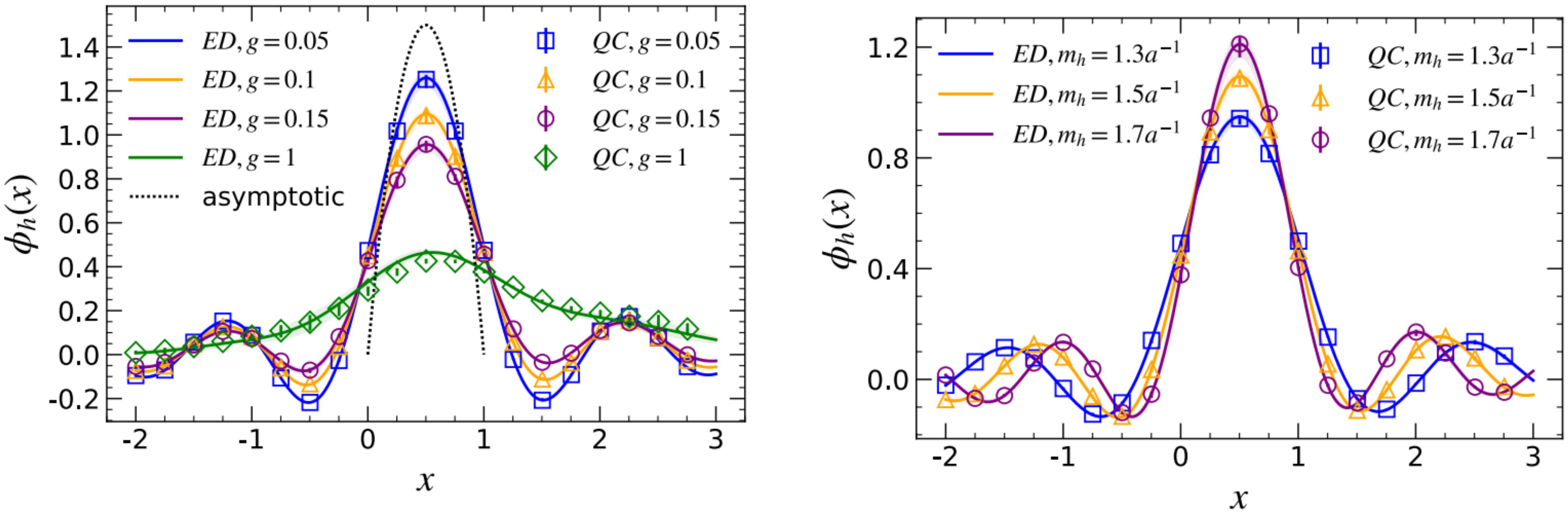
$$\sigma = f \otimes \hat{\sigma} \otimes D$$



Non-perturbative light-cone distribution amplitudes ϕ and fragmentation functions D for exclusive and inclusive process.

Results of lowest $\bar{q}q$ bound state quark LCDA in NJL model

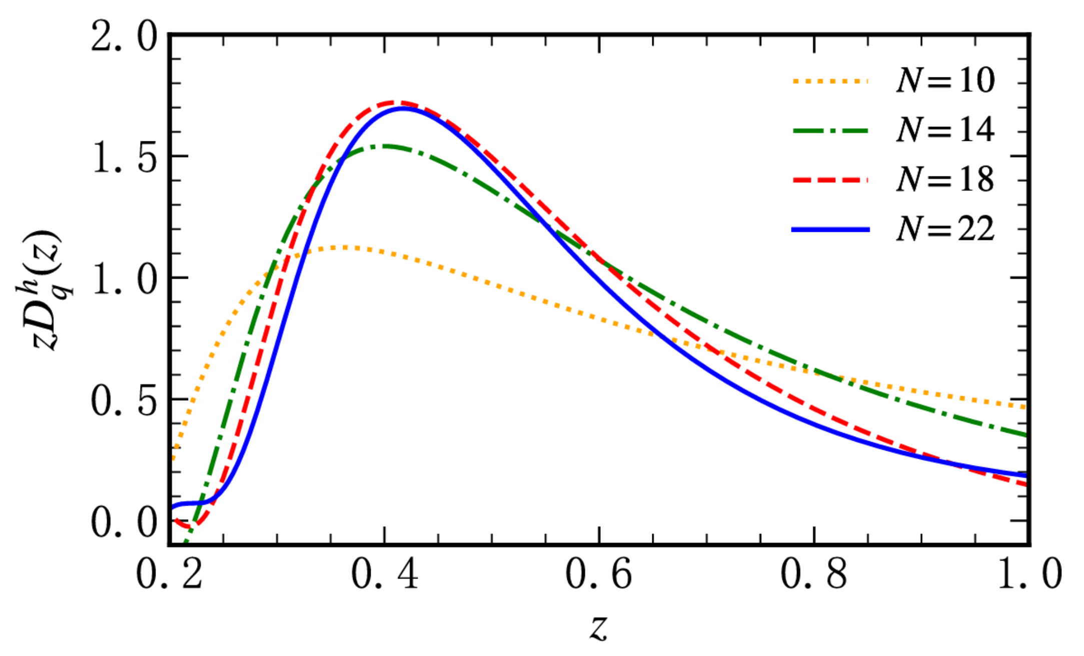
TL et al (QuNu), SCPMA (2023)



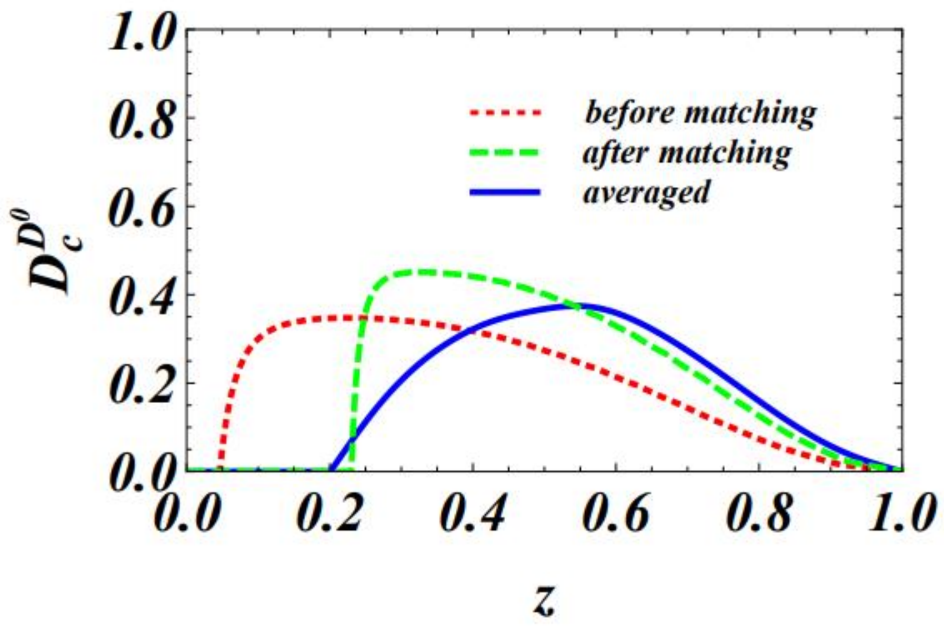
- The QC result converges to asymptotic result $6x(1-x)$ in the weak coupling limit.
- Peak gets narrower with increasing hadron mass.

Results of fragmentation function in NJL model

TL et al (QuNu), arXiv:2406.05683.



D.-J. Yang, PRD, (2020).



- Similar with the result of $D_c^{D^0}$ in [D-J. Yang, PRD,(2020)], our result also vanishes in the small z region and a peak appears in $0.4 < z < 0.6$.

Part III: Scattering amplitude from quantum computing with reduction formula

Orange technical route:

- Catch all information of scattering process
- Suitable for future fault-tolerant quantum computers.

First attempt to simulate scattering amplitude on quantum computers:

$$G_{\text{weak}} \sim \begin{cases} \left(\frac{1}{\varepsilon}\right)^{1.5+o(1)}, & d=1 \\ \left(\frac{1}{\varepsilon}\right)^{2.376+o(1)}, & d=2 \\ \left(\frac{1}{\varepsilon}\right)^{5.5+o(1)}, & d=3 \end{cases}$$

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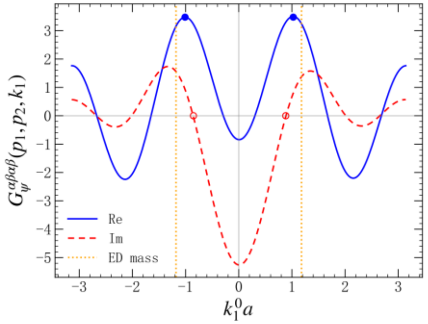
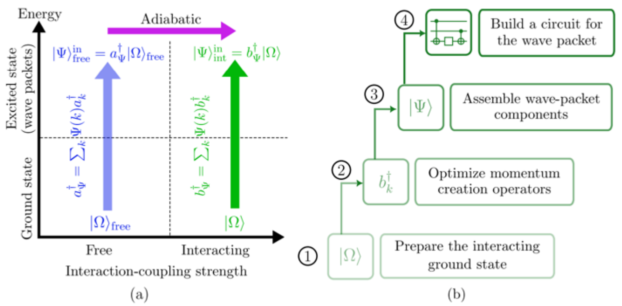
Scattering amplitude from quantum computing with reduction formula:



TL et al (QuNu), PRD, (2024)

Bound state scattering of the scalar field and gauge theories



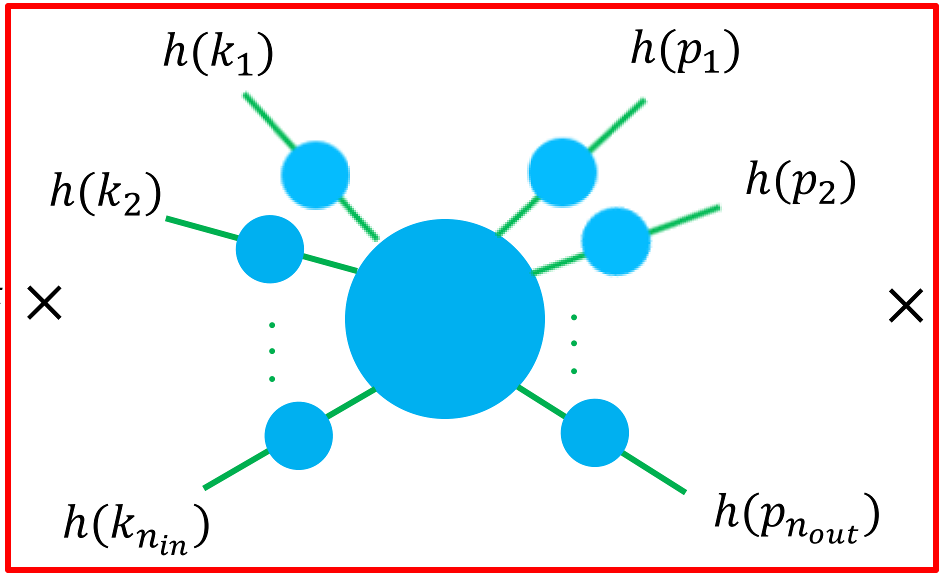
M. Turco et al, PRX Quantum, (2024). Z. Davouid et al, Quantum (2024).

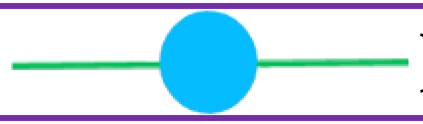
LSZ reduction formula

- We propose an alternative framework to calculate scattering amplitudes on a quantum computer based on the LSZ reduction formula.
- Using the LSZ reduction formula to calculate the scattering amplitude of

$$h(k_1) + h(k_2) + \cdots + h(k_{n_{in}}) \rightarrow h(p_1) + h(p_2) + \cdots + h(p_{n_{out}})$$

$i\mathcal{M} = R^{n_{in}+n_{out}} \times$



$\times$ ( $)^{-n_{in}-n_{out}}$

Field renormalization
$|\langle\Omega|\phi(0)|h\rangle|$

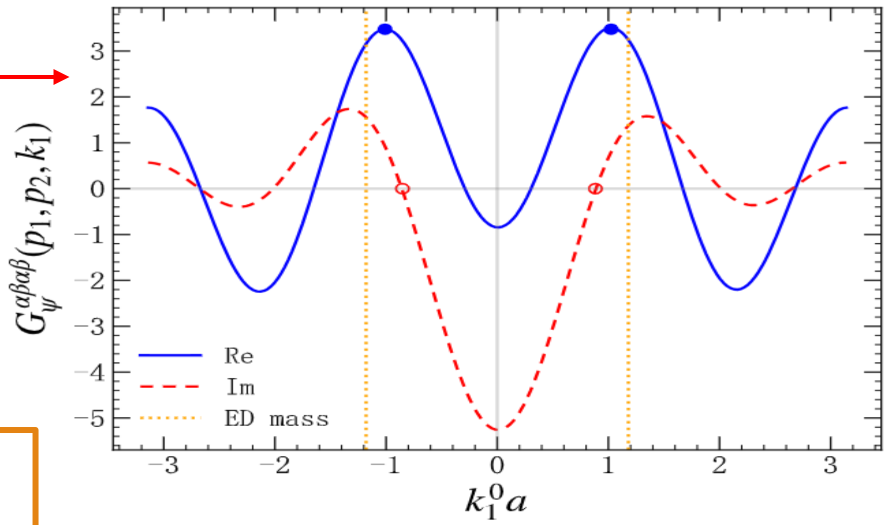
On-shell connected two-point functions

On-shell connected $n_{in} + n_{out}$-point functions

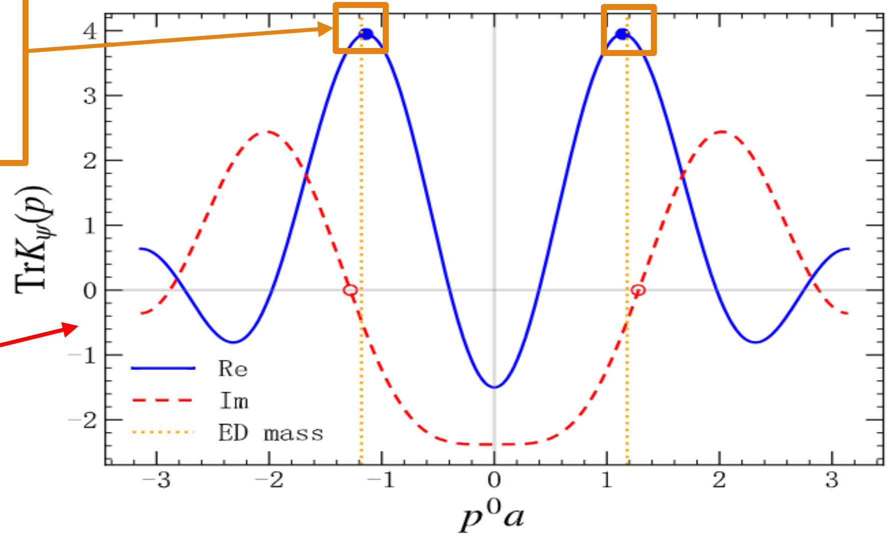
Results of NJL model

Connected four-point function $G^{\alpha\beta\alpha\beta}(p_1, p_2, k_1)$, with p_1, p_2 off shell: $p_1 = (0,0)$, $p_2 = (k_1^0, \frac{\pi}{a})$, $k_1 = (k_1^0, 0)$.

TL et al (QuNu), PRD, (2024)



Quark mass poles $i/(p^2 - m_q^2 + i\epsilon)$ of $\bar{\psi}\psi$ two-point function.
Poles position: ± 1.14;
ED quark mass: $m_q a = 1.18$.

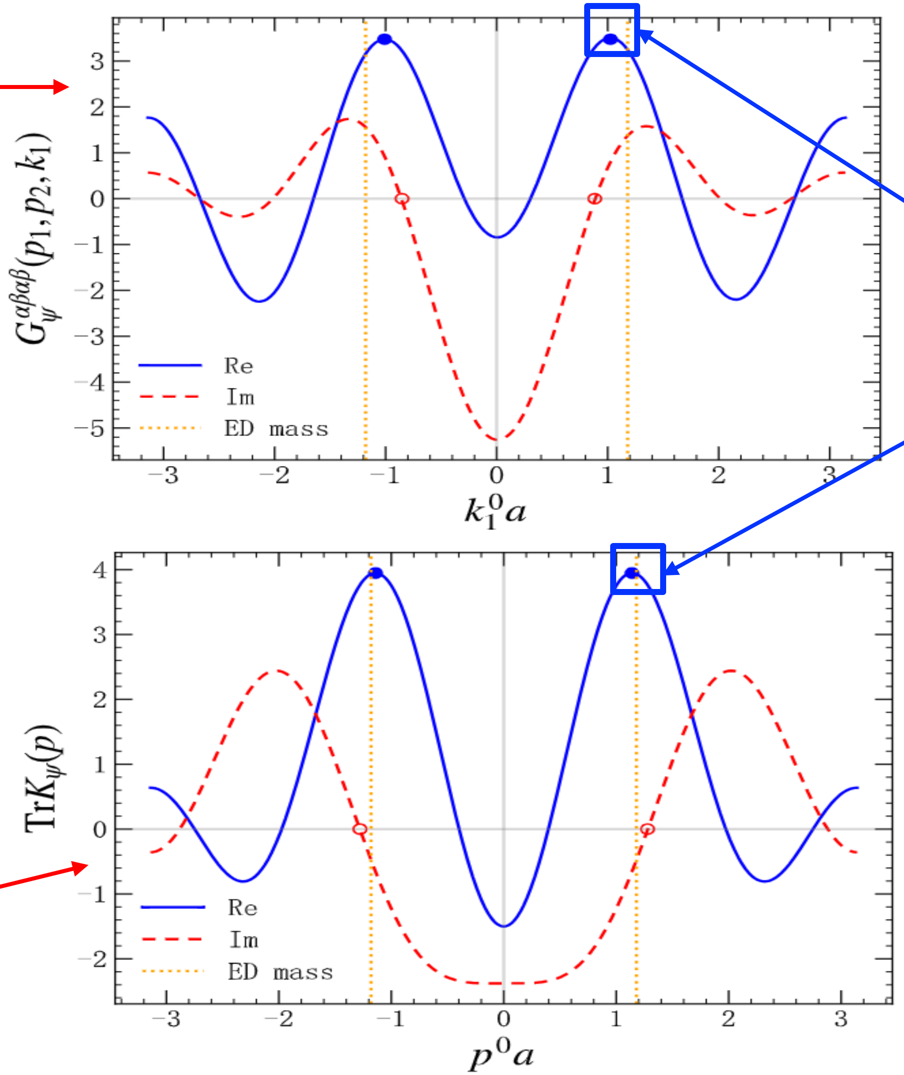


Fermion propagator with $p = (p^0 a, 0)$
$K_\psi = \int d^2x\, e^{ip\cdot x} \langle \Omega | \bar{\psi}(x)\psi(0) | \Omega \rangle$

Results of NJL model

Connected four-point function $G^{\alpha\beta\alpha\beta}(p_1, p_2, k_1)$, with p_1, p_2 off shell: $p_1 = (0,0)$, $p_2 = (k_1^0, \frac{\pi}{a})$, $k_1 = (k_1^0, 0)$.

TL et al (QuNu), PRD, (2024)



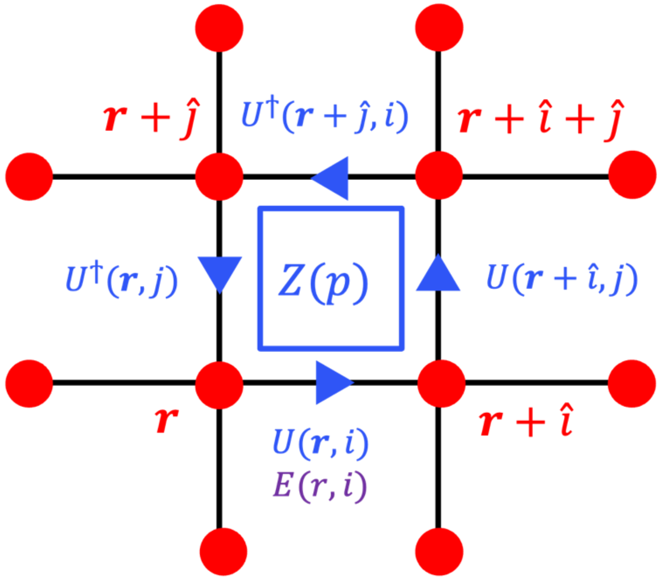
Our quantum algorithm removes the pole structure of four-point function successfully.

Fermion propagator with $p = (p^0 a, 0)$
$K_\psi = \int d^2x\, e^{ip\cdot x} \langle \Omega | \bar{\psi}(x) \psi(0) | \Omega \rangle$

Part IV: Discussions of mapping gauge fields to qubits

Review of Kogut-Susskind formalism (without gauge fixing)

J. B. Kogut, and L. Susskind, PRD, (1975)



Two constraints:

- Primary constraint: $\Pi^0 \approx 0$.
- Secondary constraint (Gauss's law): $G(E) = \partial_i E_a^i - J_a^0 \approx 0$
- Hamiltonian of the constraint system:

$$H = H_E + H_B - A_0 G(E)$$

- Quantization conditions:

$$\left[E^a, U_{ij}^\rho\right] = -\sum_k (T_\rho^a)_{ik} U_{kj}^\rho, \dots$$

How to remove the inference from the undeterminate function A^0?

- Using Gauss's law operator to project to the physical subspace:

$$G(E)|\text{Phys}\rangle = 0$$

- Hamiltonian should be gauge invariant – The eigenstate of Hamiltonian should be well-defined

$$[H, G(E)] = 0$$

Impossible triangle of K-S formalism in finite-dimensional Hilbert space

The Hilbert space of quantum computers has a finite dimension

↓

The following two conditions conflict with each other in a finite-dimensional Hilbert space:

1. $\left[E^a, U^\rho_{ij}\right] = -\sum_k \left(T^a_\rho\right)_{ik} U^\rho_{kj}, \ldots$
2. U is unitary.

↓

Broken of Gauss's law $[H, G] = 0$ or unitary. → Can we modify 1? →

Preserve Gauss's law strictly after digitization. (Including dynamical quark)

Impossible triangle

Has controllable digitization error

Unitary gauge link

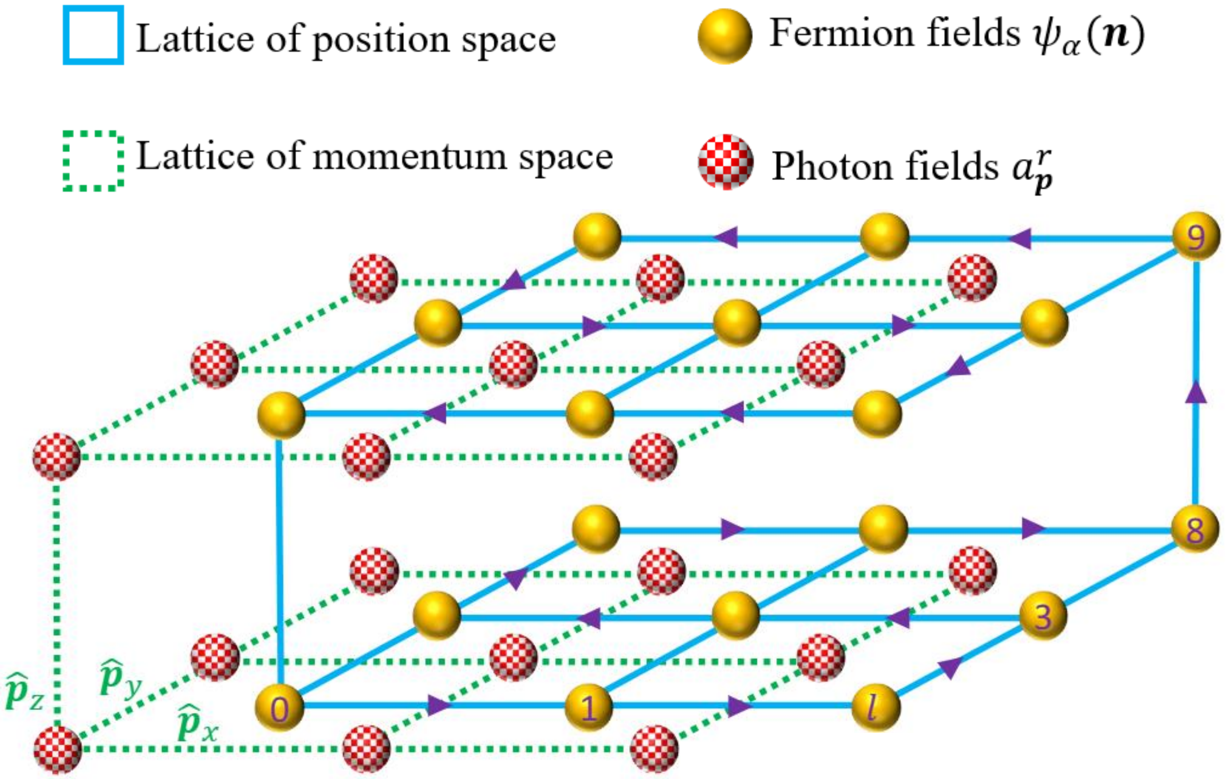
- Truncation of E basis: T. Byrnes and Y. Yamamoto, PRA, (2006). E. Zohar, J. I. Cirac, and B. Reznik, PRL, (2012)…
- Discrete subgroup method: Y. Ji, H. Lamm, and S. Zhu, PRD, (2020)…
- Fixing to the maximum tree gauge: I. D'Andrea et al., PRD, (2024)…
- Quantum link model: D. Luo et al., PRA, (2020)…
- …

The impossible triangle can be overcome by fixing to the Coulomb gauge!

Coulomb gauge QED on lattice

In CG A^0 is determined by:

$$A^0 = \int d^3y \frac{J^0(x)J^0(y)}{4\pi|x-y|}$$



TL, PRD, (2025)

$$\hat{H}_E + \hat{H}_B = \sum_{\boldsymbol{p}\neq 0} \sum_r \hat{E}_{\boldsymbol{p}} a^{r\dagger}_{\boldsymbol{p}} a^r_{\boldsymbol{p}}$$

$$\hat{H}_I = \sum_{\boldsymbol{n},i} \sum_{\boldsymbol{p}} \sum_r \frac{J^i(\boldsymbol{n})}{\sqrt{2\hat{E}_p M^3}} \left[\hat{\epsilon}^r_i a^r_{\boldsymbol{p}} e^{i\boldsymbol{p}\cdot\boldsymbol{n}} + \mathrm{H.c.}\right]$$

$$\hat{H}_V = \frac{1}{2} \sum_{\boldsymbol{m},\boldsymbol{n}} \sum_{\boldsymbol{p}} \frac{J^0(\boldsymbol{m})J^0(\boldsymbol{n})}{\hat{E}^2_{\boldsymbol{p}}} e^{-i\boldsymbol{p}\cdot(\boldsymbol{m}-\boldsymbol{n})}$$

$$\hat{H}_M = \sum_{\boldsymbol{n}} \bar{\psi}(\boldsymbol{n}) \left[-i\gamma^i \frac{\psi(\boldsymbol{n}+\hat{\imath}) - \psi(\boldsymbol{n}-\hat{\imath})}{2} + m\bar{\psi}(\boldsymbol{n})\psi(\boldsymbol{n})\right]$$

$$\hat{H}_W = \sum_{\boldsymbol{n}} -\frac{w}{2} \bar{\psi}(\boldsymbol{n}) \hat{\Delta} \psi(\boldsymbol{n})$$

- We set $a = 1$ here.
- We have M lattice sites for each special dimension.
- Wilson term $\hat{H}_W$ comes from Wilson fermion.

Overcome the impossible triangle in CG formalism

Preserve Gauss's law strictly by solving A^0 and polarization vector $\hat{\epsilon}^s(\boldsymbol{p})$ on lattice

Controllable truncation error:

- Truncation of the Fock states:

$$a_{\boldsymbol{p}}^{r\dagger}\left|\Lambda = 2^{K} - 1\right\rangle_{\boldsymbol{p},r} = 0$$

- Given truncation Λ, the error ε_s of arbitrary state $|\psi\rangle$ scales as:

$$\varepsilon_s \sim O\left(\frac{g^2 M^{3d+3} + E M^{d+1}}{\Lambda}\right)$$

Unitarity of gauge link: $\boldsymbol{U_i(n)}$:

$$U_i(n) = \exp(-igA_i(\boldsymbol{n}))$$

,where $A_i(\boldsymbol{n})$ is Hermitian.

- As a cost, the Coulomb gauge formalism **has non-local interaction terms** in the Hamiltonian.

Map the QED Hamiltonian to qubits

$$\hat{H}_E + \hat{H}_B = \sum_{\mathbf{p}\neq 0}\sum_{r} \hat{E}_{\mathbf{p}} a^{r\dagger}_{\mathbf{p}} a^{r}_{\mathbf{p}} = \sum_{\mathbf{p}\neq 0}\sum_{r}\sum_{J=0}^{K-1} 2^J \left[\frac{1}{2}(I - \sigma^3_{J,\mathbf{p},r})\right]$$

$$\hat{H}_I = \hat{H}_I^S + \hat{H}_I^A$$

$$\hat{H}_I^S = \sum_{\mathbf{n},i}\sum_{\mathbf{p}\neq 0}\sum_{r}\sum_{L=0}^{K-1} \sum_{\substack{\mu_0,\ldots,\mu_L=1,2 \\ \mu_0+\ldots+\mu_L-L-1=\text{even}}} \sum_{\mu_{L+1},\ldots,\mu_{K-1}=0,3} \frac{2^{-L} J^i(\mathbf{n})}{M^{\frac{3}{2}}\sqrt{2\hat{E}_{\mathbf{p}}}}$$

$$\times \left[\mathrm{Re}(\epsilon_i^r(\mathbf{p}))\cos(\mathbf{p}\cdot\mathbf{n}) - \mathrm{Im}(\epsilon_i^r(\mathbf{p}))\sin(\mathbf{p}\cdot\mathbf{n})\right] \mathcal{F}_{\mu_{K-1},\ldots,\mu_{L+1}} \mathcal{G}^S_{\mu_L,\ldots,\mu_0} \sigma^{\mu_{K-1}}_{K-1,\mathbf{p},r}\cdots\sigma^{\mu_{L+1}}_{L+1,\mathbf{p},r}\sigma^{\mu_L}_{L,\mathbf{p},r}\cdots\sigma^{\mu_0}_{0,\mathbf{p},r}$$

$$\hat{H}_I^A = \sum_{\mathbf{n},i}\sum_{\mathbf{p}\neq 0}\sum_{r}\sum_{L=0}^{K-1} \sum_{\substack{\mu_0,\ldots,\mu_L=1,2 \\ \mu_0+\ldots+\mu_L-L-1=\text{odd}}} \sum_{\mu_{L+1},\ldots,\mu_{K-1}=0,3} \frac{2^{-L} J^i(\mathbf{n})}{M^{\frac{3}{2}}\sqrt{2\hat{E}_{\mathbf{p}}}}$$

$$\times \left[\mathrm{Re}(\epsilon_i^r(\mathbf{p}))\sin(\mathbf{p}\cdot\mathbf{n}) + \mathrm{Im}(\epsilon_i^r(\mathbf{p}))\cos(\mathbf{p}\cdot\mathbf{n})\right] \mathcal{F}_{\mu_{K-1},\ldots,\mu_{L+1}} \mathcal{G}^A_{\mu_L,\ldots,\mu_0} \sigma^{\mu_{K-1}}_{K-1,\mathbf{p},r}\cdots\sigma^{\mu_{L+1}}_{L+1,\mathbf{p},r}\sigma^{\mu_L}_{L,\mathbf{p},r}\cdots\sigma^{\mu_0}_{0,\mathbf{p},r}$$

$$\mathcal{F}_{\mu_{K-1},\ldots,\mu_{L+1}} = \sum\nolimits_{\mu_0,\ldots,\mu_L=0,3}(-1)^{\mu_L} f_{\mu_{K-1},\ldots,\mu_0} \qquad f_{\mu_{K-1},\ldots,\mu_0} = \sum_{i_0,\ldots,i_{K-1}=0}^{1} \sqrt{\mathcal{N}(i_{K-1},\ldots,i_0)}(-1)^{i_{K-1}\mu_{K-1}} \times \ldots \times (-1)^{i_0\mu_0}$$

$$\mathcal{G}^S_{\mu_L,\ldots,\mu_0} = (-1)^{\mu_L-1}(-1)^{\left(-L-1+\sum_{J=0}^{L}\mu_J\right)/2} \qquad \mathcal{G}^A_{\mu_L,\ldots,\mu_0} = (-1)^{\mu_L-1}(-1)^{\left(-L-2+\sum_{J=0}^{L}\mu_J\right)/2}$$

Summary

- We proposed quantum algorithms for simulating PDFs, LCDAs, and FFs.
- Based on the LSZ reduction formula, we proposed that the scattering amplitude of $h_1 + h_2 + \cdots + h_{n_{in}} \to h'_1 + h'_2 + \cdots + h'_{n_{out}}$ processes can be obtained by simulating $n_{in} + n_{out}$ point functions on quantum computers.
- We proposed that using Coulomb-gauge-based lattice regularization can overcome the impossible triangle of K-S formalism.

Thank you for listening!