# Algebraic compression of quantum circuits for ~~Hamiltonian~~ simulation

Hermitian

NERSC

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# Outline and acknowledgements

1. A 3 minute **introduction** to quantum computing
2. **Hamiltonian simulation** and Trotter decompositions
3. Algebraic **compression** of Trotterized circuits for spin Hamiltonians
4. **Results** on classical and quantum hardware
5. Conclusion

**Efekan Kökcü**

**Lindsay Bassman**

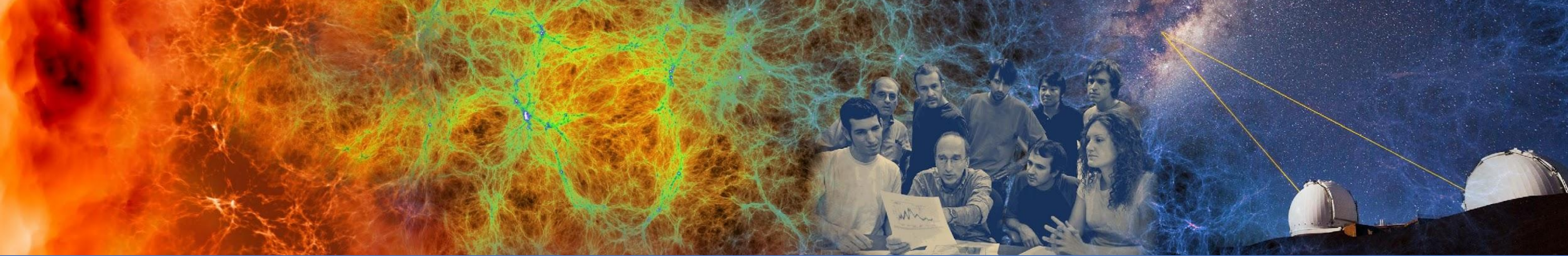
**Bert de Jong**

**Lex Kemper**

**Roel Van Beeumen**

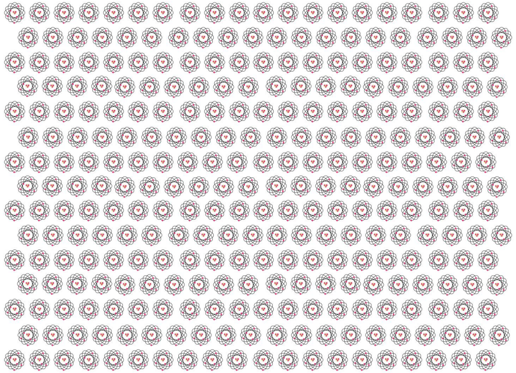
***An Algebraic Quantum Circuit Compression Algorithm for Hamiltonian Simulation***, D. Camps, E. Kökcü, L. Bassman, W. A. de Jong, A. F. Kemper, R. Van Beeumen, Accepted in SIMAX, arXiv:2108.03283

***Algebraic compression of quantum circuits for Hamiltonian evolution***, E. Kökcü, D. Camps, L. Bassman, J. K. Freericks, W. A. de Jong, R. Van Beeumen, A. F. Kemper, Phys. Rev. A 105, 032420, arXiv:2108.03282

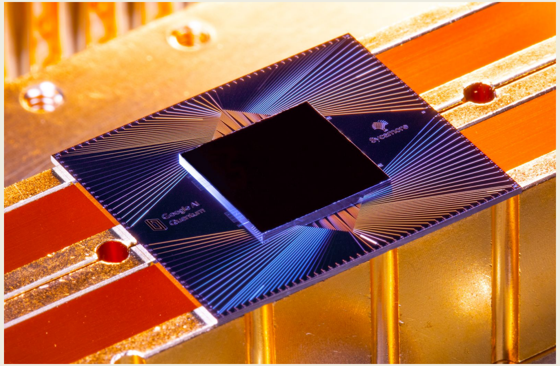


# Introduction to Quantum Computing

# Dimension of a quantum state grows exponentially with the number of particles



A complete description of a typical quantum state of just 300 qubits requires more bits than the number of atoms in the visible universe (figure from John Preskill).



Google Sycamore chip (2019)
53 qubits
2^53 ≅ 9 * 10^15 ≅ 36PB (single precision)

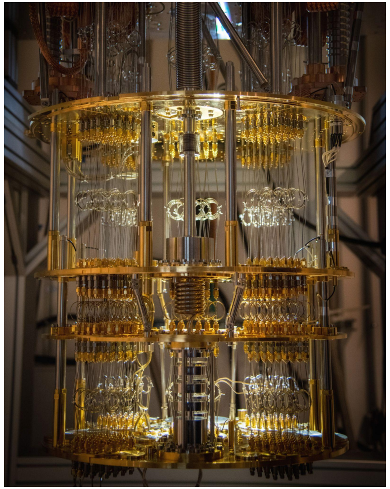
2^300 =
2037035976334486086268445688409378161051468393665936250636140449354381299763336706183397376

# Quantum computing from 10000 ft

Two things are required for quantum computation:

- An **encoding** of the data in the quantum state $|\Psi>$
- A way to **control** the evolution towards an encoding of the solution

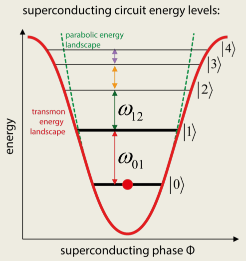
**Quantum computers are coherently controllable quantum systems**



Advanced Quantum Testbed @ Berkeley Lab

# Qubits represent quantum data

**Physics**: two-level quantum system




**Math**: 2-dimensional complex vectors with unit norm

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$|\alpha|^2 + |\beta|^2 = 1$$

**Quantum Gates**: change state of a qubit

$$|\psi\rangle - \boxed{U} - |\psi'\rangle \longrightarrow |\psi'\rangle = U|\psi\rangle$$

U is unitary

Unitary matrices preserve the norm of the vector (quantum operations are Hamiltonian time evolution)

# Multi-qubit states and quantum circuits

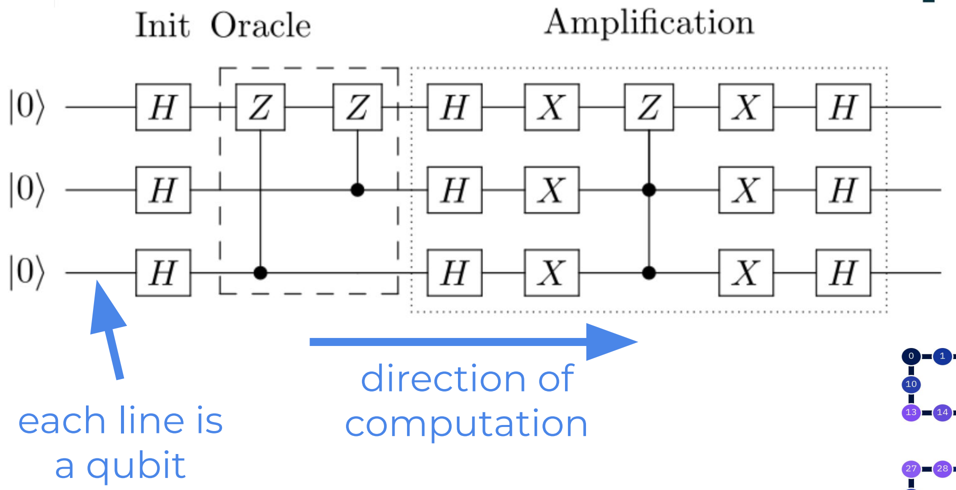
$$|00\rangle = |0\rangle \otimes |0\rangle = \begin{bmatrix}1\\0\end{bmatrix} \otimes \begin{bmatrix}1\\0\end{bmatrix} = \begin{bmatrix}1\\0\\0\\0\end{bmatrix}$$

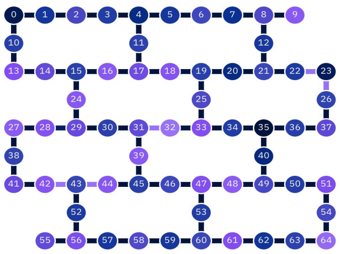
$$|01\rangle = |0\rangle \otimes |1\rangle = \begin{bmatrix}1\\0\end{bmatrix} \otimes \begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}0\\1\\0\\0\end{bmatrix}$$

$$|10\rangle = |1\rangle \otimes |0\rangle = \begin{bmatrix}0\\1\end{bmatrix} \otimes \begin{bmatrix}1\\0\end{bmatrix} = \begin{bmatrix}0\\0\\1\\0\end{bmatrix}$$

$$|11\rangle = |1\rangle \otimes |1\rangle = \begin{bmatrix}0\\1\end{bmatrix} \otimes \begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$

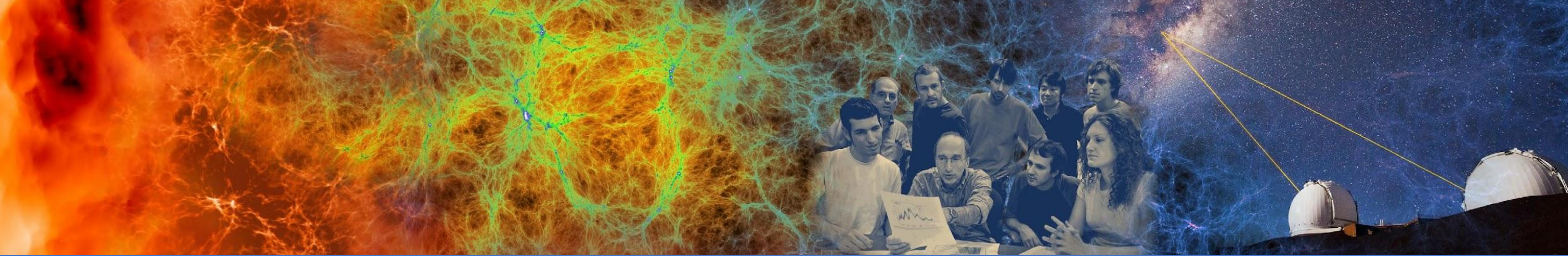
$$|\psi\rangle = \alpha_0 |00\cdots0\rangle + \alpha_1 |00\cdots1\rangle + \cdots + \alpha_{2^n-1} |11\cdots1\rangle = \begin{bmatrix}\alpha_0\\ \alpha_1\\ \vdots \\ \alpha_{2^n-1}\end{bmatrix} \in \mathbb{C}^{2^n}$$



IBMQ Brooklyn

1 qubit → 2 basis states
2 qubits → 4 basis states
....
n qubits → $2^n$ basis states



# Hamiltonian simulation and Trotterization

# Hamiltonian simulation

Simulate time evolution under Schrödinger equation for a time-dependent Hamiltonian

$$\frac{\partial}{\partial t}\psi(t) = -\mathrm{i}H(t)\psi(t)$$

$$H(t) \in \mathbb{C}^{2^N \times 2^N}$$

Hermitian matrix

Solved by applying the time-evolution operator:

$$U(t_1, t_0) = \mathcal{T} \exp\left(-\mathrm{i}\int_{t_0}^{t_1} H(t)dt\right)$$

to the initial state: $$\psi(t_1) = U(t_1, t_0)\psi(t_0)$$

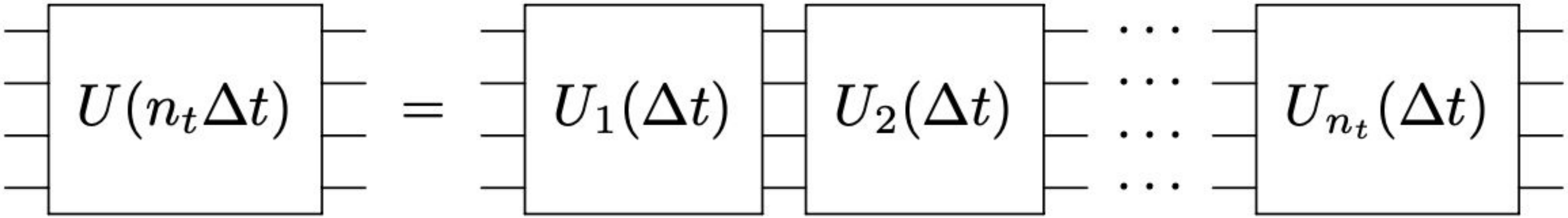
Time-independent case: $$U(t_1, t_0) = \exp\left(-\mathrm{i}(t_1 - t_0)H\right)$$

# Trotter splitting and time discretization

Trotter decomposition (or operator splitting):

$$H = A + B \qquad U(\Delta t) = \exp(-\mathrm{i}A\Delta t)\exp(-\mathrm{i}B\Delta t)$$

$$\|U(\Delta t) - \exp(-\mathrm{i}H\Delta t)\| \leq \frac{\Delta t^2}{2}\|[A, B]\|$$



# 1D Spin-$^1/_2$ Hamiltonians

Pauli spin-½ matrices: $\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $\sigma^y = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix}$, $\sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

Basis for: $\mathfrak{su}(2)$ Generators for: $\mathrm{SU}(2) = \left\{ \begin{bmatrix} \alpha & -\bar{\beta} \\ \beta & \bar{\alpha} \end{bmatrix} : \alpha, \beta \in \mathbb{C}, |\alpha|^2 + |\beta|^2 = 1 \right\}$

$$\sigma_i^\alpha := \underbrace{I \otimes \cdots \otimes I}_{i-1} \otimes \sigma^\alpha \otimes \underbrace{I \otimes \cdots \otimes I}_{N-i}$$

**Transverse field XY model:**

$$H(t) = \underbrace{\sum_{i=1}^{N-1} J_i^x(t)\, \sigma_i^x \sigma_{i+1}^x + J_i^y(t)\, \sigma_i^y \sigma_{i+1}^y}_{\text{Coupling}} + \underbrace{\sum_{i=1}^{N} h_i^z(t)\, \sigma_i^z}_{\text{External Field}}$$

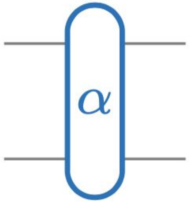
# Circuit diagrams

Single-qubit rotation over Pauli-α axis (α ∈ {x, y, z}):

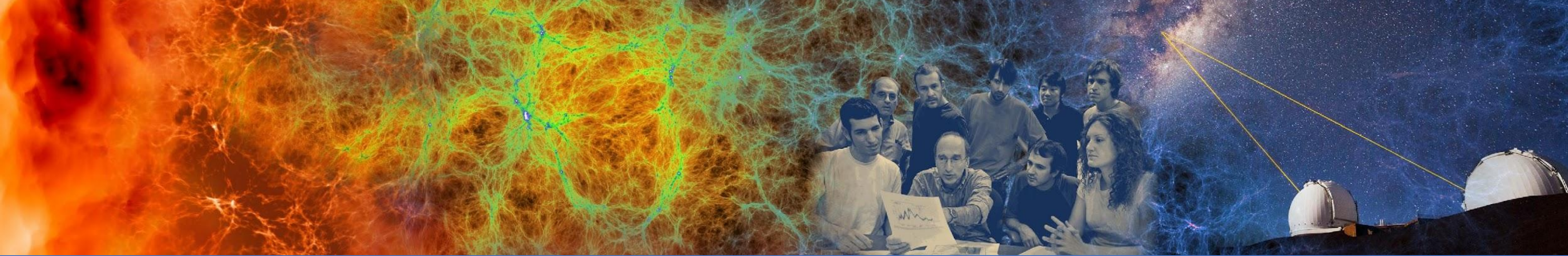
$$R^{\alpha}(\theta) := \exp(-\mathrm{i}\,\sigma^{\alpha}\,\theta/2) =$$


Two-qubit rotation over Pauli-α axis (α ∈ {x, y, z}):

$$R^{\alpha\alpha}(\theta) := \exp(-\mathrm{i}\,\sigma^{\alpha} \otimes \sigma^{\alpha}\,\theta/2) =$$




Easy operations to execute on QC: Native gate for ion traps, 2 CNOTs for superconducting



# Algebraic compression of Hamiltonian simulation circuits

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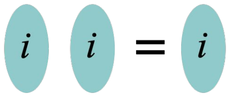
# Definition

A ***block*** is a parametrized and indexed family of operators $\mathbf{B}_i(\boldsymbol{\theta})$ that satisfy 3 properties:

- **Fusion:**

$$\mathbf{B}_i(\boldsymbol{\theta}_1)\mathbf{B}_i(\boldsymbol{\theta}_2) = \mathbf{B}_i(\hat{\boldsymbol{\theta}})$$

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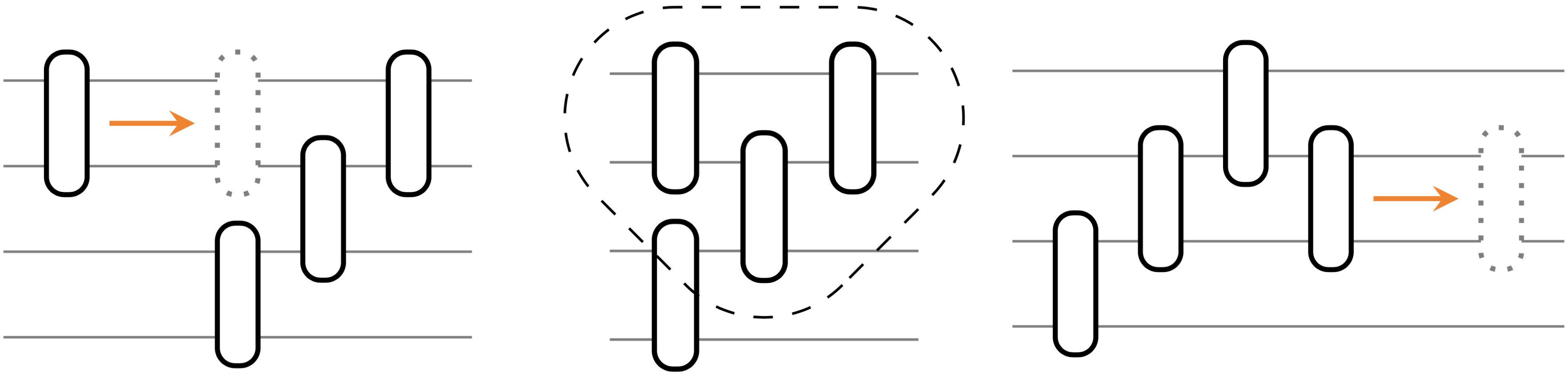
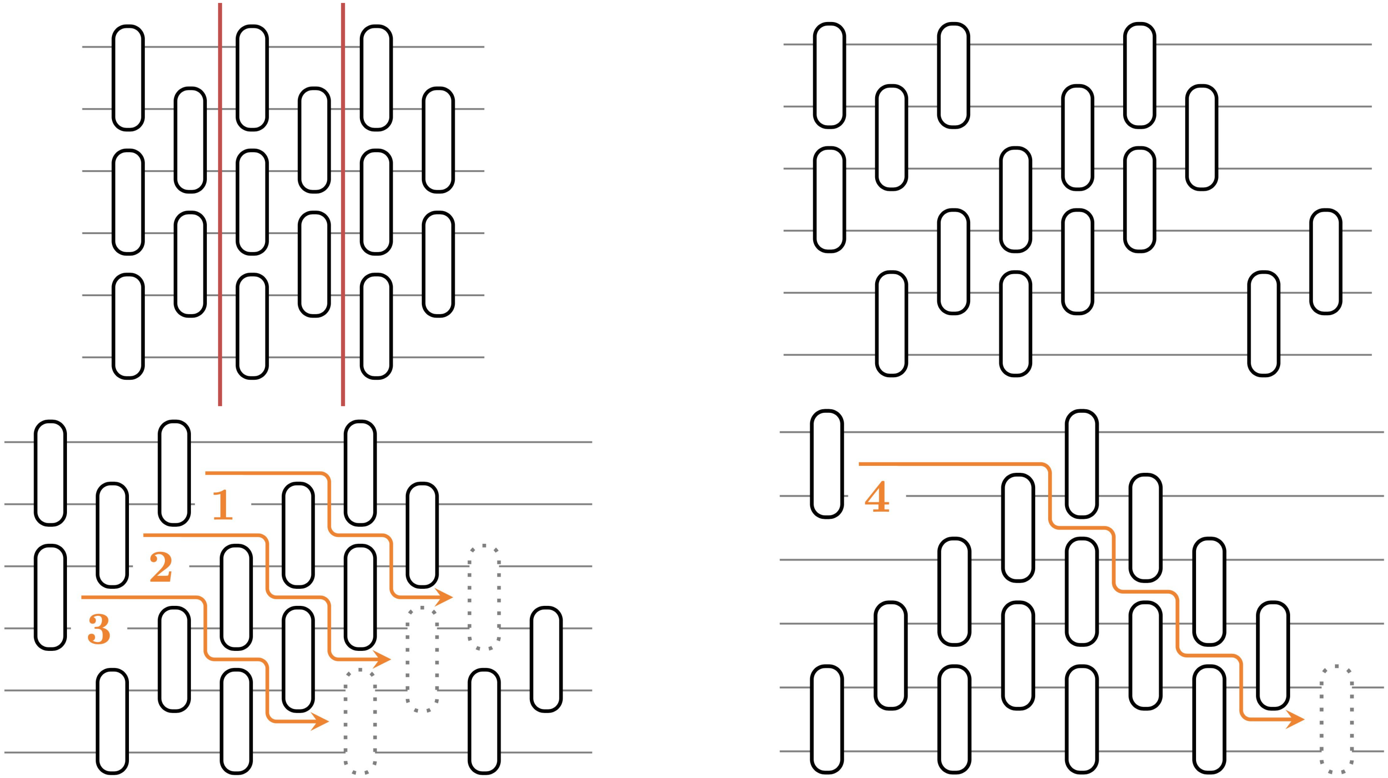
# Central mechanism in our compression algorithm



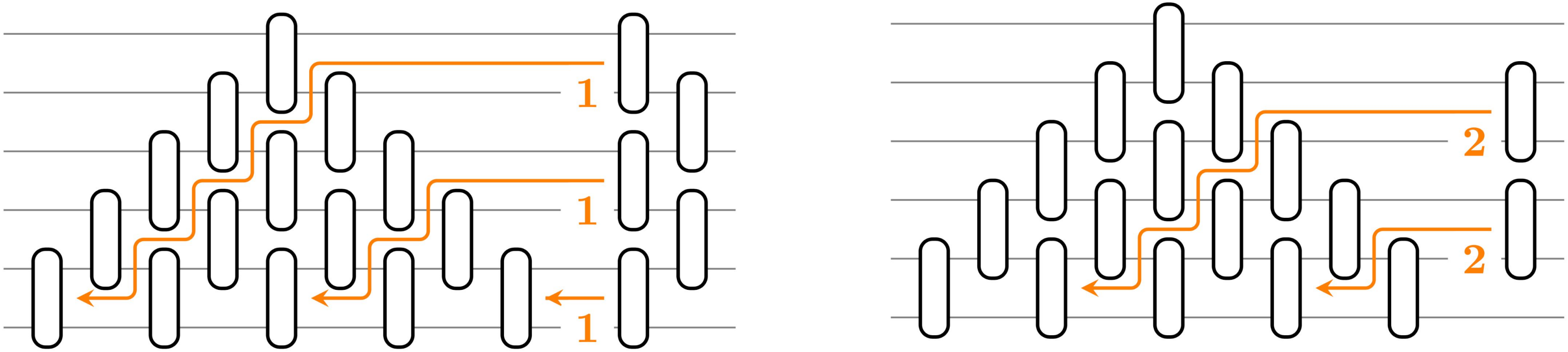
Equivalent mechanism as in *core-chasing* eigenvalue algorithms, but on operators of exponential dimension.

*Core-Chasing Algorithms for the Eigenvalue Problem*, Aurentz, Mach, Robol, Vandebril, Watkins

# Transforming squares to triangles



# Merging time-steps into triangles



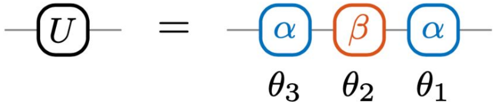

Even/odd blocks act on independent parts of the triangle. In our implementation, these are merged in parallel

# Euler decomposition and turnover of SU(2)

**Lemma: Euler decomposition**

Let α, β ∈ {x, y, z}, α≠β. Every U ∈ SU(2) can be represented as:

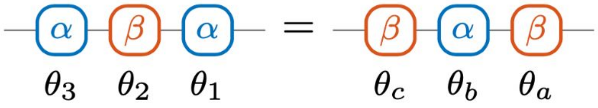
$$U = R^{\alpha}(\theta_1)\, R^{\beta}(\theta_2)\, R^{\alpha}(\theta_3),$$




**Lemma: SU(2) turnover**

Let α, β ∈ {x, y, z}, α≠β. For every $\theta_1$, $\theta_2$, $\theta_3$, there exist $\theta_a$, $\theta_b$, $\theta_c$ such that

$$R^{\alpha}(\theta_1)\, R^{\beta}(\theta_2)\, R^{\alpha}(\theta_3) = R^{\beta}(\theta_a)\, R^{\alpha}(\theta_b)\, R^{\beta}(\theta_c),$$

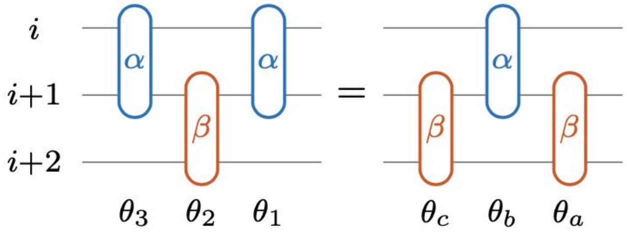


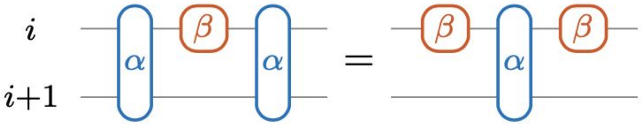

→ **We can compute the SU(2) turnover backward stable (Givens rotations)**

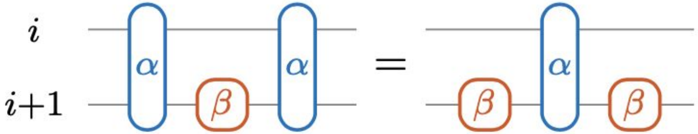
# SU(2) groups in disguise

**Lemma:**

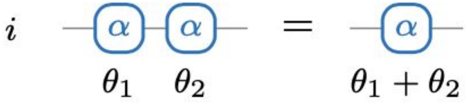
Let α, β ∈ {x, y, z}, α≠β. The following operations are also dual Euler decompositions of SU(2):

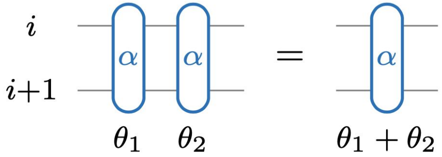



Fusion operations are trivial:



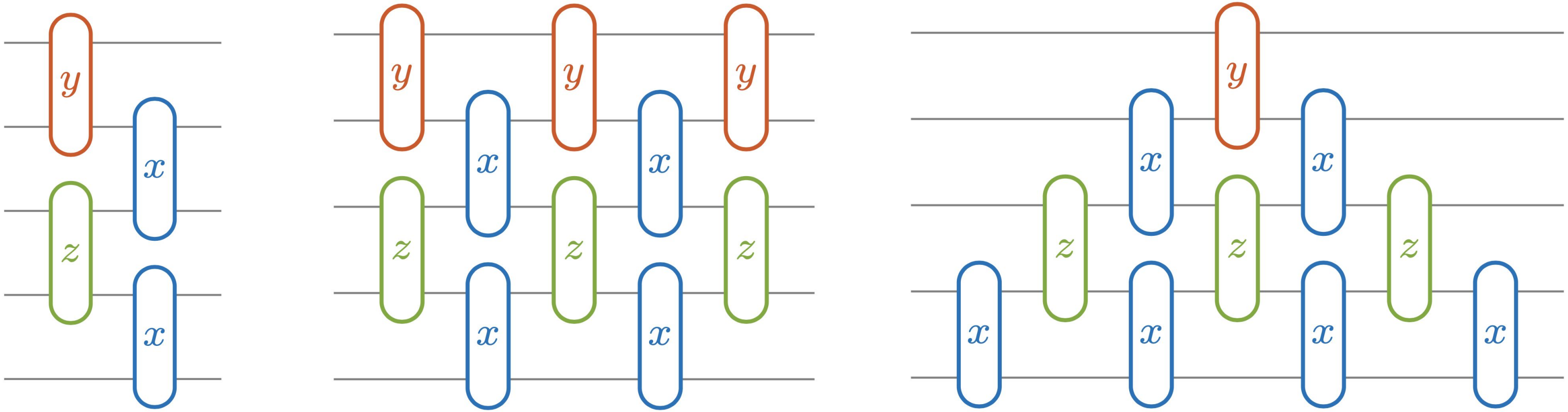



# Kitaev Chain

A Kitaev chain is a Hamiltonian of the form:

$$H(t) = \sum_{i=1}^{N-1} J_i^{\alpha_i}(t)\,\sigma_i^{\alpha_i}\sigma_{i+1}^{\alpha_i} \qquad \alpha_i \neq \alpha_{i+1}$$

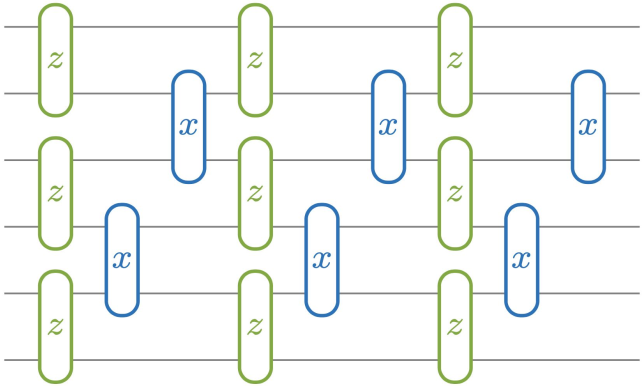
For example: $H(t) = J_1^y(t)\,\sigma_1^y\sigma_2^y + J_2^x(t)\,\sigma_2^x\sigma_3^x + J_3^z(t)\,\sigma_3^z\sigma_4^z + J_4^x(t)\,\sigma_4^x\sigma_5^x$

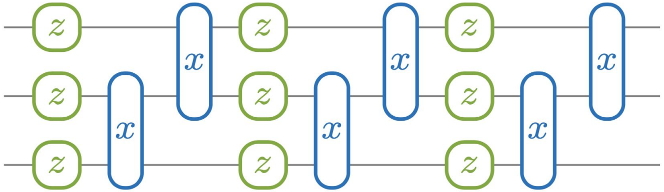


# TFIM Hamiltonian

The Transverse-Field Ising Model has the form:

$$H(t) = \sum_{i=1}^{N-1} J_i^{\alpha}(t)\, \sigma_i^{\alpha} \sigma_{i+1}^{\alpha} + \sum_{i=1}^{N} h_i^{\beta}(t)\, \sigma_i^{\beta} \qquad \alpha \neq \beta$$



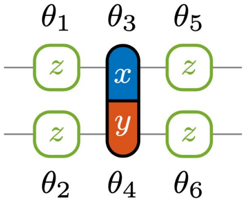


N-qubit TFIM is isomorphic to 2N-qubit Kitaev chain

# TFXY Hamiltonian

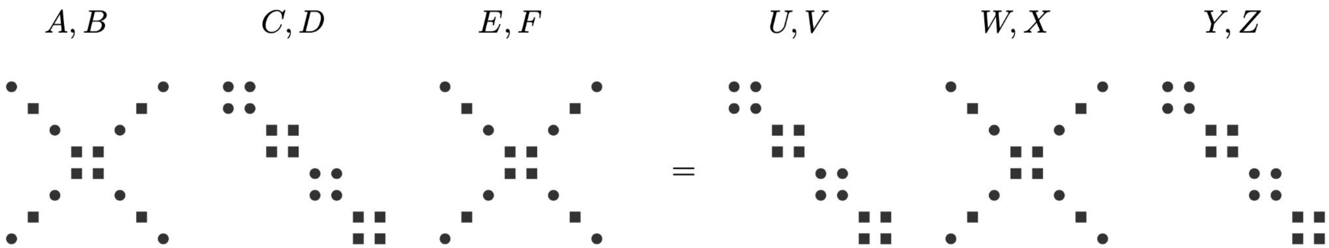
Transverse field XY model: $$H(t) = \underbrace{\sum_{i=1}^{N-1} J_i^x(t)\,\sigma_i^x\sigma_{i+1}^x + J_i^y(t)\,\sigma_i^y\sigma_{i+1}^y}_{\text{Coupling}} + \underbrace{\sum_{i=1}^{N} h_i^z(t)\,\sigma_i^z}_{\text{External Field}}$$

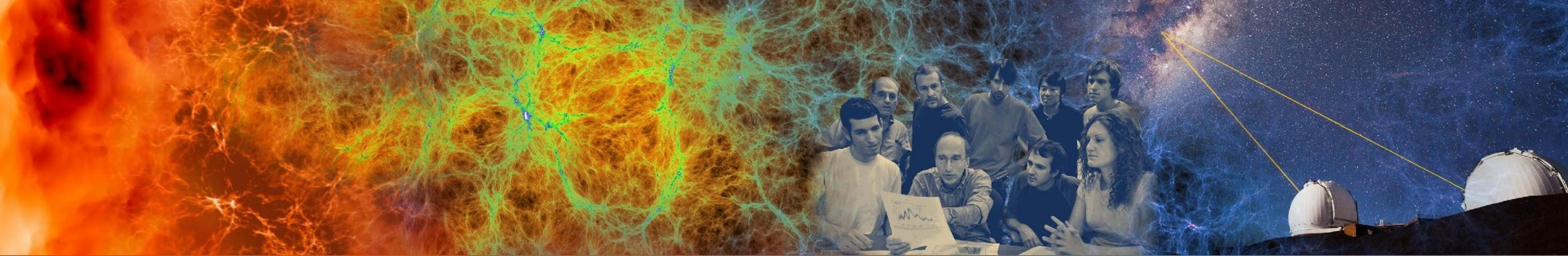
TFXY *block*:




$$= \begin{bmatrix} \alpha & & & -\bar{\delta} \\ & \beta & -\bar{\gamma} & \\ & \gamma & \bar{\beta} & \\ \delta & & & \bar{\alpha} \end{bmatrix}$$

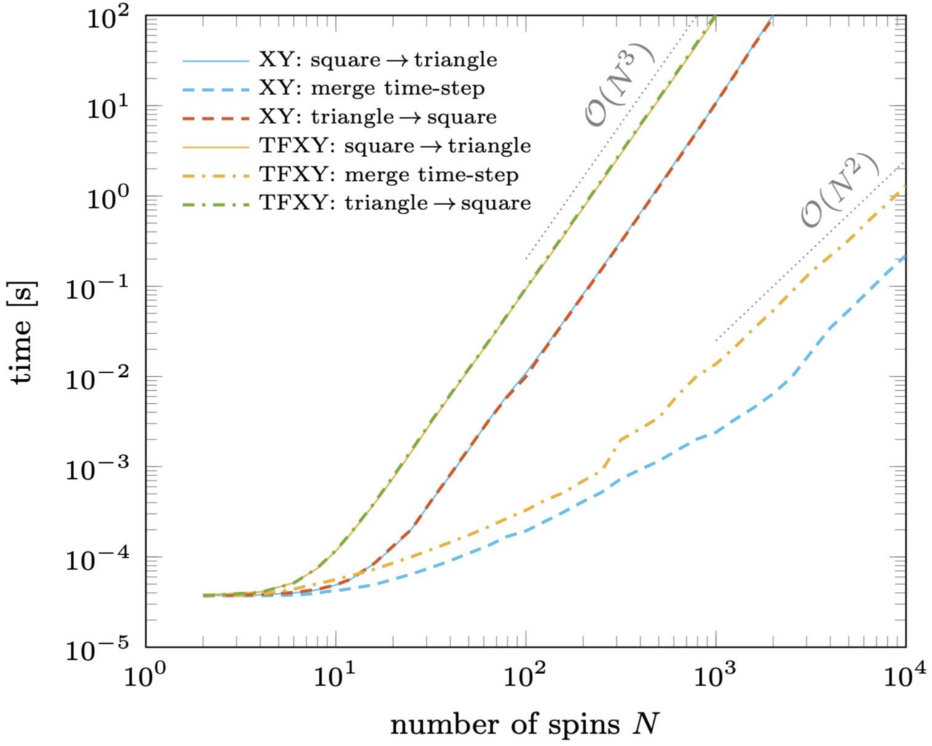
Turnover through simultaneous diagonalization



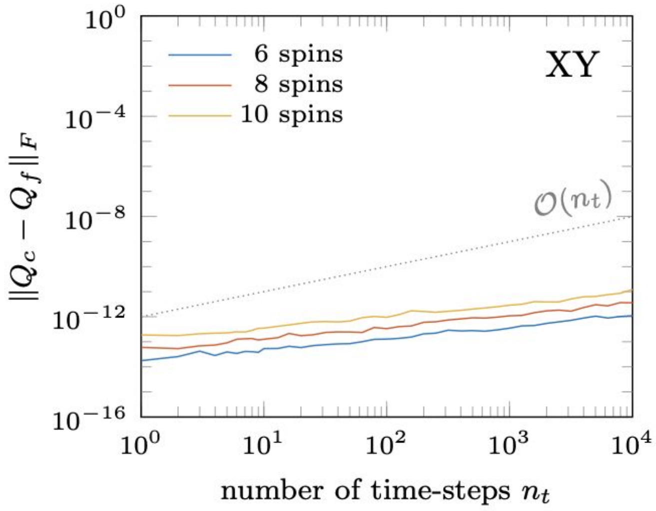


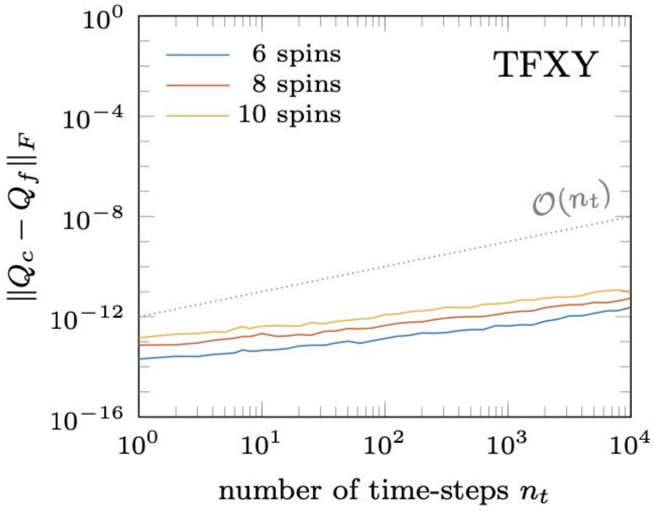
# Results

# Numerical results: timings



# Numerical results: backward error

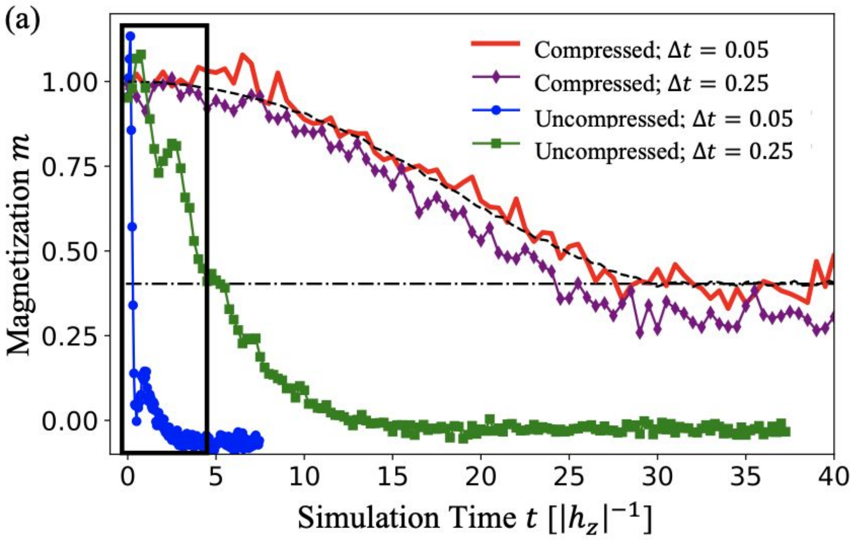


# Quantum Computer: Adiabatic State Preparation

- Time evolve TFIM in ground state from trivial state w/o coupling to more complicated ground state with coupling terms
- 5 qubit model on IBMQ Brooklyn
- Measure the average magnetization

$$H(t) = J(t)\sum_i \sigma_i^x \sigma_{i+1}^x + h\sum_i \sigma_i^z$$



# Conclusion

- Efficient and stable **classical** numerical algorithm for compression of quantum circuits for simulation of **integrable TFXY chains**
- **Enables simulation** of small systems on current generation noisy quantum hardware
  - Prepare **non-trivial states**
  - Simulate interesting physics phenomena
- Extensions to 2D non-interacting, controlled evolutions, ...

Fast Free Fermion Compiler (F3C):
[https://github.com/QuantumComputingLab](https://github.com/QuantumComputingLab)

**arXiv:2108.03282, arXiv:2108.03283**