# Quantum Computing for Heavy Quark Fragmentation (QC4HQ)


David Richards - PI

Kostas Orginos and Nobuo Sato - Co-PIs

Zhongbo Kang (UCLA) - Collaborator

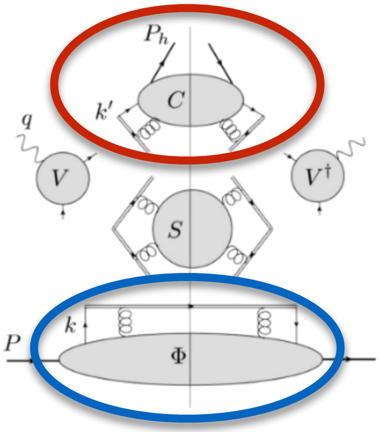
Marco Zaccheddu and Jia-Yue Zhang - Post-doctoral Fellows

# Impact and strategic value to the Laboratory's mission

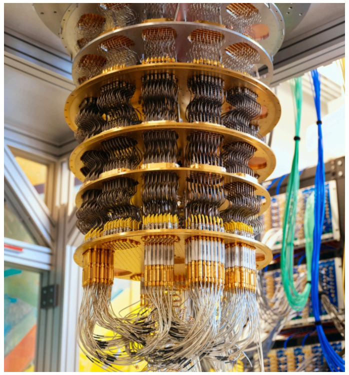
**The Problem:** How do the partons produced in experiment evolve to the final hadron(s) observed in detectors. Encapsulated in the Fragmentation Function (FF).


Parton Distribution functions: **computable on a Euclidean Lattice**

SIDIS@JLab




Fragmentation Functions: inherently time dependent and *inaccessible to a Euclidean lattice.*



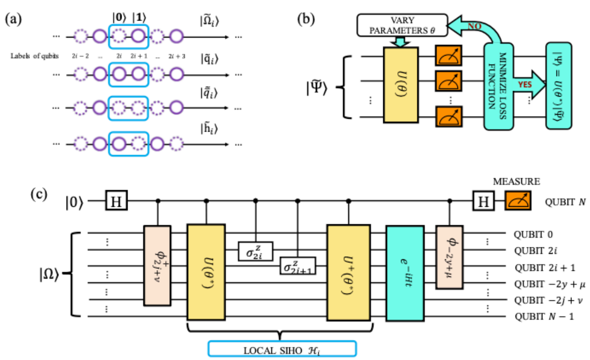
Real-time Lattice computations using a Quantum Computer

- A knowledge of fragmentation advances us to *more complete understanding of QCD*
- FFs are key to the *interpretation of data, in particular in experiments such as SIDIS*
- **Will represent a major addition to our *world-class LQCD Effort* through the study of *real-time evolution***

*Real-time lattice calculations are not part of the NP base funding*

# Level of Innovation

Since submission of LOI, two papers have appeared moving towards addressing fragmentation in 1+1D
- S.Grieninger and I.Zahed, “Quasi-fragmentation functions in the massive Schwinger model”, arXiv:2406.01891
- T.Li et al. (QuNu Collaboration), “Simulating Parton Fragmentation on Quantum Computers”, arXiv:2406.05683




NJL model - *not full field theory*

This proposal is timely

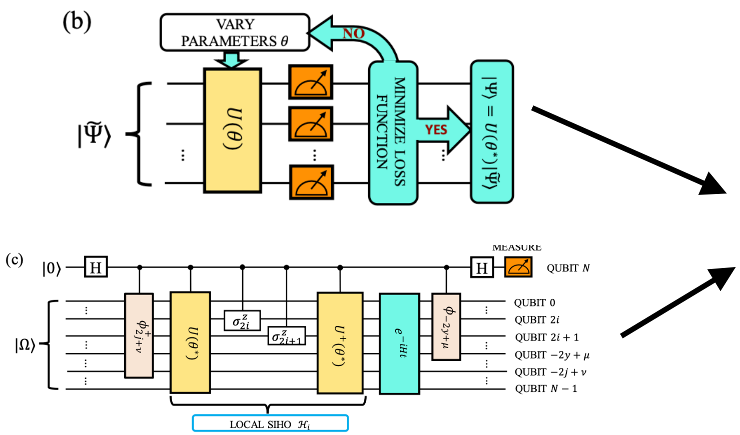
Real-time simulation of a **lattice field theory**

First-principles study of QCD in 3+1 dimensions using QC is currently beyond reach:
Study theory in 1+1 dimension that exhibits some of essential features of QCD:
- Many-body theory, i.e. allows particle creation and annihilation: lattice field theory
- Theory that admits confinement and emergence of bound states

Calculation of heavy-quark fragmentation functions in the Schwinger Model

Reduced size of Hilbert space

# Research Plan and Timeline




4. Calculation of the continuum limit and investigation of scaling/quantum advantage
5. Extension to two non-degenerate quark flavors: threshold effects

| Objective number | Milestone | FY25 | | FY26 | |
|---|---|---|---|---|---|
| | | H1 | H2 | H1 | H2 |
| 1 | Construction of Schwinger Hamiltonian; investigation of other QCD-like models | | | | |
| 2 | State preparation and its implementation in QisKIT | | | | |
| 3 | Construction of a SIHO appropriate to the Schwinger model in 1+1 dimensions | | | | |
| 4 | Investigation of fragmentation in the Schwinger model using Qiskit, and the approach to the continuum limit | | | | |
| 5 | Systematic Study of Fragmentation Functions with one heavy and one light flavor | | | | |

Outcomes

- Papers in high-impact journals
- Presentation at NP and QIS conferences
- Open release of our software

# Budget and Justification

Primarily Personpower:
- Everyone is *in-place for the two years*
- Anticipate working as a team

| Budge t ($K) | Total | FY25 | FY26 | FY27 |
|---|---|---|---|---|
| | 493.4 | 244.4 | 249 | |

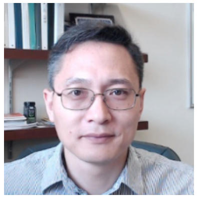
| Team Member | Role | Project Contribution | Specific Aims | Percent |
|---|---|---|---|---|
| David Richards | PI | Lead and coordinate the project | 1-5 | 25 |
| Kostas Orginos | Co-PI | Co-lead the project | 1-5 | 5 |
| Nobuo Sato | Co-PI | Co-lead the project | 1-5 | 5 |
| Marco Zaccheddu | Post-do c | Expertise in TMD factorization and fragmentation | 1-5 | 50 |
| Jia-Yia Zhang | Post-do c | Expertise in Heavy Quark physics | 1-5 | 50 |





As a team, we bring key expertise

- Lattice QCD: David Richards and Kostas Orginos
- Quantum Computing: Nobuo Sato, Kostas Orginos
- Factorization and Heavy-Quark Physics: Nobuo Sato, Marco Zaccheddu, Jia-Yia Zhang, Zhongbo Kang



Travel:
- Zhongbo Kang (UCLA) *essential to project*: budget for collaboration

# Potential for Future Funding (Beyond LDRD)

- Fermions beyond 1+1D
- TMD FFs
- Di-hadron fragmentation functions

NATIONAL QUANTUM COORDINATION OFFICE

A Report of the

National Quantum Initiative Advisory Committee

June 2023

Renewing the National Quantum Initiative: Recommendations for Sustaining American Leadership in Quantum Information Science

**RECOMMENDATION 1: The United States should renew the NQI to support U.S. quantum information science, technology, and engineering, and signal intent to extend the NQI beyond its initial ten-year authorization.**

**RECOMMENDATION 2: The United States should expand the NQI to increase support for fundamental research in quantum information science and engineering.**

The DOE's "QIS Horizons" for advanced research on QIS and NP has in the past funded a project on Parton physics, e.g. J.Vary, "Nuclei and Hadrons with Quantum Computers (NuHaQ)". This focused on a NJL light-front quantization framework.

- This project proposes to study in full a Quantum Field Theory that is more truly representative of QCD
- Therefore would present a strong case for future funding

The Variational Quantum Eigensolver (VQE) that lies at the heart of state preparation is a large-scale computational problem.

- Members of NERSC have expressed interest in the application of high-performance computing (HPC) for quantum computing
  - Opportunity for ASCR support both in terms of facilities and in terms of SciDAC-like projects

**NVIDIA Quantum**

Accelerating the future of scientific discovery.

- VQE is an increasingly large scale variational problem requiring machine learning (ML) methods
  - Development of ML methods for VQE and the development of foundational models for the AI4NP FOA

*Recall QML proposal last year*

# BACKUP

Matrix-element definition of single-hadron fragmentation function

$$D^{h/q}(z) = z \sum_X \int \frac{d\xi^+}{2\pi} e^{ik^-\xi^+}$$
$$\mathrm{Tr}\left[\langle 0|W(\infty^+,\xi^+)\psi_q(\xi^+,0^-,0_T)|P_h;X\rangle\langle P_h;X|\bar{\psi}_q(0^+,0^-,0_T)W(0^+,\infty^+)|0\rangle\gamma^-\right]$$

Sum over undetected particles

Schwinger Model

$$\mathcal{L} = -\frac{1}{4g^2}F_{\mu\nu}F^{\mu\nu} + \bar{\psi}(i\gamma^\mu D_\mu - m)\psi; \quad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$$