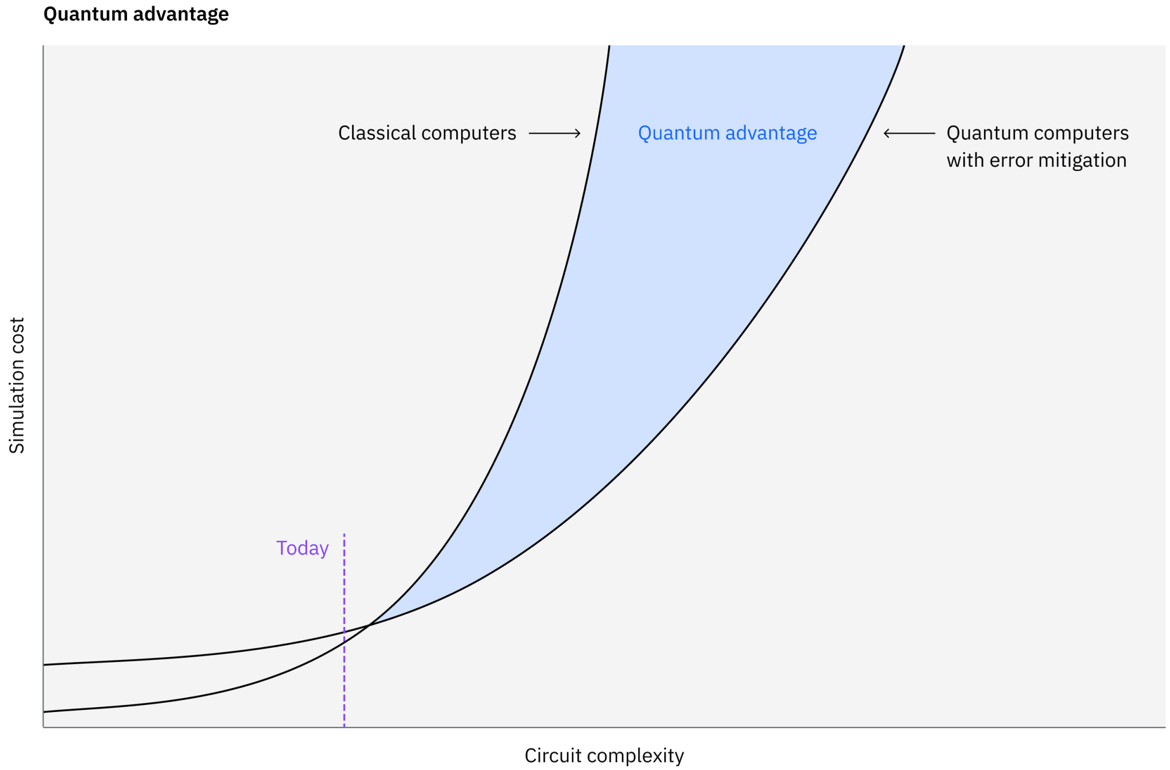
Subspaces in quantum computing and quantum machine learning

Alexander (Lex) Kemper

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

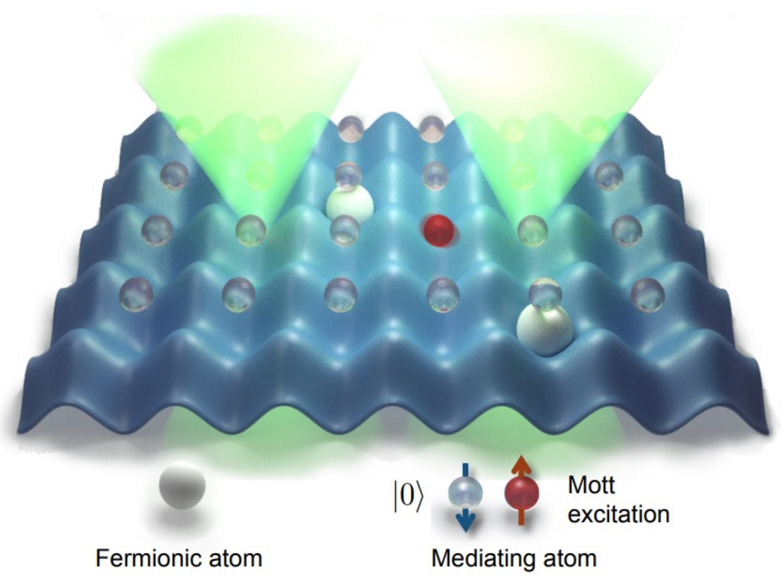
Quantum computers in 2026

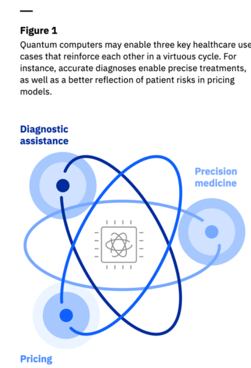


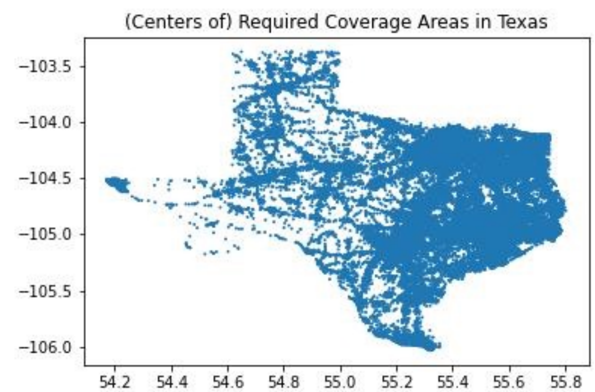
https://www.ibm.com/quantum/blog/quantum-advantage-era

Quantum computers in 2026

Bespoke quantum simulator — *Digital algorithms*







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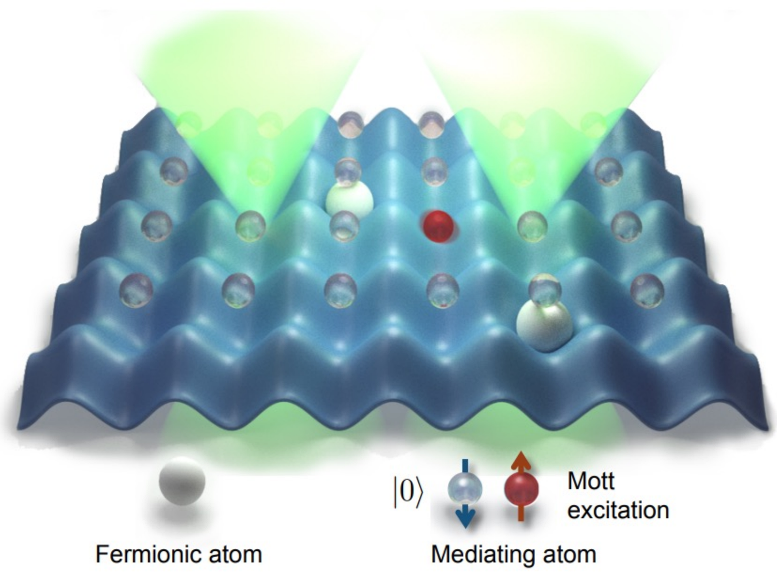
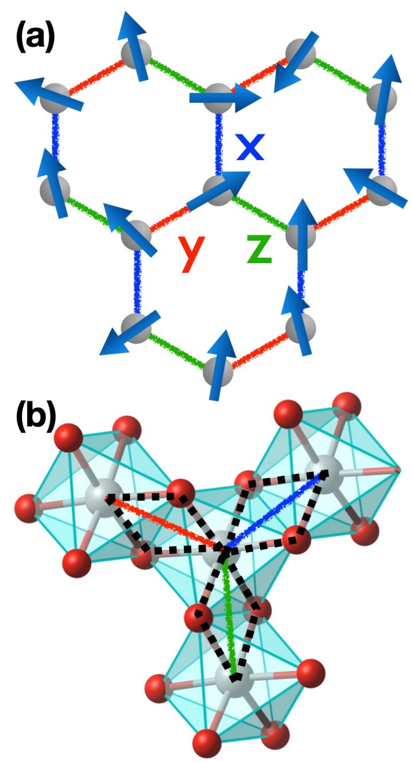
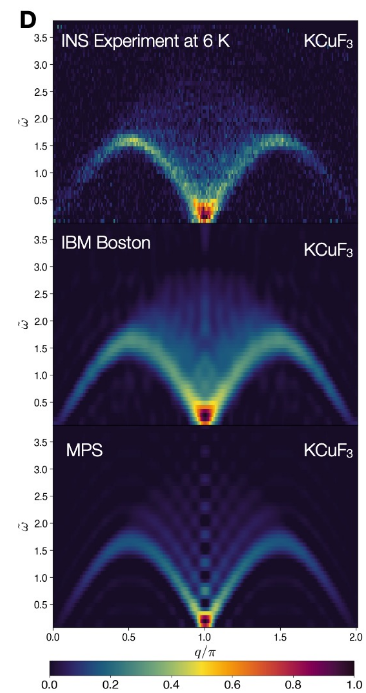
Quantum computers in 2026

Bespoke quantum simulator — *Digital algorithms*







Lee, 2603.15608

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 2026

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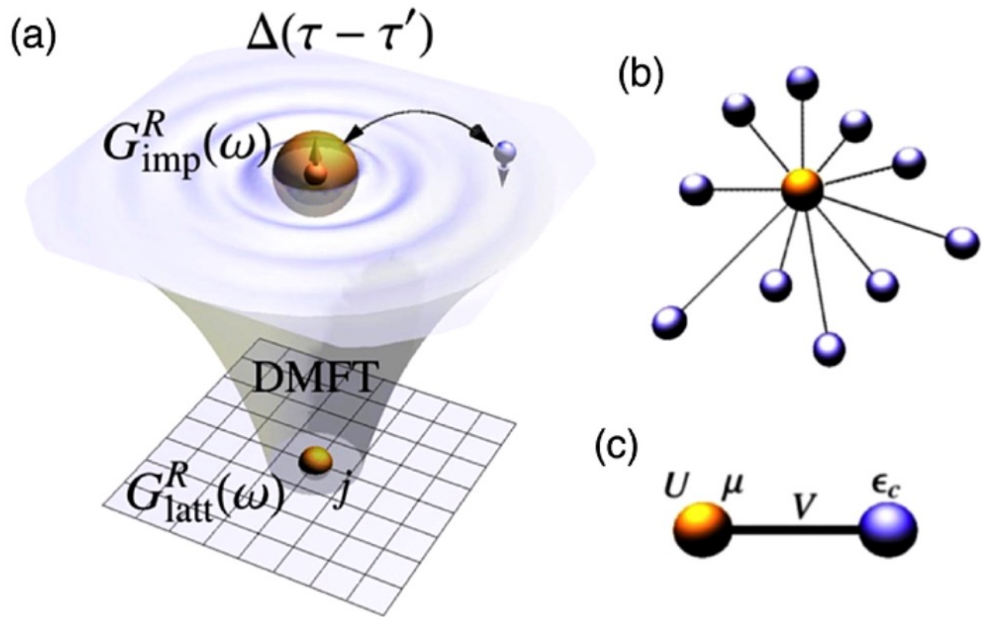
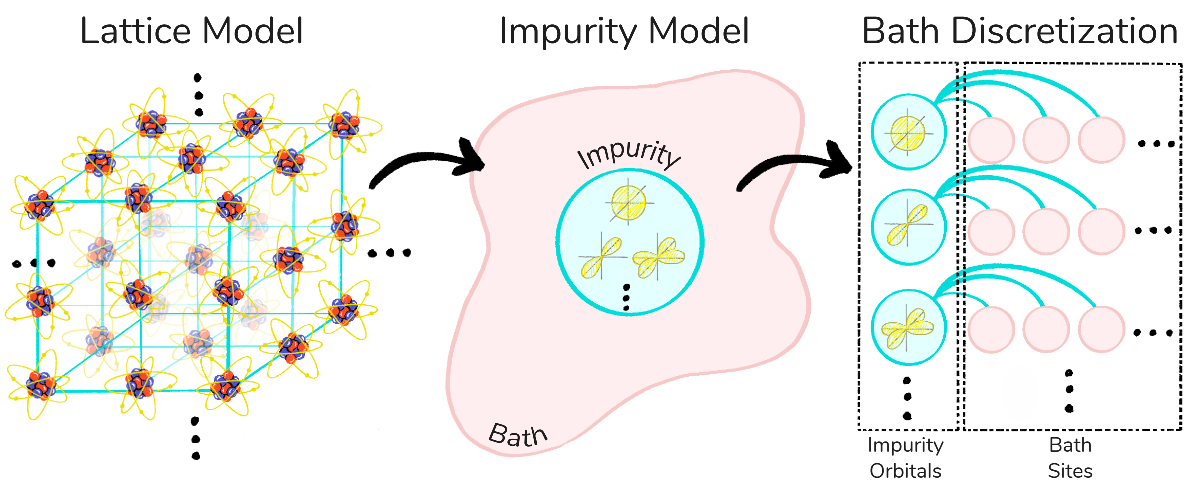


Kreula EPJ Quant. Tech. (2016)

DMFT on Quantum Computers



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

A-Z quantum simulation

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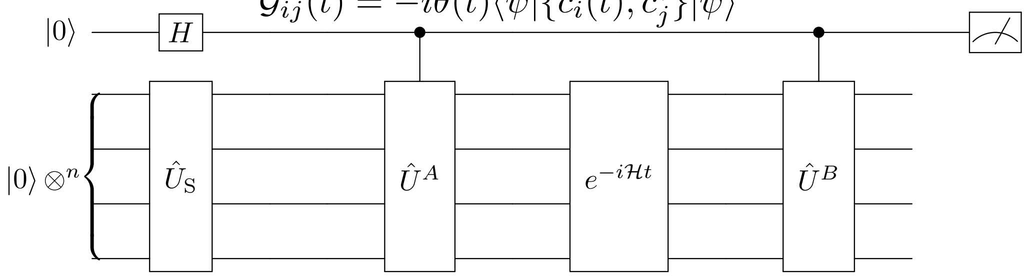


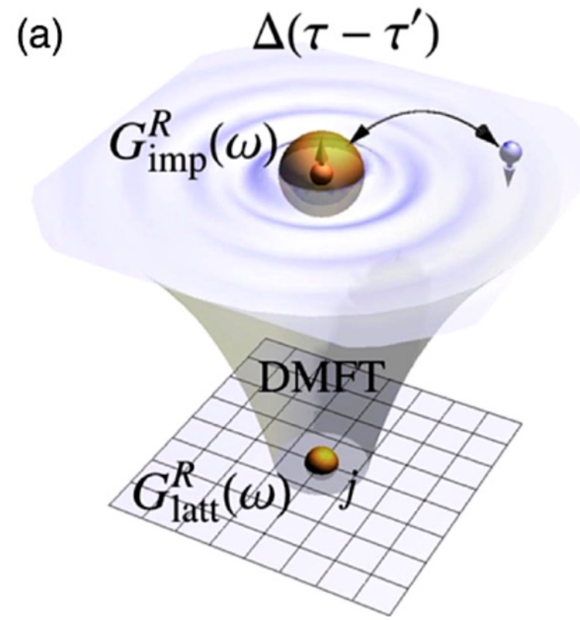
Prepare state of interest

- ☹ Circuit to prepare interacting ground state is very deep
- ☹ Variational approaches are very difficult in the presence of noise

Time evolve

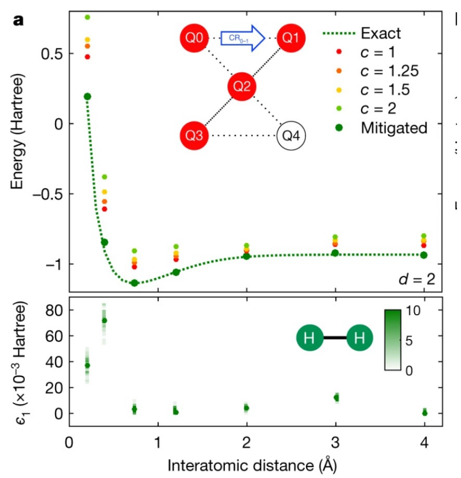
- ☹ Standard Trotter decomposition leads to deep circuits with many gates
- ☹ Alternative approaches (QSP) requires many ancillae

- ☹ Your results will be very noisy anyway



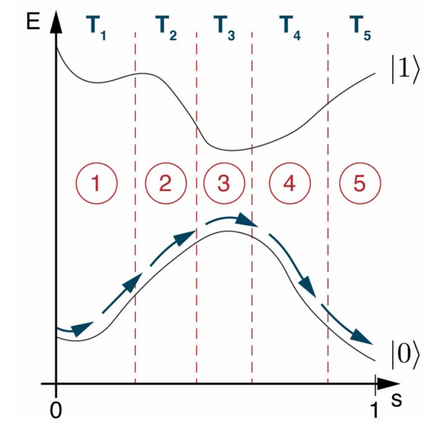
Preparing ground states

Variational Quantum Eigensolver



[Kandala, Abhinav, *et.al.*, *Nature* 549, no. 7671 (2017): 242-246.]

Adiabatic State Preparation



[Schiffer, Benjamin F., *et.al., PRX Quantum* 3, no. 2 (2022): 020347]

Barren Plateau

Larger depth circuits

Quantum Subspace Expansion

The problem: Hilbert space is unreasonably large… $|H| = 2^N$

… and diagonalization is thus difficult.

A solution:

1. Project the Hamiltonian into a smaller space spanned by some vectors $|\psi_j\rangle$
2. Solve the resulting (smaller) generalized eigenvalue problem

$$\mathcal{H}|\Psi\rangle = E\mathcal{S}|\Psi\rangle$$

3. Show (or hope) that your subspace spans the states of interest

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Quantum Subspace Expansion

Which states $|\psi_j\rangle$ to use as a subspace basis?

Krylov states (classical):

$$|\psi_j\rangle = \mathcal{H}^k|\phi_0\rangle$$

Real time evolution

$$|\psi_j\rangle = e^{-i\mathcal{H}t_j}|\phi_0\rangle$$

Cortes PRA 2022
Klymko PRXQ 2022
Stair JCTC 2022
Seki PRXQ 2021
Bespalova PRXQ 2021

Apply Pauli operators, elements of H, or creation/annihilation operators

$$|\psi_j\rangle = \mathcal{O}_j|\phi_0\rangle$$

Colless PRX 2018
McClean PRA 2017
Bharti PRA 2021
Lim QST 2021

Quantum Subspace Expansion

The problem: Hilbert space is unreasonably large… $|H| = 2^N$

… and diagonalization is thus difficult.
… although the physics we care about lives in a small corner of it.

- Ground states
- Excited states
- Thermal states

Eigenvector Continuation: Use ground/excited states of the Hamiltonian *at different parameters* to span the space of interest

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Eigenvector Continuation

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

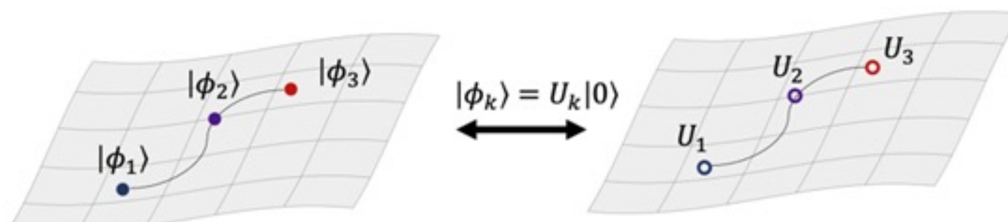
Featured in Physics

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

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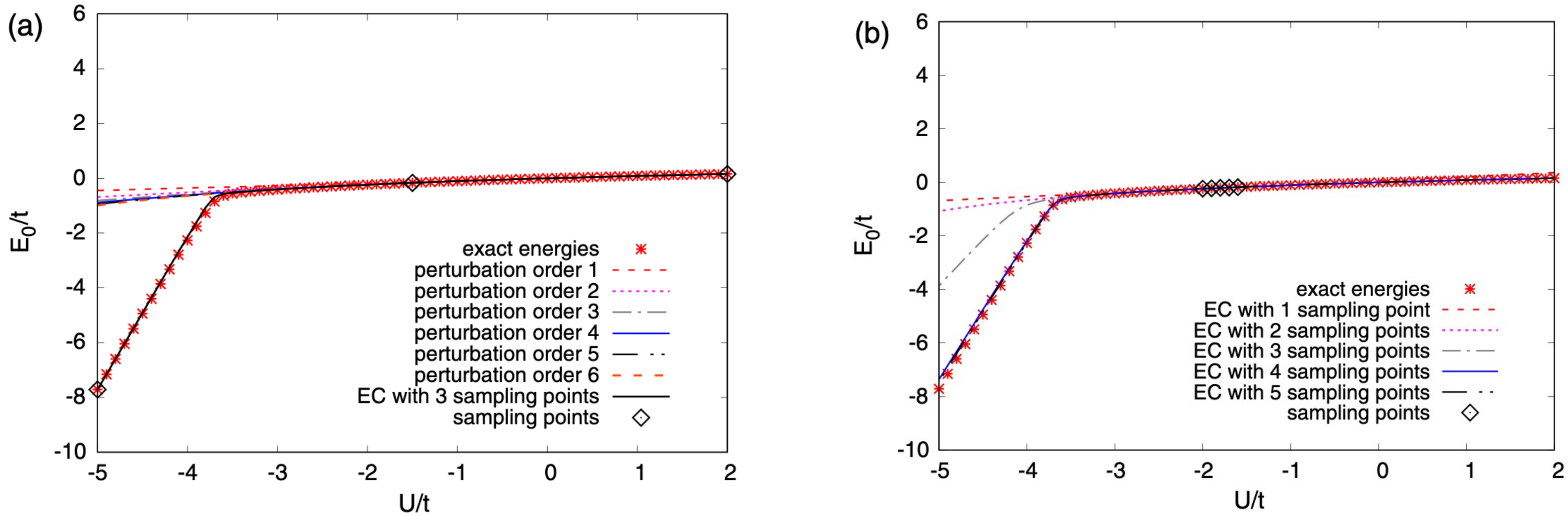

D. Frame et.al, Phys. Rev. Lett. 121, 032501

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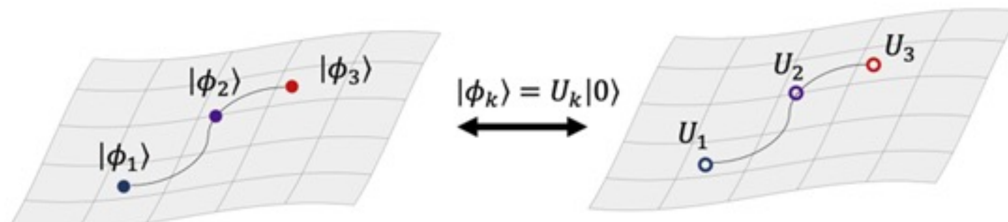


- Make a subspace using low energy states at different points in parameter space

- The spanning states do not have to have any special relation to the problem of interest

D. Frame et.al, Phys. Rev. Lett. 121, 032501
A. Francis, AFK et al., 2209.10571

Eigenvector Continuation

$$\mathcal{H}_{target} = \{H(p_0), H(p_1), \ldots H(p_n)\}$$

Choose *k* Hamiltonians at *k* parameter points

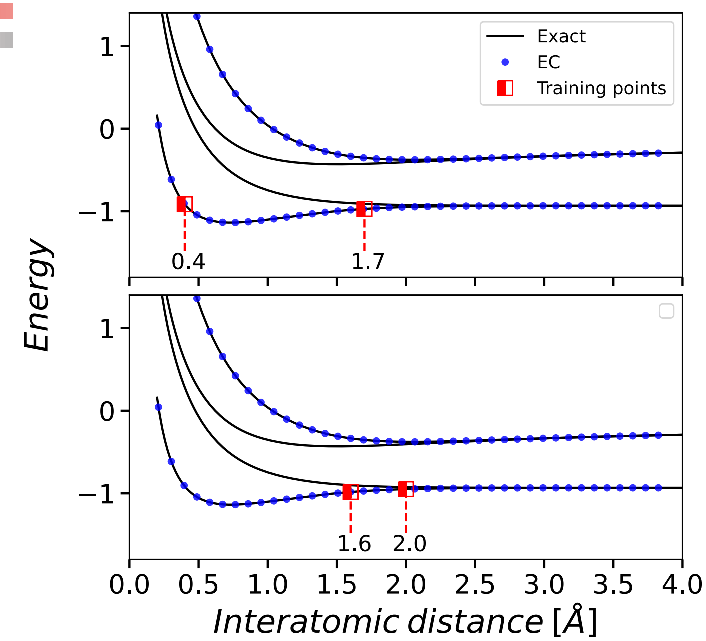
$$\{H(p_0), H(p_1), \ldots H(p_k)\}$$

Solve for ground state vector

$$\{|\phi_0\rangle, |\phi_1\rangle, \ldots |\phi_k\rangle\}$$

k Low energy state vectors

Subspace Diagonalization



Energy spectrum across the parameter range

A. Francis, AFK et al., 2209.10571

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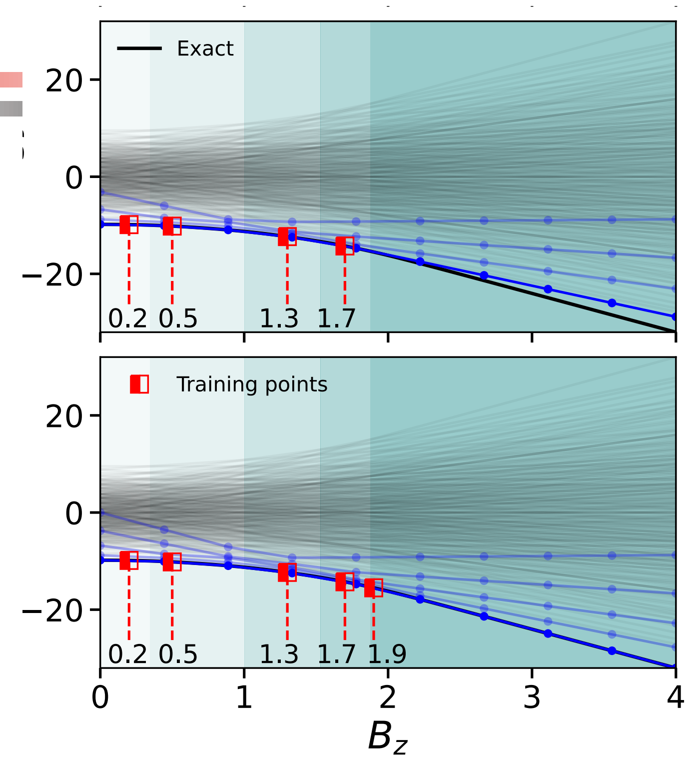

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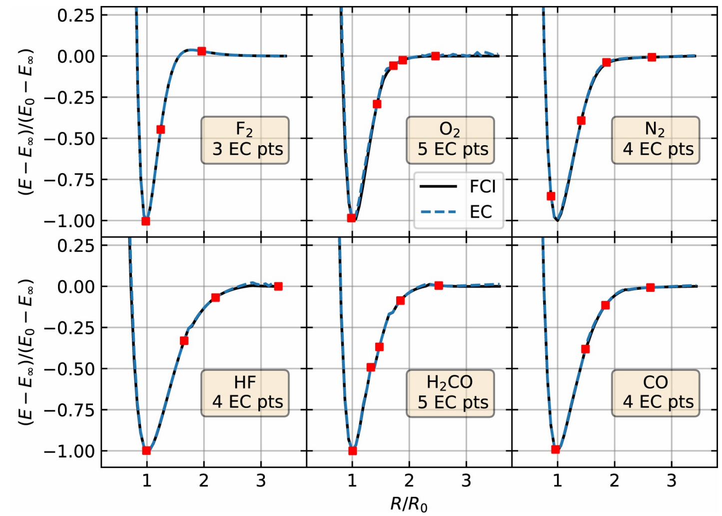


C. Mejuto-Zaera, AFK, Electron. Struct. 2023

Eigenvector Continuation

$$\mathcal{H}_{target} = \{H(p_0), H(p_1), \ldots H(p_n)\}$$

Choose *k* Hamiltonians at *k* parameter points

$$\{H(p_0), H(p_1), \ldots H(p_k)\}$$

We need low energy state vectors –
Exact ground states are not necessary!

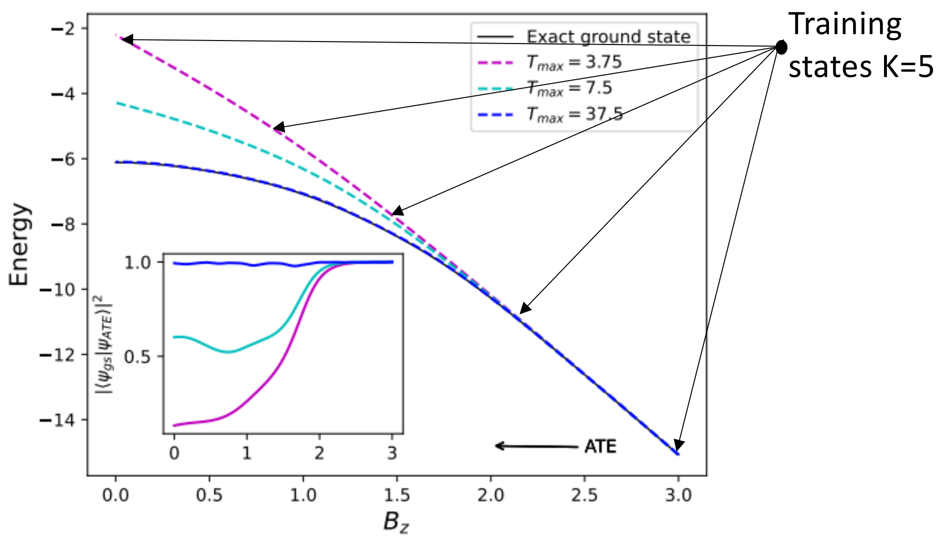
Solve for ground state vector → *We can use any state preparation method*

$$\{|\phi_0\rangle, |\phi_1\rangle, \ldots |\phi_k\rangle\}$$

k low energy state vectors

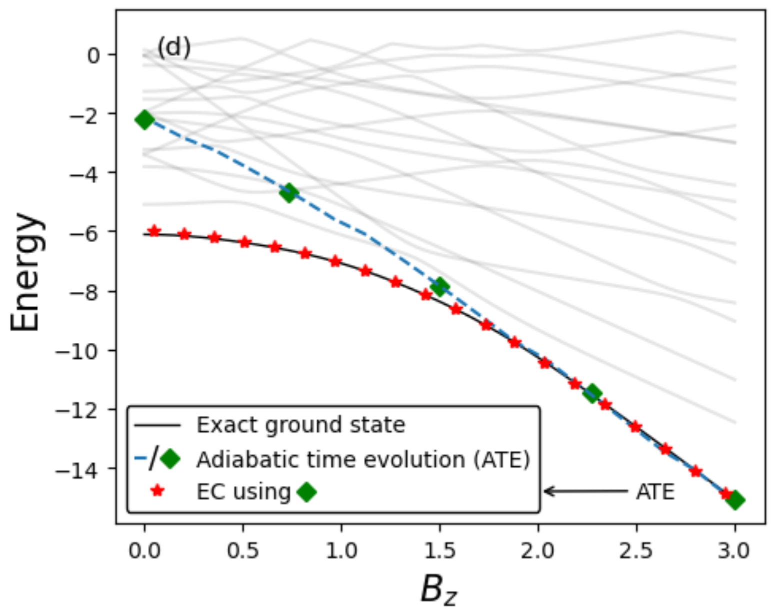
Subspace Diagonalization → Energy spectrum across the parameter range

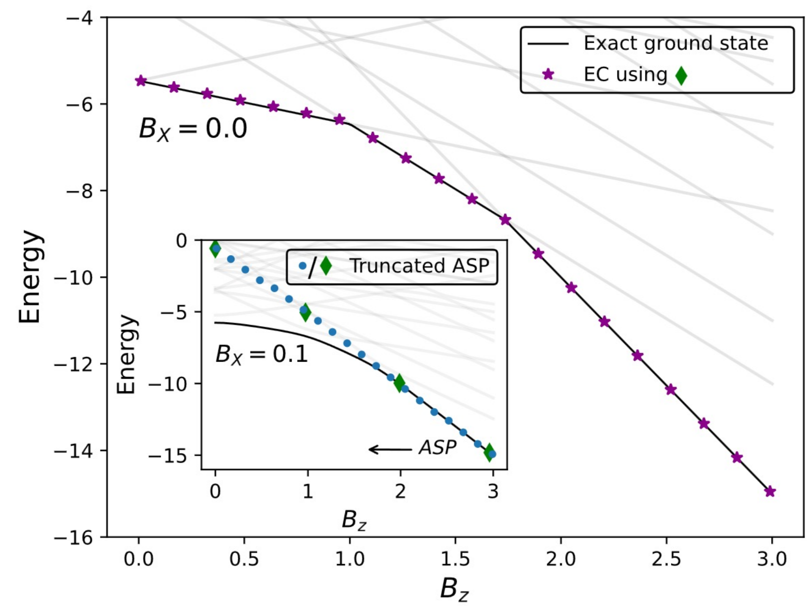
Approximate Eigenvector Continuation: Adiabatic state preparation



1D 5-site XY Model Adiabatic time evolution

Approximate Eigenvector Continuation: Adiabatic state preparation

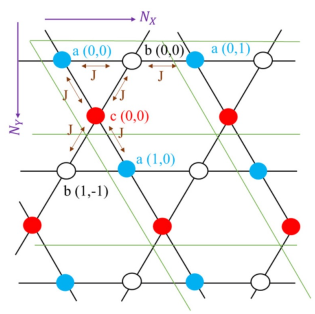


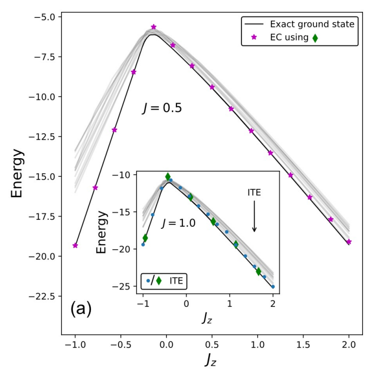


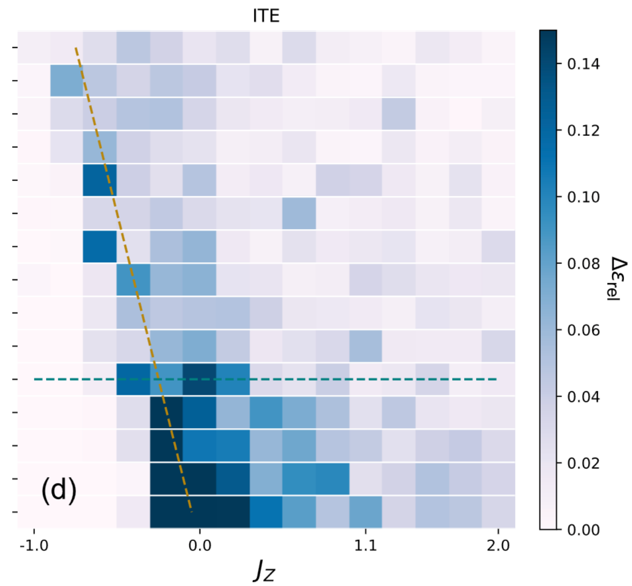
Straightforward subspace expansion -> improved results from adiabatic state preparation

Agrawal, PRA (2025), 10.1103/PhysRevA.111.032607

Approximate Eigenvector Continuation: Imaginary time evolution







Straightforward subspace expansion -> improved results from imaginary time evolution

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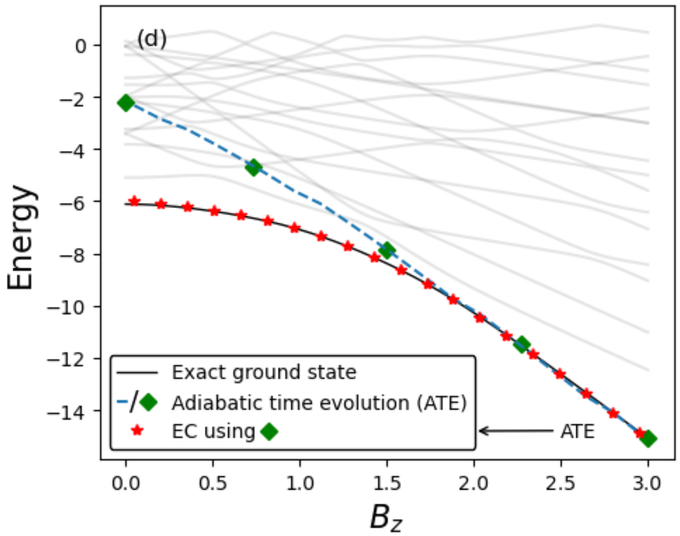
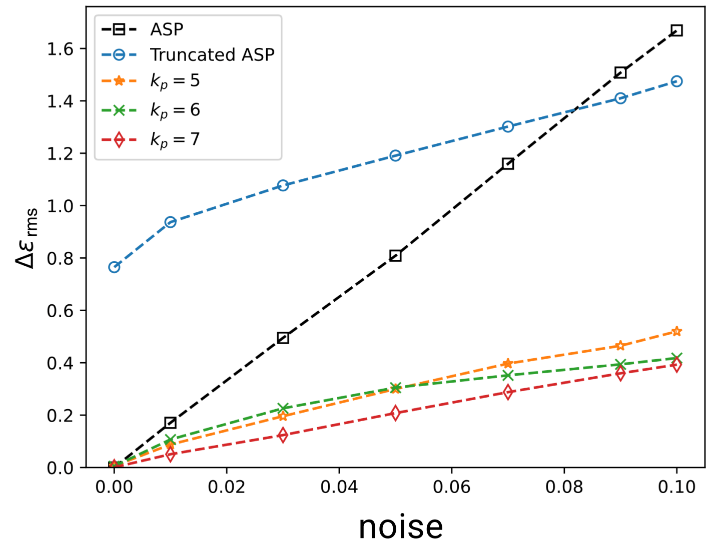
Noise resilience





Straightforward subspace expansion -> noise resilience

Agrawal, PRA (2025), [10.1103/PhysRevA.111.032607](https://doi.org/10.1103/PhysRevA.111.032607)

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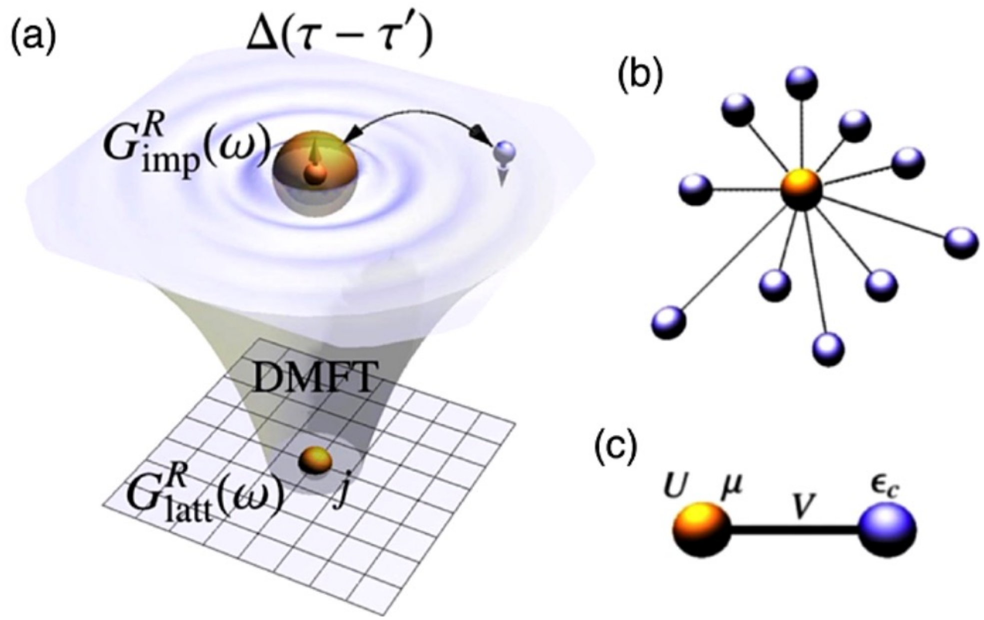
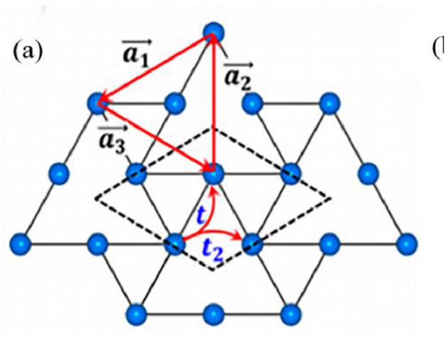
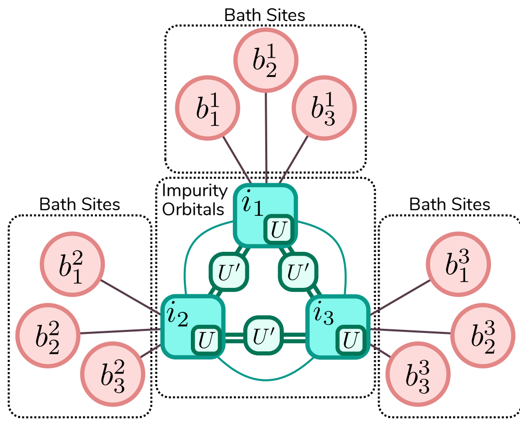
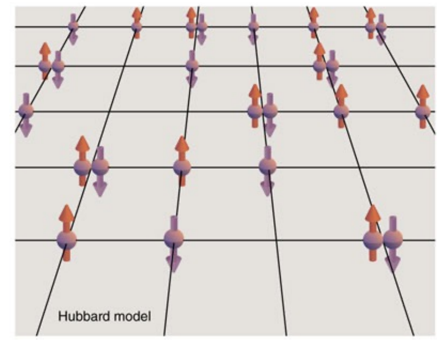


Kreula EPJ Quant. Tech. (2016)

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

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

Received: 28 November 2016 / Accepted: 6 June 2017
Published online: 31 August 2017 – © Springer-Verlag GmbH Germany 2017

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

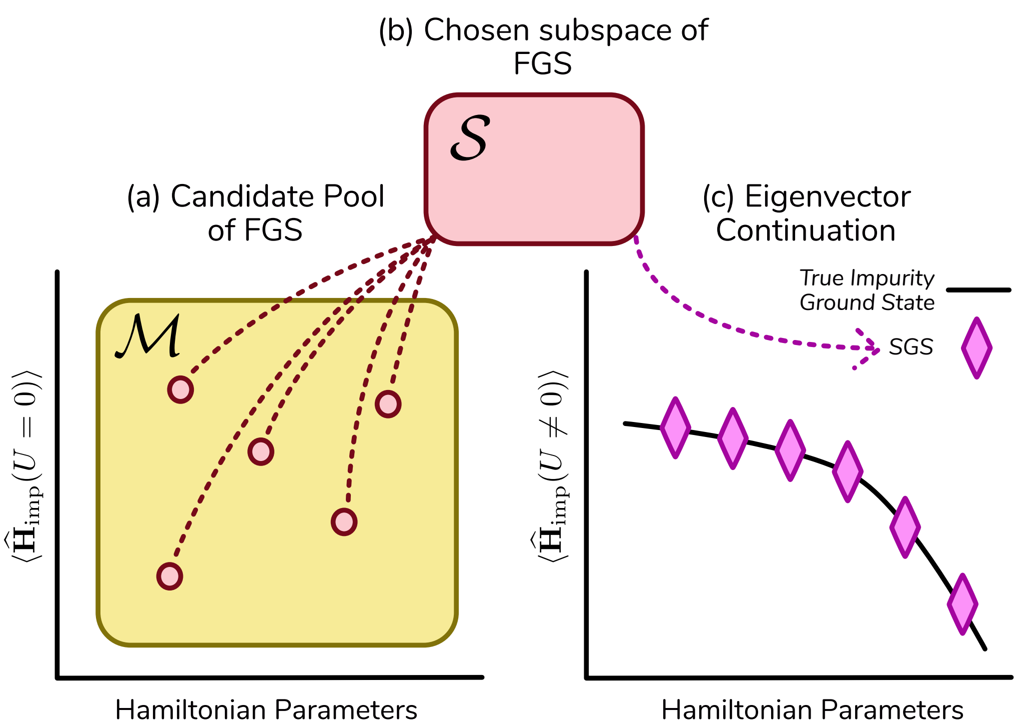
Quantum impurity models using superpositions of fermionic Gaussian states: Practical methods and applications

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

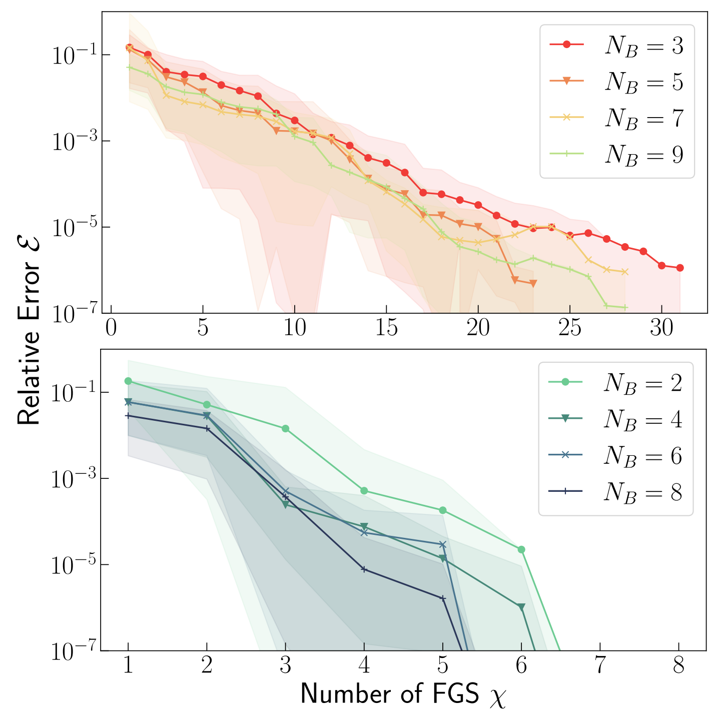
“The low energy state is represented as a superposition of exp [O(b^3)] fermionic Gaussian states.”

“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

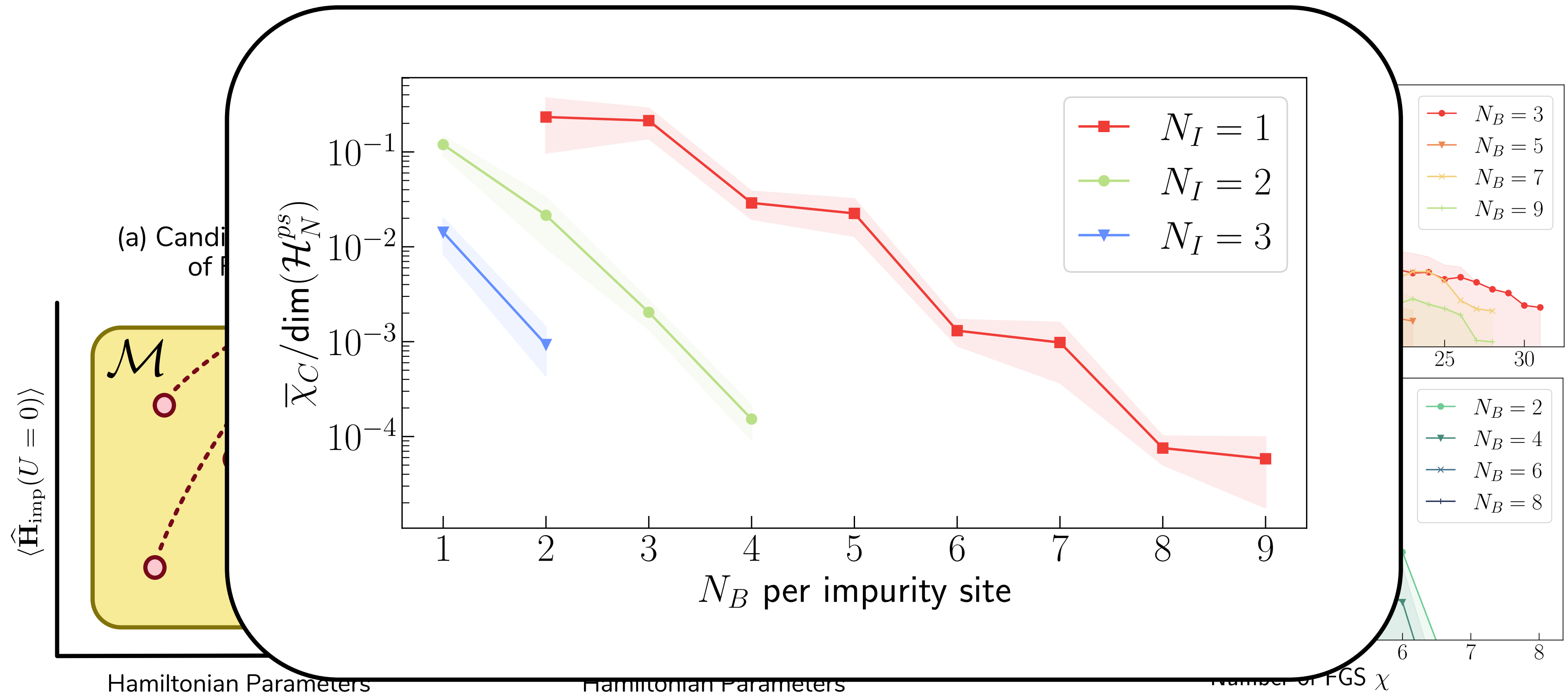


$$\widetilde{H}\vec{\alpha} = \widetilde{E}S\vec{\alpha}$$



N. Hogan, 2508.05738

Fermionic Gaussian Subspace



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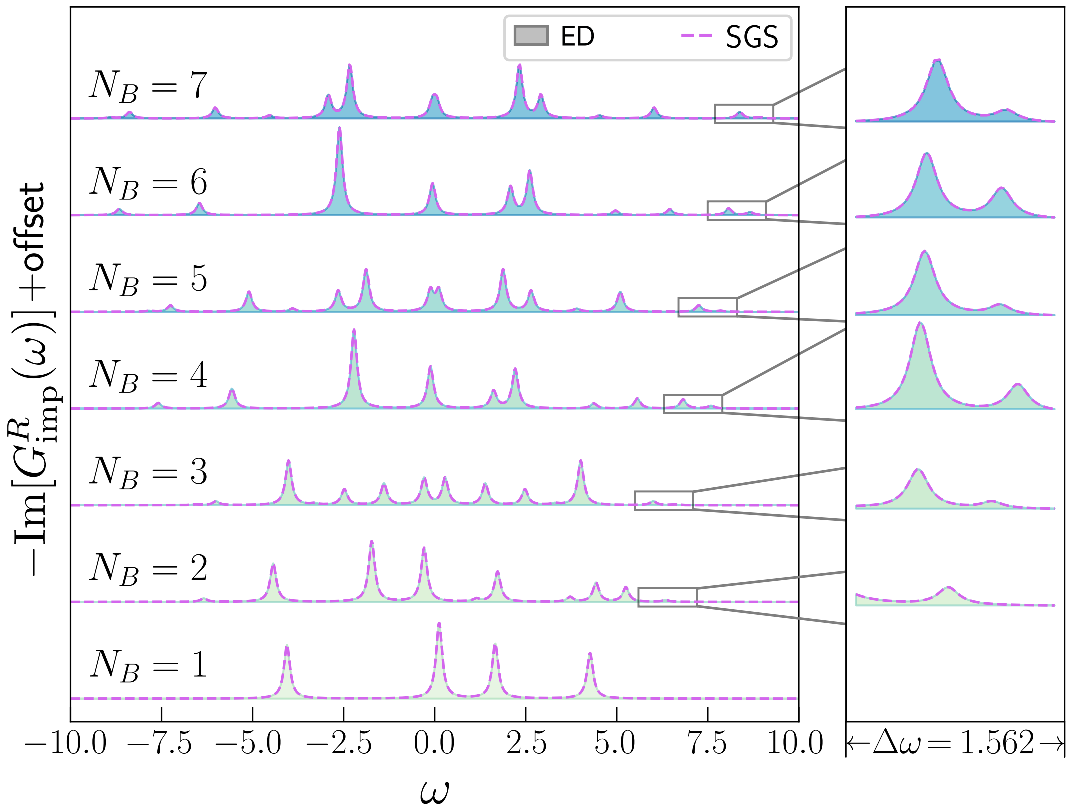


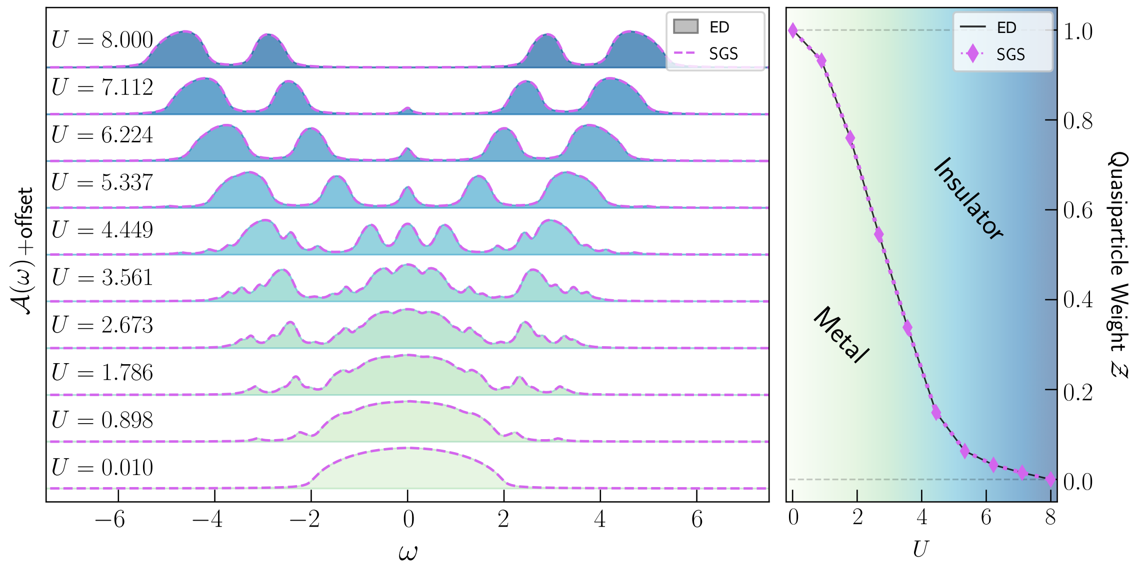
N. Hogan, 2508.05738

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)

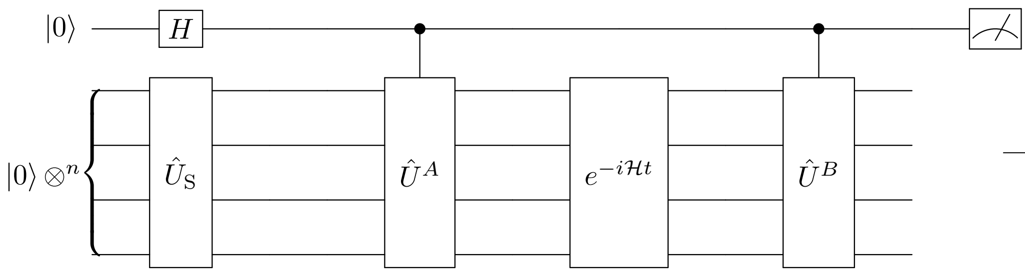
Shaded region = $|\psi\rangle$ dashed line = $\sum_{k=1}^{\chi} \alpha_k |\phi_k\rangle$



Increasing interaction strength on impurity

N. Hogan, 2508.05738

A-Z quantum simulation



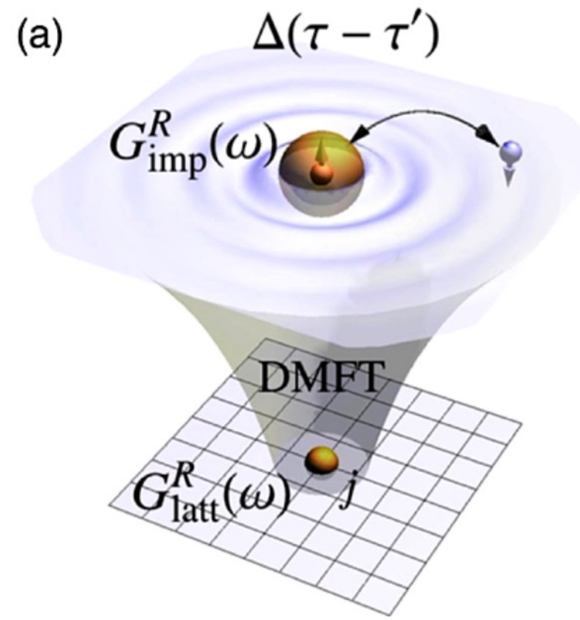
Prepare state of interest

Time evolve

- *Physics-Informed Subspace Expansions*

- *Lie-algebraic methods for time evolution*

Classical post-processing techniques



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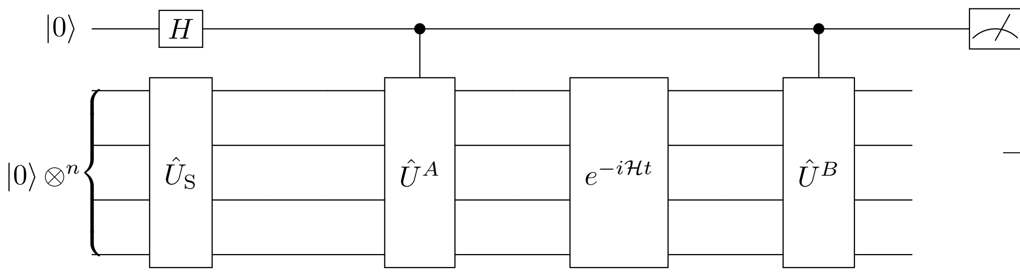

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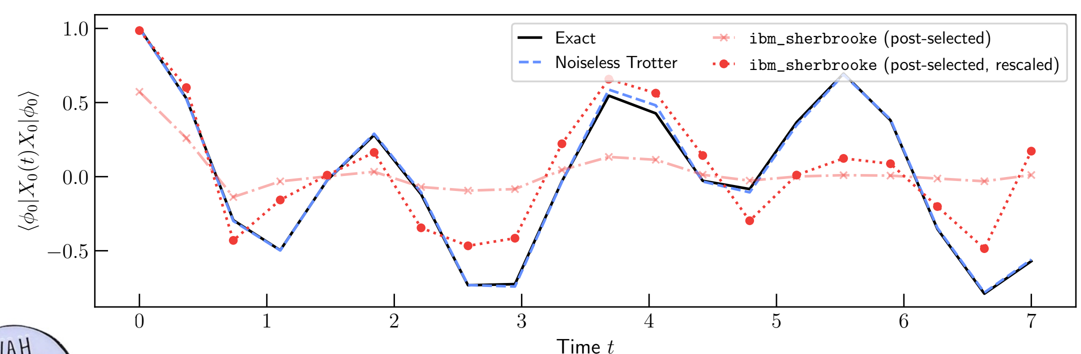
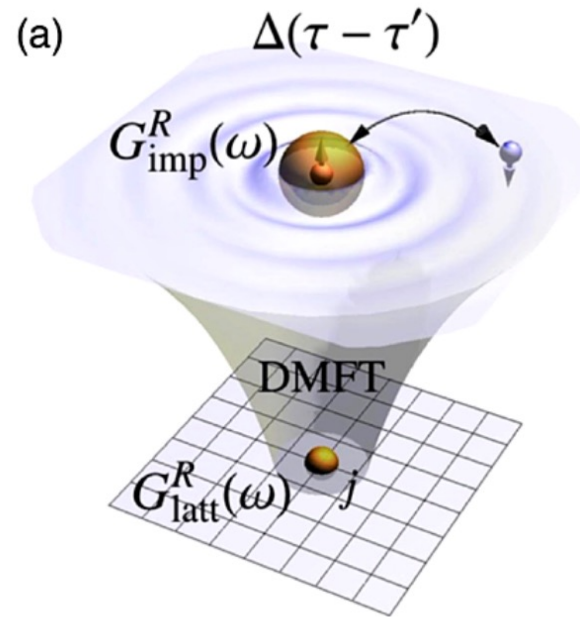




A-Z quantum simulation

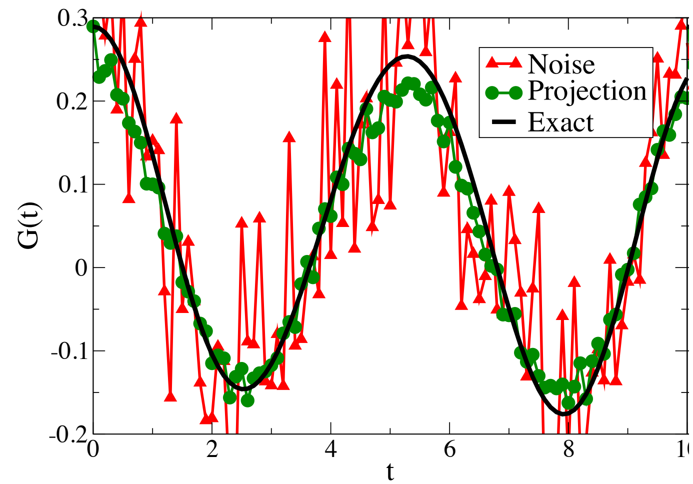
- It turns out that these are positive semi-definite (PSD) functions:

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

- Then this is a PSD matrix:

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

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



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

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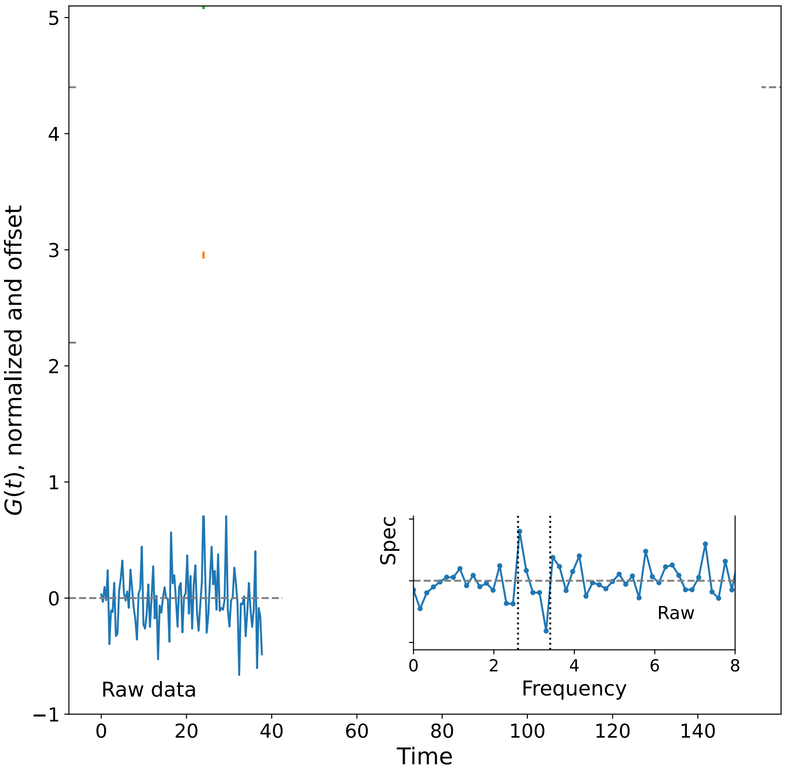

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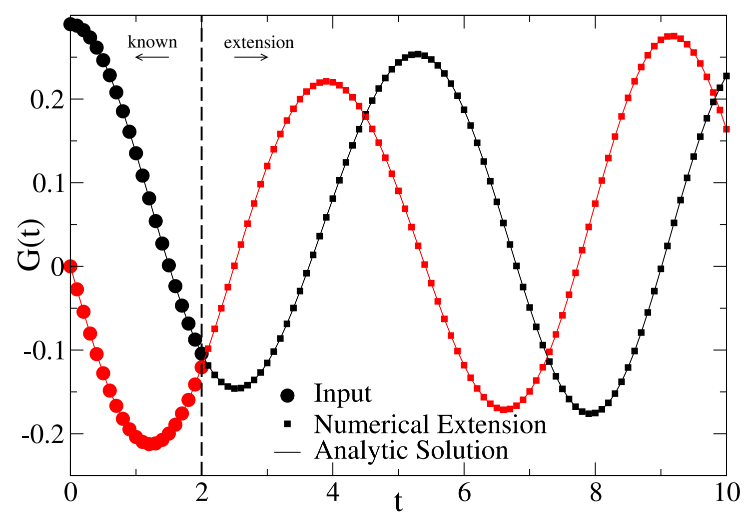

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A-Z quantum simulation

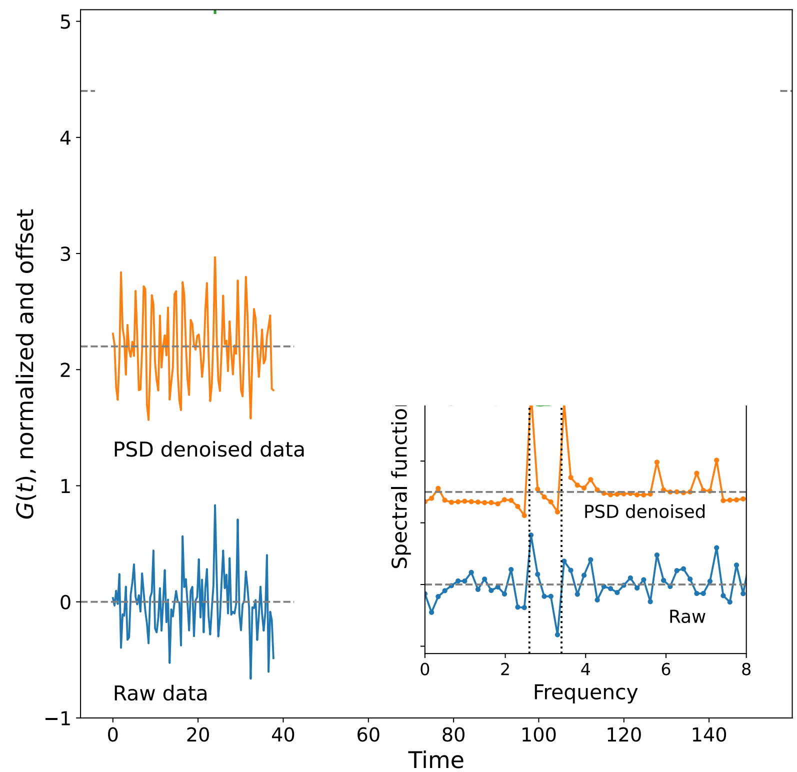
- It turns out that these are positive semi-definite (PSD) functions:

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

- Then this is a PSD matrix:

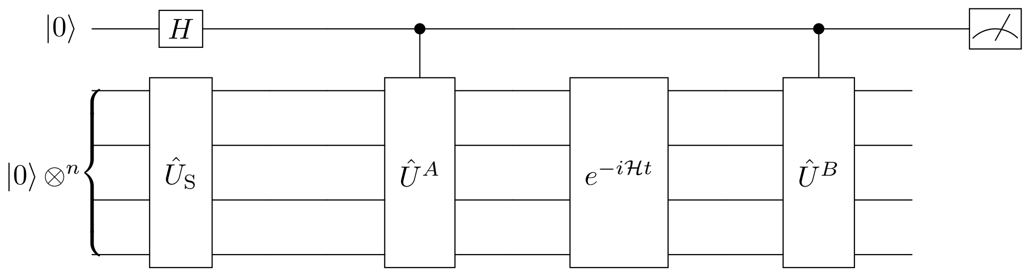
$$\underline{\mathrm{G}} = \begin{pmatrix} f_0 & f_1 & f_2 & \cdots & f_n \\ f_1^* & f_0 & f_1 & \cdots & f_{n-1} \\ f_2^* & f_1^* & f_0 & \cdots & f_{n-2} \\ \vdots & & & \ddots & \vdots \\ f_n^* & f_{n-1}^* & f_{n-2}^* & \cdots & f_0 \end{pmatrix}$$

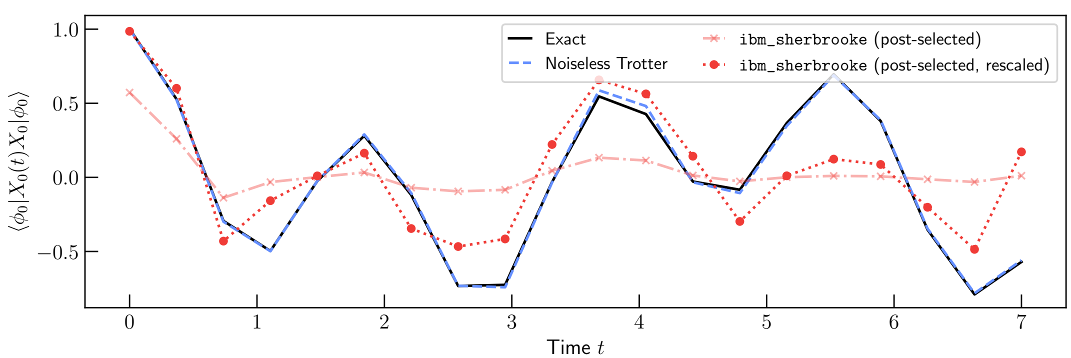
where $G_{AA}(t_i - t_j) \to f_{i-j}$

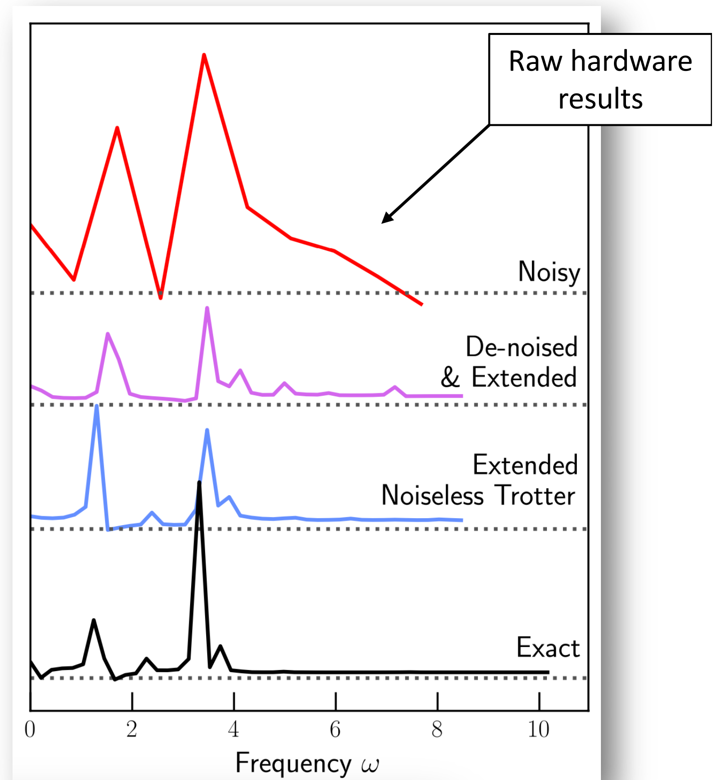


A.F. Kemper, C. Yang, E. Gull, PRL (2024)

Hardware results







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

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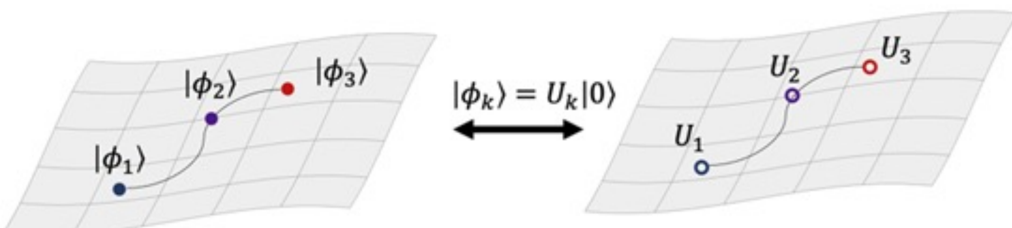
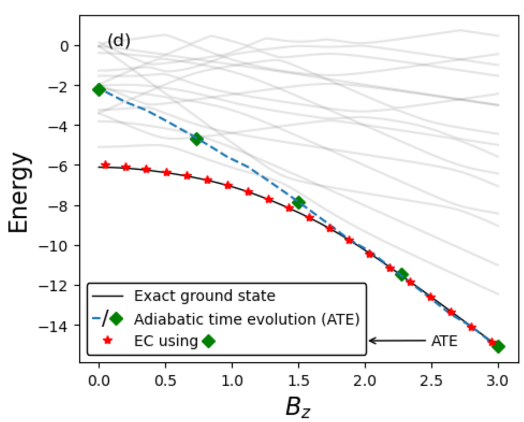
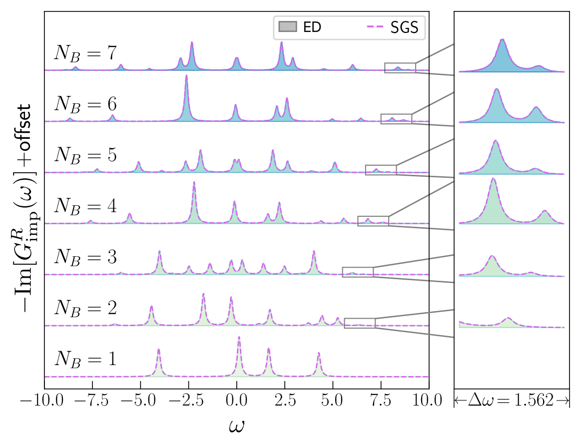
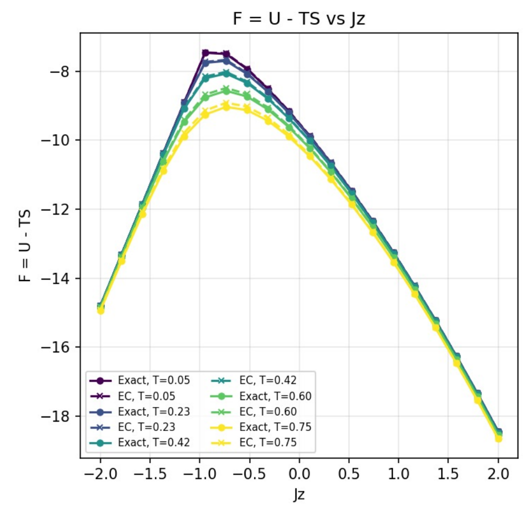
Subspaces with Eigenvector Continuation



Subspace methods can be readily added to many state preparation methods!







Agrawal 10.1103/PhysRevA.111.032607, Hogan 2508.05738

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Preparing thermal states

***Why Low-Temperature Observables*?**
•Fundamental physics Insights (like, quantum phase transitions and critical points)
•Practical applications (like, quantum material discovery)

Existing Algorithm Gaps
•QITE/QMETTS: depth blows up at low T, no reuse
•VQG: barren plateaus, no parameter-reuse strategy
•Block-encoding: optimal at high T only
•No efficient cross-parameter thermal estimation

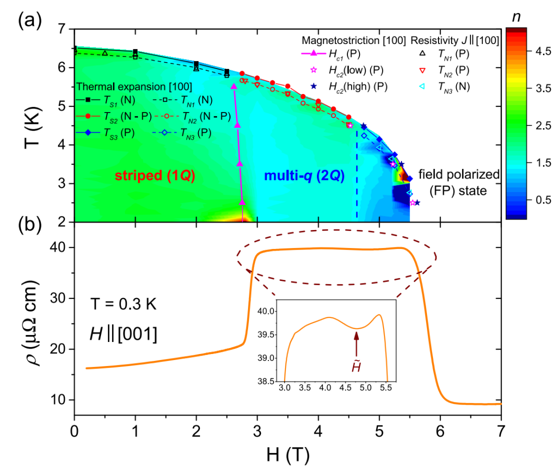

Fig. 1 Phase diagram of $CeAuSb_2$ its unusual magnetoresistance. a

Algorithm Requirements
•Efficient at low temperature (β → large)
•Parameter-reuse across Hamiltonian families
•Observable estimation without full state prep
•Scalable to early FTQC devices

[Motta M, *et. al., Nat. Phys.* **16**, 205–210(2020)] [Powers C, *et. al., Sci Rep* **13**, 1986 (2023)]
[Wang Y, *et. al.,* PRA 16, 054035(2021)] [Seo S, *et. al., Nat Comm Phys* **4,** 58 (2021)]

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Algorithm requirements

Target:

1. Low-temperature thermal states

At low-temperature, thermal state of a system Hamiltonian could be approximated with a few low-energy eigenstates, $k << |\mathcal{H}|$

$$\hat{\rho}_T = \frac{1}{Z_k} \sum_{n=0}^{k} e^{-\beta E_n} \mid E_n\rangle\langle E_n| \,, \qquad Z_k = \sum_{n=0}^{k} e^{-\beta E_n}$$

2. Low-energy states

A low-energy state could be prepared by truncated state preparation methods

3. A sufficient subspace

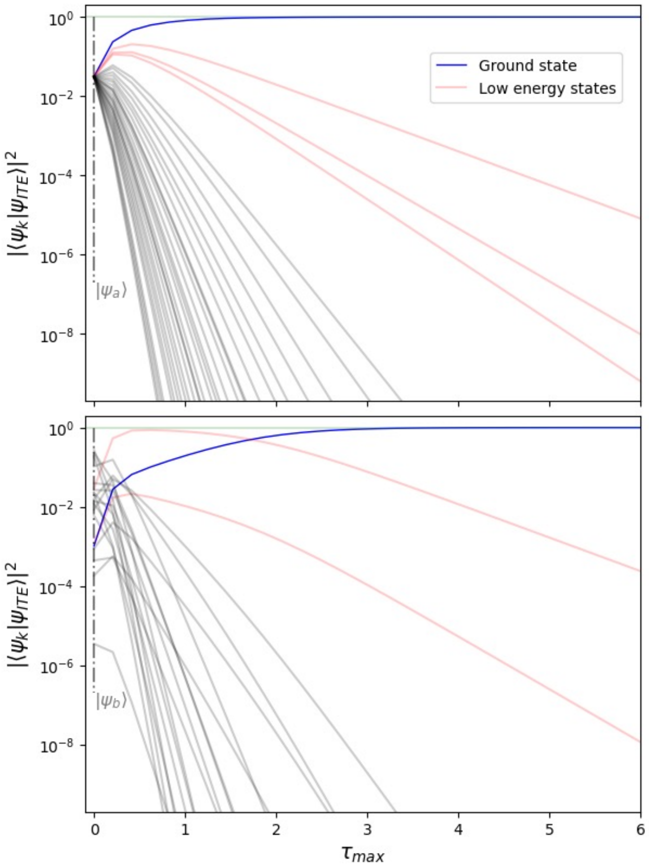
To obtain a sufficient subspace up to convergence, we could repeat the previous step

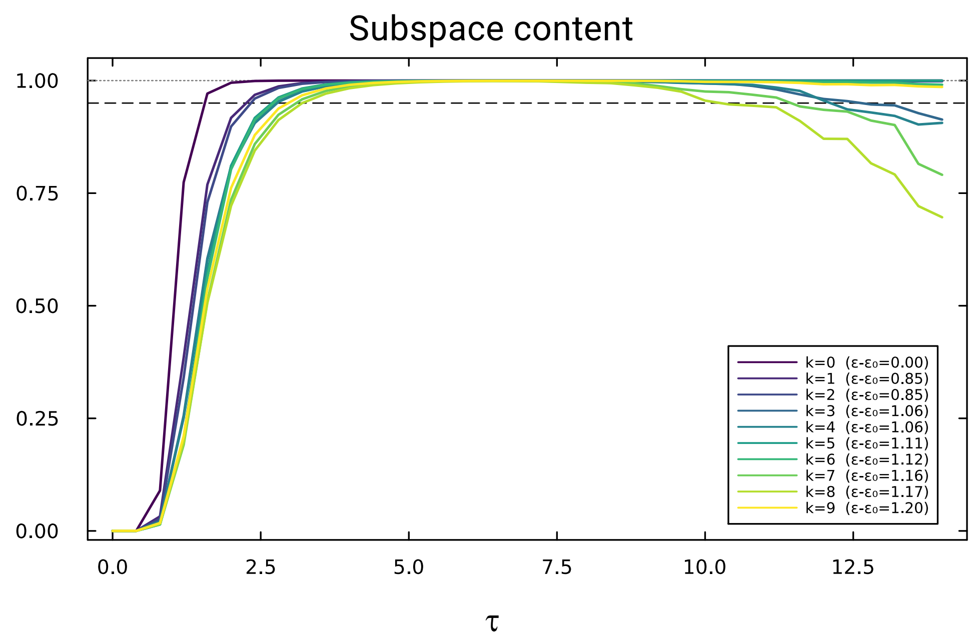
4. Resource-efficient parameter sweep

A sufficient low-energy subspace could be used for a family of Hamiltonians using techniques like Eigenvector continuation (EC)

Low-energy states : Truncated State preparation

Quantum Imaginary Time Evolution

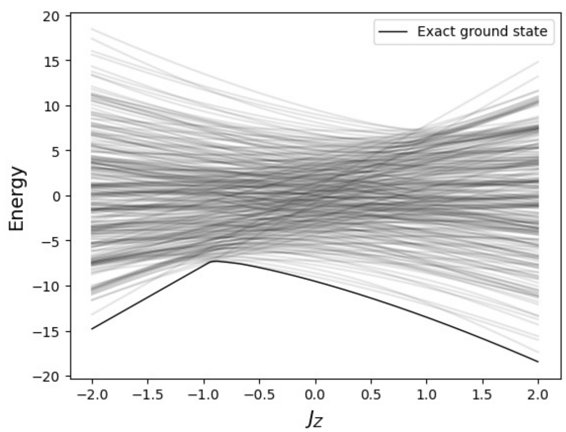




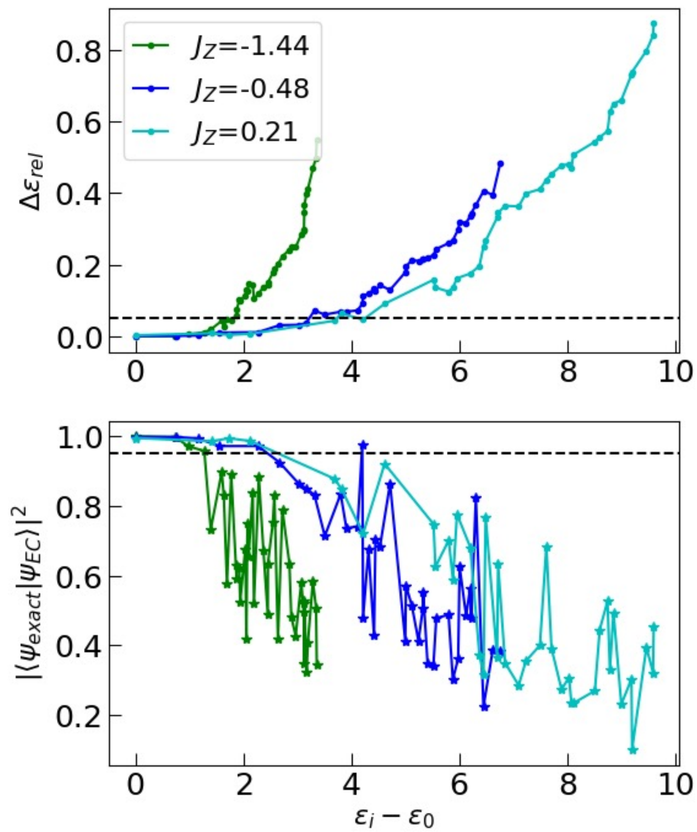
Energy gaps: “Low-temperature” is relative

“Low-temperature” Thermal States: The number of lowest eigenstates required approximate a thermal state at temperature T depends on the number of states within the energy gaps proportional to the energy corresponding to the temperature T.

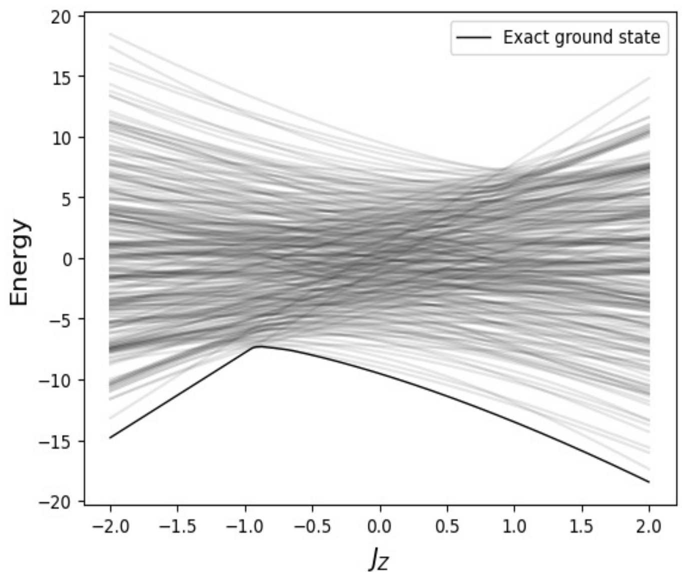
$$\mathcal{H}_{XXZ} = \sum_{i=1}^{N-1} J\,(X_i X_{i+1} + Y_i Y_{i+1}) + J_z Z_i Z_{i+1} + \sum_{k=1}^{N} B_z\, Z_k.$$



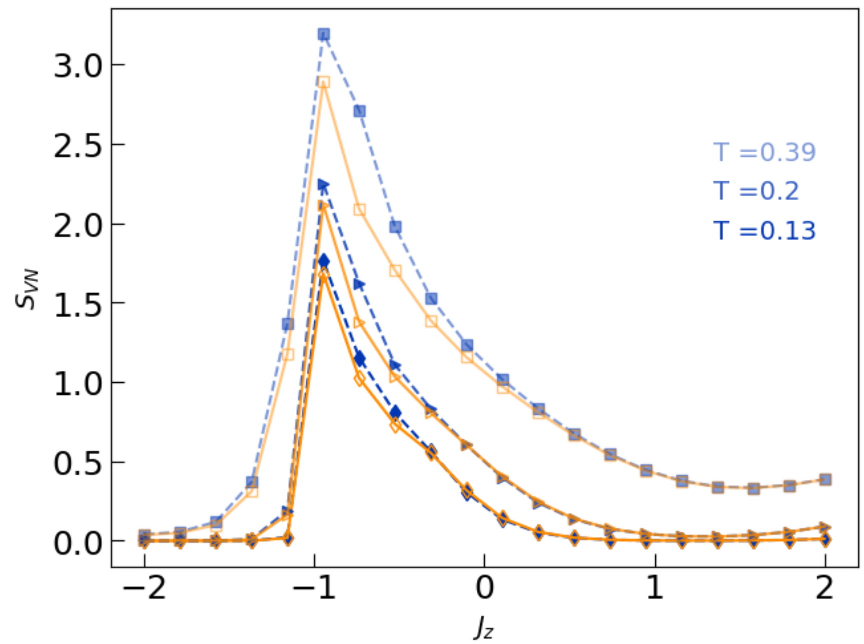
Spectrum of 1D- 8-site XXZ chain



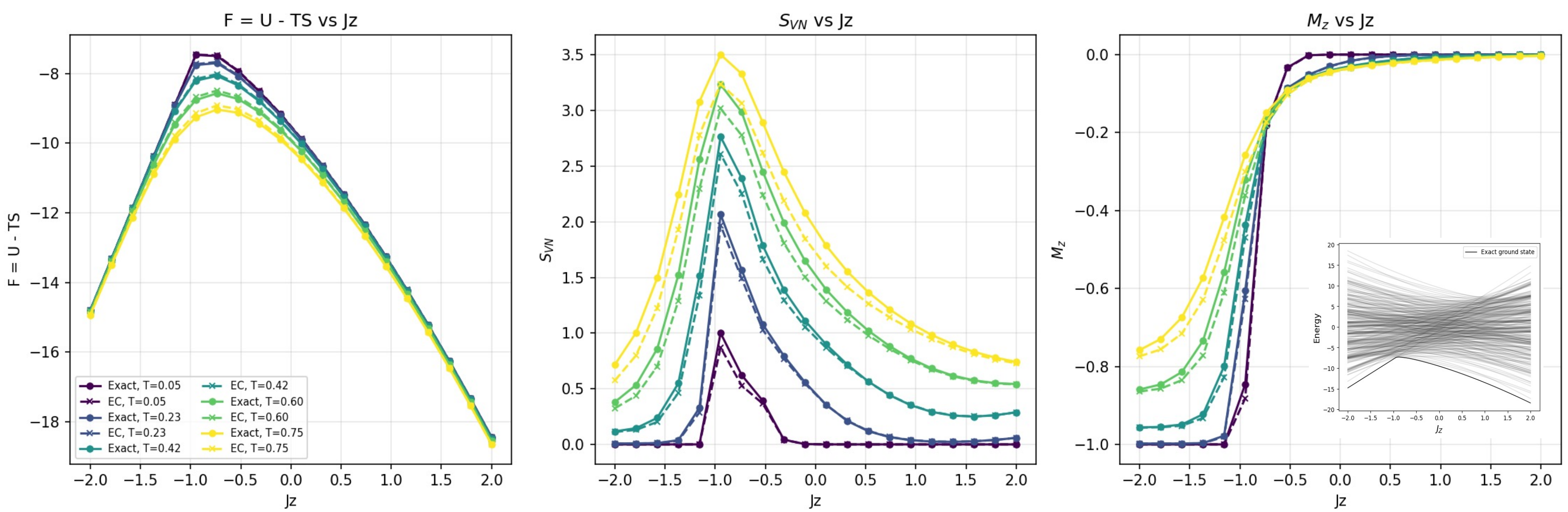
Results: Thermodynamics near phase transition for N=8



Spectrum of 1D- 8-site XXZ chain

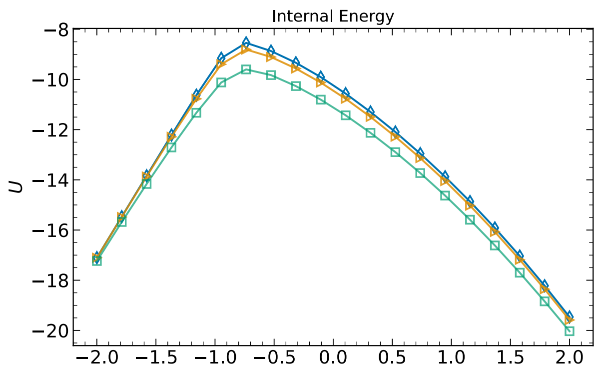


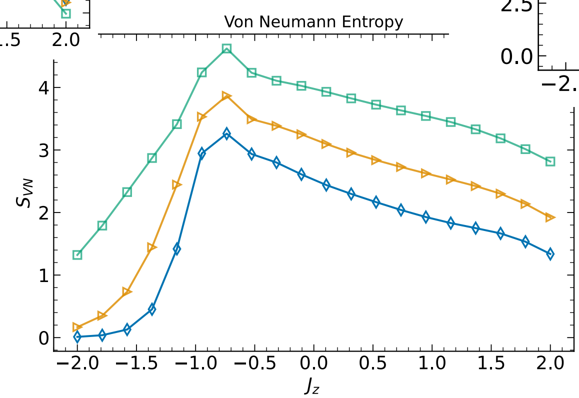
Results: Thermodynamics near phase transition for N=8

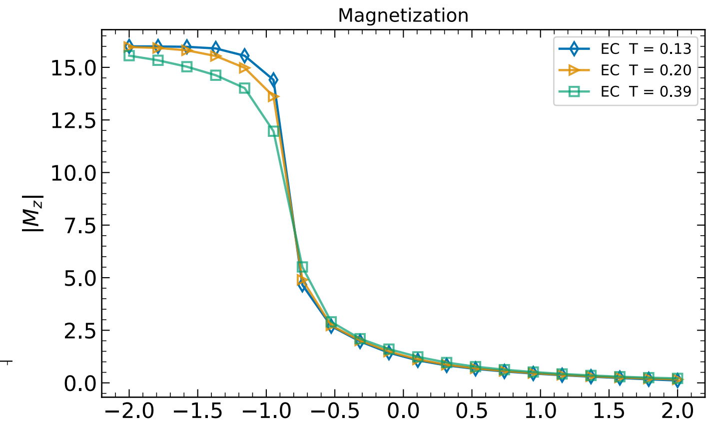


With relatively little computational effort, we can get thermal properties across the phase diagram

Results: Thermodynamics near phase transition for N=32







With relatively little computational effort, we can get thermal properties across the phase diagram even for large N

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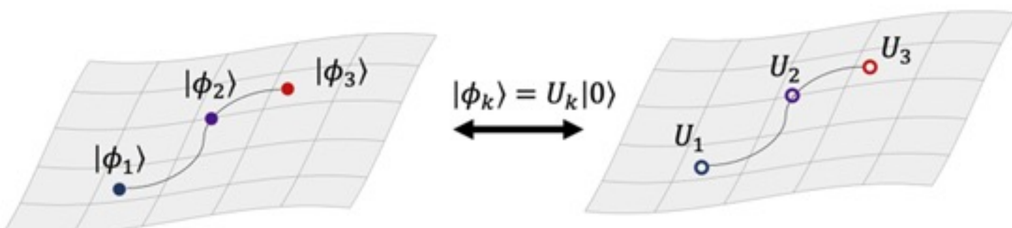
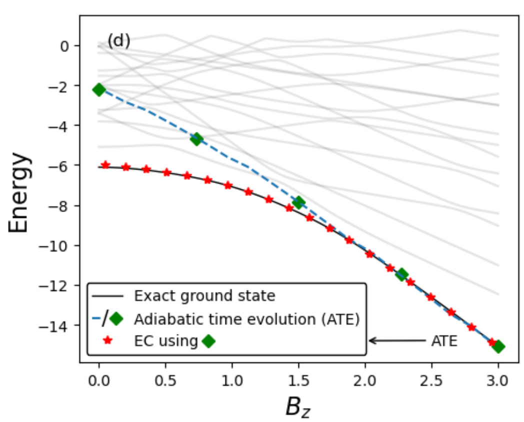
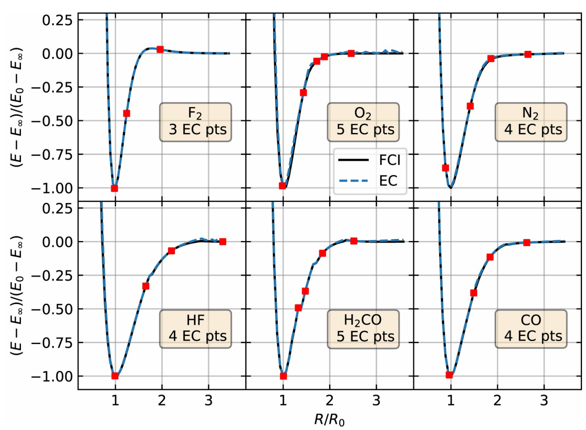
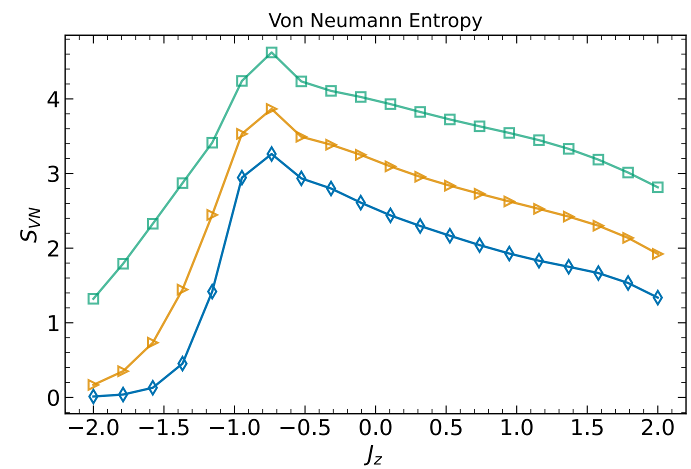
Eigenvector Continuation



Subspace methods can be readily added to many state preparation methods!







Agrawal, PRA (2025), [10.1103/PhysRevA.111.032607](https://doi.org/10.1103/PhysRevA.111.032607)