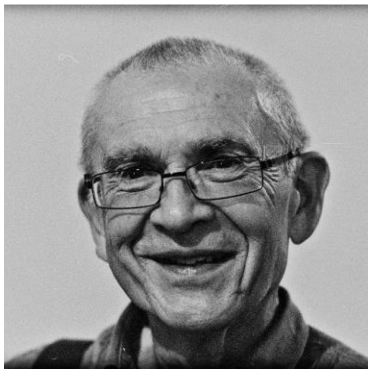
Towards practical quantum simulation of quantum field theories

M. Sohaib Alam

NASA QuAIL / USRA, Ames Research Center

C2QA Retreat, May 2023

Basic philosophy



Yuri Manin, *"Computable and Uncomputable"* (1980)

Richard Feynman, *"Simulating physics with computers"* (1982)

phenomena—the challenge of explaining quantum mechanical phenomena —has to be put into the argument, and therefore these phenomena have to be understood very well in analyzing the situation. And I'm not happy with all the analyses that go with just the classical theory, because nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy. Thank you.

OMG

T gate counts

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

(Age of the universe ~ $10^{17} s$)

[1] A. Kan and Y. Nam, "Lattice Quantum Chromodynamics and Electrodynamics on a Universal Quantum Computer", arXiv:2107.12769
[2] T. D. Cohen, H. Lamm, S. Lawrence, and Y. Yamauchi (NuQS Collaboration), Phys. Rev. D 104, 094514 (2021)

This talk

- **LCU primitives for scalar field theory[1] (C2QA)**
  - **Usable in state-of-the-art quantum simulation algorithms[2]**
  - **Simplest quantum field theory**

- **Dihedral gauge theory simulation[3] (SQMS)**
  - **Approximating gauge groups by discrete subgroups[4]**
  - **Simplest non-abelian discrete group**

[1] arXiv:23xx.xxxx, C2QA collab.
[2] "Quantum singular value transformation and beyond: exponential improvements for quantum matrix arithmetics", A. Gilyen, Y. Su, G. H. Lao, N. Wiebe, Proceedings of the 51st Annual ACM SIGACT STOC (2019)
[3] M. S. Alam, S. Hadfield, H. Lamm, A. C. Y. Li (SQMS collab.), Phys. Rev. D 105, 114501 (2022)
[4] D. C. Hackett, K. Howe, C. Hughes, W. Jay, E. T. Neil, and J. N. Simone, Digitizing gauge fields: Lattice Monte Carlo results for future quantum computers, Phys. Rev. A 99, 062341 (2019)

Linear Combination of Unitaries (LCU)

Given

$$A = \sum_{i=1}^{L} \alpha_i U_i$$

$$\alpha_i > 0$$

Construct

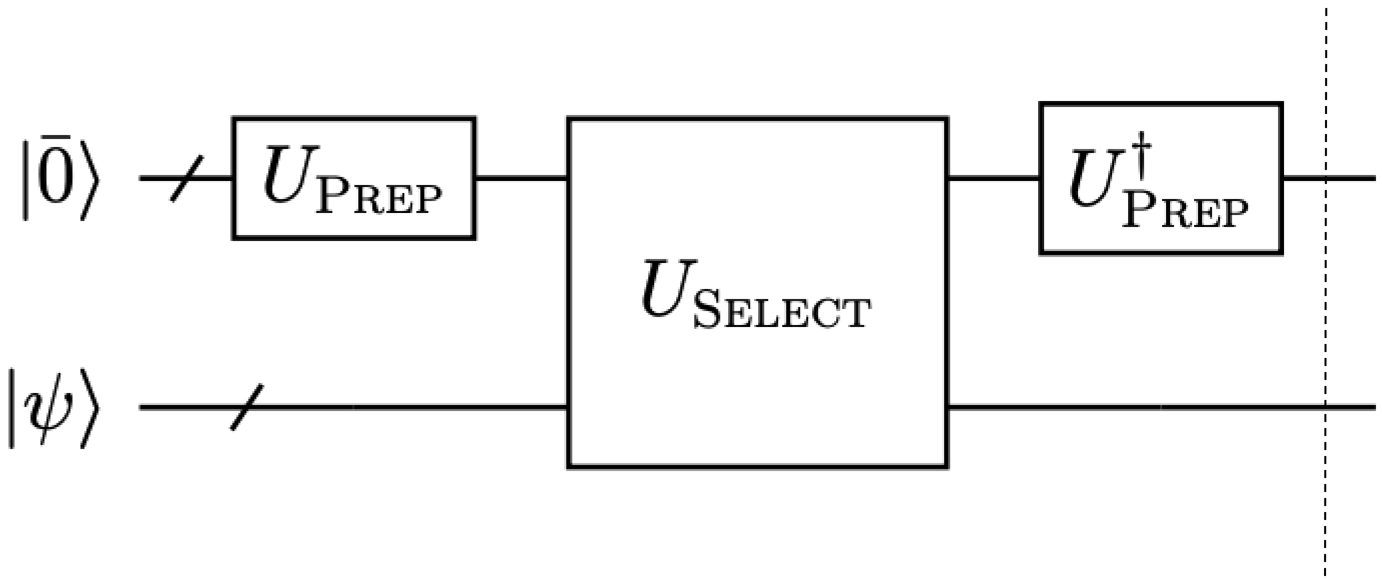
$$U_{PREP}|\bar{0}\rangle = \frac{1}{\sqrt{|\alpha|_1}} \sum_{i=1}^{L} \sqrt{\alpha_i}|i\rangle$$

$$|\alpha|_1 = \sum_{i=1}^{L} \alpha_i$$

$$U_{SELECT} = \sum_{i=1}^{L} |i\rangle\langle i| \otimes U_i$$

"Hamiltonian Simulation Using Linear Combinations of Unitary Operations", A. M. Childs, N. Wiebe, Quantum Information and Computation 12, 901-924 (2012)

Linear Combination of Unitaries (LCU)



Success probability

$$\frac{||A|\psi\rangle||^2}{||\alpha||_1^2}$$

$$\frac{1}{|\alpha|_1}|\bar{0}\rangle \otimes A|\psi\rangle + |\Phi^\perp\rangle$$

$$\left(|\bar{0}\rangle\langle\bar{0}| \otimes \mathbb{I}\right)|\Phi^\perp\rangle = 0$$

Scalar Field Theory

Discretized ϕ^4 Hamiltonian

$$H = \sum_{\vec{x}\in\Omega} a^D \left[\frac{1}{2}\Pi^2 + \frac{1}{2}||\nabla\Phi||^2 + M^2\Phi^2 + \frac{\Lambda}{4!}\Phi^4\right]$$

Simplest field theory:

- Free theory -- relativistic energy-momentum relationship (Klein-Gordon equation)
- ϕ^4 term simplest self-interaction term bounded below
- Scalar fields in nature: Higgs boson, Inflaton(?)

Scalar Field Theory

ϕ^4 Hamiltonian

$$H = \sum_{\vec{x}\in\Omega}\left[\frac{1}{2}\pi^2(x) + (m^2 + D + 1)\phi^2(\vec{x}) + \frac{\lambda}{4!}\phi^4(\vec{x}) - 2\sum_{i=1}^{D}\phi(\vec{x})\phi(\vec{x} + a\hat{x}_i)\right]$$

Rescaled variables

$$\phi = a^{\frac{D}{2}-1}\Phi, \qquad \pi = a^{\frac{D}{2}}\Pi,$$
$$m = aM, \qquad \lambda = a^{4-D}\Lambda$$

Field amplitude basis

$$\hat{\phi}|\phi\rangle = \phi|\phi\rangle$$

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

LCU with unequally sized groups of terms

$$\hat{H} = \alpha_0 \left(U_0^{(0)} + \cdots + U_{N_0-1}^{(0)} \right) + \cdots + \alpha_{M-1} \left(U_0^{(M-1)} + \cdots + U_{N_{M-1}-1}^{(M-1)} \right)$$

Let $N_{max} = \max\{N_i\}_{i=0}^{M-1}$,

$$U_{PREP} \left|\bar{0}\right\rangle = \frac{1}{\sqrt{|\alpha|_1 N_{max}}} \left(\sum_{i=0}^{M-1} \sqrt{\alpha_i N_i} \left|i\right\rangle \right) \left(\sum_{m=0}^{N_i-1} \left|m\right\rangle \right) \left(\sum_{k=0}^{\frac{N_{max}}{N_i}-1} \left|k\right\rangle \right)$$

$$U_{SELECT} = \sum_{i=0}^{M-1} \left|i\right\rangle \left\langle i\right| \otimes U_{SUB-SELECT_i}$$

$$U_{PREP}^{\dagger} U_{SELECT} U_{PREP} \left|\bar{0}\right\rangle \left|\psi\right\rangle = \left|\bar{0}\right\rangle \frac{\hat{H}}{|\alpha|_1} \left|\psi\right\rangle$$

LCU decompositions

Equal weight LCU

$$\frac{\hat{\phi}}{\Delta\phi} = \frac{1}{2}\sum_{m=0}^{2k-1} U^{(m)}$$

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

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

Unequal weight LCU[1]

$$\frac{\hat{\phi}}{\Delta\phi} = \frac{1}{2}\mathbb{I} - \frac{1}{2}\sum_{j=0}^{\log_2 2k-1} 2^j Z_j$$

$$\#\text{qubits} \sim O(\log_2 k)$$

(either way)

$$n = \frac{1}{2}\big(\underbrace{+1\cdots+1}_{k+n}\quad\underbrace{-1\cdots-1}_{k-n}\big)$$

[1] "Quantum Algorithms for Simulating the Lattice Schwinger Model", A. F. Shaw, P. Lougovski, J. R. Stryker, N. Wiebe, Quantum 4, 306 (2020)

Equal weight LCU

Use comparator (adapted from Gidney adder[1])

$$\texttt{CMP}_{A,B,C}\,|i\rangle\,|j\rangle\,|0\rangle \;=\; |i\rangle\,|j\rangle\,|j<i\rangle \;=\; |i\rangle\,|j\rangle\,|\Theta(i-j-1)\rangle$$

$O(|\Omega|\log_2 k)$ T gates

to simplify

$$U_{PREP_\phi^\dagger} U_{SELECT_\phi} U_{PREP_\phi} |\bar{0}\rangle|\psi\rangle|0\rangle_{anc}$$

$$= \left(H^{\otimes m}\texttt{CMP}^\dagger Z_{anc}\texttt{CMP}\,H^{\otimes m}\right)|\bar{0}\rangle|\psi\rangle|0\rangle_{anc}$$

$$= \left(|\bar{0}\rangle\frac{\hat{\phi}}{\phi_{max}}|\psi\rangle + |\Phi^\perp\rangle\right)|0\rangle_{anc}$$

[1] "Halving the cost of quantum addition", Craig Gidney, Quantum 2, 74 (2018)

Equal weight LCU

Other terms in the Hamiltonian

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

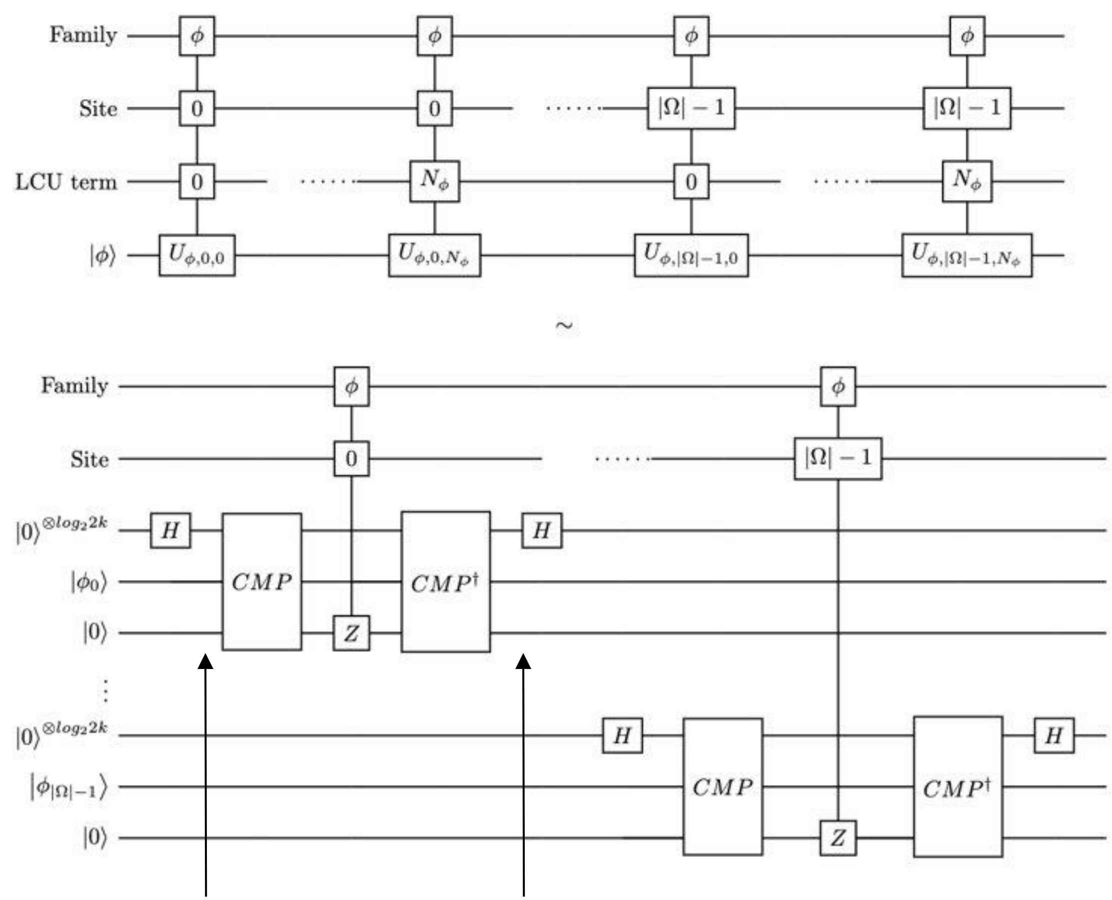
$$U^{(i)} = \sum_{j=0}^{2k-1} \left[2\Theta(k^2 + (k-j-1)^2 - i - 1) - 1\right] |j\rangle\langle j|$$

$$\pi^2 = \mathcal{F}^\dagger \phi^2 \mathcal{F}$$

$$\left(\frac{\hat{\phi}}{\Delta\phi}\right)^4 = \frac{1}{2}\sum_{i=0}^{2k^4-1} U^{(i)}, \quad \text{where}$$

$$U^{(i)} = \sum_{j=0}^{2k-1} \left[2\Theta(k^4 + (k-j-1)^4 - i - 1) - 1\right] |j\rangle\langle j|$$

Equal weight LCU



$O(|\Omega| \log_2^2 k)$ T gates

Insert $U_{initial}$ . . . and its inverse for ϕ^2, π^2, ϕ^4
(involves arithmetic and Fourier transform)

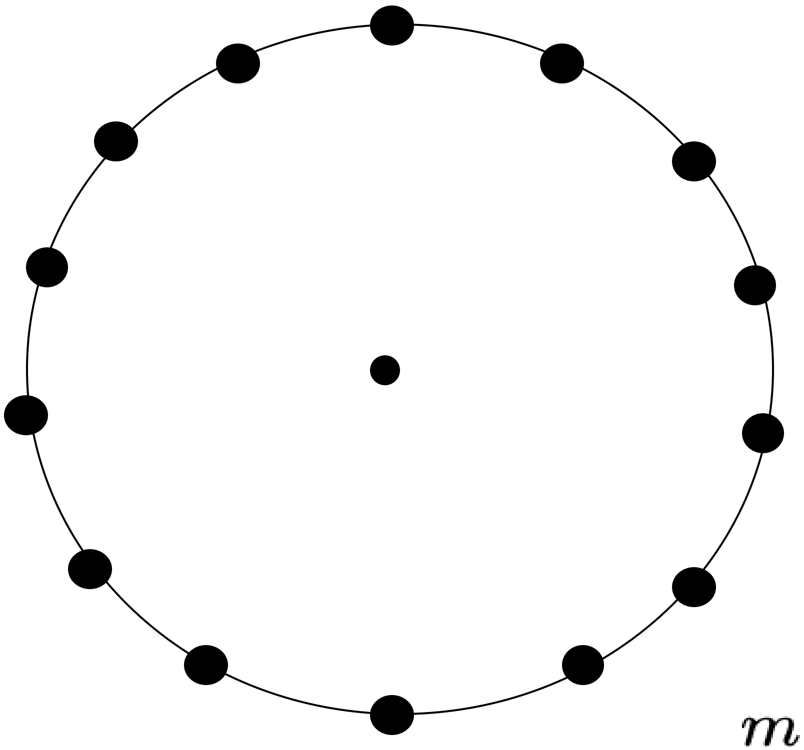
T gate complexity

$$\text{Count}(\text{T})_{\phi\phi} \sim O\left(|\Omega| D \log_2\left(|\Omega| D k\right)\right)$$

$$\text{Count}(\text{T})_{\phi^2,\pi^2,\phi^4} \sim O\left(|\Omega|(\log_2^2 k + \log_2 |\Omega|)\right)$$

$$k = \frac{\phi_{max}}{\Delta\phi} \qquad |\Omega| : \text{ Lattice size} \qquad D : \text{ spatial dimensionality}$$

Discrete Subgroups – General Idea



Approximate a continuous group by a discrete subgroup

$$U(1) \approx \mathbb{Z}_N$$

Simple example of a non-Abelian discrete group

$$D_N \sim \mathbb{Z}_N \rtimes \mathbb{Z}_2$$

Generic element

$$s^m r^k$$

$$m \in \{0,1\}\,, \quad z \in \{0,\ldots,N-1\}$$

General Methods

- **For some generic gauge group *G*,**
  - Define a *G*-register with one basis element $|g\rangle$ per group element $g \in G$
  (Hilbert space on single *G*-register $\mathcal{H}_G = \mathbb{C}G$; for *L* links on entire lattice, $\mathcal{H} = \mathbb{C}G^{\otimes L}$)
- **Define basic gates**
  - Inverse gate

$$\mathcal{U}_{-1}|g\rangle = |g^{-1}\rangle$$

  - (Left) Multiplication gate

$$\mathcal{U}_{\times}|g\rangle|h\rangle = |g\rangle|gh\rangle$$

  - Trace gate

$$\mathcal{U}_{\mathrm{Tr}}(\theta)|g\rangle = e^{i\theta \,\mathrm{Re\ Tr\ g}}|g\rangle$$

  - Fourier gate

$$\mathcal{U}_F(\theta)\sum_{g\in G} f(g)|g\rangle = \sum_{\rho\in\hat{G}} \hat{f}(\rho)_{ij}|\rho, i, j\rangle$$

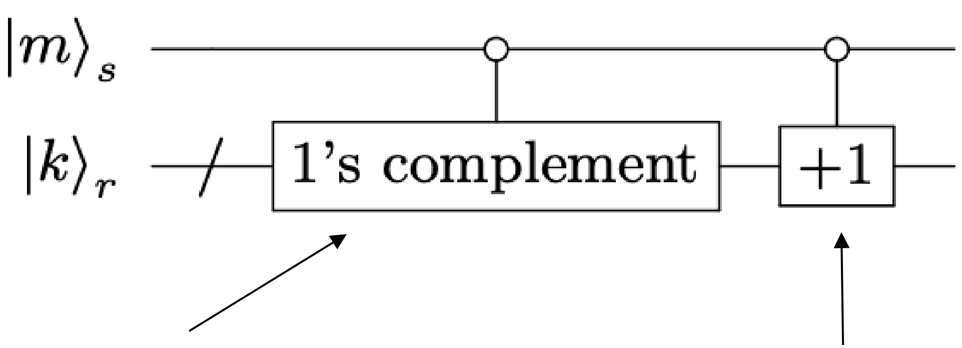
"General methods for digital quantum simulation of gauge theories", H. Lamm et al., Phys Rev D

Inverse Gate

Computing the 2's complement of k

$$\left(s^m r^k\right)^{-1} = s^m r^{Nm+(-1)^m k}$$

Equivalent to computing 1's complement, then adding 1



n CNOTs

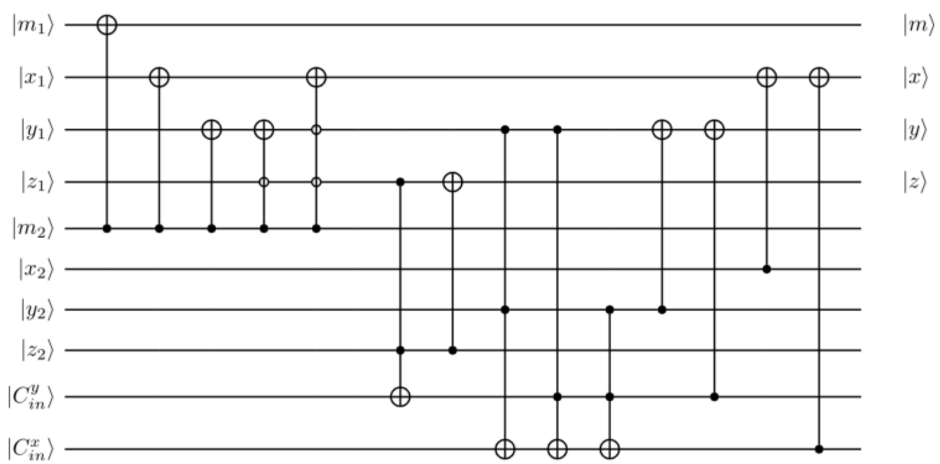
O(n) CCNOTs + const # ancillas

Multiplication Gate

$$s^{m_1} r^{k_1} \cdot s^{m_2} r^{k_2} = s^{m_1+m_2} r^{N m_2 + (-1)^{m_2} k_1 + k_2}$$

$m_2 = 0 :$ add k_1 and k_2

$m_2 = 1 :$ add 2's complement of k_1 and k_2



Example circuit for D8 multiplication gate

Sum and Carry bits in Reed-Muller form

$$S = A \oplus B \oplus C_{in}$$

$$C_{out} = AB \oplus AC_{in} \oplus BC_{in}$$

Trace Gate

Identify corresponding Hamiltonian

$$U_{\mathrm{Tr}}(\theta)\,|g\rangle = e^{i\theta\,\mathrm{Re}(\mathrm{Tr}(g))} = e^{i\theta H_{\mathrm{Tr}}} \qquad H_{\mathrm{Tr}}\,|g\rangle = \mathrm{Re}(\mathrm{Tr}(g))\,|g\rangle$$

Fundamental (2D) representation

$$\rho(g) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^m \begin{pmatrix} \omega & 0 \\ 0 & \overline{\omega} \end{pmatrix}^k \qquad \text{where} \quad \omega = e^{2\pi i/N}$$

$$\Rightarrow \qquad H_{\mathrm{Tr}} = |0\rangle\langle 0| \otimes \sum_{\ell=0}^{N-1} 2\cos(2\pi\ell/N)\,|\ell\rangle\langle\ell|$$

O(N) implementation: $U_{\mathrm{Tr}}(\theta) = \prod_{j=0}^{N} e^{i\theta a_\alpha |0\rangle\langle 0| \otimes Z_\alpha}$

Fourier Gate

Fourier transform of a representation of some finite group G

$$\hat{f}(\rho) = \sqrt{\frac{d_\rho}{N}} \sum_{g \in G} f(g)\rho(g)$$

Recursive definition

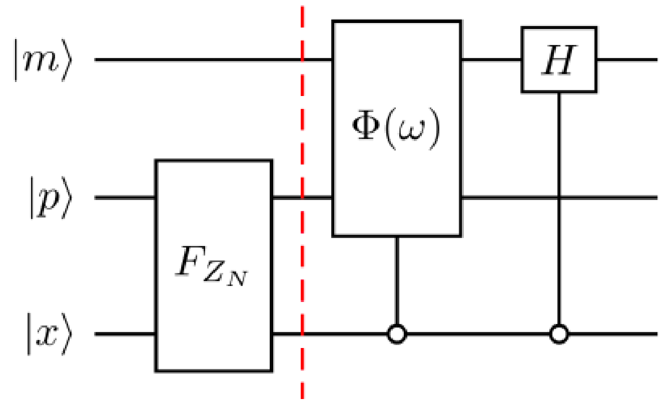
$$\sum_{g \in G} f(g)\rho(g) = \sum_{i=1}^{n} \rho(g_i)\hat{f}_i(\rho|_H)$$

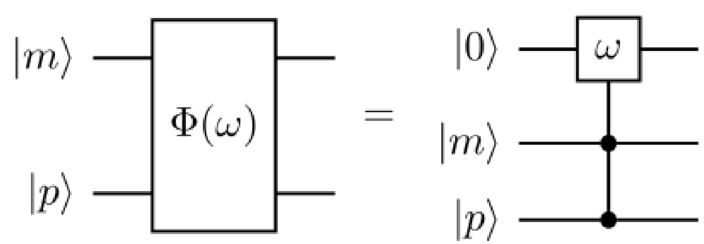
Fourier Gate

$$\sum_{g\in G} \alpha_g |g\rangle \;=\; \sum_{i=1} \sum_{h\in H} \alpha(g_i h)|g_i\rangle|h\rangle$$

$$\xrightarrow{F_H} \sum_{i=1}^{n} |g_i\rangle \left(\sum_{\tilde{h}\in\hat{H}} \hat{\alpha}_i(\tilde{h})|\tilde{h}\rangle \right)$$

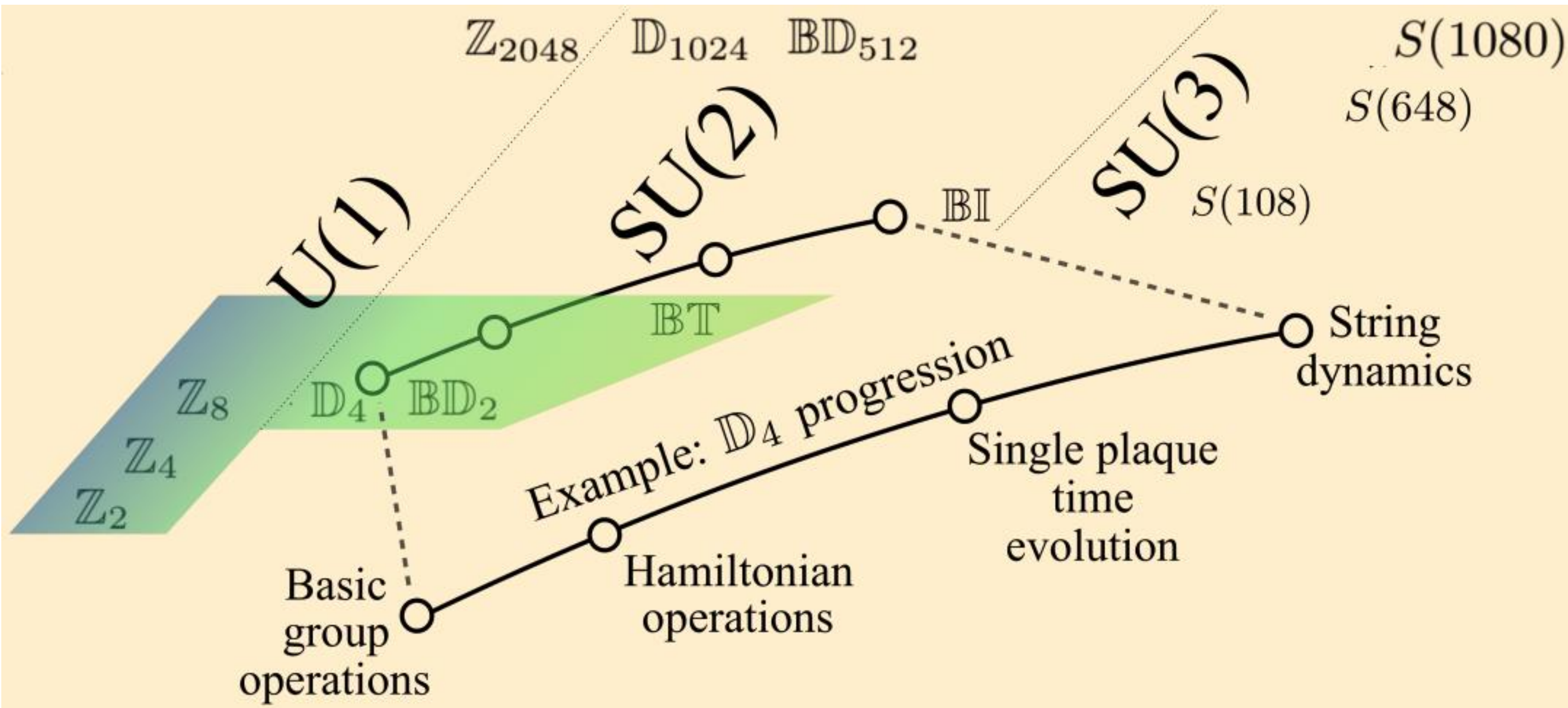
$$\xrightarrow{U} \sum_{\tilde{g}\in\hat{G}} \hat{\alpha}(\tilde{g})|\tilde{g}\rangle$$





"Efficient quantum transforms" arXiv: quant-ph/9702028 (2007), P. Hoyer

Looking ahead



Thank you!

Email: sohaib.alam@nasa.gov;
malam@usra.edu