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Lie algebraic perspectives on Hamiltonian evolution

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RPMBT XXI
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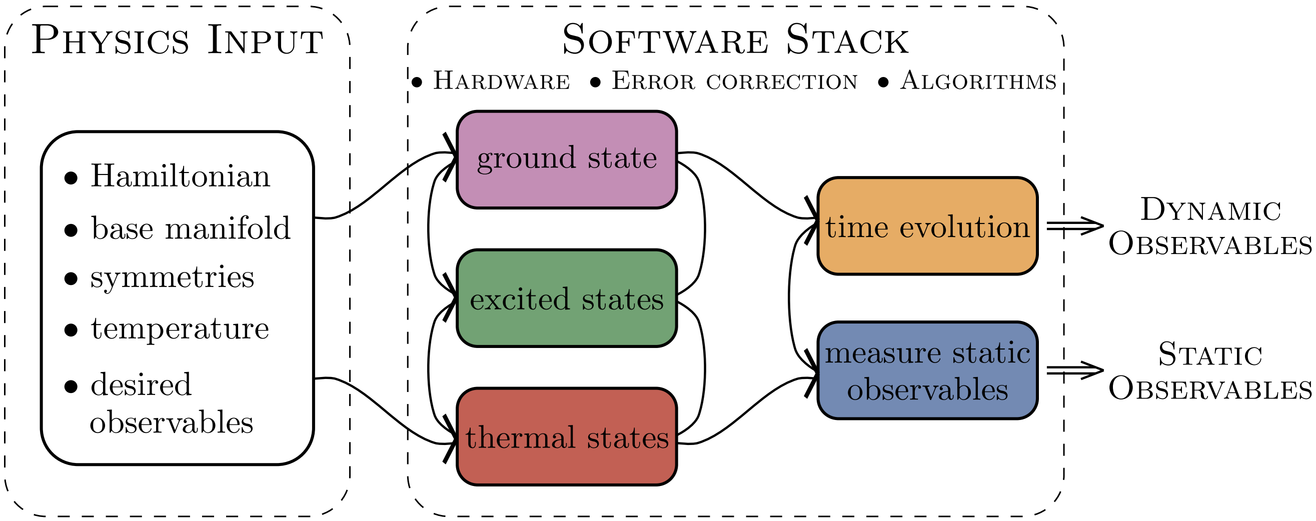
With:
Efekan Kökcü (**NCSU**)
Eugene Dumitrescu & Yan Wang (**ORNL**)
Daan Camps, Roel van Beeumen, Lindsay Bassman, Bert de Jong (**LBNL**)
Jim Freericks (**Georgetown**)

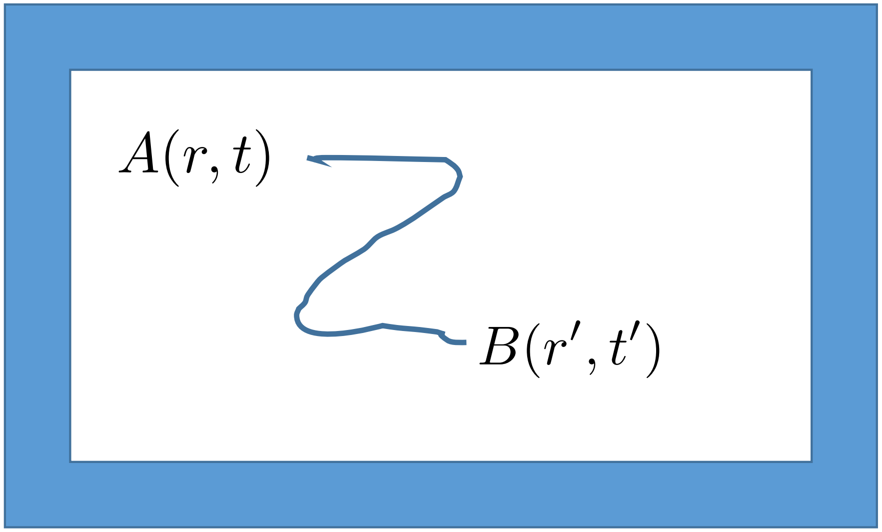
Quantum Matter meets Quantum Computing



- Experimental relevance: Measuring correlation functions
- Preparing/measuring topological states
- Driven/dissipative systems and fixed points
- Time evolution via Lie algebraic decomposition and compression
- Thermodynamics
- Physics-Informed Subspace Expansions

Low-energy excitations: correlation functions

$$\langle A(r,t) B(r',t') \rangle$$



Given some (observable) operator B at (r',t'), what is the likelihood of some (observable) operator A at (r,t)?

Low-energy excitations: correlation functions

Conductivity

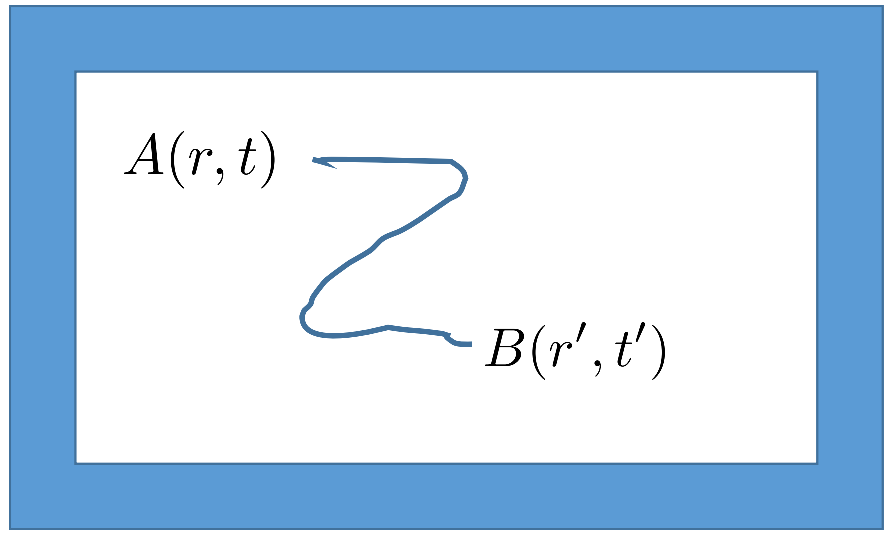
$$\langle j(r,t)j(r',t')\rangle$$

Single-particle spectra (ARPES)

$$\langle c(r,t)c^\dagger(r',t')\rangle$$

Spin-resolved neutron scattering

$$\sigma^{x,y,z}_{\alpha\beta}\langle S_\alpha(r,t)S_\beta(r',t')\rangle$$

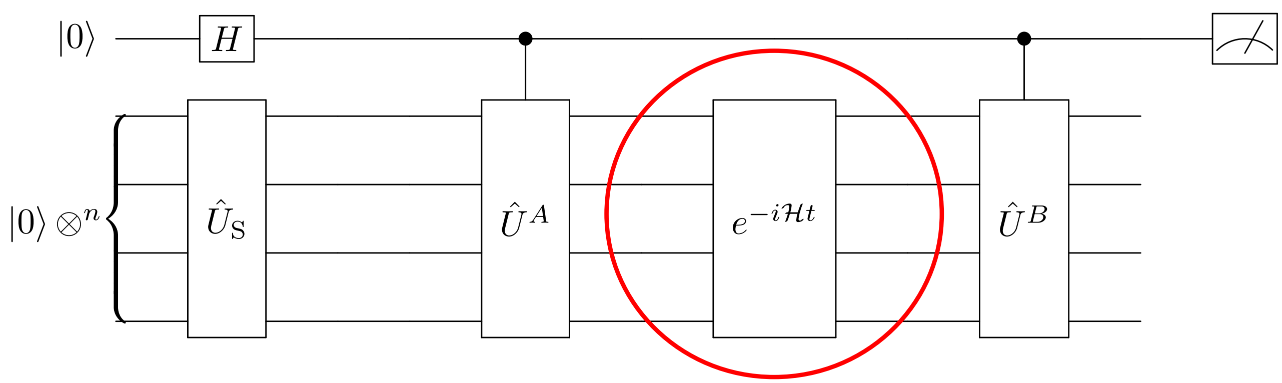


Low-energy excitations: correlation functions

Express the correlation function through the Lehmann representation:

$$C(t) = \langle \Phi | \hat{U}^B(t) \hat{U}^A(0) | \Phi \rangle = \sum_m e^{-i(E_m - E_0)t} \langle \phi_0 | U^B | m \rangle \langle m | U^A | \phi_0 \rangle \, .$$

Quantum circuit:



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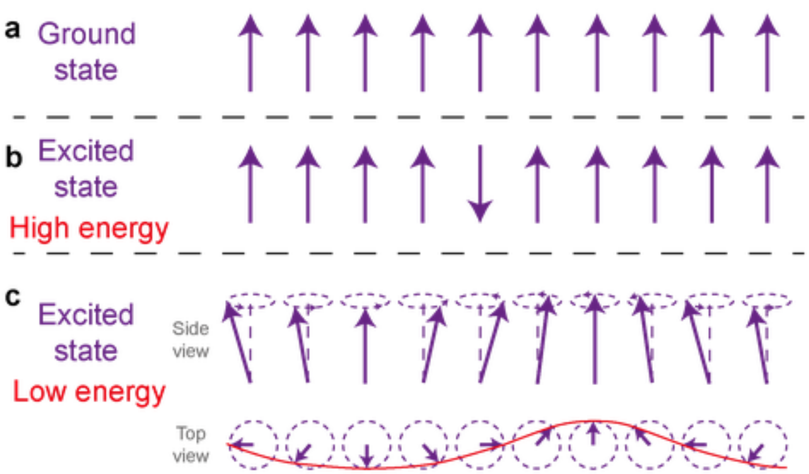
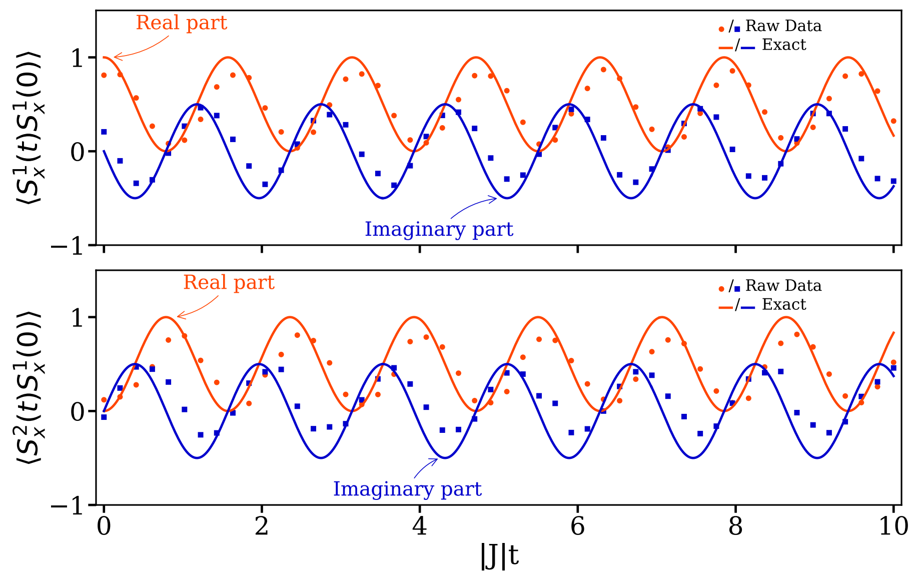
Low-energy excitations: 2-site magnons

Spin-spin correlation function for periodic Heisenberg model: Magnons!



$\uparrow\uparrow \quad \rightarrow \quad \uparrow\downarrow$

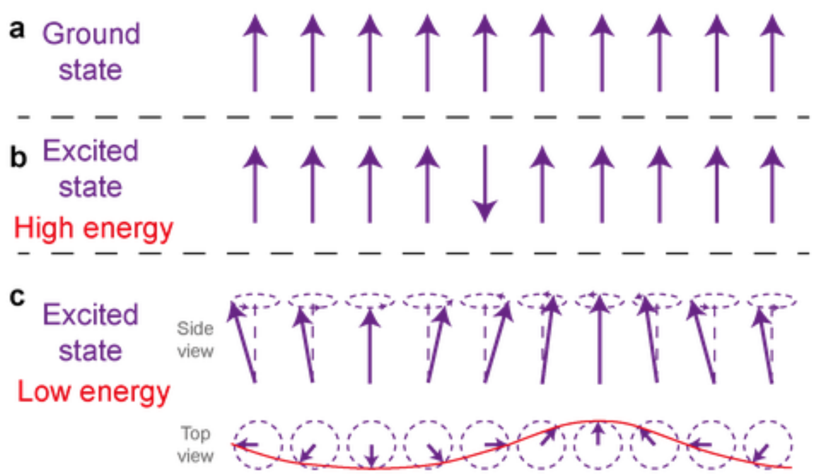


$$\hat{H} = 2SJ \sum_k (1 - \cos(k)) \hat{c}_k^\dagger \hat{c}_k$$

Data from *ibmq_tokyo*

Low-energy excitations: 4-site magnons

Spin-spin correlation function for periodic Heisenberg model $\uparrow\uparrow\uparrow\uparrow \rightarrow \uparrow\uparrow\uparrow\downarrow$



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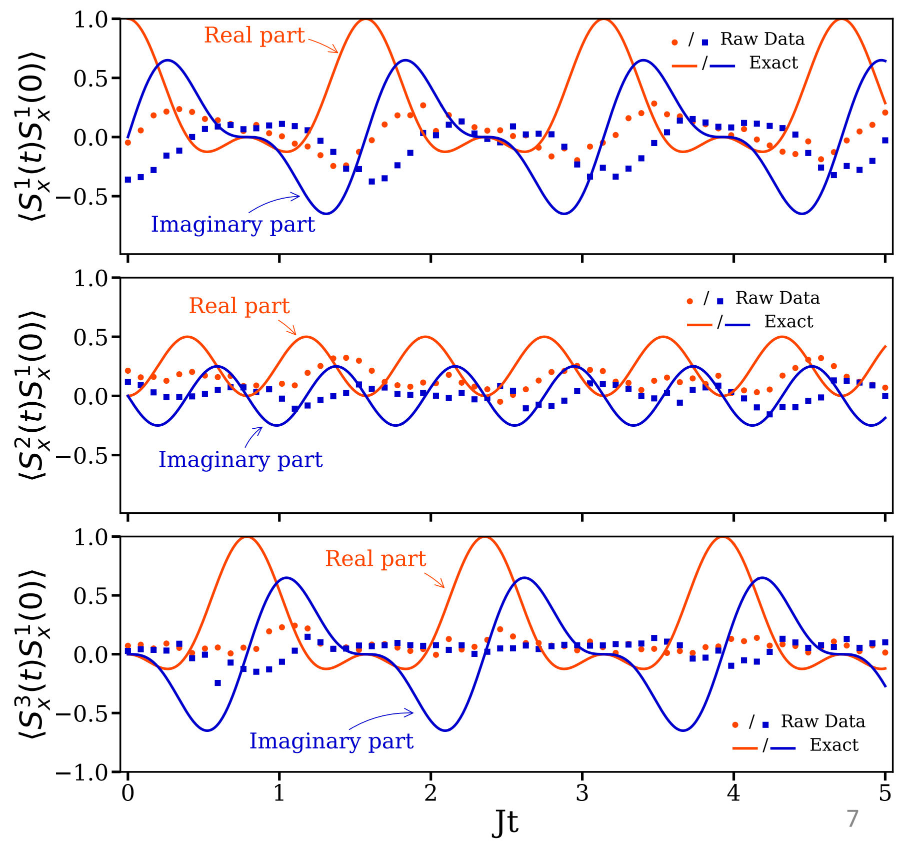

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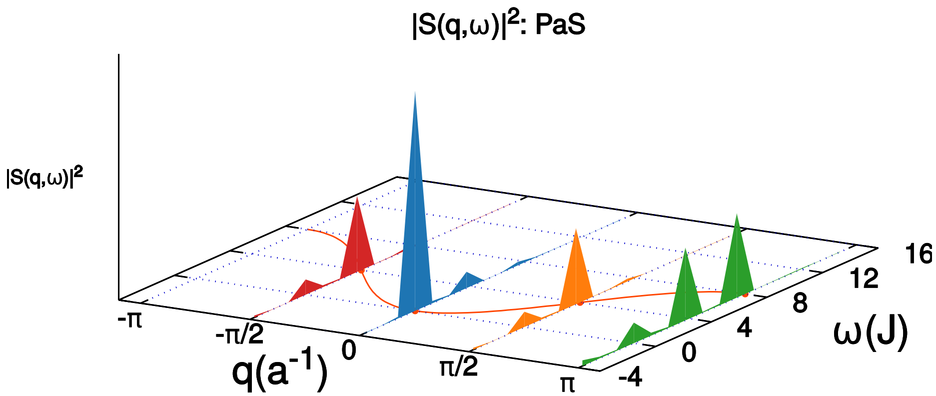

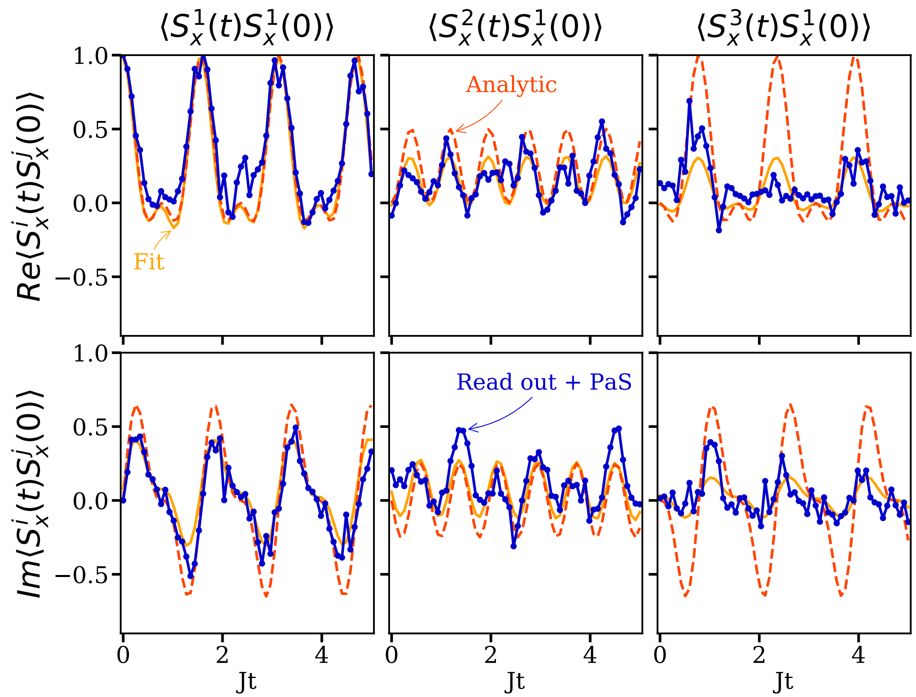

10.1103/PhysRevB.101.014411

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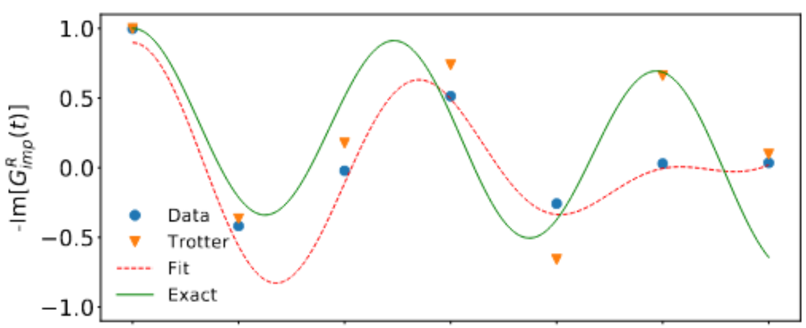
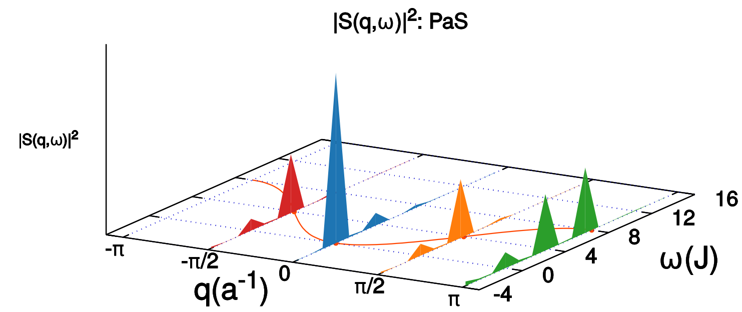
Low-energy excitations: 4-site magnons

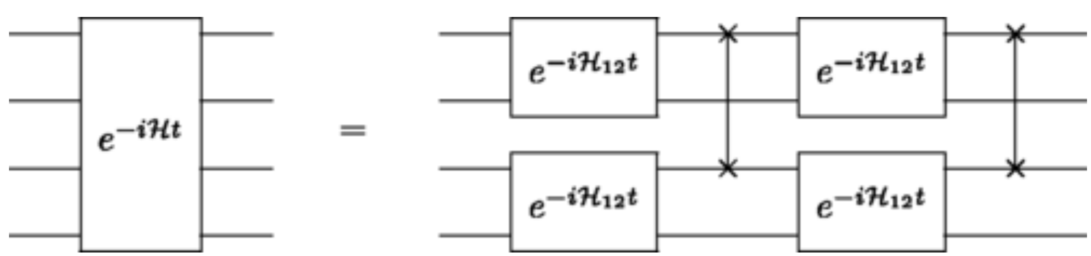
Q: Why does this work?



Keen et al., QST [10.1088/2058-9565/ab7d4c](https://doi.org/10.1088/2058-9565/ab7d4c)



A: Constant depth time evolution circuits



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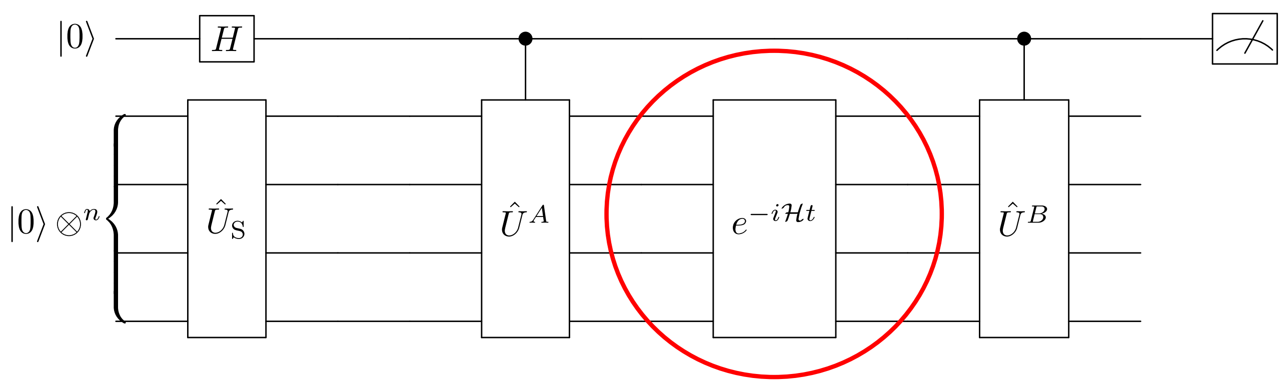
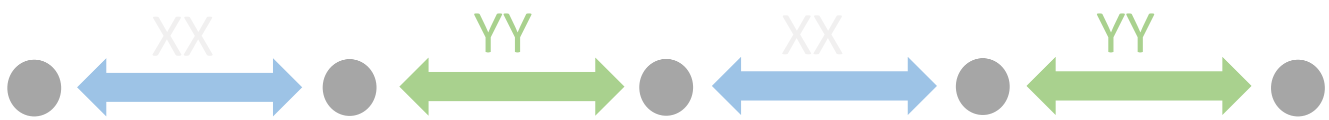
Quantum circuit:



Trotter Approximation

Consider 5 spin Kitaev chain:



$$\mathcal{H} = a\, XXIII + b\, IYYII + c\, IIXXI + d\, IIIYY$$

$$U(t) = e^{-it\mathcal{H}} \neq e^{-ita\, XXIII} e^{-itb\, IYYII} e^{-itc\, IIXXI} e^{-itd\, IIIYY}$$

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Trotter Approximation

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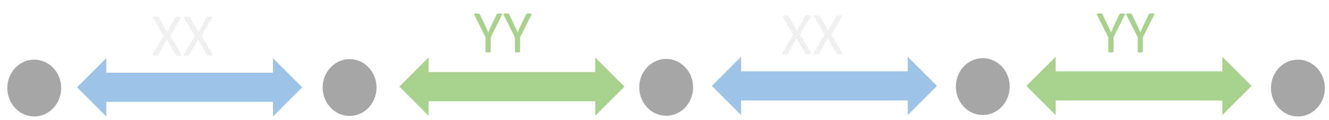

$$\mathcal{H} = a\,XXIII + b\,IYYII + c\,IIXXI + d\,IIIYY$$

$$U(\epsilon) = e^{-i\epsilon\mathcal{H}} = e^{-i\epsilon a\,XXIII} e^{-i\epsilon b\,IYYII} e^{-i\epsilon c\,IIXXI} e^{-i\epsilon d\,IIIYY} + O(\epsilon^2)$$

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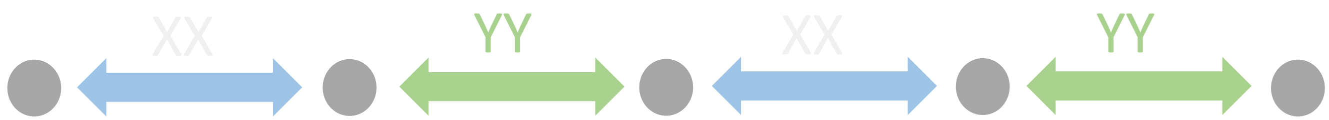

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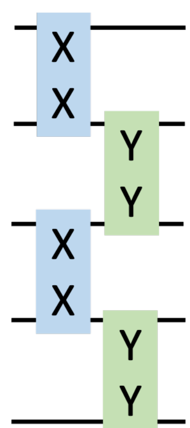

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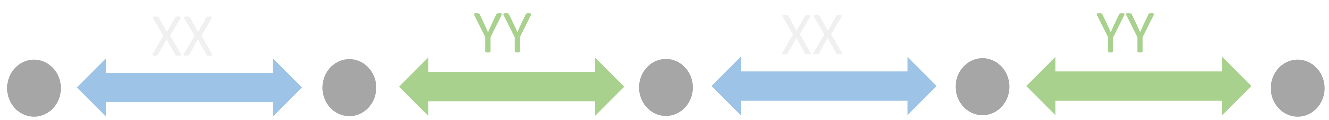

$$\mathcal{H} = a\, XXIII + b\, IYYII + c\, IIXXI + d\, IIIYY$$

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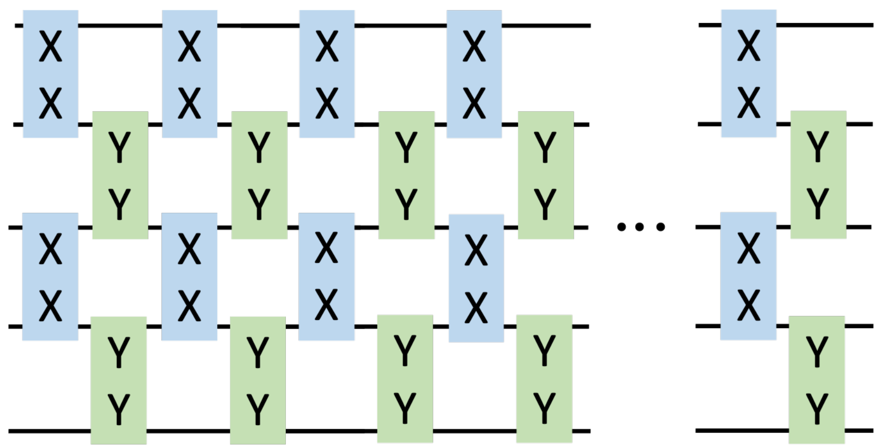
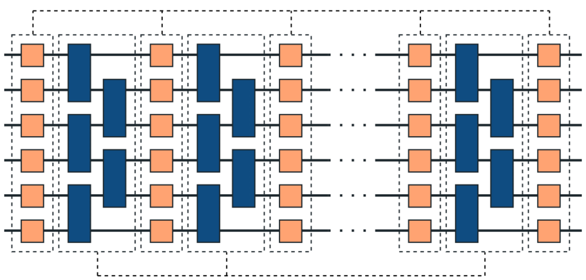
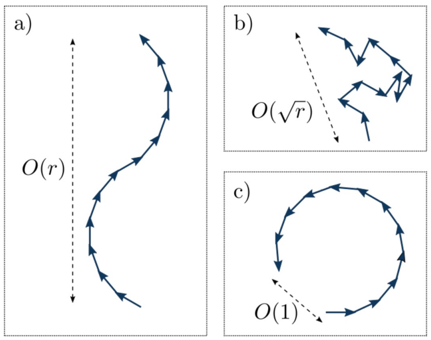
$U(t) =$



Improving Trotter Expansions

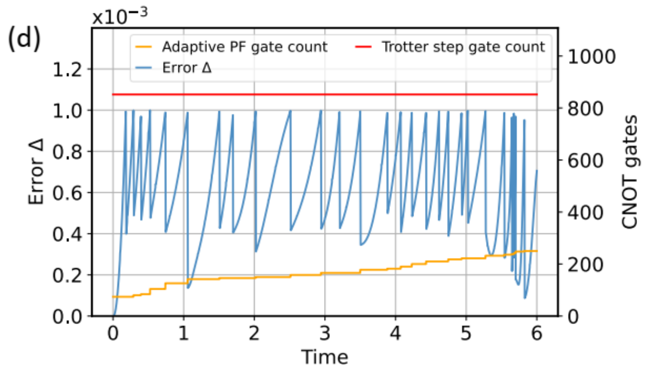
- Symmetry protection to reduce trotter error (*)





- Adaptive product formula to reduce number of trotter steps needed (**)

$$e^{-iH\delta t}|\Psi(t)\rangle \approx T(\vec{O}', \vec{\Lambda}', t)|\Psi_0\rangle$$



(*) Tran, M. C., Su, Y., Carney, D., & Taylor, J. M. (2021), PRX Quantum, 2(1), 010323.

(**) Zhang, Z. J., Sun, J., Yuan, X., & Yung, M. H. (2020), arXiv:2011.05283.

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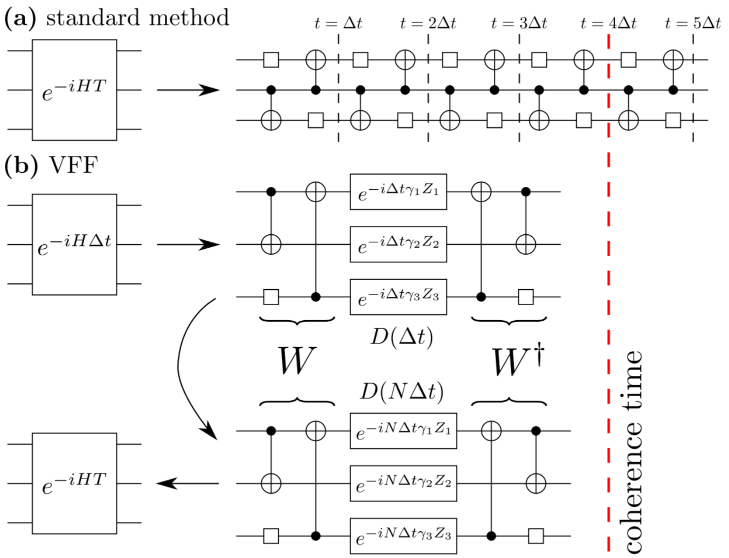
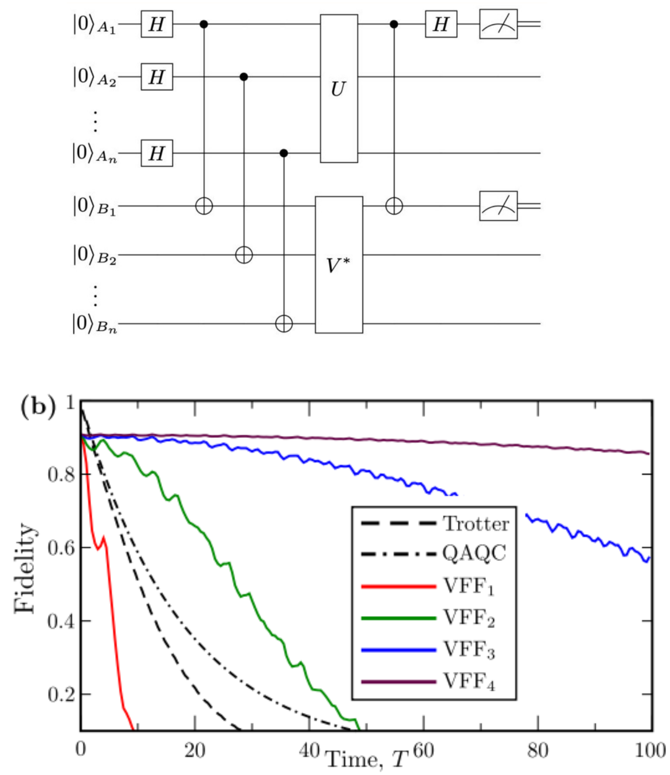
Variational Fast Forwarding

- QAQC on one trotter step to diagonalize the Hamiltonian
- then simulate for whichever simulation time you want with a fixed depth circuit!





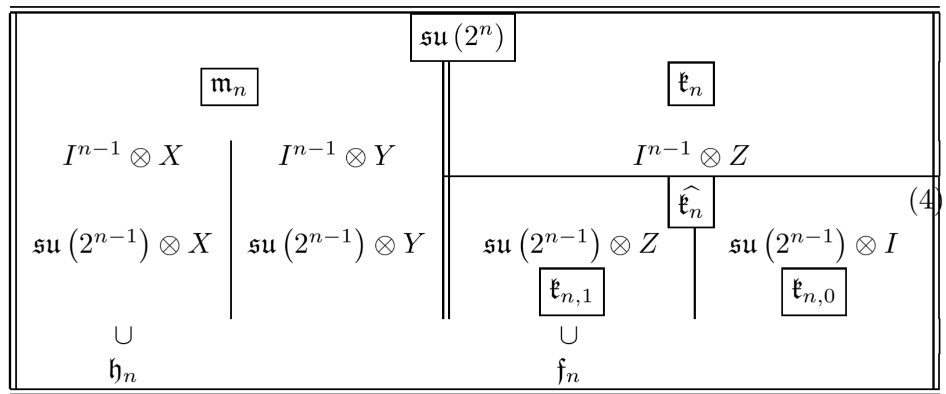
(*) Cirstoiu, C., Holmes, Z., Iosue, J., Cincio, L., Coles, P. J., & Sornborger, A. (2020), npj Quantum Information, 6(1), 1-10.

Unitary Synthesis: Cartan Decomposition

- Cartan decomposition found its application in generic unitary synthesis for quantum circuits (*,**)

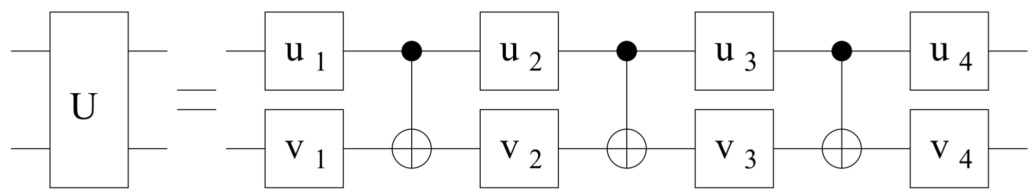
$$\mathfrak{g} = \mathfrak{m} \oplus \mathfrak{k}$$

$$\begin{aligned} [\mathfrak{k}, \mathfrak{k}] &\subset \mathfrak{k} \\ [\mathfrak{m}, \mathfrak{k}] &= \mathfrak{m} \\ [\mathfrak{m}, \mathfrak{m}] &\subset \mathfrak{k}. \end{aligned}$$



$$I^{n-1} = I^{\otimes(n-1)} = \underbrace{I \otimes .. \otimes I}_{n-1}$$

- It is optimal for SU(4) (2 qubits)! (***)



(*) N. Khaneja and S. J. Glaser, Chemical Physics 267, 11 (2001). (**) H. N. Sa Earp and J. K. Pachos, Journal of Mathematical Physics 46, 082108 (2005), doi.org/10.1063/1.2008210.

(***) G. Vidal and C. M. Dawson, Physical Review A 69, 010301 (2004).

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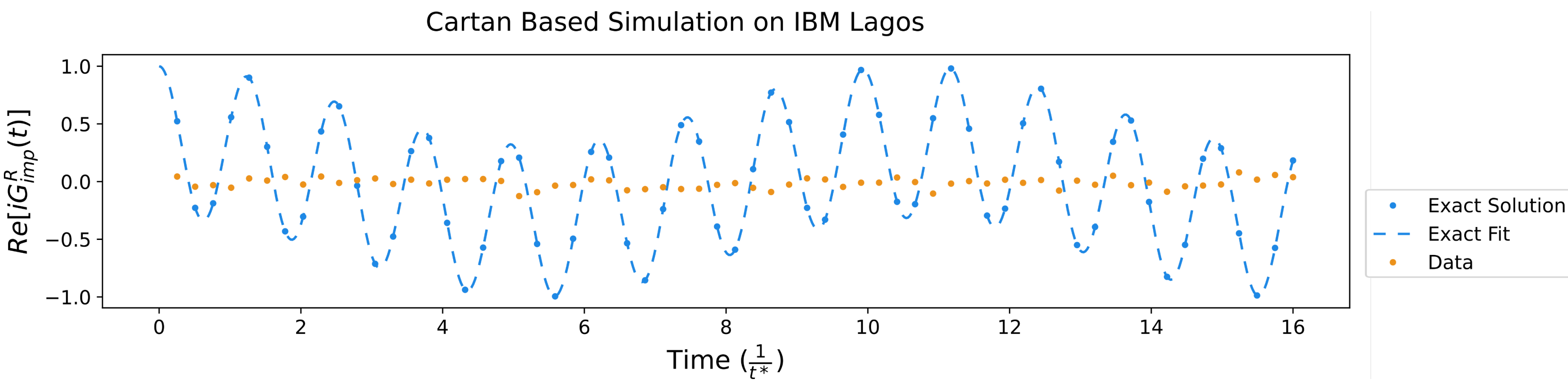
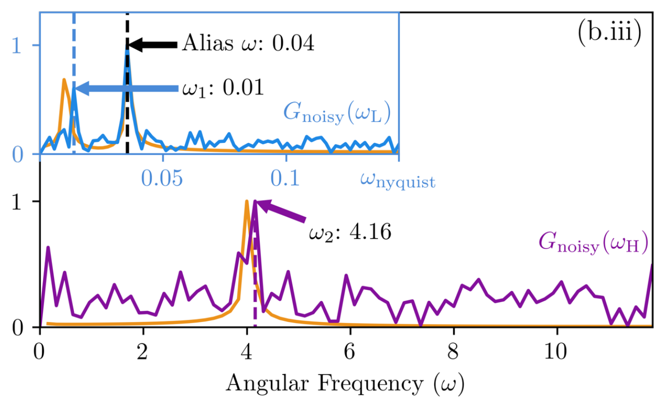
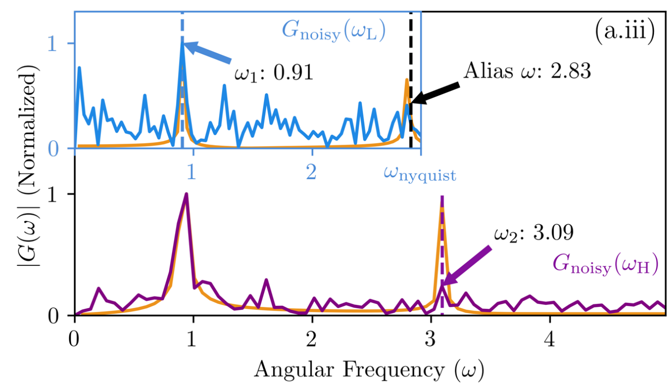
What can you do with fixed depth time evolution circuits?

[T. Steckmann et al., arXiv:2112.05688](https://arxiv.org/abs/2112.05688)

2-site Hubbard DMFT (5 qubits)







2-site Hubbard DMFT

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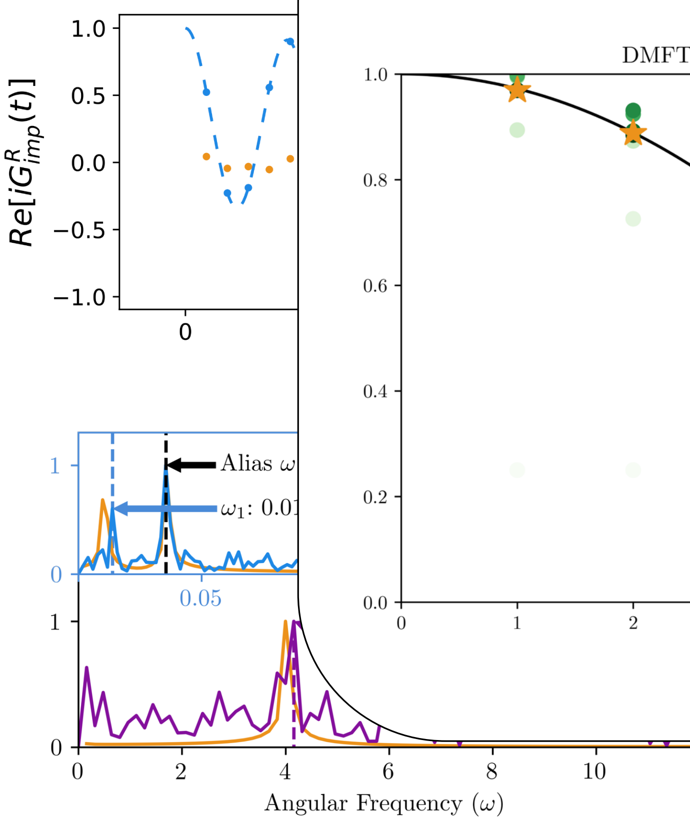
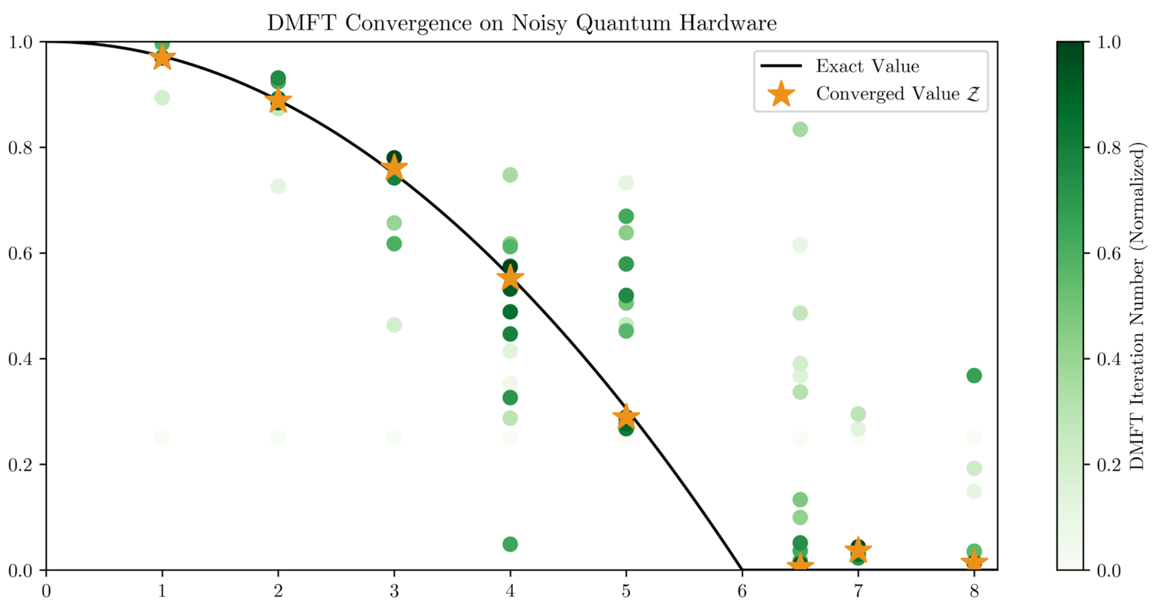
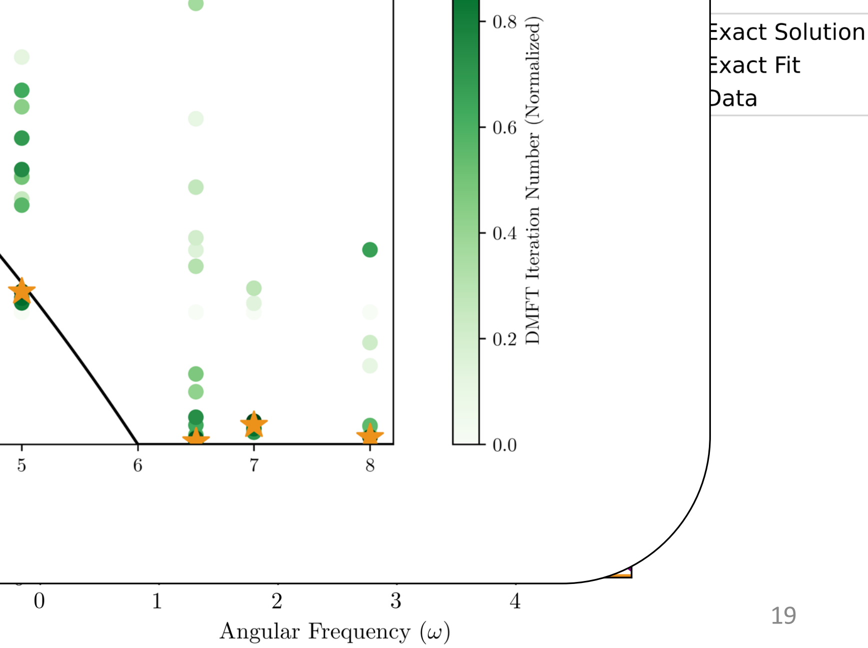


Self-consistent DMFT phase diagram showing the metal-insulator transition for 2-site Hubbard model





2 Algebraic methods for circuit compression

Cartan Decomposition

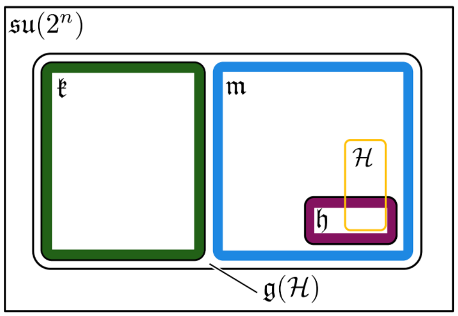
Algebraic Compression

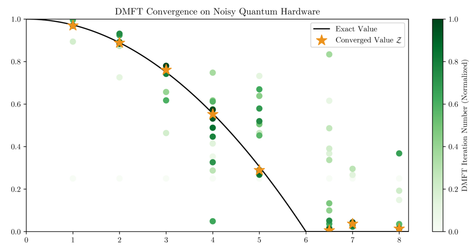
Phys. Rev. Lett. 129, 070501 (2022) , arXiv:2112.05688

Phys. Rev. A 105, 032420 (2021), SIMAX 2022 43:3, 1084-1108

2 Algebraic methods for circuit compression

Cartan Decomposition





- Produces exact, fixed depth time evolution unitaries for any model.
- Produces unitaries for linear combinations of (anti)-Hermitian operators (UCC factors).
- We have code available! https://github.com/kemperlab/cartan-quantum-synthesizer

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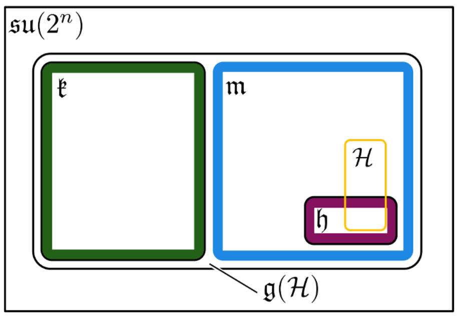

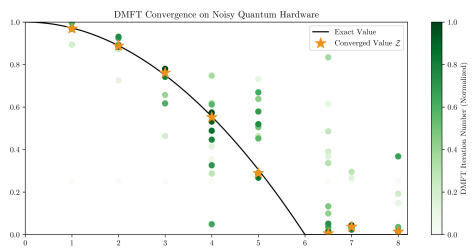

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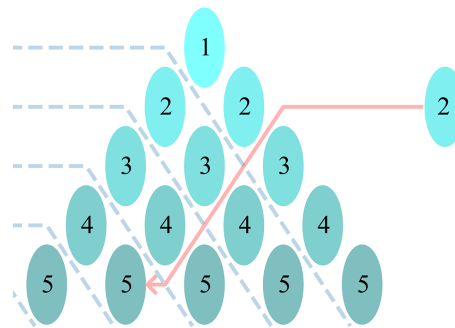

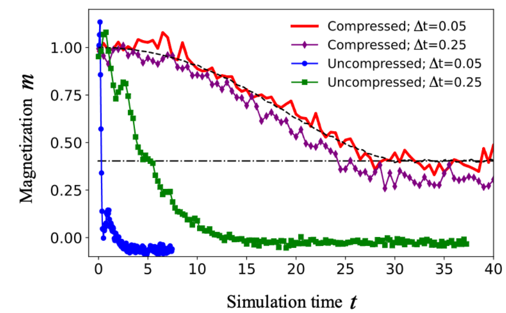

- Compressed Trotter circuits down to a shallow fixed depth circuit for 1-D nearest neighbor TFXY, TFIM, XY and Kitaev models.
- Based on 3 easy to check, local properties.
- We have code available! Check F3C, F3C++ and F3Cpy at https://github.com/QuantumComputingLab

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Approach #1: Cartan Decomposition

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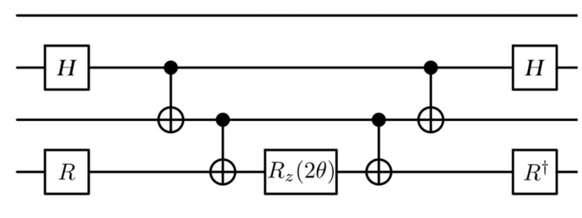
Exact simulation of a time independent spin Hamiltonian: $\mathcal{H} = \sum_j h_j \sigma^j$

Time evolution operator: $U(t) = e^{-it\mathcal{H}} = \prod_{\bar{\sigma}^i \in \mathfrak{su}(2^n)} e^{i\kappa_i \bar{\sigma}^i}$

Single exponential circuit:

$e^{i\theta IXZYI} =$



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Main Problem

Exact simulation of a time independent spin Hamiltonian: $\mathcal{H} = \sum_j h_j \sigma^j$

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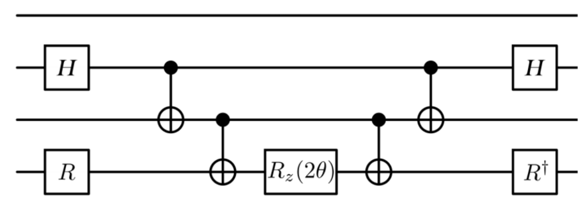

Two main issues:

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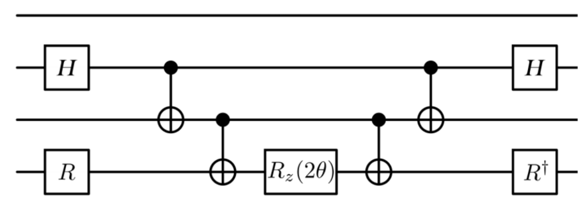

Two main issues: **1)** $4^n - 1$ many κ_i

2) What cost function? Norm of the difference?

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Hamiltonian Algebra

- We don't have to work in full $\mathfrak{su}(2^n)$

$$\mathcal{H} = \sum_j h_j \sigma^j$$

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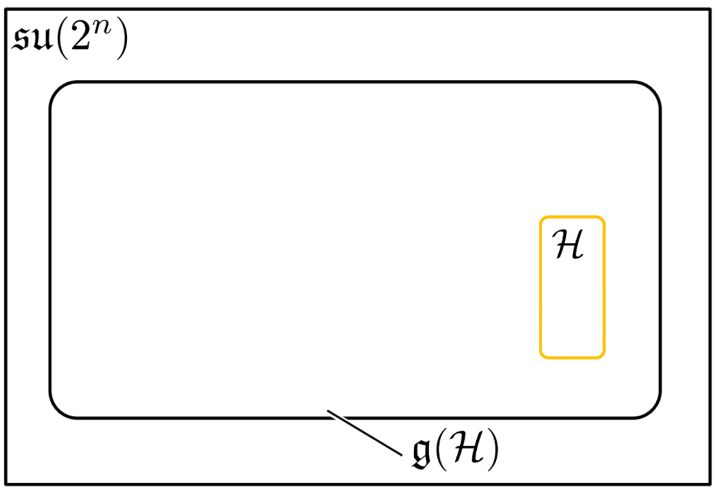
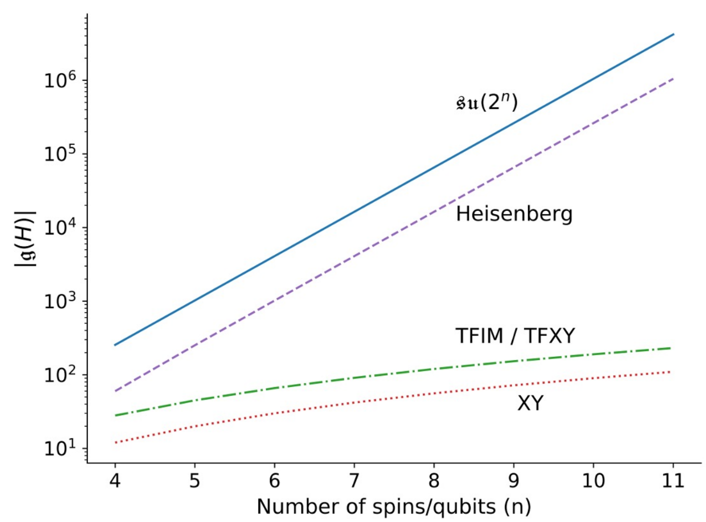
Hamiltonian Algebra

- We don't have to work in full $\mathfrak{su}(2^n)$
- Get the closure of the Pauli strings within the Hamiltonian under commutation i.e. the "Hamiltonian algebra" g(H)

$$\mathcal{H} = \sum_j h_j \sigma^j$$

$$U(t) = e^{-it\mathcal{H}} = \prod_{\substack{\cancel{\bar{\sigma}^i \in \mathfrak{su}(2^n)} \\ \bar{\sigma}^i \in \mathfrak{g}(\mathcal{H})}} e^{i\kappa_i \bar{\sigma}^i}$$





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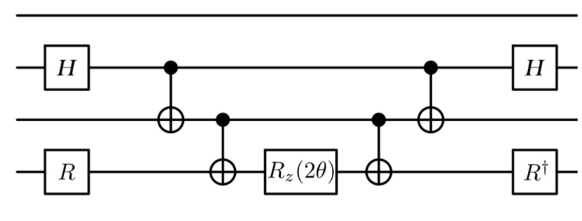
Single exponential circuit is given as: $e^{i\theta IXZYI} =$



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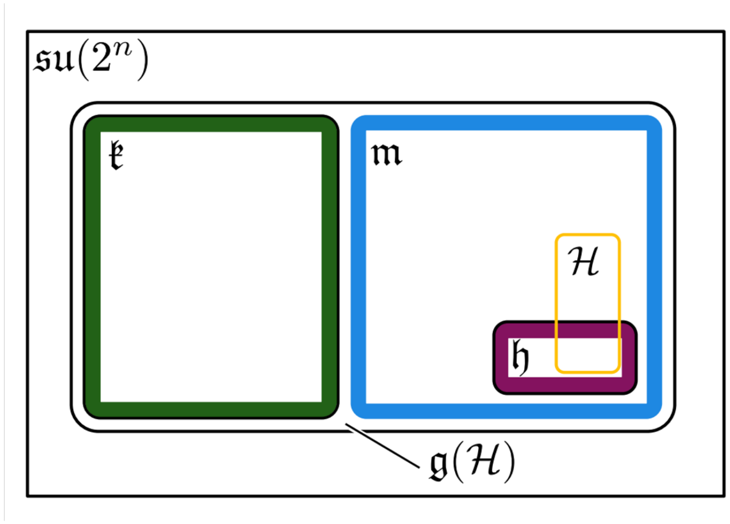
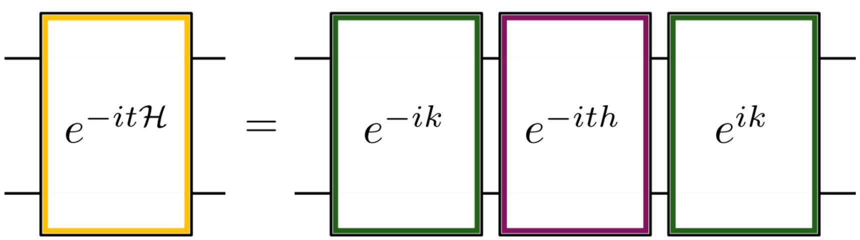
Cartan Decomposition and KHK Theorem





Have $H \in \mathfrak{m}$, and consider the following function

$$\boxed{f(K) = \langle K v K^\dagger H \rangle}$$

where

$$K = e^{\theta_1 k_1} e^{\theta_2 k_2} ... e^{\theta_{n_k} k_{n_k}}$$

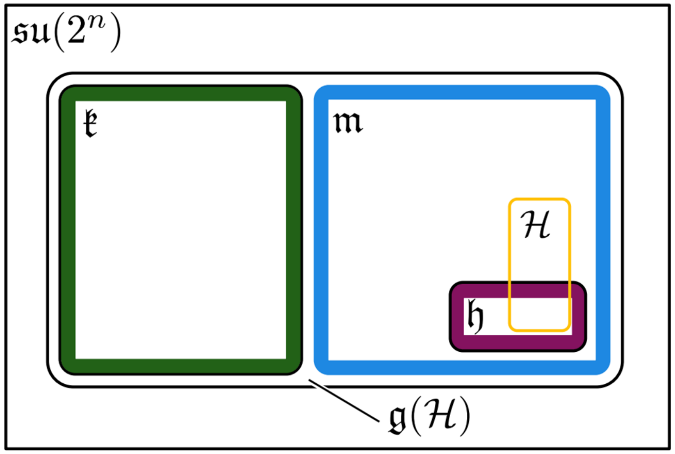
$$v = h_1 + \pi h_2 + \pi^2 h_3 + ... + \pi^{n_h - 1} h_{n_h}$$

Then for any local minimum or maximum of the function f denoted by K_0 will satisfy

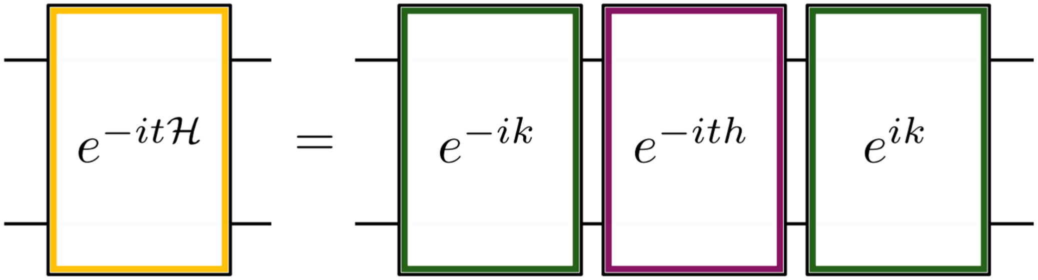
$$K_0^\dagger H K_0 \in \mathfrak{h}$$

Algorithm

1) Generate Hamiltonian algebra g(H)
2) Find a Cartan decomposition where H is in m
3) Obtain parameters via local minimum of f(K)
4) Build the circuit using K and h
5) Then simulate for any time you want!



$$f(K) = \langle K v K^\dagger, \mathcal{H} \rangle$$



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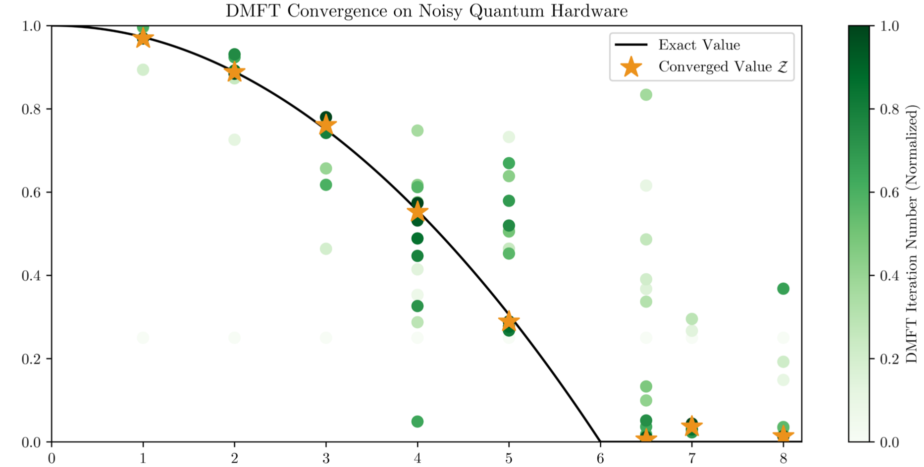
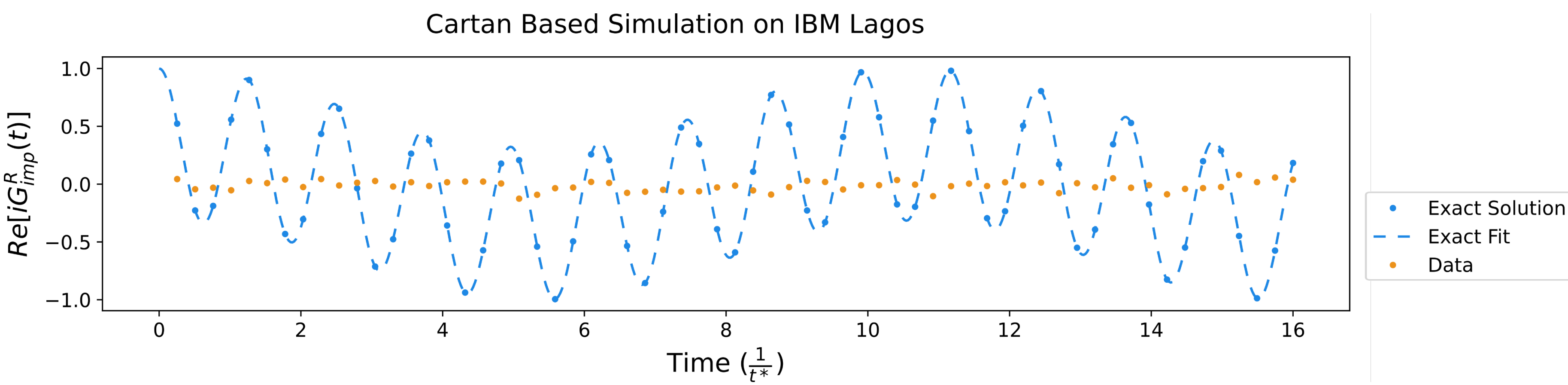
Approach #1: Cartan Decomposition

- $O(n^2)$ circuit for TFIM, TFXY, XY
- Applicable for any model
- Optimize only once for any time t
- Obtained 1st ever self-consistent DMFT Hubbard phase diagram on IBM QC.





[T. Steckmann et al., arXiv:2112.05688]

Approach #2: Algebraic Circuit Compression

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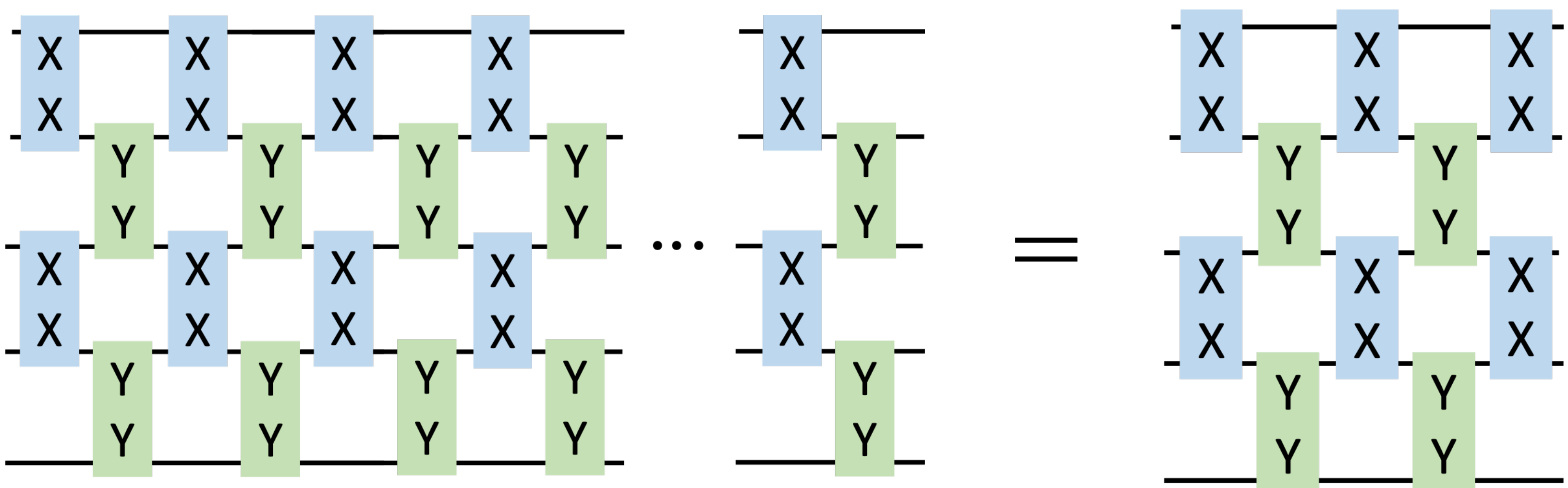
Approach #2: Algebraic Circuit Compression

- We propose a **constructive,** Lie algebra based method which leads to fixed depth circuits for several models

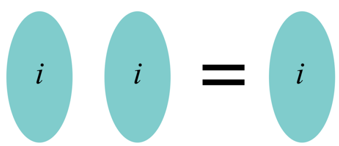
- The method is **scalable** due to its “constructive” and “local” nature.



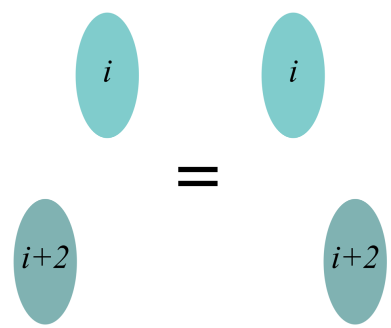
Approach #2: Algebraic Circuit Compression

We define an abstract object called “block” which satisfies:

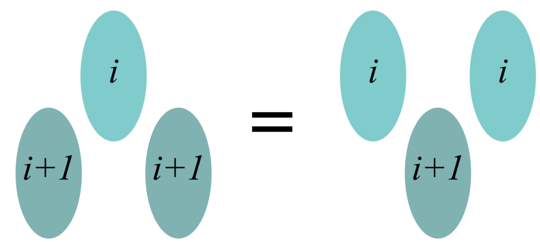
Fusion



Commutation



Turnover

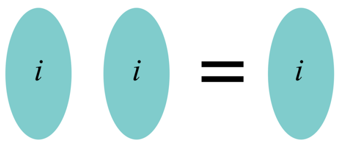


Blocks will be mapped to certain quantum gates in a model specific way.

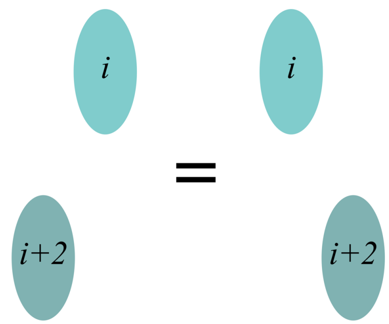
These properties are **local**! One needs to check only the neighbor gates to apply them, not the whole circuit.

Approach #2: Algebraic Circuit Compression

Fusion



Commutation



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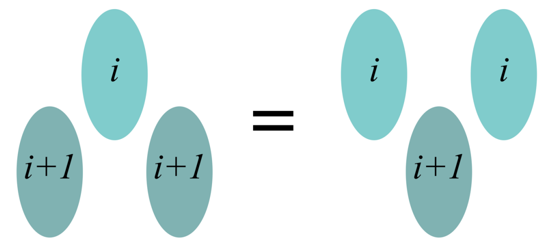
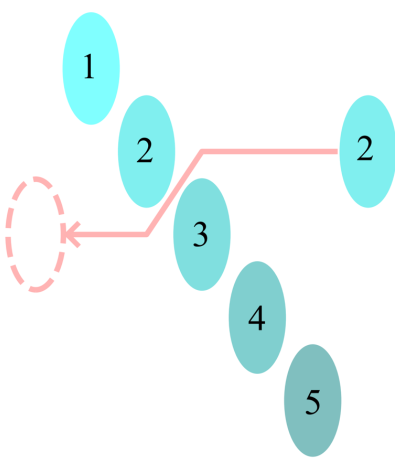
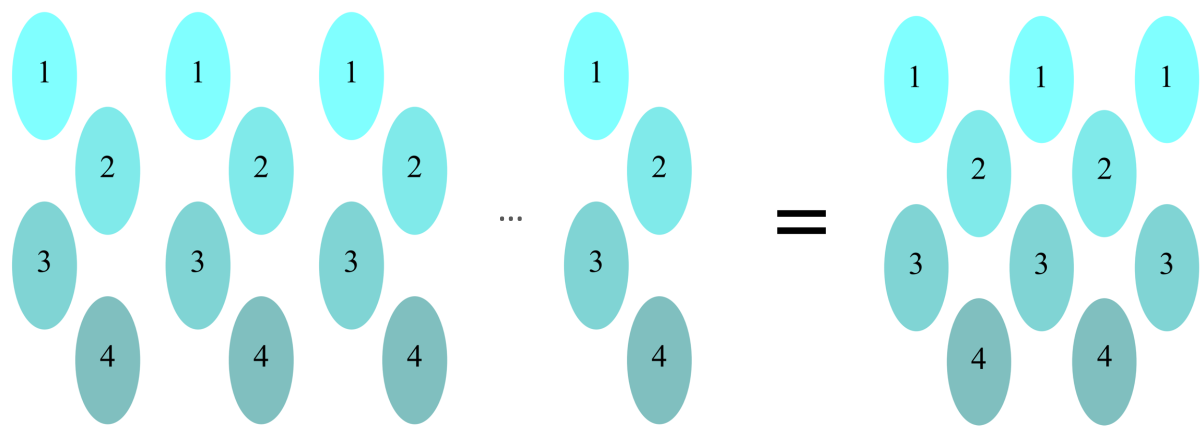
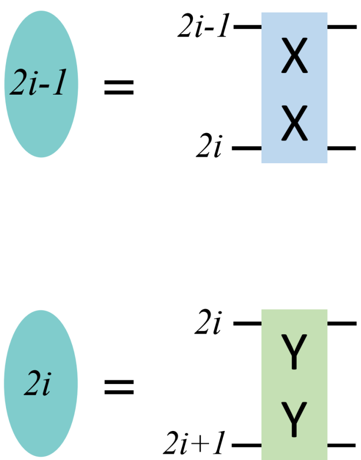






Examples

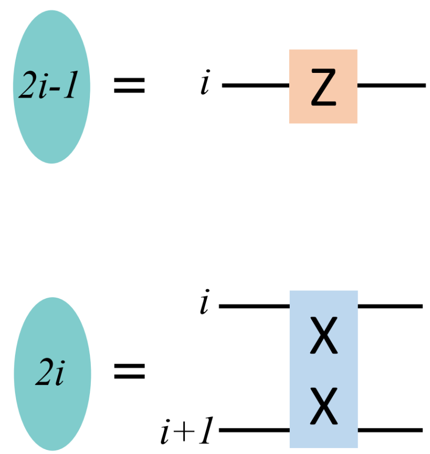
Kitaev Chain



n(n-1)/2 XX gates

n(n-1) CNOTs

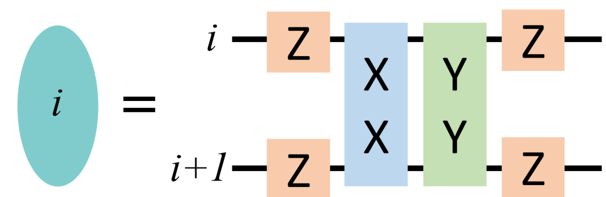
Transverse Field Ising



n(n-1) XX gates

2n(n-1) CNOTs

Transverse Field XY



n(n-1) XX gates

n(n-1) CNOTs

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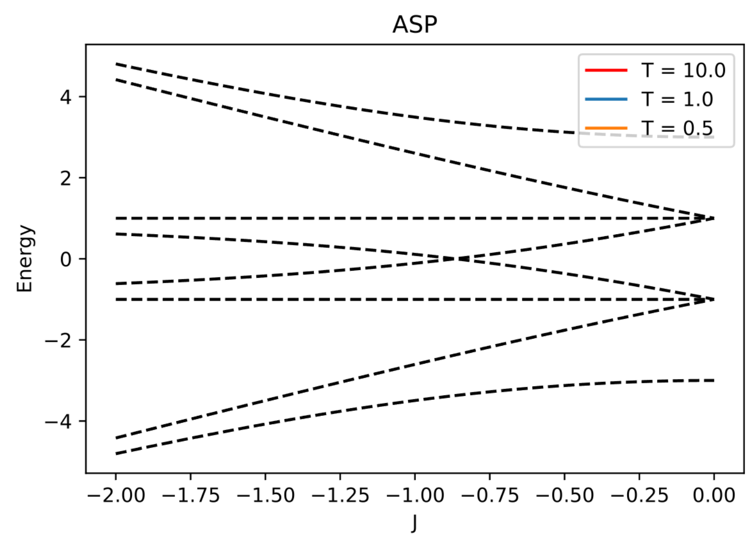
Main Example: Ising Adiabatic State Preparation

$$H = -2(X_1X_2 + X_2X_3) - (Z_1 + Z_2 + Z_3)$$



$$H = -(Z_1 + Z_2 + Z_3)$$

$$|\psi\rangle = |000\rangle$$

$$H = J(t)(X_1X_2 + X_2X_3) - (Z_1 + Z_2 + Z_3)$$

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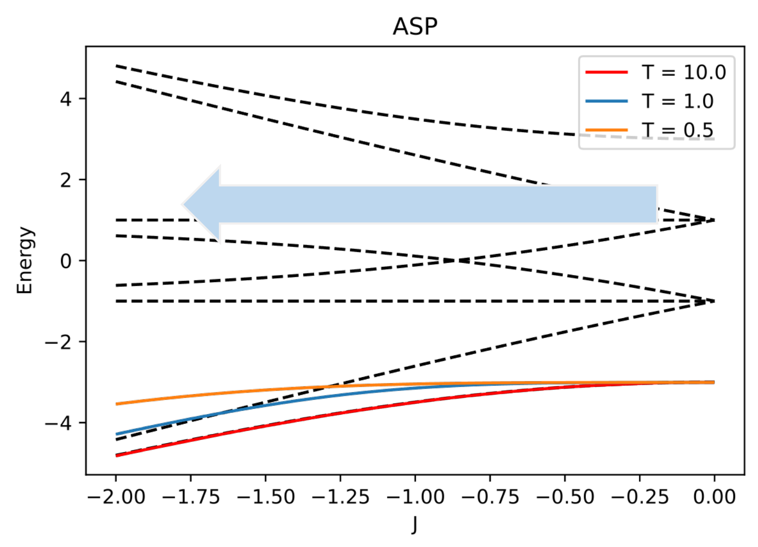

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$$H = J(t)(X_1X_2 + X_2X_3) - (Z_1 + Z_2 + Z_3)$$

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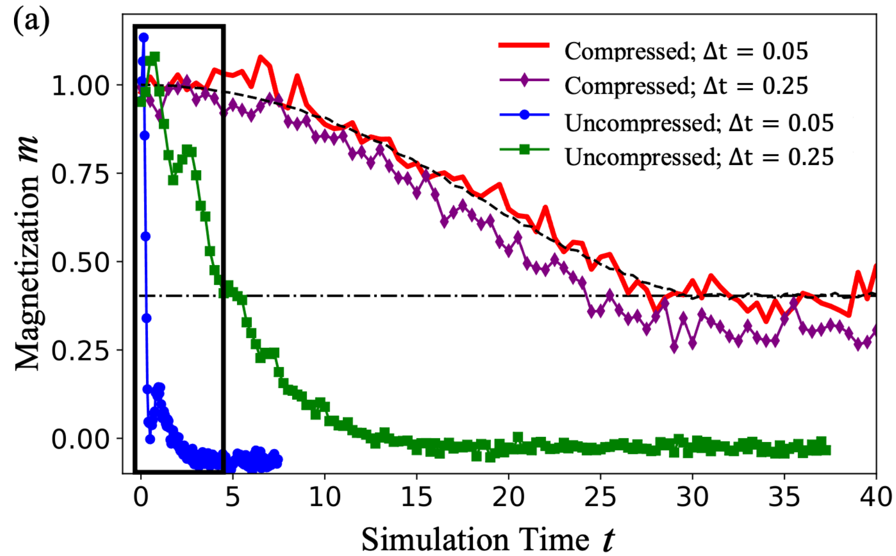
Approach #1: Algebraic Circuit Compression

$$\mathcal{H}_{ASP}(t) = J(t)\sum_{i=1}^{n-1} X_i X_{i+1} + h_z \sum_{i=1}^{n} Z_i \qquad \langle m(t) \rangle \equiv \frac{1}{n}\sum_i \sigma_i^z(t)$$

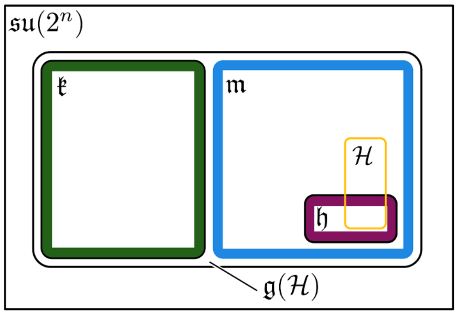


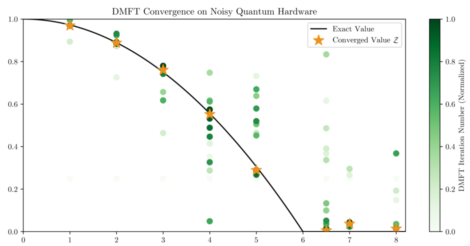
- Compressed circuits have 20 CNOT gates in total whereas Trotter circuits have increasing number of CNOTs as simulation time increases

Phys. Rev. A 105, 032420 (2021), SIMAX 2022 43:3, 1084-1108

2 Algebraic methods for circuit compression

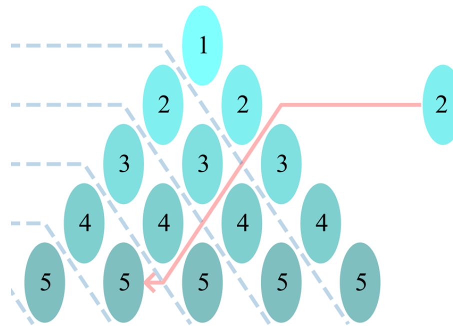
Cartan Decomposition

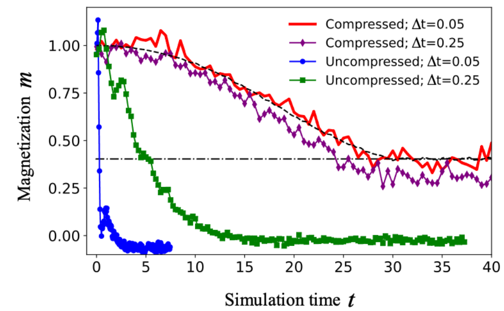




- Produces exact, fixed depth time evolution unitaries for any model.
- Produces unitaries for combinations of (anti)-Hermitian operators (UCC factors).
- We have code available! https://github.com/kemperlab/cartan-quantum-synthesizer

Algebraic Compression





- Compressed Trotter circuits down to a fixed depth circuit for 1-D nearest neighbor TFXY, TFIM, XY and Kitaev models.
- Based on 3 easy to check, local properties.
- We have code available! Check F3C, F3C++ and F3Cpy at https://github.com/QuantumComputingLab

Phys. Rev. Lett. 129, 070501 (2022) , arXiv:2112.05688

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