

Time-dependent Basis Function on Qubits (tBFq) algorithm (Hamiltonian simulation)

- Unified structure and reaction theory
- Based on successful *Ab initio* nuclear structure theory
- Non-perturbative scattering method
- Retaining full quantal coherence & entanglement
- Circumventing the exponential cost in computation resource in simulating real-time many-body dynamics

Theoretical scattering method (tBF) introduced and solved on classical computers:

W. Du, P. Yin, Y. Li, G. Chen, W. Zuo, X. Zhao and J.P. Vary, “Coulomb Excitation of Deuteron In Peripheral Collisions with a Heavy Ion,” Phys. Rev. C 97, 064620 (2018); arXiv: 1804.01156

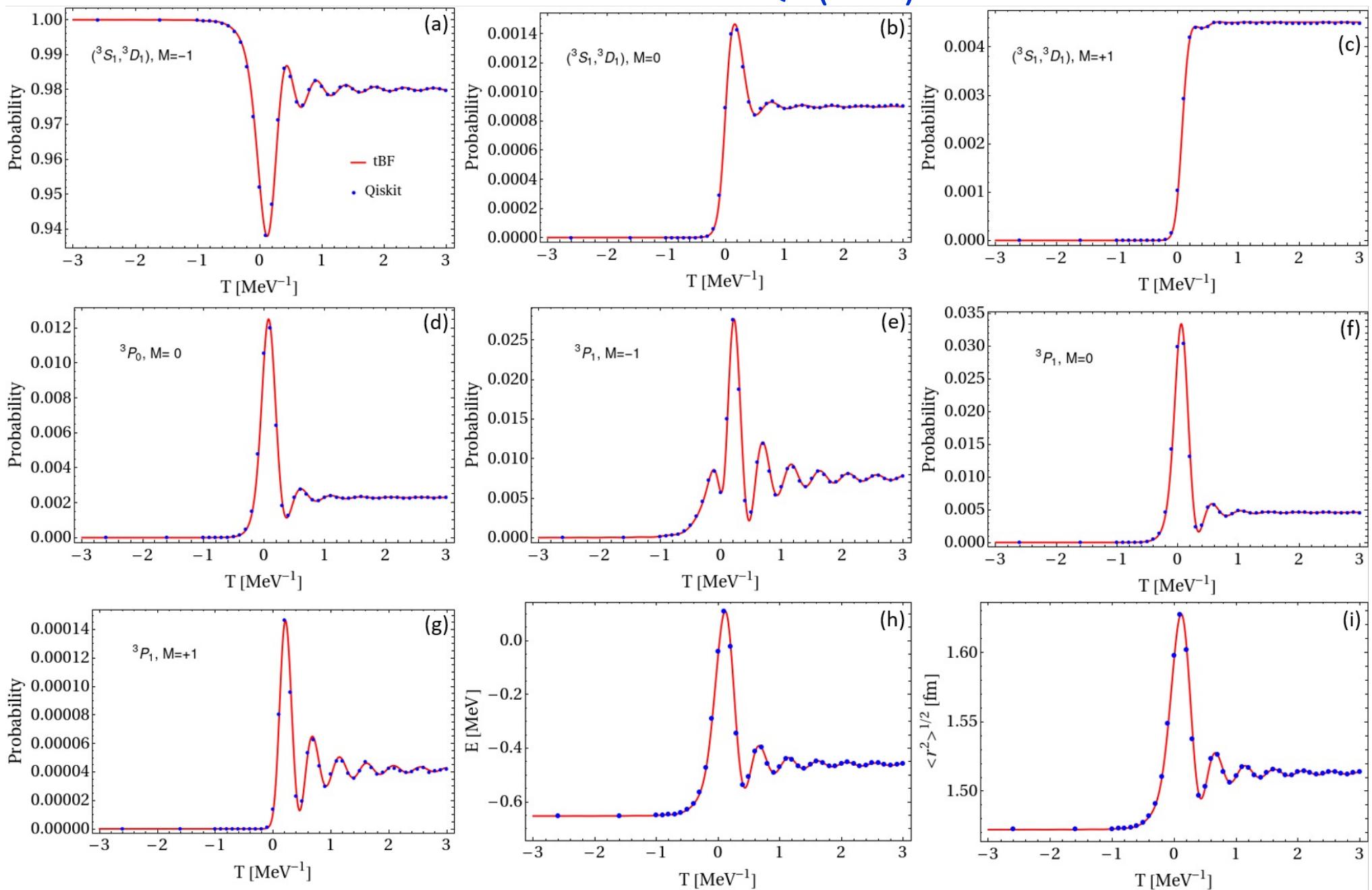
tBF solved for deuteron inelastic scattering by simulation of a quantum computer:

W. Du, J.P. Vary, X. Zhao and W. Zuo, “Quantum Simulation of Nuclear Inelastic Scattering,” Phys. Rev. A 104, 012611 (2021); arXiv: 2006.01369

tBF provides a parameter-free deuteron elastic scattering cross sections on classical computers:

P. Yin, W. Du, W. Zuo, X. Zhao and J.P. Vary, “Sub-Coulomb barrier d+208Pb scattering in a Time-dependent basis function approach,” J. Phys. G. 2022 (in press); arXiv: 1910.10586

Transition probabilities for Coulomb excitation of deuteron by ^{208}Pb on a simulated QC (dots)



Ab initio nuclear structure on quantum computer

Problem: **exponential scaling** in computing resources of quantum many-body problems

Goal: quantum algorithm for the structure and dynamics of the many-nucleon systems

Focus: to develop **input model** for the second-quantized many-nucleon Hamiltonian

Hamiltonian:
$$H = \sum_{p < q, r < s} \langle pq | H | rs \rangle a_p^\dagger a_q^\dagger a_s a_r \quad H_{pqrs} = T_{pqrs}^{\text{rel}} + V_{pqrs}^{\text{NN}} + H_{pqrs}^{\text{CM}}$$

Direct encoding scheme: one-on-one mapping between single-nucleon bases and qubits

	qubit index	0	1	2	3	4	5	6	7	8	9	10	11
neutron state	occupancy	1	0	0	0	1	0	0	0	0	0	0	0
	qubit index	12	13	14	15	16	17	18	19	20	21	22	23
proton state	occupancy	0	1	0	0	0	0	1	0	0	0	0	0

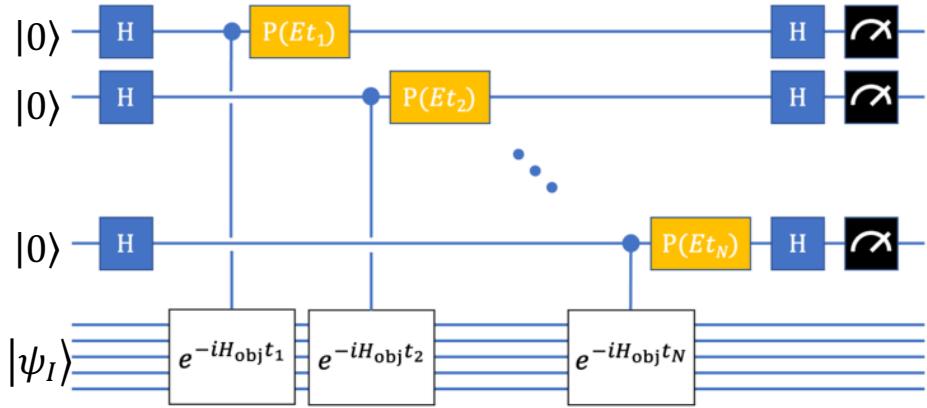
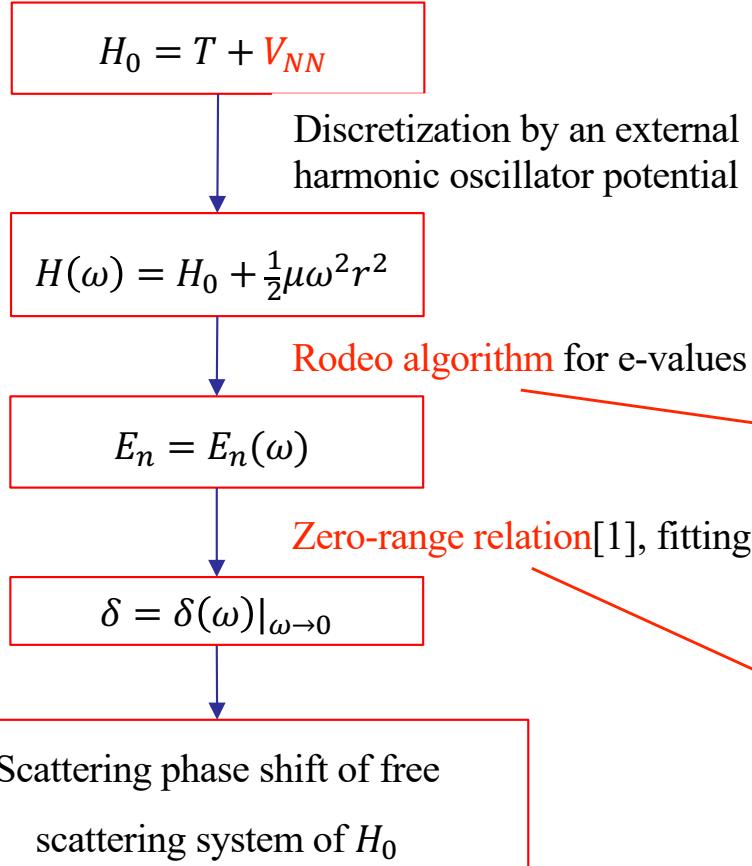
Fock state **encoded as** binary string
 $|0,4,13,18\rangle$
 $\rightarrow 100010000000\ 010000100000$

Hamiltonian input model: to construct the isometry \mathcal{T} via oracle queries

$$\begin{aligned}\mathcal{T}|\mathcal{F}\rangle|b\rangle &= |\mathcal{F}\rangle|b\rangle|\phi_{\mathcal{F},b}\rangle \\ \mathcal{T}^\dagger S \mathcal{T}|\lambda_j\rangle|0\rangle &= \left[\frac{\epsilon}{\|H\|_1} H \otimes |0\rangle\langle 0| + |0\rangle\langle 0| \otimes |1\rangle\langle 1| \right] |\lambda_j\rangle|0\rangle = \tilde{\lambda}_j |\lambda_j\rangle|0\rangle\end{aligned}$$

[Berry and Childs, Quantum Inf. Comput. 12, 29 (2012)]

Eigenvalues and phase shifts via Rodeo algorithm



The probability of the measurement 0 for m-th state:

$$P(|0\rangle, |\phi_m\rangle) = \frac{1}{4}|c_m|^2 \left| 1 + e^{i(E-E_m)t_1} \right|^2 = |c_m|^2 \left| \cos\left(\frac{E-E_m}{2}t_1\right) \right|^2$$

$$p^{2l+1} \cot \delta_l(p) = (-1)^{l+1} (2\mu\omega)^{l+\frac{1}{2}} \frac{\Gamma(\frac{2l+3}{4} - \frac{\varepsilon}{2})}{\Gamma(\frac{1-2l}{4} - \frac{\varepsilon}{2})}, \varepsilon = \frac{E}{\omega}, p = \sqrt{\mu E}$$

Demonstration problem: NN scattering phase shifts

Demonstration problem:

1. V_{NN} as spherical well potential:

$$V_{NN} = \begin{cases} -V_0, & x \leq R_0 \\ 0, & x > R_0 \end{cases}$$

$$V_0 = 48.0002 \text{ MeV}, R_0 = 1.70134 \text{ fm.}$$

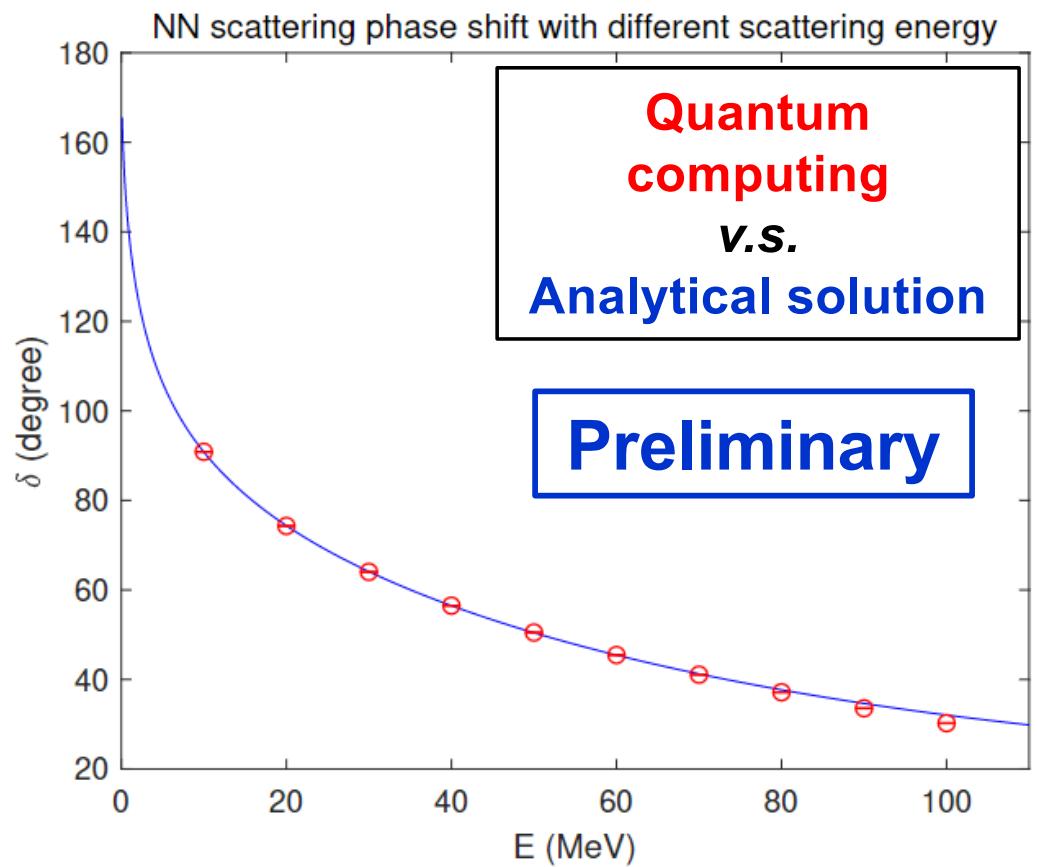
2. 3DHO basis:

$$\omega = 60 \text{ MeV}, N_{max} = 600.$$

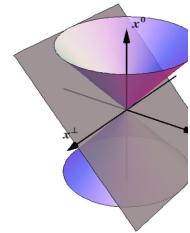
3. Analytical solution:

$$\delta = \arctan \left[\frac{k}{p} \tan(pR_0) \right] - kR_0 + n\pi$$

$$k = \sqrt{2\mu E}, p = \sqrt{2\mu(E + V_0)}.$$



[Peiyan Wang, Weijie Du et al., in preparation]



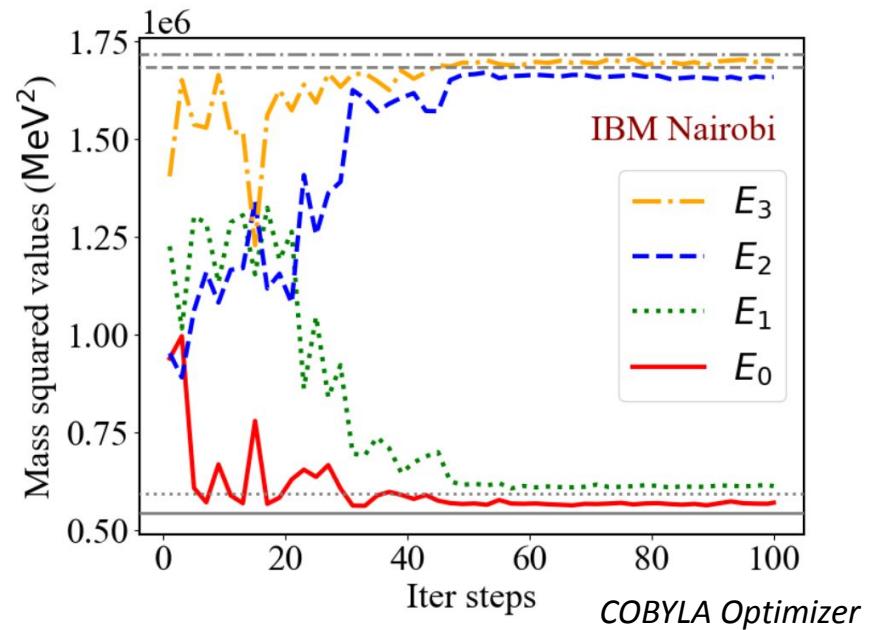
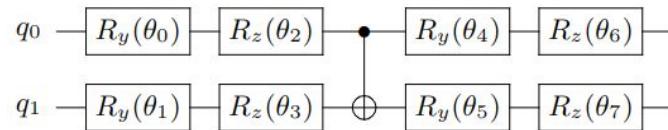
SSVQE Application to BLFQ

The SSVQE approach can be naturally applied to BLFQ hadron structure calculations, where we look at problem Hamiltonian of reduced basis representation. For example, the smallest non-trivial Hamiltonian of BLFQ light meson system:

$$\begin{aligned} H_{\text{direct}}^{(1,1)} = & 2269462 \text{ IIII} - 284243 (\text{ZIII} + \text{IIIZ}) \\ & - 850488 (\text{IZII} + \text{III}Z) \\ & + 12714 (\text{XZXI} + \text{YZYI}) \\ & - 7883 (\text{IXZX} + \text{IYZY}), \end{aligned}$$

$$\begin{aligned} H_{\text{compact}}^{(1,1)} = & 1134731 \text{ II} - 566245 \text{ IZ} \\ & + 4831 \text{ XI} + 20598 \text{ XZ}, \end{aligned}$$

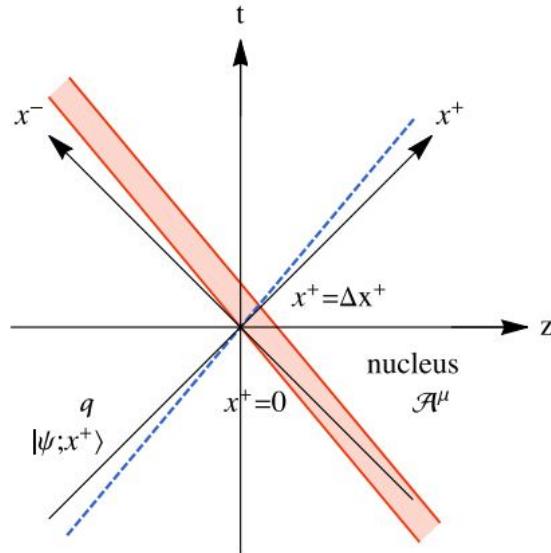
In particular, we use **compact encoding**, orthogonal basis formed by Pauli strings under trace, and **hardware-efficient heuristic ansatz**, to represent the Hamiltonian economically on quantum circuit.



Medium induced jet broadening in a quantum computer

Barata, Salgado, 2104.04661 (2021)
 Barata, Du, Li, Salgado, Qian (2022, TBA)

High-energy quark moving close to the light cone scattering on a dense nucleus medium

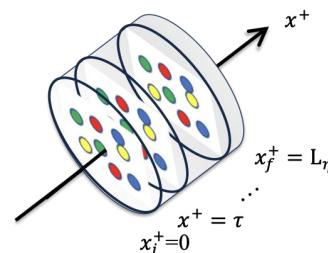


M. Li, Zhao, Maris, Chen, Y. Li, Tuchin, Vary, 2002.09757 (2020)

The light-front Hamiltonian consists of kinetic and potential term:

$$P^-(x^+) = P_{\text{KE}}^- + V_A(x^+) = \frac{p_\perp^2}{p^+} + g A(x^+) \cdot T$$

The stochastic background field uses the McLerran-Venugopalan (MV) model



$$(m_g^2 - \nabla_\perp^2) A_a^-(x^+, \mathbf{x}) = \rho_a(x^+, \mathbf{x})$$

$$\langle\langle \rho_a(x^+, \mathbf{x}) \rho_b(y^+, \mathbf{y}) \rangle\rangle$$

$$= g^2 \mu^2(\mathbf{x}) \delta_{ab} \delta^2(\mathbf{x} - \mathbf{y}) \delta(x^+ - y^+)$$

Time evolution of the probe:

$$|\psi_{L_\eta}\rangle = U(L_\eta; 0) |\psi_0\rangle$$

$$\equiv \mathcal{T}_+ e^{-i \int_0^{L_\eta} dx^+ P^-(x^+)} |\psi_0\rangle$$

$$U(L_\eta; 0) = \prod_{k=1}^{N_t} U(x_k^+; x_{k-1}^+)$$

Key QC papers/projects of our group in collaboration with other groups

Michael Kreshchuk, Shaoyang Jia, William M. Kirby, Gary Goldstein, James P. Vary and Peter J. Love,
“Simulating Hadronic Physics on NISQ devices using Basis Light-Front Quantization,”
Phys. Rev. A 103, 062601 (2021); arXiv: 2011.13443

Michael Kreshchuk, Shaoyang Jia, William M. Kirby, Gary Goldstein, James P. Vary and Peter J. Love,
“Light-Front Field Theory on Current Quantum Computers,”
Entropy 23, 597 (2021); Special Issue NISQ Technologies; arXiv: 2009.07885

Weijie Du, James P. Vary, Xingbo Zhao and Wei Zuo,
“Quantum Simulation of Nuclear Inelastic Scattering”,
Phys. Rev. A 104, 012611 (2021); arXiv: 2006.01369

Robert A.M. Basili, Wenyang Qian, Shuo Tang, Austin Castellino, Mary Eshaghian-Wilner, Ashfaq Khokhar,
Glenn Luecke and James P. Vary,
“Performance Evaluations of Noisy Approximate Quantum Fourier Arithmetic,”
2022 IPDPSW Proceedings p. 435-444; doi: 10.1109/IPDPSW55747.2022.00081; arXiv: 2112.09349

J. Barata, X. Du, M. Li, W. Qian and C. Salgado, “Medium induced jet broadening in a quantum computer,”
Phys. Rev. D 106, 074013 (2022).

Wenyang Qian, Robert Basili, Soham Pal, Glenn Luecke and James P. Vary,
“Quantum Computing for Hadron Structures,” Phys. Rev. Research (accepted); arXiv: 2112.01927

Weijie Du, James P. Vary, Xingbo Zhao and Wei Zuo,
“Ab initio nuclear structure via quantum adiabatic algorithm,” arXiv: 2105.08910

Weijie Du, et al., “An initio nuclear scattering phase shifts with quantum computers,” in preparation

Quantum Computing – Issues & Challenges

- Discovering the best QC algorithm: a research project in its own right
- New/improved QC algorithms emerging for Nuclear Structure, Reactions & Dynamics
- Need improved noise mitigation strategies for NISQ era and beyond
- Anticipating industry developments - # qubits, gate suites, topologies (“volume”)
- Trained workforce considerations: career path, sustainability
- Sharing experiences: improving exchanges with private sector

Funding Sources

DOE NP Division

DOE NP/ASCR Divisions (SciDAC/UNEDF SciDAC/NUCLEI)

DOE ASCR Division INCITE Awards on Leadership Class Supercomputers

DOE ASCR Division NERSC Annual Awards