BERKELEY LAB
Bringing Science Solutions to the World

U.S. DEPARTMENT OF ENERGY
Office of Science

Quantum simulation: Cracking the exponential wall

Michael Kreshchuk, LBNL

September 23, 2022

Tufts University

Argonne NATIONAL LABORATORY

BROOKHAVEN NATIONAL LABORATORY

IOWA STATE UNIVERSITY

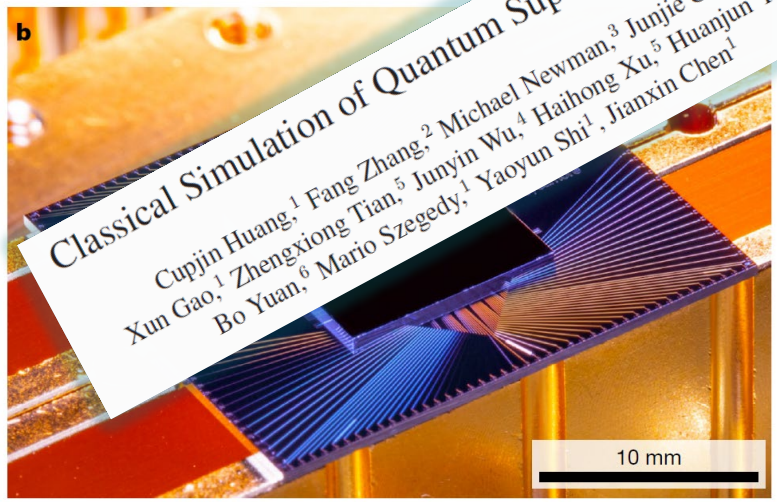
Quantum Computers: the era of rapid progress

Article

Quantum supremacy using a pr… able superconducting processo…

Classical Simulation of Quantum Supremacy Circuits

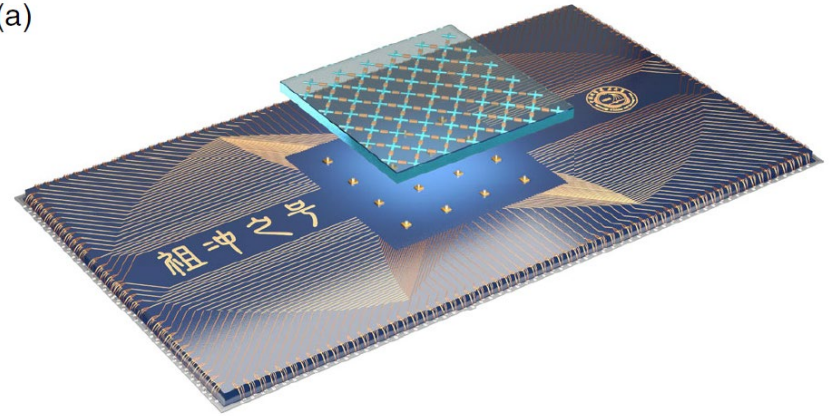
Cupjin Huang,[1] Fang Zhang,[2] Michael Newman,[3] Junjie Cai,[4] Xun Gao,[1] Zhengxiong Tian,[5] Junyin Wu,[4] Haihong Xu,[5] Huanjun Yu,[5] Bo Yuan,[6] Mario Szegedy,[1] Yaoyun Shi[1], Jianxin Chen[1]



Strong Quantum Computational Advantage Using a Superconducting Quantum Processor

Yulin Wu,[1,2,3] Wan-Su Bao,[4] Sirui Cao,[1,2,3] Fusheng Chen,[1,2,3] Ming-Cheng Chen,[1,2,3] Xiawei Chen,[2] Tung-Hsun Chung,[1,2,3] Hui Deng,[1,2,3] Yajie Du,[2] Daojin Fan,[1,2,3] Ming Gong,[1,2,3] Cheng Guo,[1,2,3] Chu Guo,[1,2,3] Shaojun Guo,[1,2,3] Lianchen Han,[1,2,3] Linyin Hong,[5] He-Liang Huang,[1,2,3,4] Yong-Heng Huo,[1,2,3] Liping Li,[2] Na Li,[1,2,3] Shaowei Li,[1,2,3] Yuan Li,[1,2,3] Futian Liang,[1,2,3] Chun Lin,[6] Jin Lin,[1,2,3] Haoran Qian,[1,2,3] Dan Qiao,[2] Hao Rong,[1,2,3] Hong Su,[1,2,3] Lihua Sun,[1,2,3] Liangyuan Wang,[2] Shiyu Wang,[1,2,3] Dachao Wu,[1,2,3] Yu Xu,[1,2,3] Kai Yan,[2] Weifeng Yang,[5] Yang Yang,[2] Yangsen Ye,[1,2,3] Jianghan Yin,[2] Chong Ying,[1,2,3] Jiale Yu,[1,2,3] Chen Zha,[1,2,3] Cha Zhang,[1,2,3] Haibin Zhang,[2] Kaili Zhang,[1,2,3] Yiming Zhang,[1,2,3] Han Zhao,[2] Youwei Zhao,[1,2,3] Liang Zhou,[5] Qingling Zhu,[1,2,3] Chao-Yang Lu,[1,2,3] Cheng-Zhi Peng,[1,2,3] Xiaobo Zhu,[1,2,3] and Jian-Wei Pan[1,2,3]

(a)



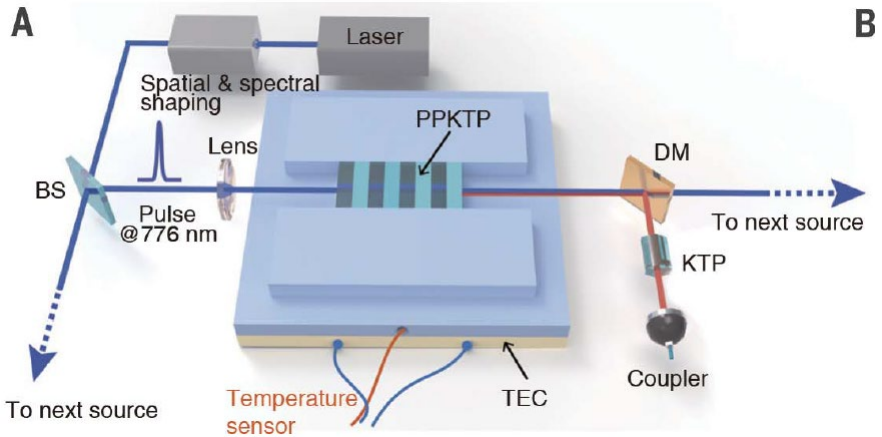
- ✓ Prototypes
- ✓ Supremacy
- ✗ Advantage
- ✓ “Quantum” > “Nano”

Quantum Computers: why care?

QUANTUM COMPUTING

Quantum computational advantage using photons

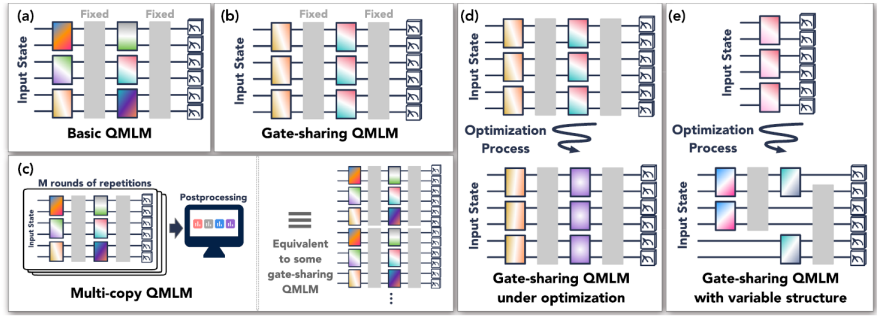
Han-Sen Zhong[1,2]*, Hui Wang[1,2]*, Yu-Hao Deng[1,2]*, Ming-Cheng Chen[1,2]*, Li-Chao Peng[1,2], Yi-Han Luo[1,2], Jian Qin[1,2], Dian Wu[1,2], Xing Ding[1,2], Yi Hu[1,2], Peng Hu[3], Xiao-Yan Yang[3], Wei-Jun Zhang[3], Hao Li[3], Yuxuan Li[4], Xiao Jiang[1,2], Lin Gan[4], Guangwen Yang[4], Lixing You[3], Zhen Wang[3], Li Li[1,2], Nai-Le Liu[1,2], Chao-Yang Lu[1,2]†, Jian-Wei Pan[1,2]†



Generalization in quantum machine learning from few training data

Received: 12 April 2022
Accepted: 4 August 2022

Matthias C. Caro[1,2], Hsin-Yuan Huang[3,4], M. Cerezo[5,6], Kunal Sharma[7], Andrew Sornborger[5,8], Lukasz Cincio[9] & Patrick J. Coles[9]

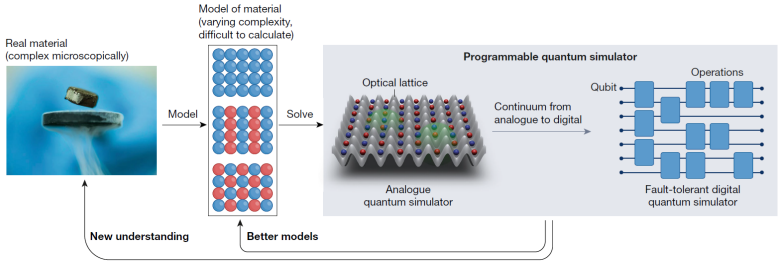


Perspective

Practical quantum advantage in quantum simulation

https://doi.org/10.1038/s41586-022-04940-6
Received: 1 July 2021
Accepted: 7 June 2022

Andrew J. Daley[1], Immanuel Bloch[2,3,4], Christian Kokail[5,6], Stuart Flannigan[1], Natalie Pearson[1], Matthias Troyer[7] & Peter Zoller[5,6]



Quantum Computers and Quantum Computation

Quantum Computer:
A highly controllable quantum system, which naturally stores superpositions of quantum states.

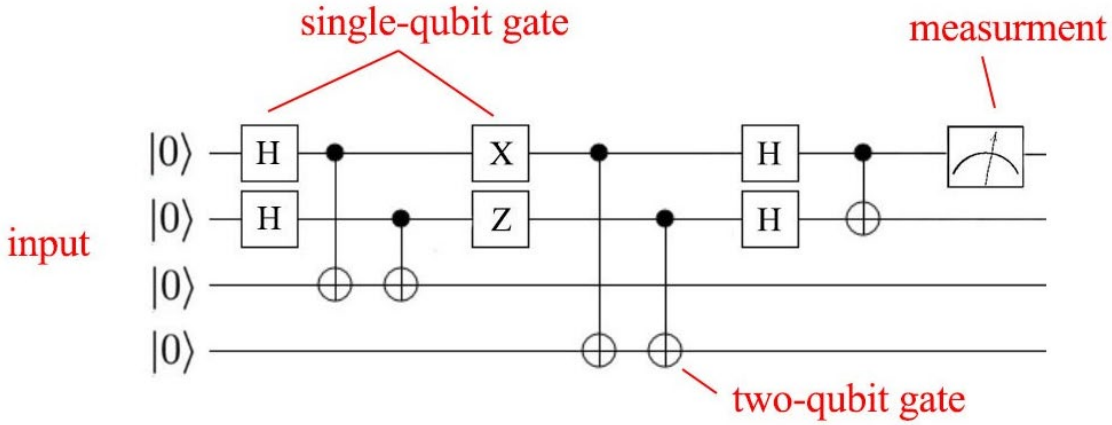
Basic example:

$$|\Psi_{\text{phys}}\rangle = \alpha|\uparrow\uparrow\downarrow\uparrow\downarrow\cdots\rangle + \beta|\uparrow\downarrow\downarrow\uparrow\uparrow\cdots\rangle + \cdots$$
$$|\Psi_{\text{qubit}}\rangle = \alpha|11010\ldots\rangle + \beta|10011\ldots\rangle + \cdots$$

$|\Psi_{\text{phys}}\rangle$ — state of a spin chain, state of a molecule in the second-quantized formalism, ect.

$|\Psi_{\text{qubit}}\rangle$ — state in the quantum computer.

Depending on hardware, one can implement 1-, 2-, or many-qubit gates, which are used to manipulate $|\Psi_{\text{qubit}}\rangle$ with local or non-local elementary operations.



Efficient quantum simulation:

- N physical DOFs $\mapsto \lesssim \mathrm{poly}(\mathrm{N})$ qubits.
- Number of gates $\lesssim \mathrm{poly}(\mathrm{N}, \mathrm{t}, \epsilon)$.
- Number of circuit runs $\lesssim \mathrm{poly}(\mathrm{N}, \mathrm{t}, \epsilon)$.

Quantum Simulation: recap

Preliminary steps, which determine the type of quantum simulation:

- Choice the physical system.
- Choice of observables : Spectroscopy? Real-time dynamics? Thermalization?
- Choice of the physical model: Ab initio? Effective?
- Discretizing the model: Spatial coordinates? Field variables? Gauge DOFs?

Intermediate step:

- Mapping physical DOFs onto qubits: various ways of encoding fermions and bosons in the QC.

Quantum simulation!

Quantum Simulation of LF QFT

For several reasons LF QFT is highly appealing as starting point for quantum simulation:

LF QFT Features	Advantages for Quantum Simulation
Linear EoM → few DOFs	Lower qubit count*
LF momentum > 0 → few DOFs are occupied	Lower qubit count**
Efficient basis choice → early truncation	Lower qubit count
Observables are easy to extract from the LFWF	Measurements are easy to design
Trivial vacuum	Good initial state is readily available,
Valence sector calculations give good results	and this state is easy to prepare

A number of complications exist as well:

LF QFT Features	Issues / open questions for Quantum Simulation
Bases with non-local interactions are typically used	# of Hamiltonian terms increases; non-local gates
The renormalized many-body formulations of $3+1D$ gauge theories are under development	Starting point not defined yet. QCs are likely to only be useful for simulating many-body problems
HEP scattering applications are under development	Harder to advertise

Quantum Simulation of LF QFT: why many-body

Quantum Simulation is likely to only become useful if the full many-body setting is considered:

	# of single-particle states ("modes")	# of occupied states	Hilbert space dimension	Sparse	# of qubits	# gates
Valence	$N = K\Lambda_\perp^2$	$\sim 2,3,\ldots$	$\binom{N}{2,3} = \mathrm{poly}(N)$	X	$\sim N$ or $\sim K$	$\mathrm{poly}(N)$
Full		$\sim K$	$\exp(N)$	✓	$\sim N$ or $\sim K$	$\mathrm{poly}(N)$

In fact, limiting the calculation to sectors of a fixed number of particles on a QC comes with an additional cost — many-body simulation is a natural application of QCs.

LF many-body formulations	Comments
Sector-dependent renormalization	Hard to adopt to QC, as modes in all states are treated uniformly
Pauli-Villars	Quantum Simulation of non-Hermitian Hamiltonians is in its infancy
RGPEP	$a_t = U_s a U_s^\dagger$ may be naturally implemented on a QC

Quantum Simulation of LF QFT: compact encoding

Consider DLCQ in $3+1D$. While $N = K\Lambda_\perp^2$, the number of occupied modes in a Fock state $\sim K$.

$$\left|n_1^{m_1}, n_2^{m_2}, \ldots, n_N^{m_N}\right\rangle$$

Since $n_j > 0$ and $\sum_j n_j m_j = K$, at most K occupancies can be nonzero.

In the *direct encoding* schemes, one uses $\sim N = K\Lambda_\perp^2$ qubits to **store occupancies of all modes**:

$$\underbrace{\underbrace{0101010101010101011010101\ldots}_{\text{Fermions — one qubit per mode}}\underbrace{1110\ldots}\underbrace{0011\ldots}\underbrace{1010\ldots}\underbrace{0100\ldots}\underbrace{0001\ldots}\ \ldots}_{\text{Bosons — several qubits per mode}}$$
$$K\Lambda_\perp^2 \text{ modes total}$$

In the *compact encoding* scheme, ones uses $\sim K\log(K+\Lambda_\perp)$ qubits to **store momenta and occupancies of occupied modes only**:

$$\underbrace{\underbrace{110110\ldots}_{n_1}\underbrace{00110\ldots}_{m_1}}_{1^{st}\text{ occupied mode}}\underbrace{\underbrace{110110\ldots}_{n_2}\underbrace{00110\ldots}_{m_2}}_{2^{nd}\text{ occupied mode}}\ldots$$
$$K \text{ occupied modes}$$

Quantum Simulation of LF QFT: price for non-locality

The position representation is unique in the sense that it preserves locality of operators:

$$H = \sum_{\mathbf{x}\in\Omega} a^d \left[\frac{1}{2}\pi(\mathbf{x})^2 + \frac{1}{2}\left(\nabla_a \phi\right)^2(\mathbf{x}) + \frac{1}{2}m_0^2\phi(\mathbf{x})^2 + \frac{\lambda_0}{4!}\phi(\mathbf{x})^4 \right]$$

$$\left(\nabla_a \phi\right)^2(\mathbf{x}) = \sum_{j=1}^{d} \left(\frac{\phi(\mathbf{x} + a\hat{r}_j) - \phi(\mathbf{x})}{a} \right)^2$$

Each term in the Hamiltonian is represented by a constant number of elementary operators, therefore the total **number of terms is proportional to the lattice size N.**

However, switching to any other basis, such as

$$\phi(\mathbf{x}) \quad = \quad \sum_{\mathbf{p}\in\Gamma} \frac{1}{L^d} e^{i\mathbf{p}\cdot\mathbf{x}} \sqrt{\frac{1}{2\omega(\mathbf{p})}} \left(a_{\mathbf{p}} + a^{\dagger}_{-\mathbf{p}} \right)$$

immediately increases the number of terms to N^3 (momentum basis) or N^4 (other bases), and also requires one to do a lot of non-local quantum operations.

Quantum Simulation of LF QFT: initial state

Knowledge of a state having $1/\mathrm{poly}(N)$ overlap with the true GS would be a huge advantage!

Note that Theorem 8 does not require the knowledge of the energy gap!

Since the valence sector Hilbert space has dimension polynomial in the problem size, even the basis vector with largest amplitude would suffice as an initial state for an efficient quantum GS preparation algorithm.

Near-optimal ground state preparation

Lin Lin[1,2] and Yu Tong[1]

3 Algorithm with *a priori* ground energy bound

With the approximate projector developed in the previous section we can readily design an algorithm to prepare the ground state. We assume we have the Hamiltonian H given through its block-encoding as in the last section. If we are further given an initial state $|\phi_0\rangle$ prepared by a unitary U_I, i.e. $U_I|0^n\rangle = |\phi_0\rangle$, and the promises that for some known $\gamma > 0$, μ, and Δ, we have

(P1) Lower bound for the overlap: $|\langle\phi_0|\psi_0\rangle| \geq \gamma$,

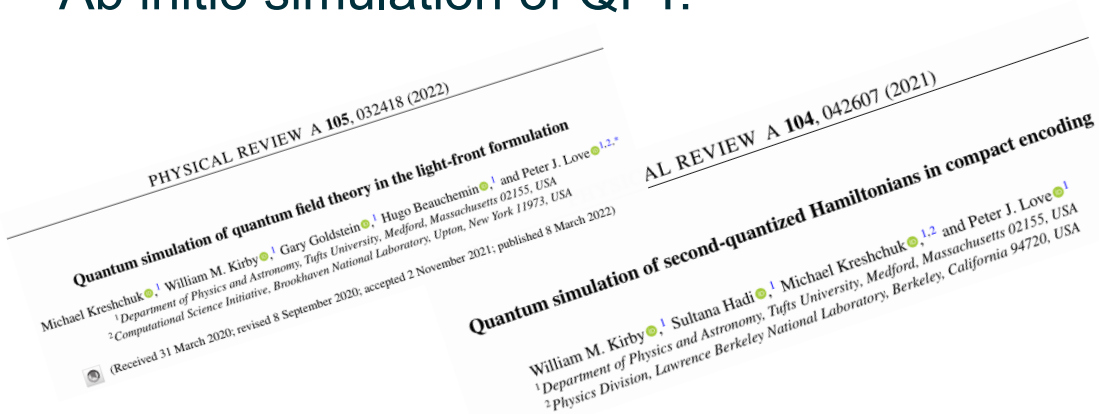
~~(P2) Bounds for the ground energy and spectral gap: $\lambda_0 \leq \mu - \Delta/2 < \mu + \Delta/2 \leq \lambda_1$.~~

Theorem 8 (Ground energy). *Suppose we have Hamiltonian $H = \sum_k \lambda_k |\psi_k\rangle\langle\psi_k| \in \mathbb{C}^{N\times N}$, where $\lambda_k \leq \lambda_{k+1}$, given through its $(\alpha, m, 0)$-block-encoding U_H. Also suppose we have an initial state $|\phi_0\rangle$ prepared by circuit U_I, as well as the promise (P1). Then the ground energy can be estimated to precision h with probability $1-\vartheta$ with the following costs:*

1. *Query complexity:* $\mathcal{O}\left(\frac{\alpha}{\gamma h}\log\left(\frac{\alpha}{h}\right)\log\left(\frac{1}{\gamma}\right)\log\left(\frac{\log(\alpha/h)}{\vartheta}\right)\right)$ *queries to* U_H *and* $\mathcal{O}\left(\frac{1}{\gamma}\log\left(\frac{\alpha}{h}\right)\log\left(\frac{\log(\alpha/h)}{\vartheta}\right)\right)$ *queries to* U_I,
2. *Number of qubits:* $\mathcal{O}(n+m+\log(\frac{1}{\gamma}))$,
3. *Other one- and two- qubit gates:* $\mathcal{O}\left(\frac{m\alpha}{\gamma h}\log\left(\frac{\alpha}{h}\right)\log\left(\frac{1}{\gamma}\right)\log\left(\frac{\log(\alpha/h)}{\vartheta}\right)\right)$.

Quantum Simulation of LF QFT: Developments

- Ab initio simulation of QFT:


PHYSICAL REVIEW A **105**, 032418 (2022)

Quantum simulation of quantum field theory in the light-front formulation

Michael Kreshchuk, William M. Kirby, Gary Goldstein, Hugo Beauchemin, and Peter J. Love

[1]Department of Physics and Astronomy, Tufts University, Medford, Massachusetts 02155, USA
[2]Computational Science Initiative, Brookhaven National Laboratory, Upton, New York 11973, USA

(Received 31 March 2020; revised 8 September 2020; accepted 2 November 2021; published 8 March 2022)

AL REVIEW A **104**, 042607 (2021)

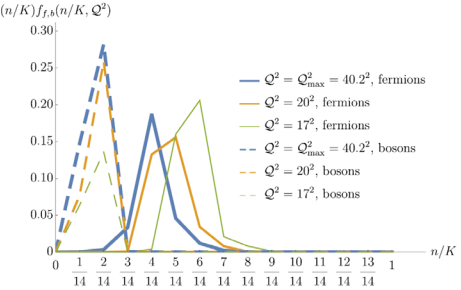
Quantum simulation of second-quantized Hamiltonians in compact encoding

William M. Kirby, Sultana Hadi, Michael Kreshchuk, and Peter J. Love

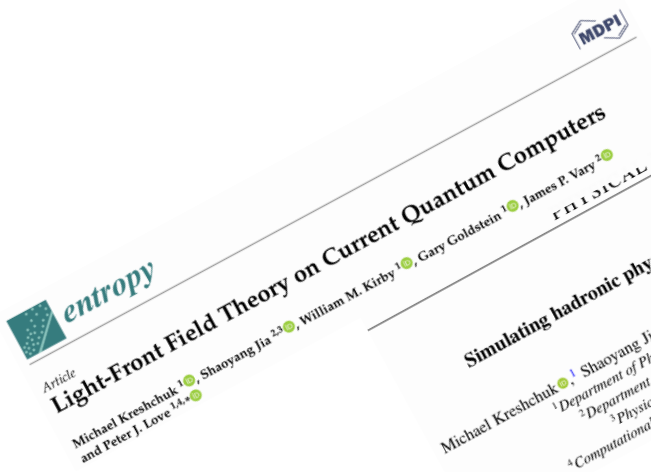
[1]Department of Physics and Astronomy, Tufts University, Medford, Massachusetts 02155, USA
[2]Physics Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

$$Q \leq \overbrace{2K}^{\text{number of occupied fermion/antifermion modes}} \overbrace{\left[\underbrace{\lceil \log_2 K \rceil + 2\lceil \log_2 \Lambda_\perp \rceil}_{\text{momentum}} + \underbrace{1}_{\text{helicity}} + \underbrace{\lceil \log_2 n_f \rceil}_{\text{flavors}} + \underbrace{\lceil \log_2 n_c \rceil}_{\text{colors}}\right]}^{\text{fermion/antifermion modes}}$$

$$+ \overbrace{\underbrace{K}_{\text{number of occupied boson modes}} \left[\underbrace{\lceil \log_2 K \rceil + 2\lceil \log_2 \Lambda_\perp \rceil}_{\text{momentum}} + \underbrace{\lceil \log_2 K \rceil}_{\text{occupancy}} + \underbrace{1}_{\text{helicity}} + \underbrace{\lceil \log_2 (n_c^2 - 1) \rceil}_{\text{colors}}\right]}^{\text{boson modes}}$$



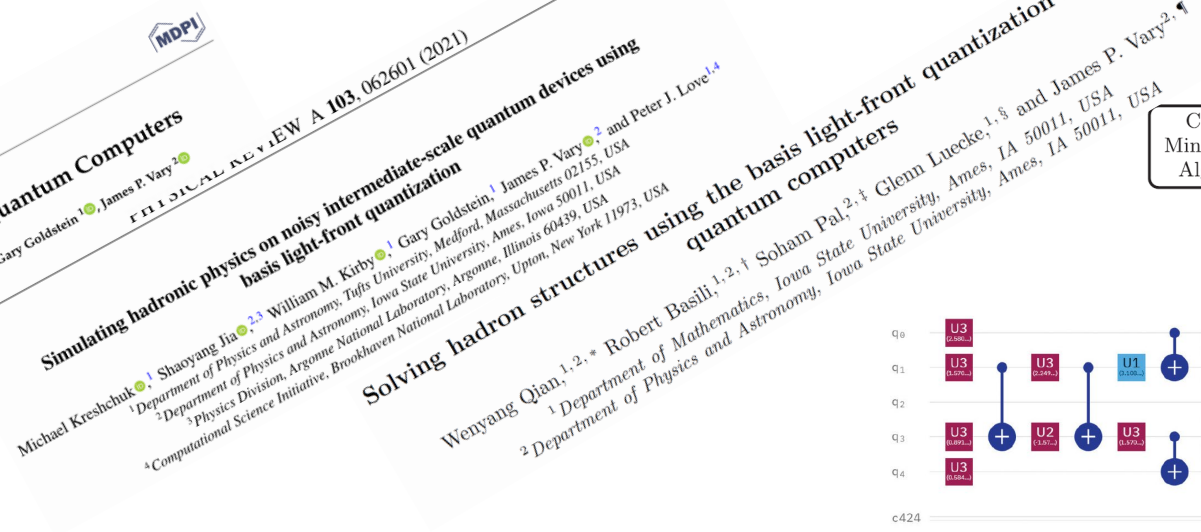
- Effective field theories, benchmarking existing QCs:


entropy

Article

Light-Front Field Theory on Current Quantum Computers

Michael Kreshchuk, Shaoyang Jia, William M. Kirby, Gary Goldstein, James P. Vary and Peter J. Love


MDPI

PHYSICAL REVIEW A **103**, 062601 (2021)

Simulating hadronic physics on noisy intermediate-scale quantum devices using basis light-front quantization

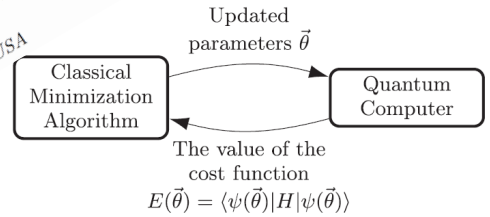
Michael Kreshchuk, Shaoyang Jia, William M. Kirby, Gary Goldstein, James P. Vary, and Peter J. Love

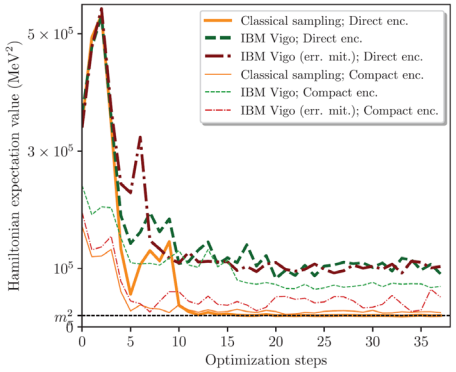
[1]Department of Physics and Astronomy, Tufts University, Medford, Massachusetts 02155, USA
[2]Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA
[3]Physics Division, Argonne National Laboratory, Argonne, Illinois 60439, USA
[4]Computational Science Initiative, Brookhaven National Laboratory, Upton, New York 11973, USA

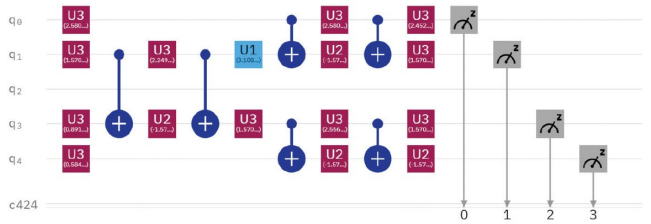
Solving hadron structures using the basis light-front quantization approach on quantum computers

Wenyang Qian, Robert Basili, Soham Pal, Glenn Luecke, and James P. Vary

[1]Department of Mathematics, Iowa State University, Ames, IA 50011, USA
[2]Department of Physics and Astronomy, Iowa State University, Ames, IA 50011, USA







Quantum Simulation of LF QFT: Ongoing Work

How does one simulate scattering events within the LF framework?

- Light-heavy particle scattering / scattering in strong background fields: tBLFQ.

$$P^-_{QCD}\,|\beta\rangle = P^-_{\beta}\,|\beta\rangle \qquad |\psi; x^+\rangle_I = \sum_{\beta} c_\beta(x^+)\,|\beta\rangle \qquad i\frac{\partial}{\partial x^+}\,|\psi; x^+\rangle_I = \frac{1}{2}V_I(x^+)\,|\psi; x^+\rangle_I$$

  Similar idea, but in application to nuclear physics:

Quantum simulation of nuclear inelastic scattering

Weijie Du,[1,2,3,*] James P. Vary,[2] Xingbo Zhao,[1,3] and Wei Zuo[1,3]

- What about the HEP scattering of particles of comparable sizes?

  Conventional approach in quantum simulation: represent particles by wave packets.

  Can we instead use the fact that within the LF formalism we actually use the most fundamental definition of a particle in QFT — the eigenstate of H_{full}?

Quantum Simulation of LF QFT: Eigenstate-based scattering

- Inspiration #0, free theory:

$$|p_1, p_2\rangle = a^\dagger_{p_1} a^\dagger_{p_2} |0\rangle$$

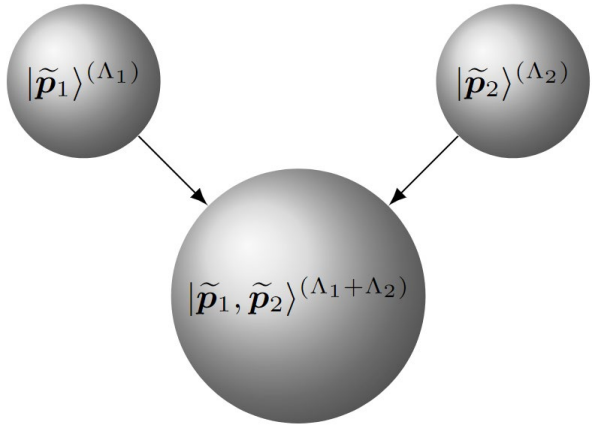
- Inspiration #1:

All-charm tetraquark in front form dynamics

Zhongkui Kuang (邝中奎),[1,2,3,*] Kamil Serafin,[1,2,†] Xingbo Zhao,[1,2,3,‡] and James P. Vary[4,§]

$$|\psi_M\rangle = \int_{12} P^+_M \tilde{\delta}_{12.P_M} \psi_M(12) b^\dagger_1 d^\dagger_2 |0\rangle$$

$$|\psi_{AB}\rangle = \int_{13} P^+_A \tilde{\delta}_{13.P_A} \psi_A(13) b^\dagger_1 d^\dagger_3 \times \int_{24} P^+_B \tilde{\delta}_{24.P_B} \psi_B(24) b^\dagger_2 d^\dagger_4 |0\rangle$$



Unlike the free case, while the incoming particles are the eigenstates of the theories with corresponding cutoffs, the combined state is not an eigenstate.

- Promoting this idea to the full many-body setting:

$$A^\dagger_K = (\mathcal{U}_K)(a^\dagger_K)(\mathcal{U}_K)^\dagger$$

Here $\mathcal{U}_K$ is the adiabatic interaction turn-on operator, **with modes only up to K included**.

$$\begin{aligned} |K_1, K_2\rangle &\propto \\ &= (A^\dagger_{K_1})(A^\dagger_{K_2})|\text{vac}\rangle \\ &= \mathcal{U}_{K_1} a^\dagger_{K_1} \mathcal{U}^\dagger_{K_1} \mathcal{U}_{K_2} a^\dagger_{K_2} \mathcal{U}^\dagger_{K_2} |\text{vac}\rangle \\ &= \mathcal{U}_{K_1} a^\dagger_{K_1} \mathcal{U}^\dagger_{K_1} \mathcal{U}_{K_2} a^\dagger_{K_2} |\text{vac}\rangle \end{aligned}$$

Quantum Simulation of LF QFT: Eigenstate-based scattering

- At any fixed K, the adiabatic turn-on operator $\mathcal{U}_K$ can be found via the "Full Unitary Couple Cluster" procedure, i.e. by seeking for it in the form

$$\mathcal{U}_K = \mathrm{e}^{-i\mathcal{V}_K} \qquad \mathcal{V}_K = \sum_{r,s=1}^{K} \sum_{\substack{\mathsf{i}_1,\mathsf{i}_2\ldots,\mathsf{i}_r,\\ \mathsf{j}_1,\mathsf{j}_2\cdots,\mathsf{j}_s}} \theta_{\mathsf{i}_1,\ldots,\mathsf{i}_r,\mathsf{j}_1,\ldots,\mathsf{j}_s} a^\dagger_{\mathsf{i}_1}\ldots a^\dagger_{\mathsf{i}_r} a_{\mathsf{j}_1}\ldots a_{\mathsf{j}_s}$$

  and demanding that

$$\mathcal{U}_K|\mathcal{F}_n^{\{K'\}}\rangle = U_{K'}|\mathcal{F}_n^{\{K'\}}\rangle \quad \text{for } K' \leq K$$

  where $U_{K'}$ is the matrix relating the free (Fock states) and interacting eigenbases at K'.

  In other words, we require that $\mathcal{U}_K$ acts as the adiabatic interaction turn-on operator in sectors of harmonic resolution up to K'.

Quantum Simulation of LF QFT: Eigenstate-based scattering

- If a quantum circuit for adiabatic interaction turn-on can be implemented efficiently, then implementing $A_K^\dagger = (\mathcal{U}_K)(a_K^\dagger)(\mathcal{U}_K)^\dagger$ is easily doable.
- In all of the above not renormalization was assumed.

$(A_3^\dagger)^2|\text{vac}\rangle$

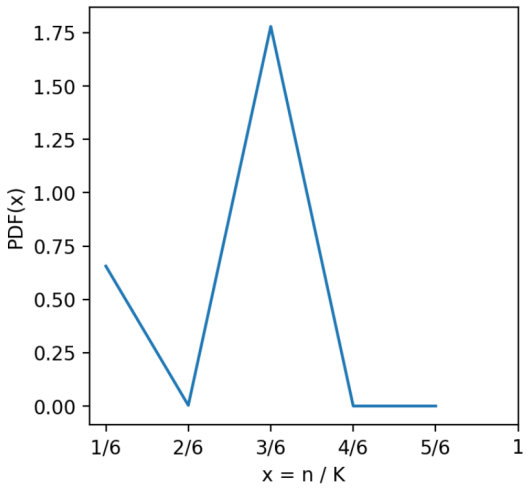


Figure 6. Parton distribution function $\text{PDF}(x = n/K, t = 0)$, as defined in (61), for the initial state $|i\rangle = \left|[K = 3, 0]^2\right\rangle$ from (59c). Shown is the exact result obtained by classical simulation and usage of the Full UCC method.

$e^{-i\mathcal{H}t}(A_3^\dagger)^2|\text{vac}\rangle$

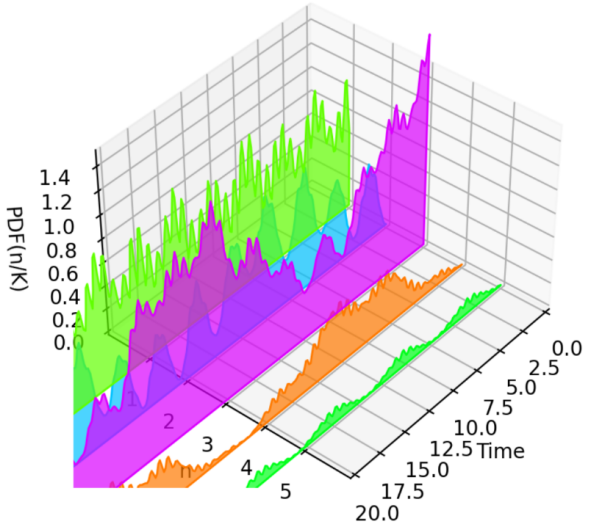


Figure 7. Time-dependent parton distribution function $\text{PDF}(x = \mathsf{n}/K, t)$ for the state $|i\rangle = \left|[K = 3, 0]^2\right\rangle$ from (59c). Shown is the exact result obtained by classical simulation and usage of the Full UCC method. The plot illustrates how the higher-LF-momentum modes $(\mathsf{n} = 4, 5)$ participate in the time evolution of the state $|i\rangle = \left|[K = 3, 0]^2\right\rangle$, in which only the $\mathsf{n} = 1, 2, 3$ modes were initially occupied.

Summary

- Quantum Simulation motivates the development of the full many-body formulations of LF QFT.
  - Which one is more suitable for QCs?
  - Toy examples!
- LF formulation allows for efficient basis choices, which also complicates the Hamiltonian operator.
  - Compare with lattice ET?
  - Align with projected capabilities of future QCs.
- Scattering:
  - Examples of tBLFQ, eigenstate-based.
  - Relation to renormalized theories?

Thank You!