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# Scattering Processes from Quantum Simulation Algorithms for Scalar Field Theories

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UNIVERSITY OF TORONTO

# Outline

1. Motivation
2. Scalar Field Theory
3. Quantum Simulation
4. Trotterization
5. LCU Decomposition
6. Conclusion

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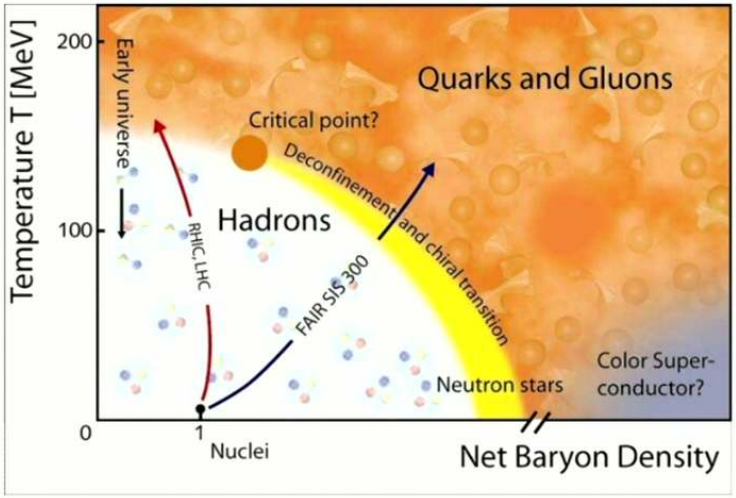
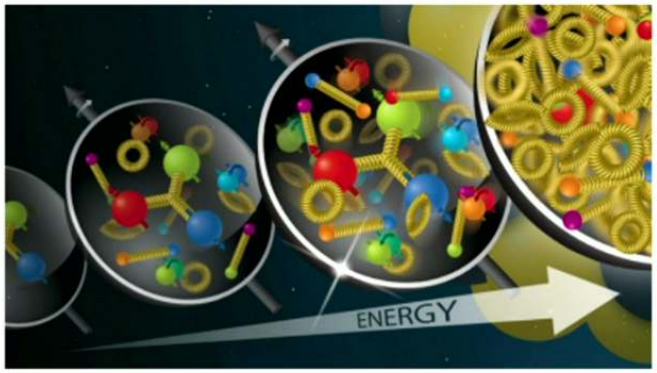
# Motivation: Eventual Physics Objectives

- **Scattering and S-Matrix**
  - Resolving high energy particle interactions and calculating transition amplitudes between multi-particle asymptotic states in strongly coupled regimes.
- **Dense Quantum Matter**
  - Interested in finite density phases of matter, a difficult classical problem, and relevant to early universe structure.
- **Real-Time Dynamics**
  - Accessing transport coefficients, structure functions, and non-equilibrium evolution beyond the limitations of Euclidean time analytic continuation.



# Unique Problems to Simulating Field Theories

- **Relativistic Theories**
  - Typically require a Lorentz invariant theory with time and space on equal footing.
- **Bosonic Quantum Number**
  - The bosonic part of theories lack U(1) number conservation, requiring large Hilbert spaces.
- **Representing Gauge Degrees of Freedom**
  - An open problem to faithfully and efficiently give a Hamiltonian representation of gauge fluctuations.



# Motivation: Quantum Simulation of Quantum Field Theories

- Lattice field theory offers a non-perturbative approach to study strongly interacting quantum field theories.
- Simulating dynamics requires an exponential amount of resources.
- Finite density is challenging due to the sign problem.
- Even current quantum algorithms are infeasible at present.

| Gauge Group | T-Gates: Transport Coefficients | T-Gates: Heavy-Ion Collisions |
|---|---|---|
| $U(1)$ | $7.35 \times 10^{17}$ | $7.19 \times 10^{23}$ |
| $SU(2)$ | $2.83 \times 10^{34}$ | $3.71 \times 10^{40}$ |
| $SU(3)$ | $3.01 \times 10^{49}$ | $3.22 \times 10^{55}$ |

Computational time $10^{17}$s: Age of Universe

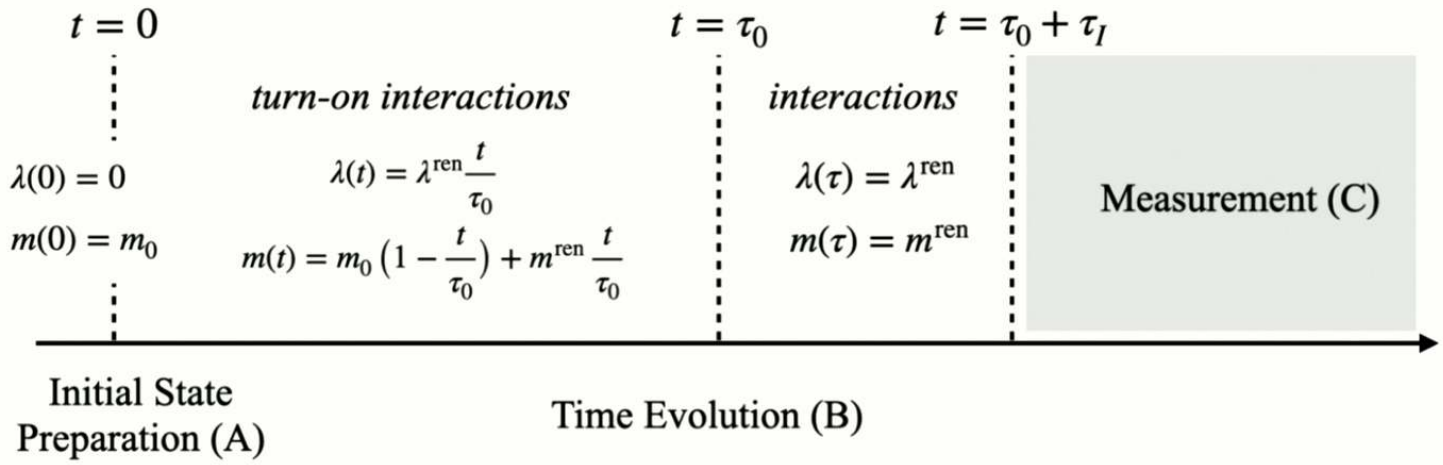
A. Kan and A. Nam (arXiv:2107.12769), T. Cohen,et. al. (NuQS Collaboration) PRD 104, 0954514 (2021)

# $\phi^4$ Theory

$$H = \int d^d x \left[ \frac{1}{2}\pi(\mathbf{x})^2 + \frac{1}{2}(\nabla\phi(\mathbf{x}))^2 + \frac{1}{2}m^2\phi(\mathbf{x})^2 + \lambda\phi(\mathbf{x})^4 \right]$$

- Toy theory with a non-interacting limit.
- $\phi^4$ is a simple interaction that's bounded below.
- Scalar fields in nature: Higgs boson, order parameters in phase transitions.
- Lessons learned might be extendable to other field theories, Sine-Gorden, gauge theories, etc.

# Jordan-Lee-Preskill Approach



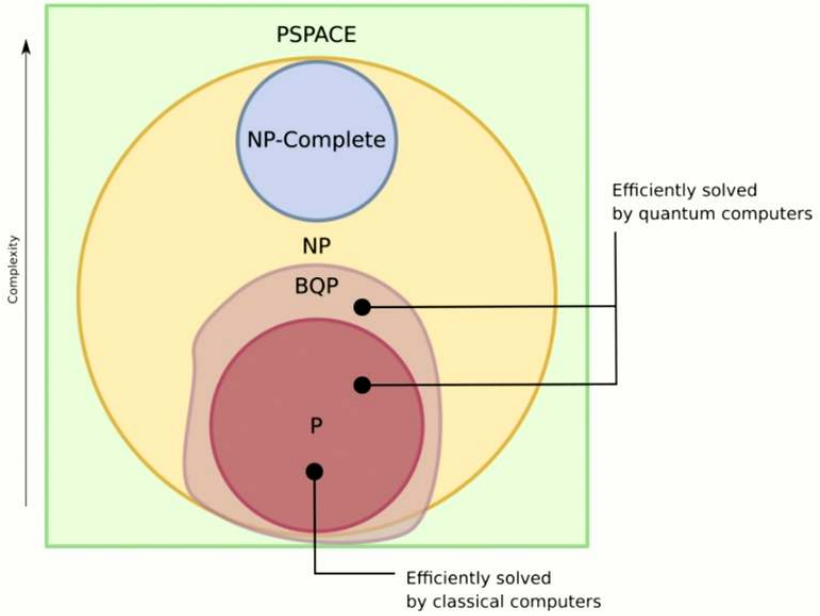

Jodan, Lee, Preskill, Science 336, 6085 (2012). Figure from: J. Barata, et. al. PRA 103, 042410 (2021)

# The Jordan-Lee-Preskill Protocol

- **Framework:** First comprehensive algorithm for simulating $\phi^4$ theory on a digital quantum computer in polynomial time.
- **The Protocol Steps:**
  1. **Discretization:** Map the field theory to a spatial lattice with spacing $a$ and volume $\Omega$.
  2. **Vacuum Prep:** Prepare the ground state $|\Omega_0\rangle$ of the free Hamiltonian ($H_0$).
  3. **Wavepacket Creation:** Apply filter operators to create non-interacting particle excitations.
  4. **Adiabatic Evolution:** Slowly turn on the interaction $\lambda(t)$ and shift mass $m(t)$ to transition from the free to the interacting theory.
  5. **Scattering:** Evolve the state under $H_{int}$ for time $t$.
  6. **Measurement:** Adiabatically turn off interactions and measure the final state in the free basis.

# Quantum Complexity of Scattering

- Computing a VEV of $\phi^4$ theory as a binary decision problem is BQP complete (JKLP 2017)
- Computing arbitrary $S-$matrix elements is NEEXP (full state tomography).
- Arbitrary state preparation and ground state determination is QMA-hard
- We'd like to compute physical quantities somewhere in between.




S. Aaronson, "The limits of quantum computers." Scientific American 298, no. 3 (2008)

# Efficient Methods to Measure (some) Scattering

- Energy quantization with finite volume (without interactions)

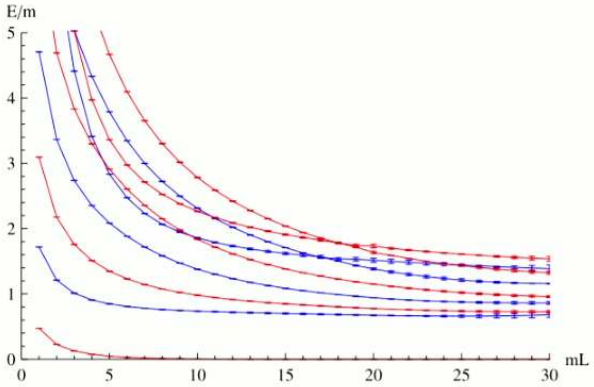
$$p_i = \frac{2\pi n_i}{L}, \quad n_i \in \mathbb{Z}, \quad E = \sum_{i=1,2} \left( m^2 + \frac{4\pi^2 n_i^2}{L^2} \right)^{1/2},$$

- Scattering phase can be related to energy shifts (with interactions)

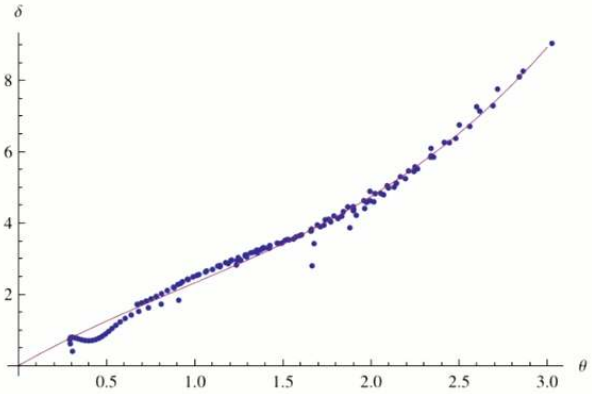
$$\begin{aligned} \frac{2\pi n_1}{L} &= p_1 - \tfrac{i}{L} \log S(p_1, p_2); \\ \frac{2\pi n_2}{L} &= p_2 - \tfrac{i}{L} \log S(p_2, p_1). \end{aligned} \tag{1}$$

- Applicable to higher dimensions (Lüscher formalism) and possibly inelastic scattering.
- Quantum utility depends on the computational difficulty of computing energies.
- Different bases may be useful at different energy scales.

# Extracting Scattering Phases via the Lüscher Method




The volume-dependent energy levels $E_n(L)$ are extracted from the finite-size spectrum.




The discrete energies determine the interacting momenta $p_n$ to construct the continuous phase shift.

$$S(\theta) = \pm \prod_j \frac{\sinh(\theta) + i\sin(\beta_j)}{\sinh(\theta) - i\sin(\beta_j)} \times \exp\left[ - \int_{-\infty}^{\infty} \frac{d\theta'}{2\pi i} \frac{\log f(\theta')}{\sinh(\theta - \theta' + i\epsilon)} \right].$$

Z. Bajnok and M. Lajer, Truncated Hilbert space approach to the 2d $\phi^4$ theory, J. High Energy Phys. 2016, 50 (2016)

# Field Basis

- Rescaled Lattice Hamiltonian

$$H_{amp} = \sum_{\mathbf{x}\in\Omega} \left[ \frac{1}{2}\Pi^2(\mathbf{x}) + \frac{1}{2}(M^2 + d + 1)\Phi^2(\mathbf{x}) + \frac{\Lambda}{4!}\Phi^4(\mathbf{x}) - \sum_{i=1}^{d} \Phi(\mathbf{x})\Phi(\mathbf{x} + a\hat{x}_i) \right]$$

- Using rescaled lattice variables

$$\Phi := a^{\frac{d}{2}-1}\phi, \quad \Pi := a^{\frac{d}{2}}\pi$$
$$M := am, \qquad \Lambda := a^{4-d}\lambda$$

- Field representation

$$\frac{\hat{\Phi}}{\Delta\Phi} = \begin{pmatrix} -k+1 & & & & \\ & \ddots & & & \\ & & 0 & & \\ & & & \ddots & \\ & & & & k \end{pmatrix}$$

# Occupation Basis

- Field Decompositon

$$\phi(\mathbf{x}) = \sum_{\mathbf{p}\in\Gamma} \frac{1}{L^d} e^{i\mathbf{p}\cdot\mathbf{x}} \sqrt{\frac{1}{2\omega_{\mathbf{p}}}} (a_{\mathbf{p}} + a^\dagger_{-\mathbf{p}}); \quad \pi(\mathbf{x}) = \sum_{\mathbf{p}\in\Gamma} \frac{-i}{L^d} e^{i\mathbf{p}\cdot\mathbf{x}} \sqrt{\frac{\omega_{\mathbf{p}}}{2}} (a_{\mathbf{p}} - a^\dagger_{-\mathbf{p}})$$

- Non-Interacting Hamiltonian

$$: H_0 := \frac{1}{|\Omega|} \sum_{\mathbf{p}} \omega_{\mathbf{p}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}}$$

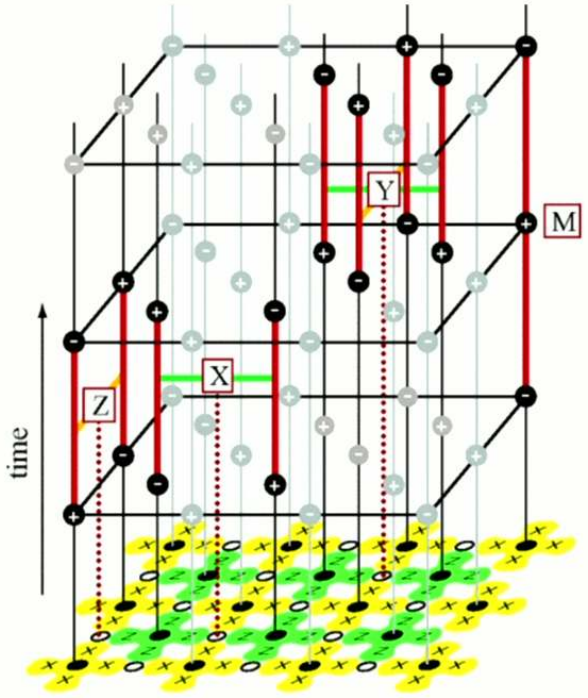
- Interacting Hamiltonian

$$H_\lambda = \frac{\lambda}{4!|\Omega|^3} \sum_{\{\mathbf{p}_i\}} \frac{1}{4\sqrt{\omega_{\mathbf{p}_1}\omega_{\mathbf{p}_2}\omega_{\mathbf{p}_3}\omega_{-(\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_3)}}}$$

$$\left\{ \left(a_{\mathbf{p}_1} + a^\dagger_{-\mathbf{p}_1}\right) \left(a_{\mathbf{p}_2} + a^\dagger_{-\mathbf{p}_2}\right) \left(a_{-\mathbf{p}_3} + a^\dagger_{\mathbf{p}_3}\right) \left(a_{(\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_3)} + a^\dagger_{-(\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_3)}\right) \right\}$$

# Fault Tolerant Implementation

- Consider a fault-tolerant implementation of quantum computing consisting of
  - A surface code to implement Clifford operations
  - "magic"-state distillation to implement $T$ gates, for universal computation.
- $T$ gates come from a "factory" using 15-qubit Reed-Mueller repitition code.
- Total computation time $10^5$ seconds, $10^7$ physical qubits.




A. Fowler, et. al, PRA 86,032324 (2012)

# Theory of Trotterization

- Trotter-Suzuki formula

$$e^{-it\hat{H}} = e^{-it\sum_n \hat{H}_n} = \lim_{K\to\infty} \left( \prod_n e^{-i\frac{t}{K}\hat{H}_n} \right)^K$$

- Can bound the error on the simulation through the Trotter error of this truncation.
- Mature theory of Trotter error, see Childs, et. al., Weibe, PRX (2021).
- More nuanced approachs, such as QDRIFT with randomized unitaries can improve bounds.

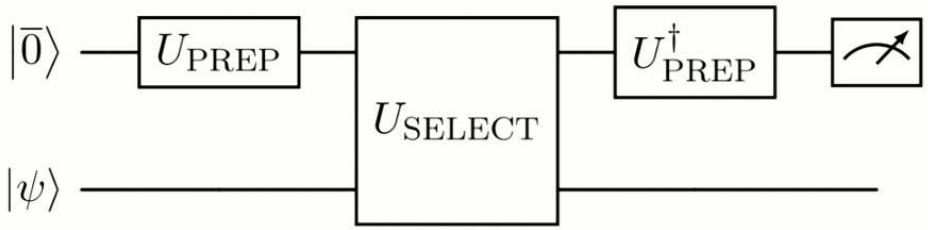
# Linear Combination of Unitaries

- Given an operator of the form $H_i = \sum_{j=1}^{M_i} h_{ij} U_{ij}$, such that $\lambda_i = \sum_j |h_{ij}|$
- The sum of unitaries may not be unitary, although we can "block-encode" in a larger unitary.
- We can construct

$$U_{\mathrm{PREP},i} |0\rangle^{\log M_i} = \sum_{j=1}^{M_i} \sqrt{\frac{h_{ij}}{\lambda_i}} |j\rangle \tag{2}$$

$$U_{\mathrm{SELECT,i}} = \sum_{j=1}^{M_i} |j\rangle \langle j| \otimes U_{ij} \tag{3}$$

# LCU Circuit




- This maps the state to

$$U_{H_i}|\overline{0}\rangle_a|\psi\rangle_s = \frac{1}{\lambda_i}|\overline{0}\rangle_a H_i|\psi\rangle_s + |\perp\rangle_{as}$$

- Could be made arbitrarily likely with Oblivious Amplitude Amplification.

# Quantum Singular Value Transformation

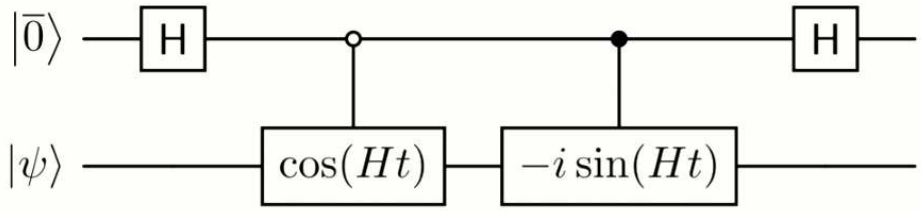
- How can we apply polynomials of our block encoded Hamiltonian ?

$$U = U_{\text{PREP}} U_{\text{SELECT}} U_{\text{PREP}}^{\dagger} = \begin{bmatrix} H & \cdot \\ \cdot & \cdot \end{bmatrix} \longrightarrow \begin{bmatrix} \text{Poly}(H) & \cdot \\ \cdot & \cdot \end{bmatrix}$$

- In particular, the time evolution operator

$$e^{-iHt} = \cos(Ht) - i \sin(Ht)$$

# QSVT for Hamiltonian Simulation




- Jacobi-Anger expansion

$$\cos(xt) = J_0(t) + 2\sum_{n=1}^{\infty}(-1)^n J_{2n}(t)T_{2n}(x)$$

$$\sin(xt) = 2\sum_{n=0}^{\infty}(-1)^n J_{2n+1}(t)T_{2n+1}(x)$$

- $J_i(x)$ Bessel function, $T_i(x)$ Chebyshev polynomial

# Qubit Mapping of Occupation Basis

- Consider a unary encoding of the the occupation basis

$$\begin{aligned} |p,n\rangle &= |0_{1,0},\ldots,0_{p-1,N};0_{p,0},\ldots,0_{p,n-1},1_{p,n},0_{p,n+1},\ldots,0_{p,N};0_{p+1,0},\ldots 0_{V,N}\rangle \\ &= \left(\otimes_{j=1}^{p-1}|0_{j,0}\ldots,0_{j,N}\rangle\right)\bigotimes|0_{p,0},\ldots 1_{p,n}\ldots,0_{p,N}\rangle\bigotimes\left(\otimes_{j=p+1}^{|\Omega|}|0_{j,0}\ldots,0_{j,N}\rangle\right). \end{aligned}$$

- This allows for an explicit qubit mapping

$$\begin{aligned} a_{\mathbf{p}}^{\dagger} &= \sum_n \sqrt{n+1}\left(\sigma_n^-\sigma_{n+1}^+\right)_{\mathbf{p}} \\ a_{\mathbf{p}} &= \sum_n \sqrt{n+1}\left(\sigma_n^+\sigma_{n+1}^-\right)_{\mathbf{p}}, \end{aligned}$$

- With the convenient form

$$a_{\mathbf{p}}+a_{\mathbf{p}}^{\dagger} = \frac{1}{2}\sum_n \sqrt{n+1}\left(X_nX_{n+1}+Y_nY_{n+1}\right)_{\mathbf{p}}.$$

# Decomposition of the Interaction

- Consider for example, the case where all $3$ momentum modes of the interaction are distinct

$$H_\lambda = \frac{\lambda}{4!|\Omega|^3} \sum_{\mathbf{p}\in S_{4\mathbf{p}}} \prod_{p_i\in\mathbf{p}} \frac{1}{\sqrt{2w_{p_i}}} \left[\left(a_{\mathbf{p}_i} + a^\dagger_{\mathbf{p}_i}\right)\right]$$

- This has a qubit mapping to

$$\begin{aligned} H_{1\varphi} &= \frac{\lambda}{24|\Omega|^3} \sum_{\mathbf{p}\in S_{4\mathbf{p}}} \prod_{p_i\in\mathbf{p}} \frac{1}{\sqrt{2w_{p_i}}} \left(\sum_n \frac{1}{2}\sqrt{n+1}\left(X_{p_i,n}X_{p_i,n+1} + Y_{p_i,n}Y_{p_i,n+1}\right)\right) \\ &= \frac{\lambda}{96\cdot 16|\Omega|^3} \sum_{\mathbf{p}\in S_{4\mathbf{p}}} \sum_{\vec{n}\in S_{4\vec{n}}} \prod_{(p_j,n_j)\in(\mathbf{p},\vec{n})} \sqrt{\frac{n_j+1}{w_{p_j}}}\left(X_{p_j,n_j}X_{p_j,n_j+1} + Y_{p_j,n_j}Y_{p_j,n_j+1}\right) \end{aligned}$$

# Trotterization of Occupation Basis

- You can bound the error of exponentiating such a Hamiltonian using the following Trotter-Suzuki bounds

$$\left\| e^{-iH\tau} - \mathscr{S}_p(\tau) \right\| \in O\left(\widetilde{\alpha}_{comm}\tau^3\right), \tag{4}$$

- Asymptotic bounds on commutator error given by

$$\widetilde{\alpha}_{comm} \in O\left(\frac{\lambda^2 N^6}{M^5}\right) . \tag{5}$$

- Improved bounds could be found with

$$\widetilde{\alpha}_{comm} \leq 2^{p-(p'+1)} \sum_{\gamma_{i_1},\gamma_{i_2},\ldots,\gamma_{i_{p'+1}}} \left\| [H_{\gamma_{p'+1}}, [\ldots [H_{\gamma_3}, [H_{\gamma_2}, H_{\gamma_1}]] \ldots]] \right\| \left( \sum_{\gamma=1}^{\Gamma} \|H_\gamma\| \right)^{p-p'} \quad [$$

# Computational Complexity of QSVT

- Truncate the expansion at $2n, 2n+1$ up to error $\epsilon$.
- Query Complexity $(n)$ to the "walk" operator

$$\mathcal{O}\left(|\alpha|_1 t + \frac{\log(1/\epsilon)}{\log\left(e + \frac{\log(1/\epsilon)}{|\alpha|_1 t}\right)}\right)$$

- $|\alpha_1|$ is the $\ell_1$ norm of $H$.

# Walk Operator for QSVT (Qubitization)

- Consider the Szegedy Walk Operator

$$W = \left(2U_{PREP}|0\rangle\langle 0|U_{PREP}^{\dagger} \otimes \mathbb{I} - \mathbb{I}\right) \cdot U_{SELECT}$$

$$W = \oplus_n \begin{pmatrix} \frac{E_n}{|\alpha|} & \sqrt{1-\left(\frac{E_n}{|\alpha|}\right)^2} \\ -\sqrt{1-\left(\frac{E_n}{|\alpha|}\right)^2} & \frac{E_n}{|\alpha|} \end{pmatrix} = \oplus_n e^{-i \arccos(E_n/|\alpha|)Y}$$

- Quantum Phase estimation gives eigenvalues of the Hamiltonian (simpler than time evolution).

# equal-weight LCU Decomposition (Algorithm I)

- Operator decomposition with equal coefficents for each of the unitaries in the decomposition of a Hamiltonian term.

$$\frac{\hat{\Phi}}{\Delta\Phi} = \frac{1}{2}\sum_{i=0}^{2k-1} U^{(i)}, \quad \text{where}$$

$$U^{(i)} = -\sum_{j=0}^{i-1} |j\rangle\langle j| + \sum_{j=i}^{2k-1} |i\rangle\langle i| = \sum_{j=0}^{2k-1} \left[2\Theta(j-i)-1\right] |j\rangle\langle j|$$

- Finite-difference term for example

$$-\frac{\hat{\Phi}_a\hat{\Phi}_b}{(\Delta\Phi)^2} = \frac{1}{4}\sum_{i_a,j_a=0}^{2k-1}\sum_{i_b,j_b=0}^{2k-1} \left[2\Theta(j_a-i_a)-1\right]\left[1-2\Theta(j_b-i_b)\right] |j_a\rangle\langle j_a| \otimes |j_b\rangle\langle j_b|$$

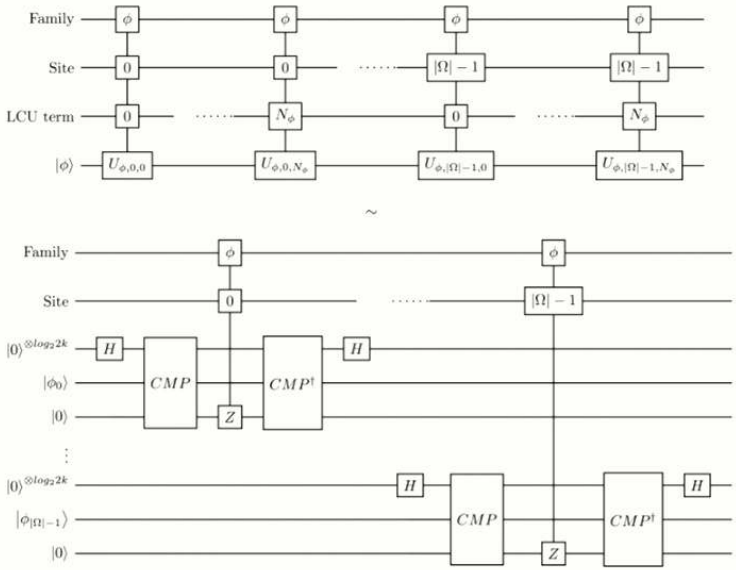
# LCU Decomposition of additional Hamiltonian Terms

- $$\left(\frac{\hat{\Phi}}{\Delta\Phi}\right)^2 = \frac{1}{2}\sum_{i=0}^{2k^2-1} U^{(i)}, \quad \text{where}$$
$$U^{(i)} = \sum_{j=0}^{2k-1}\left[2\Theta\left(k^2+(k-j-1)^2-i-1\right)-1\right]|j\rangle\langle j|$$

- $$\left(\frac{\hat{\Phi}}{\Delta\Phi}\right)^4 = \frac{1}{2}\sum_{i=0}^{2k^4-1} U^{(i)}, \quad \text{where}$$
$$U^{(i)} = \sum_{j=0}^{2k-1}\left[2\Theta\left(k^4+(k-j-1)^4-i-1\right)-1\right]|j\rangle\langle j|$$

# Quantum Circuits for equal-weight LCU

- The "family" register controls which of the four families of terms in the Hamiltonian we want to apply.
- The "site" register controls which of the lattice sites we want to apply the operator to.
- The "LCU term" register controls which of the unitaries we wish to apply.



# LCU with binary decomposition (Algorithm III)

- The field basis admits an even compacter representation as **Z** operators.

$$\frac{\Phi}{\Delta\Phi} = -\frac{1}{2}\sum_{j=0}^{\log_2 k} 2^j \mathrm{Z}_j - \frac{1}{2} \tag{7}$$

- Hamiltonian Terms can be constructed as

$$\left(\frac{\Phi}{\Delta\Phi}\right)^2 = \left(\frac{\Phi}{\Delta\Phi} + \frac{\mathbb{I}}{2}\right)^2 - \left(\frac{\Phi}{\Delta\Phi} + \frac{\mathbb{I}}{2}\right) + \frac{\mathbb{I}}{4}$$

$$= \frac{1}{6}\left(2^{2\log_2 k+1} + 1\right)\mathbb{I} + \sum_{j=0}^{\log_2 k-1}\sum_{k>j}^{\log_2 k} 2^{j+k-1}\mathrm{Z}_j\mathrm{Z}_k + \frac{1}{2}\sum_{j=0}^{\log_2 k} 2^j \mathrm{Z}_j$$

# LCU with binary decomposition (Algorithm III)

- Finite Difference Term

$$H_{\phi''} = \sum_{\substack{\mathbf{x},\mathbf{x}' \\ (\mathbf{x},\mathbf{x}')\in E_D}} \sum_{j,j'} \beta_{jj'} \left(Z_j\right)_{\mathbf{x}} \left(Z_{j'}\right)_{\mathbf{x}'}$$

- Likewise for conjugate momentum

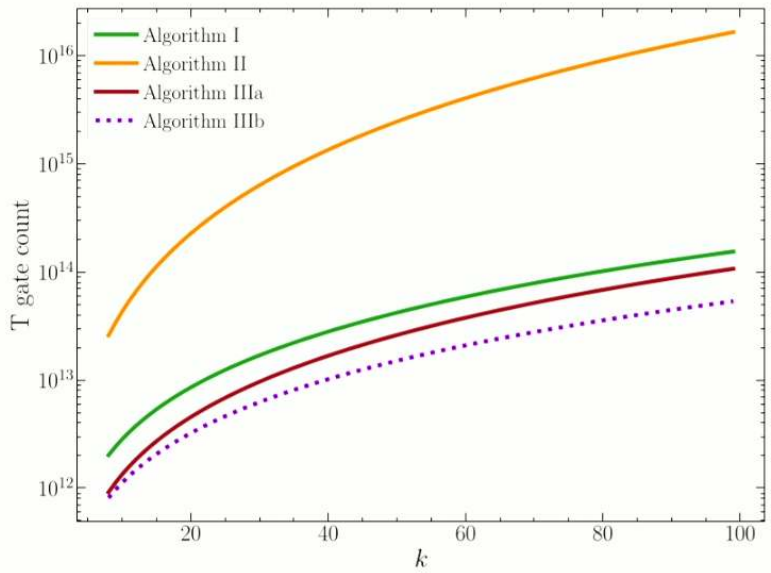
$$H_\pi = \sum_{\mathbf{x}\in\Omega} H_{\pi\mathbf{x}} := \sum_{\mathbf{x}\in\Omega} \frac{1}{2}\Pi^2(\mathbf{x}) = \sum_{\mathbf{x}\in\Omega} \mathcal{F}\left(\gamma_0 \mathbb{I} + \sum_j \gamma_j Z_j + \sum_{j,k} \gamma_{jk} Z_j Z_k\right) \mathcal{F}^\dagger$$

# Primitives for binary decomposition LCU

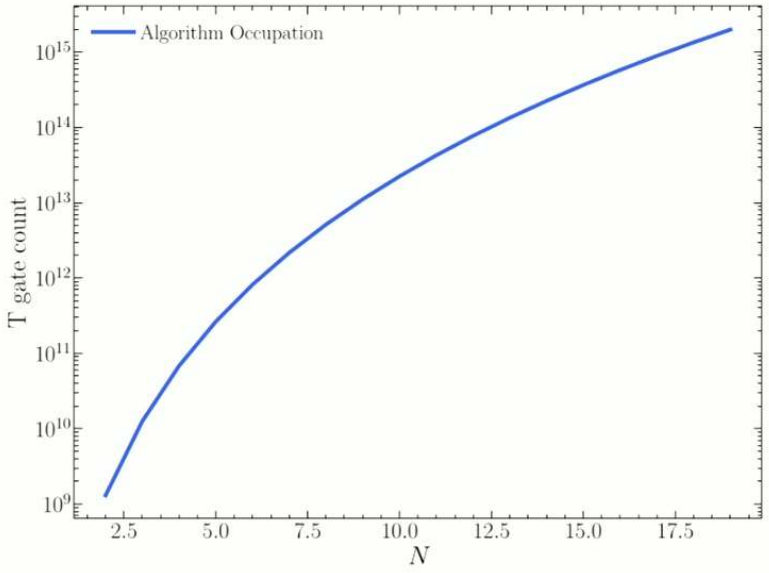
- $$\mathrm{PREP}_{1\vec{x}}\,|0\rangle^{1+\log_2(L_1+L_2)} = \frac{1}{\mathcal{N}_{1\vec{x}}}\left(\sum_{j=1}^{L_1}\sqrt{\alpha_j}|j,0\rangle + \sum_{j'=L_1+1}^{L_1+L_2}\sqrt{\alpha_{j'}}\,|j',0\rangle + \sum_{j=1}^{L_1}\sqrt{\gamma_j}|j,1\rangle + \sum_{j'=L_1+1}^{L_1+L_2}\sqrt{\gamma_{j'}}\,|j',0\rangle\right)$$

- $$\mathrm{SELECT}_{1\vec{x}}\,|j,0\rangle|\psi\rangle \to |j,0\rangle Z_j|\psi\rangle$$
$$\mathrm{SELECT}_{1\vec{x}}\,|j,1\rangle|\psi\rangle \to |j,1\rangle \mathcal{F} Z_j \mathcal{F}^\dagger|\psi\rangle$$

# T Gate Cost in 'Energy' basis.



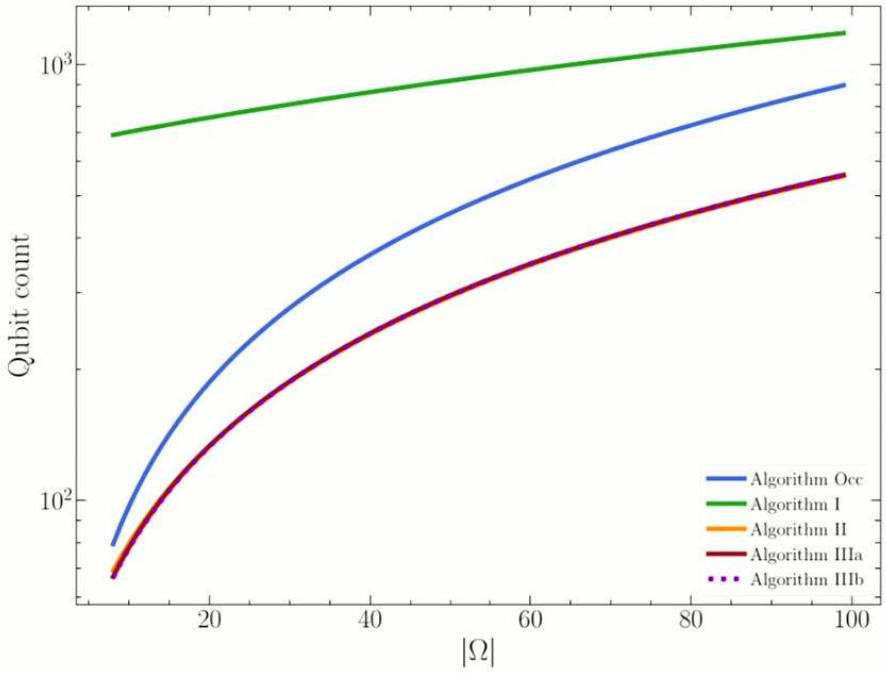

(a) $\mathcal{O}(|\Omega|^2(k^2\Lambda + kM^2)/\epsilon)$




(b) $\mathcal{O}(\lambda N^7|\Omega|^3/(M^{5/2}\epsilon^{3/2}))$

# Total Qubit Cost

- Costs depend upon the basis and the representation of the fields.
- LCU methods can (but are not guaranteed to) be more efficient.
- The binary decomposition LCU require the fewest qubits .



# Conclusion

1. We extend the Lusher formalism to the quantum simulation framework.
2. Challenge: The QSim community needs new innovative approaches for realistic measurements.
3. We provide detailed and optimized circuit development for simulating scalar field theory.
4. Challenge: The QSim community needs to continue to consider all error propagation and costs when developing protocols.