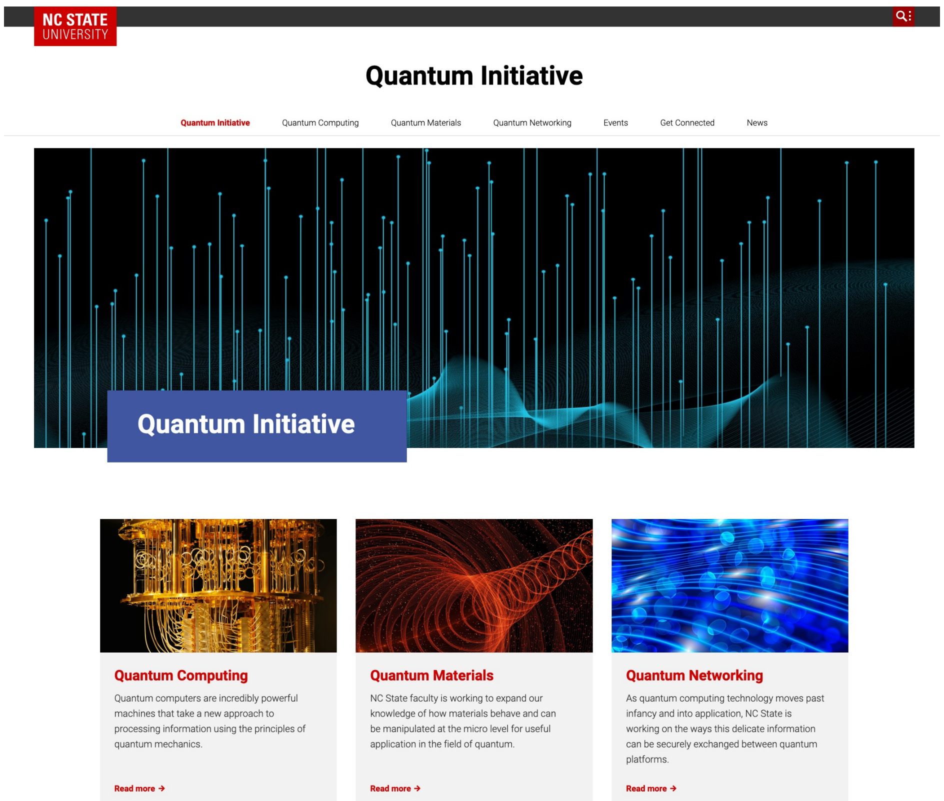
Quantum Information for Quantum Materials

Alexander (Lex) Kemper

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

Dirac Quantum Discussions @ FSU
02/25/2025



https://quantum.ncsu.edu/

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Quantum Computing
Algorithms
Error mitigation/correction
System software
Applications

Quantum Networking
Single-photon emitters/detectors
Distributed entanglement
Networking protocols
Distributed quantum computing

Education
Courses – within and across disciplines
Certificates, Degree programs
Seminars, Workshops, Conferences
Student engagement, clubs

Quantum Materials
Perovskites
Organic LEDs
Quantum dots
Novel superconductors

Industry Engagement
IBM QIC
SBIR/STTR
Short courses, invited speakers
QED-C

NC Quantum Institute

https://quantum.ncsu.edu/

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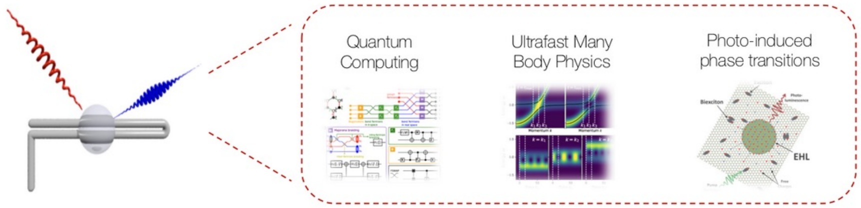


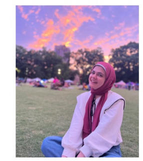
Kemper Lab

Quantum materials in and out of equilibrium.

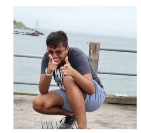
Current members


Alexander (Lex) Kemper
Principal investigator


Anjali Agrawal
Graduate Researcher


Heba Labib
Graduate Researcher


Norman Hogan
Graduate Researcher


Arvin Kushwaha
Undergraduate Researcher


Omar Alsheikh
Graduate Researcher


Goksu Toga
Postdoctoral Researcher

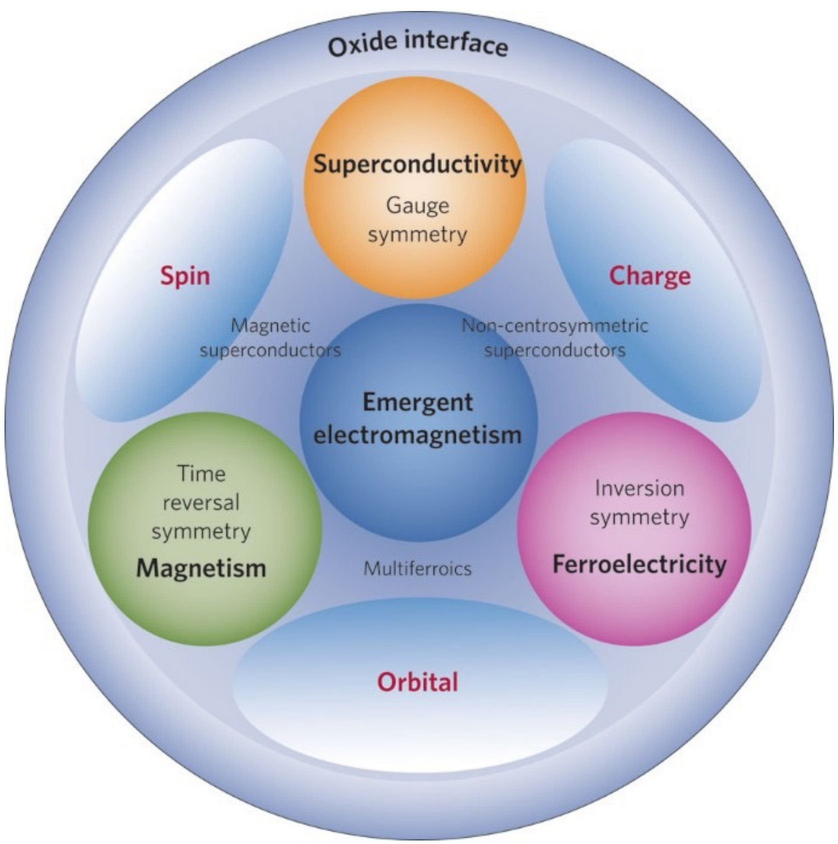

João C. Getelina
Postdoctoral Researcher


Your Name
New lab member

Collaborations with:

- Bojko Bakalov (NCSU Math)
- Marco Cerezo, Martin de la Rocca (LANL)
- Jim Freericks (Georgetown)
- Daan Camps, Roel van Beeumen, Bert de Jong, Akhil Francis (LBNL)
- Thomas Steckmann (UMD)
- Yan Wang, Eugene Dumitrescu (ORNL)
- Emanuel Gull (U. Michigan)
- Itay Hen (U. Southern California)

Quantum Information and Quantum Materials



H. Hwang, 10.1038/nmat3223

JoP D: Special Issue on Quantum Materials and Emerging Phenomena

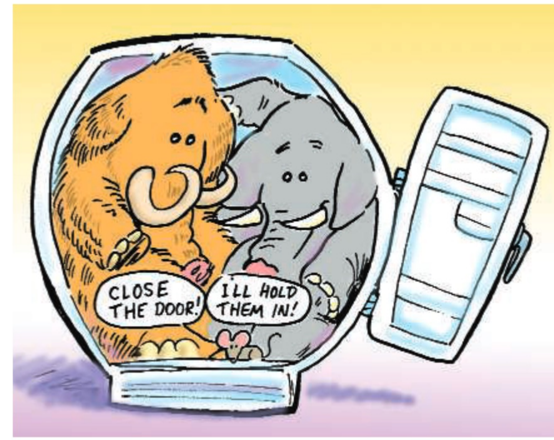
Quantum Information and Quantum Materials

PHYSICS

Is There Glue in Cuprate Superconductors?

Philip W. Anderson

Many theories about electron pairing in cuprate superconductors may be on the wrong track.



"We have a mammoth and an elephant in our refrigerator—do we care much if there is also a mouse?"

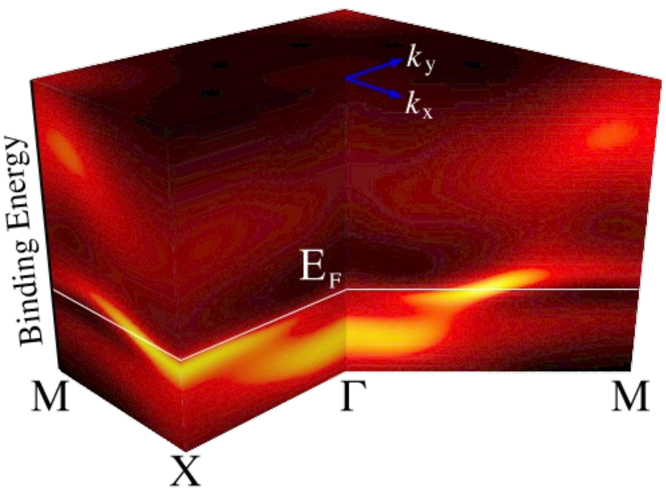
10.1126/science.1140970

Q: What do you do with a quantum state once you've prepared one?

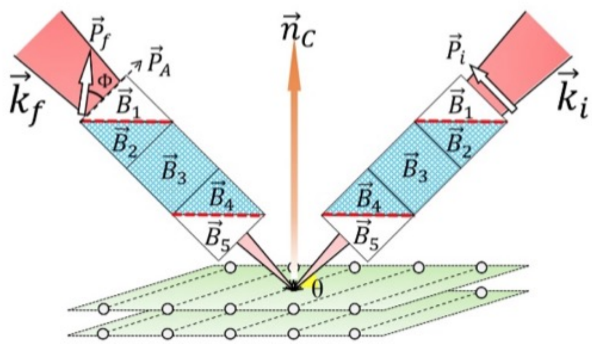
A: You measure its excitations.

Measuring Excitations

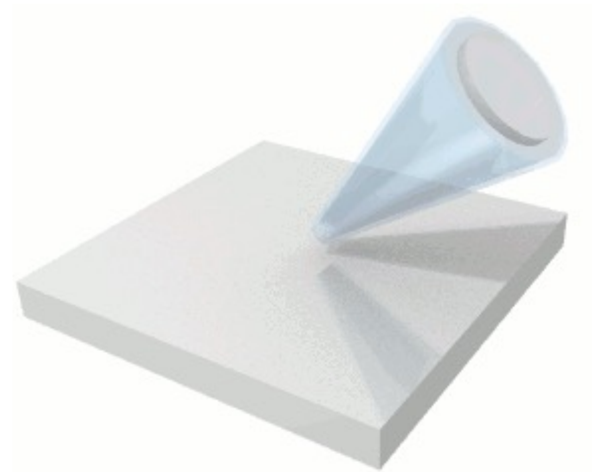
Figures courtesy of Devereaux/Shen group and ORNL



Angle-resolved Photoemission (ARPES)

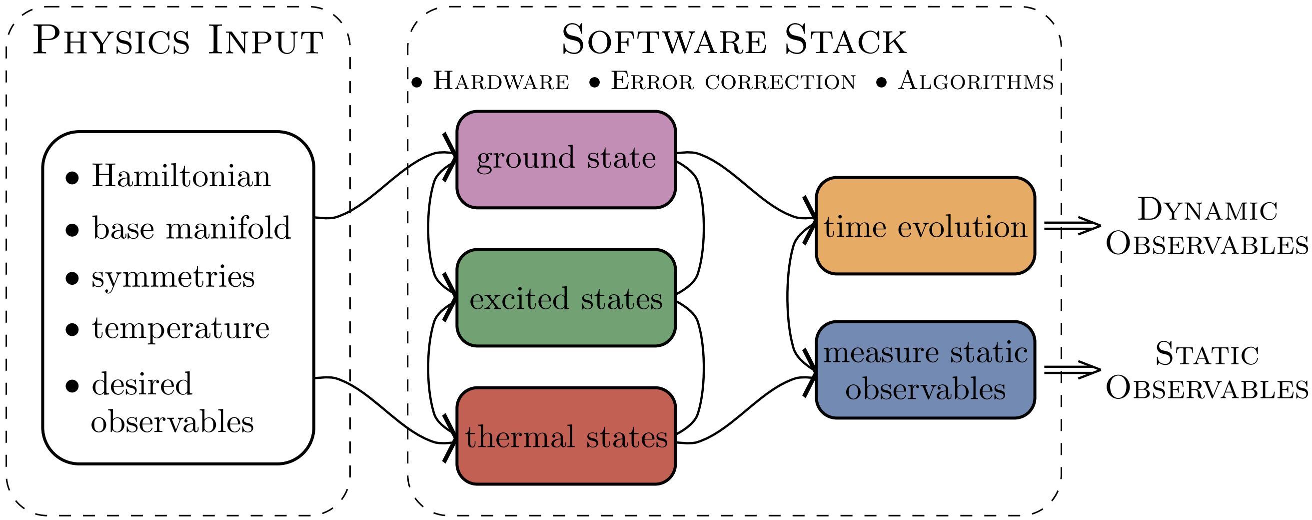


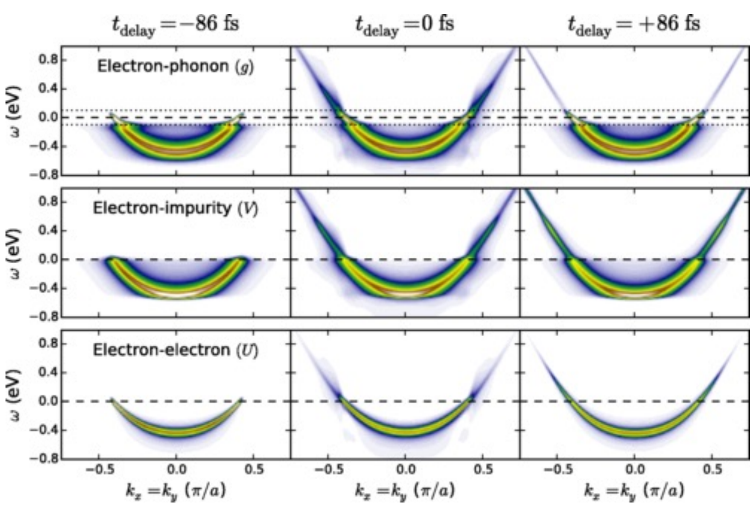
Neutron Scattering



Time-resolved ARPES

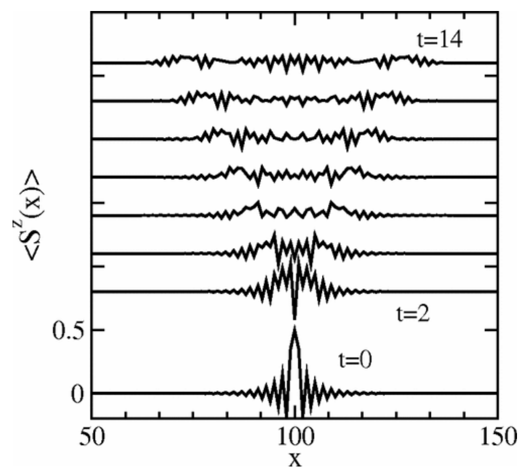
A-Z quantum simulation





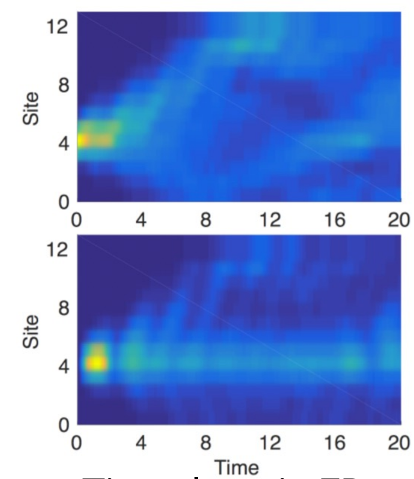
Non-Equilibrium Green's functions

Phys. Rev. X 8, 041009 (2018)



Time domain DMRG

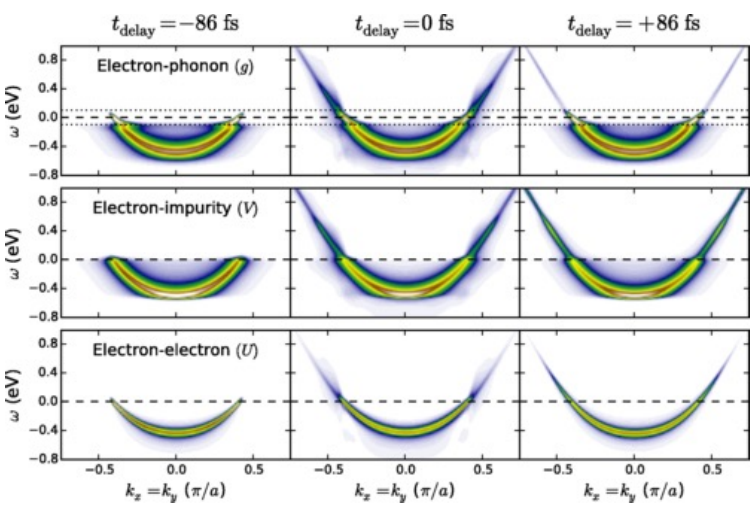
Phys. Rev. Lett. 93, 076401 (2004)



Time domain ED

Johnston & Kemper, unpublished

All these techniques eventually reach a barrier.



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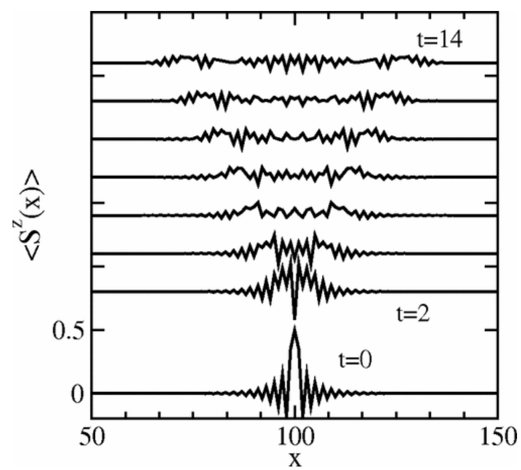

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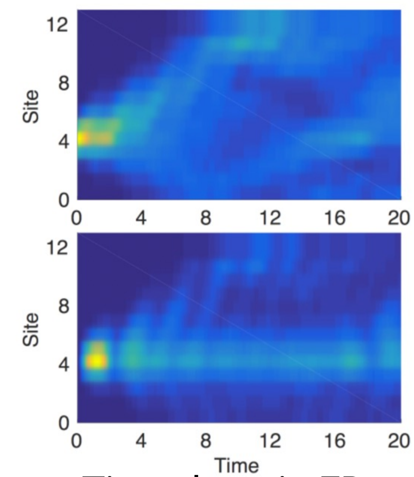

Time domain ED

Johnston & Kemper, unpublished

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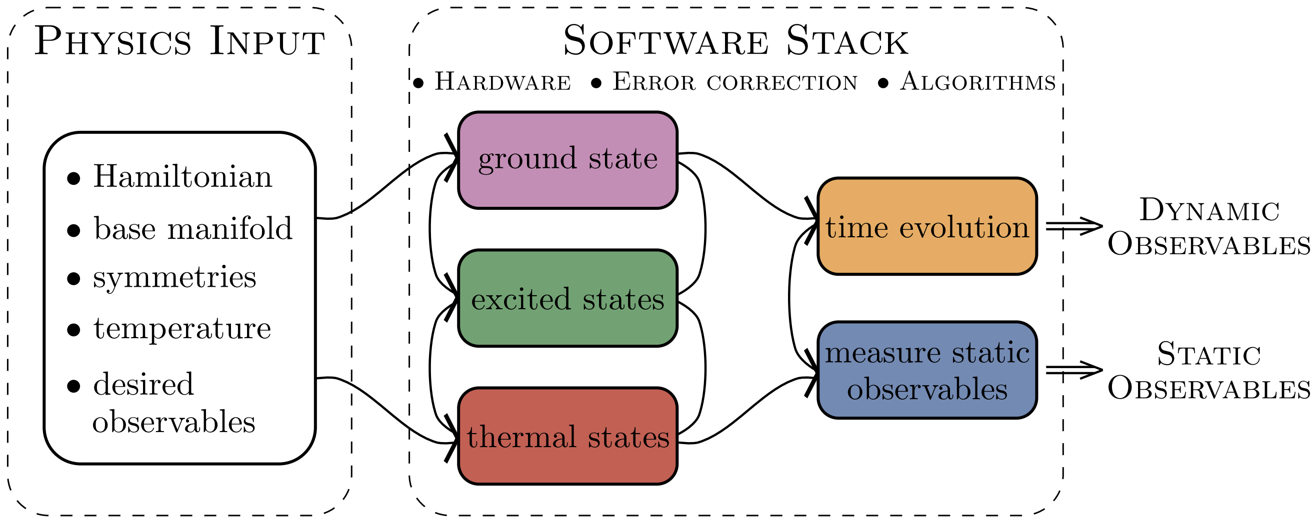
A-Z quantum simulation



Bespoke quantum simulator — *Digital algorithms*

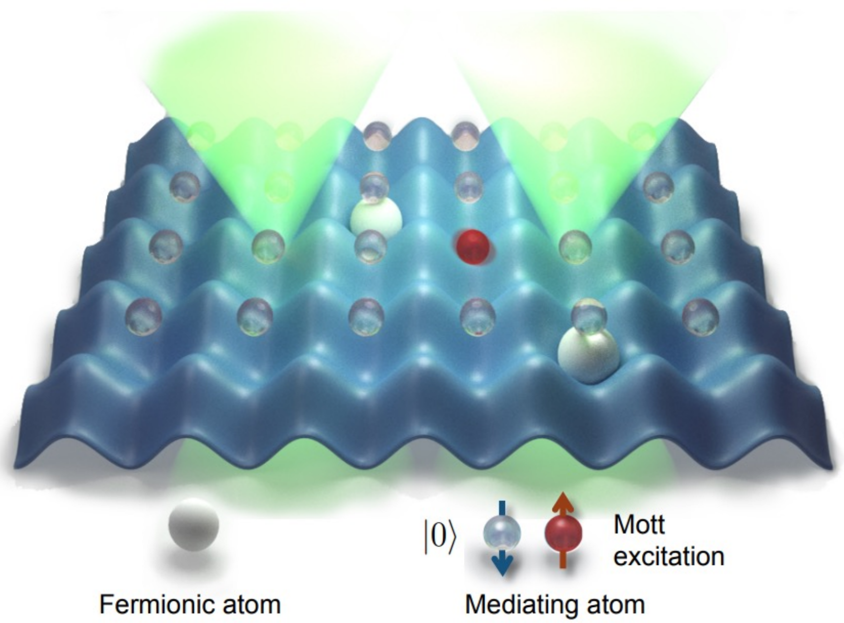
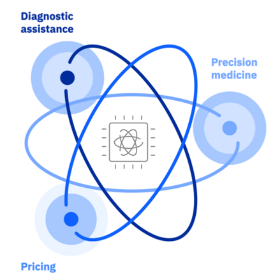
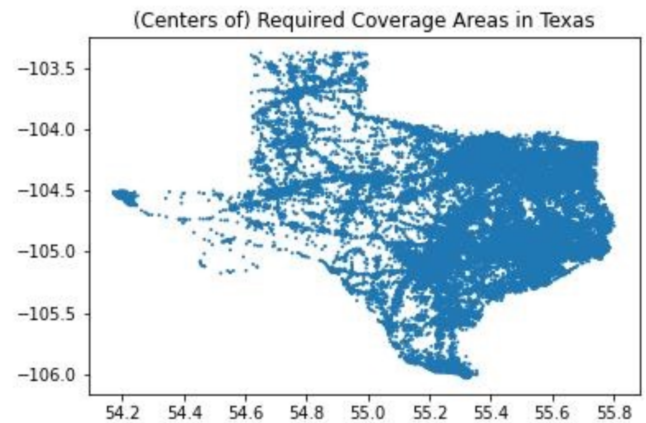
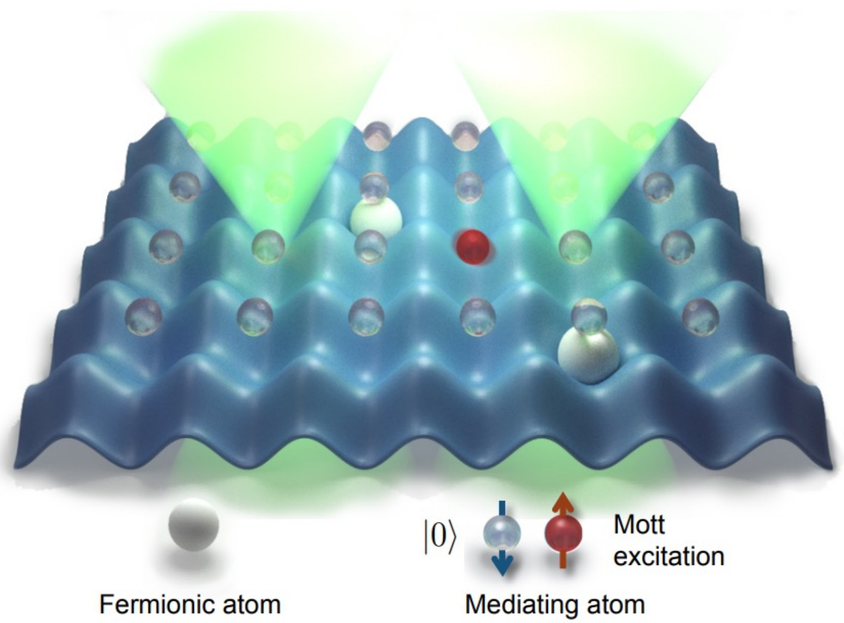


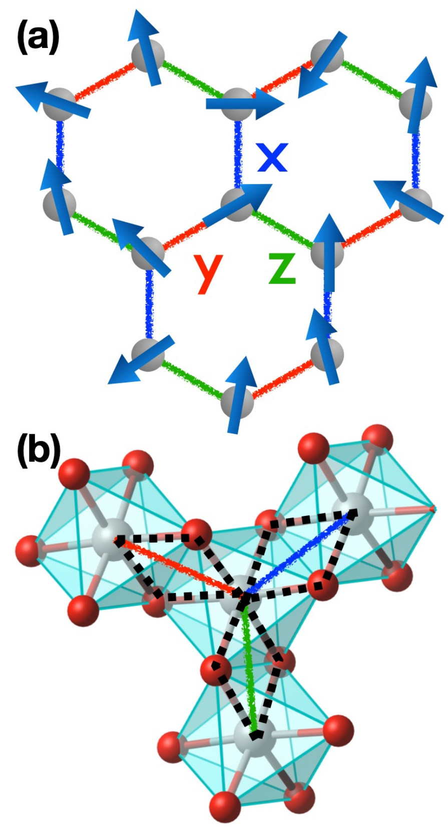
Figure 1
Quantum computers may enable three key healthcare use cases that reinforce each other in a virtuous cycle. For instance, accurate diagnoses enable precise treatments, as well as a better reflection of patient risks in pricing models.





Bespoke quantum simulator — *Digital algorithms*





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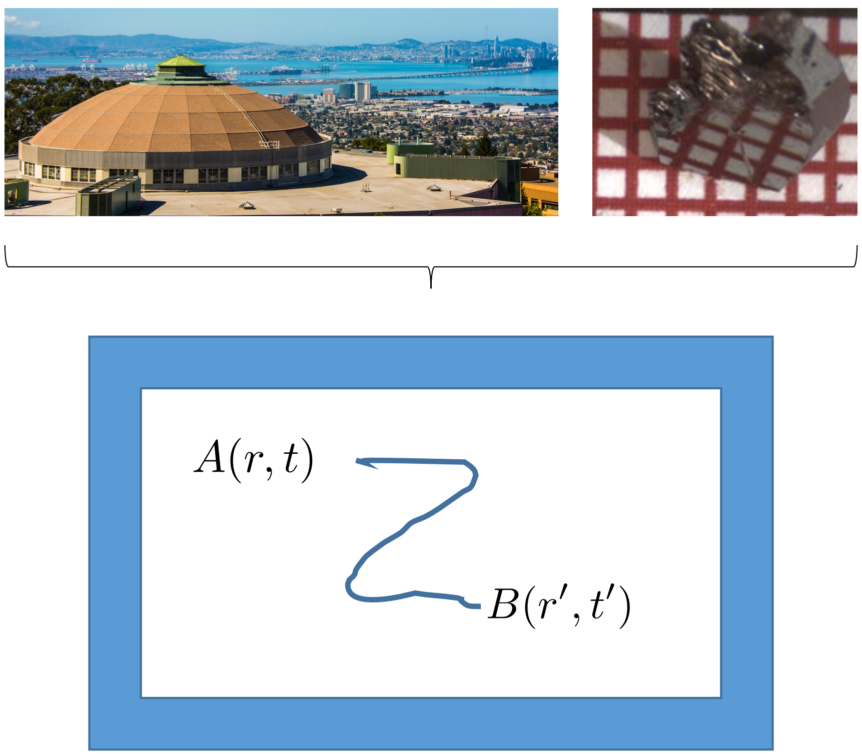
Correlation functions

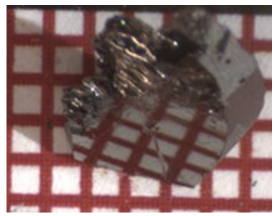


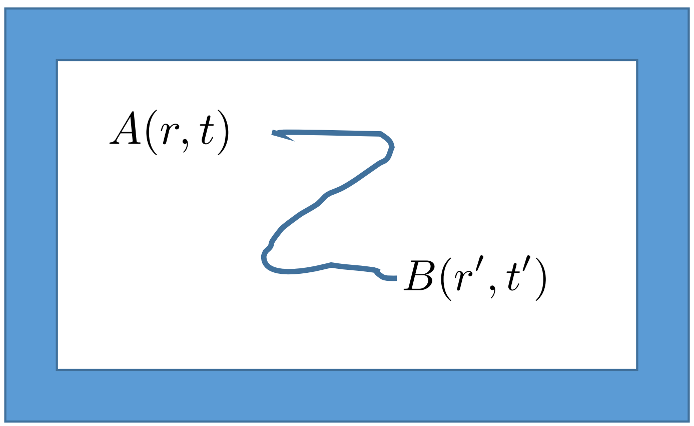
$$\langle A(r,t)B(r',t')\rangle$$

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

Optical conductivity, γ/X-ray scattering, photoemission, neutron scattering, Raman, IR absorption, etc.

Correlation functions





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

Interfere with ground state

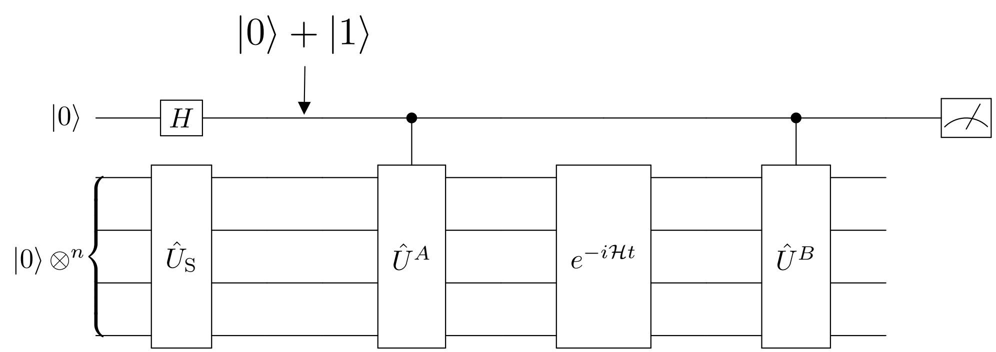
Complete expectation value

Apply excitation B

Time evolve

Apply excitation A

Prepare state of interest



Somma, Simulating physical phenomena by quantum networks (2002)

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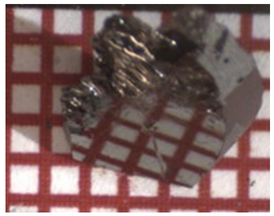
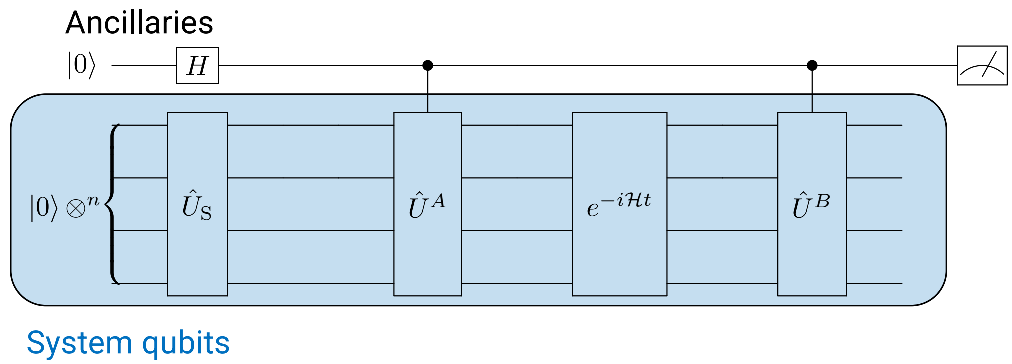
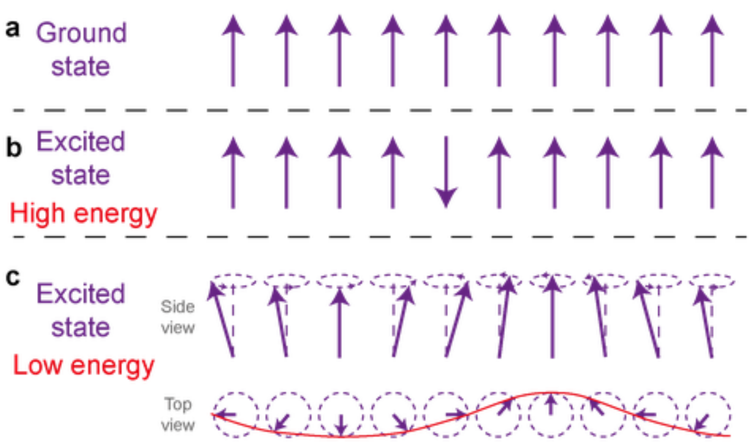
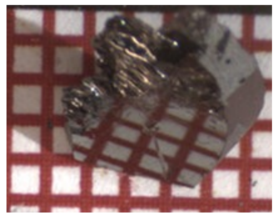
Correlation functions

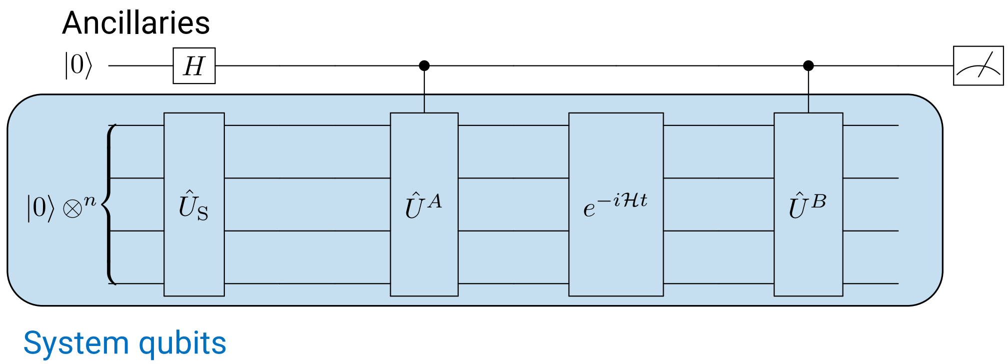




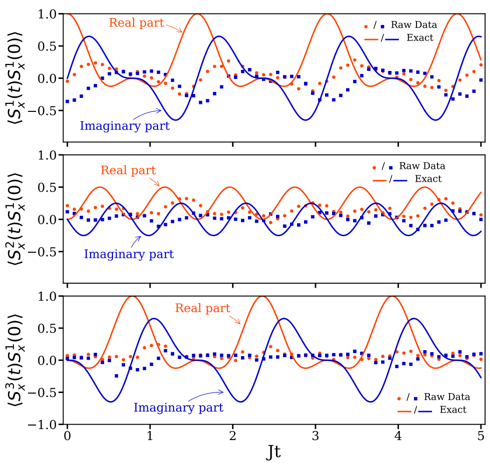


Correlation functions



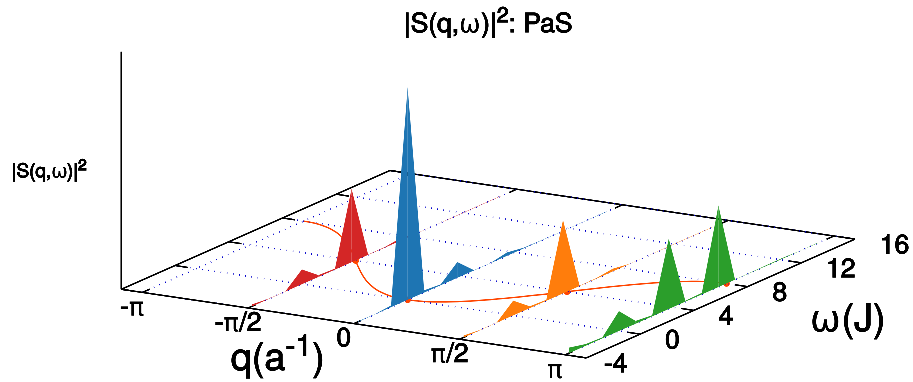


Raw data (2019)

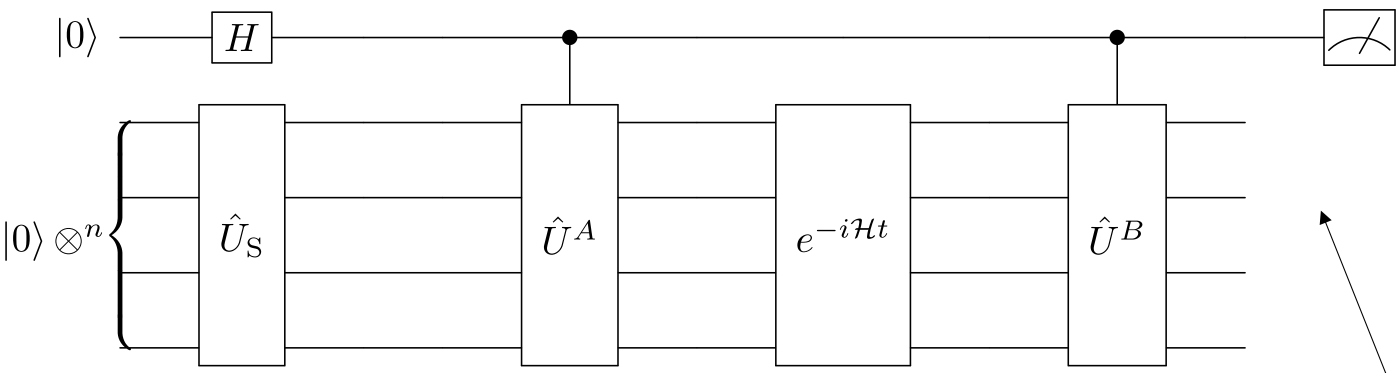


$$\langle A(r,t)B(r',t')\rangle$$

Error mitigation



A-Z quantum simulation



Classical post-processing techniques

Prepare state of interest

- *Physics-Informed Subspace Expansions*
- *Barren optimization plateaus*

Time evolve

- *Lie-algebraic methods for time evolution*
- *Open quantum system evolution*

Dynamical response functions

- *Correlation functions*
- *Open quantum system Green's functions*
- *Dynamical Mean Field Theory*

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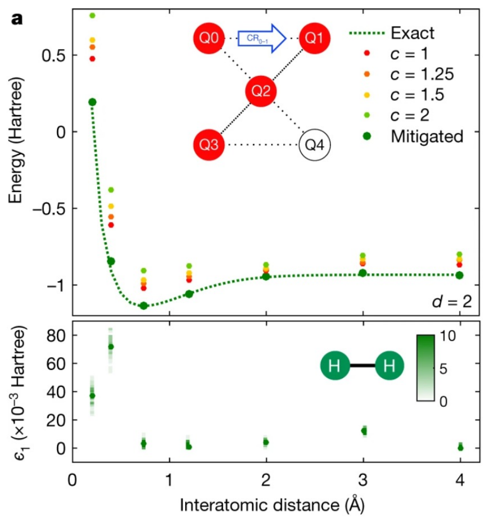
A-Z quantum simulation

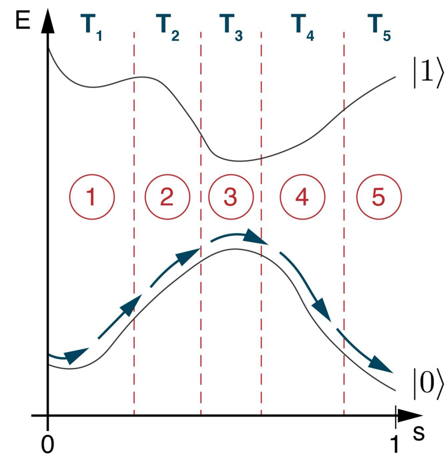
Variational Quantum Eigensolver



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

Barren Plateau

Adiabatic State Preparation



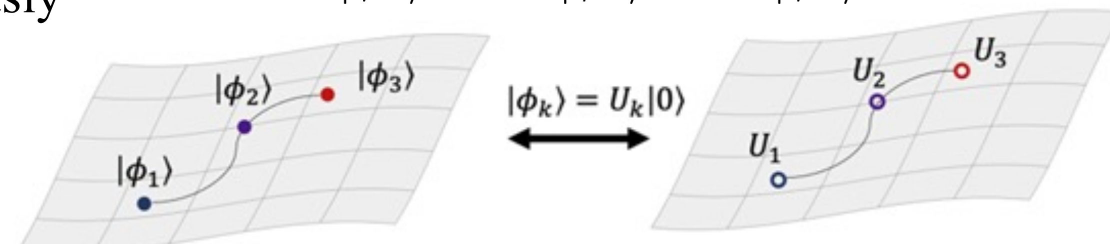
[Schiffer, Benjamin F., *et.al.*, *PRX Quantum* 3, no. 2 (2022): 020347]

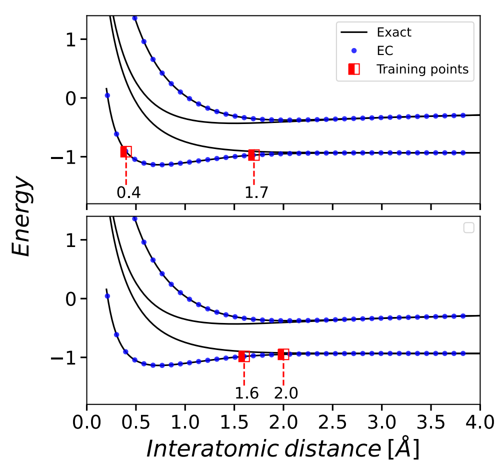
Larger depth circuits

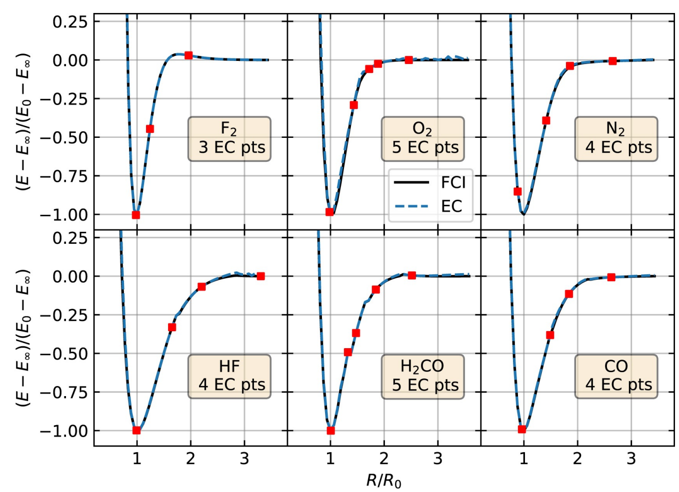
A-Z quantum simulation

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

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







arXiv:2209.10571

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

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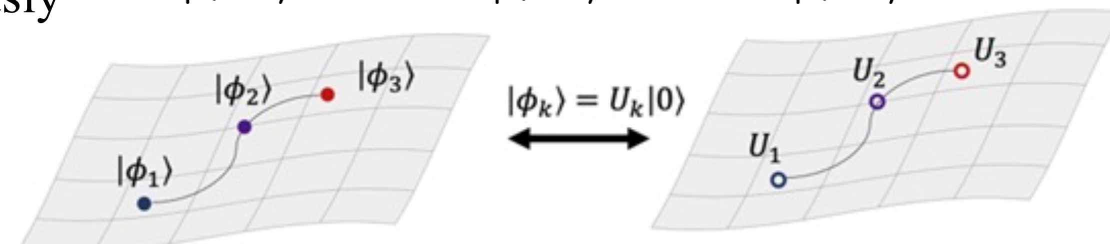
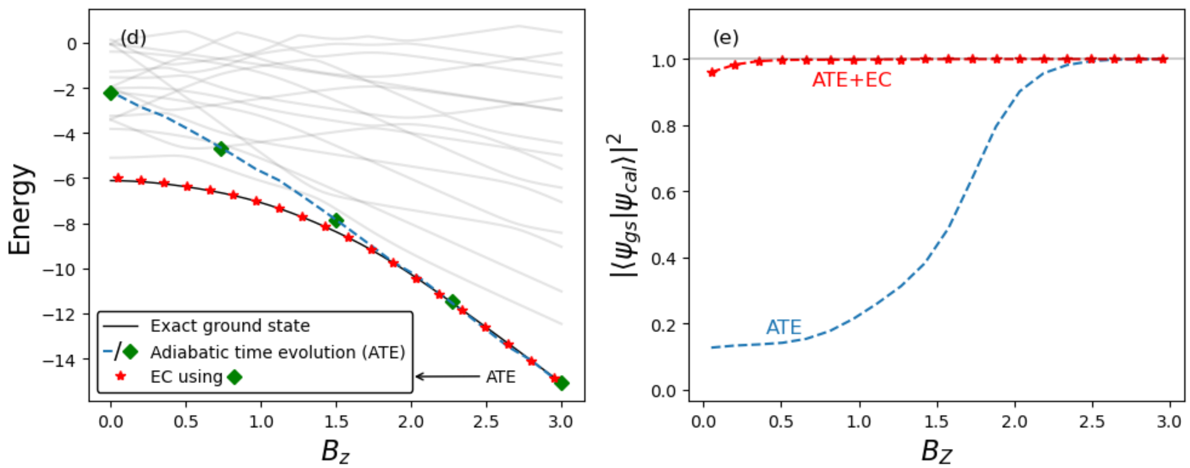
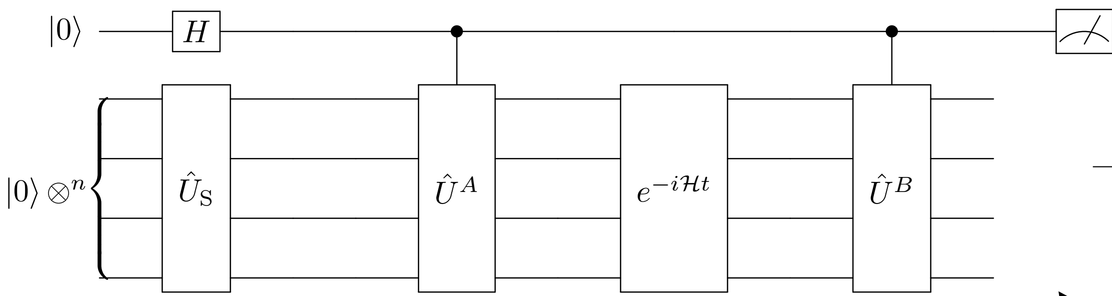




Agrawal, arXiv:2406.17037, to appear in PRB

A-Z quantum simulation



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Dynamical response functions

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Driven dissipative systems

PHYSICAL REVIEW B **102**, 125112 (2020)

Driven-dissipative quantum mechanics on a lattice: Simulating a fermionic reservoir on a quantum computer

Lorenzo Del Re,[1,2] Brian Rost,[1] A. F. Kemper,[3] and J. K. Freericks[1]

Why?

- The driven dissipative many-body system is one of the frontiers of quantum mechanics.
- New ultrafast pump/probe experiments and nonequilibrium ultracold atomic gases provide real data on these systems
- Theory on conventional computers remains restricted to short times only.

Driven dissipative systems

PHYSICAL REVIEW B **102**, 125112 (2020)

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Hamiltonian + Reservoir

$\Downarrow$

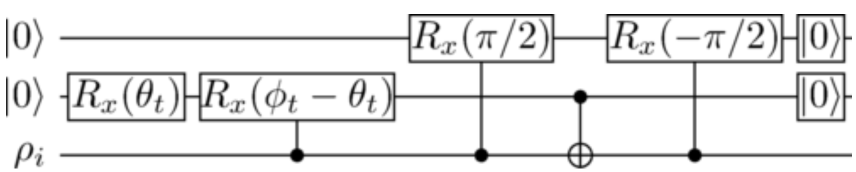
Master equation

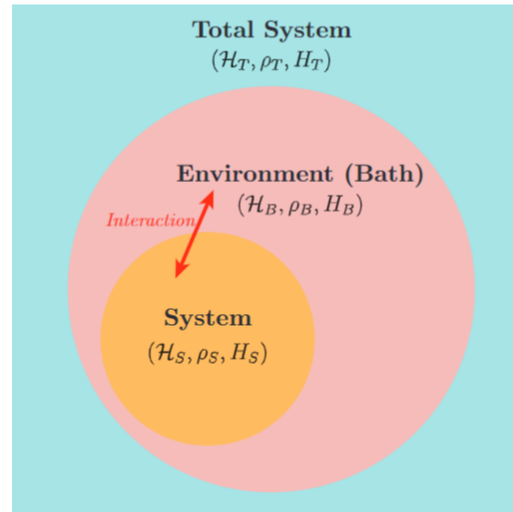
$\Downarrow$

Kraus map

$\Downarrow$

Quantum circuit





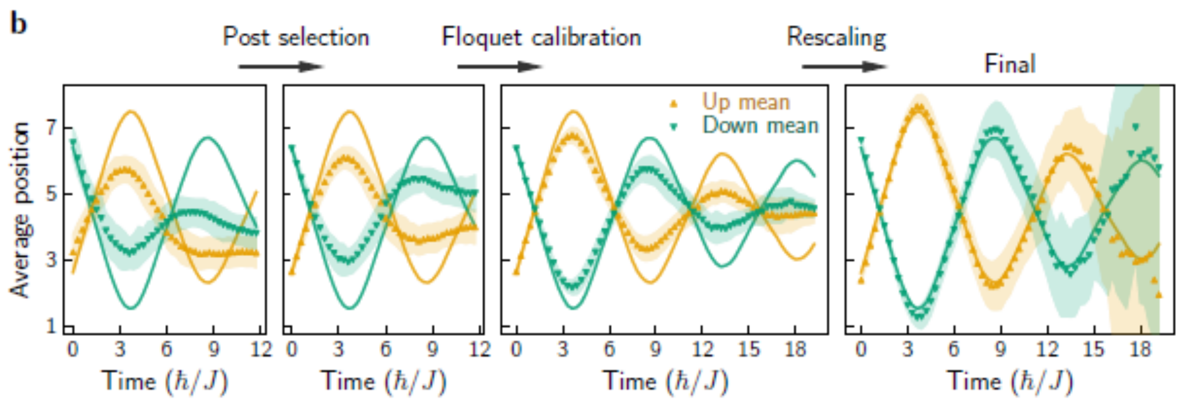
$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar}\left[\hat{H}, \hat{\rho}\right] + \sum_{i=x,y,z}\left(\hat{L}_i \hat{\rho} \hat{L}_i^\dagger - \frac{1}{2}\{\hat{L}_i^\dagger \hat{L}_i, \hat{\rho}\}\right),$$

$$\Phi(\rho) = \sum_i B_i \rho B_i^*.$$

Conventional time evolution (Trotter)

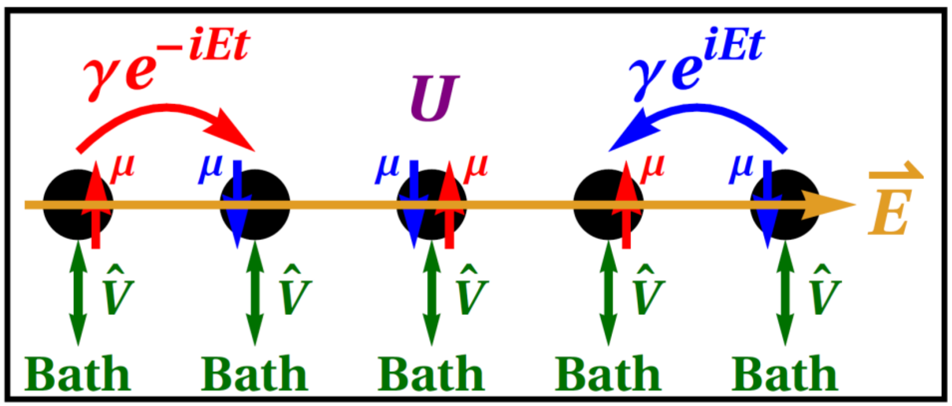
Observation of separated dynamics of charge and spin in the Fermi-Hubbard model

Google AI Quantum and collaborators*
(Dated: October 19, 2020)

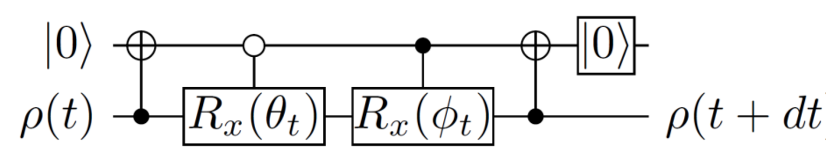


They achieve 55 Trotter steps, but the data starts to look bad after 25-30 steps
It requires significant error mitigation.

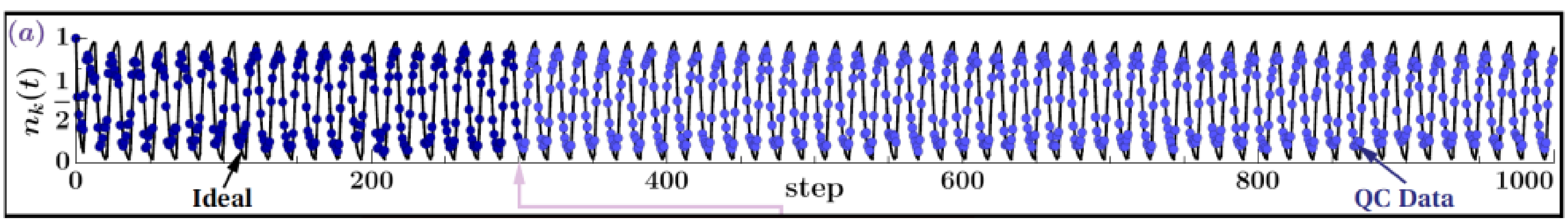
Driven-dissipative fermion model



Non-interacting limit, $U = \mu = 0$

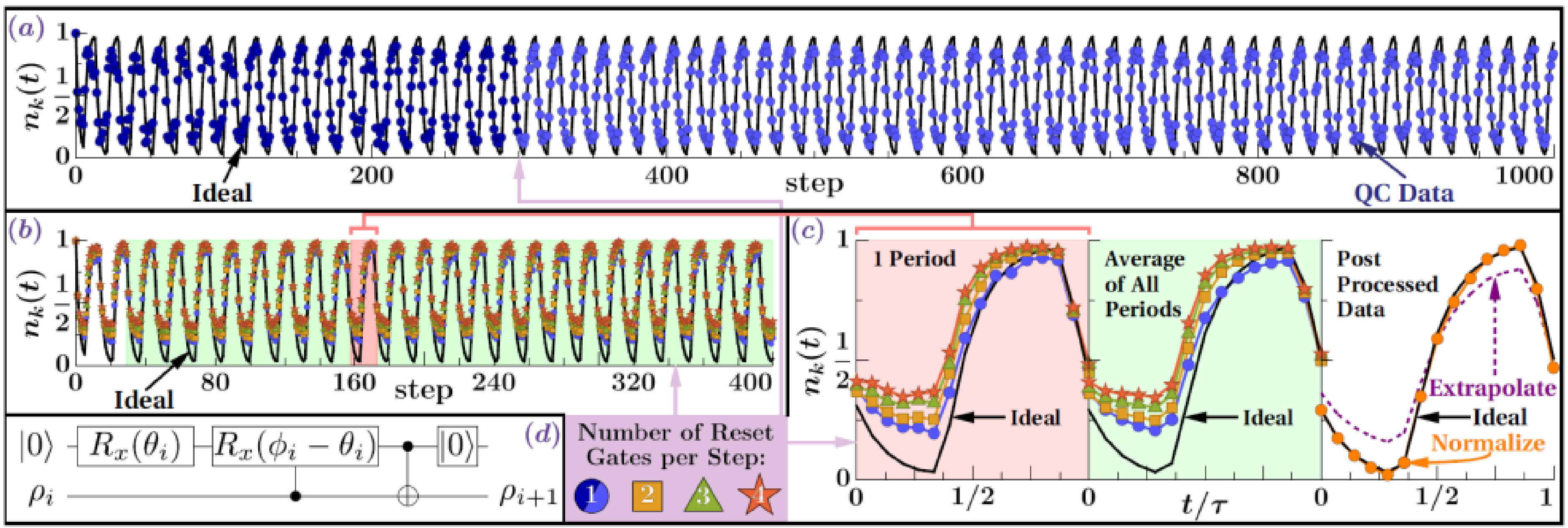


1. Kraus operators derived from master equation
2. System, bath details encoded in θ_t and ϕ_t
3. Time evolution done by iterating circuit
4. Density, current, energy, ...etc.



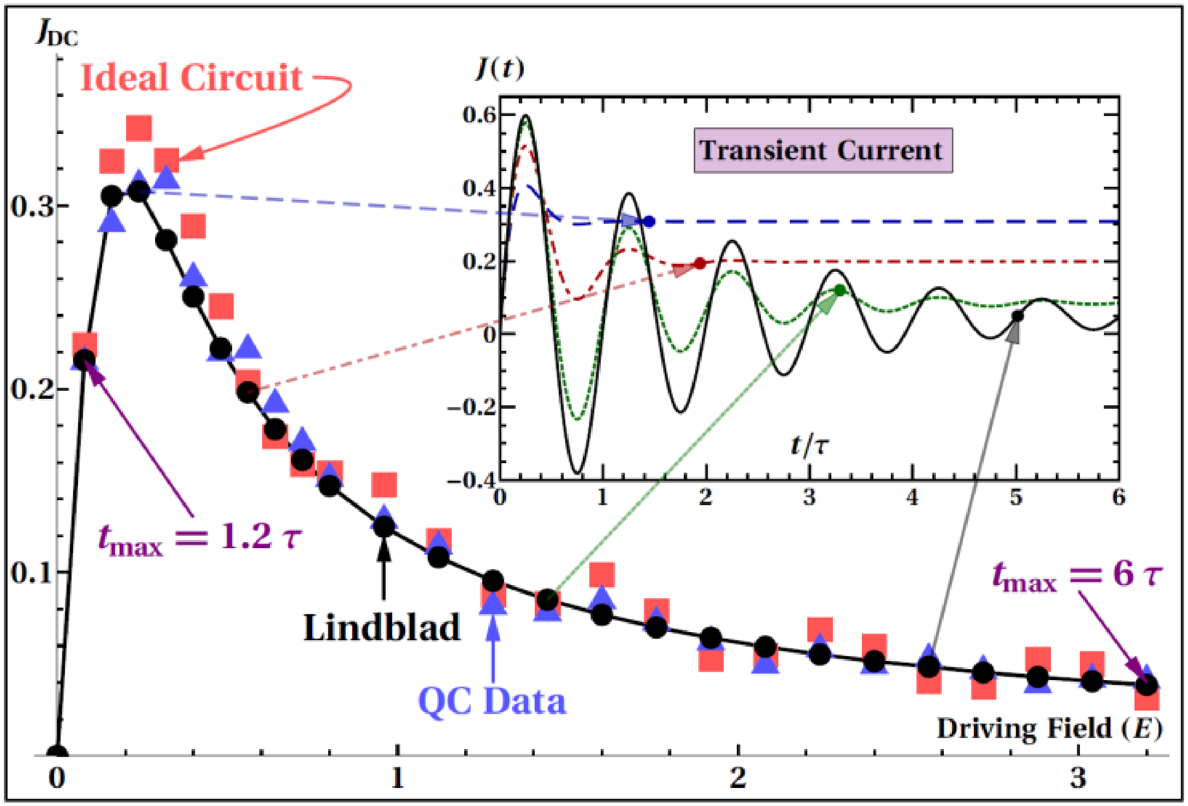
Rost, AFK, et al. NPJQI 2025

Results: density



Rost, AFK, et al. NPJQI 2025

Results: dc-current vs driving field



Rost, AFK, et al. NPJQI 2025

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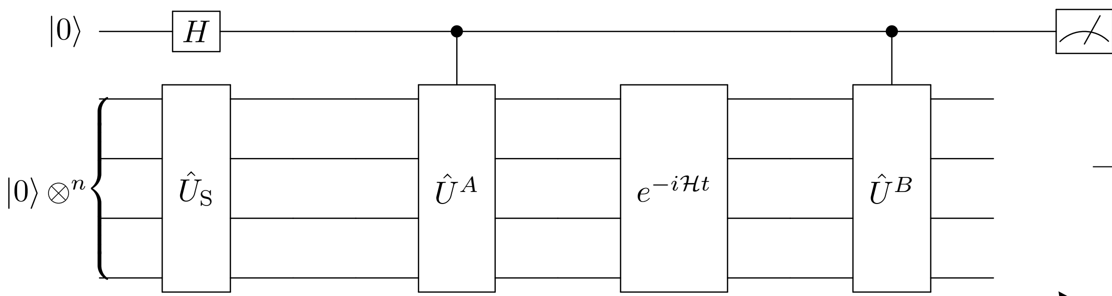
A-Z quantum simulation



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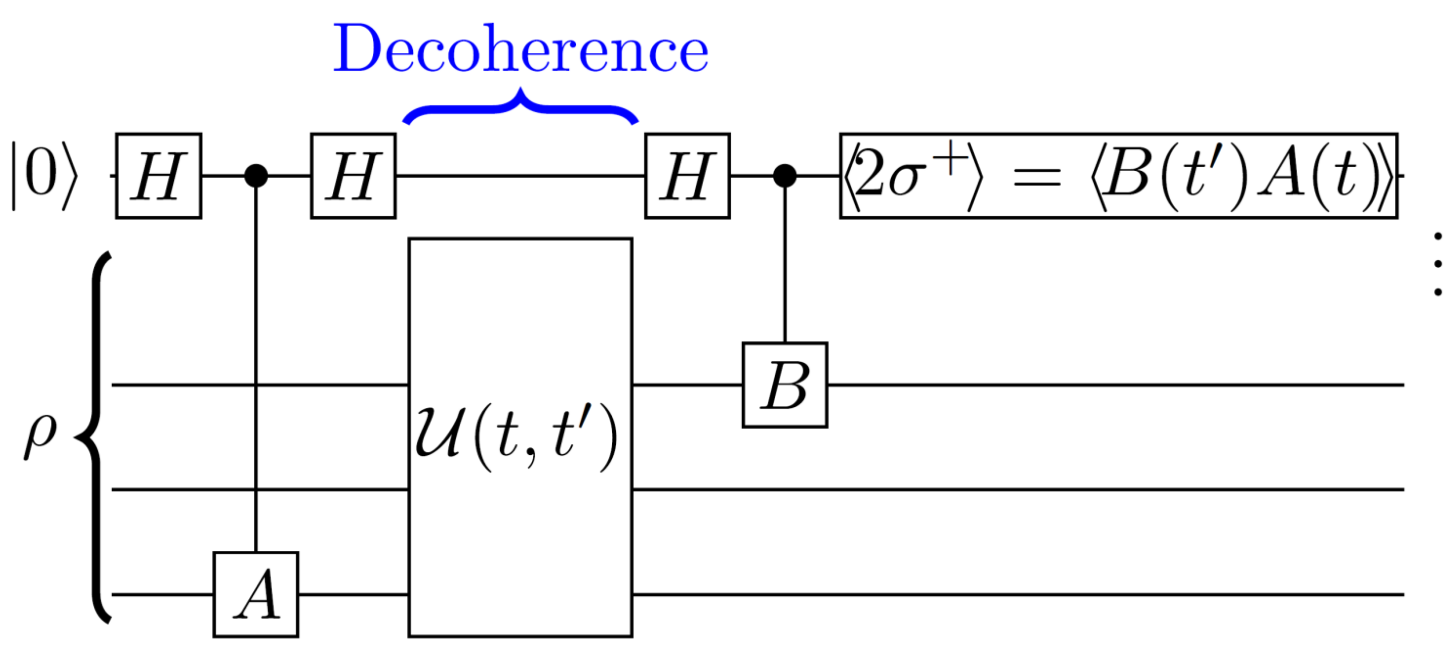
A-Z quantum simulation

Robust Measurements of *n*-Point Correlation Functions of Driven-Dissipative Quantum Systems on a Digital Quantum Computer

Lorenzo Del Re,[1,2] Brian Rost,[1] Michael Foss-Feig,[3] A. F. Kemper,[4] and J. K. Freericks[1]



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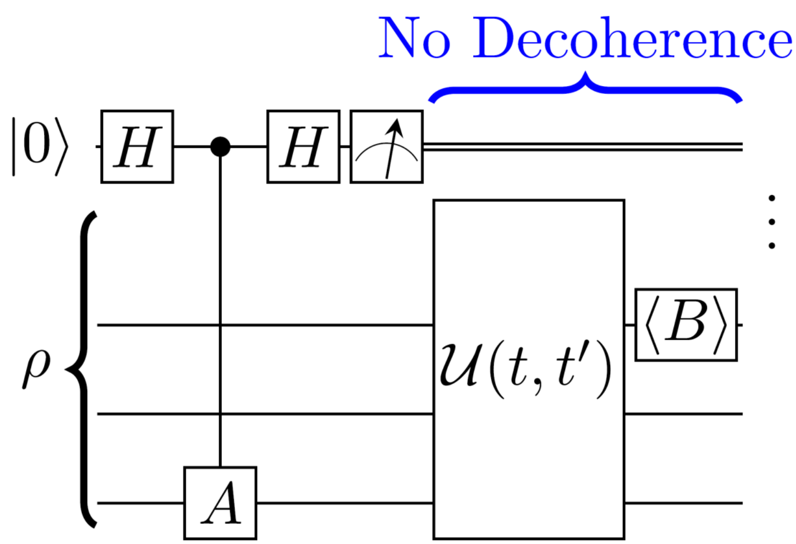
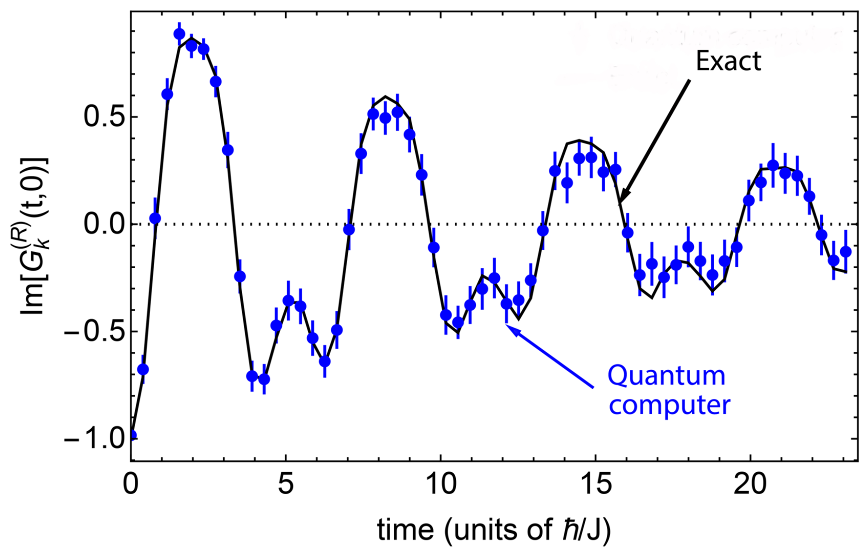
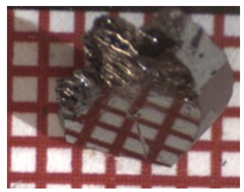
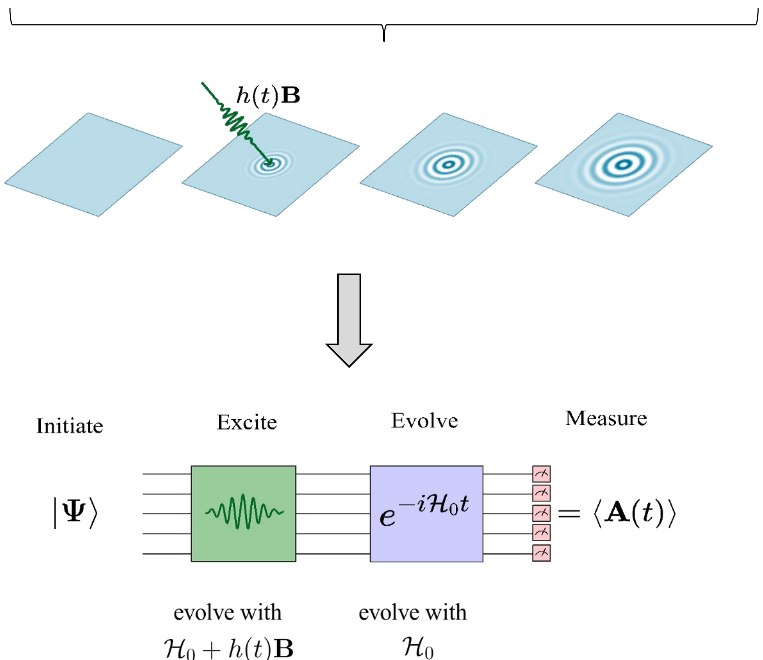




A-Z quantum simulation

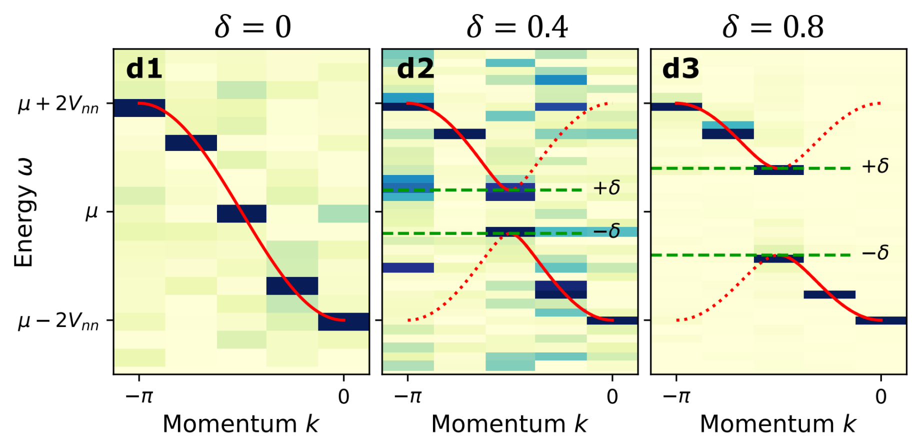




A linear response framework for simulating bosonic and fermionic correlation functions illustrated on quantum computers

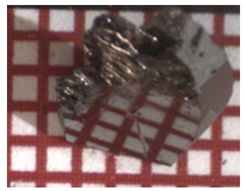
Efekan Kökcü,[1] Heba A. Labib,[1] J. K. Freericks,[2] and A. F. Kemper[1,*]
[1] *Department of Physics, North Carolina State University, Raleigh, North Carolina 27695, USA*
[2] *Department of Physics, Georgetown University, 37th and O Sts. NW, Washington, DC 20057 USA*
(Dated: February 22, 2023)

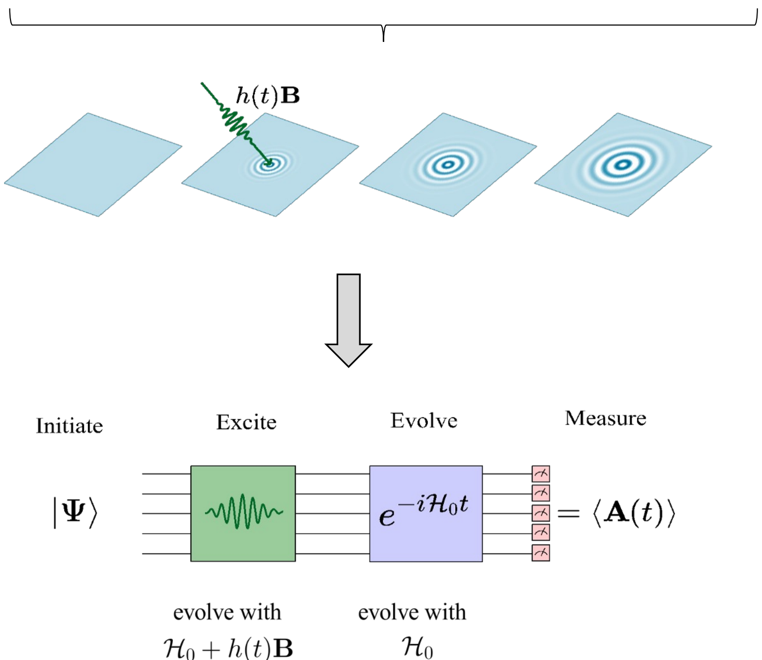
1. Make the excitation part of the quantum simulation
2. Post-process the data to get the response functions



Kökcü et al., Nat. Comm. 2024

A-Z quantum simulation





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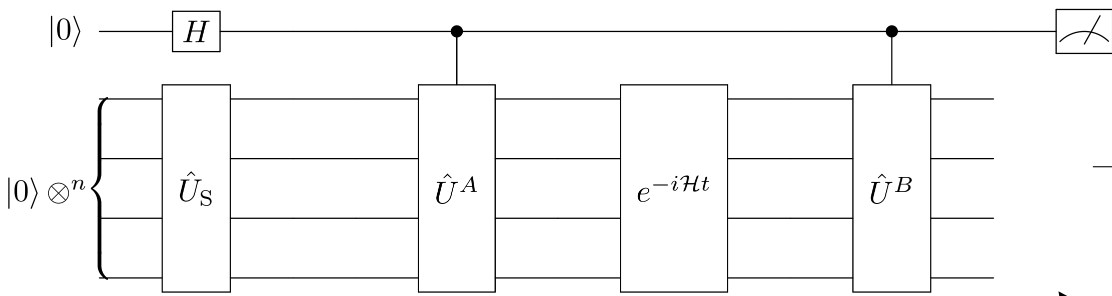
(Dated: February 22, 2023)

Benefits

- Any operator A,B you desire (as long as it is Hermitian*)
- No ancillas/controlled operations needed
- Many correlation functions at the same time
- Less post-processing (less noise)
- Frequency/momentum selective

Kökcü et al., Nat. Comm. 2024

A-Z quantum simulation



Classical post-processing techniques

Prepare state of interest

Time evolve

Dynamical response functions

- *Physics-Informed Subspace Expansions*
- *Barren optimization plateaus*

- *Lie-algebraic methods for time evolution*
- *Open quantum system evolution*

- *Correlation functions*
- *Open quantum system Green's functions*
- *Dynamical Mean Field Theory*

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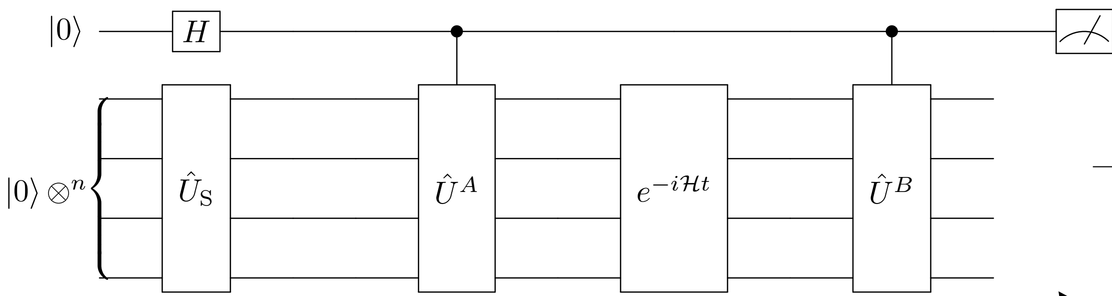
A-Z quantum simulation



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A-Z quantum simulation

$|0\rangle$

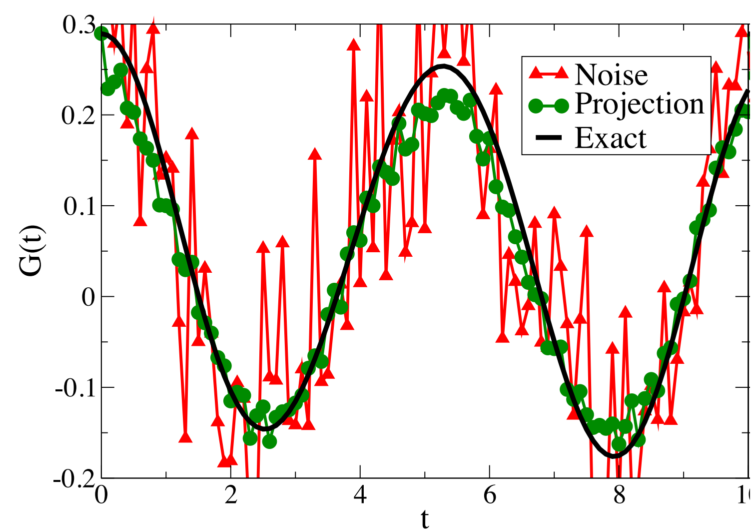
- It turns out that these are positive semi-definite (PSD) functions:

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

- 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 et al., PRL (2024)

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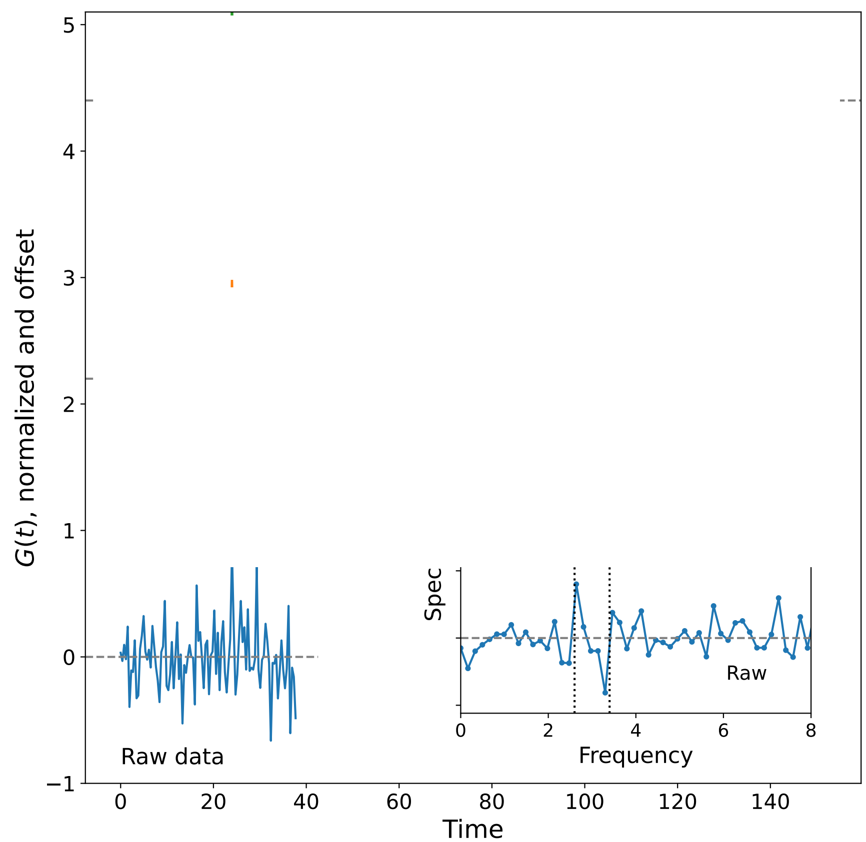

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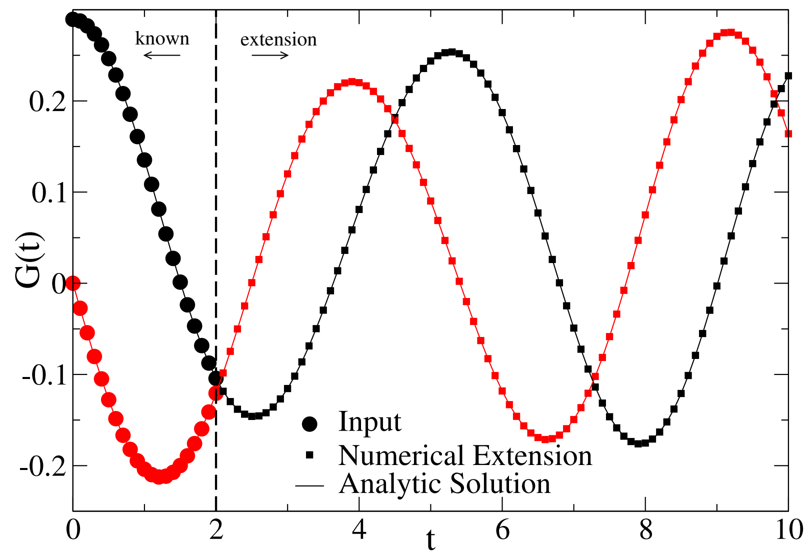

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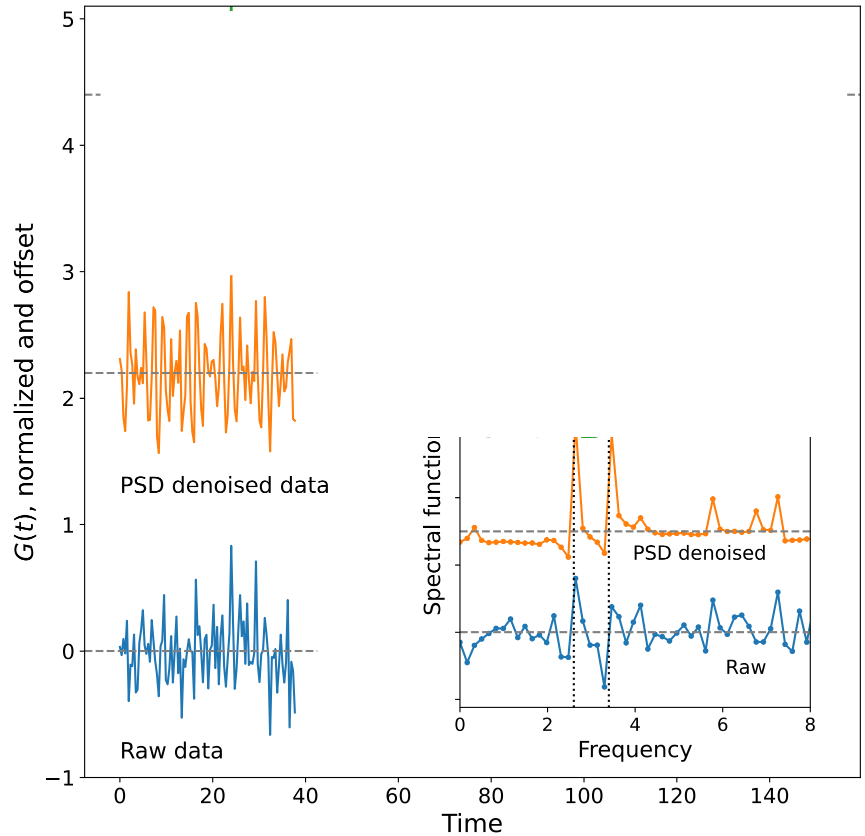

A.F. Kemper et al., PRL (2024)

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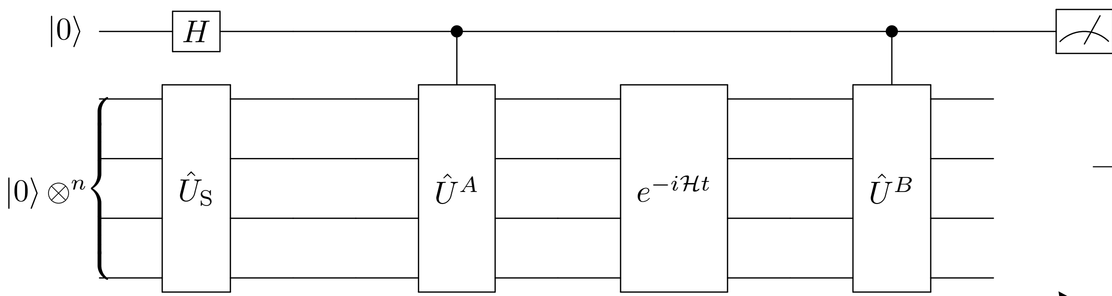

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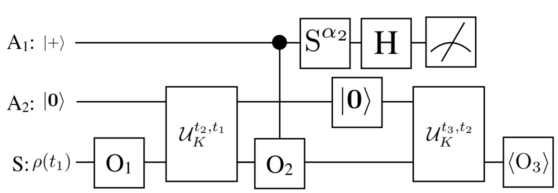
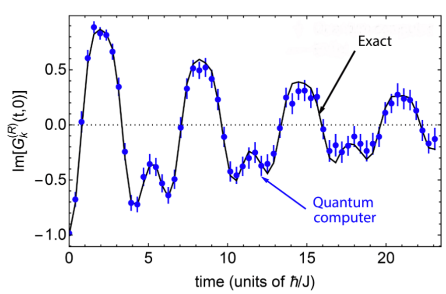
(A few) Quantum Algorithm(s) for correlation functions

Robust measurements of n-point correlation functions of driven-dissipative quantum systems on a digital quantum computer

Lorenzo Del Re,[1,2] Brian Rost,[1] Michael Foss-Feig,[3] A. F. Kemper,[4] and J. K. Freericks[1]
[1]*Department of Physics, Georgetown University, 37th and O Sts., NW, Washington, DC 20057, USA*
[2]*Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany*
[3]*Quantinuum, 303 S. Technology Ct, Broomfield, Colorado 80021, USA*
[4]*Department of Physics, North Carolina State University, Raleigh, North Carolina 27695, USA*
(Dated: April 27, 2022)





(Anti-)Commutators, open/dissipative

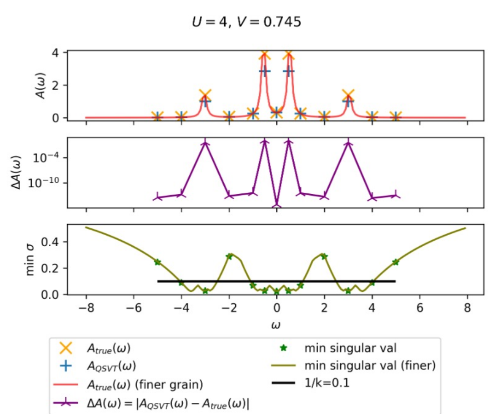
L. Del Re, B. Rost, M. Foss-Feig, AFK, J.K. Freericks
2204.12400

Quantum Computed Green's Functions using a Cumulant Expansion of the Lanczos Method

Gabriel Greene-Diniz,[1,*] David Zsolt Manrique,[1] Kentaro Yamamoto,[2] Evgeny Plekhanov,[1] Nathan Fitzpatrick,[1] Michal Krompiec,[1] Rei Sakuma,[3] and David Muñoz Ramo[1]
[1]*Quantinuum, Terrington House, 13-15 Hills Road, Cambridge CB2 1NL, UK*
[2]*Quantinuum K.K., Otemachi Financial City Grand Cube 3F, 1-9-2 Otemachi, Chiyoda-ku, Tokyo, Japan*
[3]*Materials Informatics Initiative, RD Technology & Digital Transformation Center, JSR Corporation, 3-103-9, Tonomachi, Kawasaki-ku, Kawasaki, 210-0821, Kanagawa, Japan.*
(Dated: September 19, 2023)

Calculating the Single-Particle Many-body Green's Functions via the Quantum Singular Value Transform Algorithm

Alexis Ralli,[1,2,*] Gabriel Greene-Diniz,[1] David Muñoz Ramo,[1] and Nathan Fitzpatrick[1,†]
[1]*Quantinuum 13-15 Hills Road, CB2 1NL Cambridge United Kingdom*
[2]*Centre for Computational Science Department of Chemistry, University College London, WC1H 0AJ United Kingdom*
(Dated: July 26, 2023)



PRL **111**, 147205 (2013) PHYSICAL REVIEW LETTERS week ending 4 OCTOBER 2013

Probing Real-Space and Time-Resolved Correlation Functions with Many-Body Ramsey Interferometry

Michael Knap,[1,2,*] Adrian Kantian,[3] Thierry Giamarchi,[3] Immanuel Bloch,[4,5] Mikhail D. Lukin,[1] and Eugene Demler[1]
[1]*Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA*
[2]*ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138, USA*
[3]*DPMC-MaNEP, University of Geneva, 24 Quai Ernest-Ansermet CH-1211 Geneva, Switzerland*
[4]*Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, 85748 Garching, Germany*
[5]*Fakultät für Physik, Ludwig-Maximilians-Universität München, 80799 München, Germany*
(Received 2 July 2013; revised manuscript received 18 September 2013; published 4 October 2013)

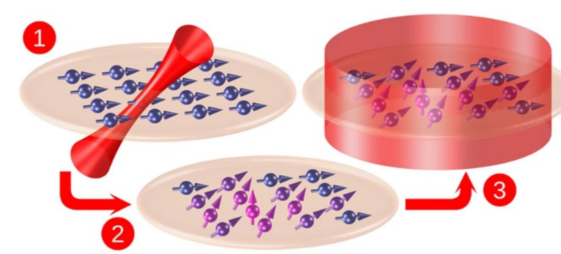


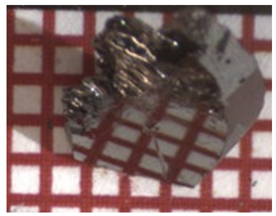
FIG. 1 (color online). Many-body Ramsey interferometry consists of the following steps: (1) A spin system prepared in its ground state is locally excited by $\pi/2$ rotation; (2) the system evolves in time; (3) a global $\pi/2$ rotation is applied, followed by the measurement of the spin state. This protocol provides the dynamic many-body Green's function.

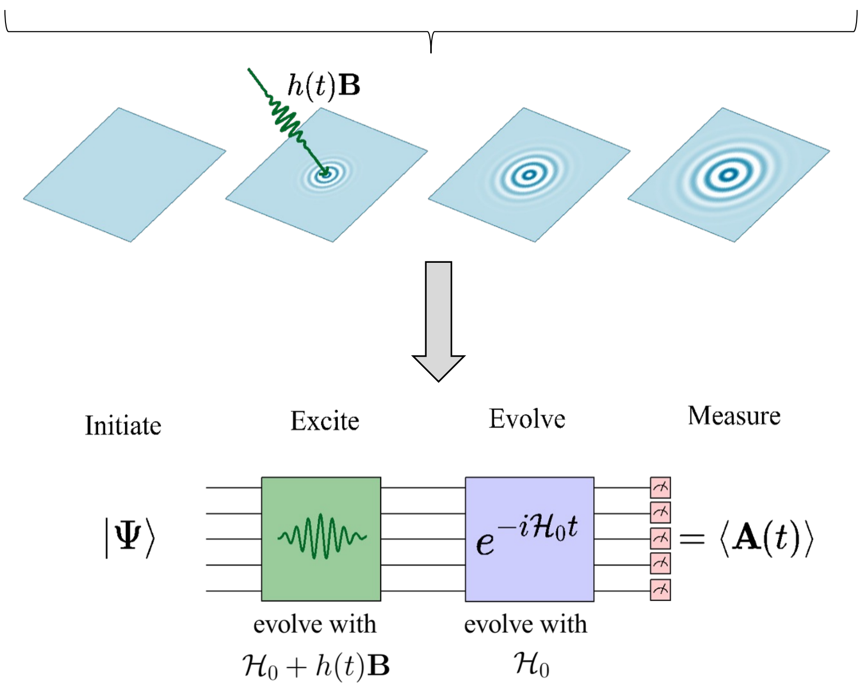
Commutators

10.1103/PhysRevLett.111.147205

Linear Response

Kokcu, Nat Comm 2024





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(Dated: February 22, 2023)

1. Make the excitation part of the quantum simulation

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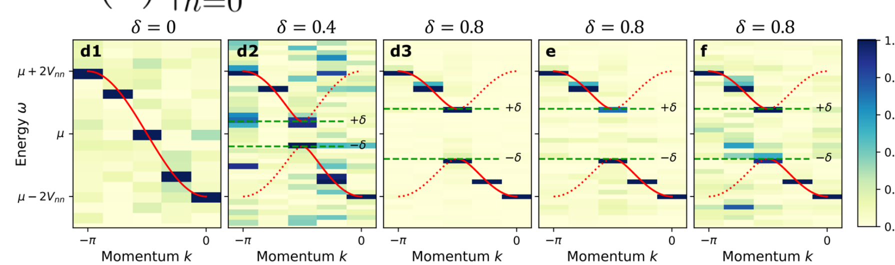
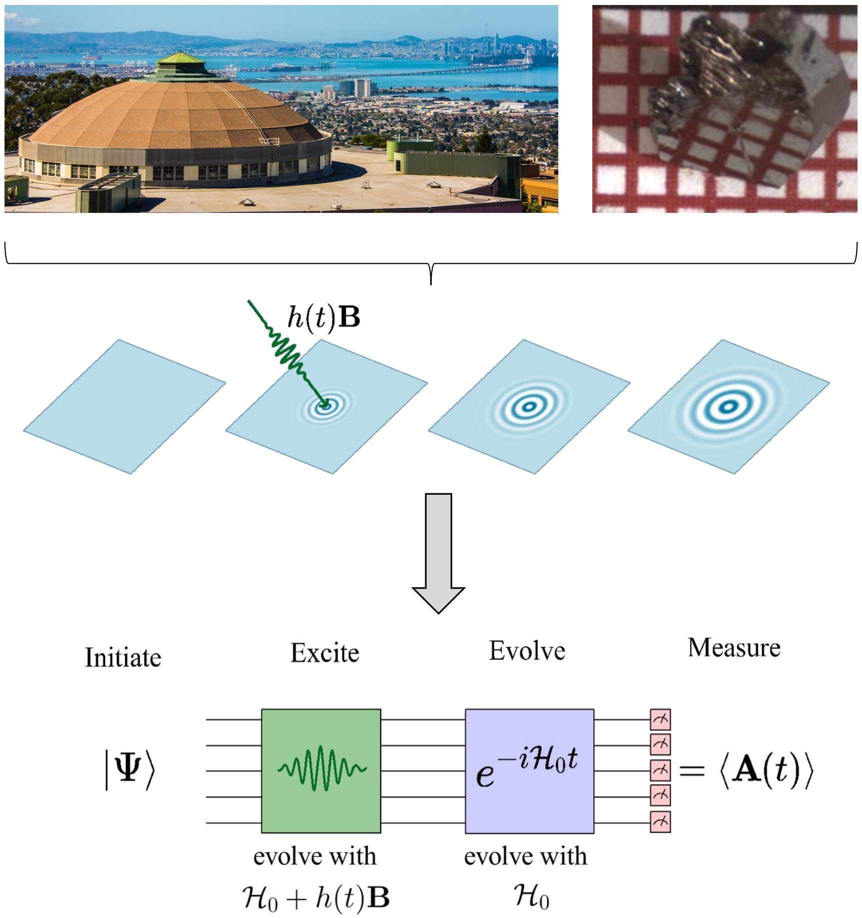
$$\left.\frac{\delta A(t)}{\delta h(t')}\right|_{h=0} = -i\theta(t-t')\langle\psi_0|[\mathbf{A}(t), \mathbf{B}(t')]|\psi_0\rangle$$



Linear Response

Kokcu, Nat Comm 2024



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- Any operator A,B you desire (as long as it is Hermitian*)
- No ancillas/controlled operations needed
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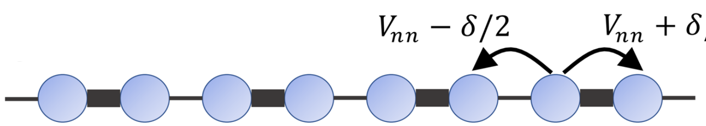
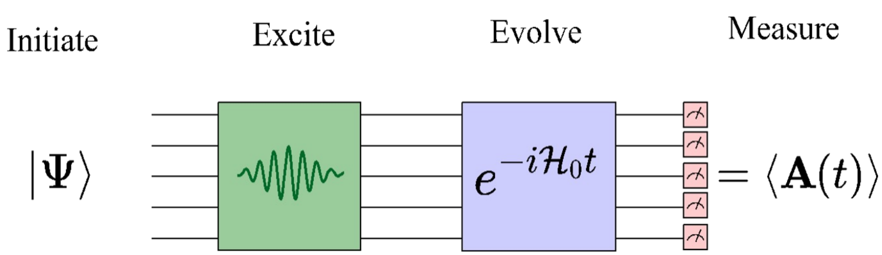
Linear Response -> Green's function

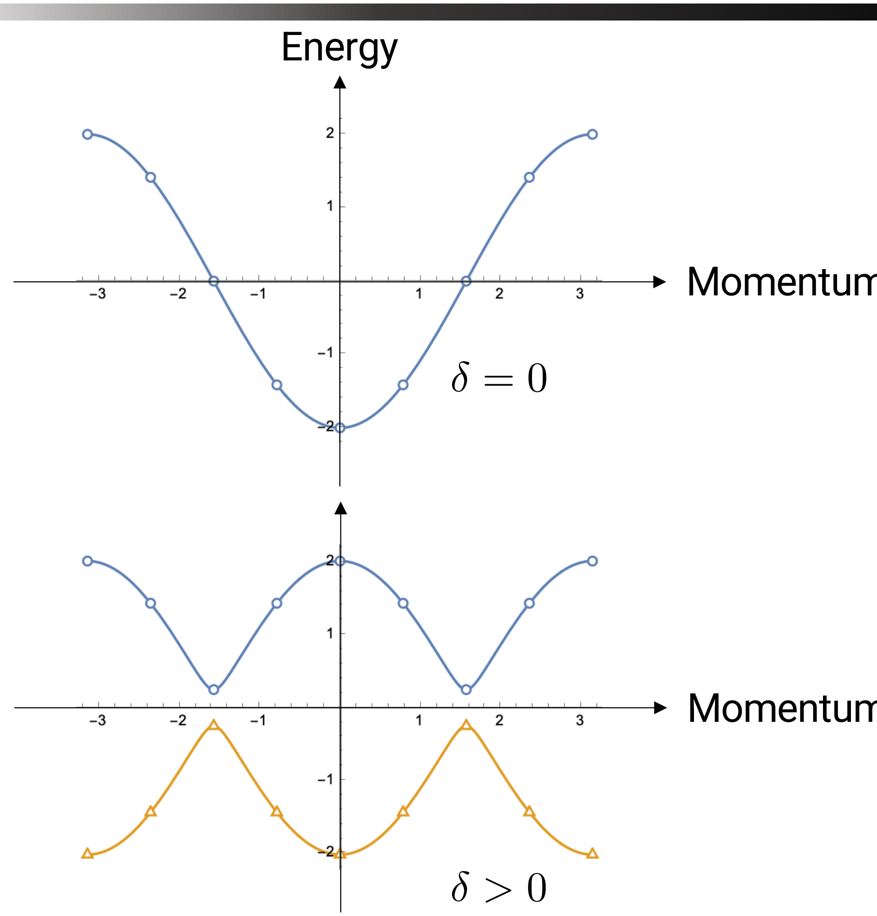
Su-Schrieffer-Heeger model for polyacetylene



$$\mathcal{H}_0 = -\sum_{\langle i,j \rangle} \left[V_{nn} + (-1)^i \, \delta/2 \right] c_i^\dagger c_j - \mu \sum_i c_i^\dagger c_i$$



$$G^R(r_i, t; r_j, t') = -i\theta(t - t') \, \langle \psi_0 | \{ c_i(t), c_j^\dagger(t') \} | \psi_0 \rangle$$



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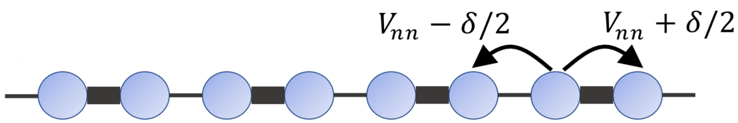

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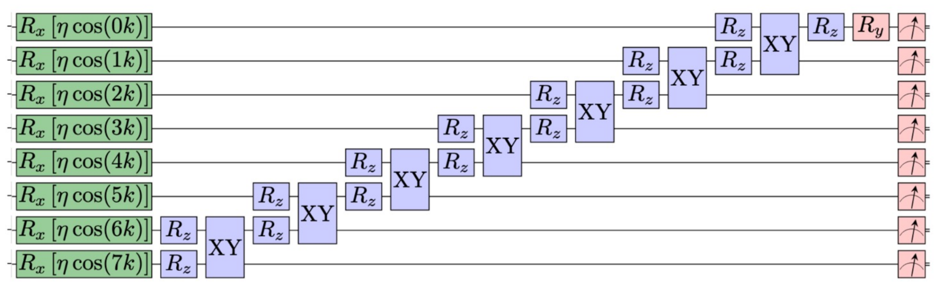
Compressed circuit run on *ibm_auckland*



$$\mathbf{B} = \sum_i 2\cos(kr_i) \left[c_i + c_i^\dagger \right]$$

Choose **B** to create a momentum eigenstate

$$G_k^R(t) = -i\theta(t) \langle \psi_0 | \{ c_k(t), c_k^\dagger(0) \} | \psi_0 \rangle$$

Linear Response -> Green's function

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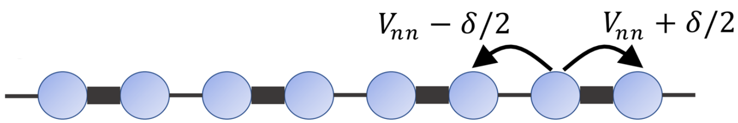

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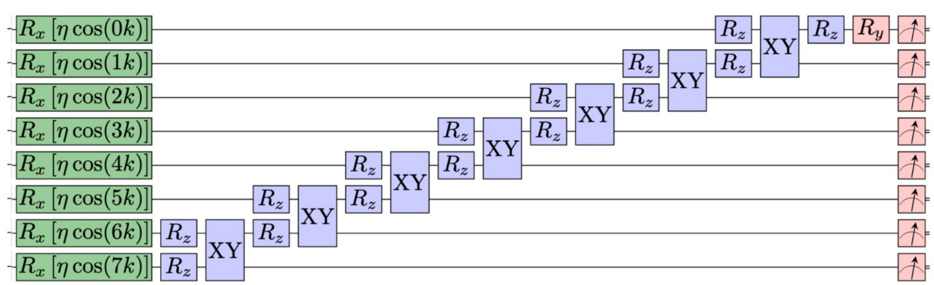

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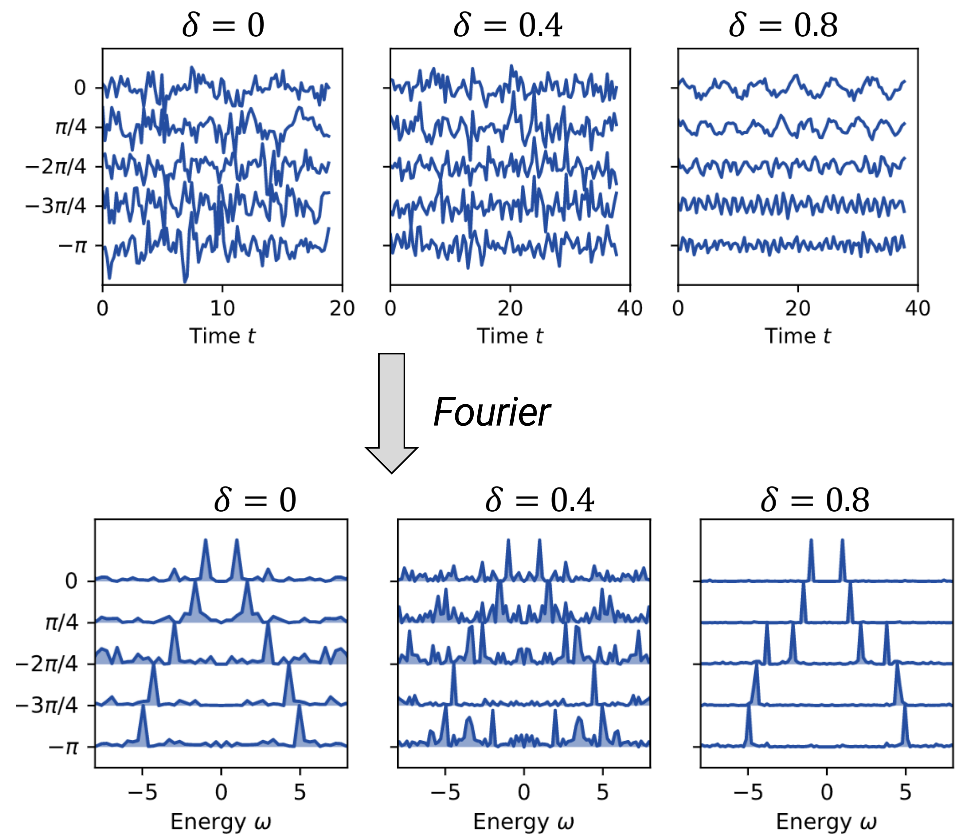

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Linear Response -> Green’s function

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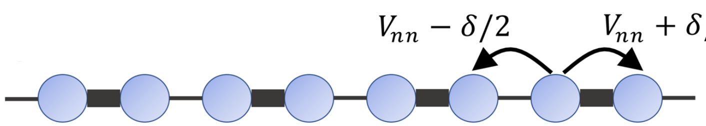

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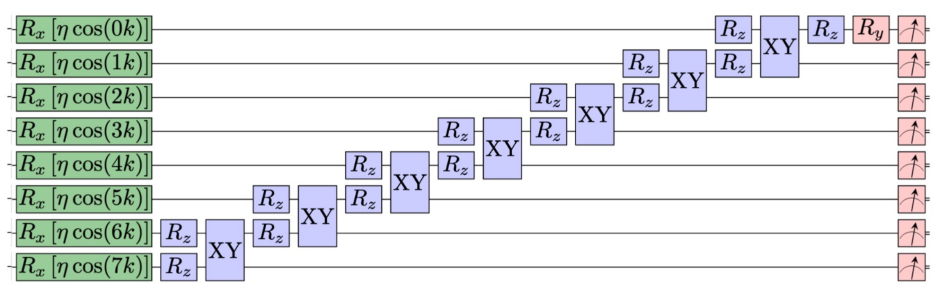

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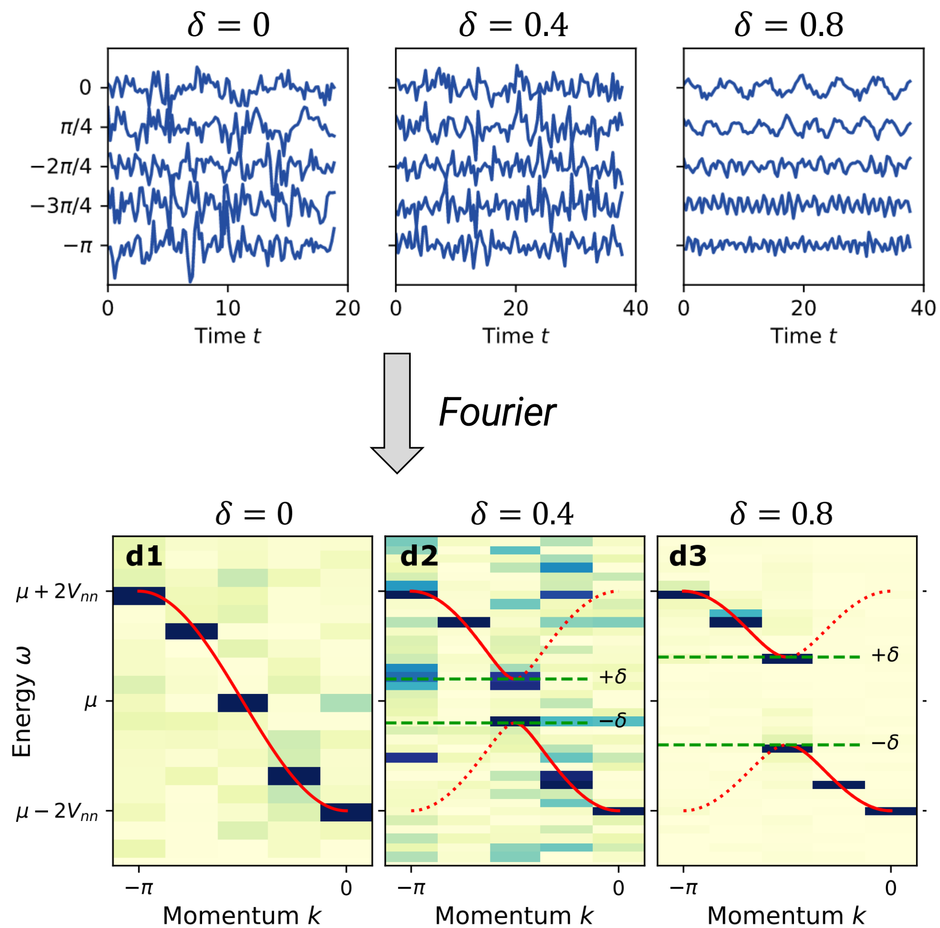

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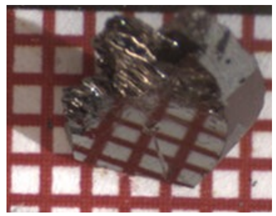
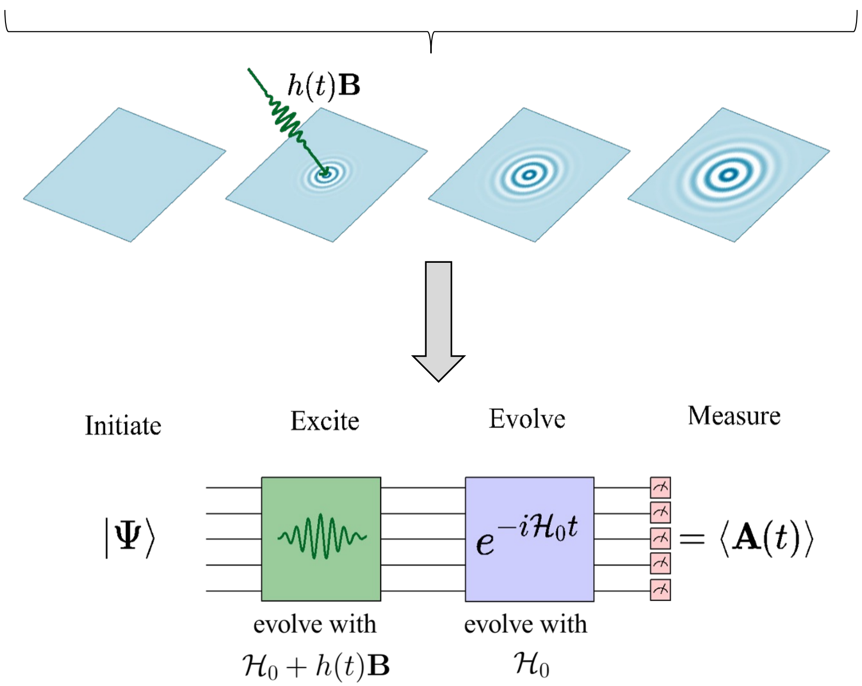
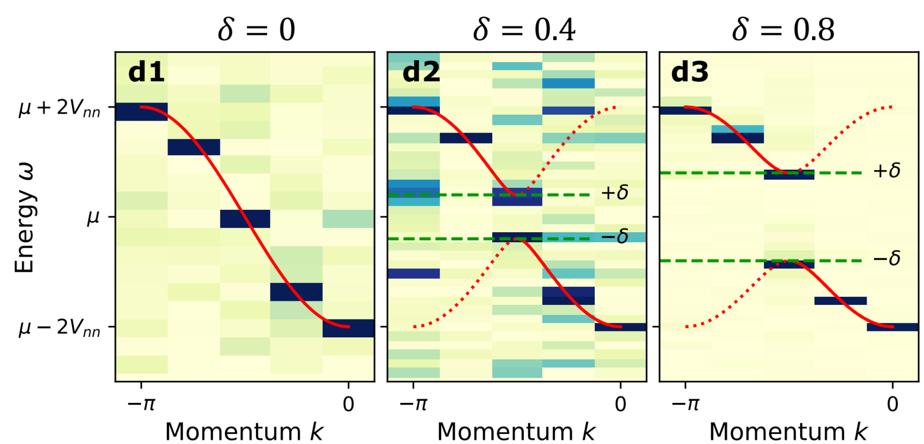




- Ancilla free
- Momentum and frequency selectivity
- Both bosonic and fermionic correlators
- More noise robust compared to existing methods



E. Kökcü. H.Labib. J.K. Freericks. AFK.. Nature Communications 15. 3881 (2024)

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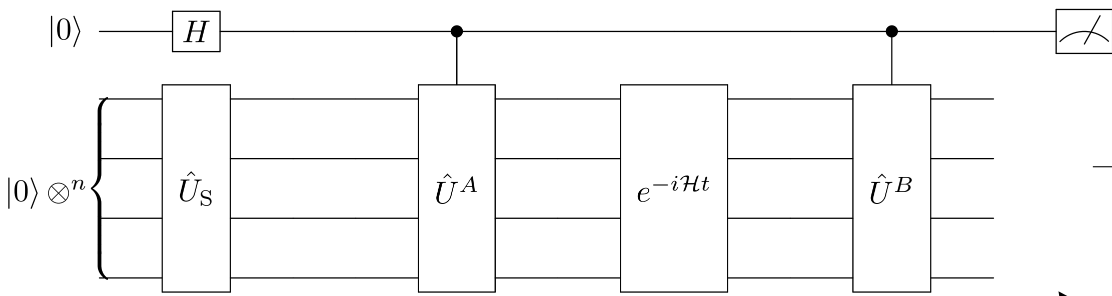
A-Z quantum simulation



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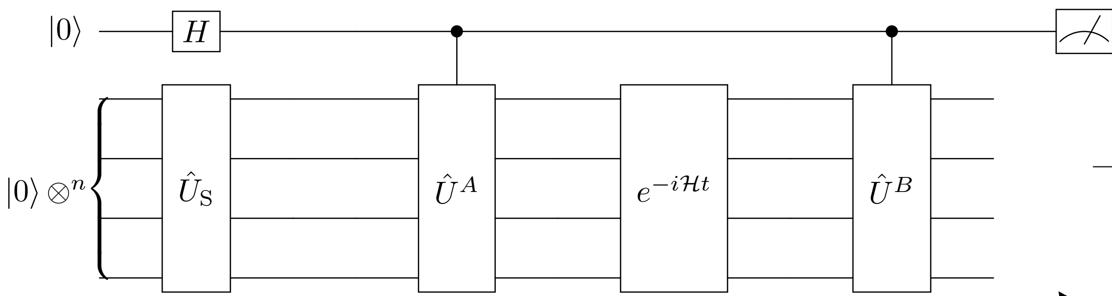

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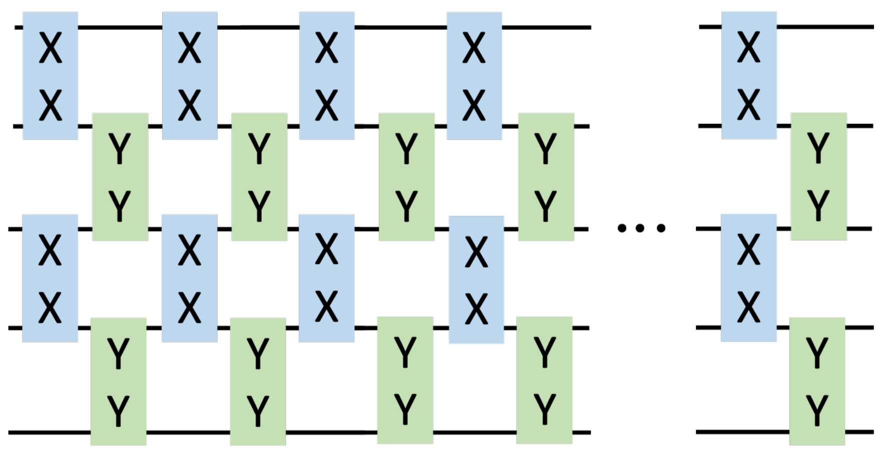
A-Z quantum simulation

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

$U(t) =$ 

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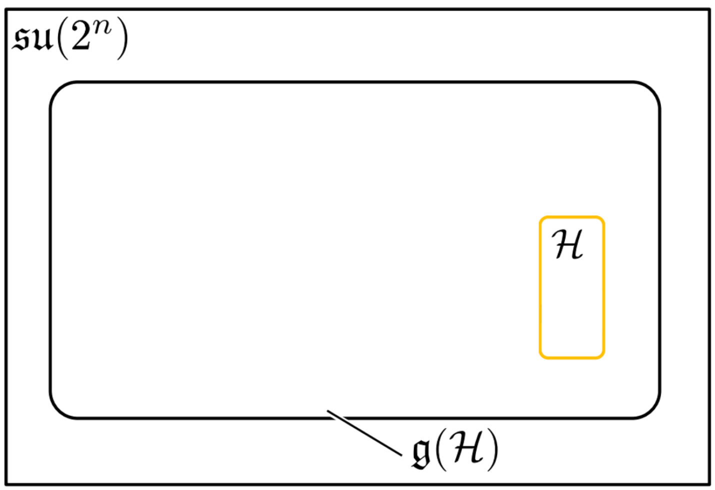
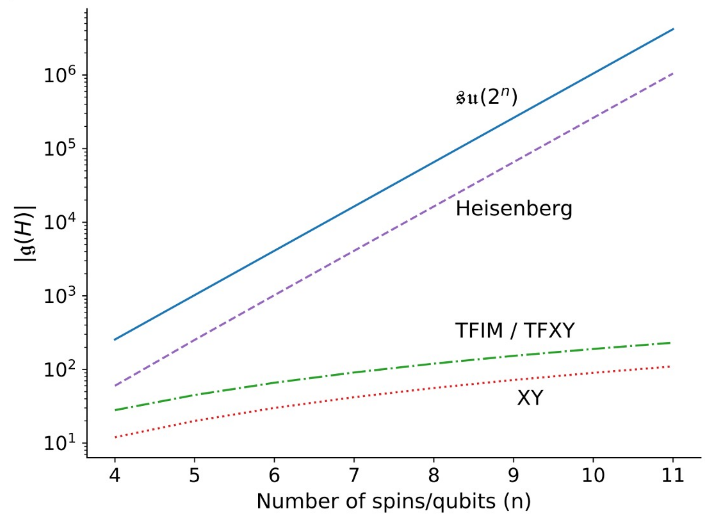
$$\mathrm{DLA} := \mathrm{span}\left\{[a_{i_1}, [a_{i_2}, [\cdots [a_{i_r}, a_j] \cdots]]]\right\}$$





NC STATE UNIVERSITY

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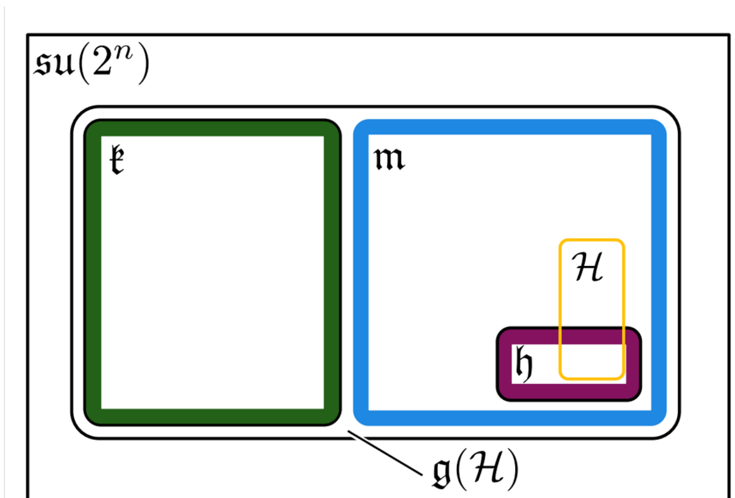

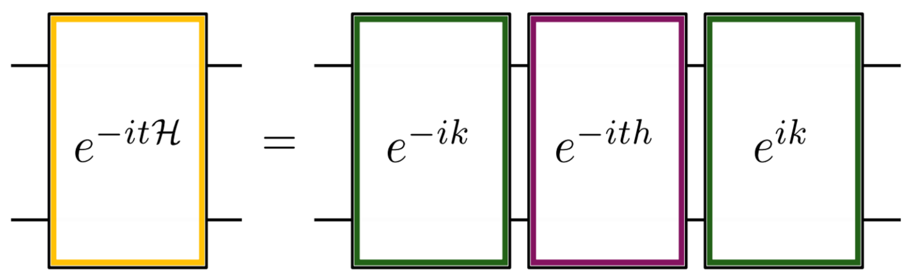

E. Kökcü et al., Phys. Rev. Lett. (2022)

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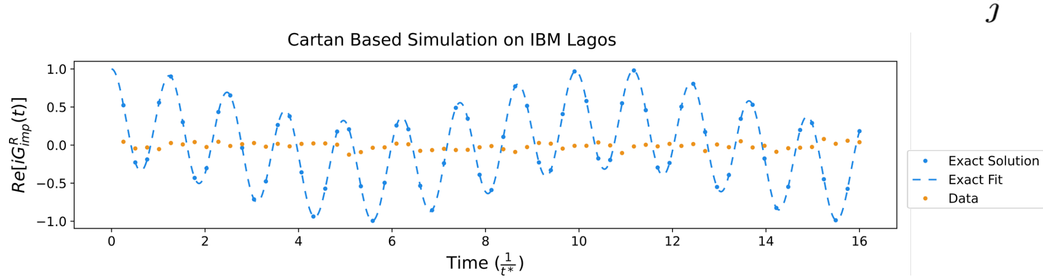

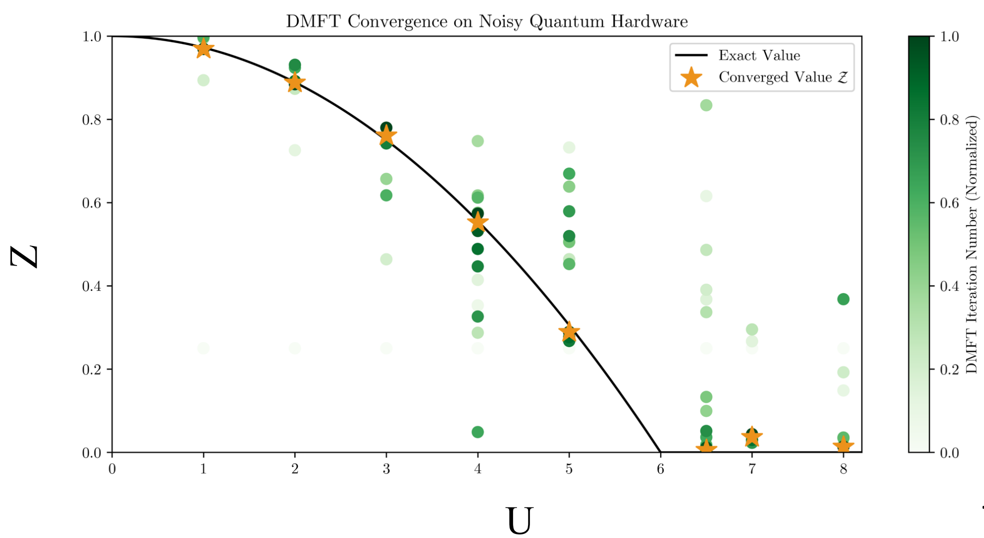

T. Steckmann et al., PRR (2023)

NC STATE UNIVERSITY

Further improvements via mathematics

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

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

Kemper, Yang, Gull, PRL 2024

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

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Kemper, Yang, Gull, PRL 2024

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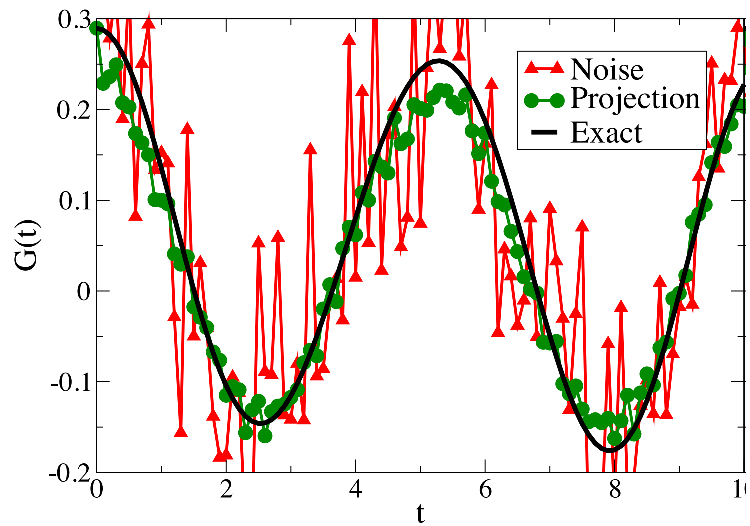
- What can I do with this?



Kemper, Yang, Gull, PRL 2024

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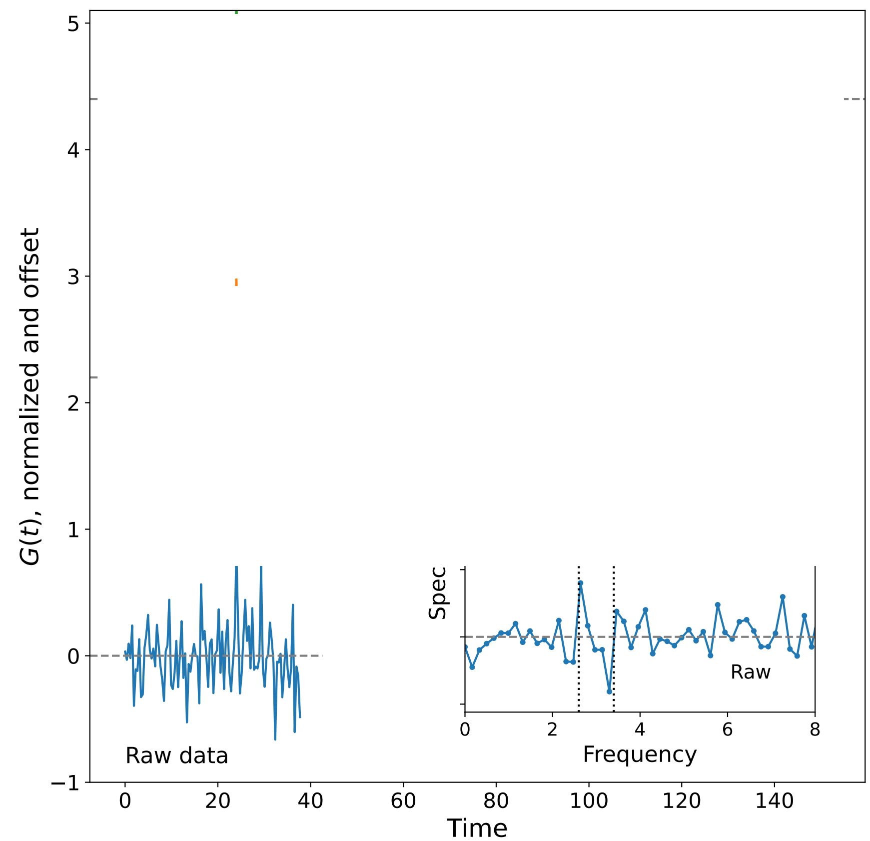

Kemper, Yang, Gull, PRL 2024

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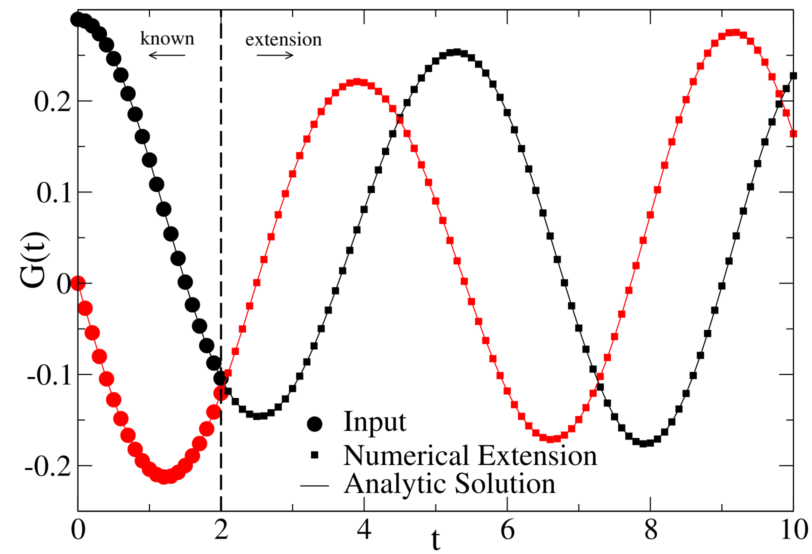
- What else can I do with this?



Kemper, Yang, Gull, PRL 2024

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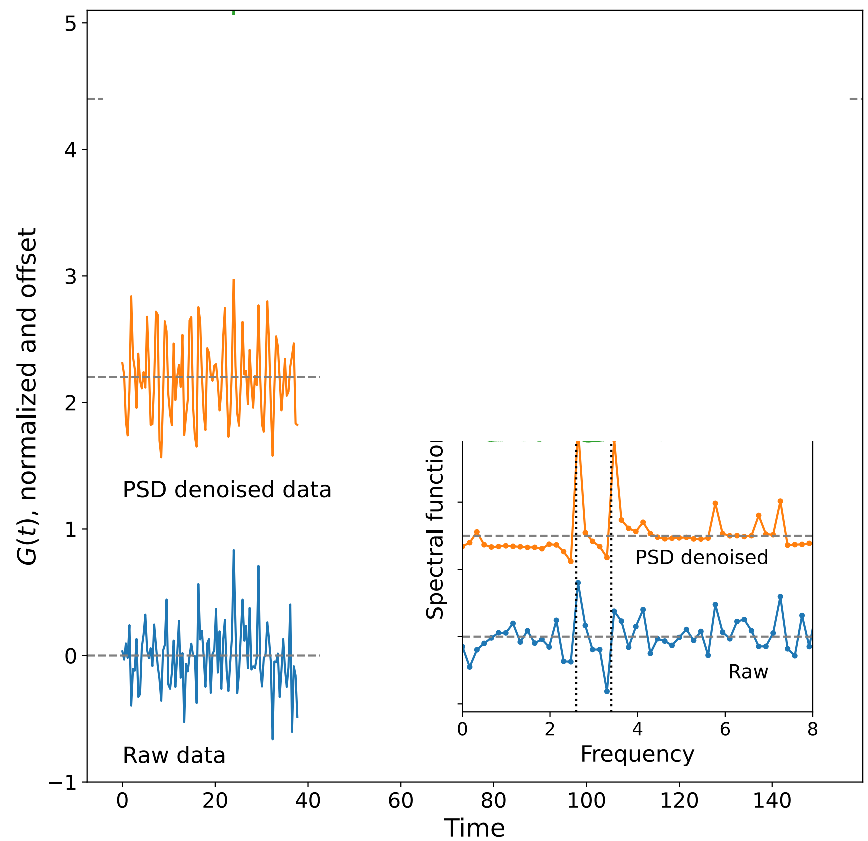
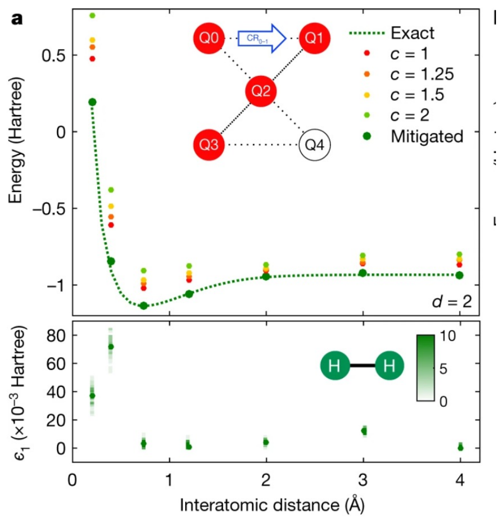


Kemper, Yang, Gull, PRL 2024

Preparing ground states

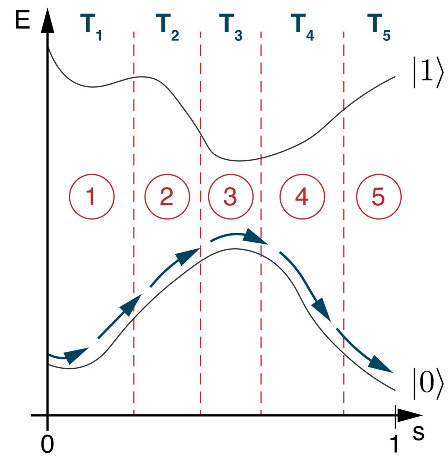
Variational Quantum Eigensolver



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

Barren Plateau

Adiabatic State Preparation



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

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

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.

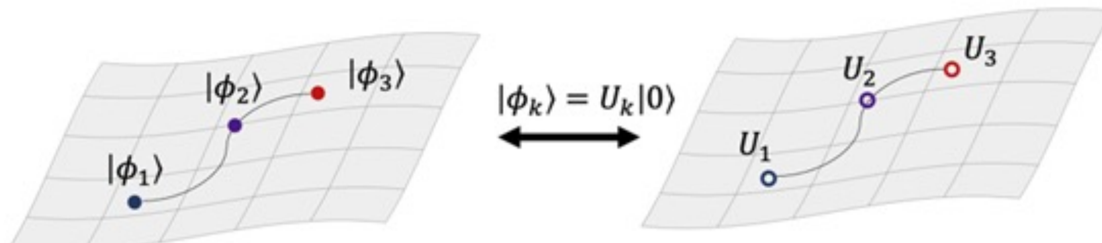
- Ground states
- Excited states
- Thermal states

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

Eigenvector Continuation

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

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



Using this:

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

- Use quantum state preparation techniques to get low energy states

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

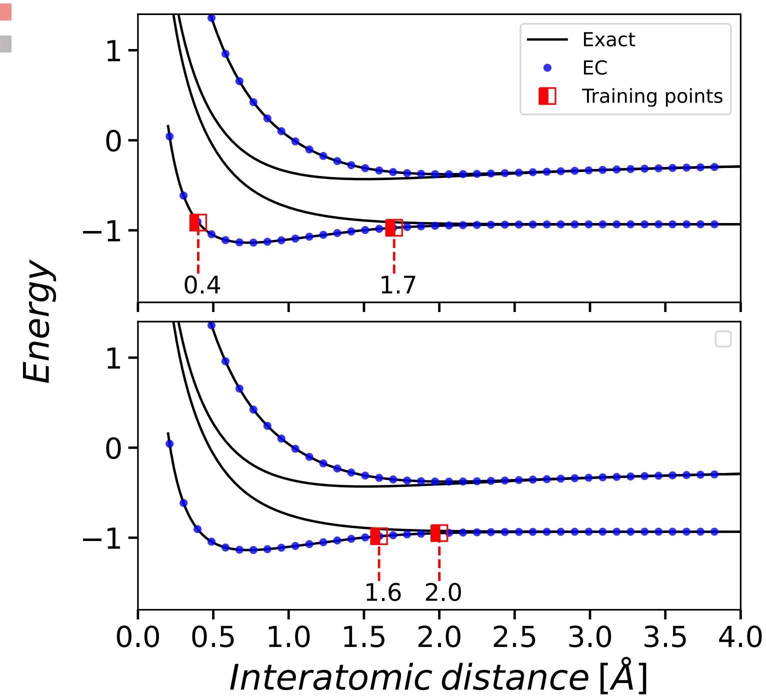
$$\{H(p_0), H(p_1), \ldots H(p_k)\}$$

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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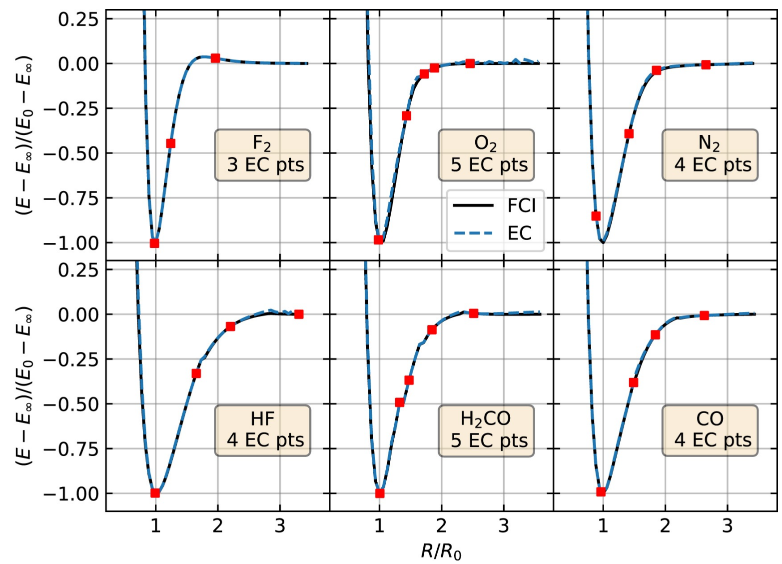

C. Mejuto-Zaera, AFK, Electron. Struct. 2023

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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

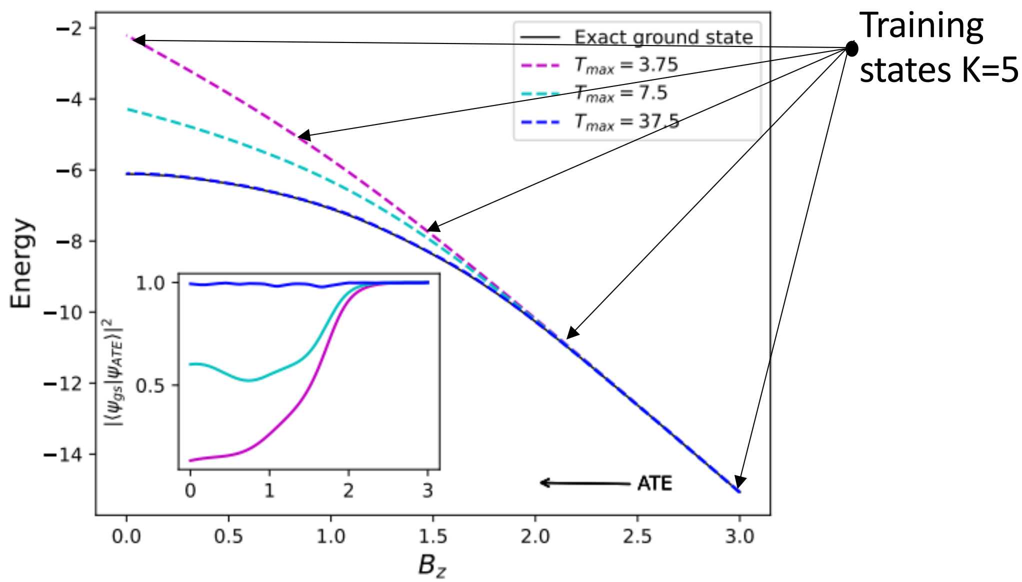
Energy spectrum across the parameter

Approximate Eigenvector Continuation

dt = 0.05; dB_Z/dt = 0.15
750 time steps
RMS error < 0.09

Adiabatic time evolution

dt = 0.05; dB_Z/dt = 1.5
75 time steps
RMS error > 2.1



1D 5-site XY Model Adiabatic time evolution

Approximate Eigenvector Continuation

dt = 0.05; dB_Z/dt = 0.15
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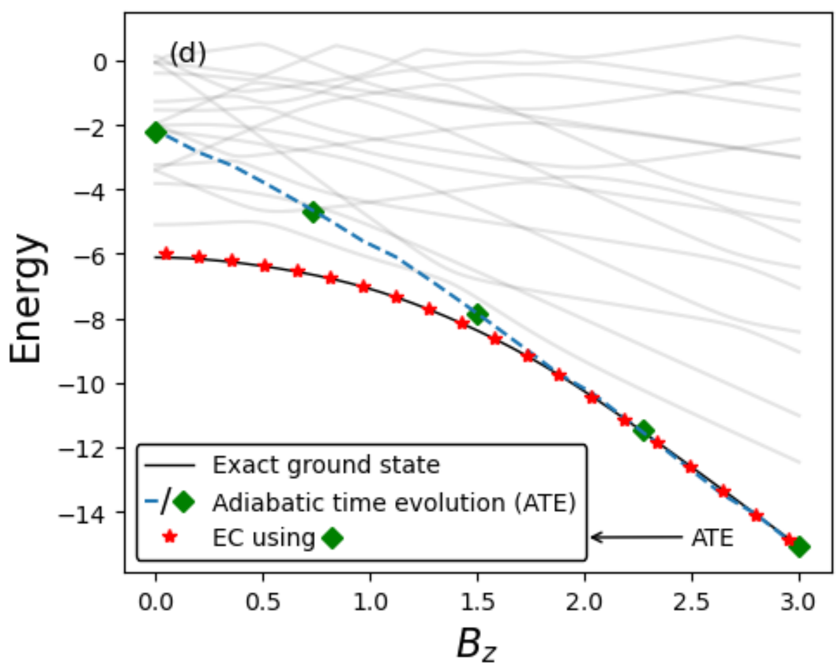
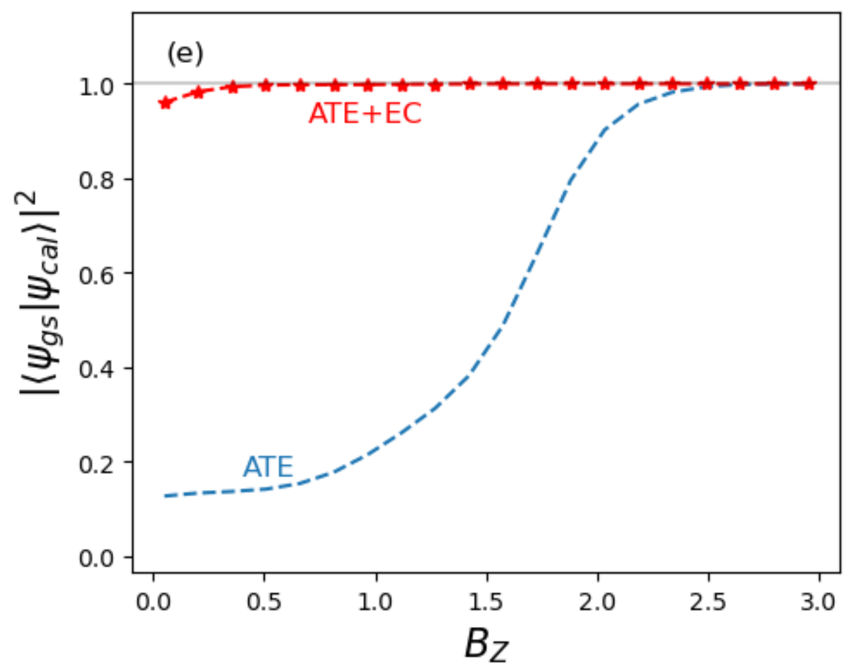
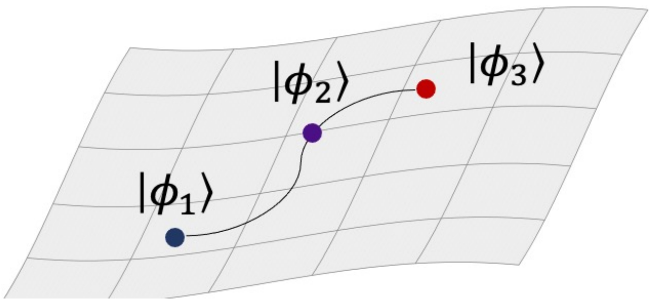
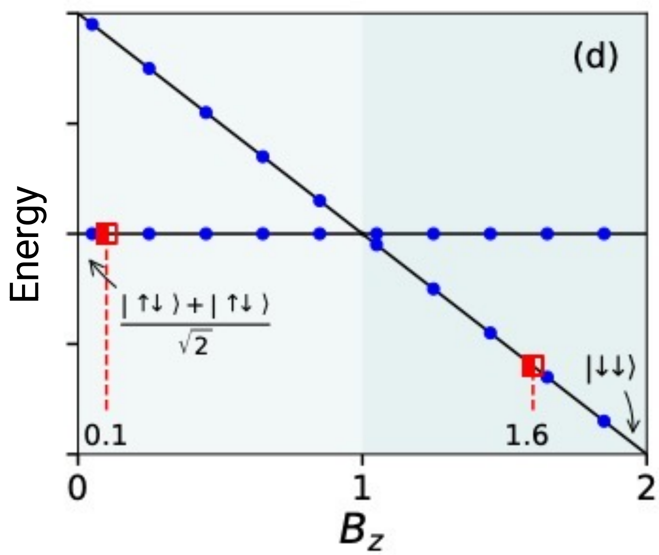




Eigenvector Continuation



$$\mathcal{H} = X_1X_2 + Y_1Y_2 + B_z(Z_1 + Z_2)$$



Choose two training points:

$$B_z < 1: \quad |\psi\rangle = \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}}$$

$$B_z > 1: \quad |\psi\rangle = |\downarrow\downarrow\rangle$$

These span the full subspace!

- Only needed 2 sets of measurements
- Covers 2 different magnetization sectors

Eigenvector Continuation

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

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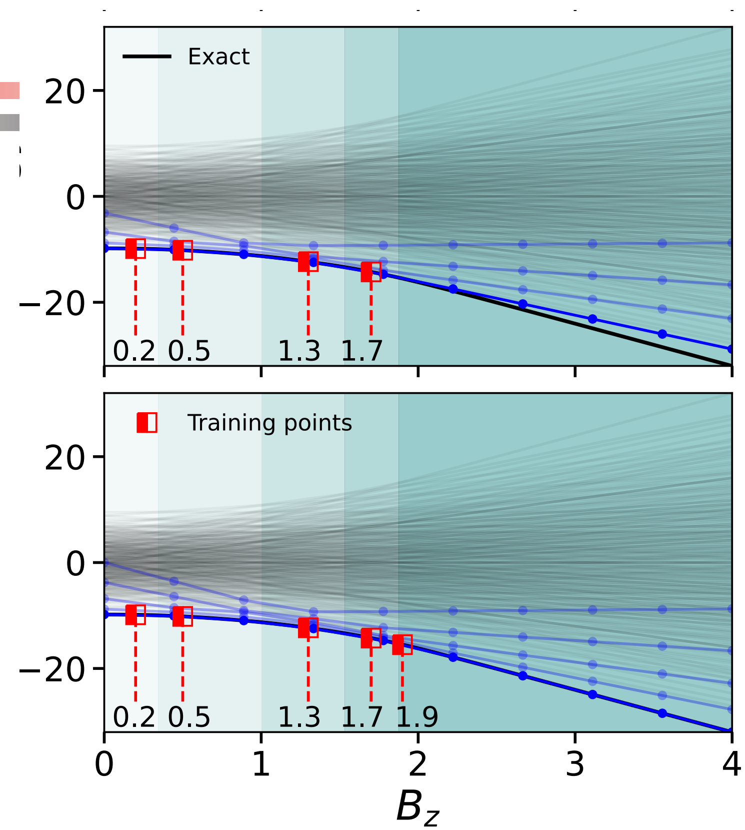
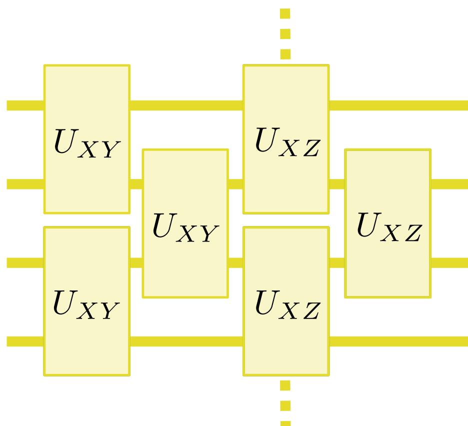


Energy spectrum across the parameter range

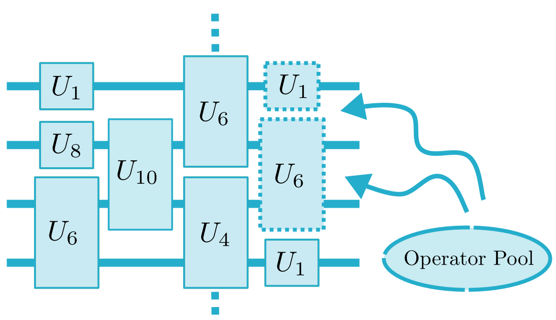
A. Francis, AFK et al., 2209.10571

Lie algebraic methods for quantum computing

Time evolution



Variational ansätze



Dynamical Lie algebras

Given a set of operators a_i (either in the operator pool or Hamiltonian)

Their Dynamical Lie Algebra expresses all the operators that can be generated by this set

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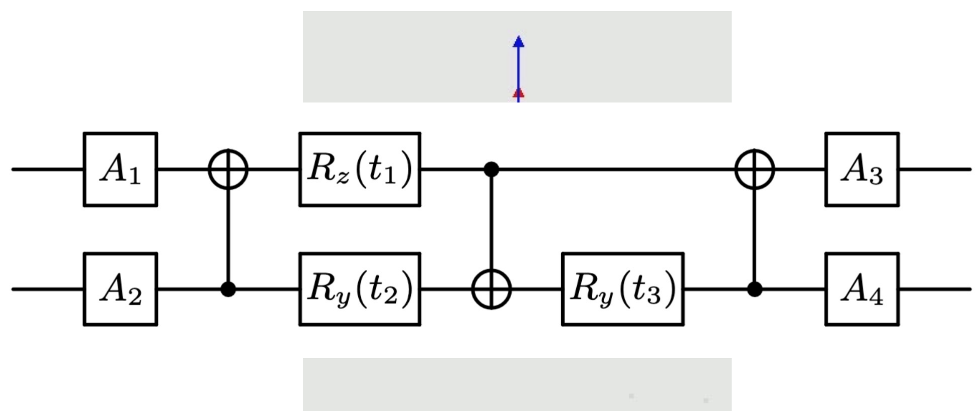

Lie algebraic methods for quantum computing

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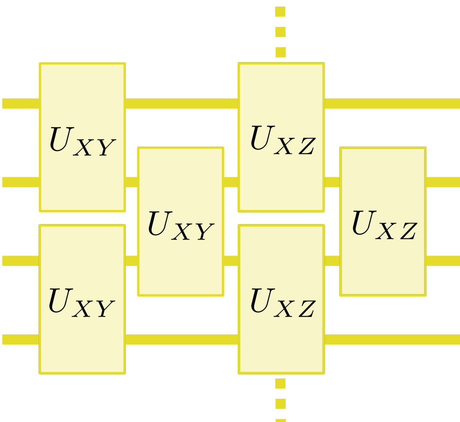

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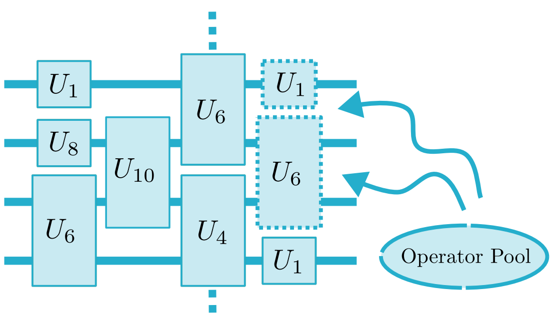
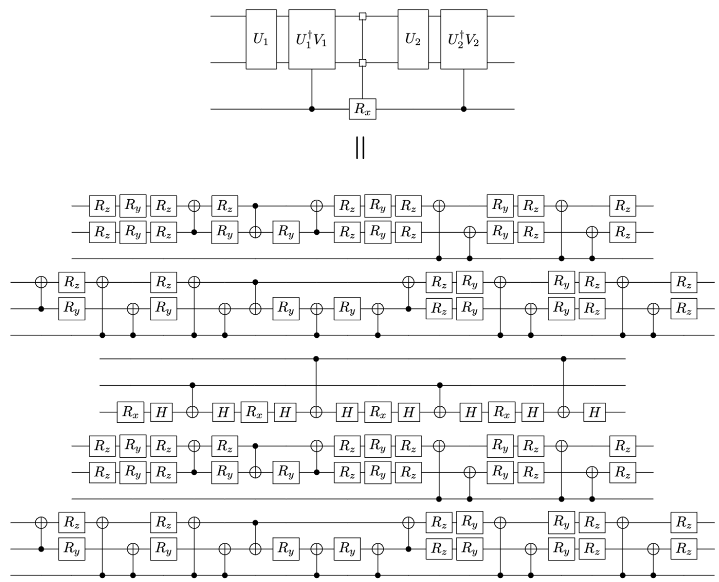


Constructive Quantum Shannon Decomposition from Cartan Involutions

Byron Drury, Peter Love



Lie algebraic methods for quantum computing

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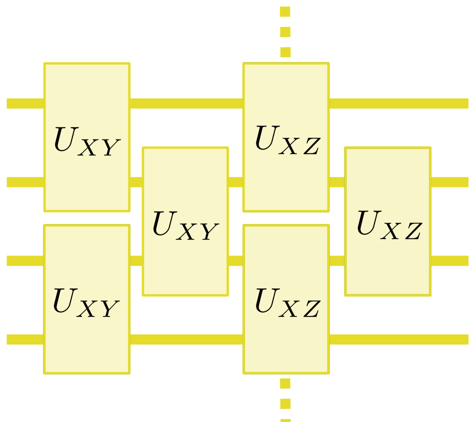

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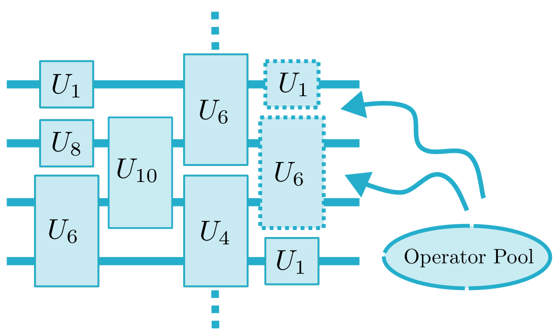
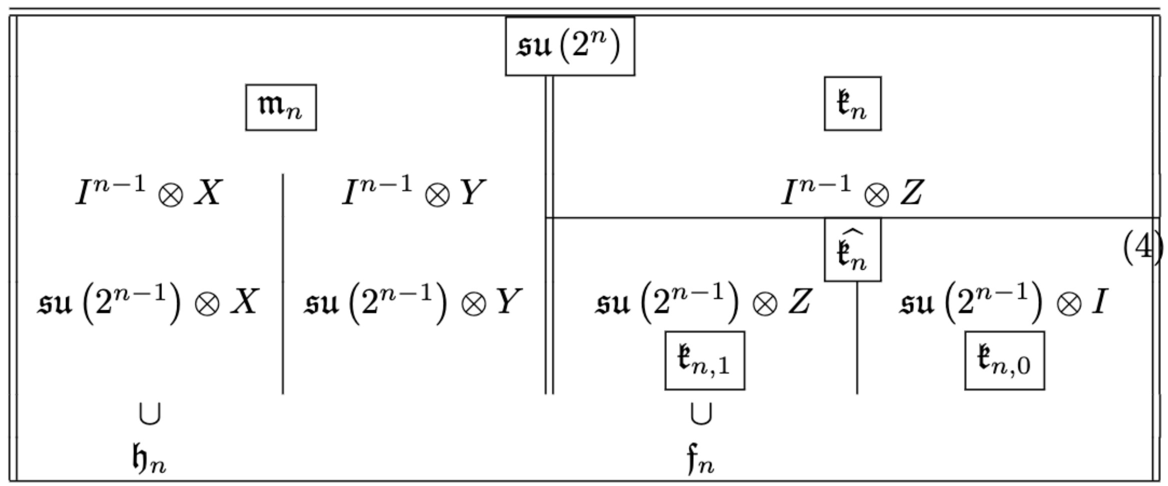


A constructive algorithm for the Cartan decomposition of $SU(2^N)$

Henrique N. Sá Earp[1] and Jiannis K. Pachos[2]



N. Khaneja and S. J. Glaser, Chemical Physics 267, 11 (2001)

Lie algebraic methods for quantum computing

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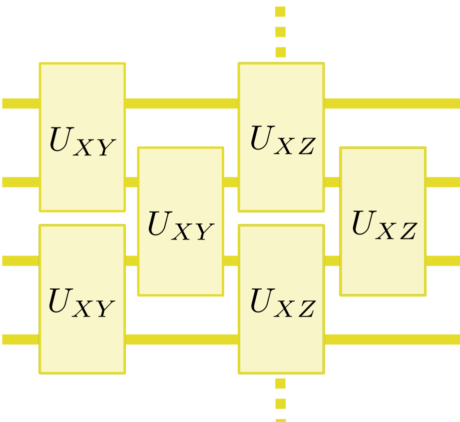

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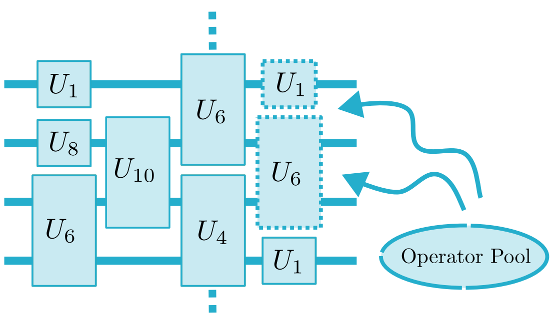

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Cartan decomposition for exact time evolution

Kökcü, PRL 2022

Circuit compression

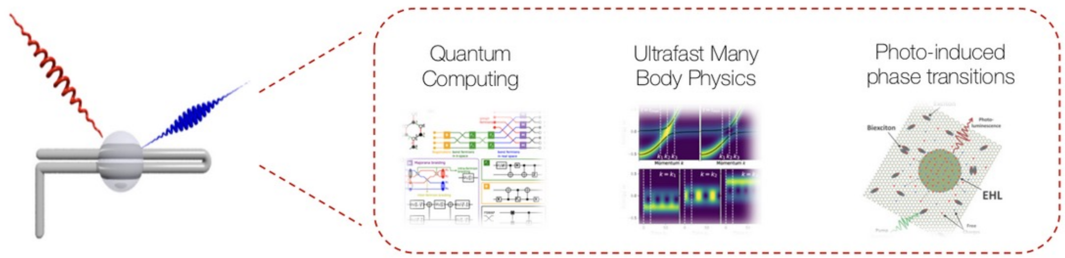
Kökcü, PRA 2022
Camps, SIMAX 2022
Kökcü, arXiv:2303.09538

Unified Framework for Barren plateaus in VQA

Ragone, arXiv:2309.09342

Complete (DLA) classification of 1-d nearest neighbor spin models

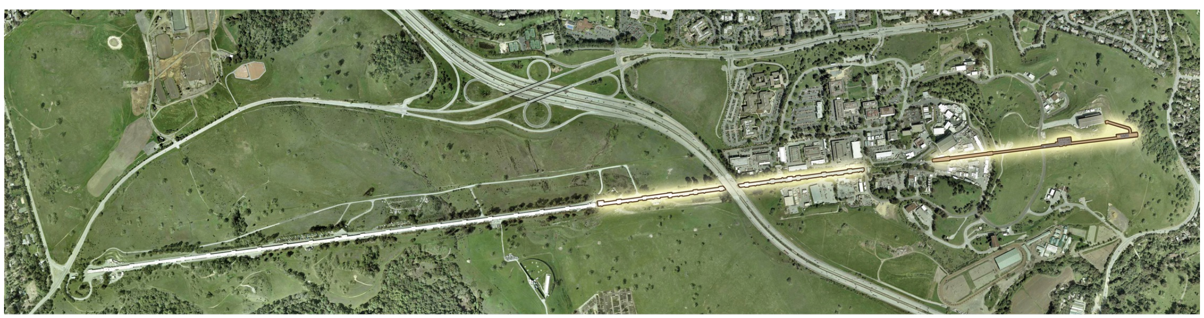
Wiersema, arXiv:2309.05690

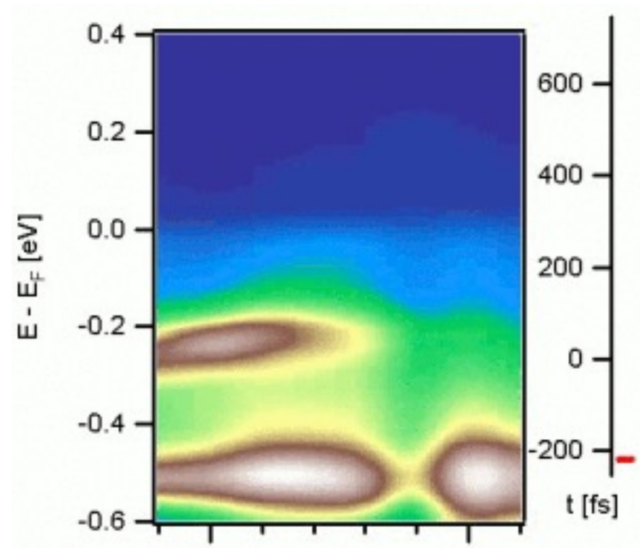


Kemper Lab

Quantum materials in and out of equilibrium.

Time-resolved experiments





Shen group (Stanford)

Main Problem

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

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

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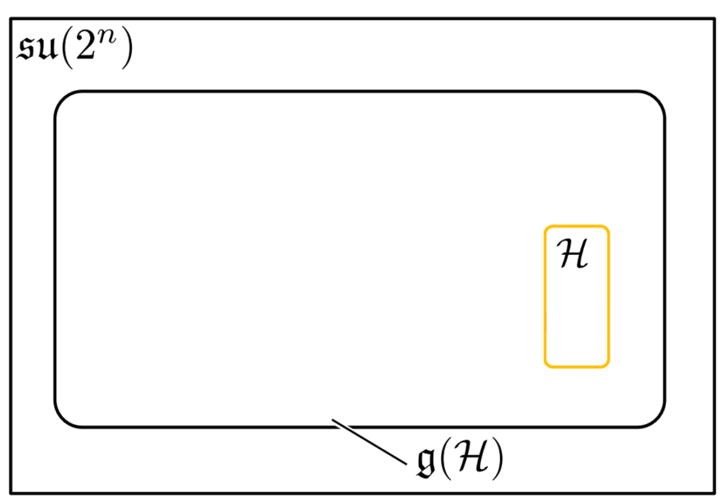
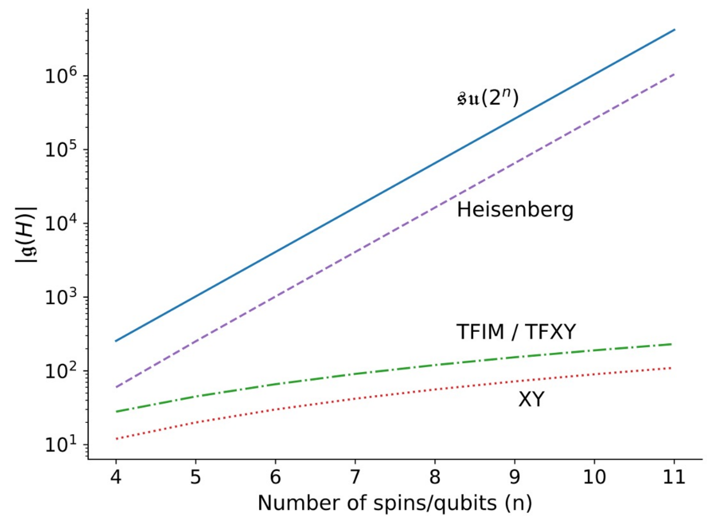




$$\mathfrak{a}_0(n) = \mathrm{span}\{X_j X_{j+1}\}_{1\le j\le n-1} \cong \mathfrak{u}(1)^{\oplus(n-1)}, \quad \dim = n-1,$$

$$\mathfrak{a}_1(n) = \mathrm{span}\{X_i Z_{i+1}\cdots Z_{j-1} Y_j\}_{1\le i<j\le n} \cong \mathfrak{so}(n), \quad \dim = \frac{n(n-1)}{2},$$

$$\mathfrak{a}_2(n) = \mathrm{span}\{X_i Z_{i+1}\cdots Z_{j-1} Y_j\}_{1\le i<j\le n} \oplus \mathrm{span}\{Y_i Z_{i+1}\cdots Z_{j-1} X_j\}_{1\le i<j\le n}$$
$$\cong \mathfrak{so}(n)\oplus\mathfrak{so}(n), \quad \dim = n(n-1),$$

$$\mathfrak{a}_3(n) \cong \begin{cases} \mathfrak{so}(2^{n-2})^{\oplus 4}, & \dim = 2^{n-1}(2^{n-2}-1), \quad n\equiv 0 \mod 8, \\ \mathfrak{so}(2^{n-1}), & \dim = 2^{n-2}(2^{n-1}-1), \quad n\equiv \pm 1 \mod 8, \\ \mathfrak{su}(2^{n-2})^{\oplus 2}, & \dim = 2^{2n-3}-2, \quad n\equiv \pm 2 \mod 8, \\ \mathfrak{sp}(2^{n-2}), & \dim = 2^{n-2}(2^{n-1}+1), \quad n\equiv \pm 3 \mod 8, \\ \mathfrak{sp}(2^{n-3})^{\oplus 4}, & \dim = 2^{n-1}(2^{n-2}+1), \quad n\equiv 4 \mod 8, \end{cases}$$

$$\mathfrak{a}_4(n) \cong \mathfrak{a}_2(n),$$

$$\mathfrak{a}_5(n) \cong \begin{cases} \mathfrak{so}(2^{n-2})^{\oplus 4}, & \dim = 2^{n-1}(2^{n-2}-1), \quad n\equiv 0 \mod 6, \\ \mathfrak{so}(2^{n-1}), & \dim = 2^{n-2}(2^{n-1}-1), \quad n\equiv \pm 1 \mod 6, \\ \mathfrak{su}(2^{n-2})^{\oplus 2}, & \dim = 2^{2n-3}-2, \quad n\equiv \pm 2 \mod 6, \\ \mathfrak{sp}(2^{n-2}), & \dim = 2^{n-2}(2^{n-1}+1), \quad n\equiv 3 \mod 6, \end{cases}$$

$$\mathfrak{a}_6(n) \cong \mathfrak{a}_7(n) \cong \mathfrak{a}_{10}(n) \cong \begin{cases} \mathfrak{su}(2^{n-1}), & \dim = 2^{2n-2}-1, \quad n \text{ odd}, \\ \mathfrak{su}(2^{n-2})^{\oplus 4}, & \dim = 2^{2n-2}-4, \quad n\ge 4 \text{ even}, \end{cases}$$

$$\mathfrak{a}_8(n) \cong \mathfrak{so}(2n-1), \quad \dim = (n-1)(2n-1),$$

$$\mathfrak{a}_9(n) \cong \mathfrak{sp}(2^{n-2}), \quad \dim = 2^{n-2}(2^{n-1}+1),$$

$$\mathfrak{a}_{11}(n) = \mathfrak{a}_{16}(n) = \mathfrak{so}(2^n), \quad \dim = 2^{n-1}(2^n-1), \quad n\ge 4,$$

$$\mathfrak{a}_k(n) = \mathfrak{su}(2^n), \quad \dim = 2^{2n}-1, \quad k = 12,17,18,19,21,22, \quad n\ge 4,$$

$$\mathfrak{a}_{13}(n) = \mathfrak{a}_{20}(n) \cong \mathfrak{a}_{15}(n) \cong \mathfrak{su}(2^{n-1})\oplus\mathfrak{su}(2^{n-1}), \quad \dim = 2^{2n-1}-2,$$

$$\mathfrak{a}_{14}(n) \cong \mathfrak{so}(2n), \quad \dim = n(2n-1),$$

$$\mathfrak{b}_0(n) = \mathrm{span}\{X_i\}_{1\le i\le n} \cong \mathfrak{u}(1)^{\oplus n}, \quad \dim = n,$$

$$\mathfrak{b}_1(n) = \mathrm{span}\{X_i, X_j X_{j+1}\}_{1\le i\le n,\ 1\le j\le n-1} \cong \mathfrak{u}(1)^{\oplus(2n-1)}, \quad \dim = 2n-1,$$

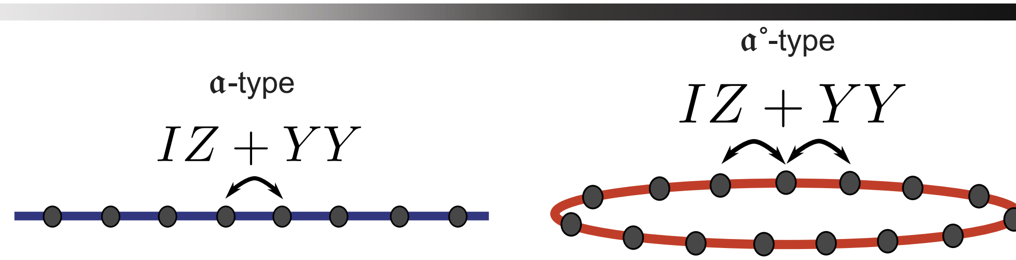
$$\mathfrak{b}_2(n) = \mathfrak{a}_9(n)\oplus\mathrm{span}\{X_1\} \cong \mathfrak{sp}(2^{n-2})\oplus\mathfrak{u}(1), \quad \dim = 2^{n-2}(2^{n-1}+1)+1,$$

$$\mathfrak{b}_3(n) = \mathrm{span}\{X_i, Y_i, Z_i\}_{1\le i\le n} \cong \mathfrak{su}(2)^{\oplus n}, \quad \dim = 3n,$$

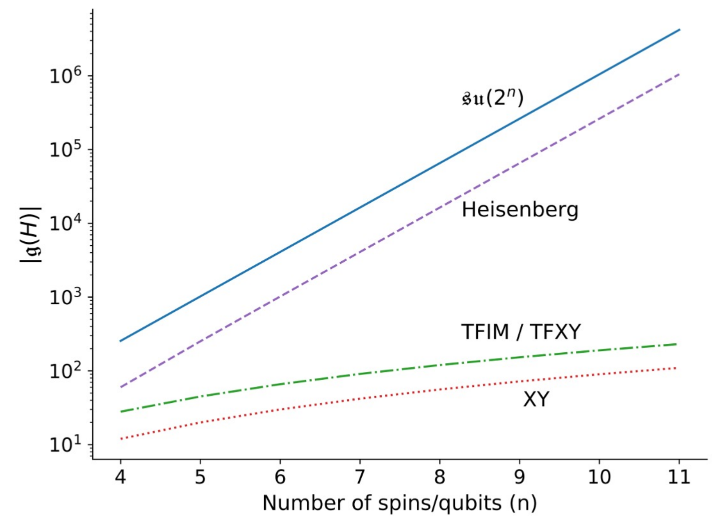
$$\mathfrak{b}_4(n) = \mathfrak{a}_{15}(n)\oplus\mathrm{span}\{X_1\} \cong \mathfrak{su}(2^{n-1})\oplus\mathfrak{su}(2^{n-1})\oplus\mathfrak{u}(1), \quad \dim = 2^{2n-1}-1.$$

List of unique dynamical Lie algebras

Roeland Wiersema, et al. , arXiv preprint arXiv:2309.05690 (2023).



$$\mathrm{DLA} := \mathrm{span}\{[a_{i_1}, [a_{i_2}, [\cdots [a_{i_r}, a_j]\cdots]]]\}$$



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Main Problem

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

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

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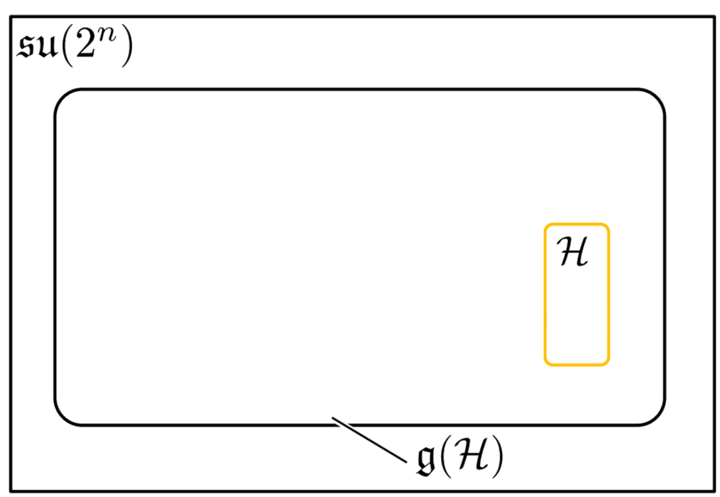

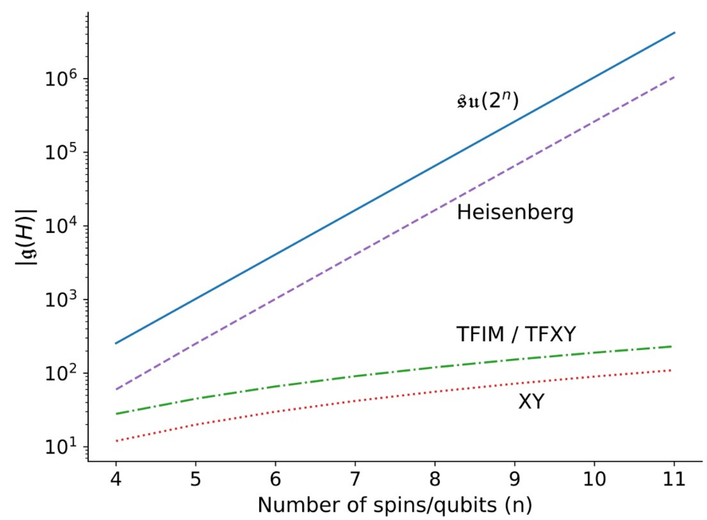

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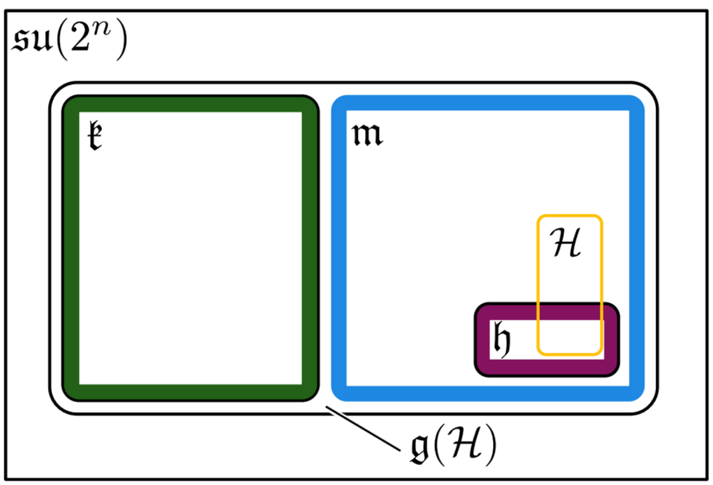
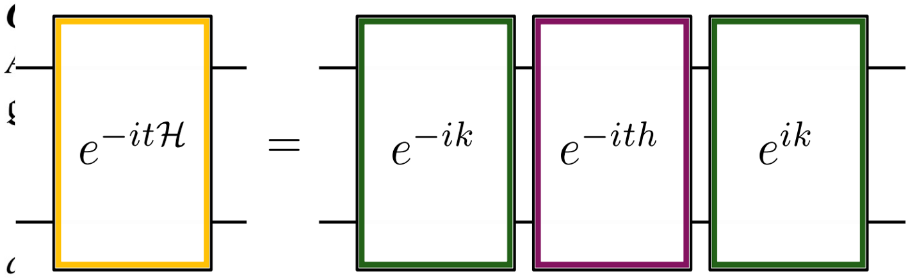


Definition 1 *Consider a compact semi-simple Lie subgroup*

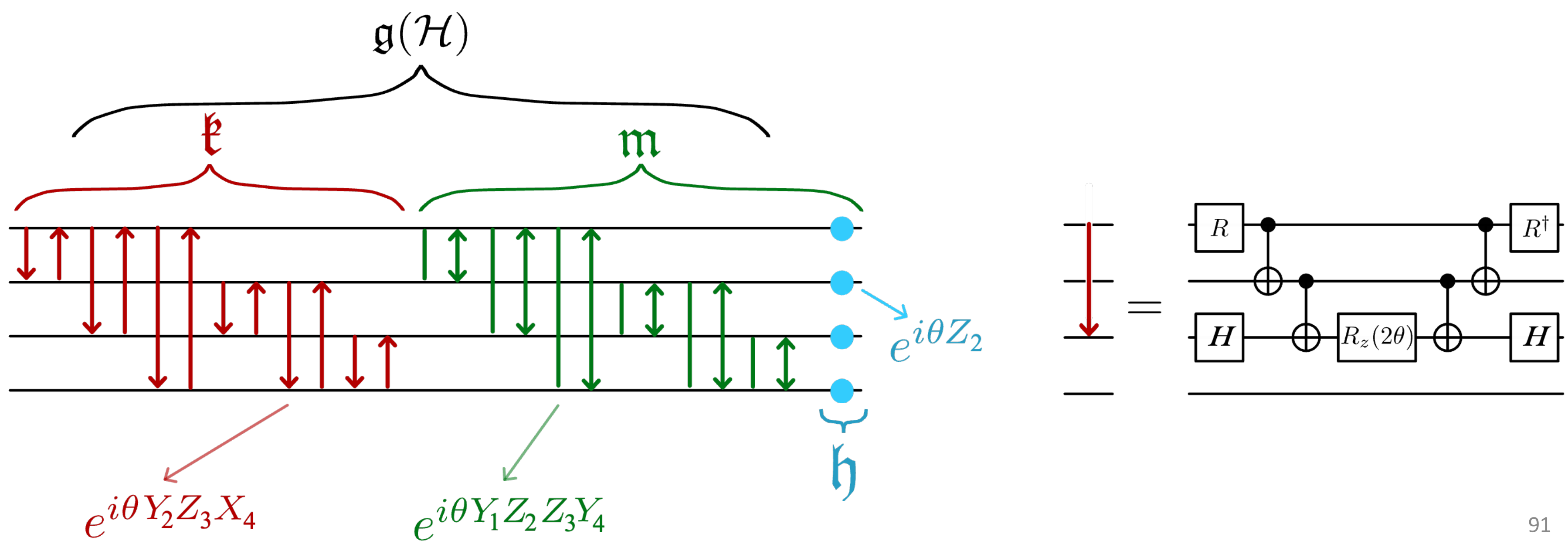


sition is defined as one of the maximal Abelian subalgebras of $\mathfrak{m}$*, and denoted as* $\mathfrak{h}$.

Illustrative Example: TFXY model

- Let us consider a TFXY chain: $$\mathcal{H} = \sum_{i=1}^{n-1} \left(X_i X_{i+1} + Y_i Y_{i+1} \right) + \sum_{i=1}^{n} b_i Z_i$$

$$\mathfrak{g}(\mathcal{H}) = \ \mathrm{span}\left\{ H_i, [H_i, H_j], \left[[H_i, H_j], H_k\right], \ldots \right\}$$



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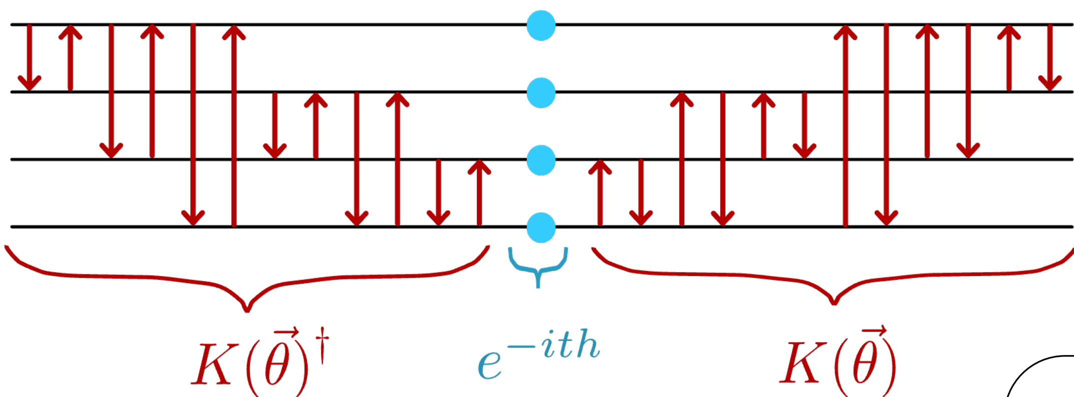
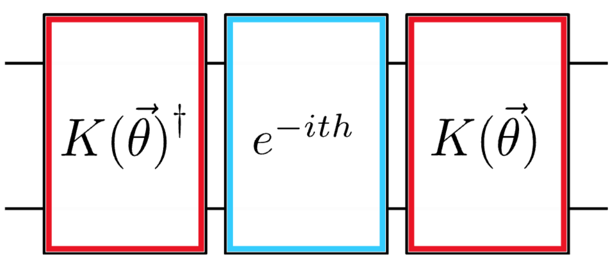


$$K(\vec{\theta}) = \prod_i e^{i\theta_i k_i}$$

We need to find $\vec{\theta} = \{\theta_i\}$



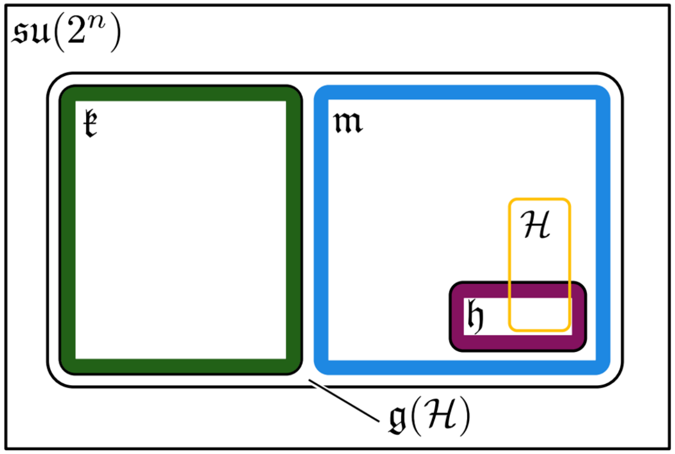
$$f(K) = \mathrm{Tr}\left[vK^\dagger H K \right]$$

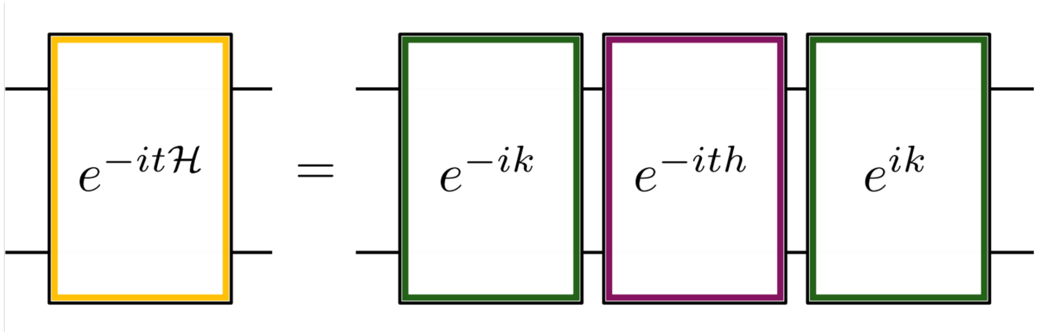
$$v = h_1 + \pi h_2 + \pi^2 h_3 + \ldots + \pi^{n_h - 1} h_{n_h}$$

Find a <u>local</u> minimum of this function

Algorithm

1) Generate Hamiltonian algebra $\mathbf{g}(H)$
2) Find a Cartan decomposition where H is in $\boldsymbol{m}$
3) Obtain parameters via local minimum of $f(K)$
4) Build the circuit using K and h
5) Then simulate for any t





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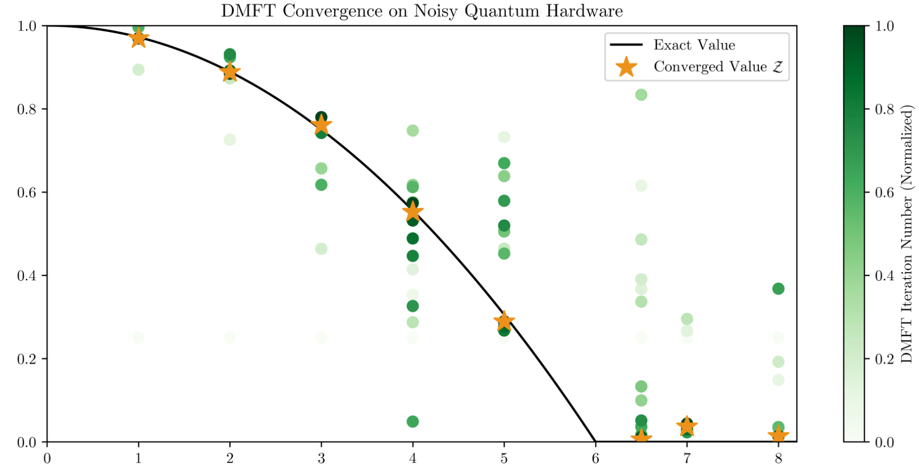
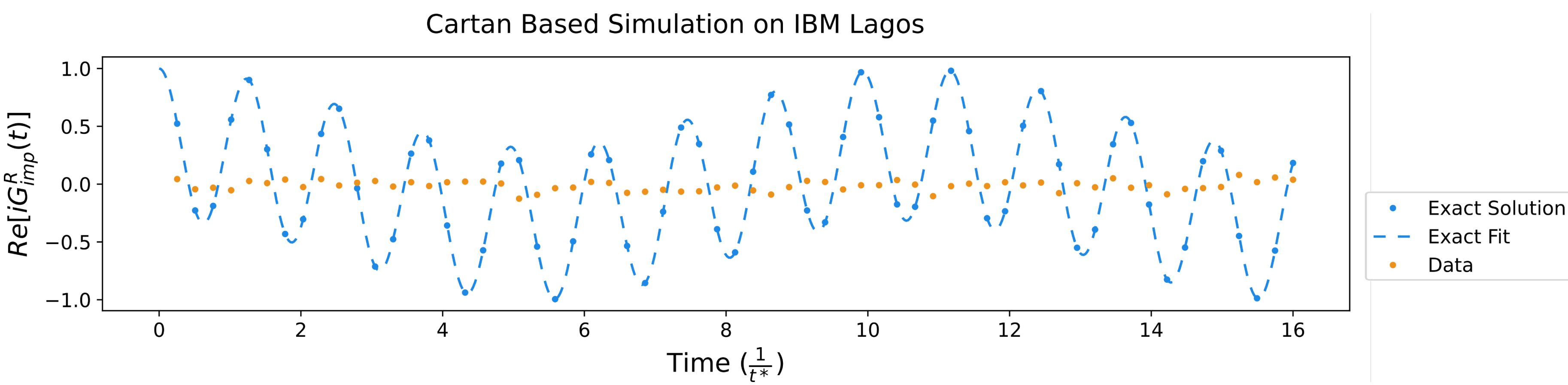
Cartan Decomposition

- $O(n^2)$ 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.

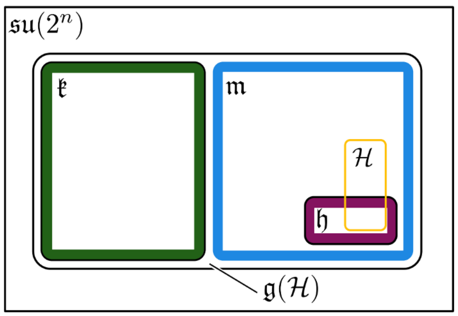


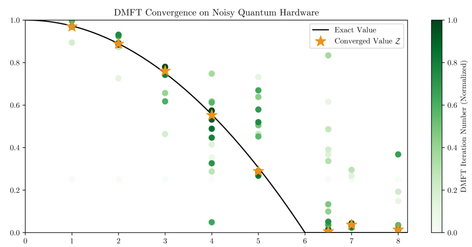


T. Steckmann, Phys Rev Research (2023)

2 Algebraic methods for circuit generation

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

Iterative Cartan Decomposition

Kökcü PRL (2022) , Steckmann PRR (2023)

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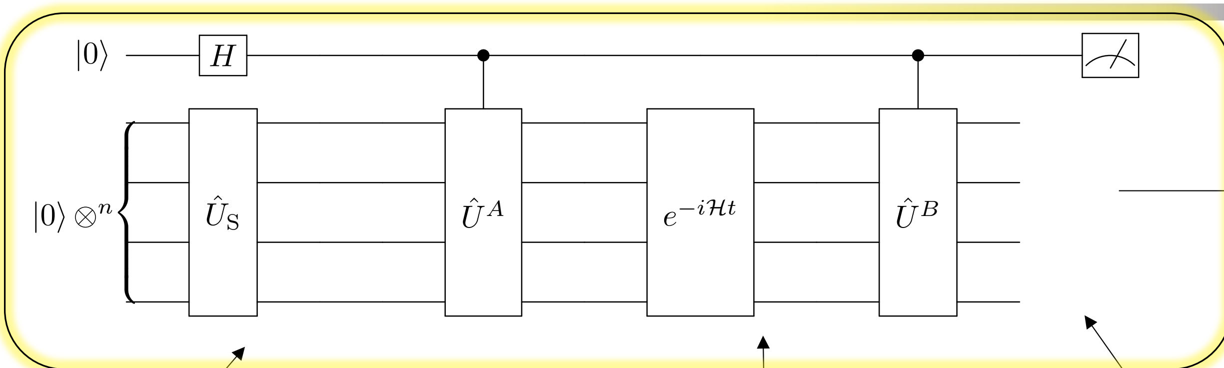
A-Z quantum simulation



Classical post-processing techniques

Prepare state of interest

Time evolve

Dynamical response functions

- *Physics-Informed Subspace Expansions*

- *Lie-algebraic methods for time evolution*
- *Open quantum system evolution*

- *Neutron scattering (magnon) spectra*
- *Open quantum system Green's functions*
- *Dynamical Mean Field Theory*

A-Z quantum simulation