Electronic version of this talk

Lie algebraic perspectives on Hamiltonian evolution

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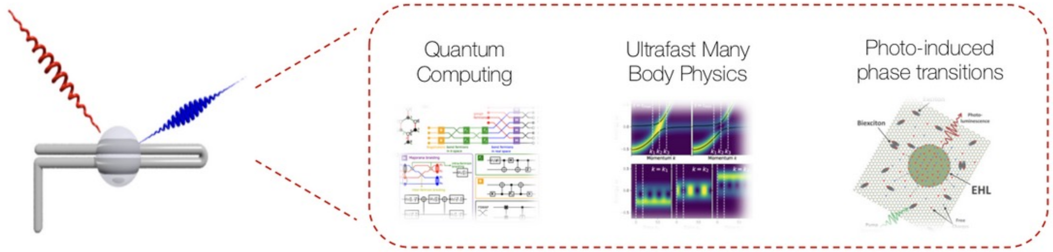
RPMBT XXI
09/12/2022

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

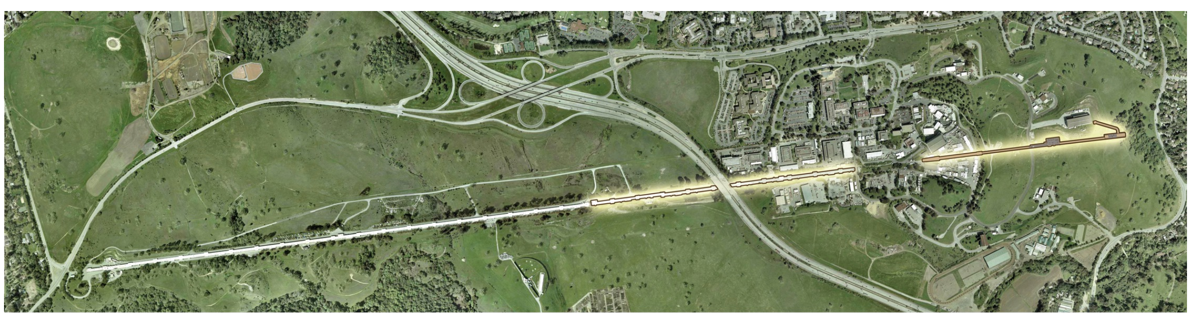
Why quantum computing for condensed matter?

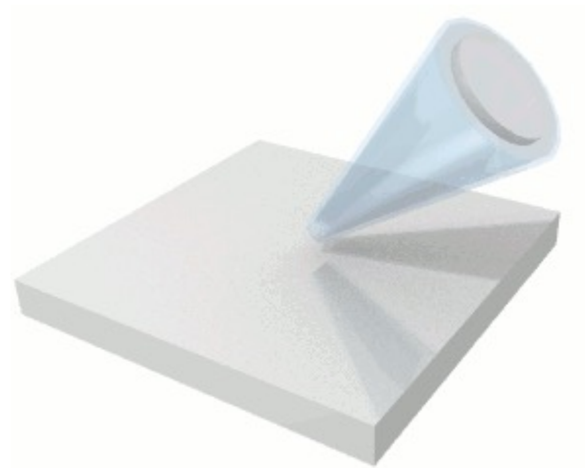


Kemper Lab

Quantum materials in and out of equilibrium.

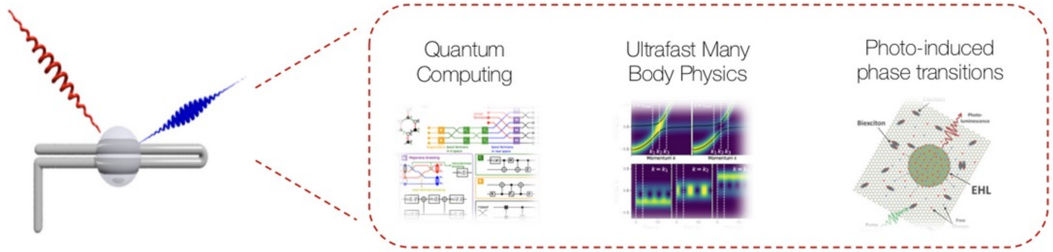
Time-resolved experiments





Shen group (Stanford)

Why quantum computing for condensed matter?



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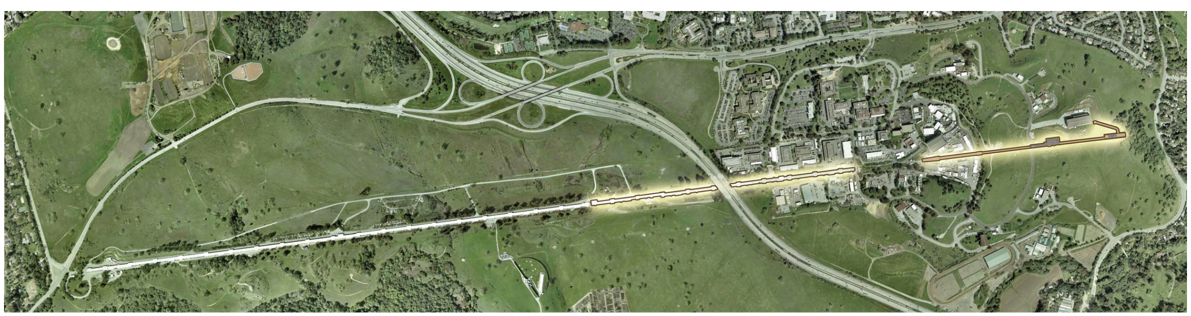
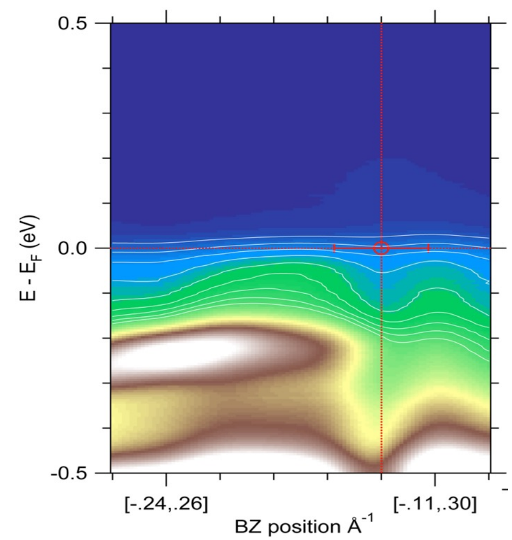


$ErTe_3$



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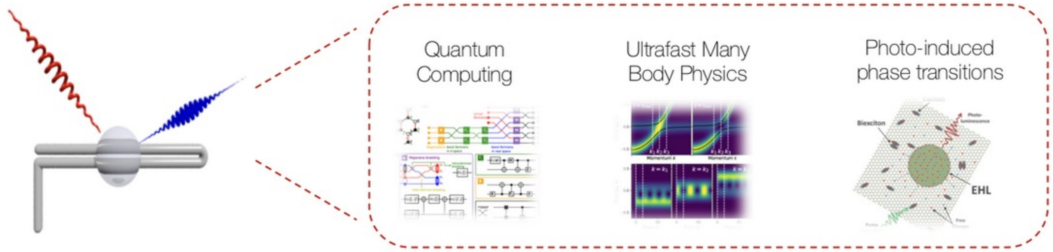

Kemper Lab

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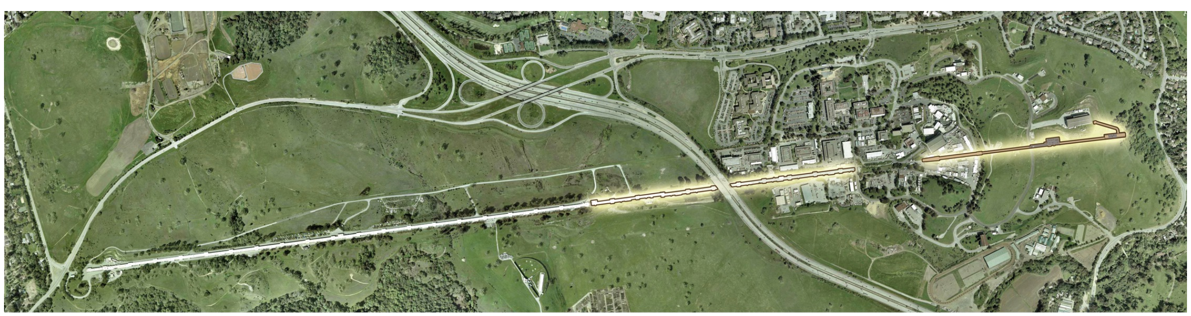

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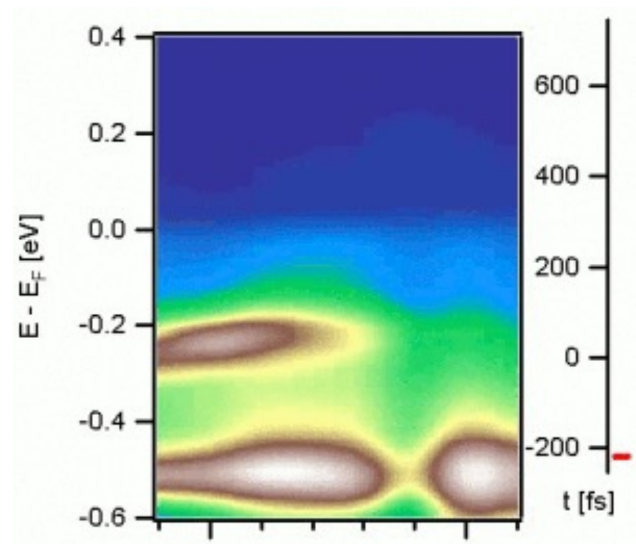

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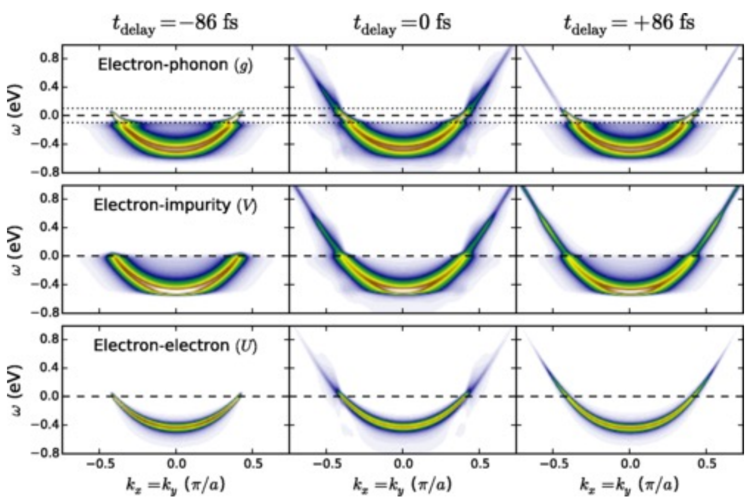
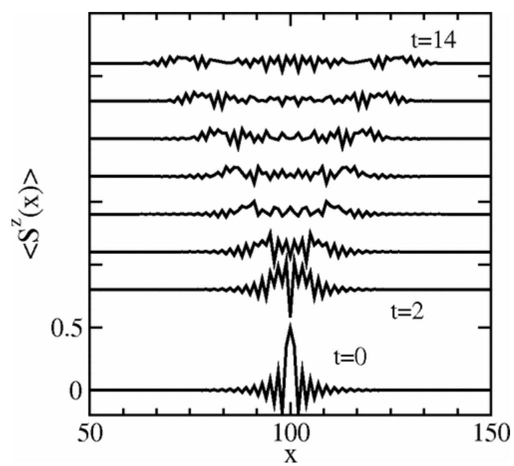


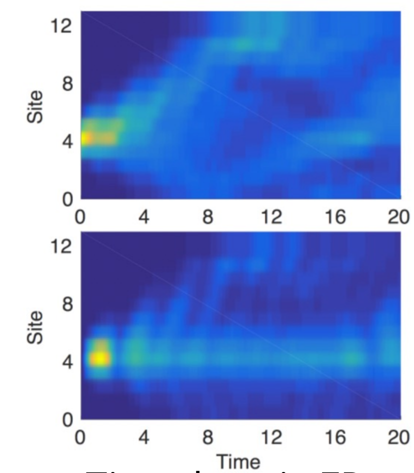
Non-Equilibrium Green's functions

Phys. Rev. X 8, 041009 (2018)



Time domain DMRG

Phys. Rev. Lett. 93, 076401 (2004)

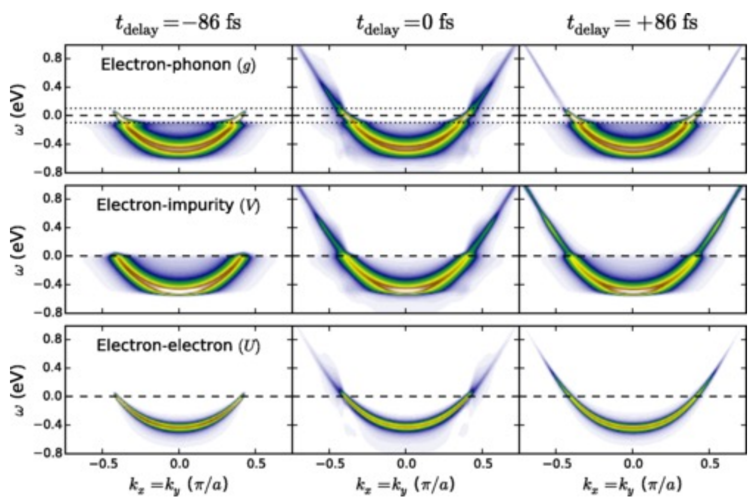


Time domain ED

Johnston & Kemper, unpublished

Why quantum computing for condensed matter?

All these techniques eventually reach a barrier.



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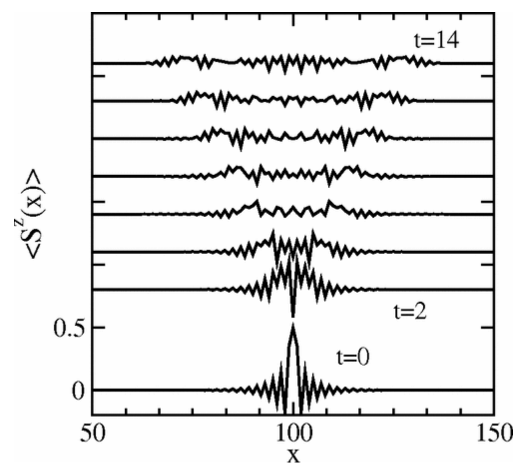

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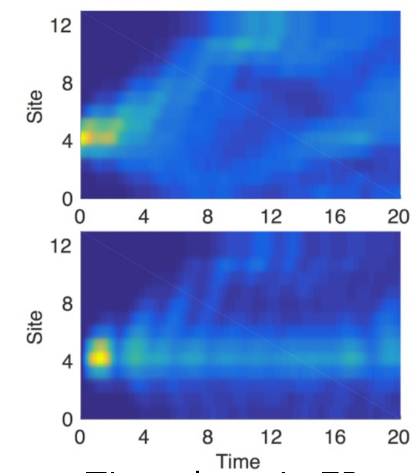

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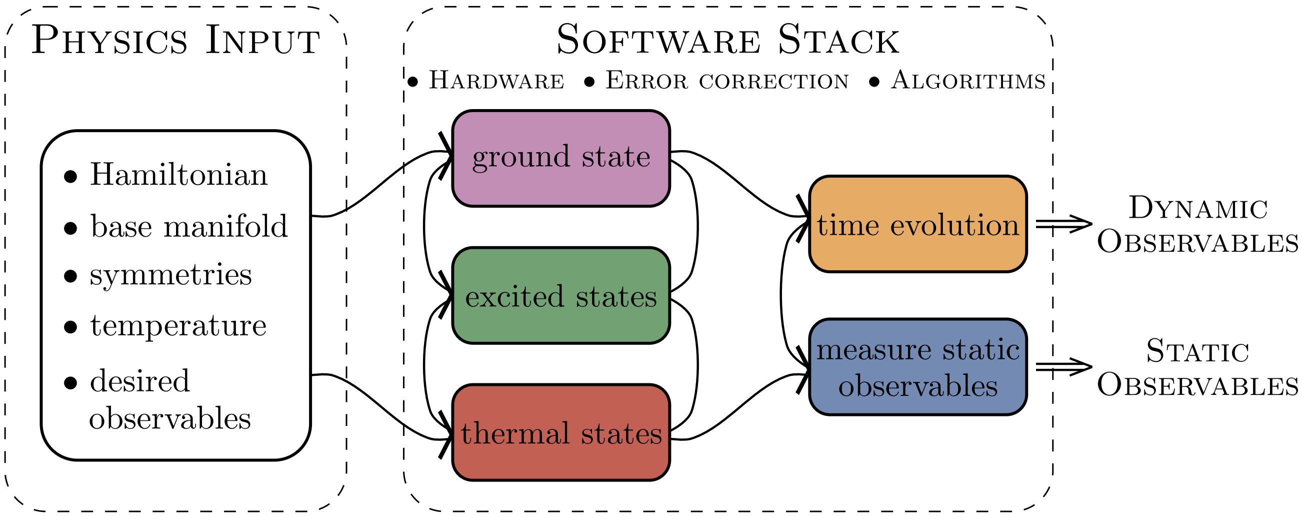
Johnston & Kemper, unpublished

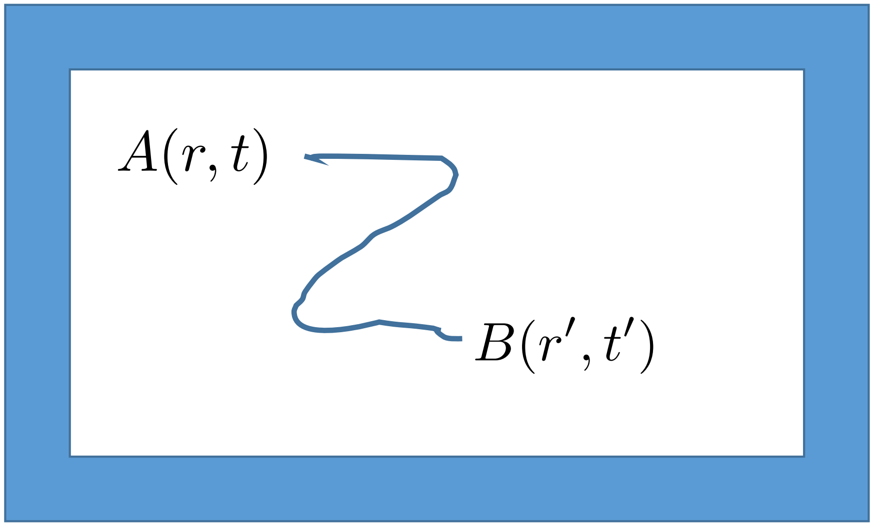
Quantum Matter meets Quantum Computing



- Experimental relevance: Measuring correlation functions
- Measuring exact integer Chern numbers for topological states
- Driven/dissipative systems and fixed points (1000 Trotter steps)
- Time evolution via Lie algebraic decomposition and compression
- Thermodynamics via Lee-Yang Zeros
- 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

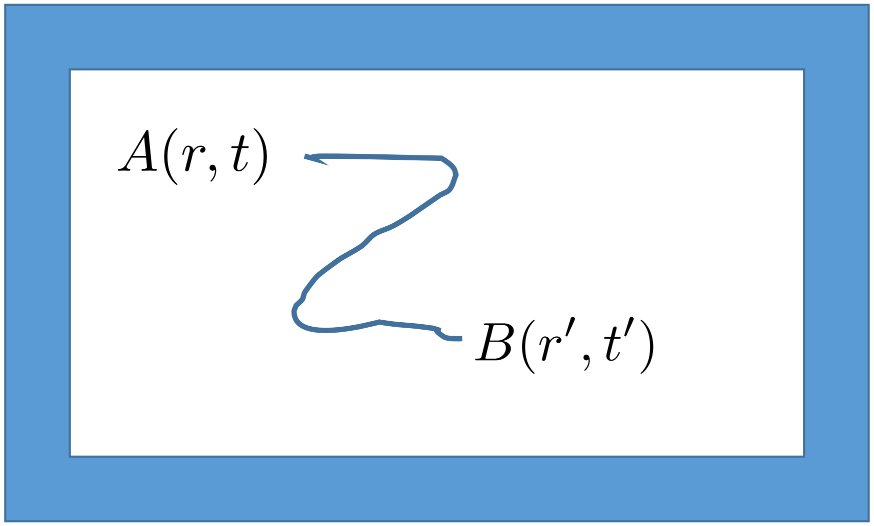
$$\langle j(r,t) j(r',t') \rangle$$

Single-particle spectra (ARPES)

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

Spin-resolved neutron scattering

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

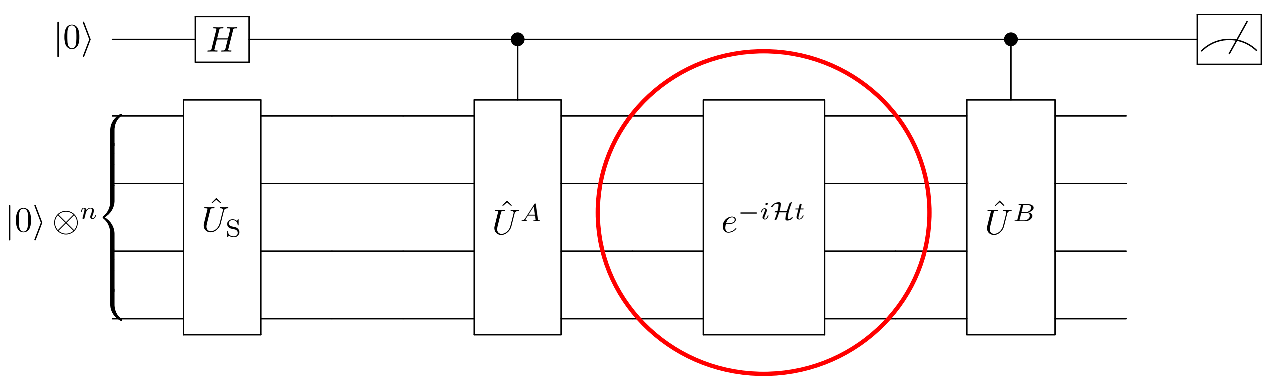


Low-energy excitations: correlation functions

Express the correlation function through the Lehmann representation:

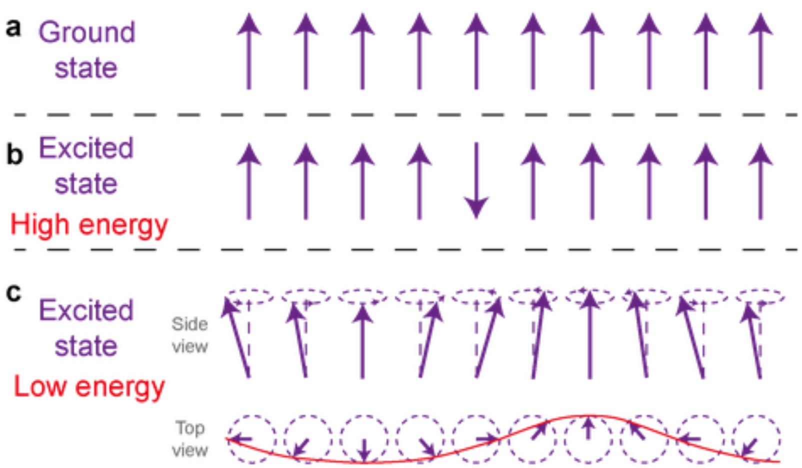
$$C(t) = \langle\Phi|\hat{U}^B(t)\hat{U}^A(0)|\Phi\rangle = \sum_m e^{-i(E_m - E_0)t} \langle\phi_0| U^B |m\rangle \langle m| U^A |\phi_0\rangle \, .$$

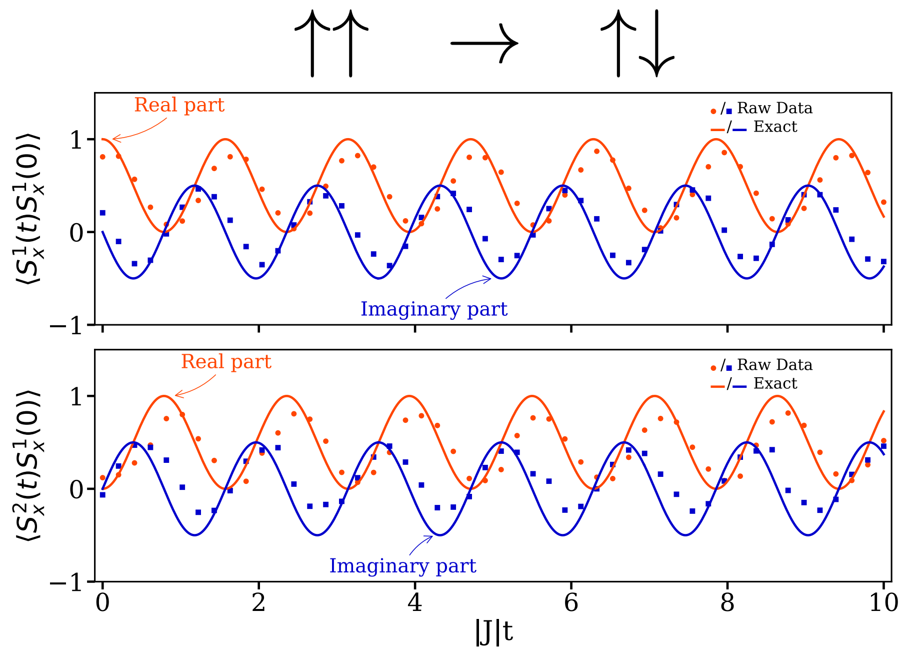
Quantum circuit:



Low-energy excitations: 2-site magnons

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



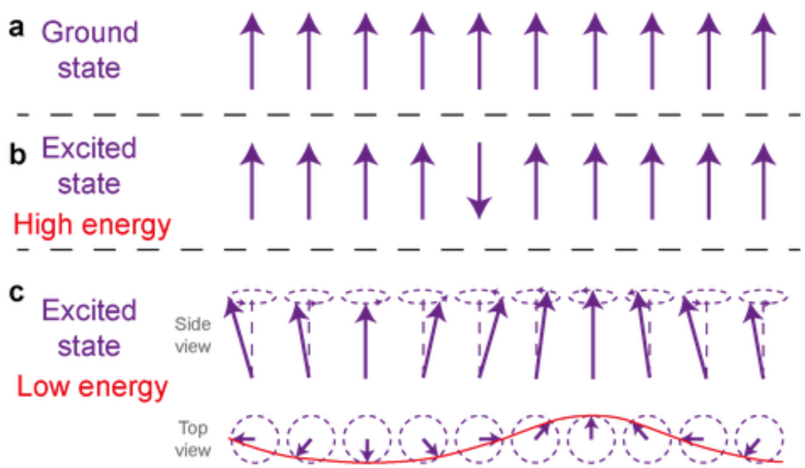


$$\hat{H} = 2SJ\sum_k(1-\cos(k))\hat{c}_k^\dagger\hat{c}_k$$

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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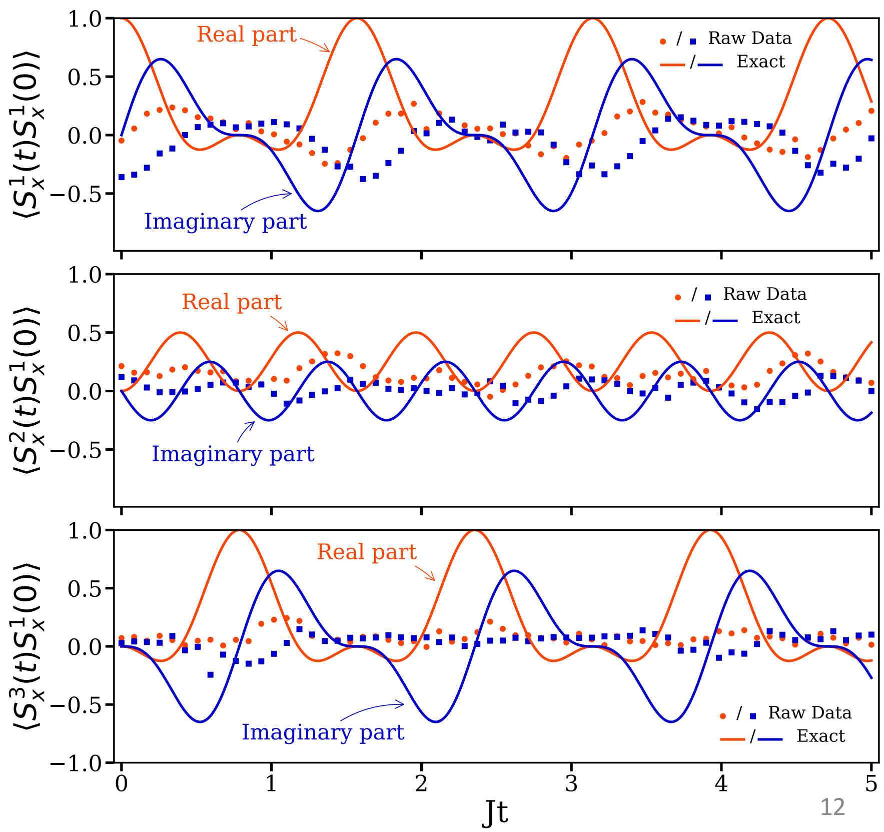
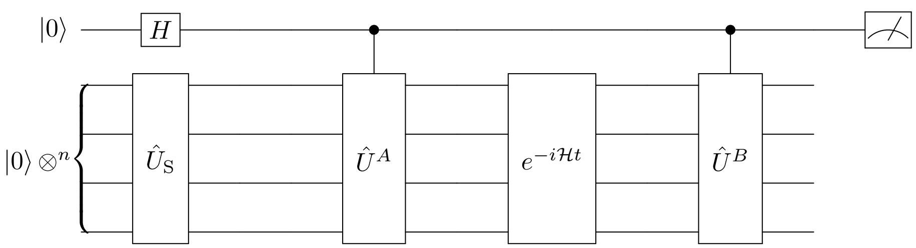
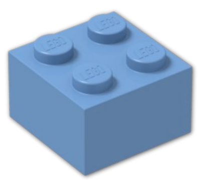


Data from *ibmq_tokyo*

Quantum Compiling





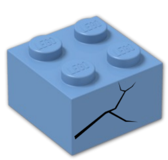
Single Qubit Gates

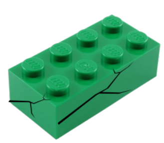
+

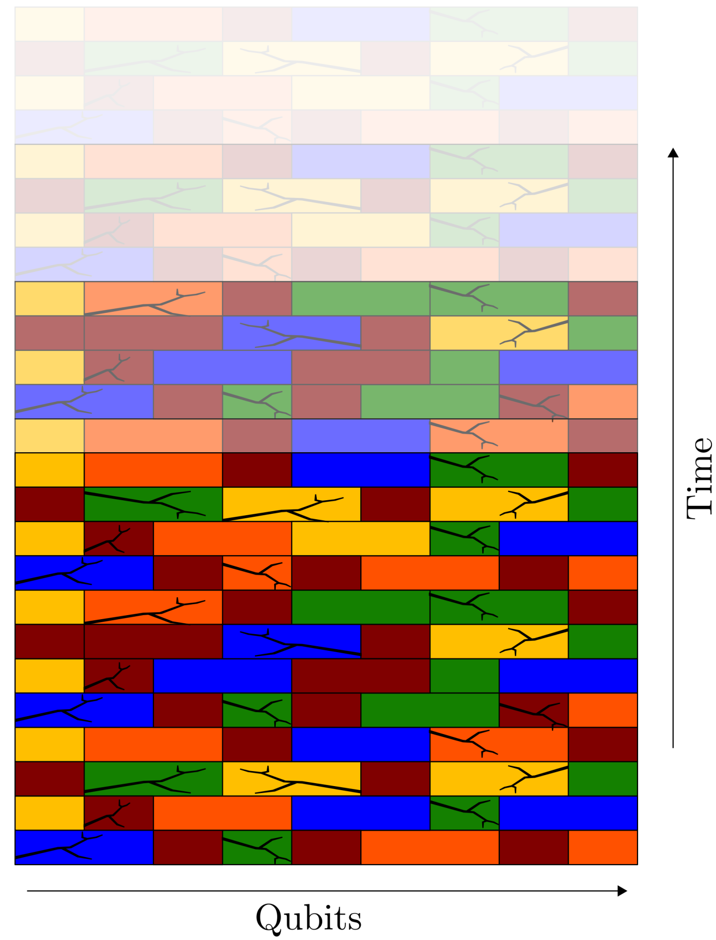
Two Qubit Gate

= Anything!*

*Actual Gates

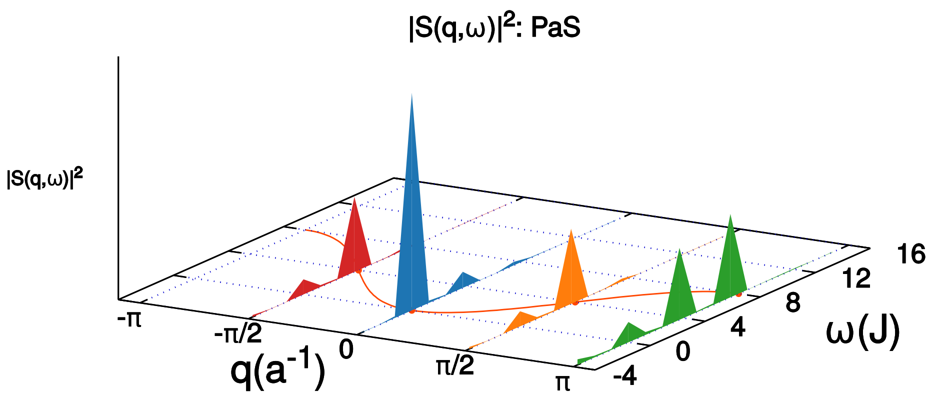


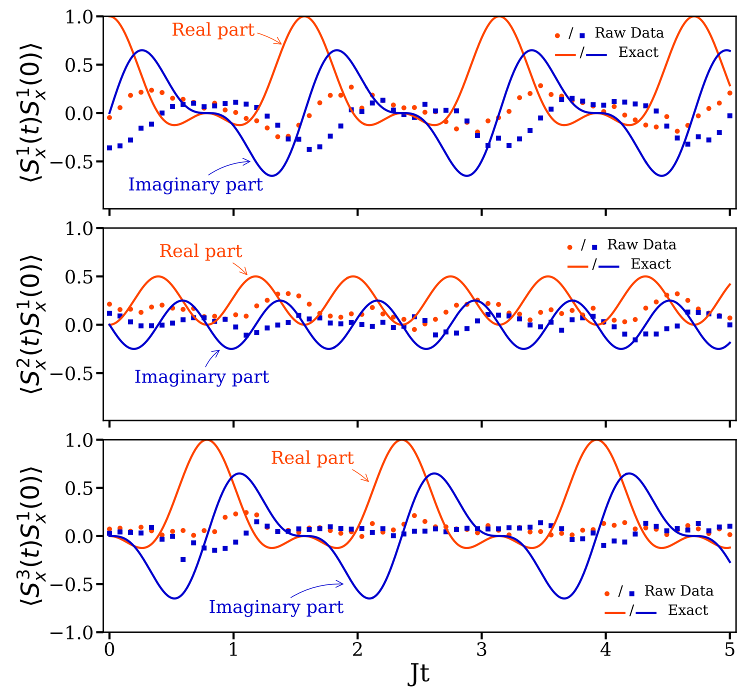




Low-energy excitations: 4-site magnons

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

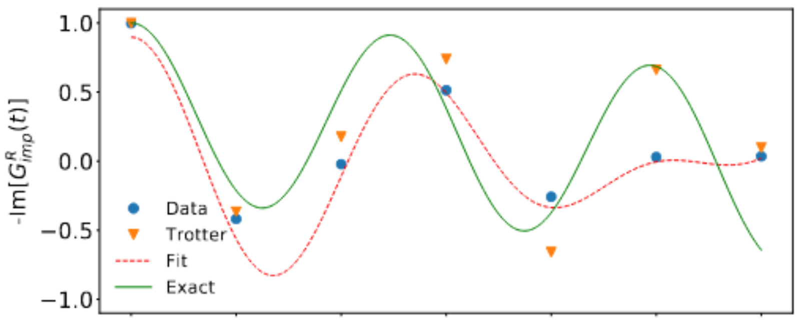




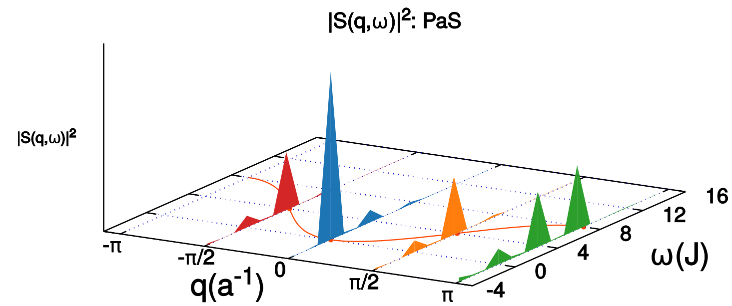
10.1103/PhysRevB.101.014411

Low-energy excitations: 4-site magnons

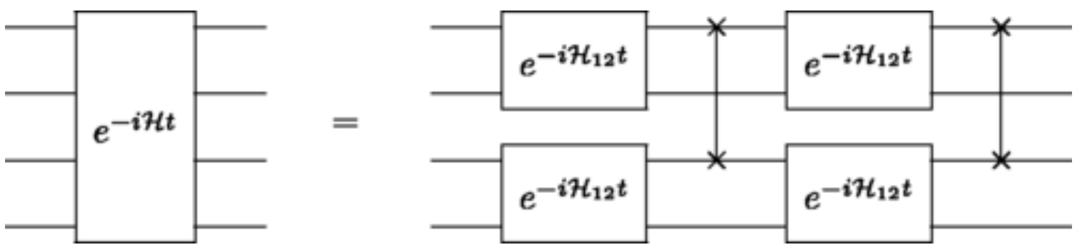
Q: Why does this work?



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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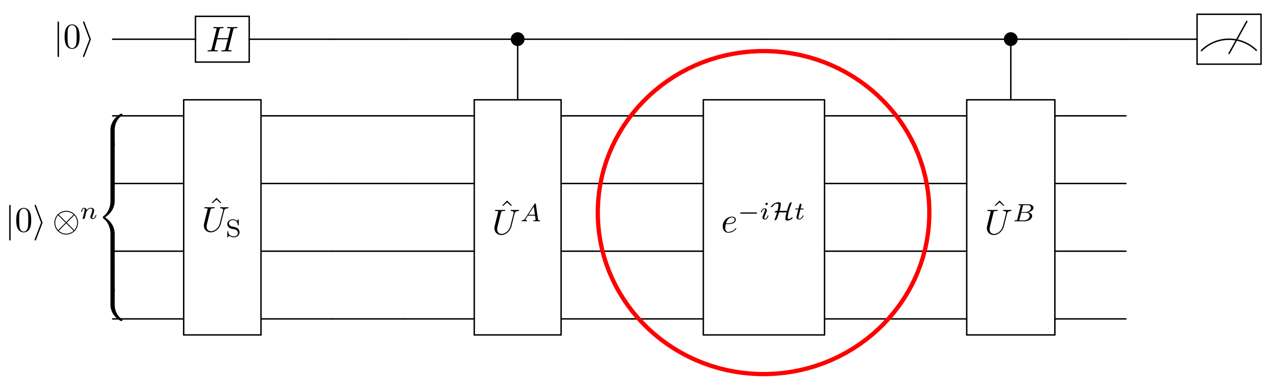
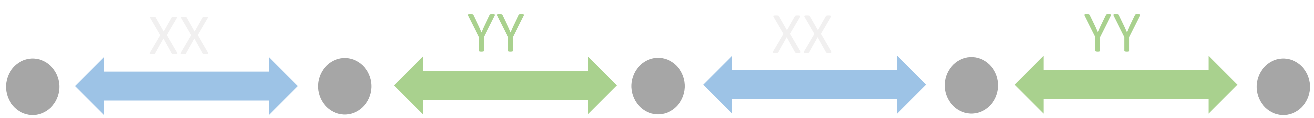
Quantum circuit:



Trotter Approximation

Consider 5 spin Kitaev chain:

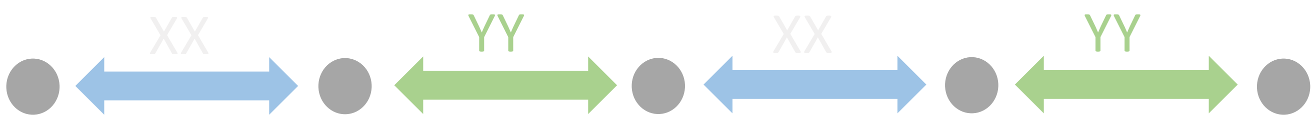


$$\mathcal{H} = a\,XXIII + b\,IYYII + c\,IIXXI + d\,IIIYY$$

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

Trotter Approximation

Consider 5 spin Kitaev chain:



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

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

Trotter Approximation

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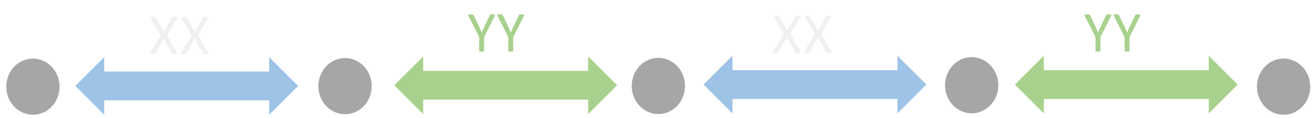

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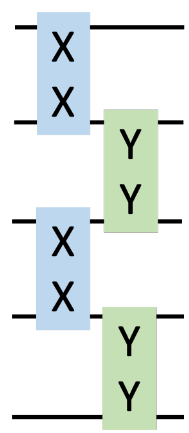

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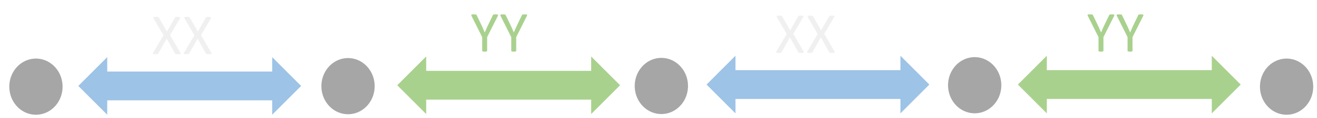

$$\mathcal{H} = a\, XXIII + b\, IYYII + c\, IIXXI + d\, IIIYY$$

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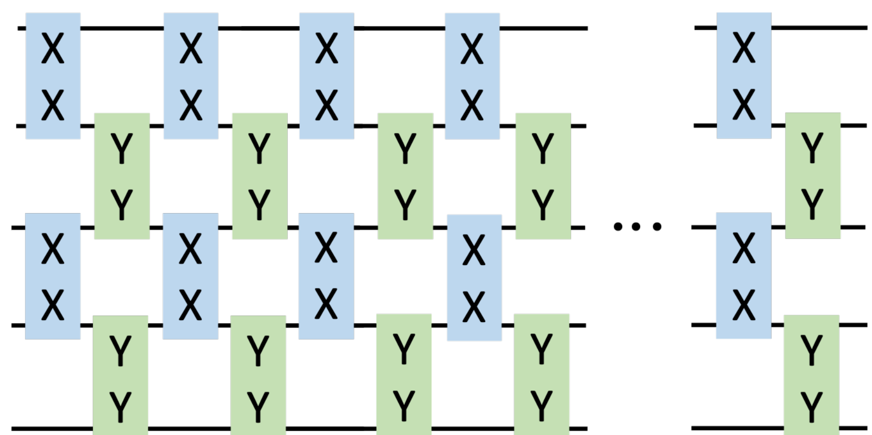
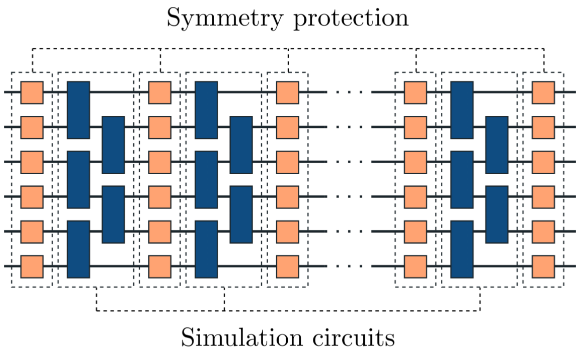
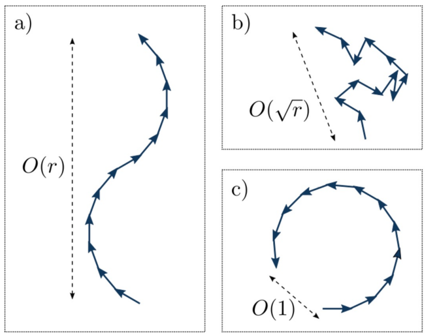
$U(t) =$ 

Improving Trotter Expansions

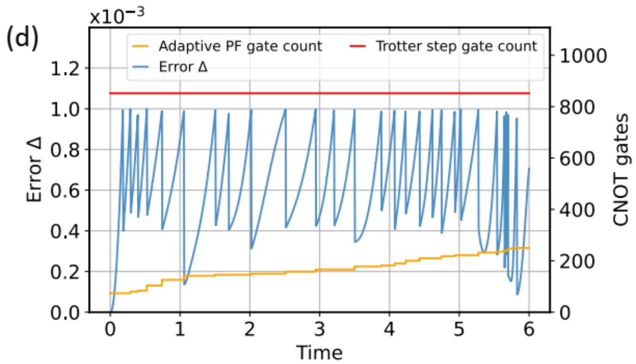
- Symmetry protection to reduce trotter error (*)





- 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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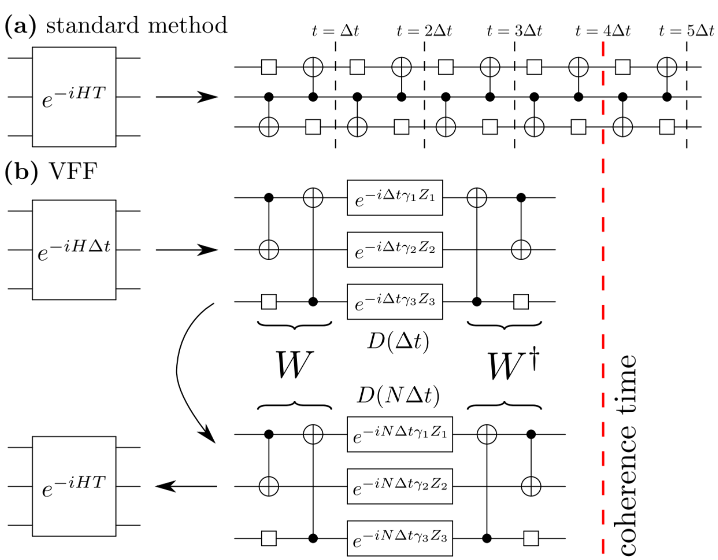
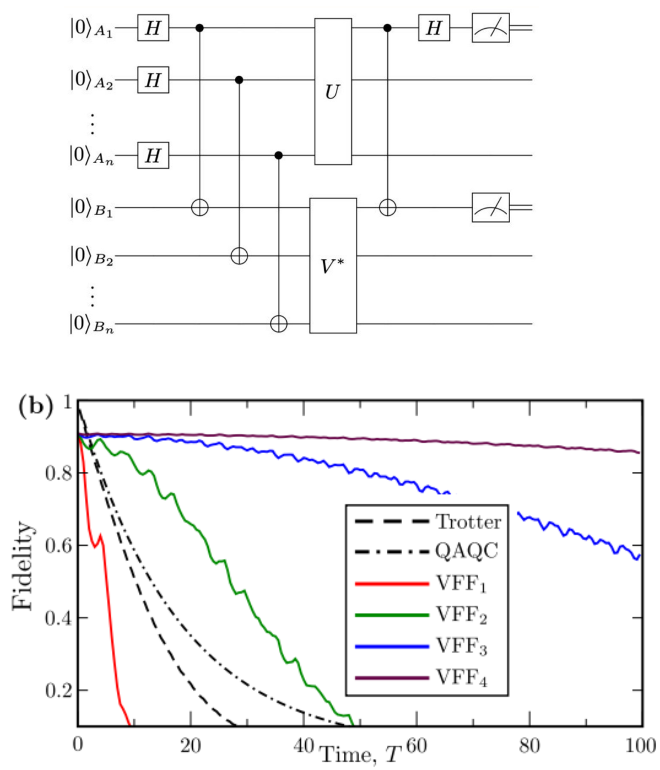
Variational Fast Forwarding

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





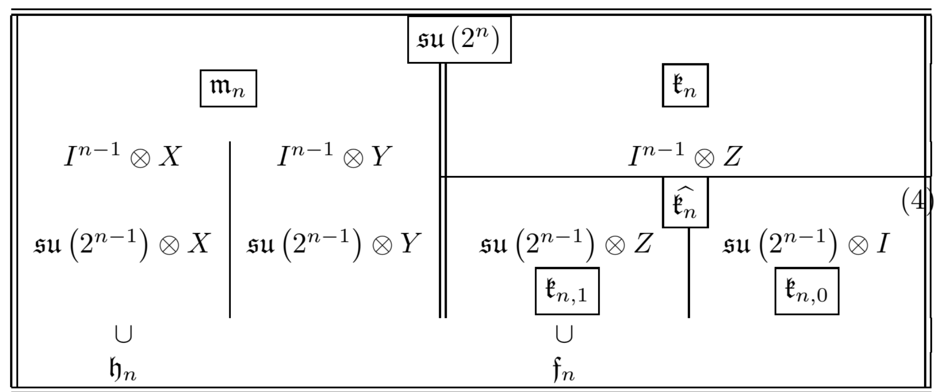
(*) Cirstoiu, C., Holmes, Z., Iosue, J., Cincio, L., Coles, P. J., & Sornborger, A. (2020), npj Quantum Information, 6(1), 1-10.

Unitary Synthesis: Cartan Decomposition

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

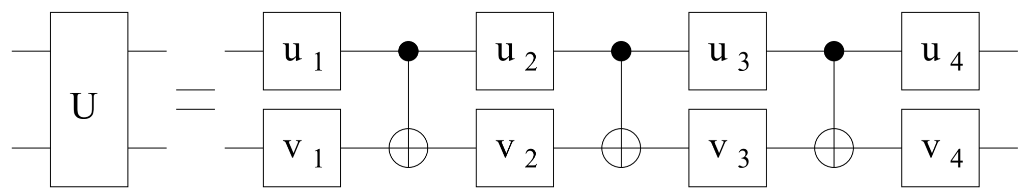
$$\mathfrak{g} = \mathfrak{m} \oplus \mathfrak{k}$$

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



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

- 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).

What can you do with fixed depth time evolution circuits?

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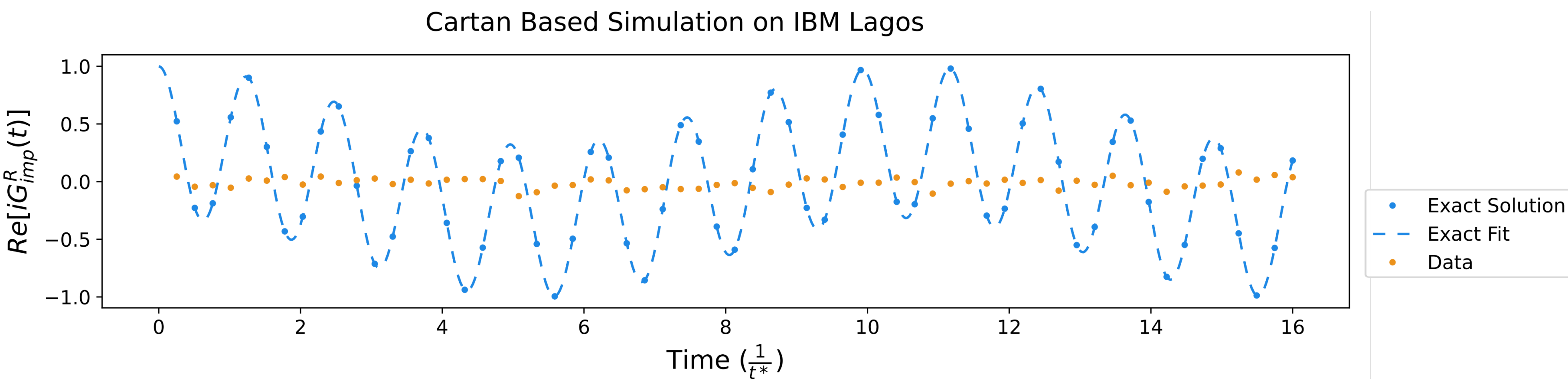
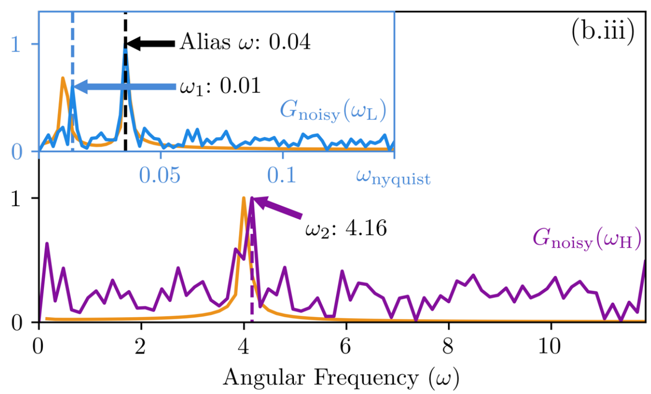
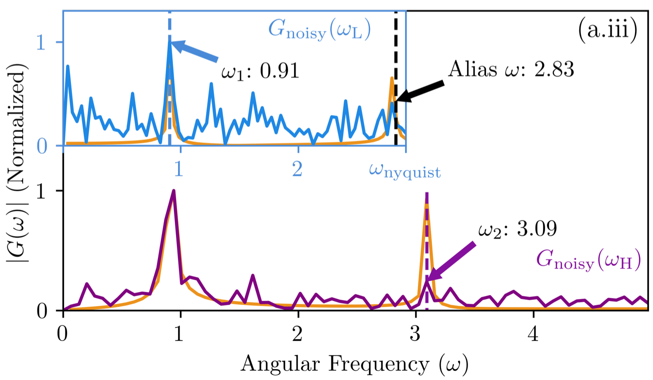
[T. Steckmann et al., arXiv:2112.05688]

2-site Hubbard DMFT (5 qubits)



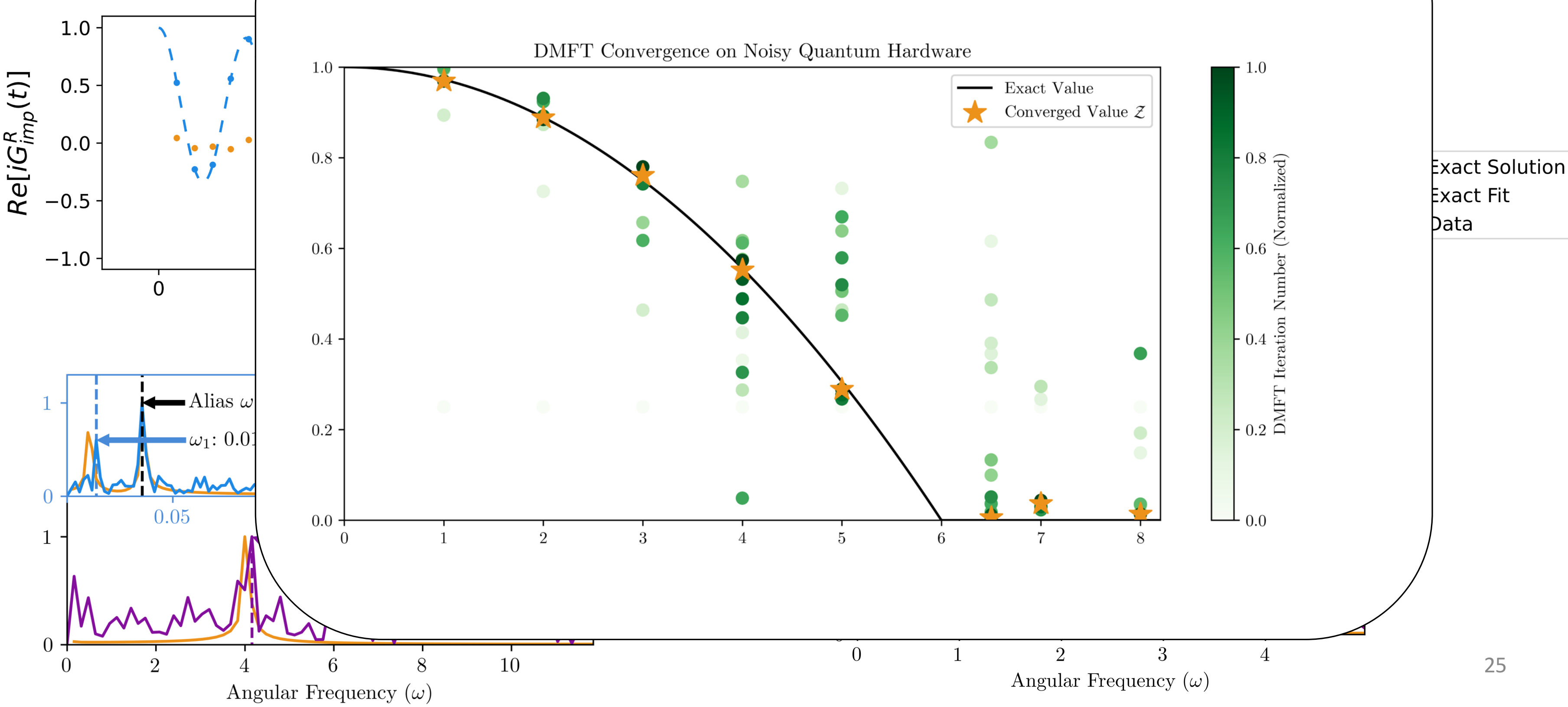




2-site Hubbard DMFT

T. Steckmann et al., arXiv:2112.05688

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



2 Algebraic methods for circuit compression

Cartan Decomposition

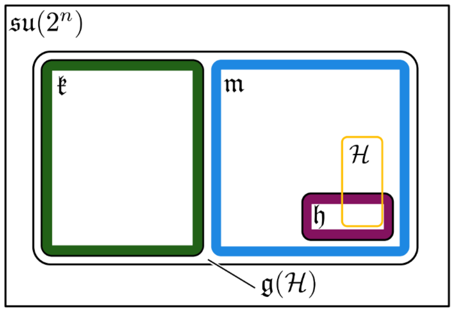
Algebraic Compression

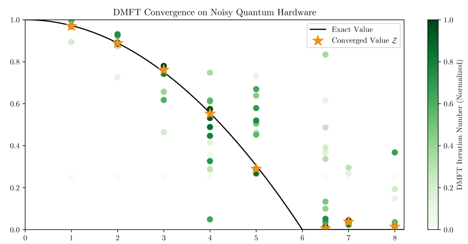
Phys. Rev. Lett. 129, 070501 (2022) , arXiv:2112.05688

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

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

Algebraic Compression

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

2 Algebraic methods for circuit compression

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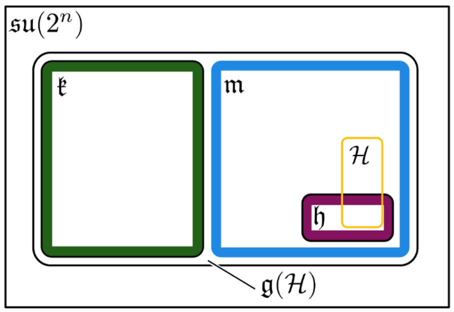
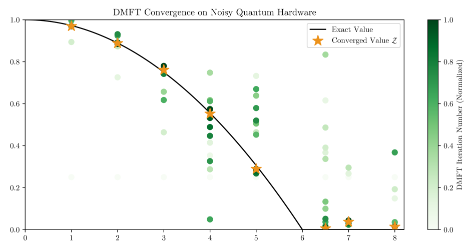
Cartan Decomposition

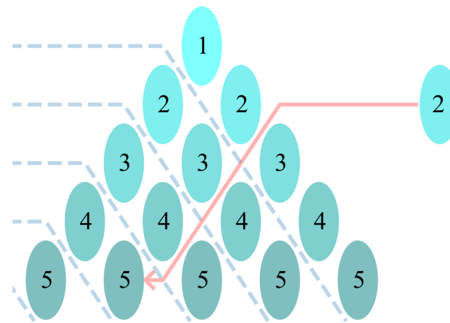


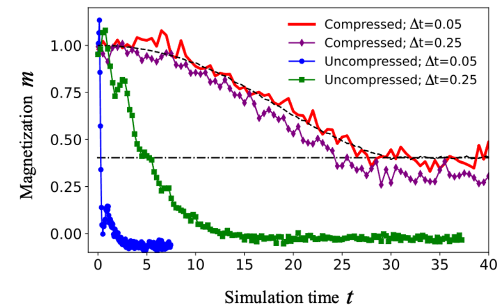


- Produces exact, fixed depth time evolution unitaries for any model.
- Produces unitaries for linear combinations of (anti)-Hermitian operators (UCC factors).
- We have code available! https://github.com/kemperlab/cartan-quantum-synthesizer

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

Algebraic Compression





- 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

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

Approach #1: Cartan Decomposition

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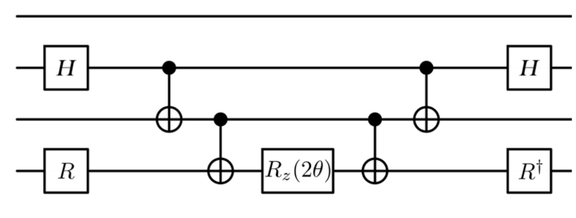
Main Problem

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: $e^{i\theta IXZYI} =$



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 $\mathfrak{su}(2^n)$

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

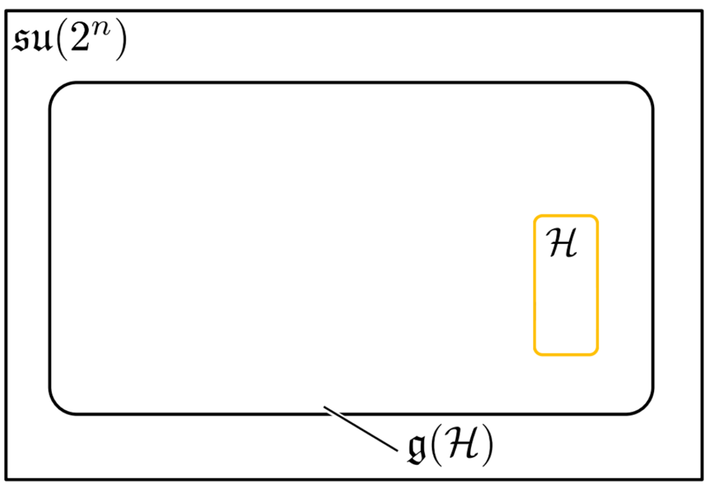
$$U(t) = e^{-it\mathcal{H}} = \prod_{\bar{\sigma}^i \in \mathfrak{su}(2^n)} e^{i\kappa_i \bar{\sigma}^i}$$

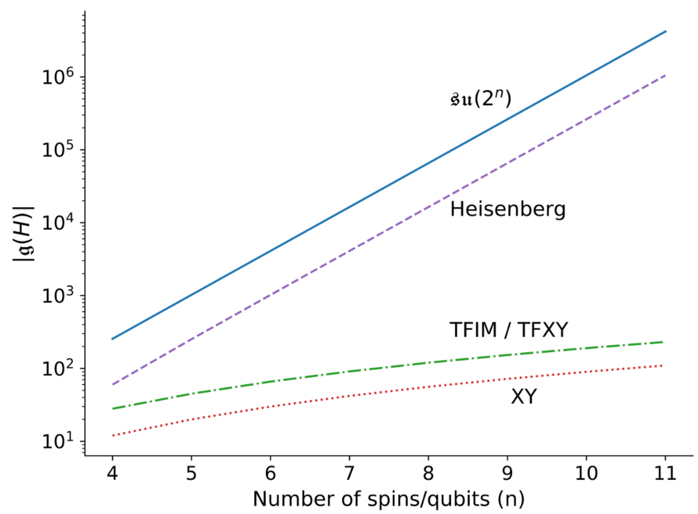
Hamiltonian Algebra

- 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)

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

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





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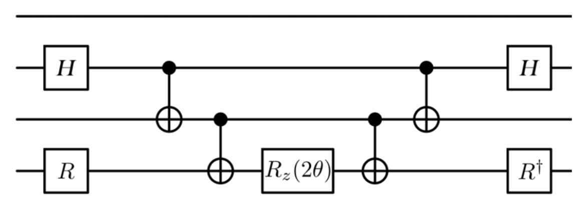
Single exponential circuit is given as: $e^{i\theta IXZYI} =$



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

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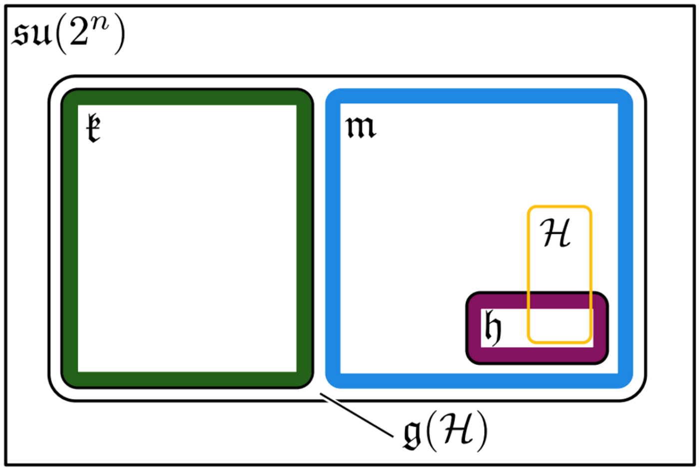
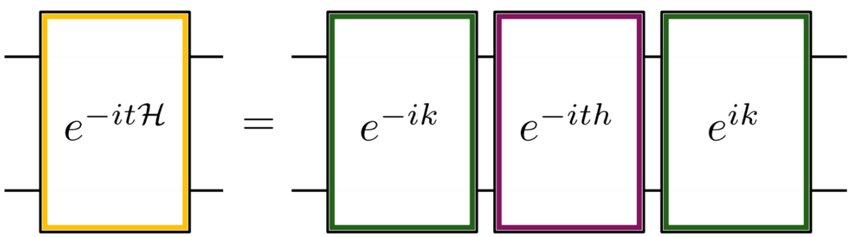
Cartan Decomposition and KHK Theorem





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

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

where

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

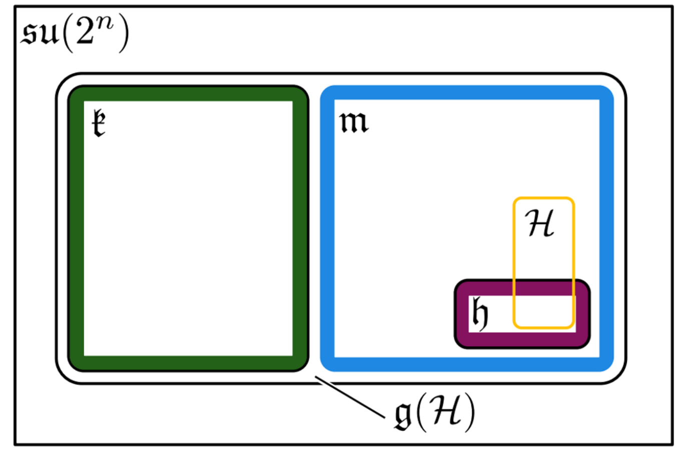
$$v = h_1 + \pi h_2 + \pi^2 h_3 + ... + \pi^{n_h - 1} h_{n_h}$$

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

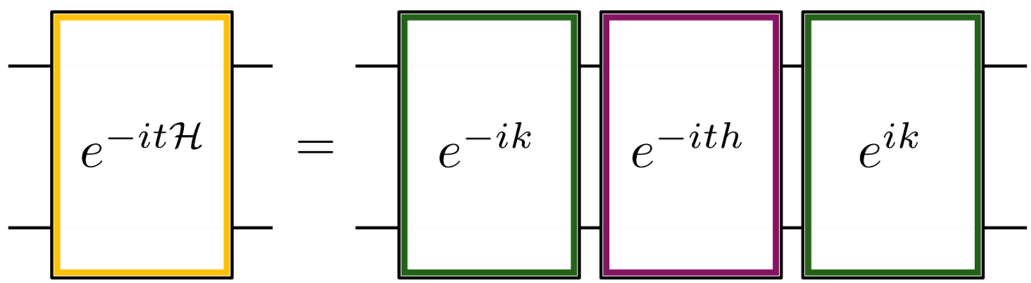
$$K_0^{\dagger} H K_0 \in \mathfrak{h}$$

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!

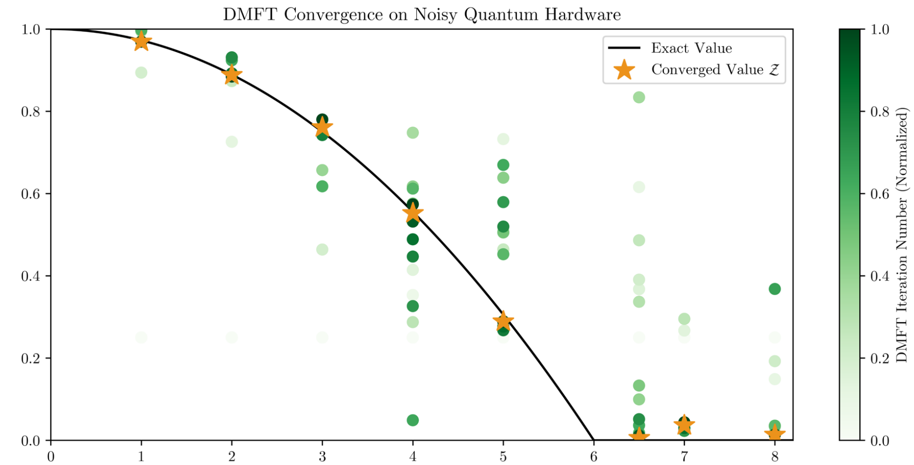


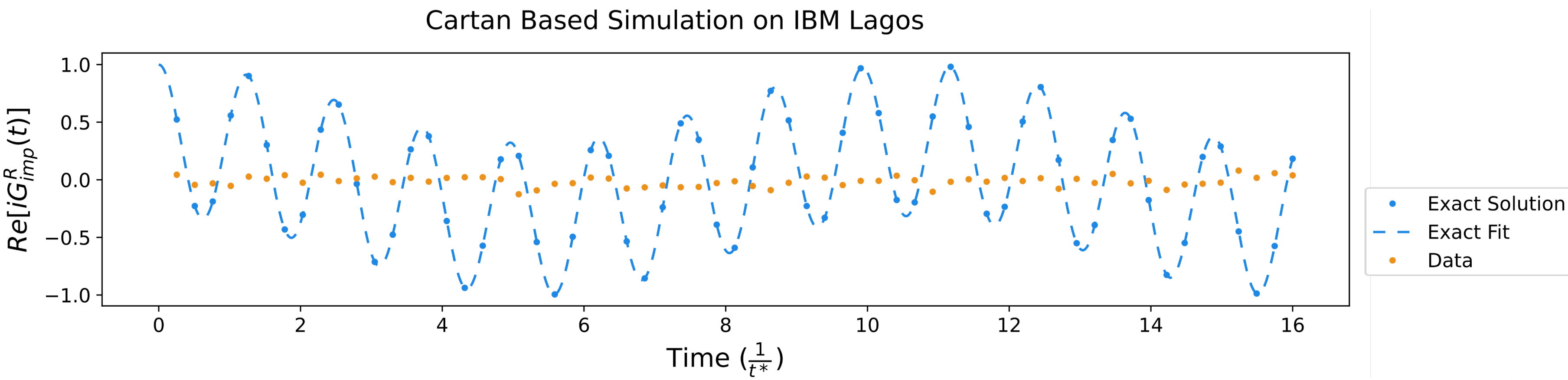
$$f(K) = \langle K v K^{\dagger}, \mathcal{H} \rangle$$



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.





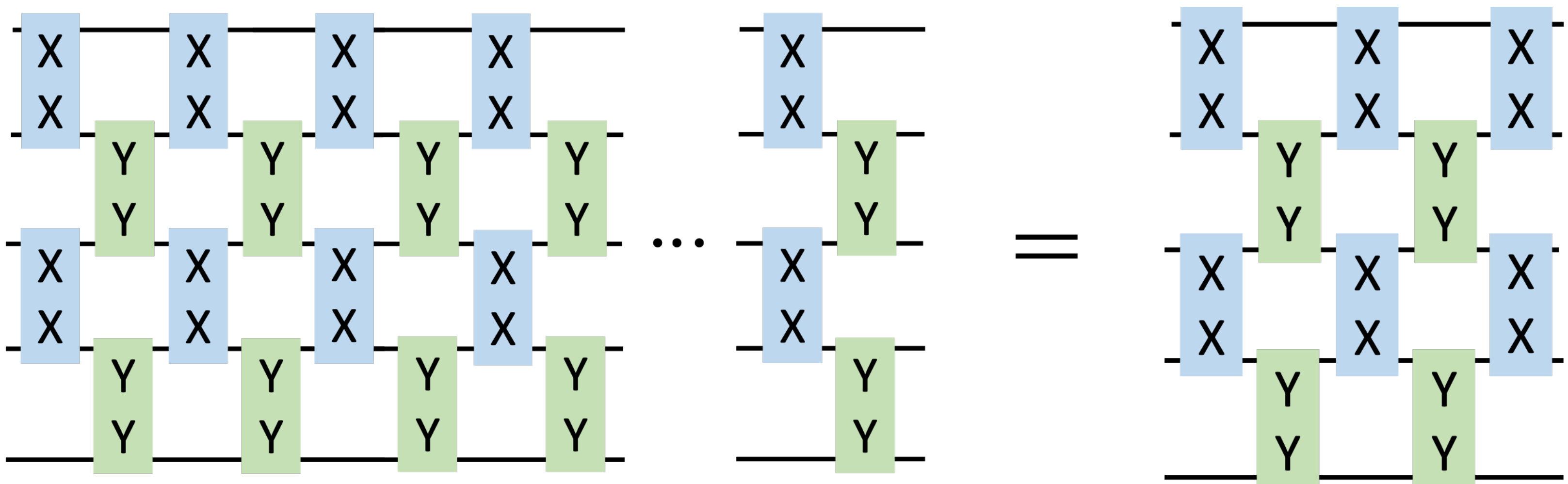
T. Steckmann et al., arXiv:2112.05688

Approach #2: Algebraic Circuit Compression

Approach #2: Algebraic Circuit Compression

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

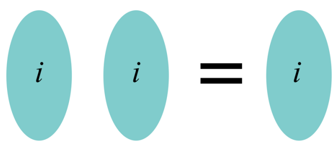
- The method is **scalable** due to its "constructive" and "local" nature.



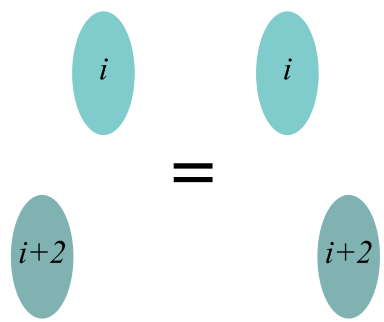
Approach #2: Algebraic Circuit Compression

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

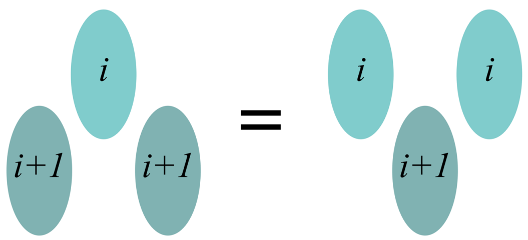
Fusion



Commutation



Turnover

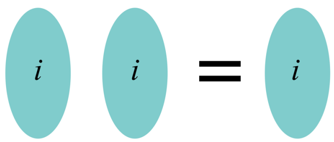


Blocks will be mapped to certain quantum gates in a model specific way.

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



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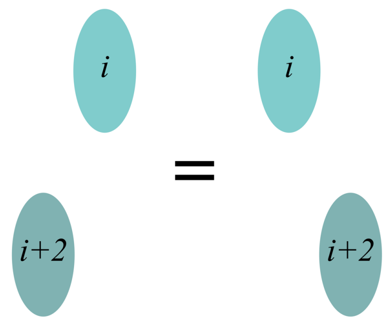

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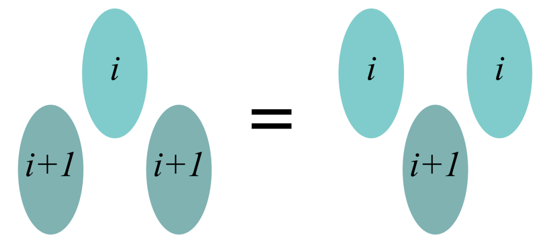

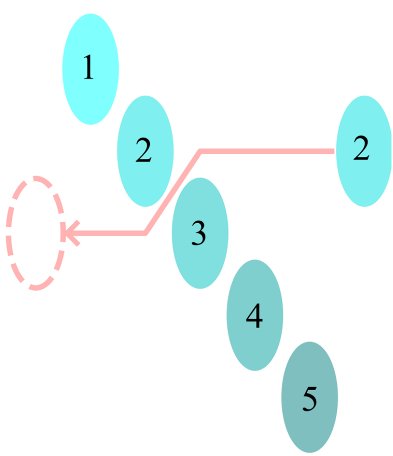

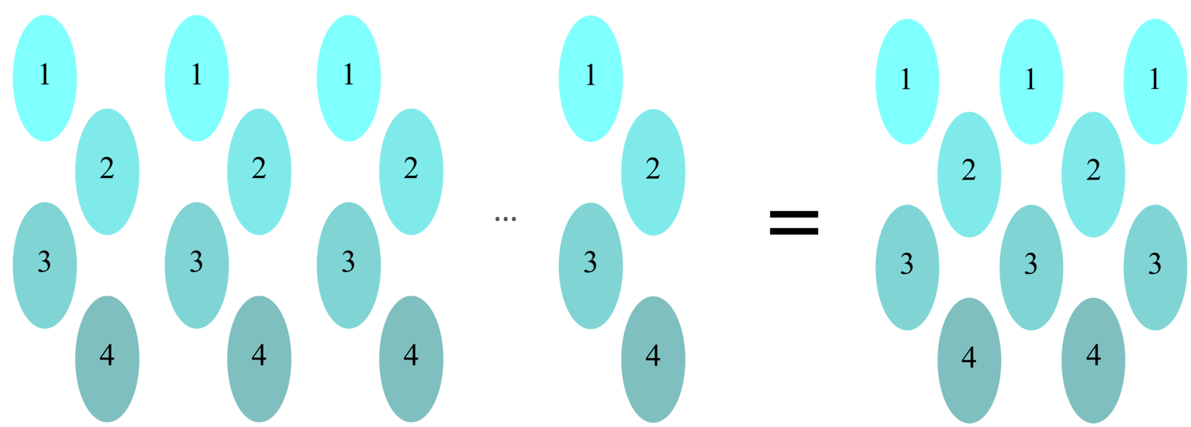

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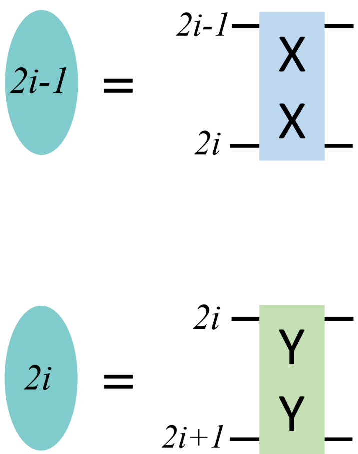
Examples

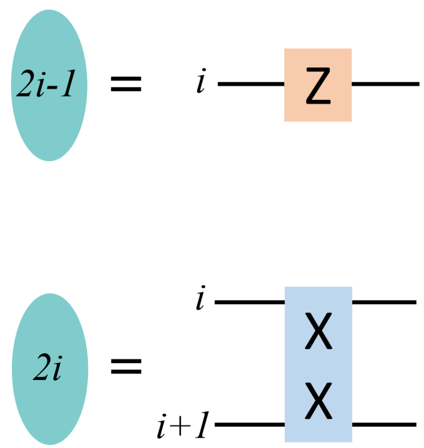
Kitaev Chain



n(n-1)/2 XX gates

n(n-1) CNOTs

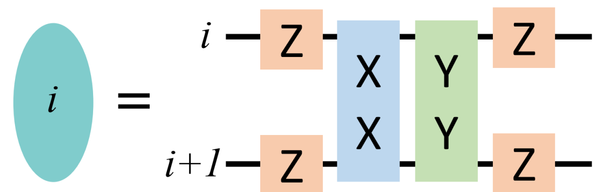
Transverse Field Ising



n(n-1) XX gates

2n(n-1) CNOTs

Transverse Field XY

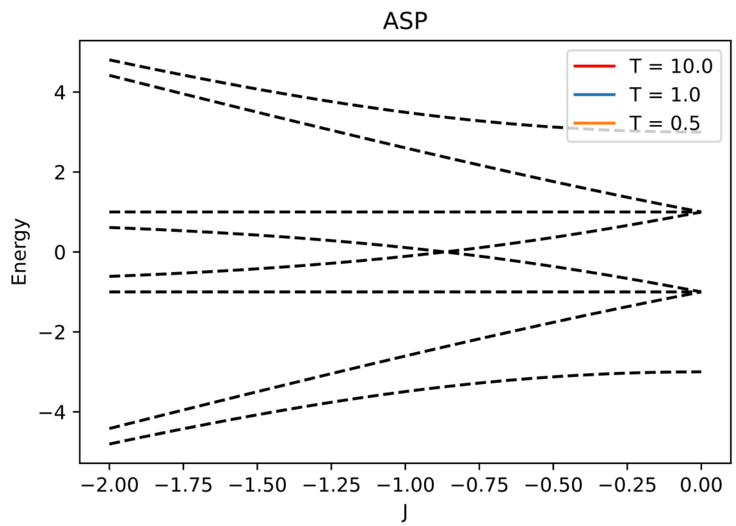


n(n-1) XX gates

n(n-1) CNOTs

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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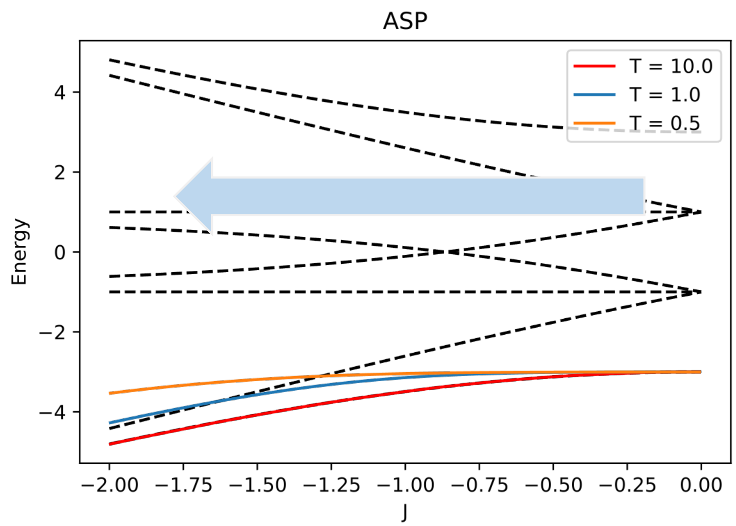

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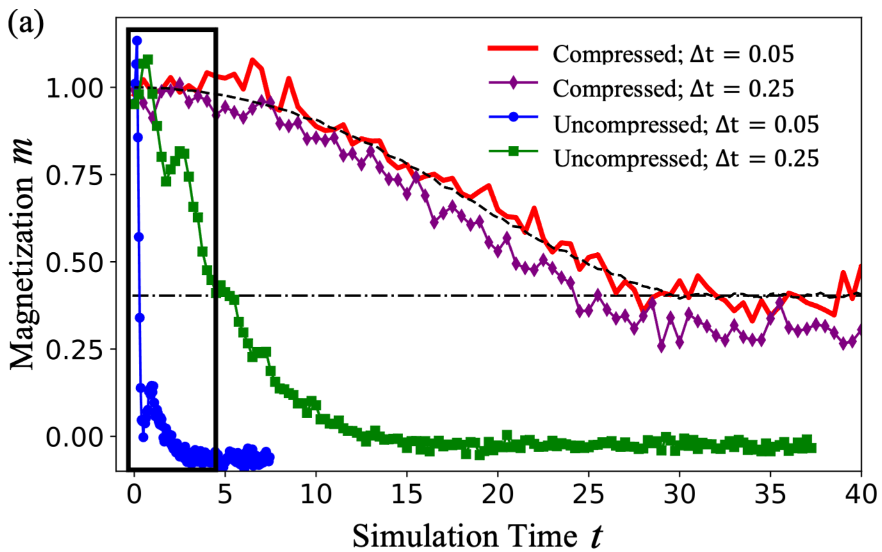
Approach #1: Algebraic Circuit Compression

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



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

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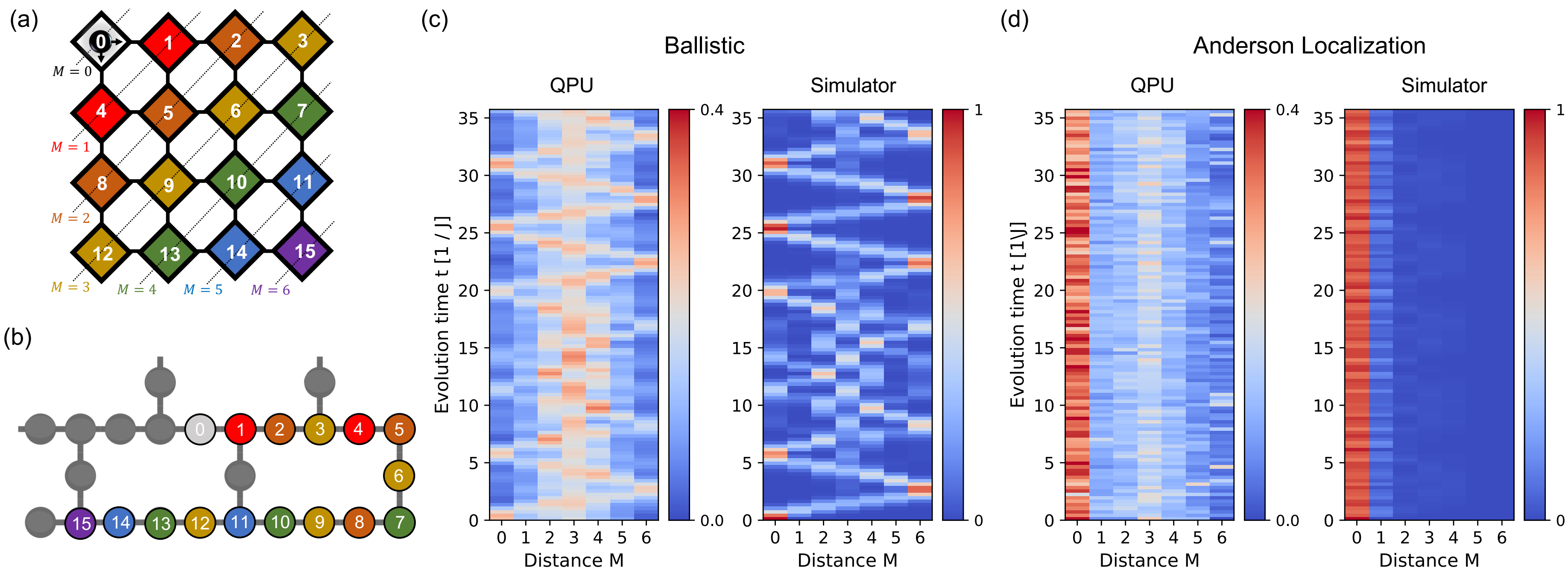
Approach #1: Algebraic Circuit Compression (preliminary)



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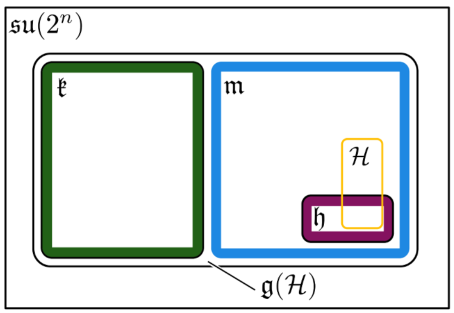
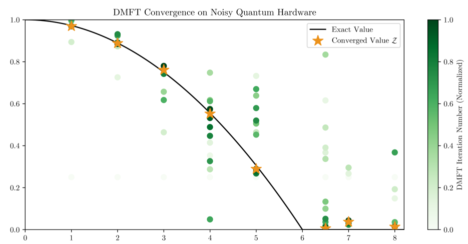
2 Algebraic methods for circuit compression

Electronic version of this talk

Cartan Decomposition





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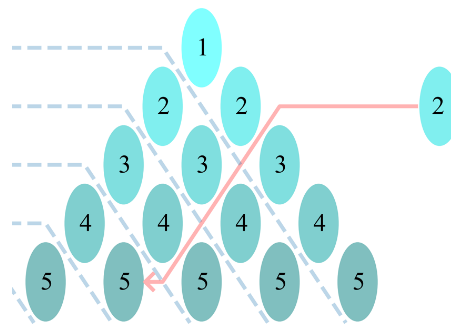

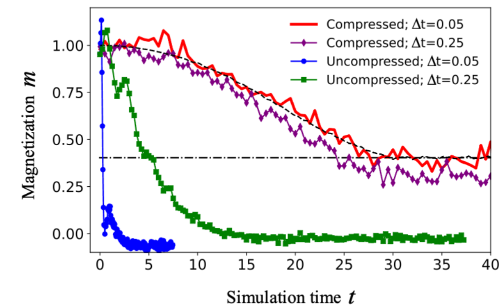

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