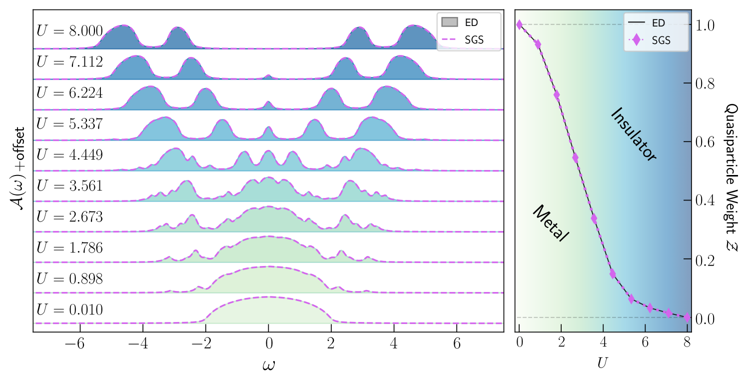
Towards early quantum advantage with impurity embedding methods

Alexander (Lex) Kemper

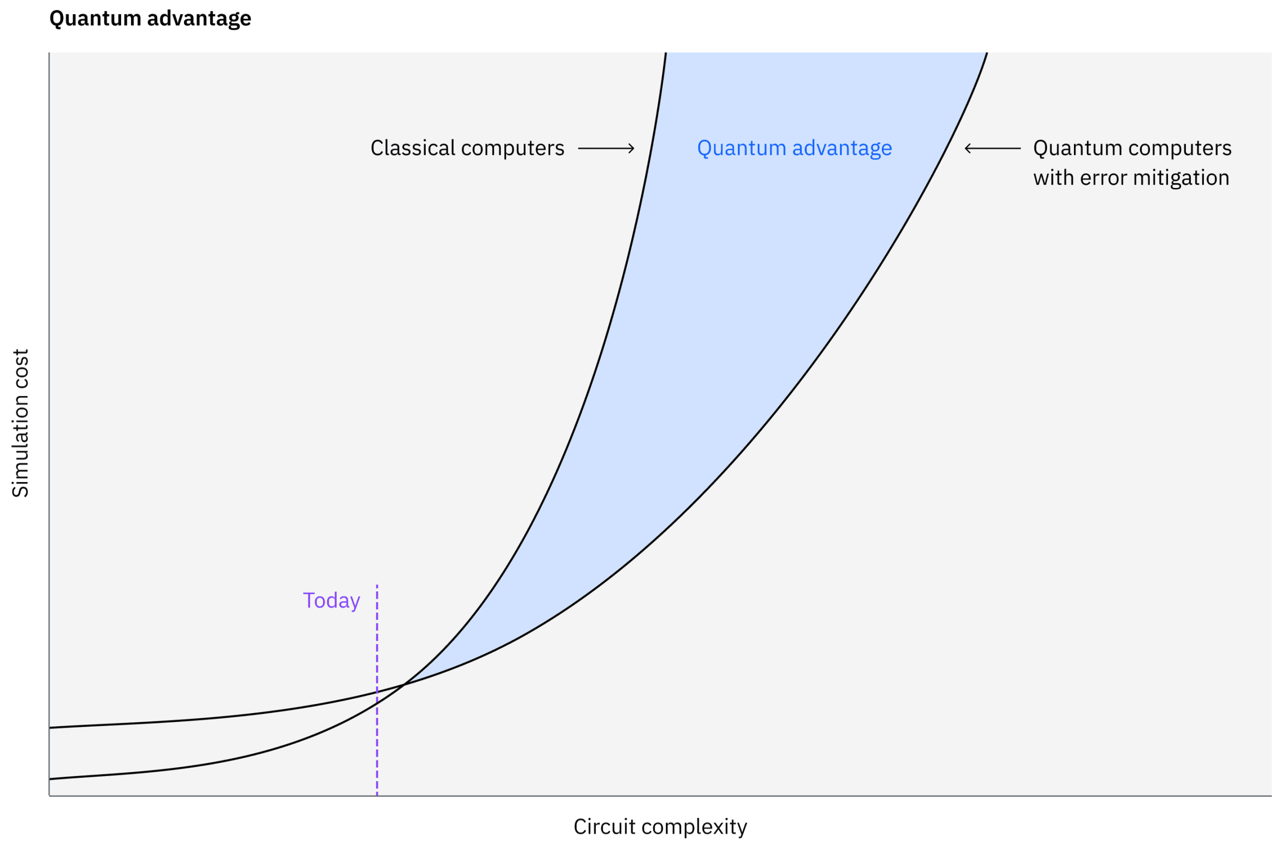
Department of Physics
North Carolina State University
https://go.ncsu.edu/kemper-lab

BNF2026
IPAM
02-17-2026



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 2026



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

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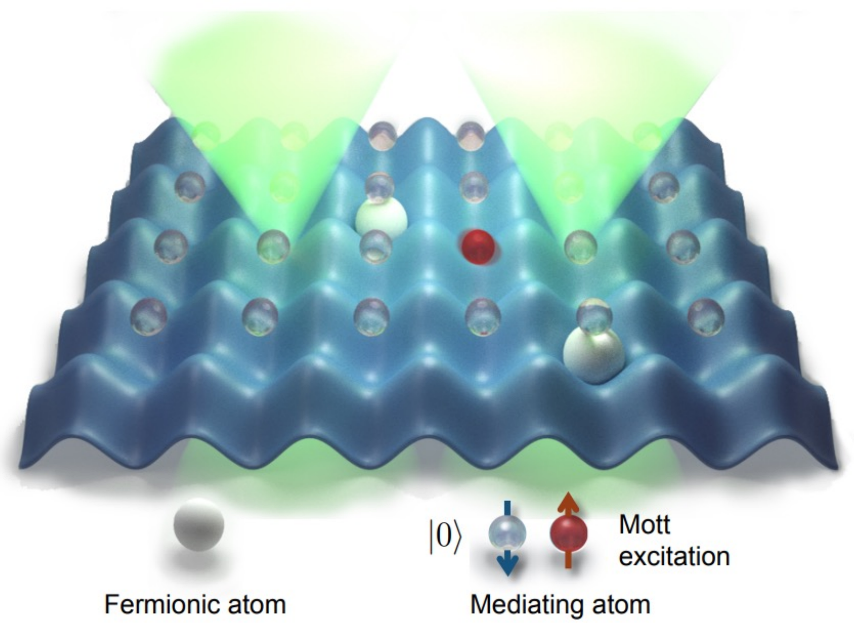
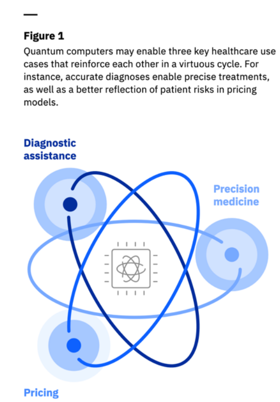
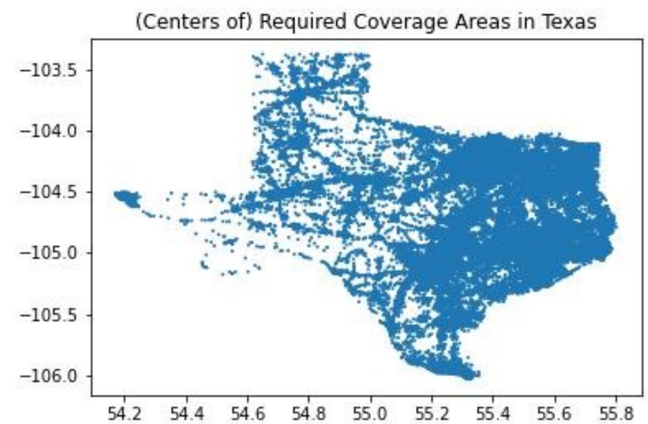
Quantum computers in 2026

Bespoke quantum simulator *Digital algorithms*

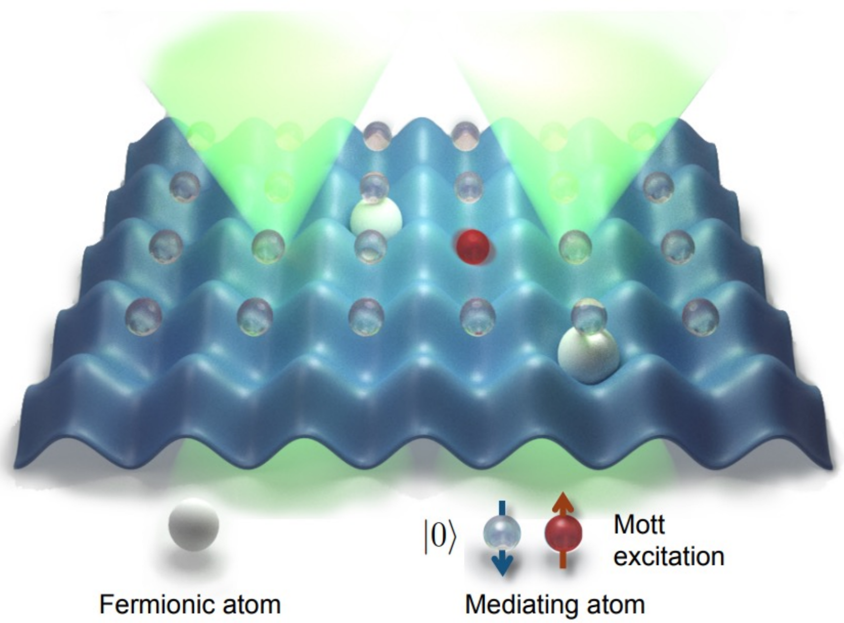


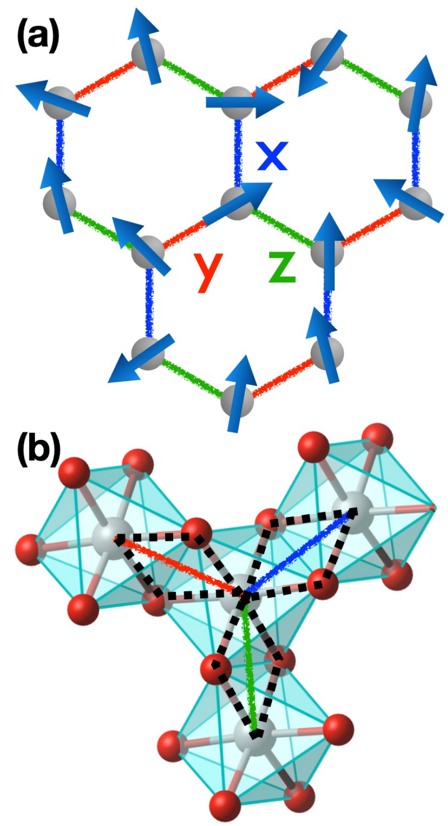




Quantum computers in 2026

Bespoke quantum simulator — *Digital algorithms*





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Quantum computers in 2026

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

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Quantum computers in 2026

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

What about fault tolerance?

To bridge to fault tolerance, we need a problem that is

- Relevant/interesting from small to large problem sizes
- Can be used to interface with non-QC folks
- Runs on a few qubits (< 100) but can scale to larger sizes
- Doesn't require long qubit coherence times but can make use of them

Quantum computers in 2025

Lex' de
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phys

To

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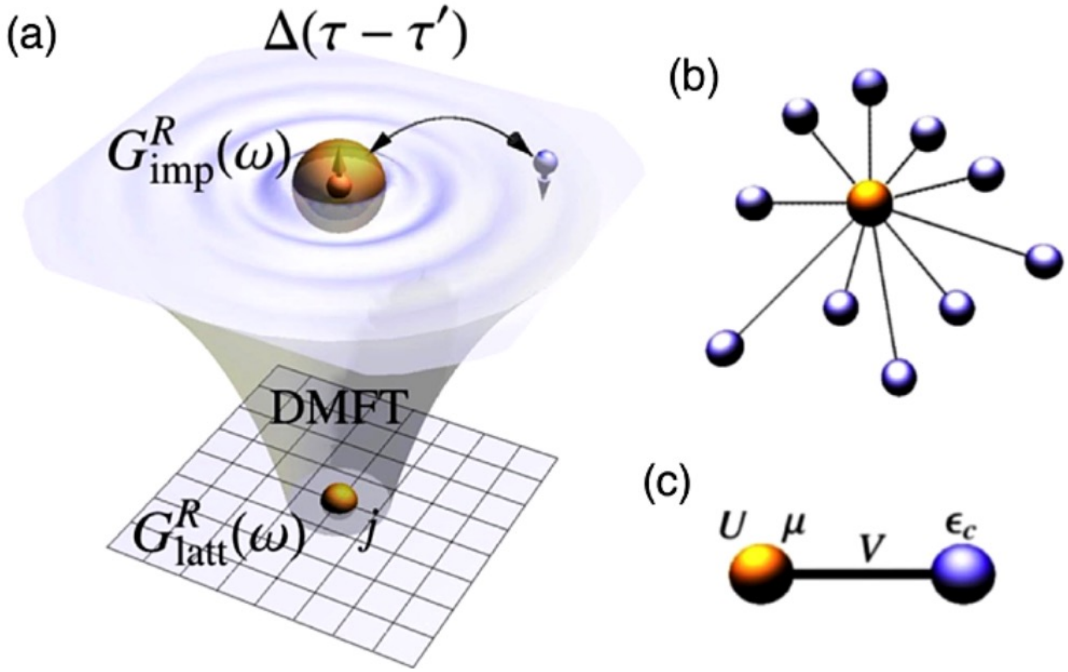
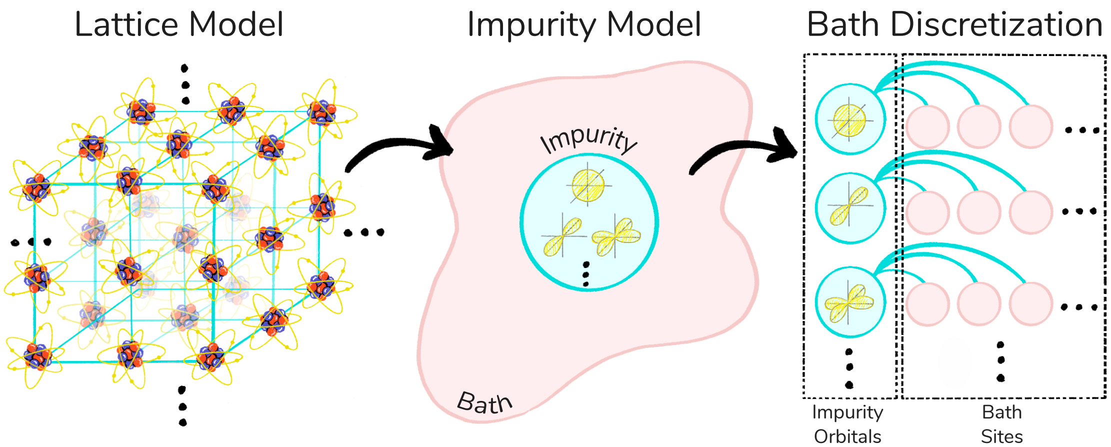


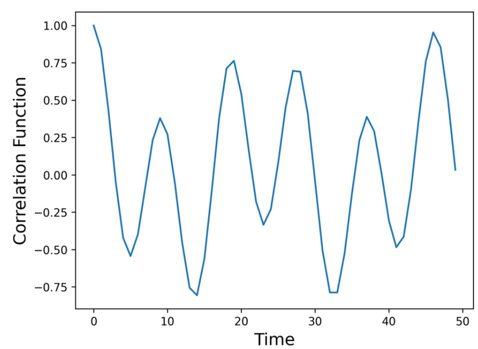
Kreula EPJ Quant. Tech. (2016)

DMFT

Dynamical Mean Field Theory (DMFT)



Updating the parameters of the bath…



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

DFT + DMFT

Electronic structure of $SrVO_3$

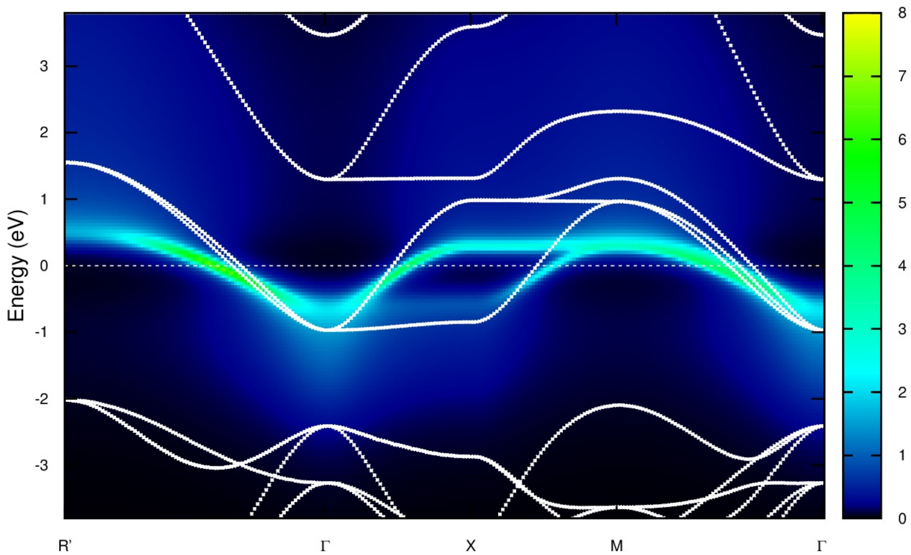
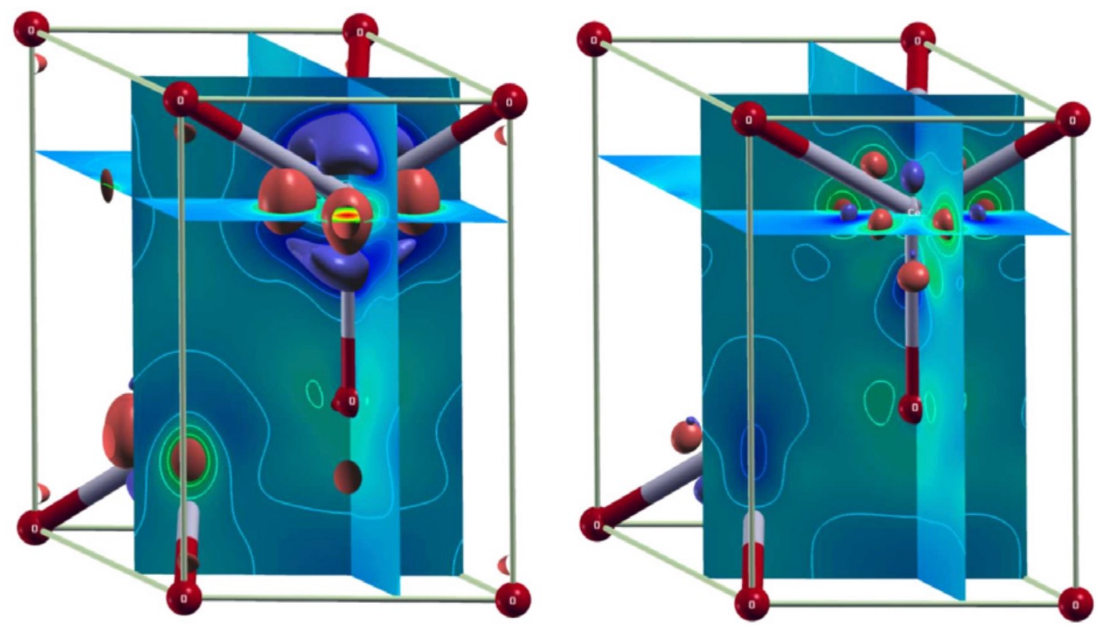


FIG. 1. LDA band structure for $SrVO_3$.

PHYSICAL REVIEW B 77, 205112 2008

Local density of Pu_2O_3



J. Phys.: Condens. Matter 24 (2012) 075604

DMFT

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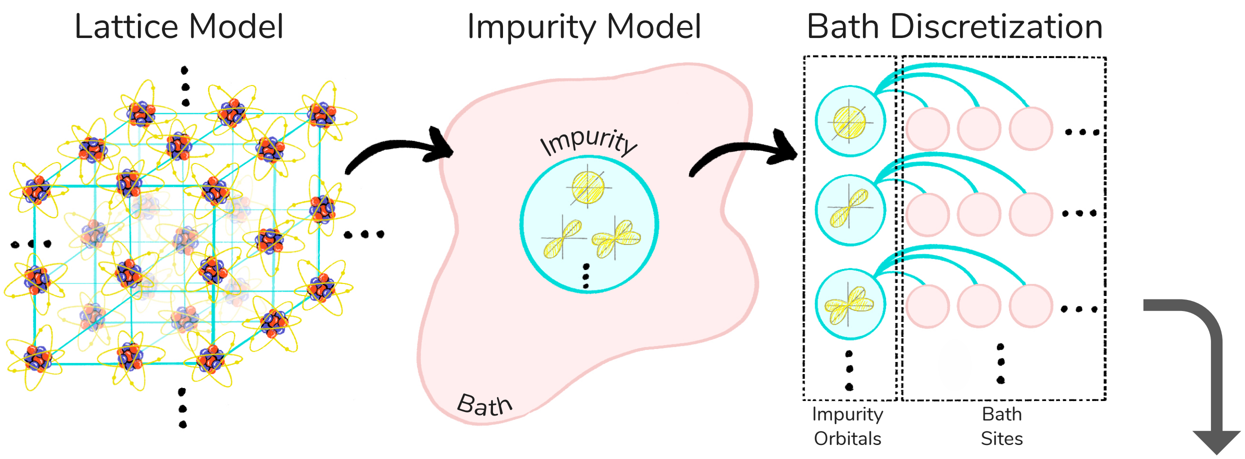

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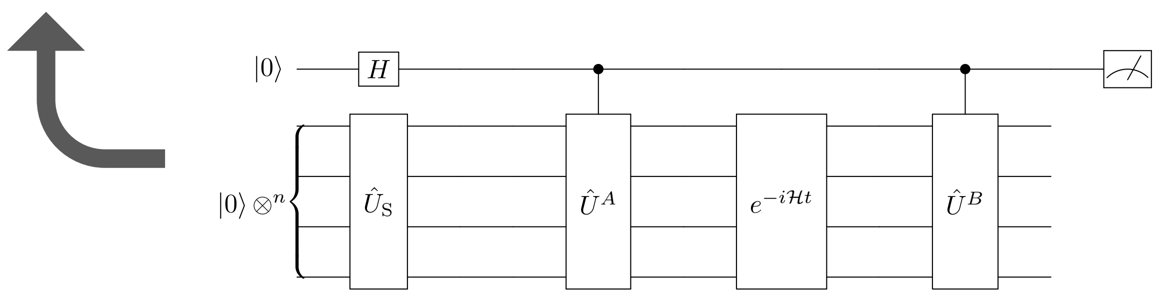
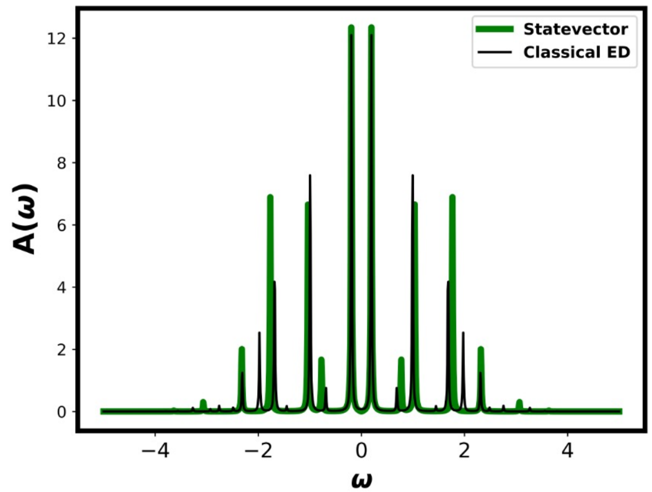
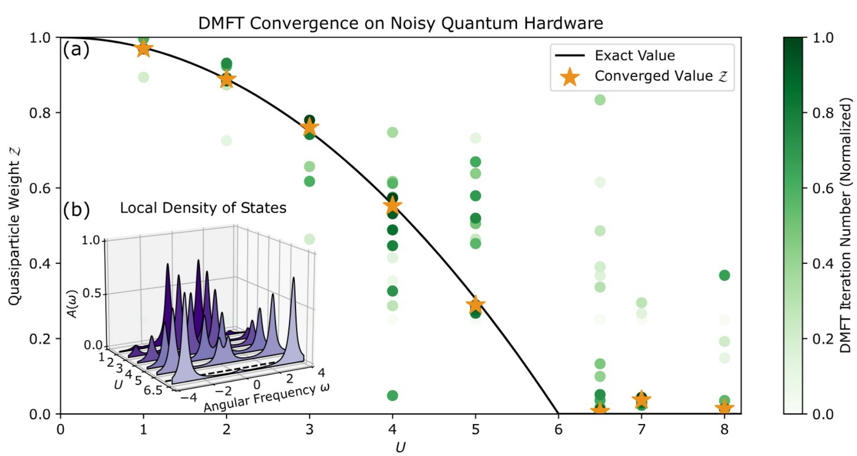


$t), c_j^\dagger\}|\psi\rangle$

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

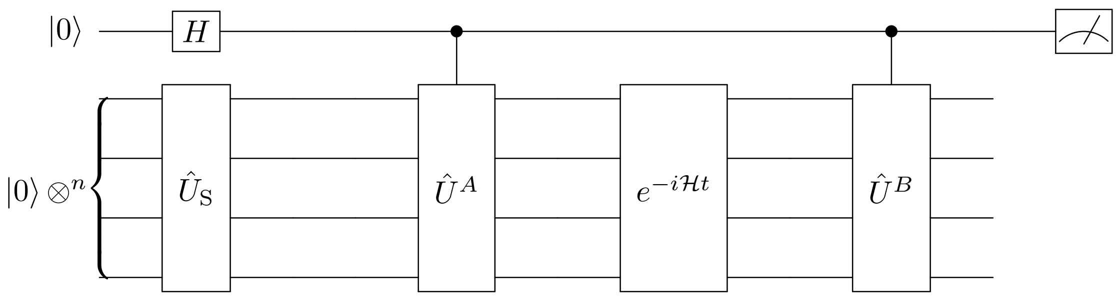
DMFT on Quantum Computers





- 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)
- **Hogan arXiv (2025)**

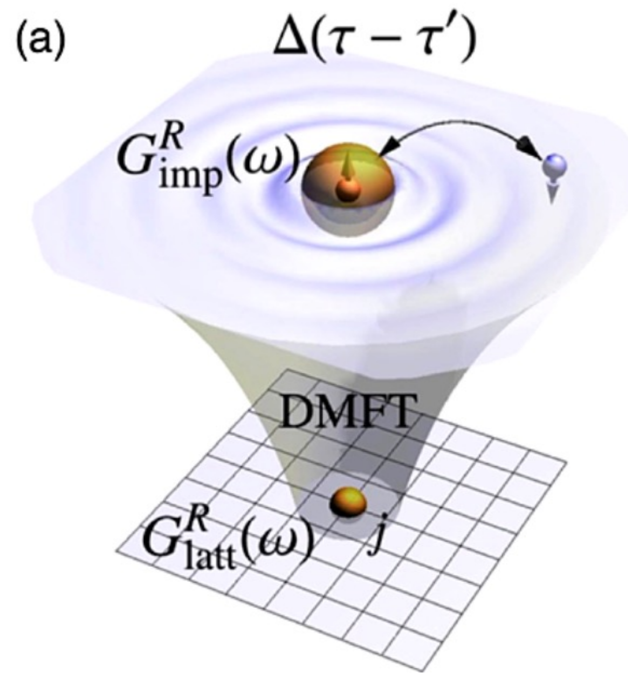
A-Z quantum simulation



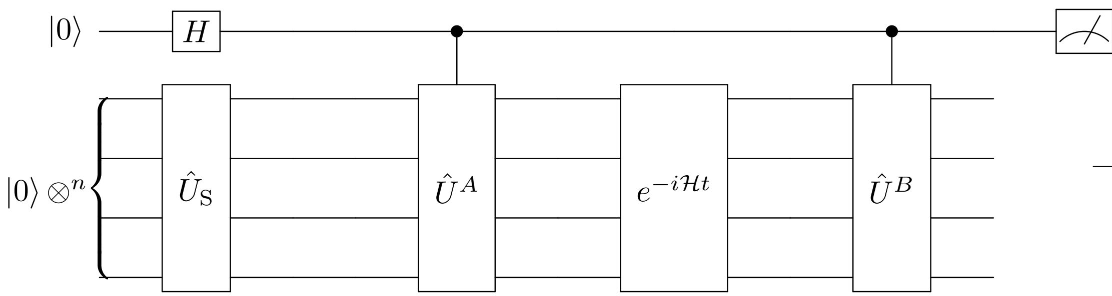
Prepare state of interest

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



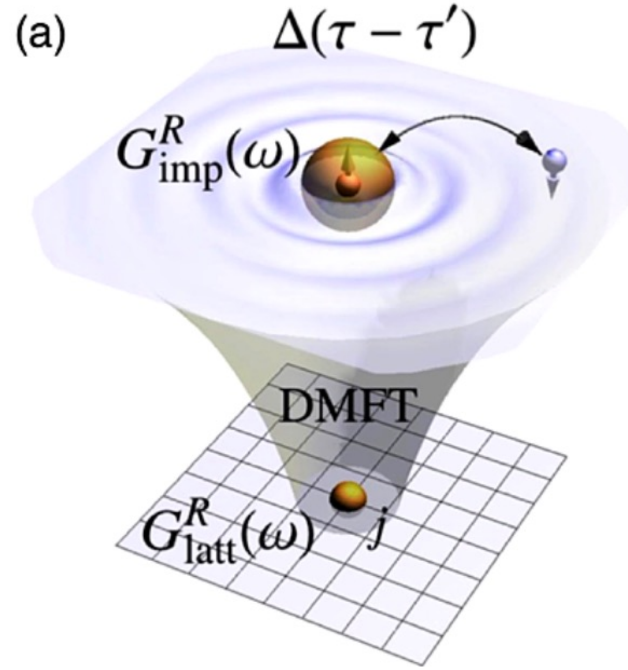
Prepare state of interest

Time evolve

Classical post-processing techniques

- *Physics-Informed Subspace Expansions*

- *Lie-algebraic methods for time evolution*



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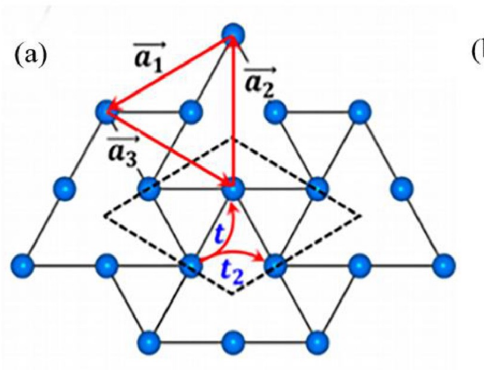
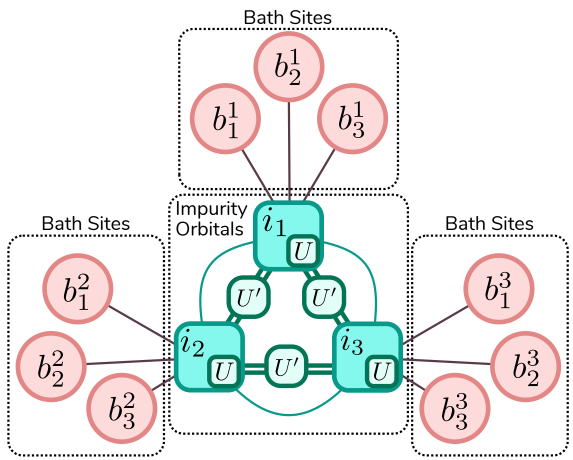
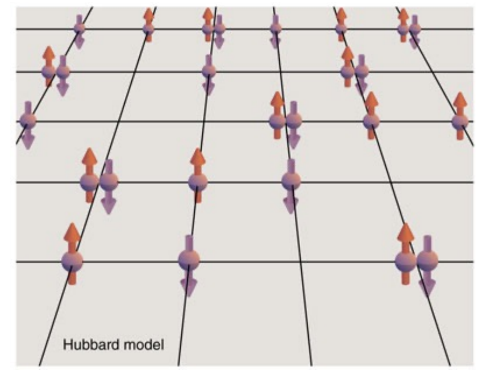
Ground state preparation: Fermionic Gaussian Subspace



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*

$$|\psi\rangle \approx \sum_{k=1}^{\chi} \alpha_k |\phi_k\rangle$$

Bravyi & Gosset (2016)
Boutin & Bauer (2021)

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

Ground state preparation: Eigenvector Continuation

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

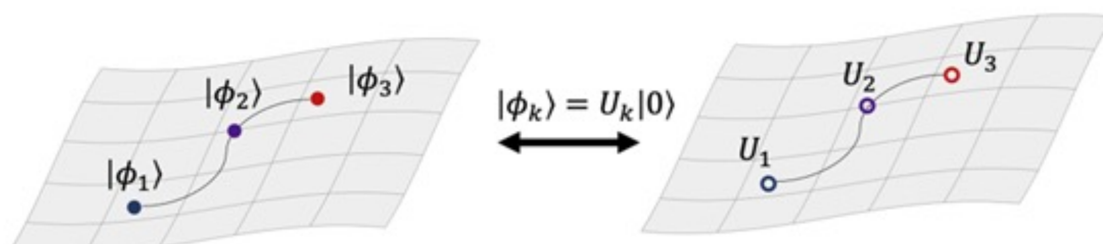
Featured in Physics

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.

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



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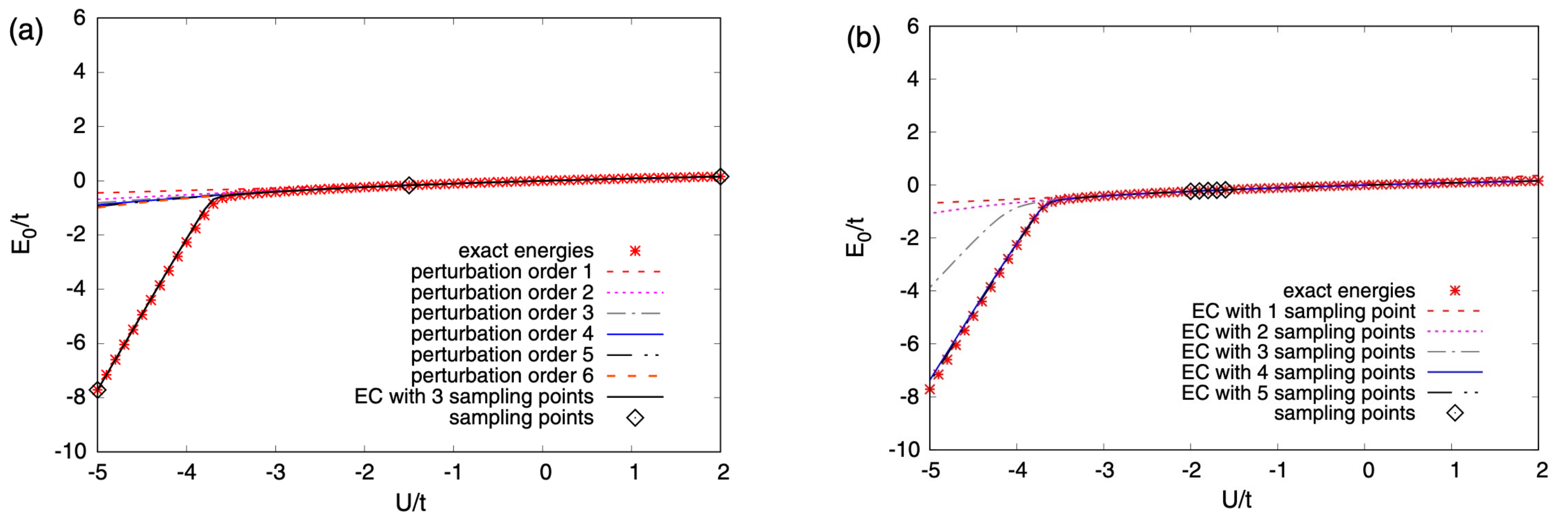

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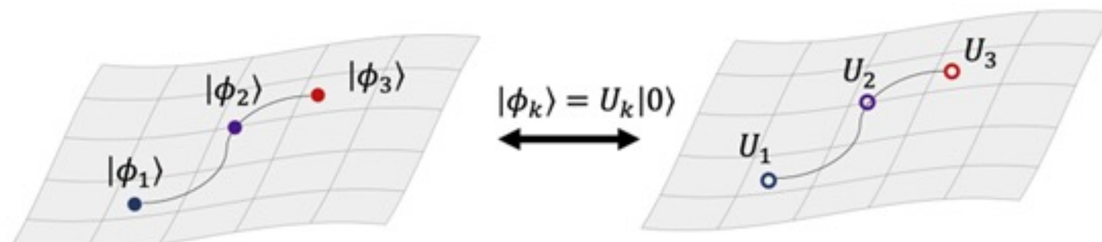
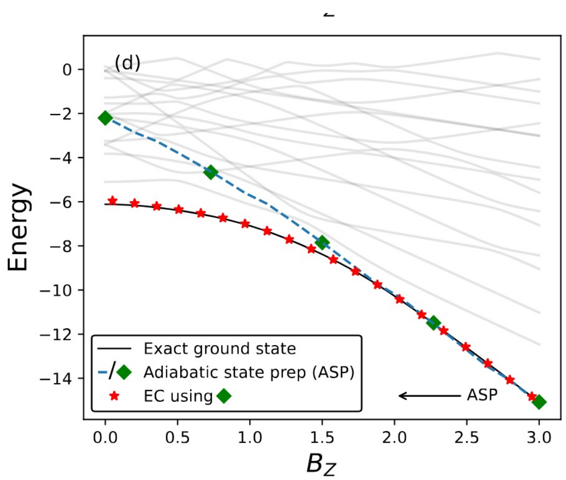
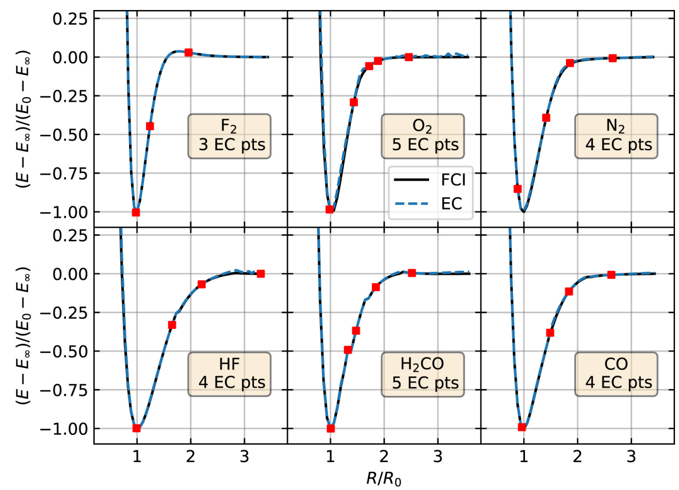






A. Agrawal, AFK et al. Phys. Rev. A 111, 032607 (2025)

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

Eigenvector Continuation

Representing the impurity ground state:

[1] 10.1007/s00220-017-2976-9
[2] 10.1103/PhysResearch.3.033188
[3] arXiv:2406.17037
[4] arXiv:2209.10571

- Sum of Gaussian states [1,2]

$$|\psi\rangle \approx \sum_{k=1}^{\chi} \alpha_k |\phi_k\rangle$$

Hard to represent

Easy to represent (characterized by 1RDMs)

- Subspace diagonalization & Eigenvector Continuation [3,4]

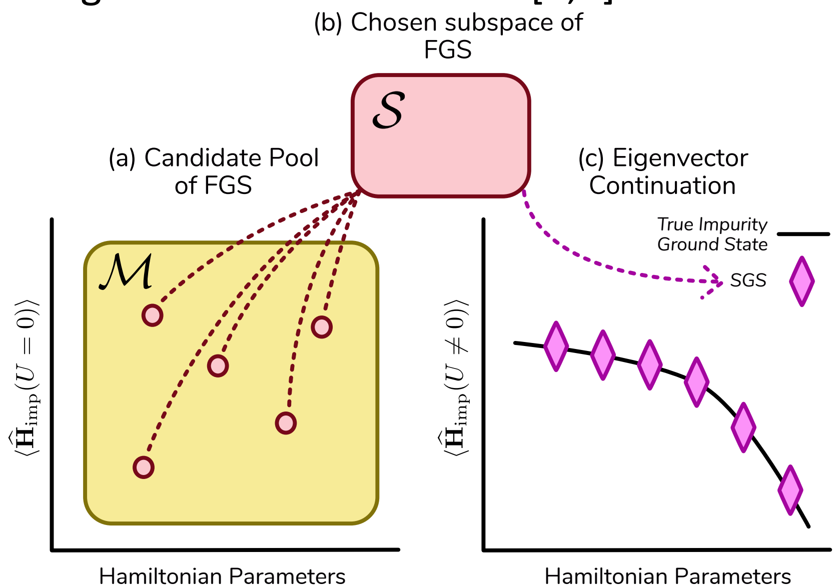
$$\widehat{H}|\psi\rangle = E|\psi\rangle$$

$$\downarrow$$

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

$$\widetilde{H}_{ij} = \langle\phi_i|\hat{H}|\phi_j\rangle$$

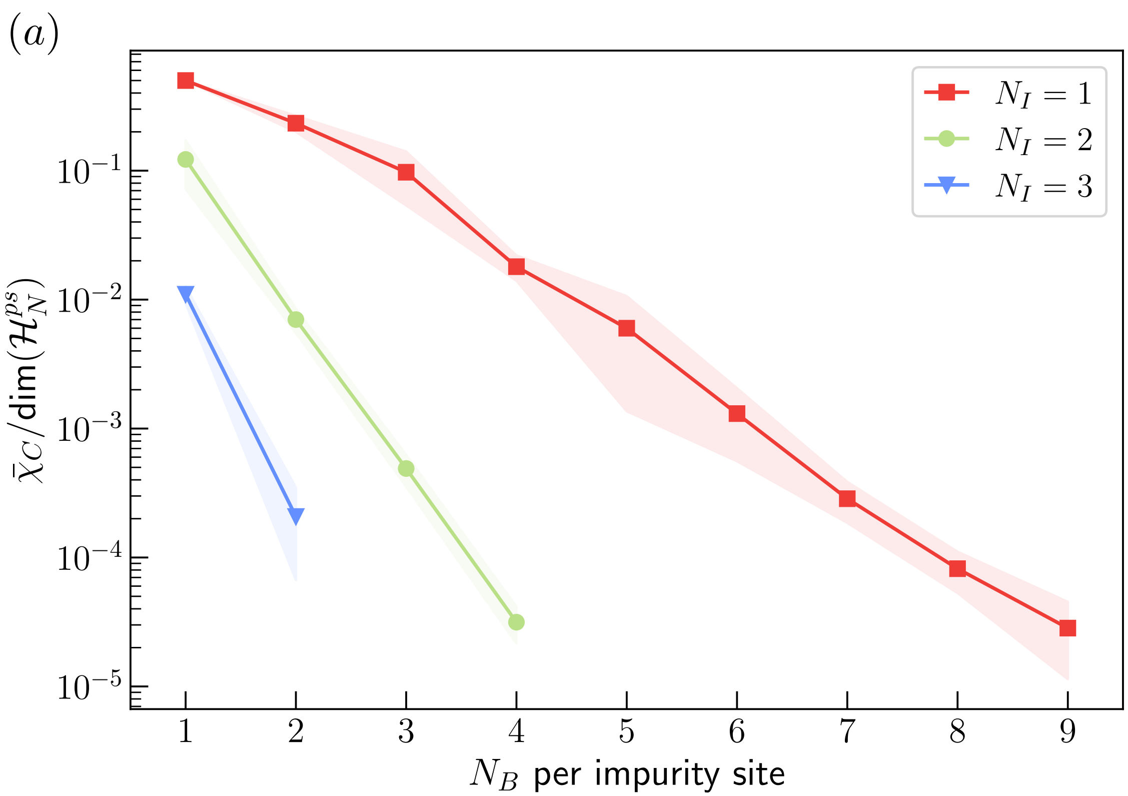
$$S_{ij} = \langle\phi_i|\phi_j\rangle$$

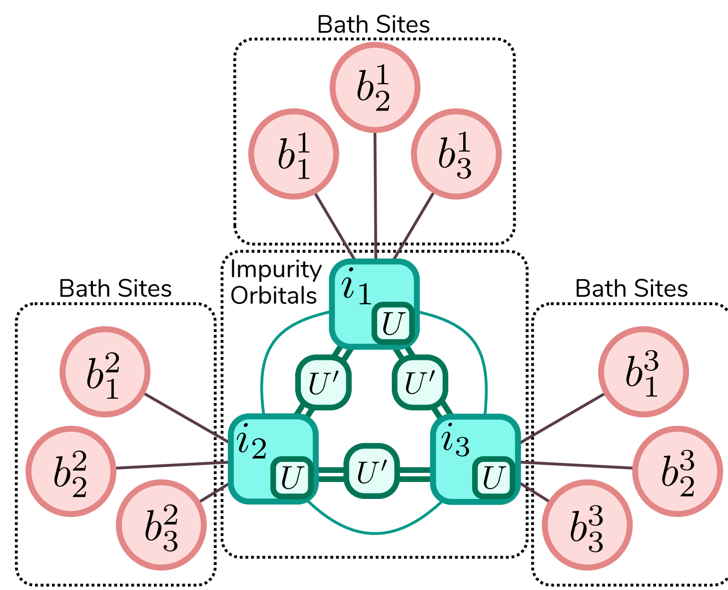


All of this can be done efficiently on a classical computer!

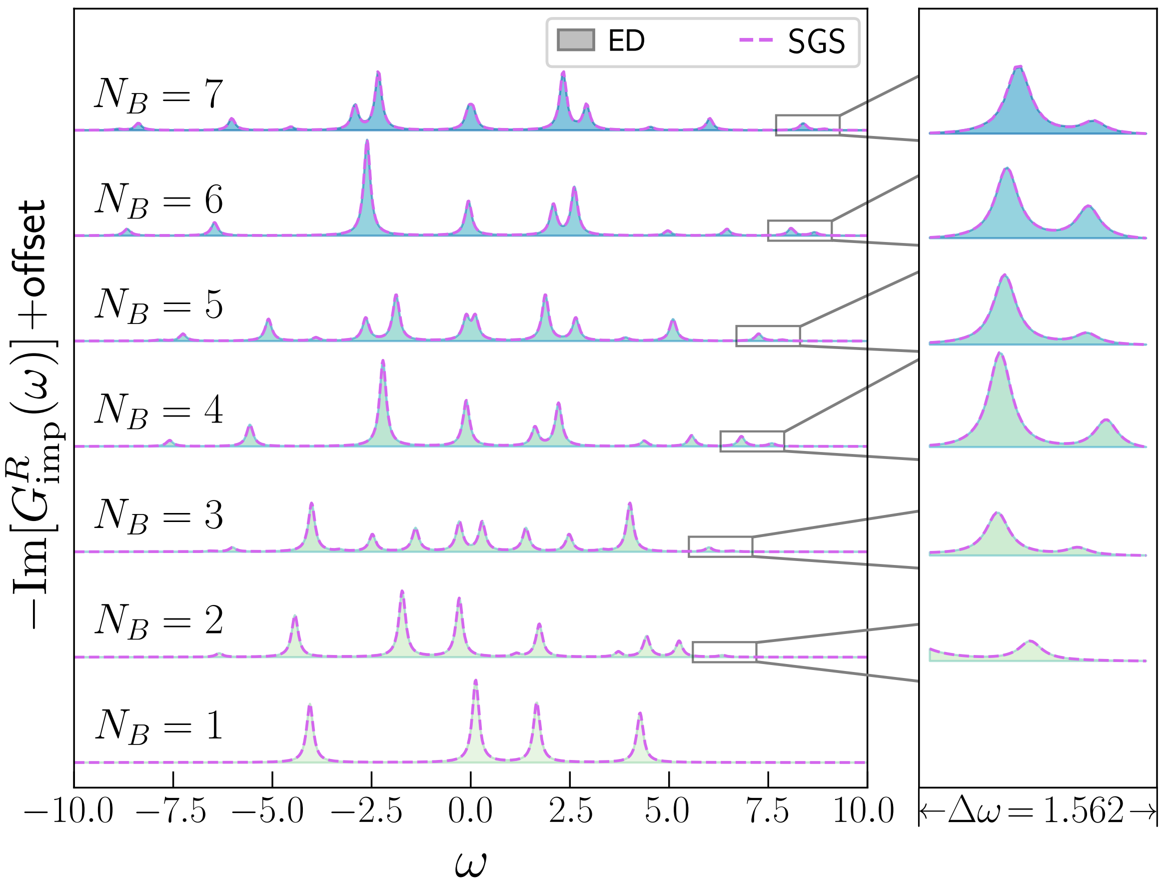
Eigenvector Continuation

How many fermionic Gaussian states are needed?





Fermionic Gaussian Subspace

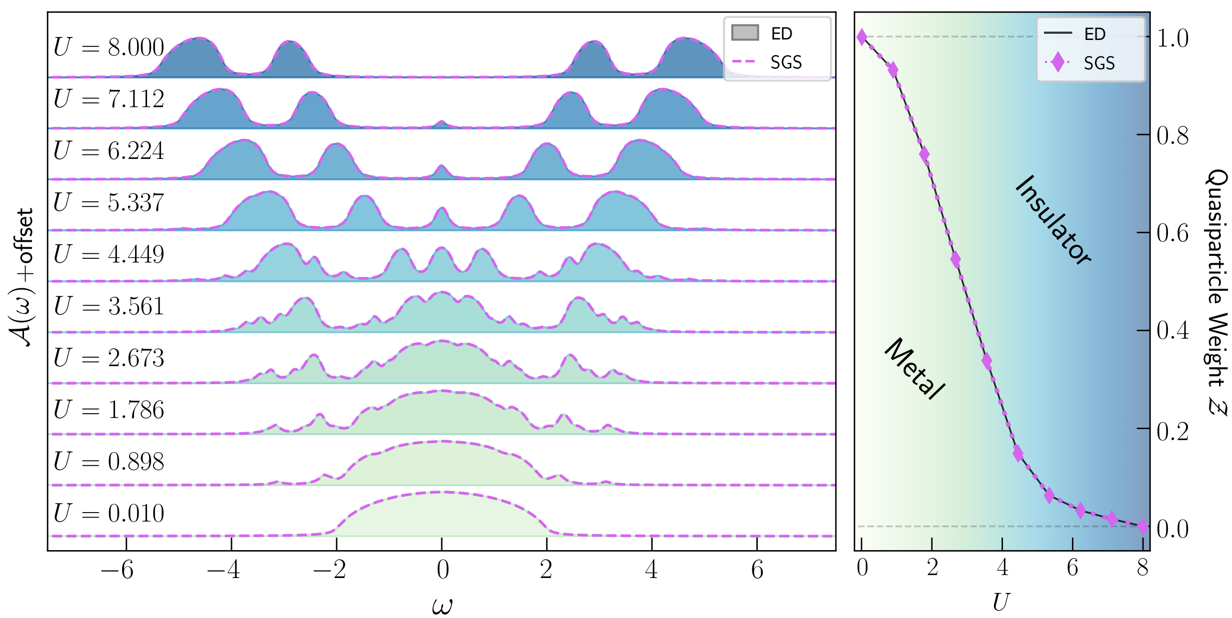


Fermionic Gaussian Subspace

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

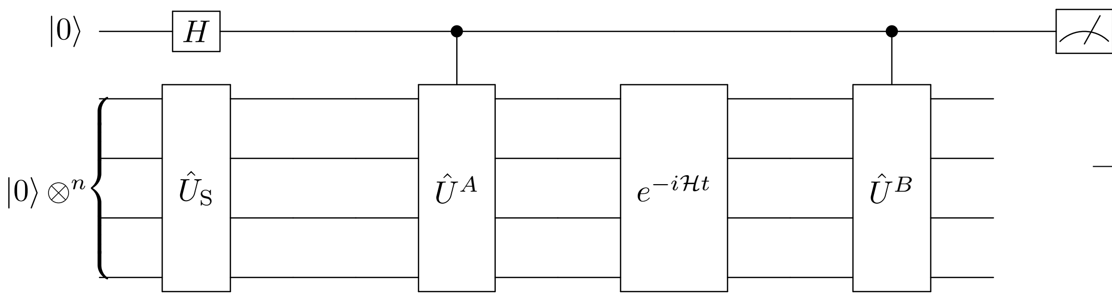
- DMFT using sum of Gaussian states (SGS) (Hubbard Model w/ Bethe lattice)

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



Increasing interaction strength on impurity

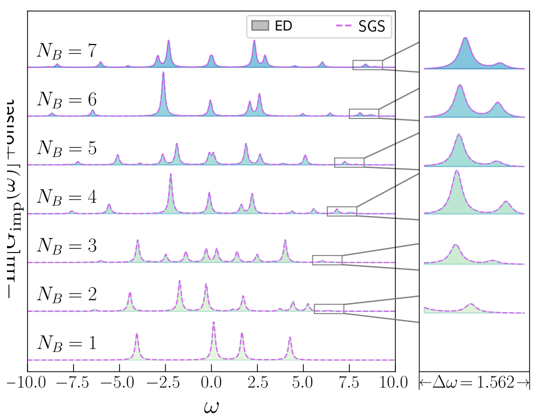
A-Z quantum simulation



Classical post-processing techniques

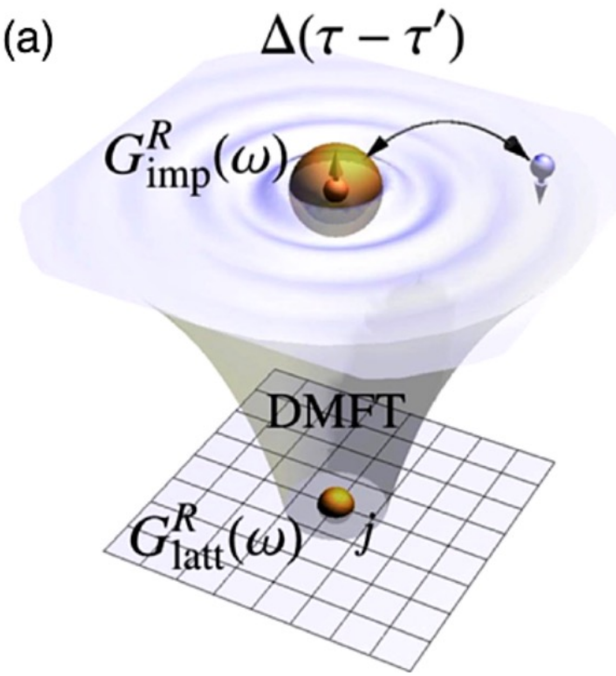
Prepare state of interest using subspace of free fermionic states

Time evolve



- *Lie-algebraic methods for time evolution*

(a)

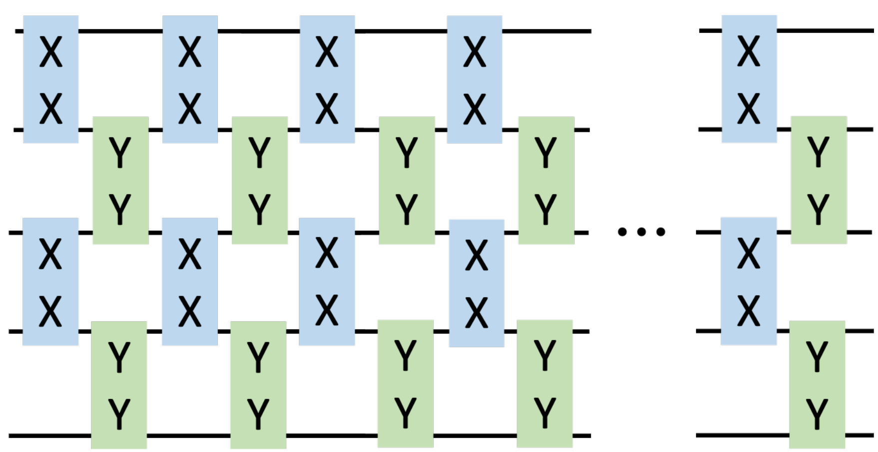


Time evolution

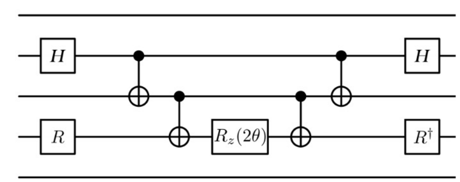
Simulation of a time independent spin Hamiltonian:

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

$$U(t) =$$

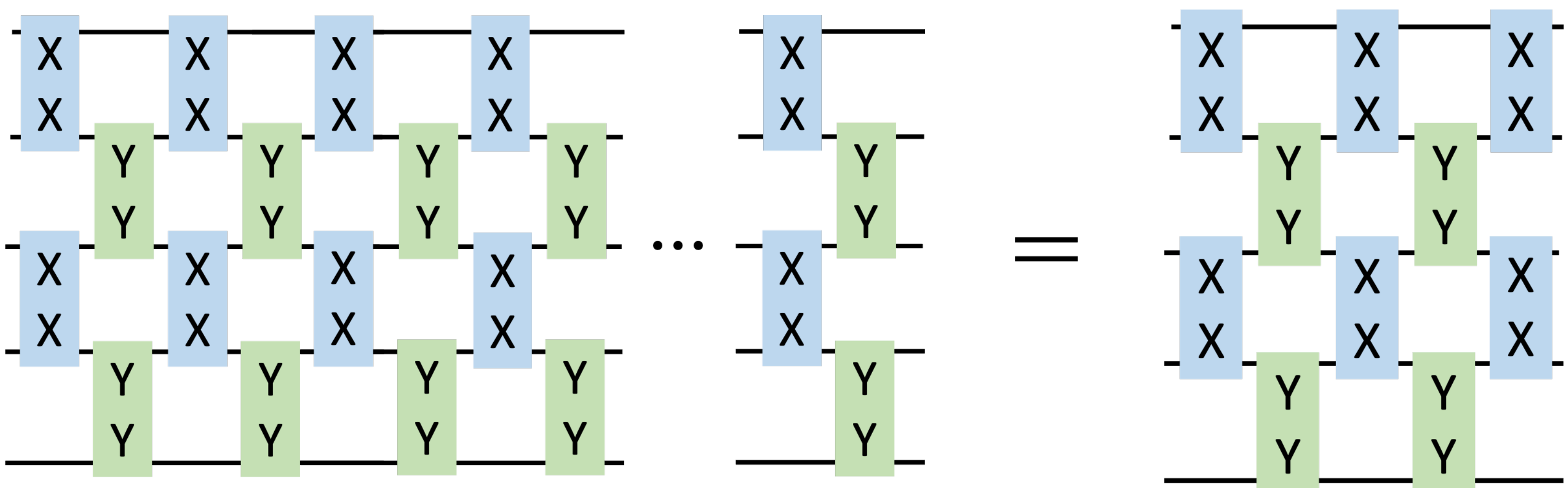


$$e^{i\theta IXZYI} =$$



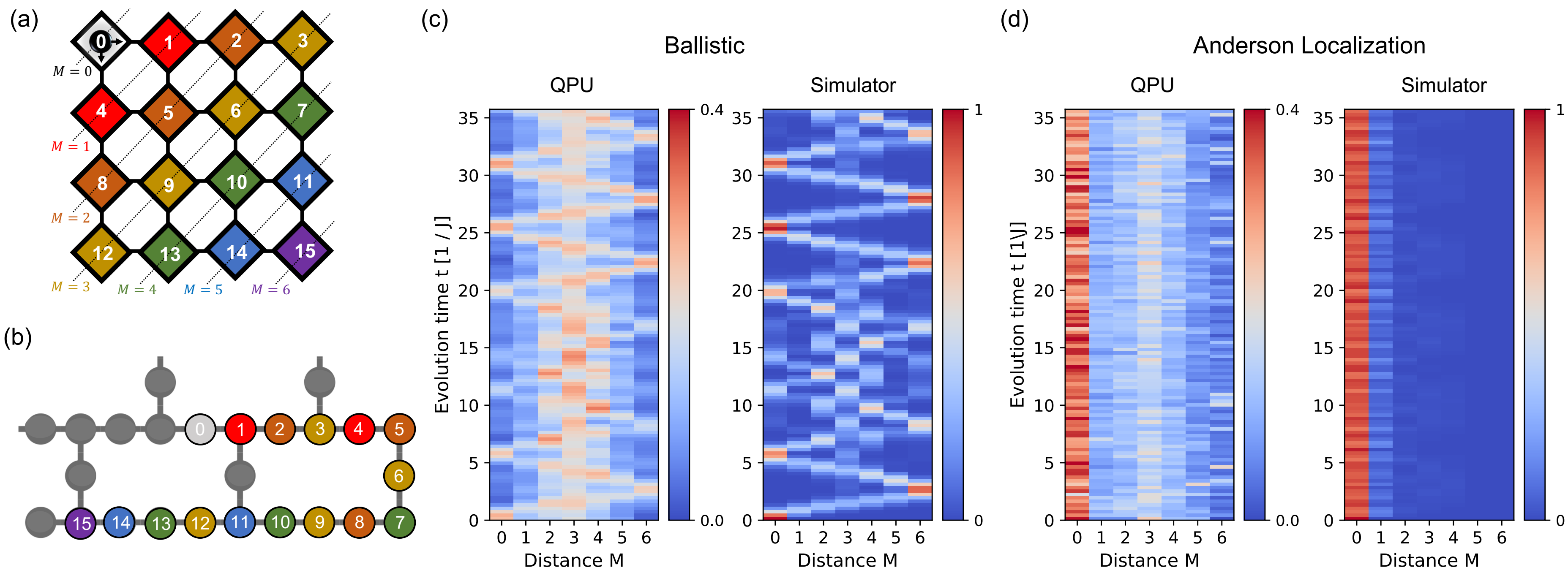
Algebraic Circuit Compression

- 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.



Phys. Rev. A 105, 032420 (2021), SIMAX 2022 43:3, 1084-1108, 2303.09538

Algebraic Circuit Compression



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Partial Compression

Time evolving the impurity ground state

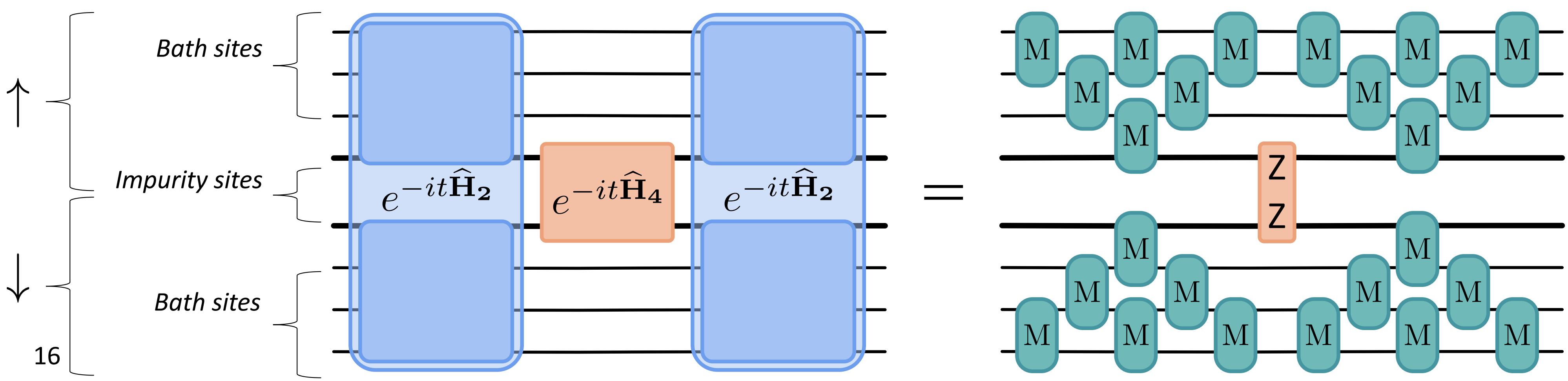
- Compression of free-fermionic circuits for fixed-depth time evolution [1,2]
  - Evolving longer in time is a matter of tuning some gate angles
- ***Partial compression*** for impurity models:

[1] 10.1103/PhysRevLett.129.070501
[2] 10.1103/PhysRevA.105.032420
[3] 10.1137/21M1439298
[4] arXiv:2303.09538
[5] arXiv:2508.05738

M = match gate

ZZ = impurity interaction

Example: 1 trotter step



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Partial Compression

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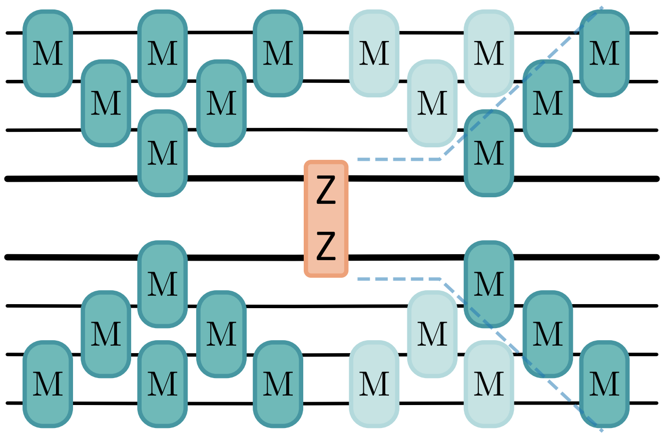

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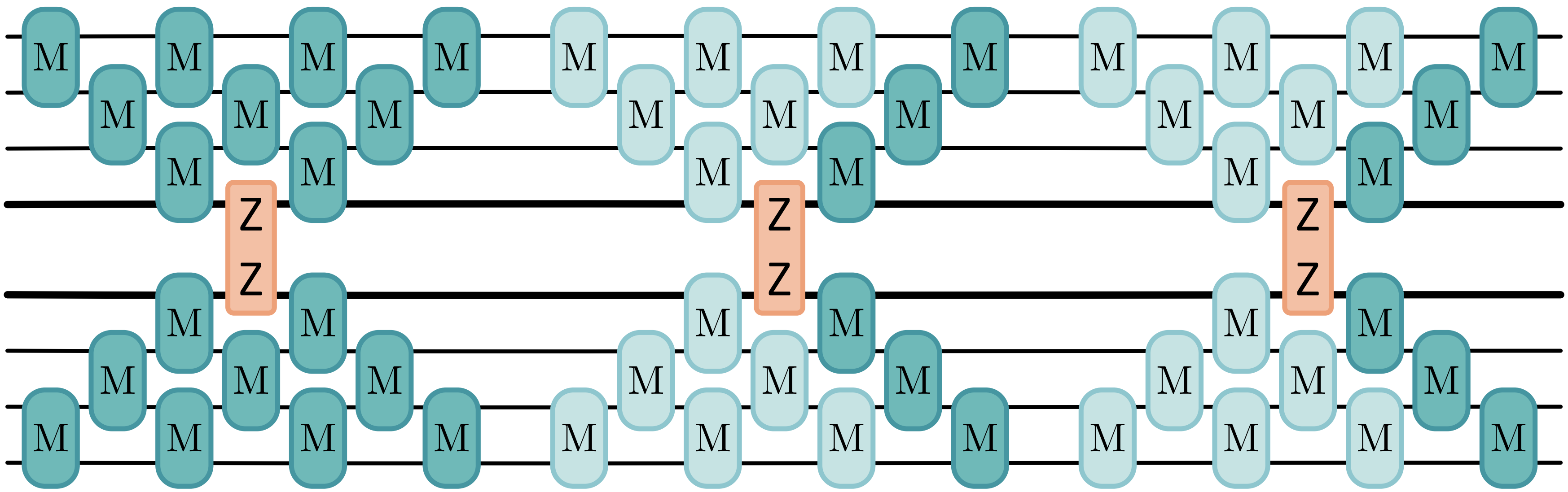
Further example: 3 trotter steps



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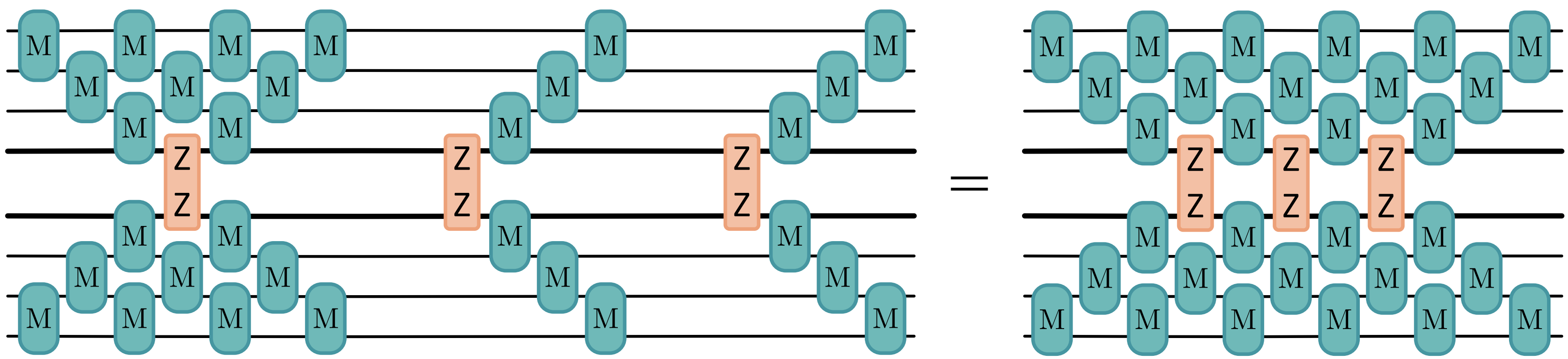
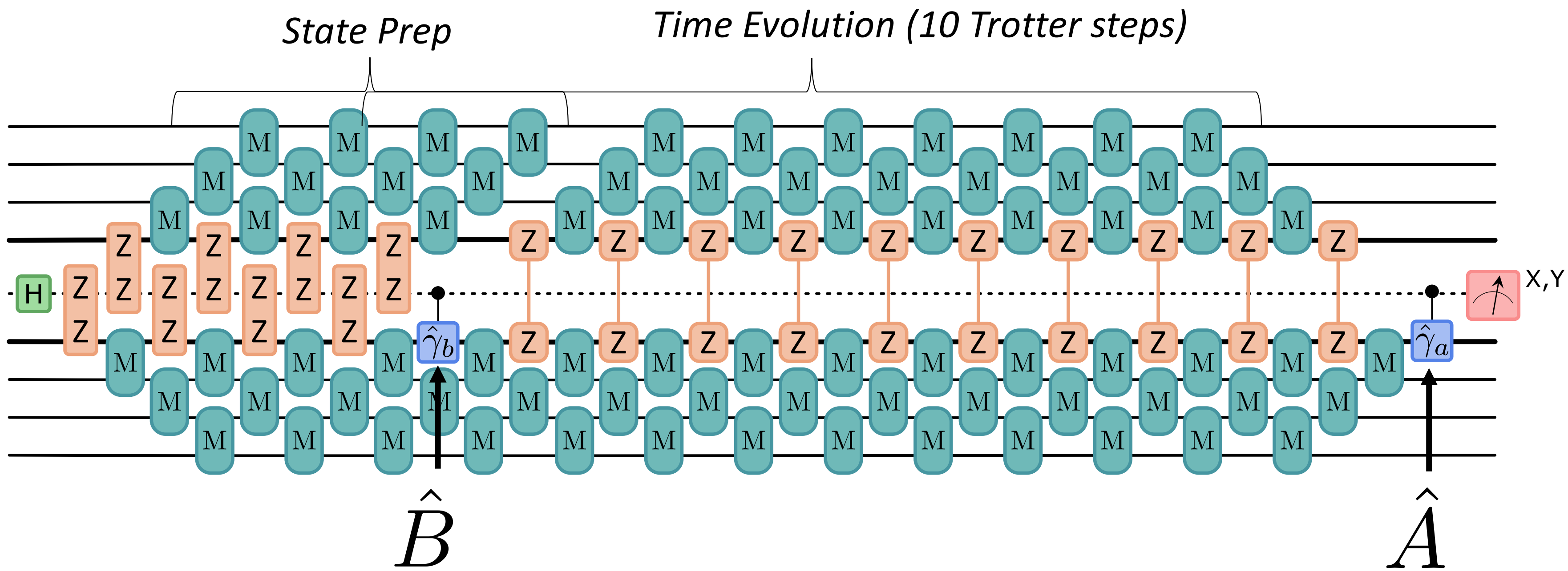


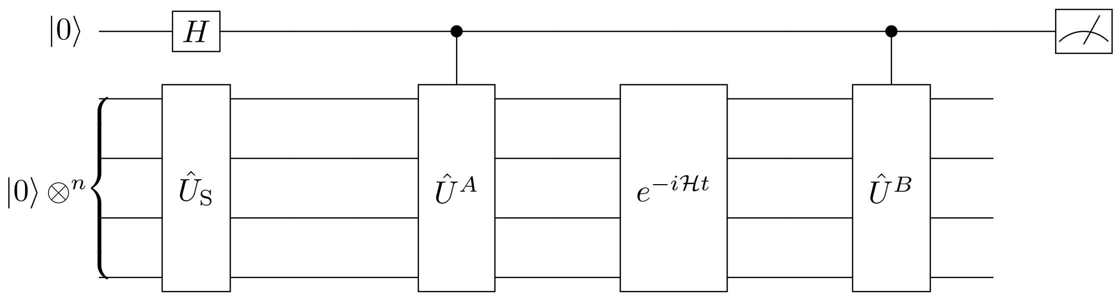
Partial Compression

Having Gaussian states to represent our impurity ground state naturally assists partial compression!

$$\langle\psi|\hat{A}(t)\hat{B}|\psi\rangle \approx \sum_{i,j}^{\chi}\langle\phi_i|\hat{A}(t)\hat{B}|\phi_j\rangle$$

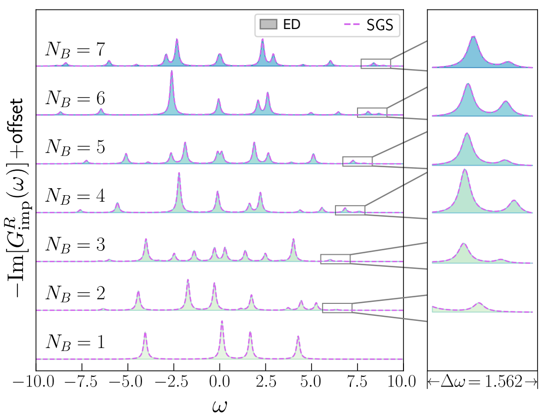


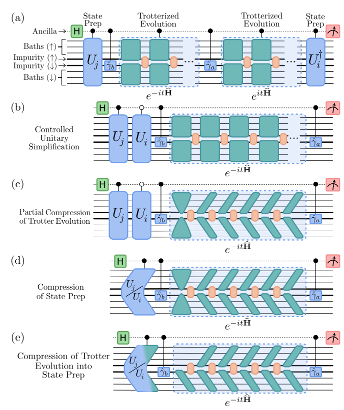
A-Z quantum simulation

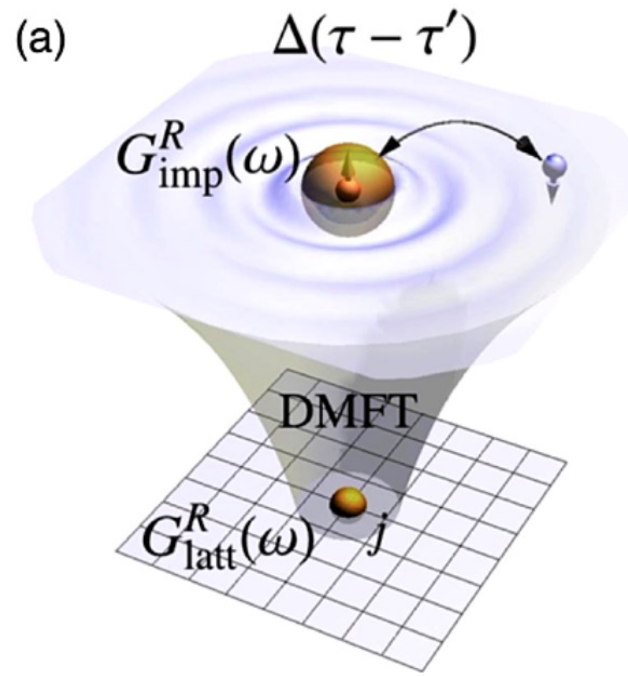


Prepare state of interest
using subspace of free fermionic states

Time evolve
using circuit compression







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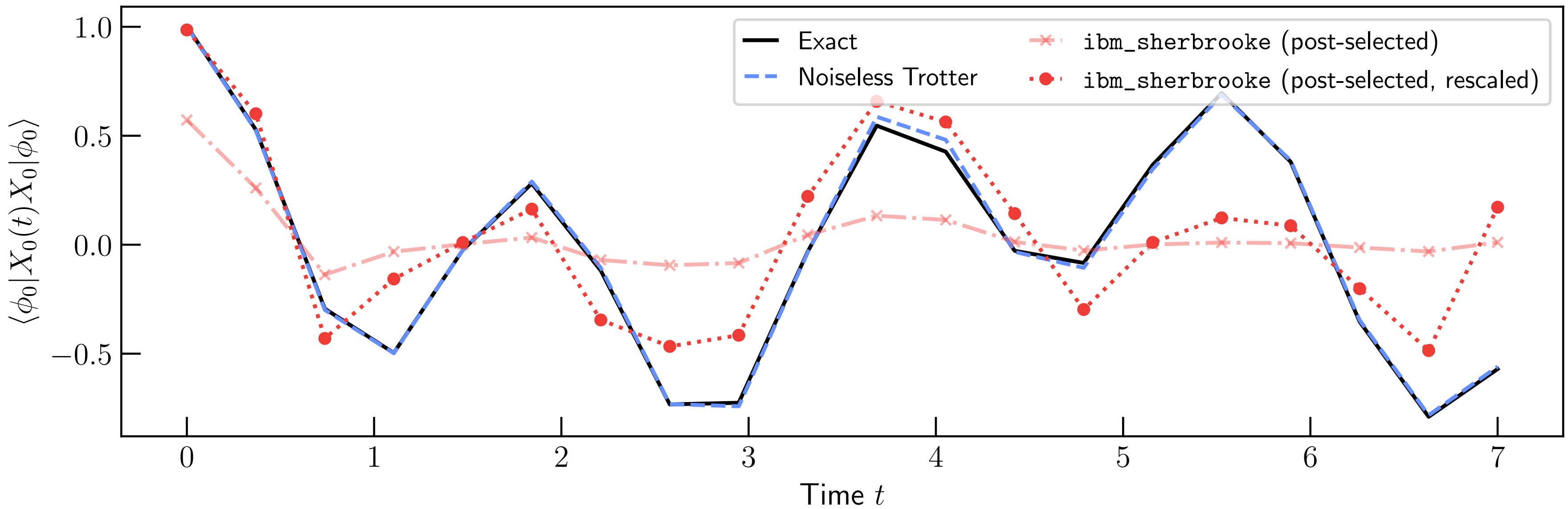
Hardware results



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

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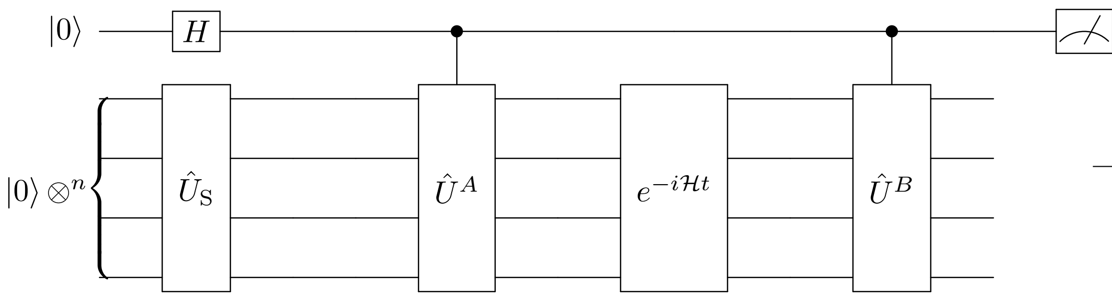
A-Z quantum simulation



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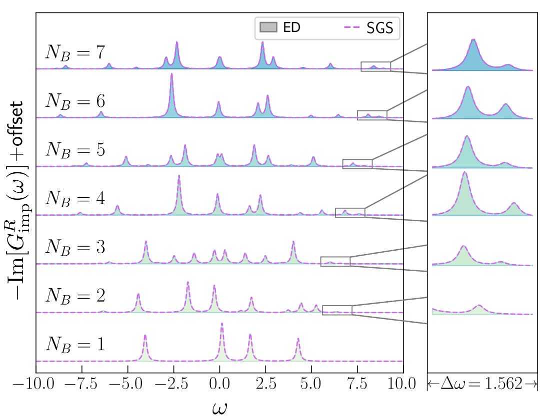
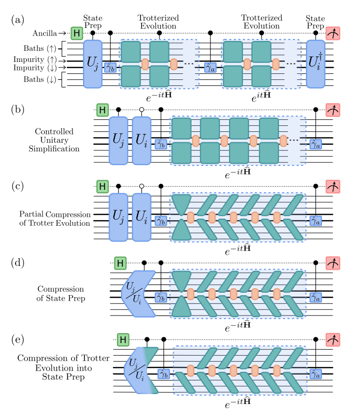
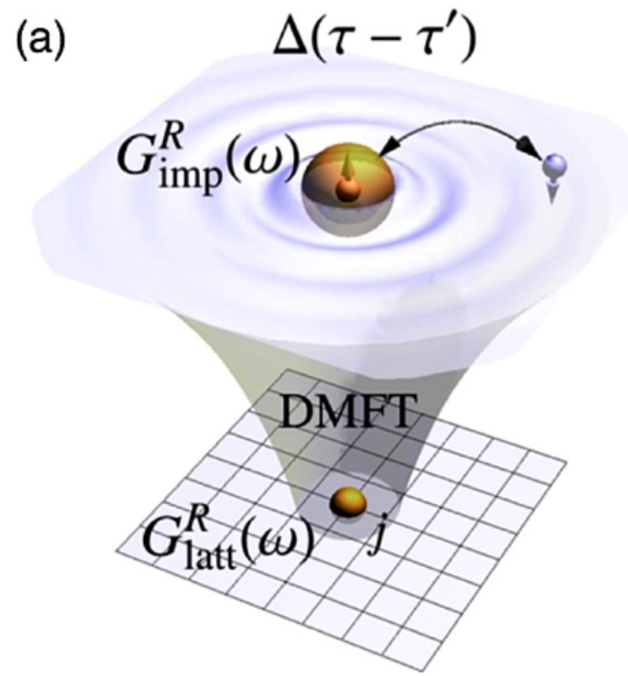
using circuit compression







A-Z quantum simulation

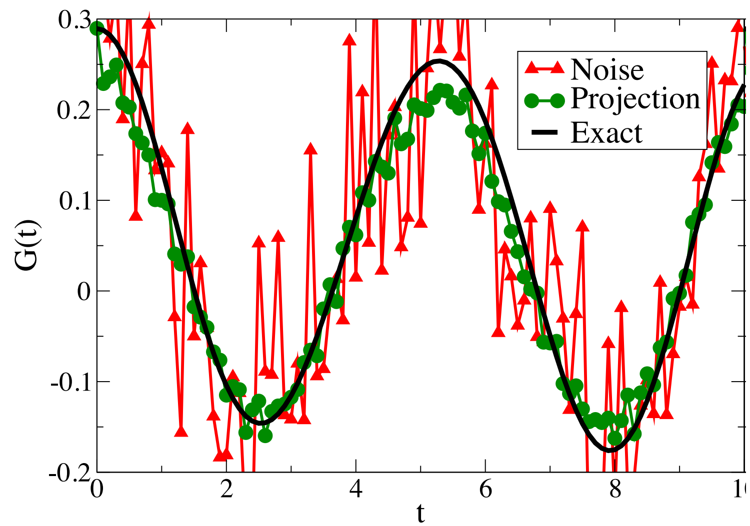
- It turns out that these are positive semi-definite (PSD) functions:

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

- 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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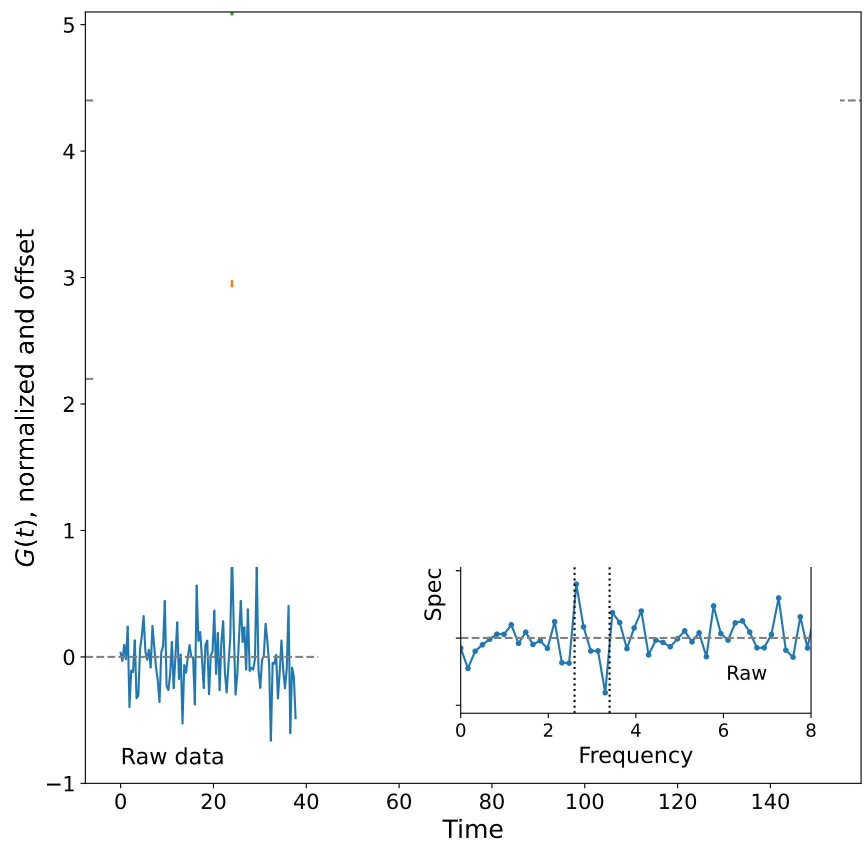

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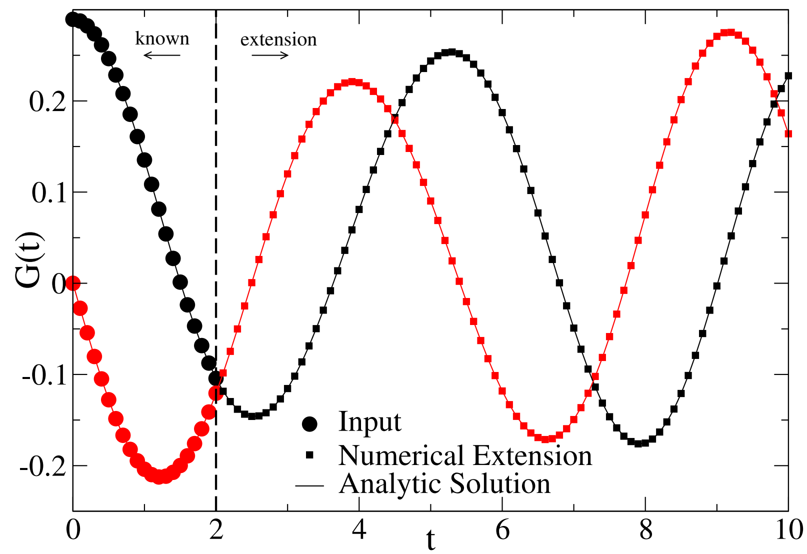

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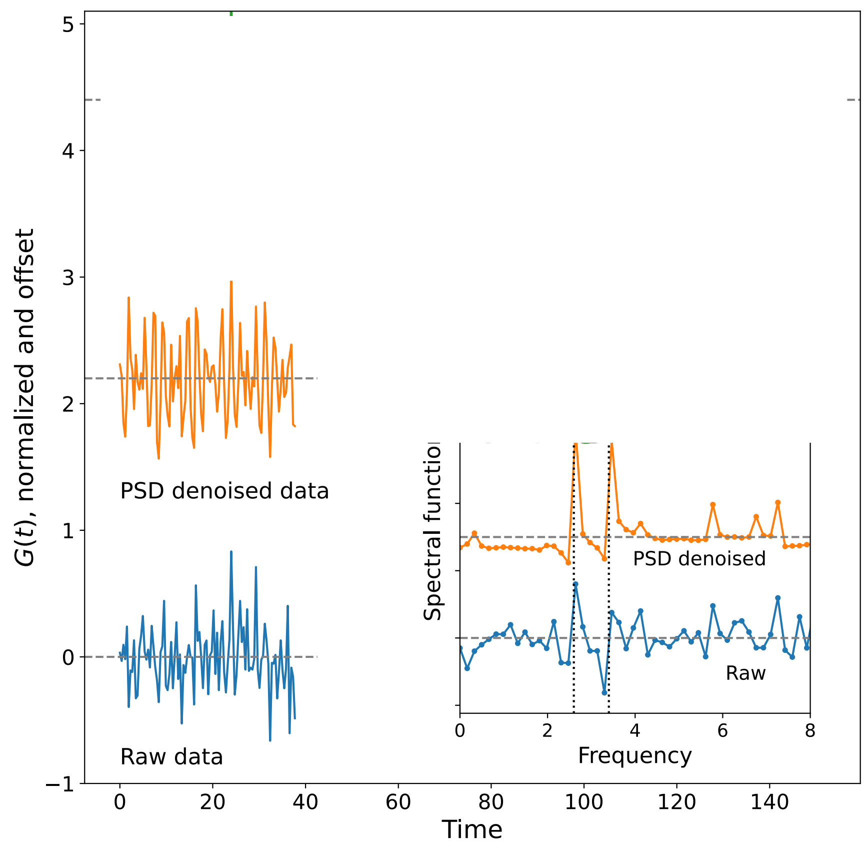

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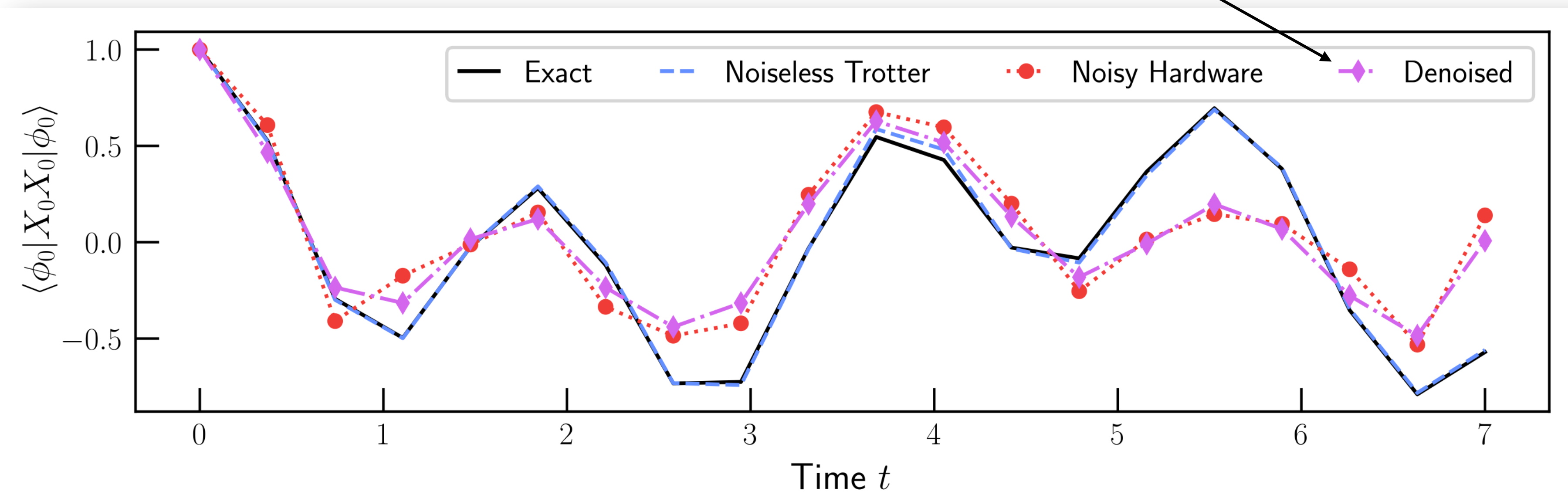
Hardware results

- 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])



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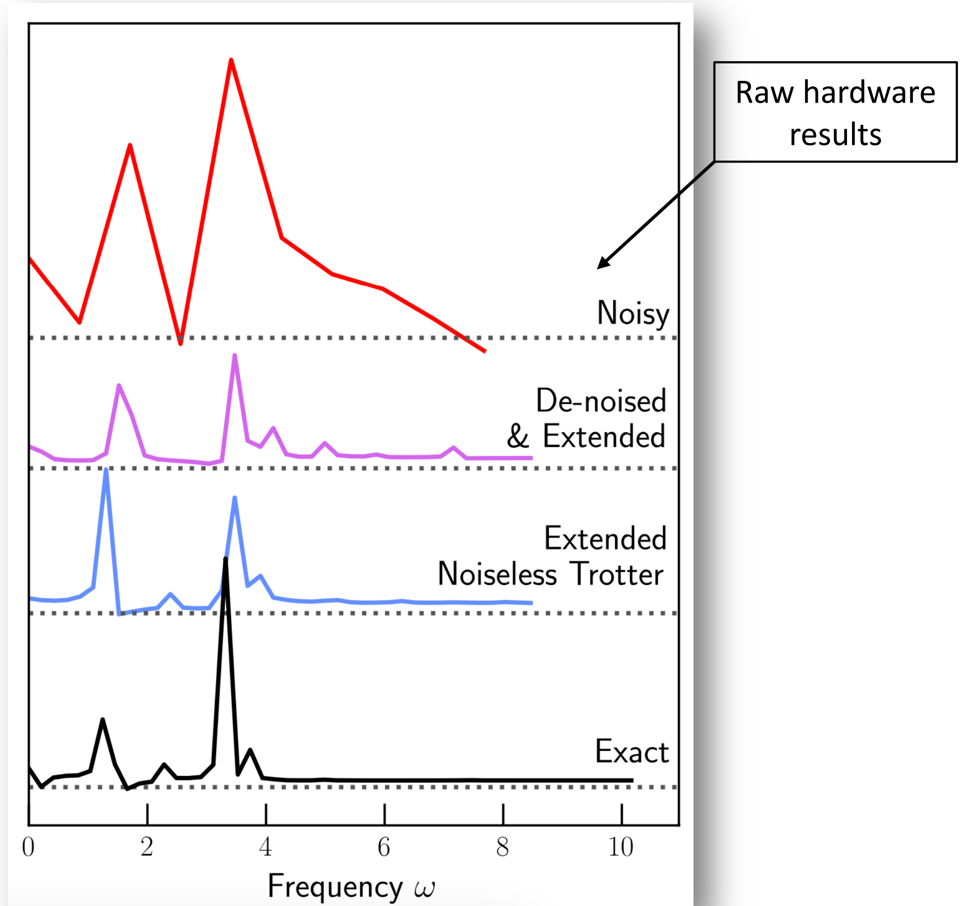
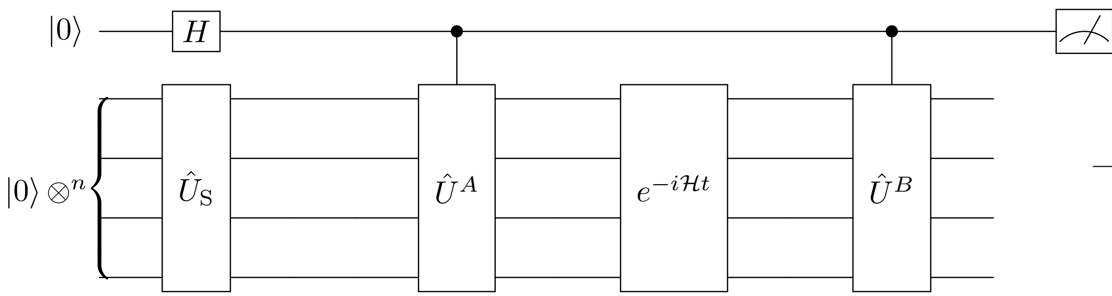


NC STATE UNIVERSITY

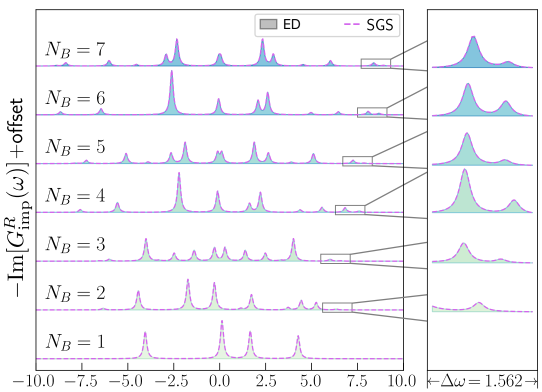
DMFT on Quantum Computers – a path to quantum advantage

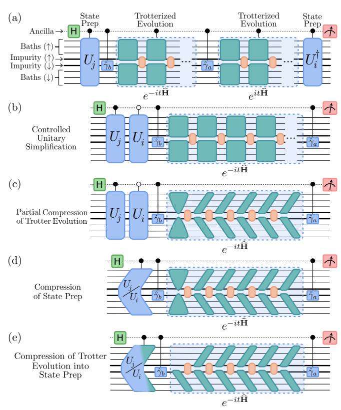


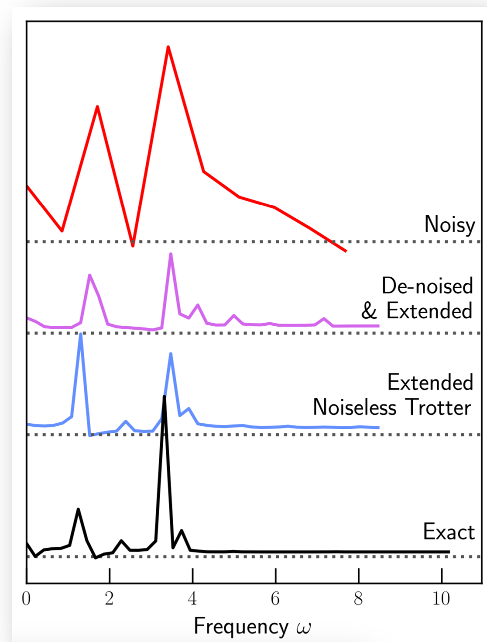
Classical post-processing technique based on PSD projection

Prepare state of interest using subspace of free fermionic states

Time evolve using circuit compression







N. Hogan et al., 2508.05738