A quantum computing approach to efficiently simulating correlated materials using impurity models and DMFT

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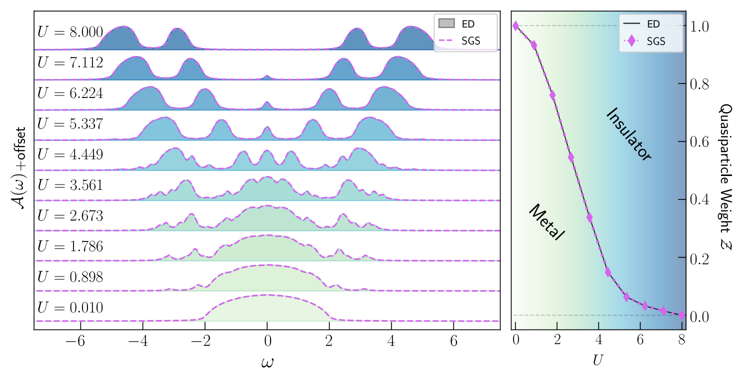
North Carolina State University
https://go.ncsu.edu/kemper-lab

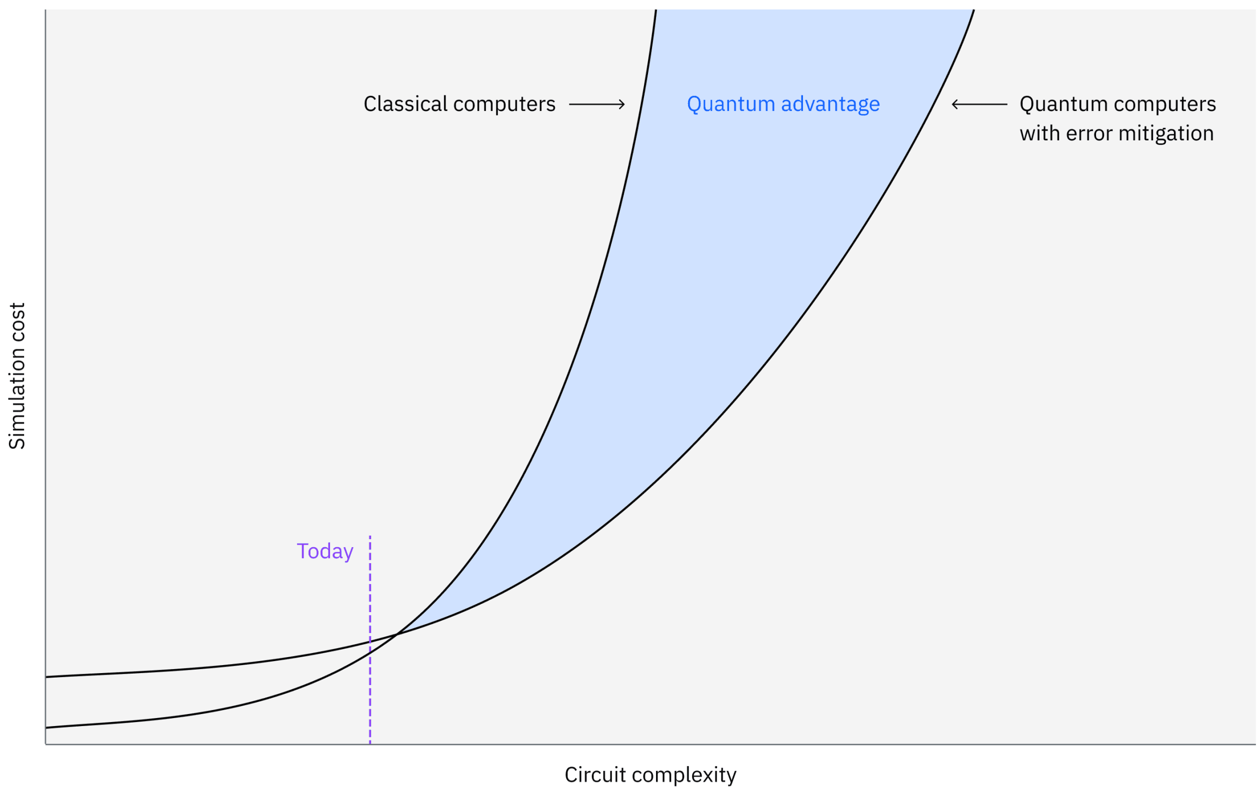
CCDS25
08-09-2025



[N. Hogan, E. Kökcü, T. Steckmann, L. Doak, C. Mejuto-Zaera, D. Camps, R. van Beeumen, W.A. de Jong, A.F. Kemper, 2508.05738](#)

Quantum computers in 2025

Quantum advantage



https://www.ibm.com/quantum/blog/quantum-advantage-era

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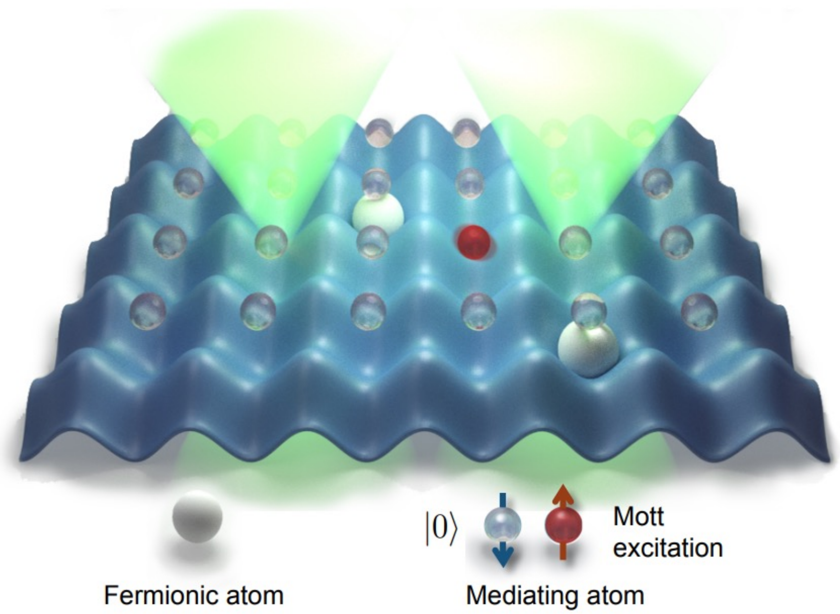
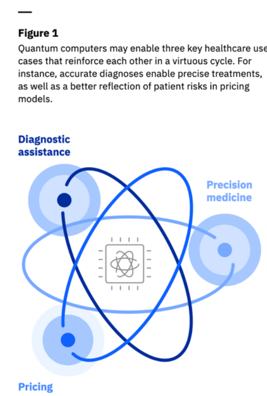
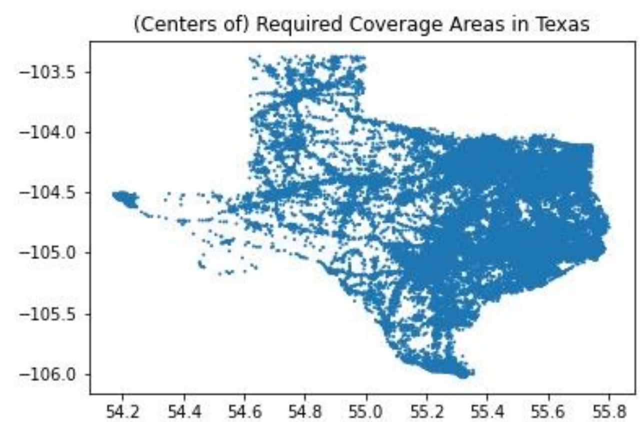
Quantum computers in 2025

Bespoke quantum simulator — *Digital algorithms*

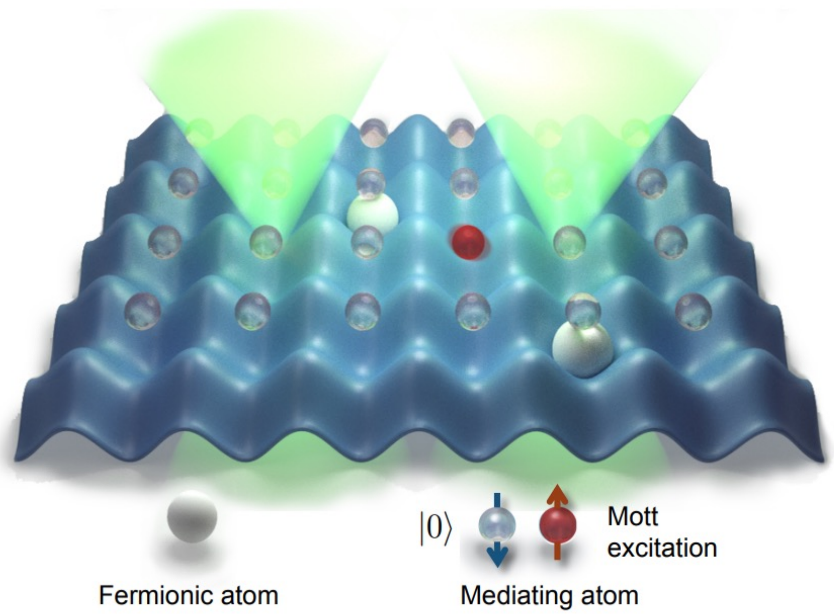


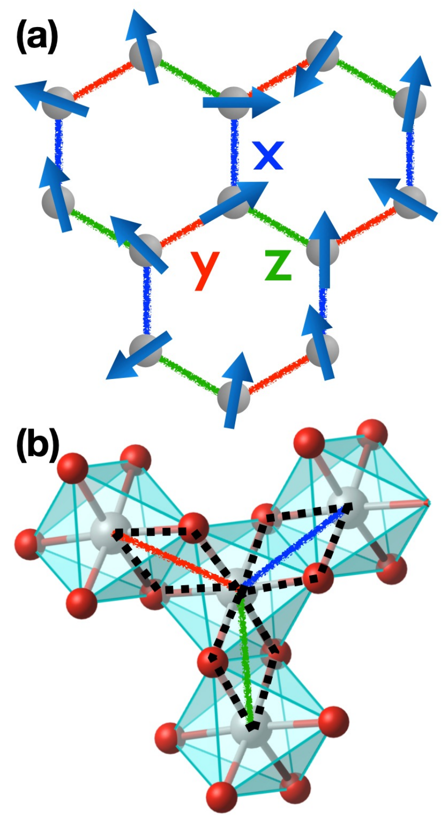




Quantum computers in 2025

Bespoke quantum simulator *Digital algorithms*





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Quantum computers in 2025

Lex' definition of quantum advantage: when I can use a quantum computer to answer a question relevant to condensed matter physicists.

To get to a quantum advantage, we need a problem that is

- Relevant/interesting
- Can be used to interface with non-QC folks
- Runs on a few qubits (< 100)
- Doesn't require long qubit coherence times

Quantum computers in 2025

Lex' de
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phys

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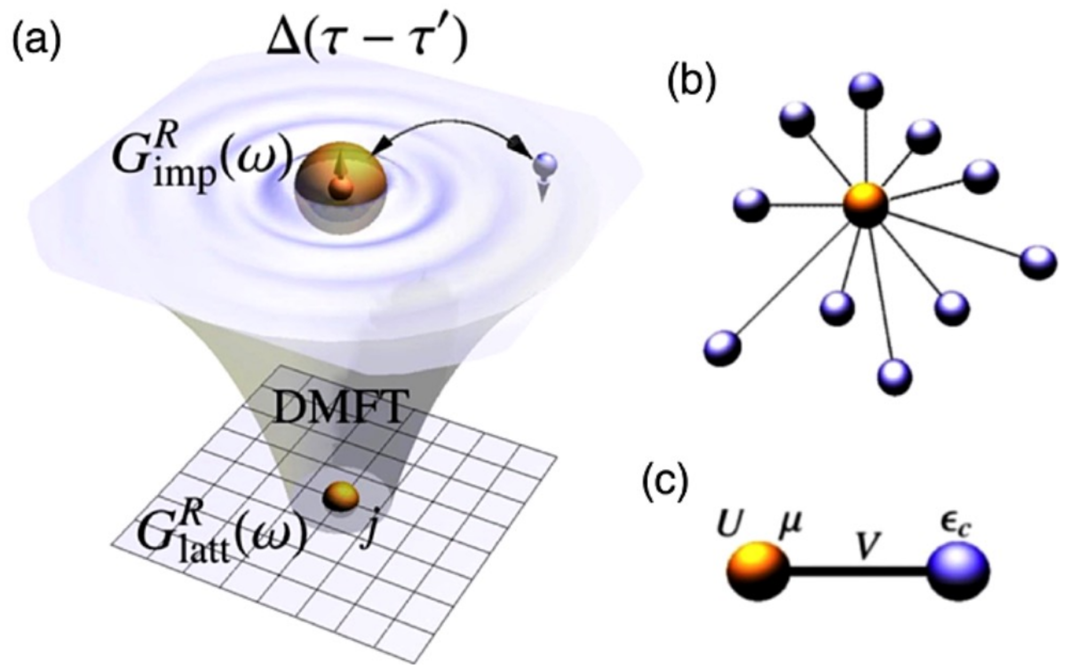

Kreula EPJ Quant. Tech. (2016)

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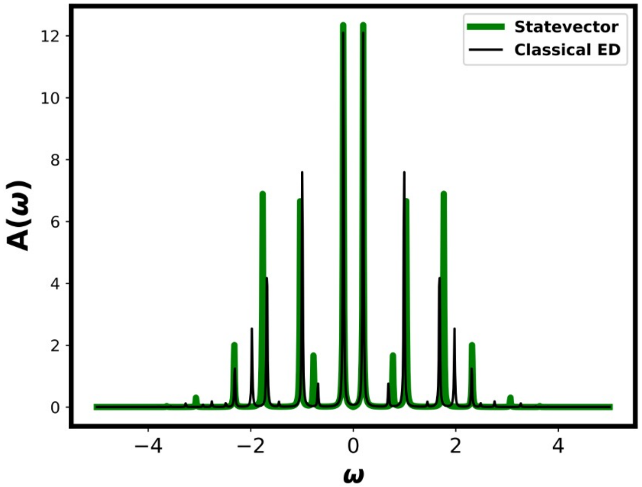
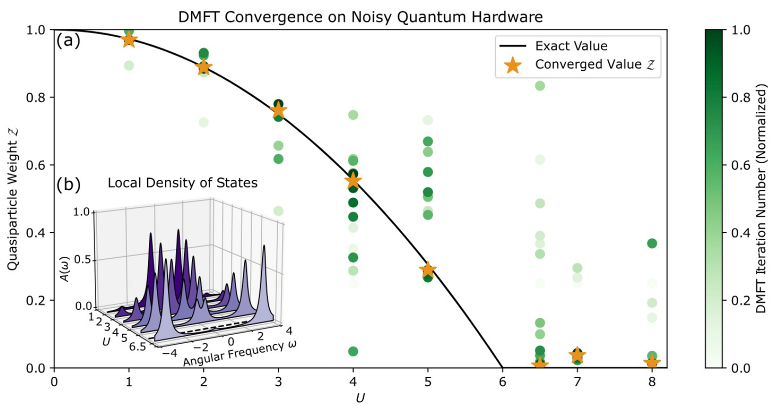
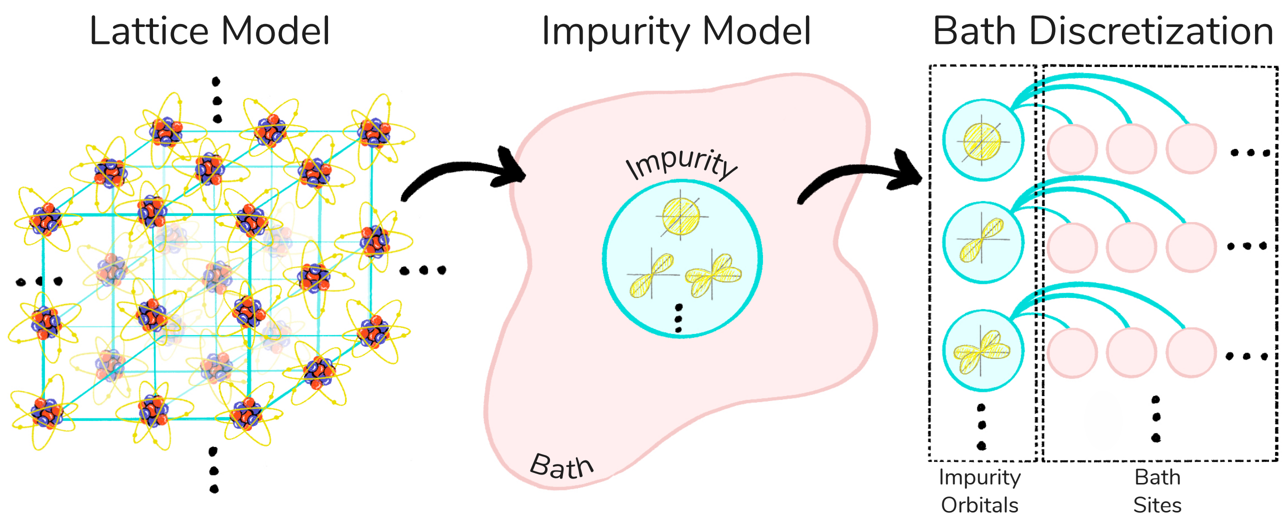
DMFT on Quantum Computers





- Bauer PRX (2016)
- Kreula, EPJ QT (2016)
- Rungger arXiv (2019)
- Keen QST (2020)
- Besserve PRB (2022)
- Jamet arXiv (2022)
- Steckmann PRR (2023)
- Nie PRL (2024)
- Selisko arXiv (2024)
- Greene-Diniz Quantum (2024)
- Jamet APL Quantum (2025)

DMFT on Quantum Computers



$$\mathcal{G}_{ij}(t) = -i\theta(t)\langle\psi|\{c_i(t), c_j^\dagger\}|\psi\rangle$$

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Correlation functions

The Rules

1. You may only use unitary operations
2. More qubits = bad
3. More operations = bad
4. Complex qubit operations = bad
5. Your results will be very noisy anyway

$$e^{iE_0 t}\langle\phi_0|Be^{-i\mathcal{H}t}A|\phi_0\rangle$$

Interfere with ground state

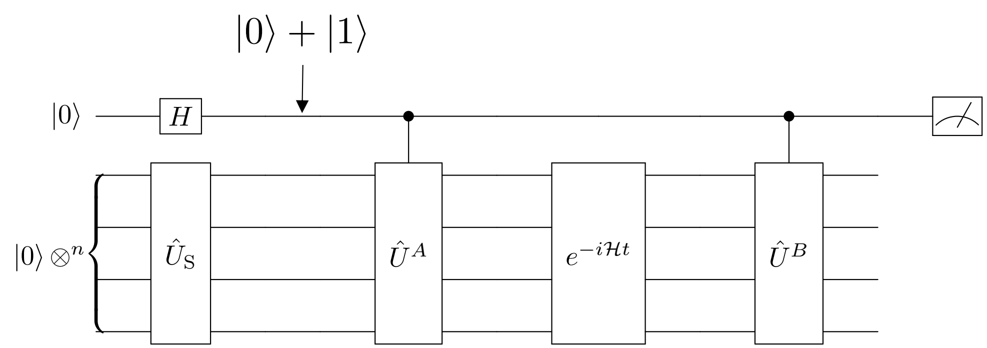
Complete expectation value

Apply excitation B

Time evolve

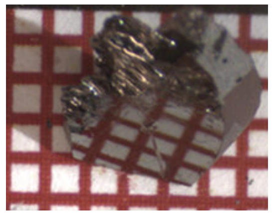
Apply excitation A

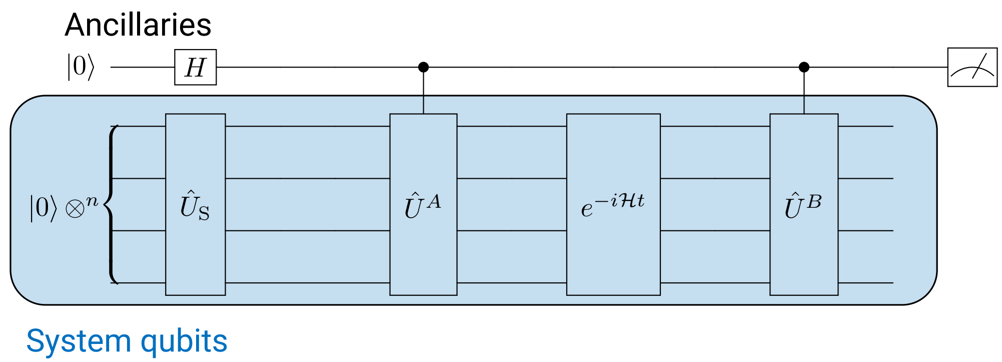
Prepare state of interest

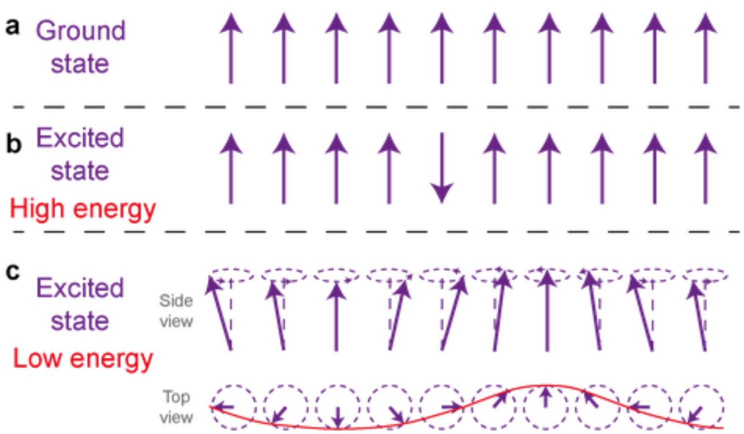


Somma, Simulating physical phenomena by quantum networks (2002)

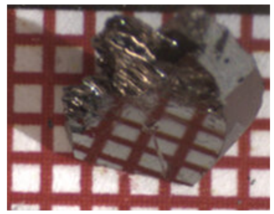
Correlation functions



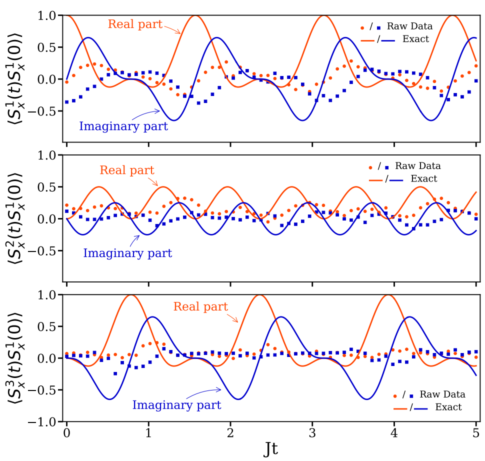




Correlation functions

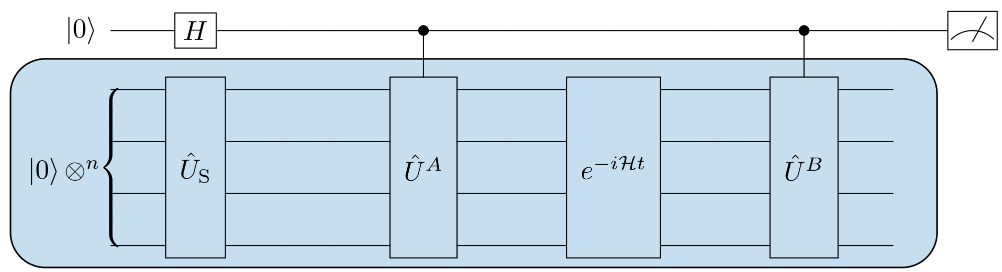


Raw data (2019)



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

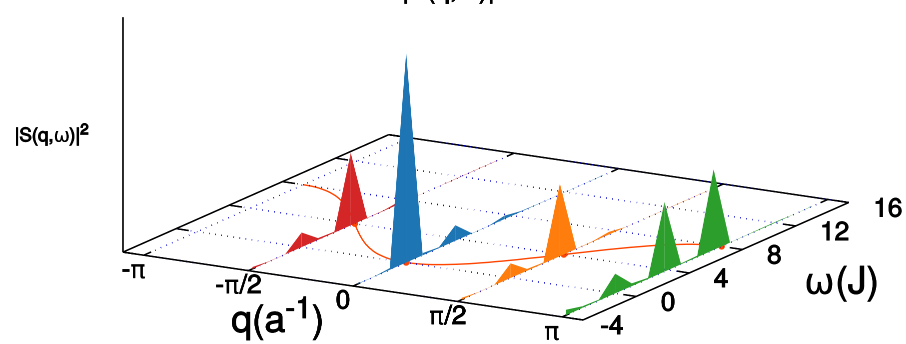
Ancillaries



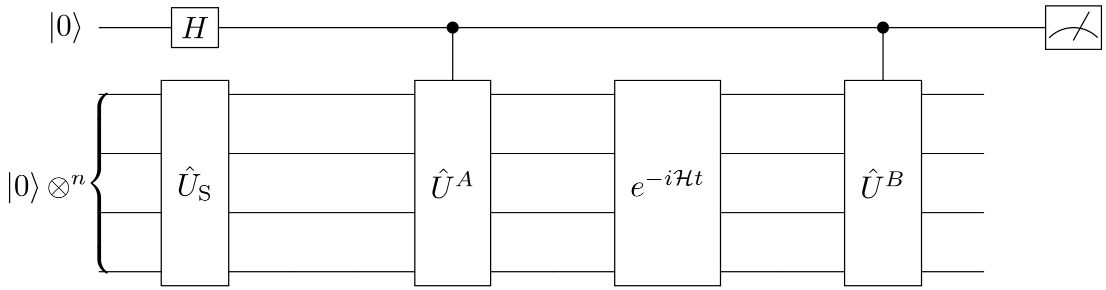
System qubits

Error mitigation

|S(q,ω)|²: PaS



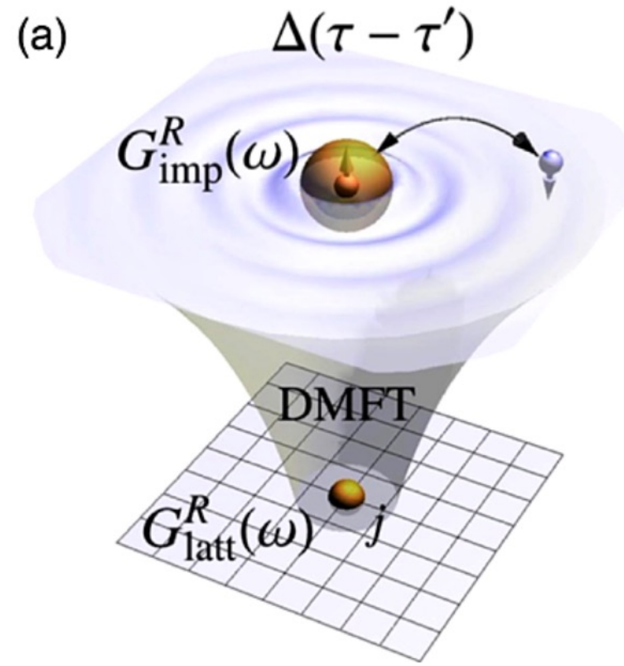
A-Z quantum simulation



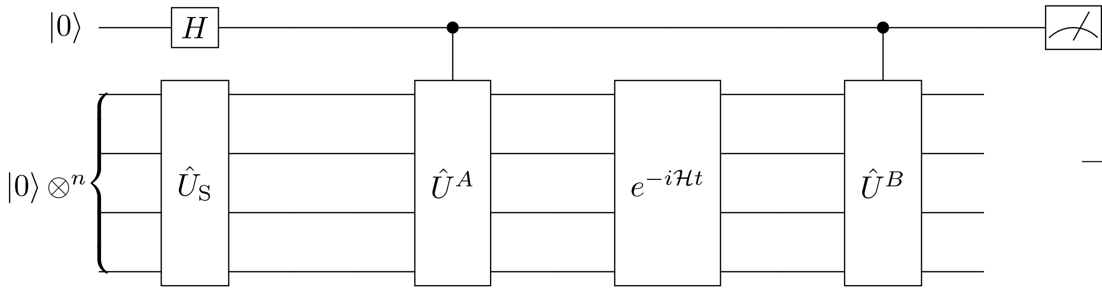
Prepare state of interest

Time evolve

- 🙁 Circuit to prepare interacting ground state is very deep
- 🙁 Variational approaches are very difficult in the presence of noise
- 🙁 Standard Trotter decomposition leads to deep circuits with many gates
- 🙁 Alternative approaches (QSP) requires many ancillae
- 🙁 Your results will be very noisy anyway



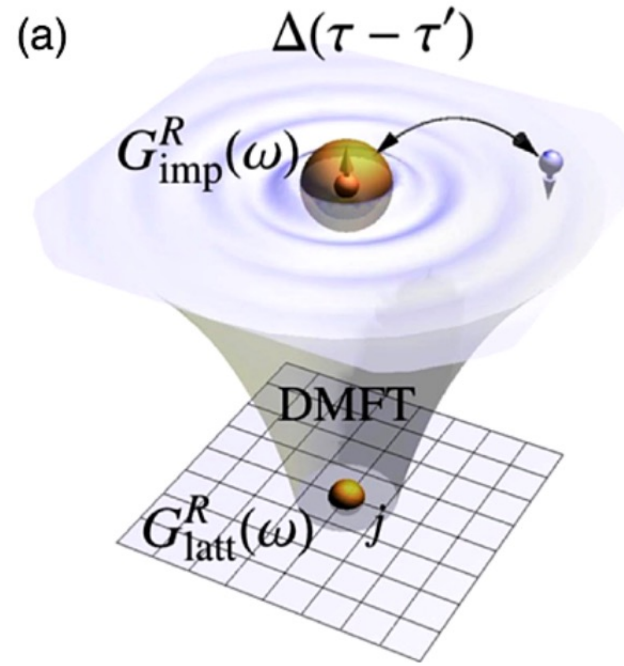
A-Z quantum simulation



Prepare state of interest

Time evolve

Classical post-processing techniques



- *Physics-Informed Subspace Expansions*

- *Lie-algebraic methods for time evolution*

Eigenvector Continuation

PHYSICAL REVIEW LETTERS **121,** 032501 (2018)

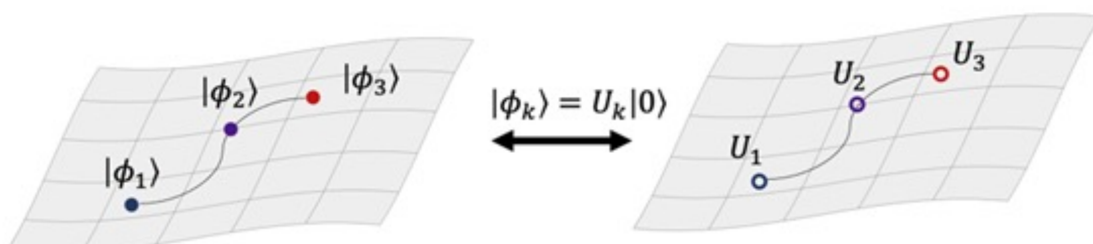
Featured in Physics

Eigenvector Continuation with Subspace Learning

Dillon Frame,[1,2] Rongzheng He,[1,2] Ilse Ipsen,[3] Daniel Lee,[4] Dean Lee,[1,2] and Ermal Rrapaj[5]

- Ground state varies continuously in a parameter space and is spanned by a few low energy state vectors.

$$|\phi_3\rangle = \alpha_1|\phi_1\rangle + \alpha_2|\phi_2\rangle$$



Eigenvector Continuation

PHYSICAL REVIEW LETTERS **121,** 032501 (2018)

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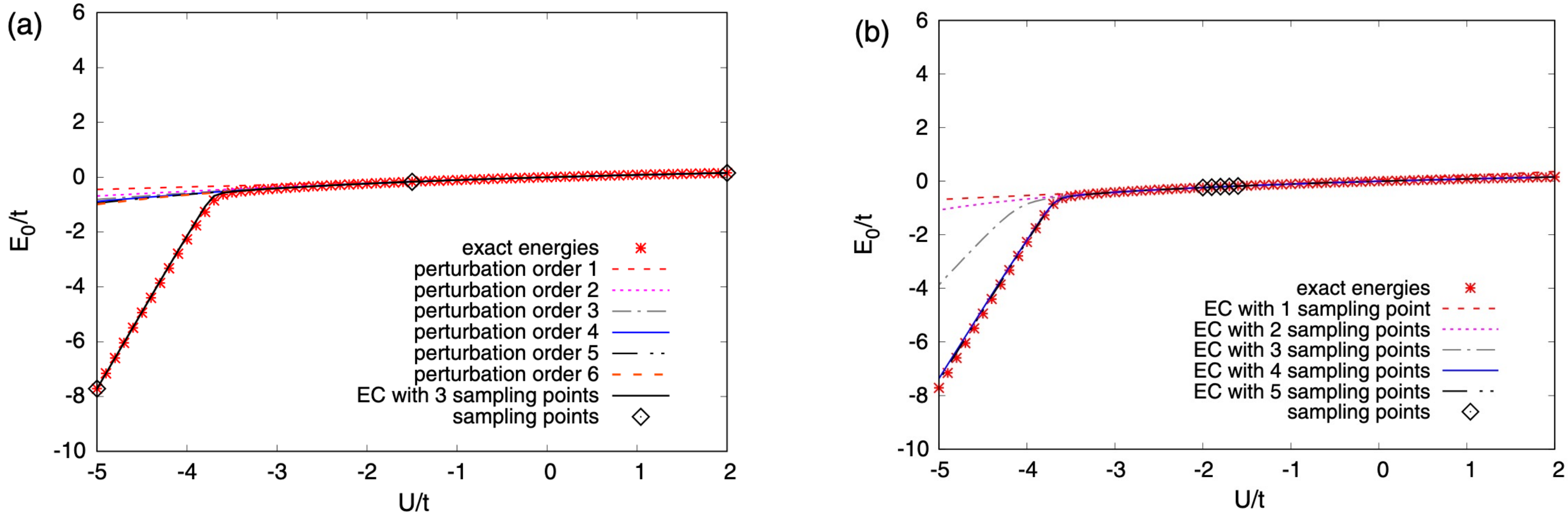

Eigenvector Continuation

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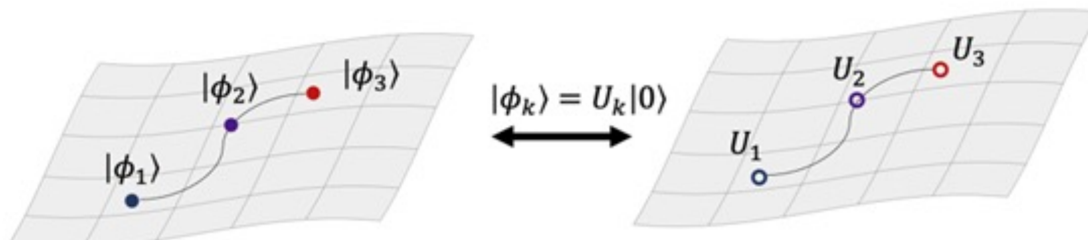
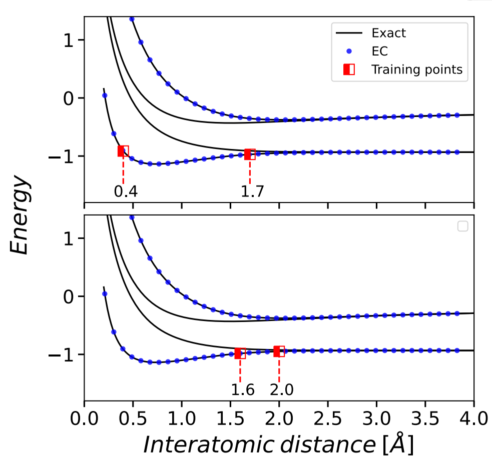
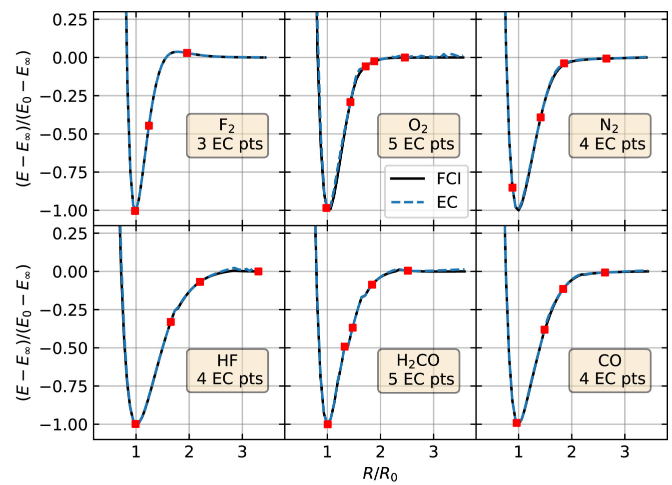




arXiv:2209.10571



C. Mejuto-Zaera et al., Electron. Struct. 2023

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Fermionic Gaussian Subspace

Commun. Math. Phys. 356, 451–500 (2017)
Digital Object Identifier (DOI) 10.1007/s00220-017-2976-9

Communications in **Mathematical Physics**

CrossMark

Complexity of Quantum Impurity Problems

Sergey Bravyi, David Gosset

IBM T.J. Watson Research Center, Yorktown Heights, NY, USA. E-mail: sbravyi@us.ibm.com; dngosset@us.ibm.com

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Published online: 31 August 2017 – © Springer-Verlag GmbH Germany 2017

PHYSICAL REVIEW RESEARCH **3**, 033188 (2021)

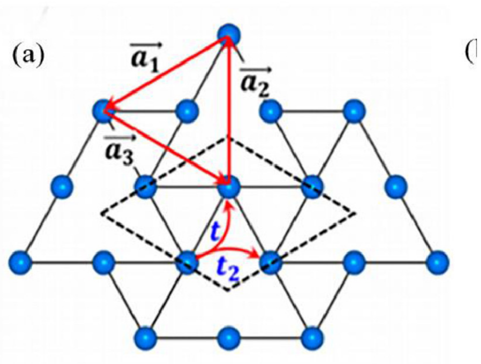
Quantum impurity models using superpositions of fermionic Gaussian states: Practical methods and applications

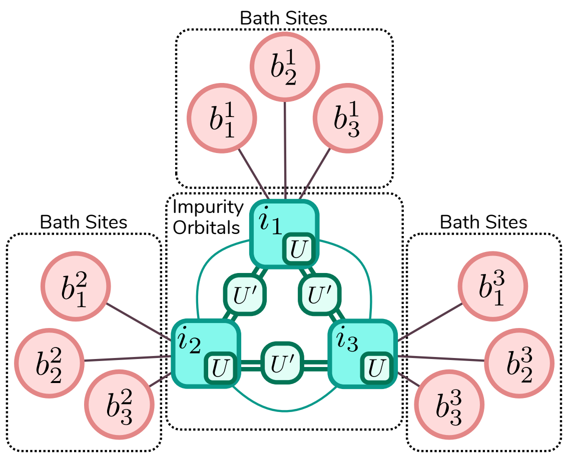
Samuel Boutin and Bela Bauer
Station Q, Microsoft Corporation, Santa Barbara, California 93106 USA

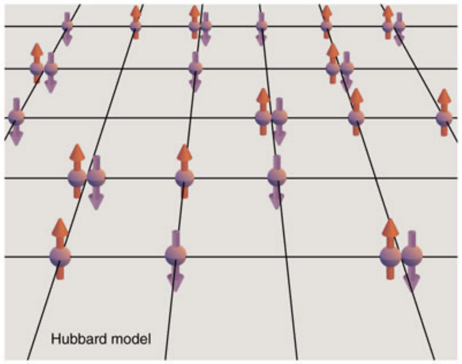
“The low energy state is represented as a superposition of exp [O(b^3)] fermionic Gaussian states.”

“Quantum impurity models provide a natural arena for studying the complexity of fermionic systems in an intermediate regime interpolating between the free and the fully interacting cases.”

Fermionic Gaussian Subspace







Free fermions *Impurity model* *Fully interacting*

Complexity

Advantages of a basis based on fermionic gaussian states:

- Polynomially sized calculations to find the ground state
- Easy to prepare on QC
- One basis set spans the necessary space across entire DMFT phase diagam

Image credit: 10.1016/j.chphma.2022.04.009, American Scientist

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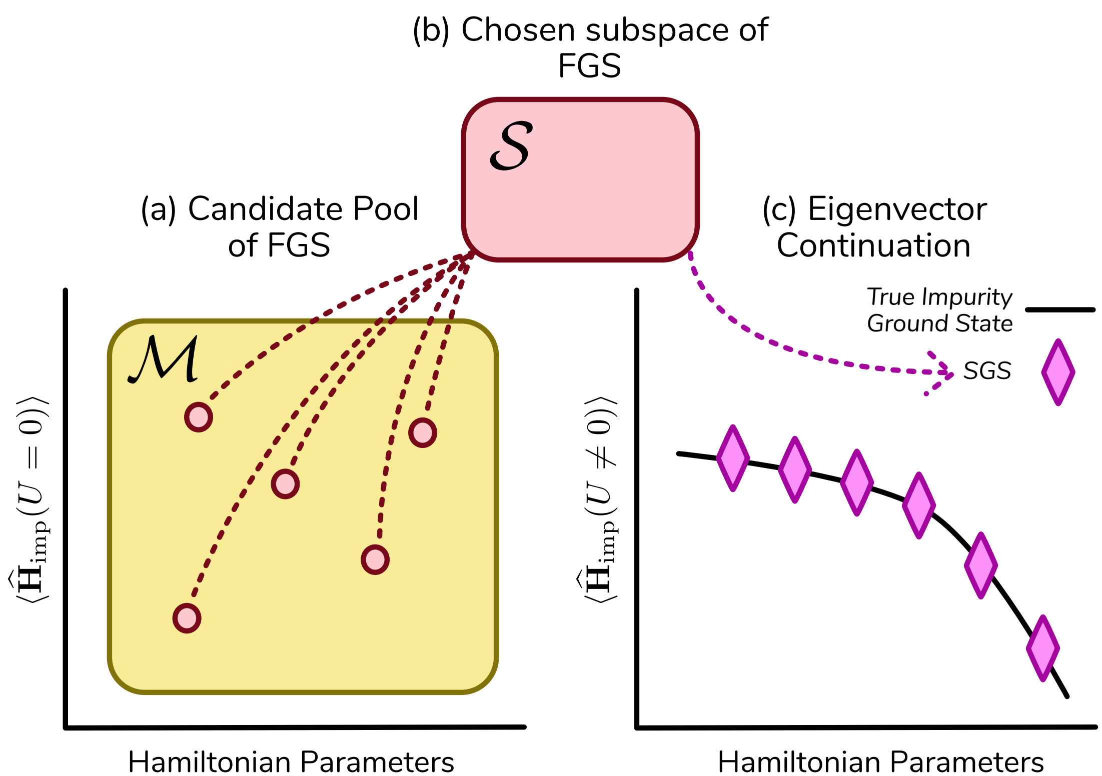
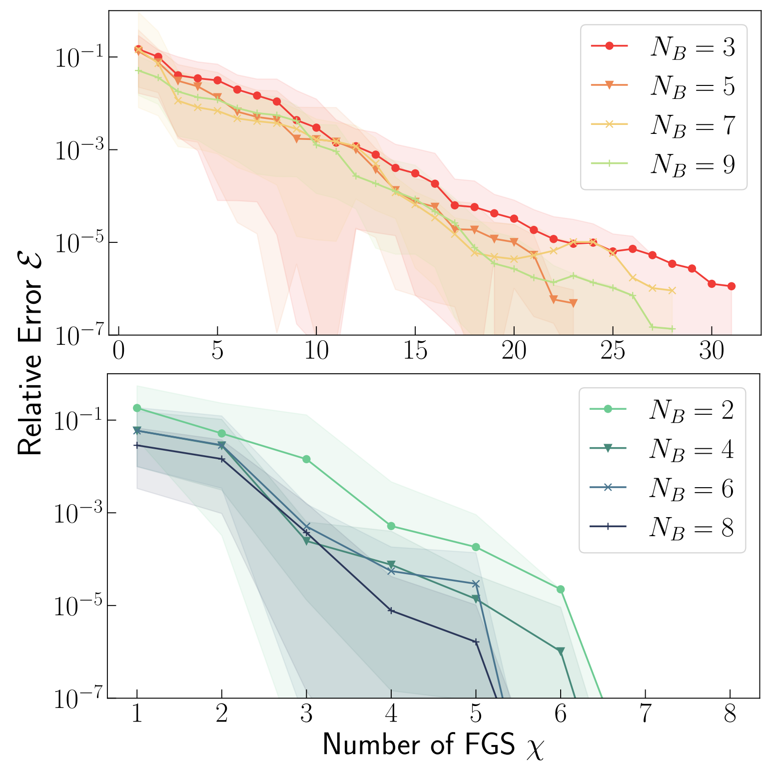
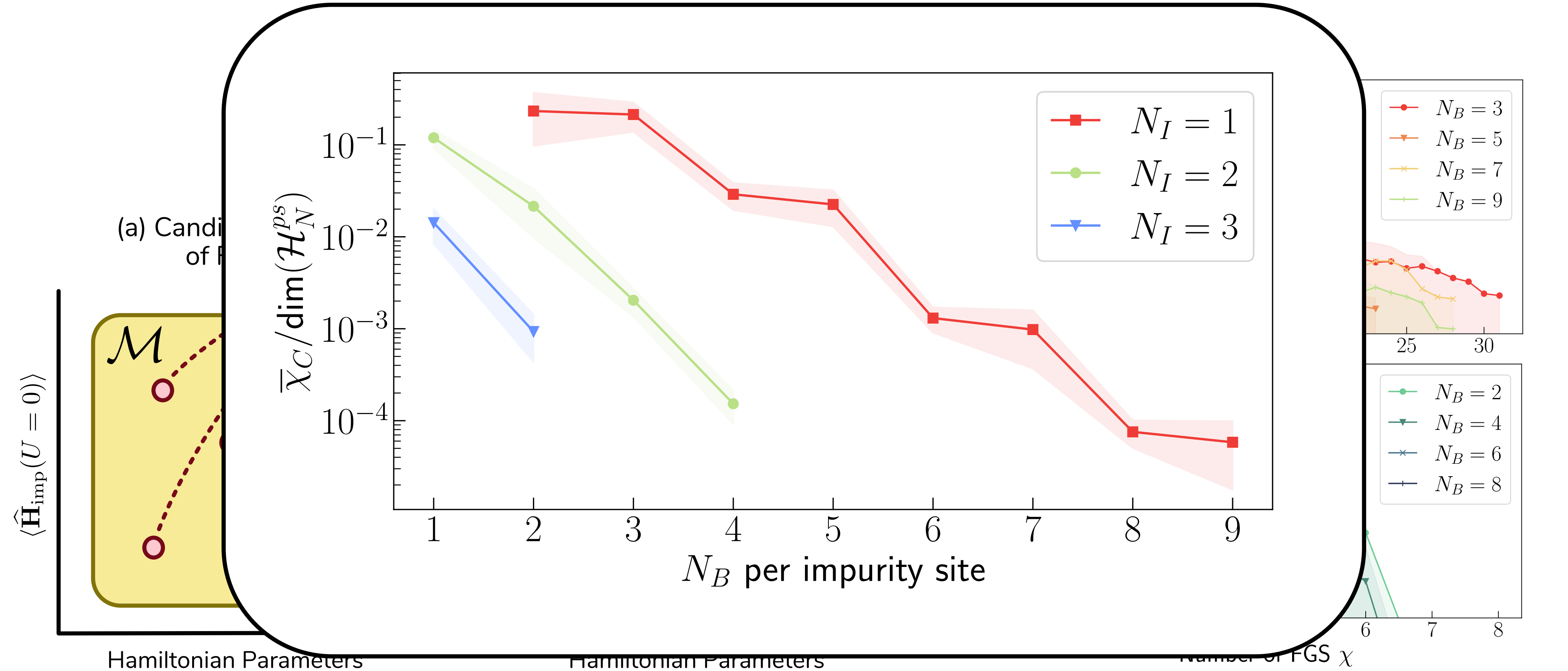
Fermionic Gaussian Subspace



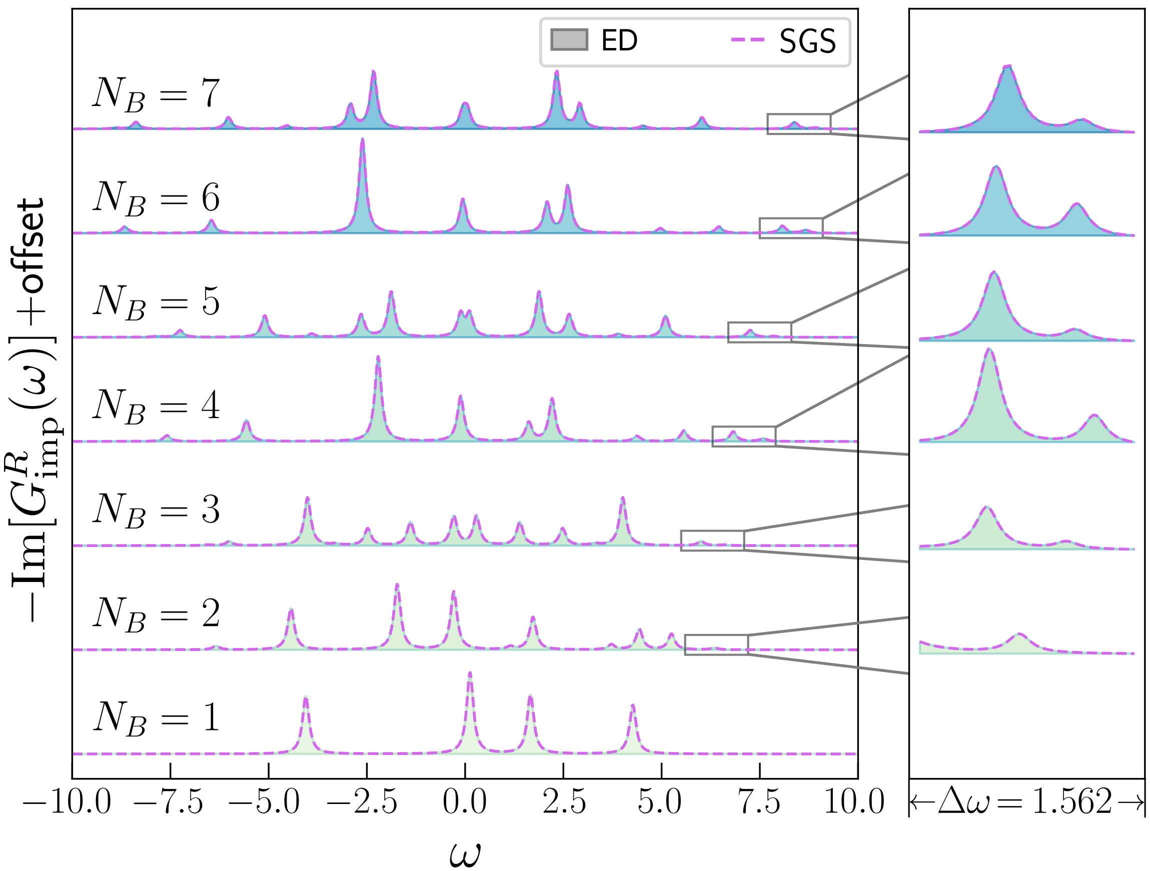
$$\widetilde{H}\vec{\alpha} = \widetilde{E}S\vec{\alpha}$$



Fermionic Gaussian Subspace



Fermionic Gaussian Subspace



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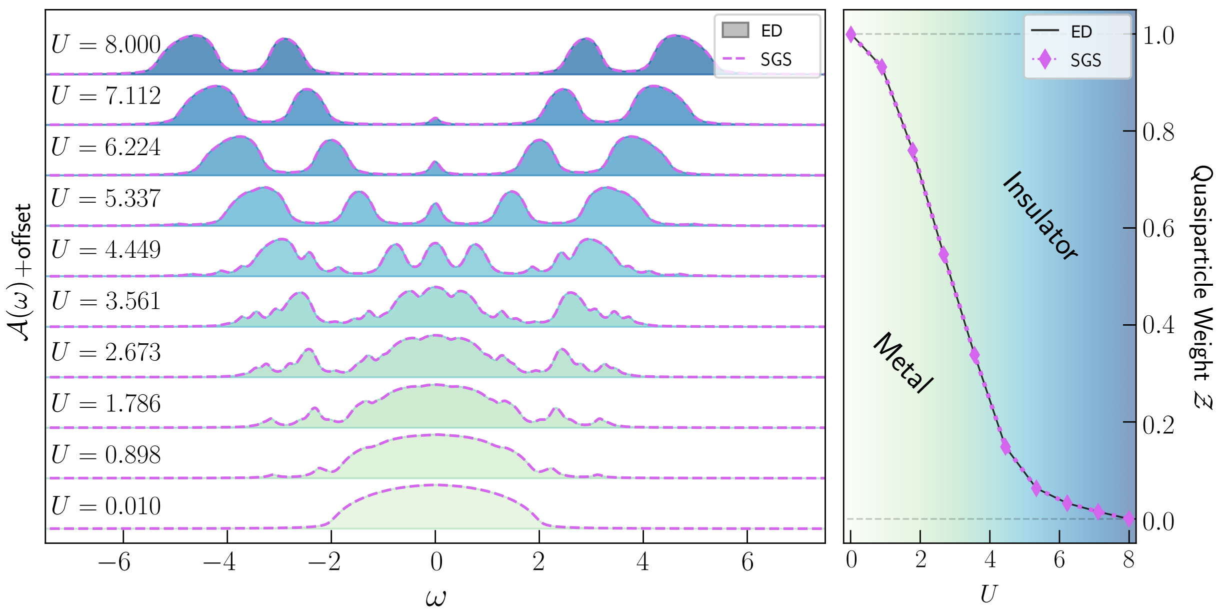
Fermionic Gaussian Subspace

Now that we have the tools, let's see how it works:

- DMFT using sum of Gaussian states (SGS) (Hubbard Model w/ Bethe lattice)

Shaded region = $|\psi\rangle$ dashed line = $\sum_{k=1}^{\chi} \alpha_k |\phi_k\rangle$



Increasing interaction strength on impurity

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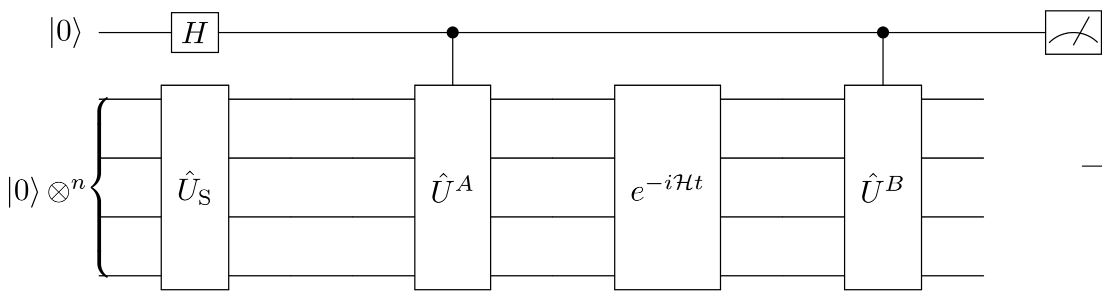
A-Z quantum simulation



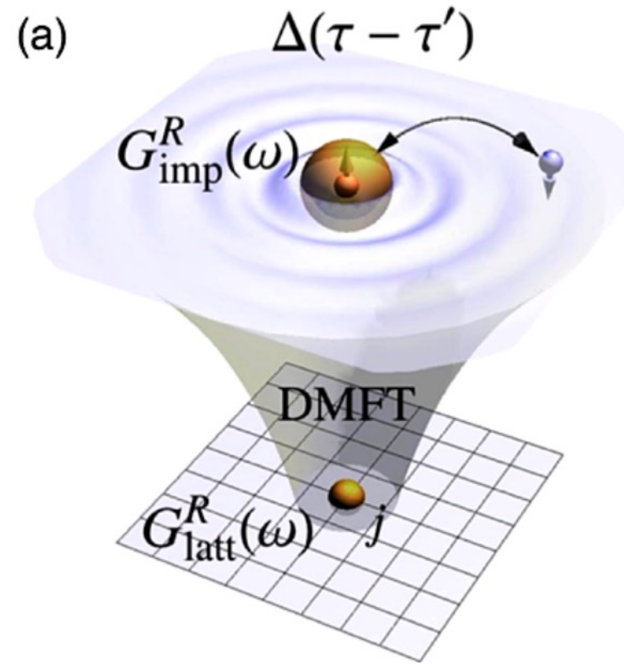
Prepare state of interest

Time evolve

Classical post-processing techniques

- *Physics-Informed Subspace Expansions*

- *Lie-algebraic methods for time evolution*

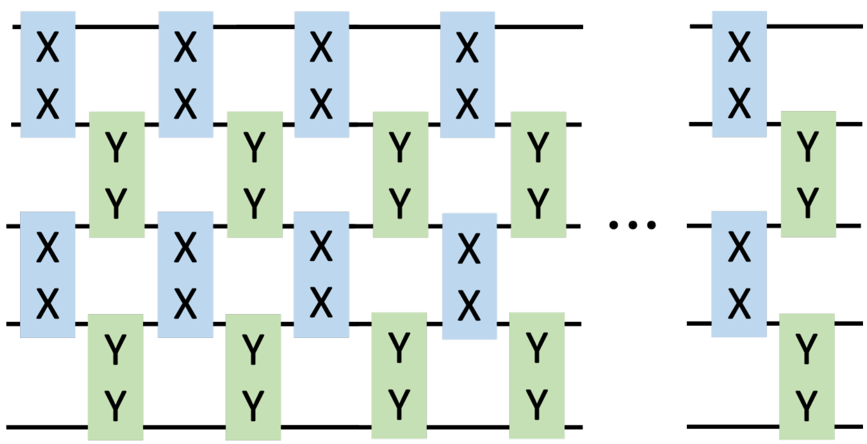


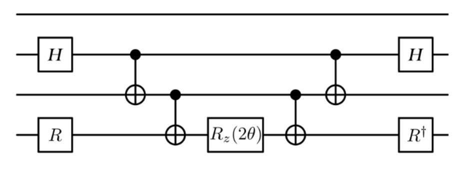
Time evolution

Simulation of a time independent spin Hamiltonian:

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

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

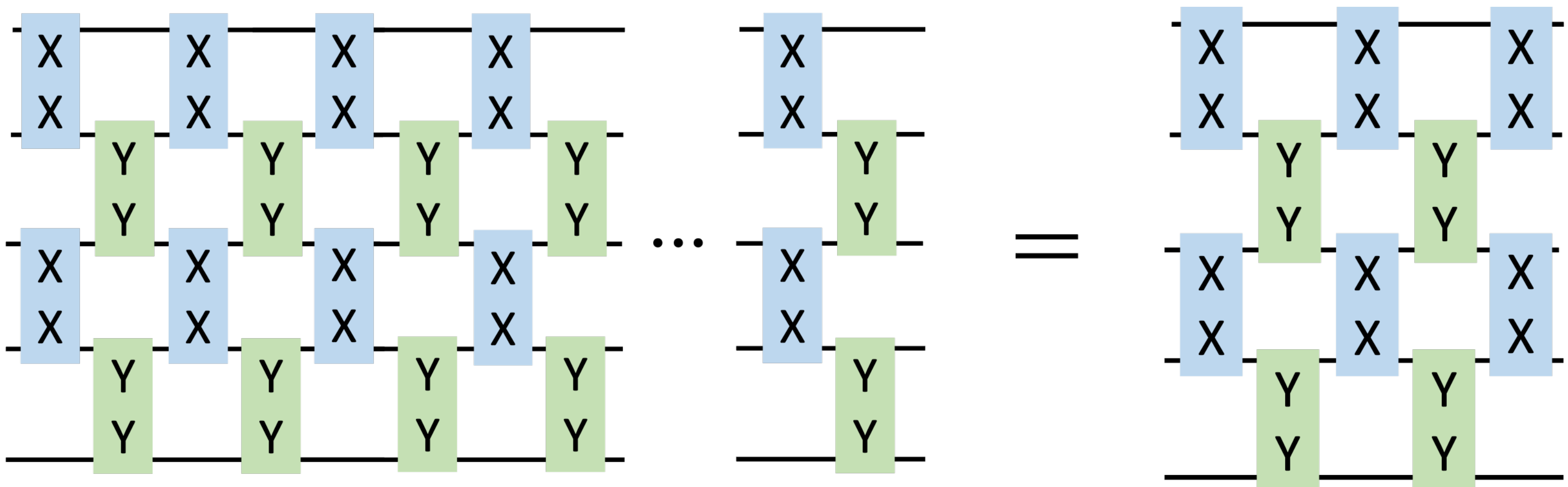
$U(t) =$ 

$e^{i\theta IXZYI} =$ 

Algebraic Circuit Compression

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

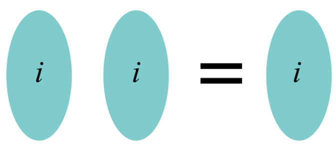
- The method is **scalable** due to its "constructive" and "local" nature.



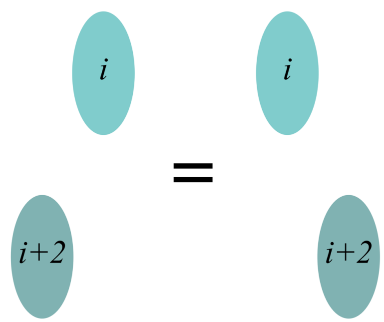
Algebraic Circuit Compression

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

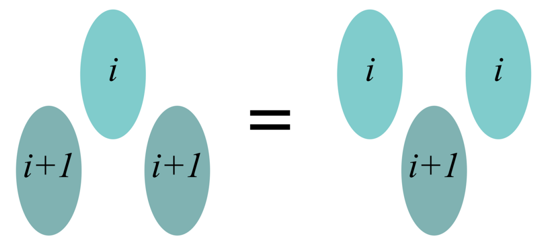
Fusion



Commutation

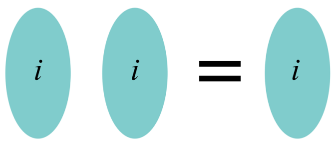


Turnover

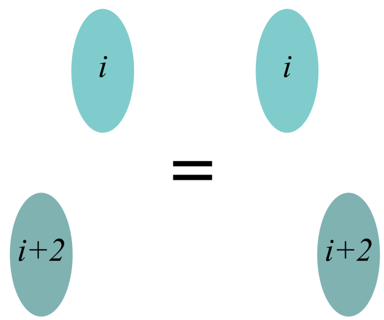


Algebraic Circuit Compression

Fusion



Commutation



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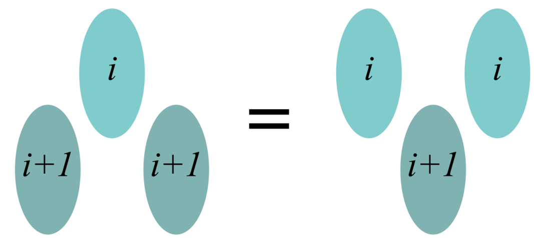
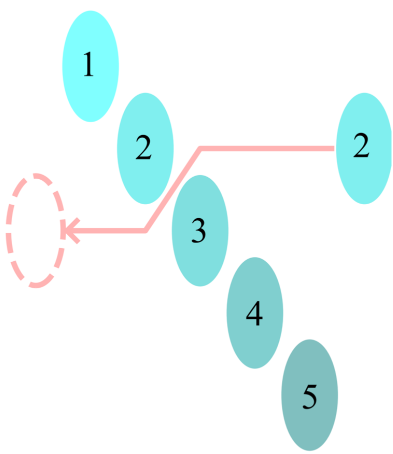
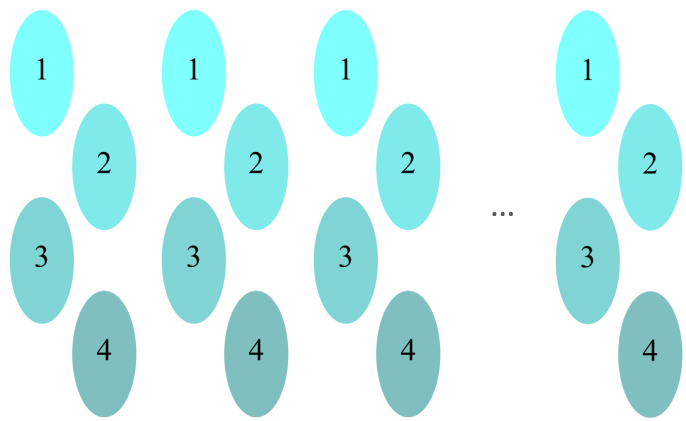
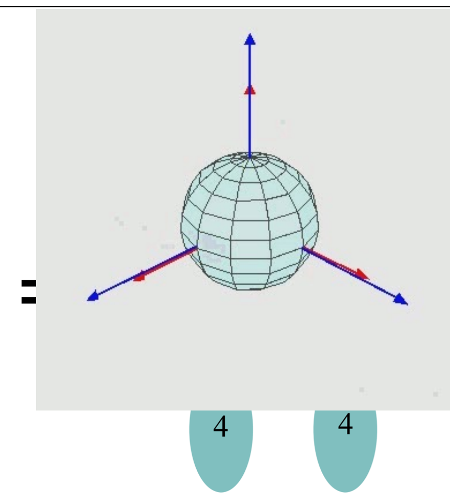


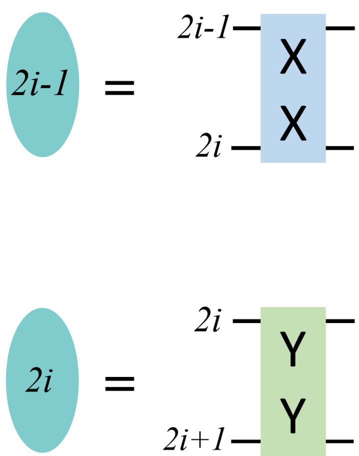




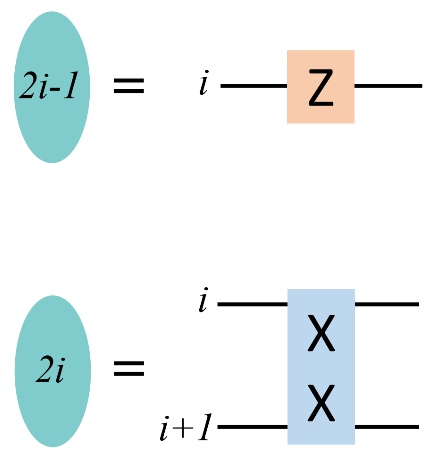


Free Fermion Blocks

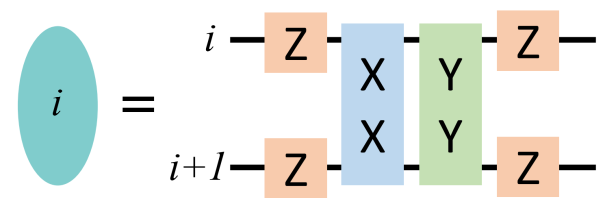
Kitaev Chain



Transverse Field Ising

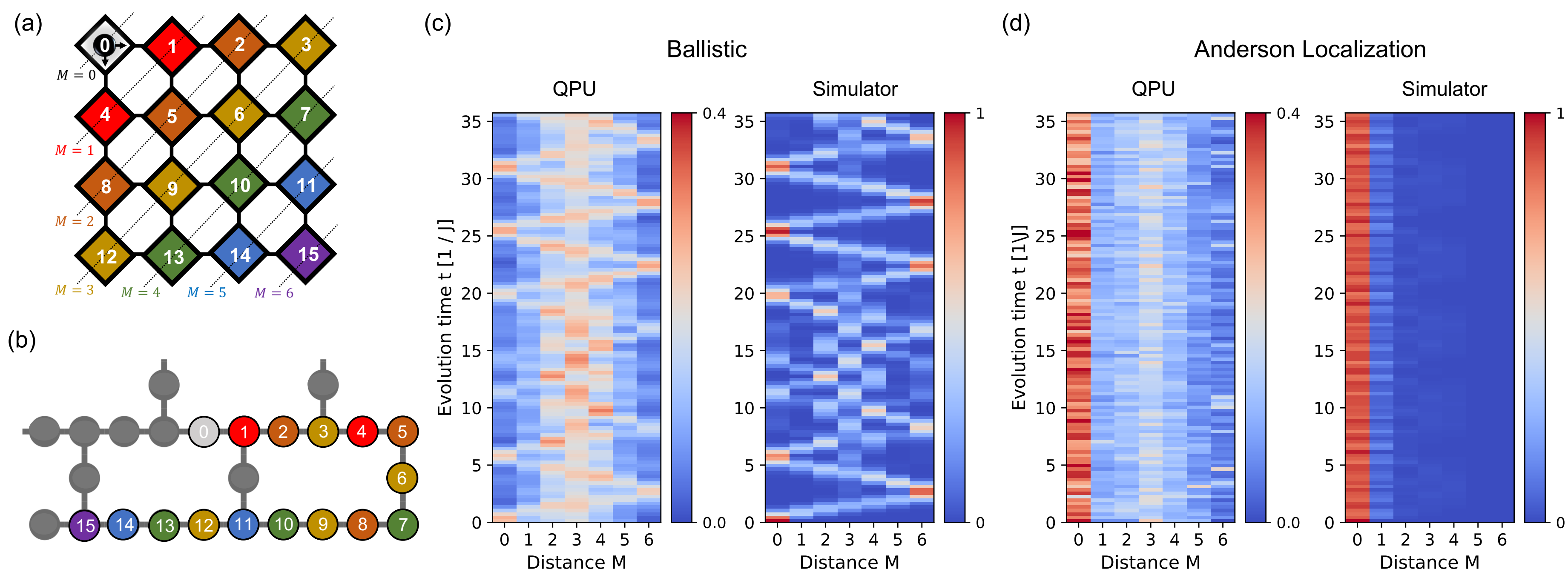


Transverse Field XY



$$\mathcal{H} = -t \sum_i \left[X_i X_{i+1} + Y_i Y_{i+1}\right] + h \sum_i Z_i$$

Approach #1: Algebraic Circuit Compression (preliminary)



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

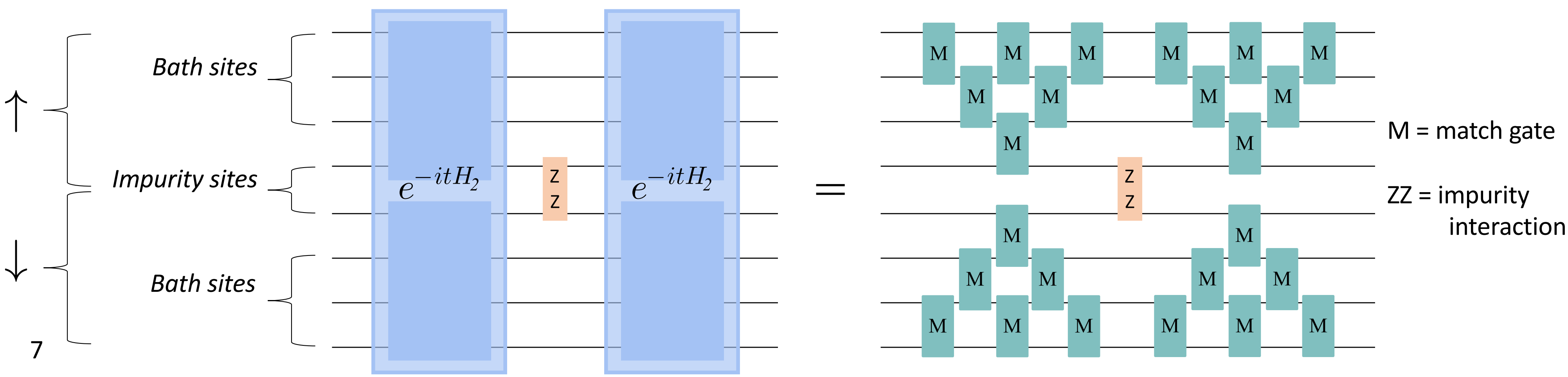
Simulating the Impurity Model on a Quantum Computer

Time evolving the impurity ground state

- ***Partial compression*** for impurity models:

[1] 10.1103/PhysRevLett.129.070501
[2] arXiv:2303.09538

Example: 1 trotter step



Simulating the Impurity Model on a Quantum Computer

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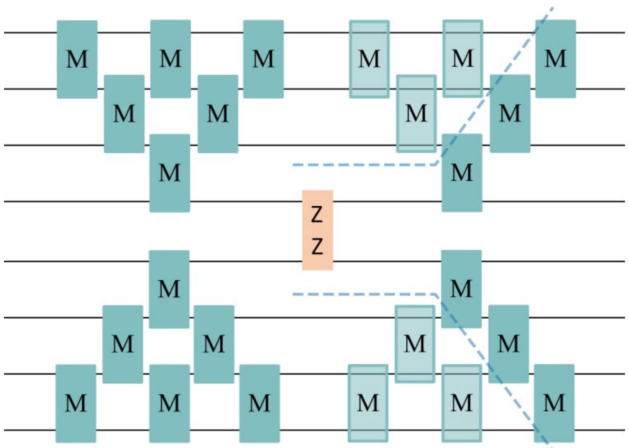
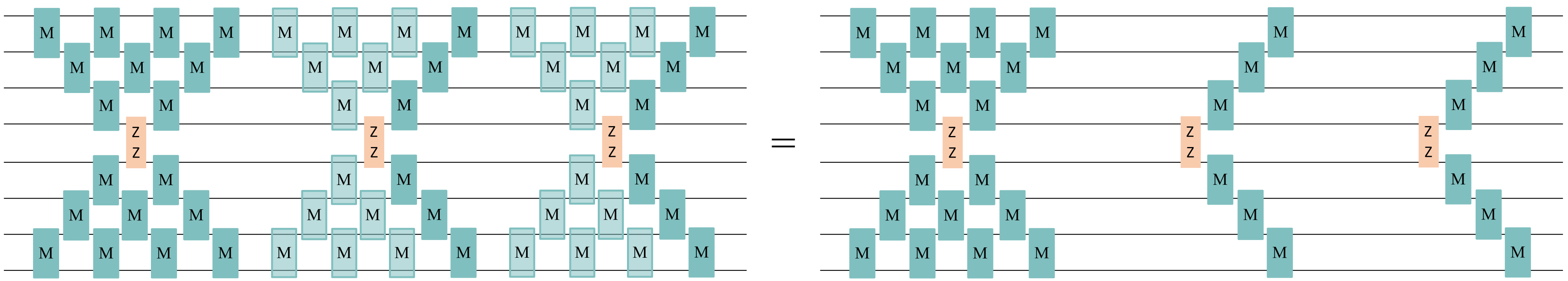


Simulating the Impurity Model on a Quantum Computer

[1] 10.1103/PhysRevLett.129.070501
[2] arXiv:2303.09538

Further example: 3 trotter steps



Simulating the Impurity Model on a Quantum Computer

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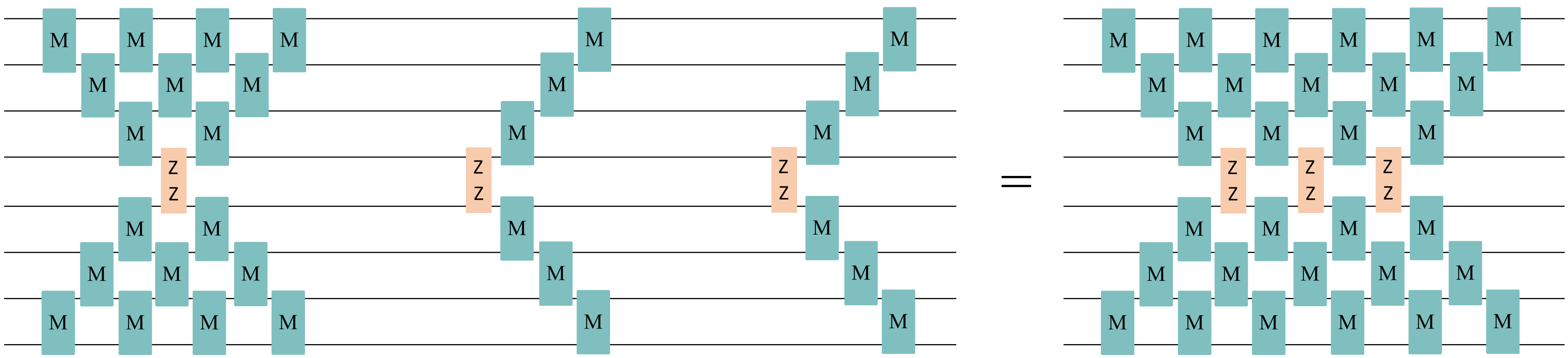
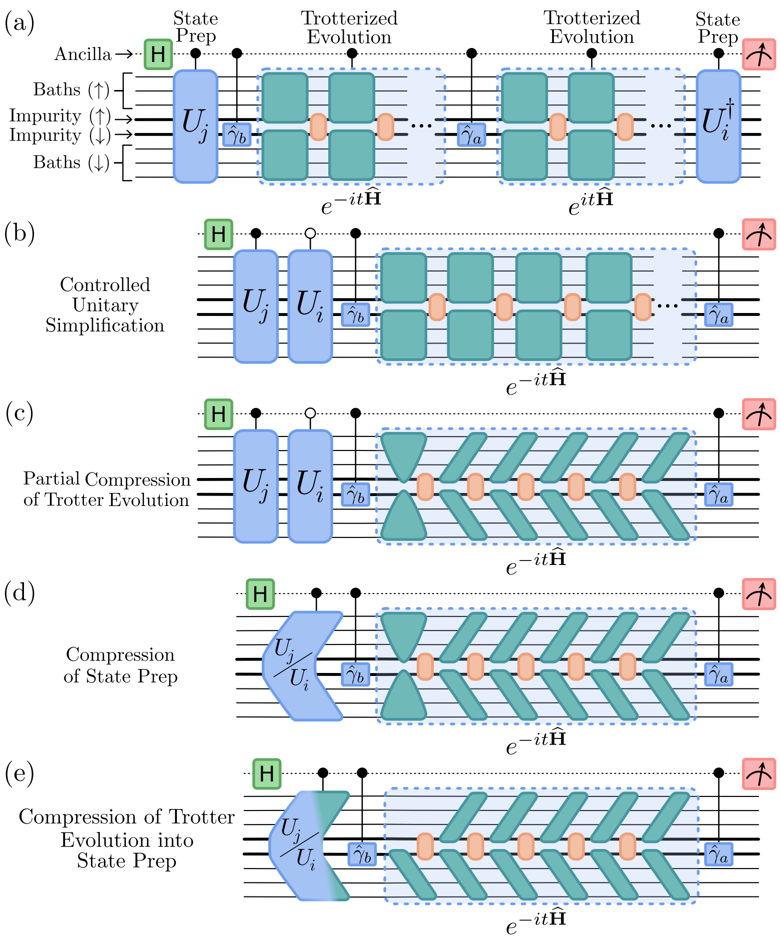


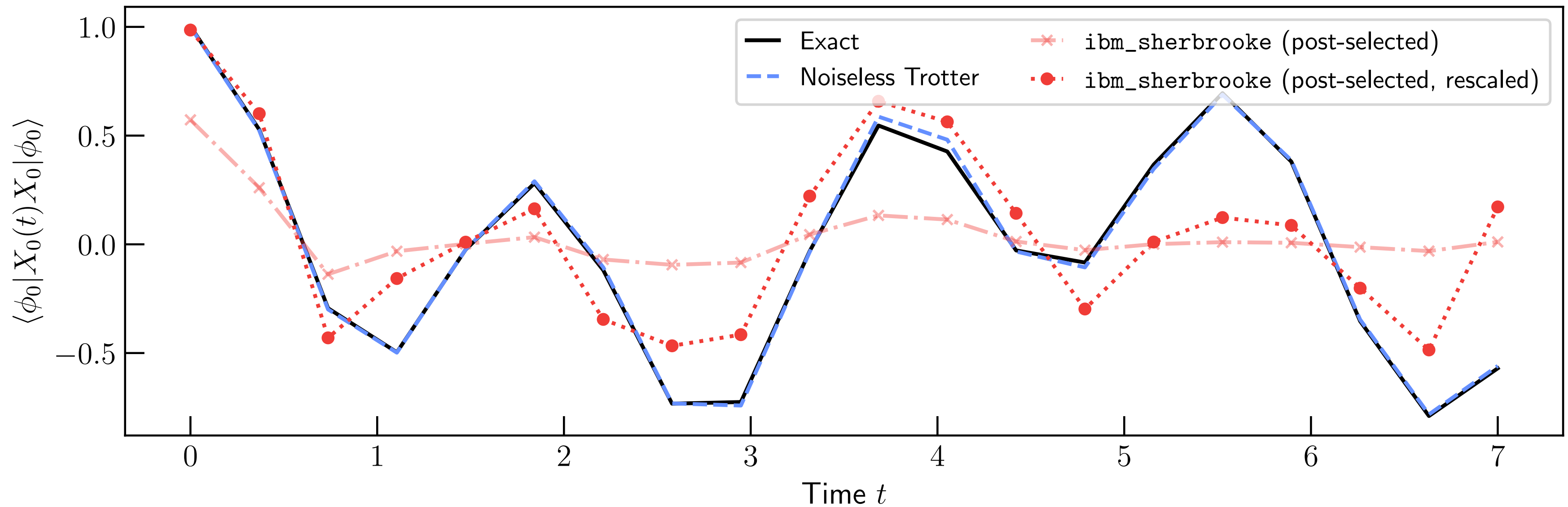
Simulating the Impurity Model on a Quantum Computer



The Rules

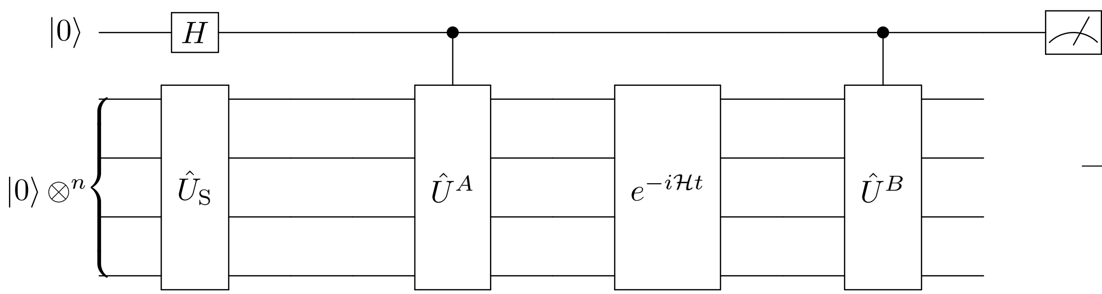
1. You may only use unitary operations
2. More qubits = bad
3. More operations = bad
4. Complex qubit operations = bad
5. Your results will be very noisy anyway

Hardware results



$$\mathcal{G}_{00}(t) = -i\theta(t)\langle \phi_0 | \{c_0(t), c_0^\dagger\} | \phi_0 \rangle$$

A-Z quantum simulation



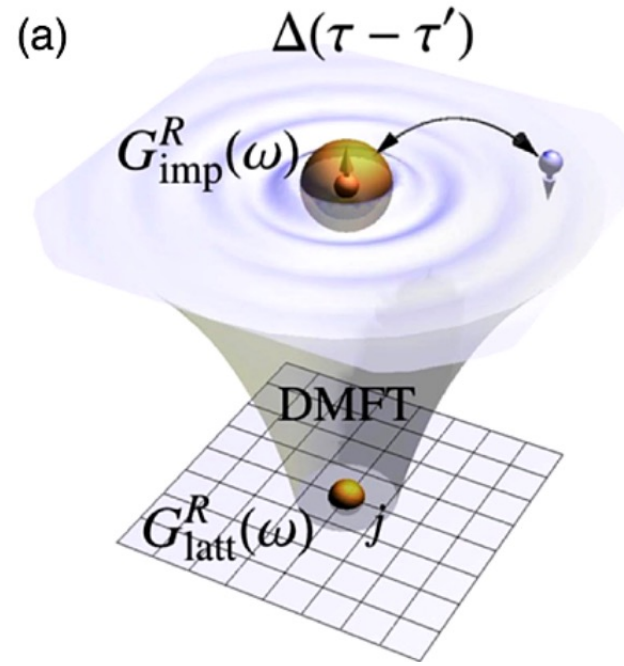
Prepare state of interest

Time evolve

Classical post-processing techniques

- *Physics-Informed Subspace Expansions*

- *Lie-algebraic methods for time evolution*



A-Z quantum simulation

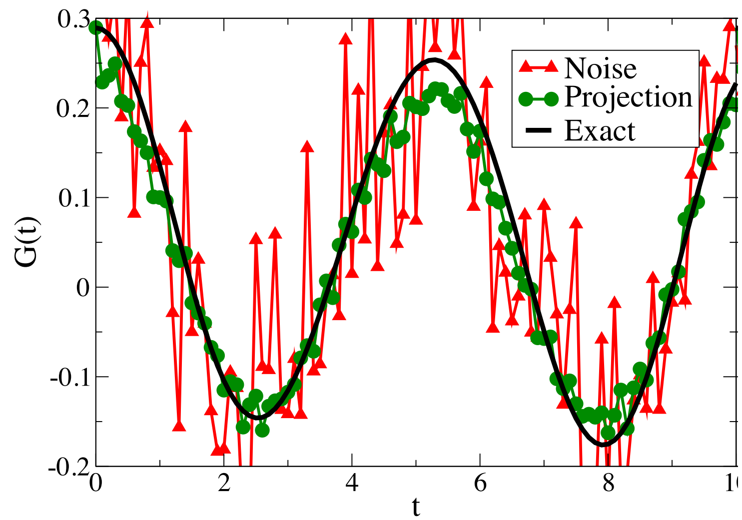
- It turns out that these are positive semi-definite (PSD) functions:

$$G_{AA}(t-t') = \mathrm{Tr}\left[\rho A(t)^\dagger A(t')\right]$$

- Then this is a PSD matrix:

$$\underline{\mathrm{G}} = \begin{pmatrix} f_0 & f_1 & f_2 & \cdots & f_n \\ f_1^* & f_0 & f_1 & \cdots & f_{n-1} \\ f_2^* & f_1^* & f_0 & \cdots & f_{n-2} \\ \vdots & & & \ddots & \vdots \\ f_n^* & f_{n-1}^* & f_{n-2}^* & \cdots & f_0 \end{pmatrix}$$

where $G_{AA}(t_i - t_j) \to f_{i-j}$



A.F. Kemper, C. Yang, E. Gull, PRL (2024)

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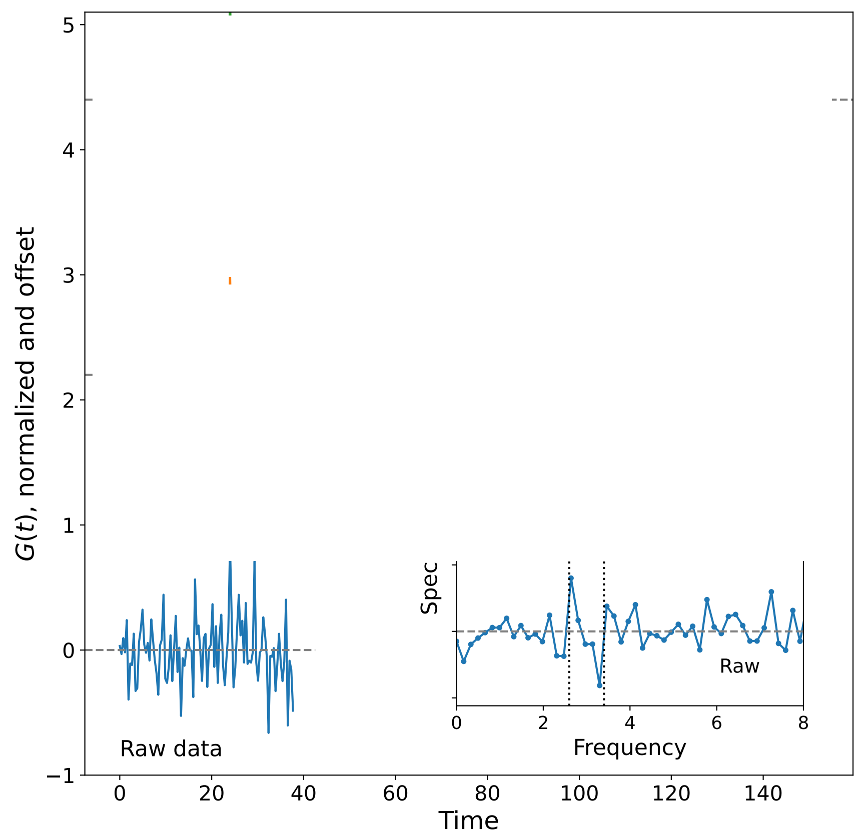

A.F. Kemper, C. Yang, E. Gull, PRL (2024)

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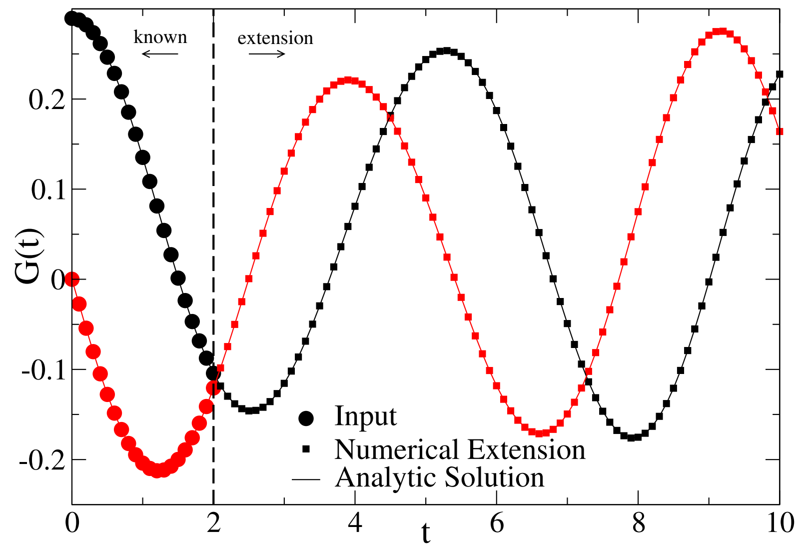

A.F. Kemper, C. Yang, E. Gull, PRL (2024)

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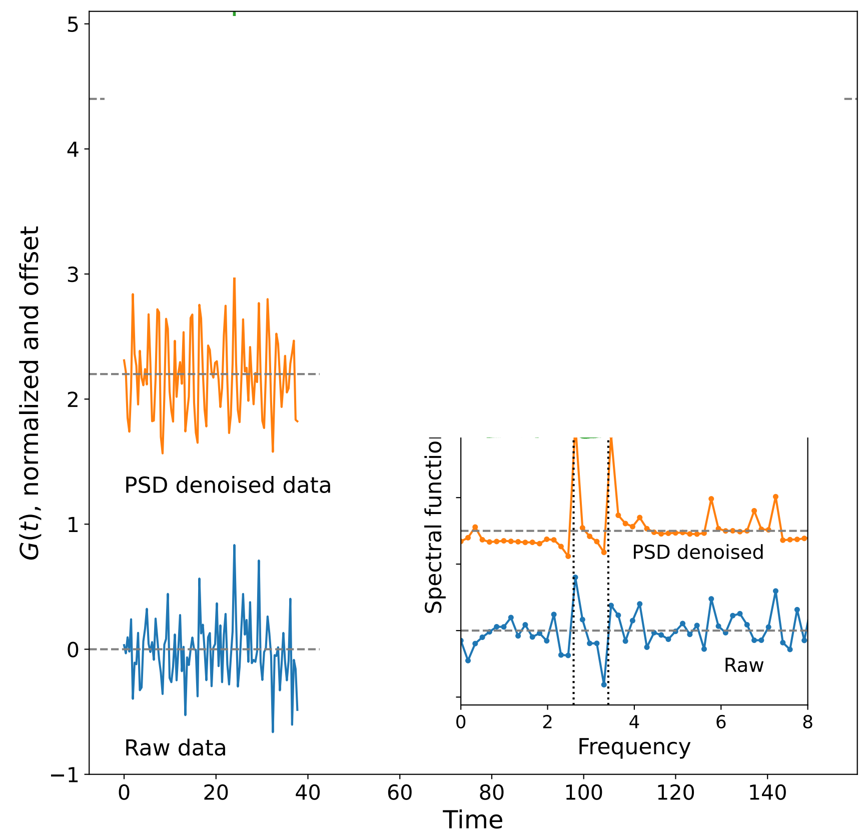
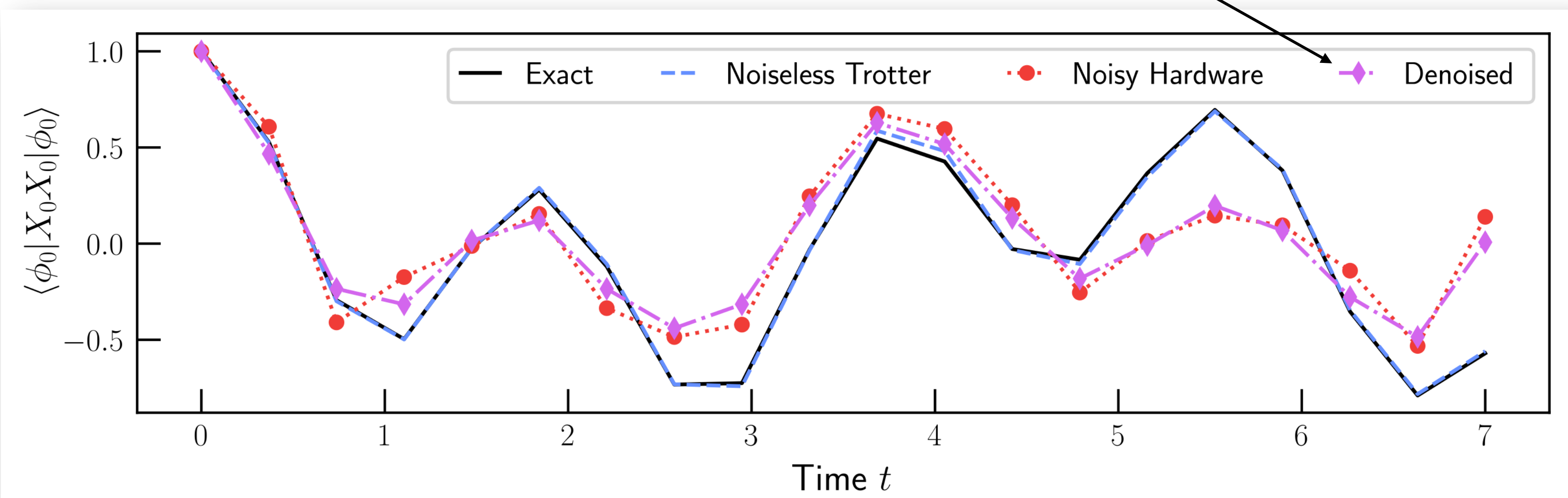


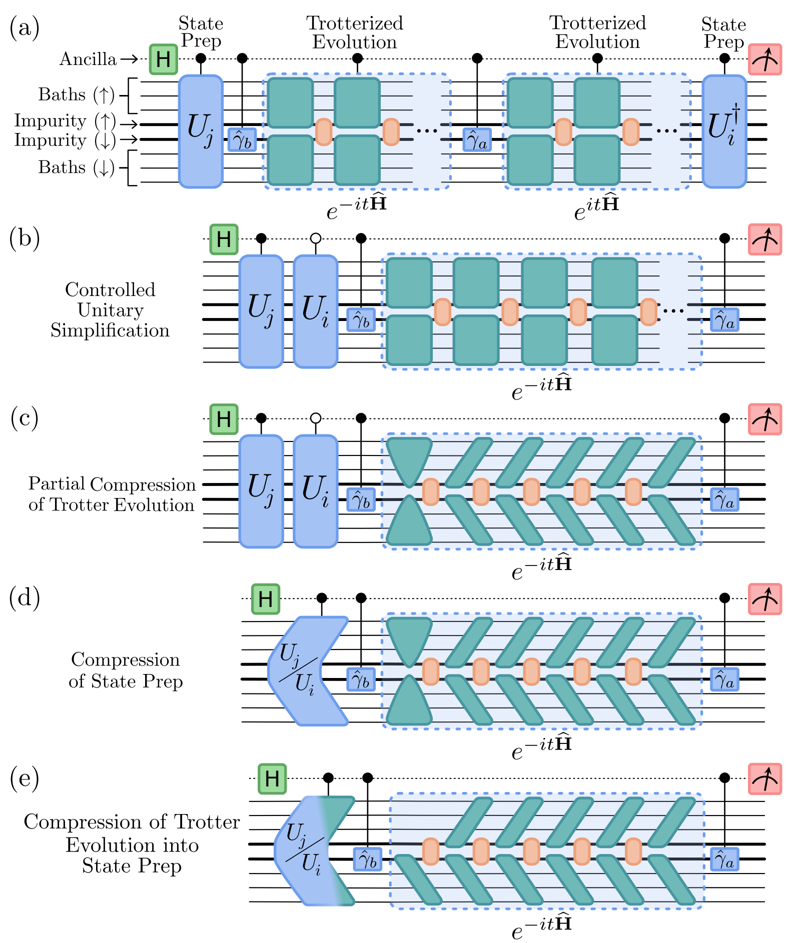
A.F. Kemper, C. Yang, E. Gull, PRL (2024)

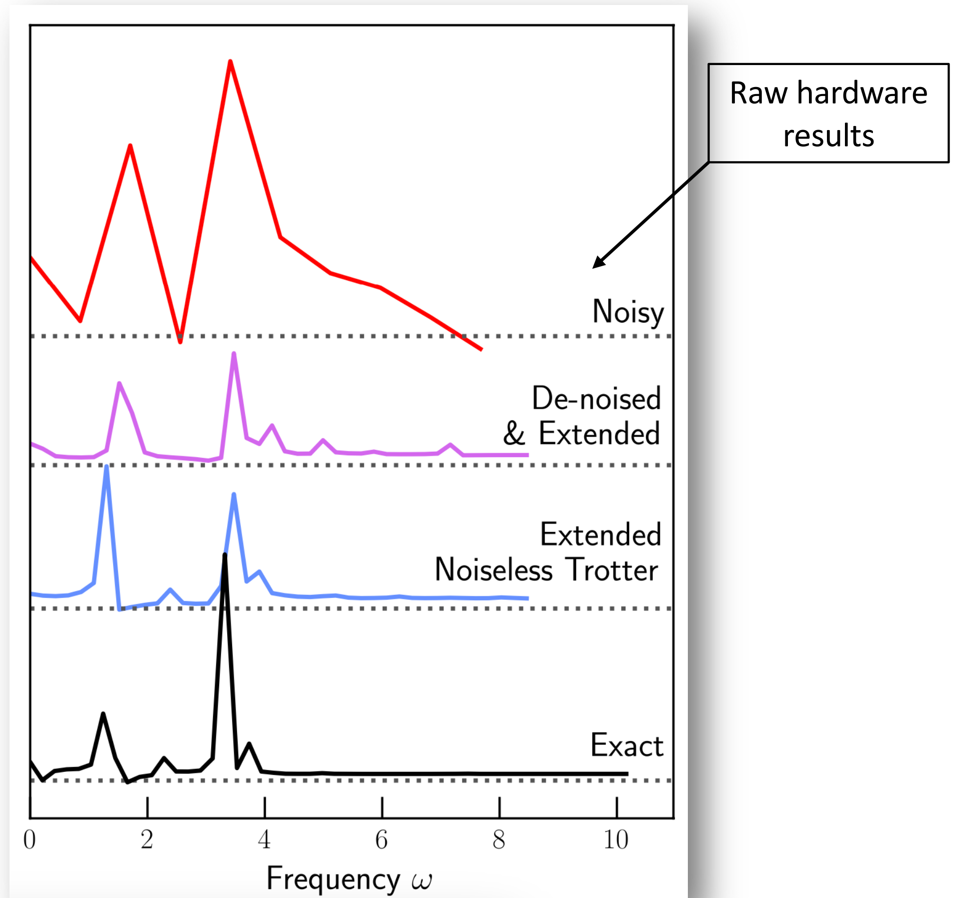
Hardware results

- Evaluation of correlation functions on a quantum computer (ibm_sherbrooke)
  - Shallow circuits + error mitigation = signal we can work with
  - Signal-processing used (post-selecting results, PSD de-noising [10.1103/PhysRevLett.132.160403])

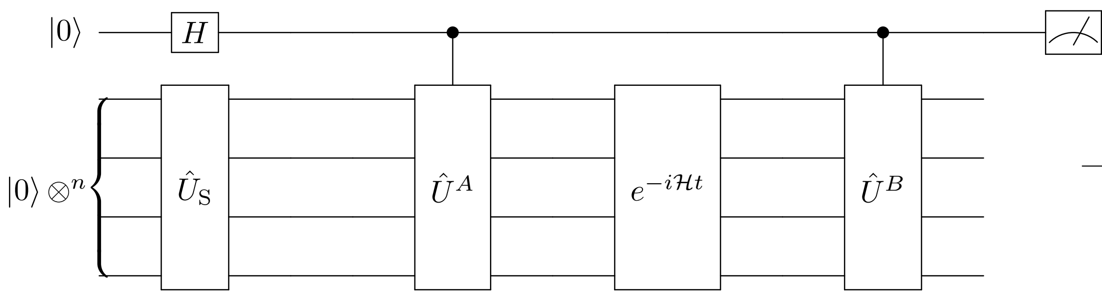


Hardware results





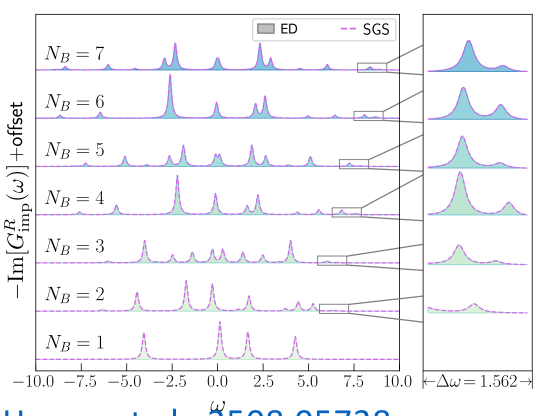
DMFT on Quantum Computers – a path to quantum advantage

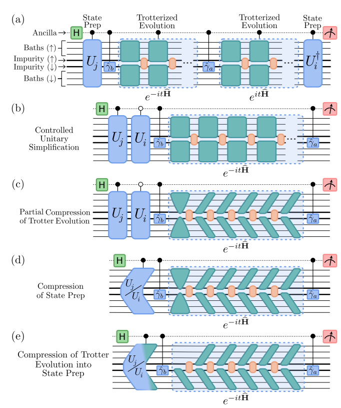


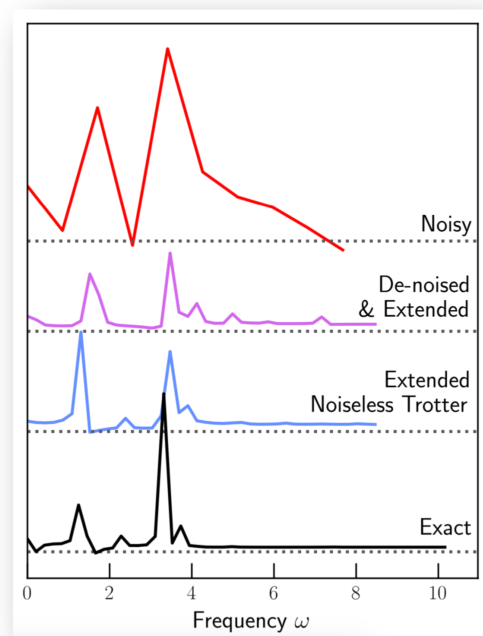
Classical post-processing technique based on PSD projection

Prepare state of interest using subspace of free fermionic states

Time evolve using circuit compression







N. Hogan et al., 2508.05738