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Quantum Information and Quantum Materials

Alexander (Lex) Kemper

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

SEQC
10/30/2024

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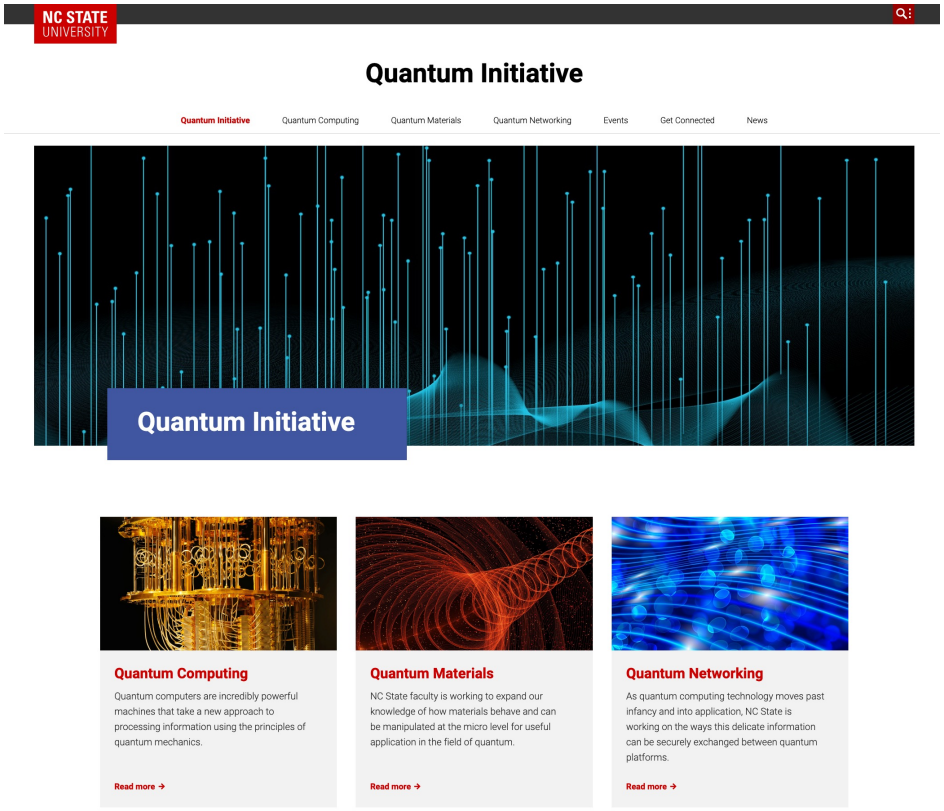

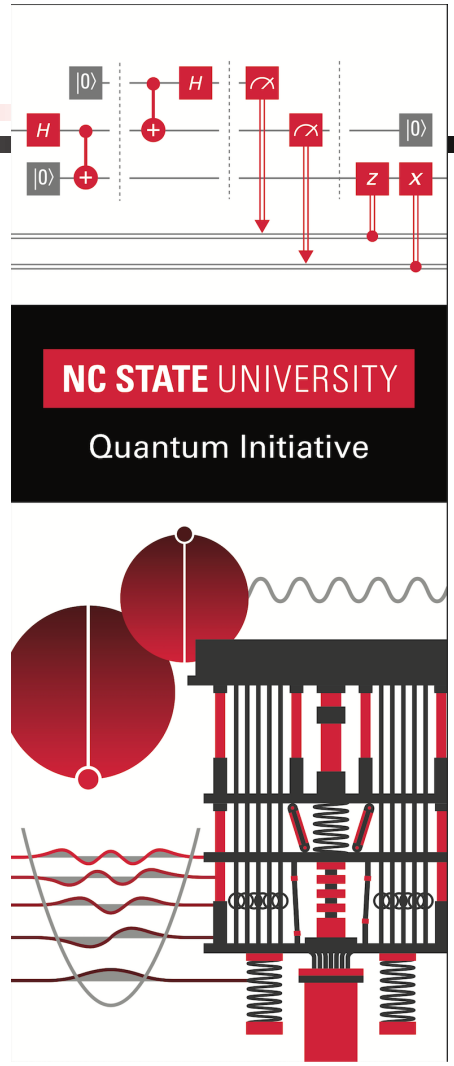

https://quantum.ncsu.edu/

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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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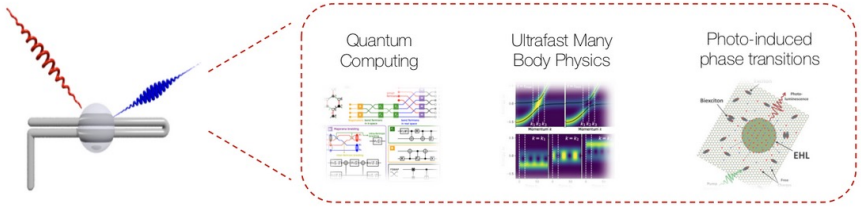


Kemper Lab

Quantum materials in and out of equilibrium.

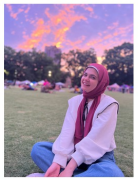
Collaborations with:

- 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)

Current members

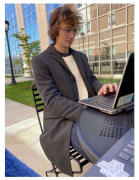
Alexander (Lex) Kemper
Principal investigator

Anjali Agrawal
Graduate Researcher



Heba Labib
Graduate Researcher

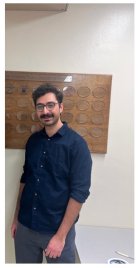
Norman Hogan
Graduate Researcher



Ethan Blair
Undergraduate Researcher

Arvin Kushwaha
Undergraduate Researcher

Omar Alsheikh
Graduate Researcher



Goksu Toga
Postdoctoral Researcher

Your Name
New lab member

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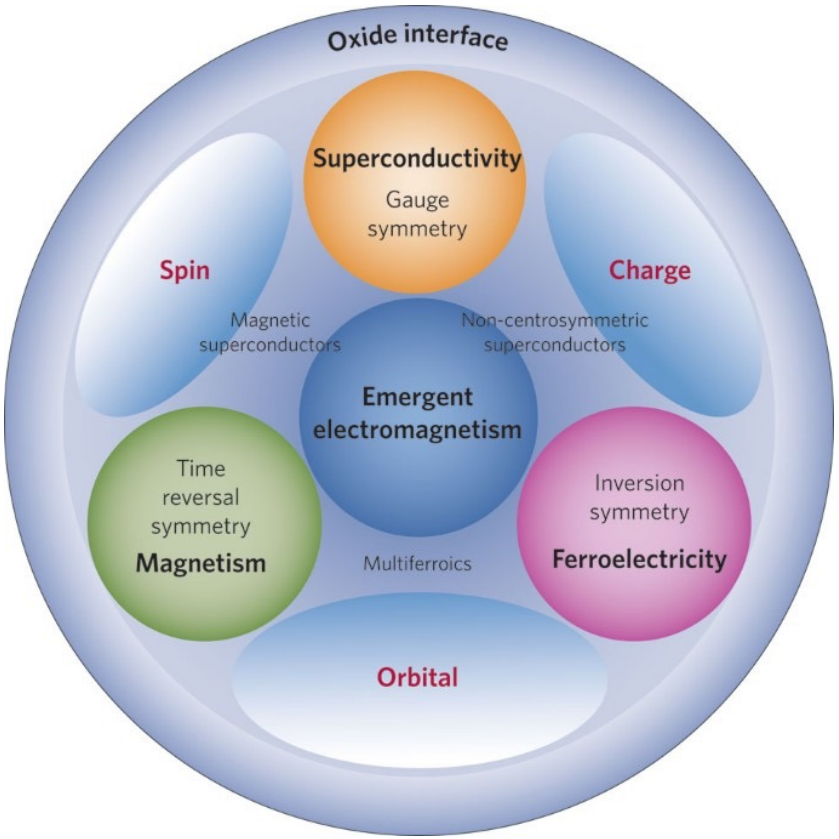
Quantum Information and Quantum Materials



H. Hwang, 10.1038/nmat3223

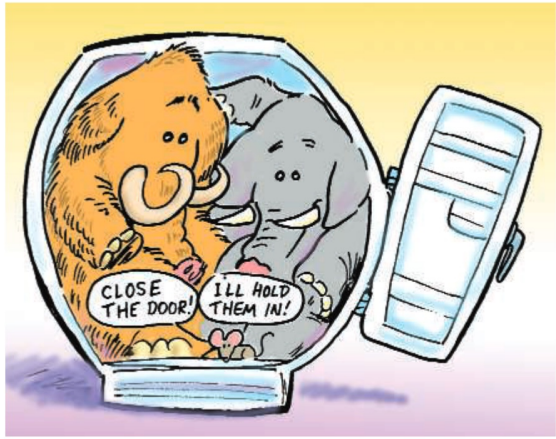
JoP D: Special Issue on Quantum Materials and Emerging Phenomena

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

H. Hwang, 10.1038/nmat3229

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

A: You measure its excitations.

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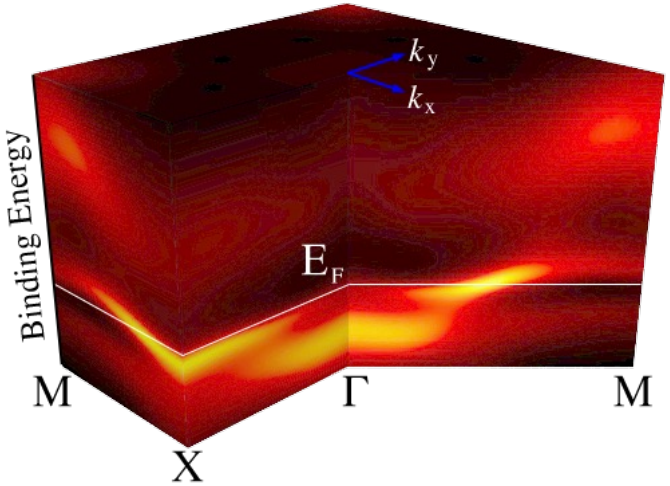
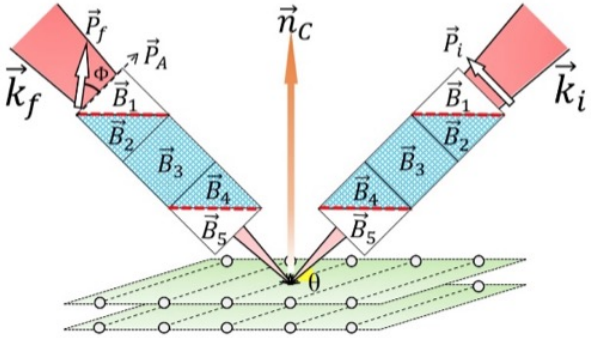
Measuring Excitations

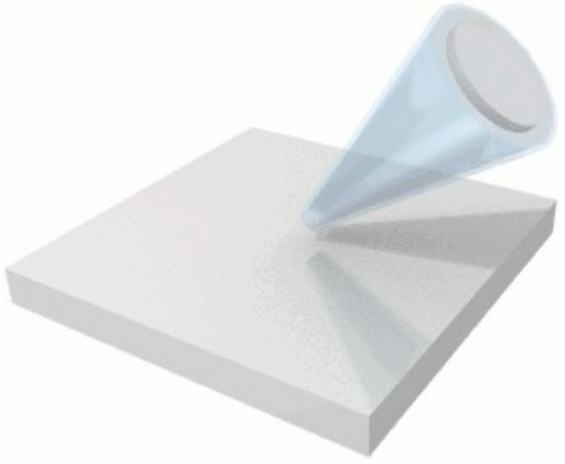
Figures courtesy of Devereaux/Shen group and ORNL



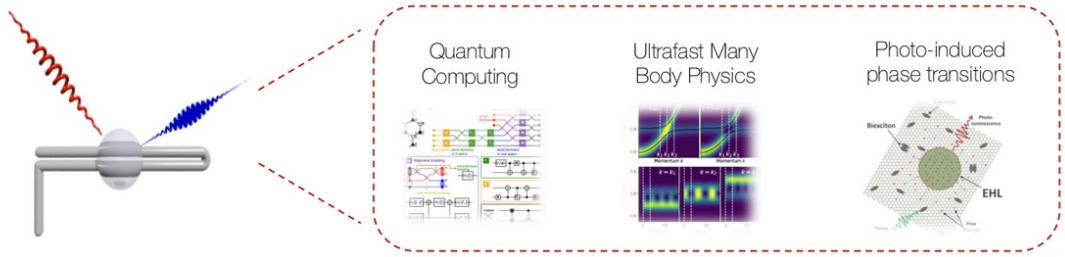
Angle-resolved Photoemission (ARPES)



Neutron Scattering



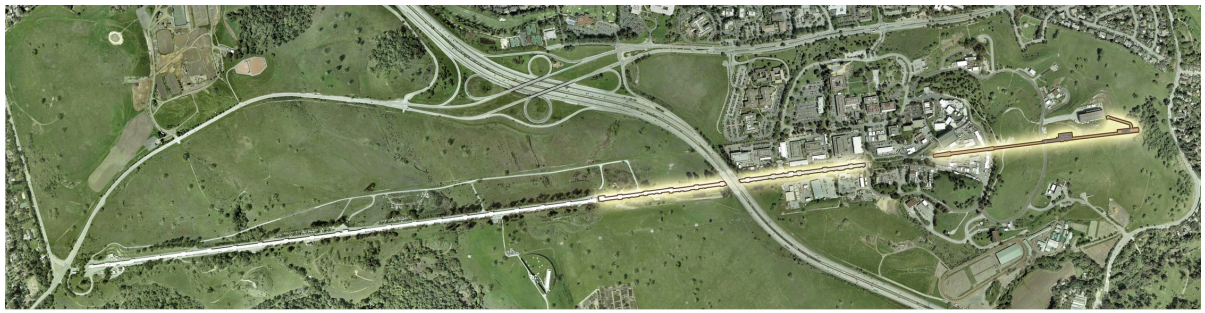
Time-resolved ARPES

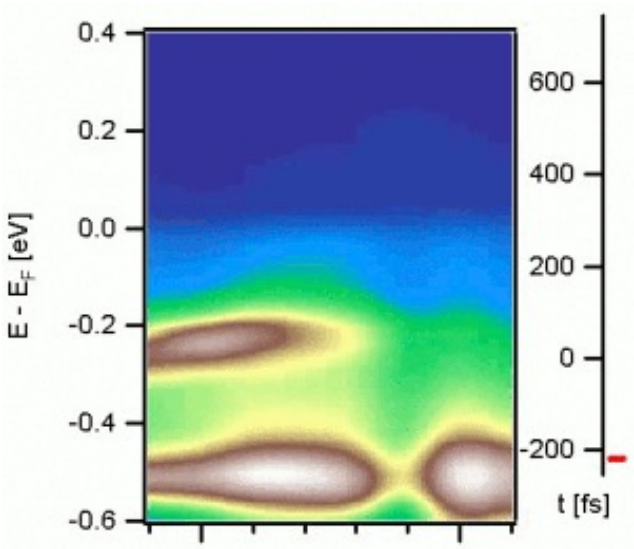


Kemper Lab

Quantum materials in and out of equilibrium.

Time-resolved experiments





Shen group (Stanford)

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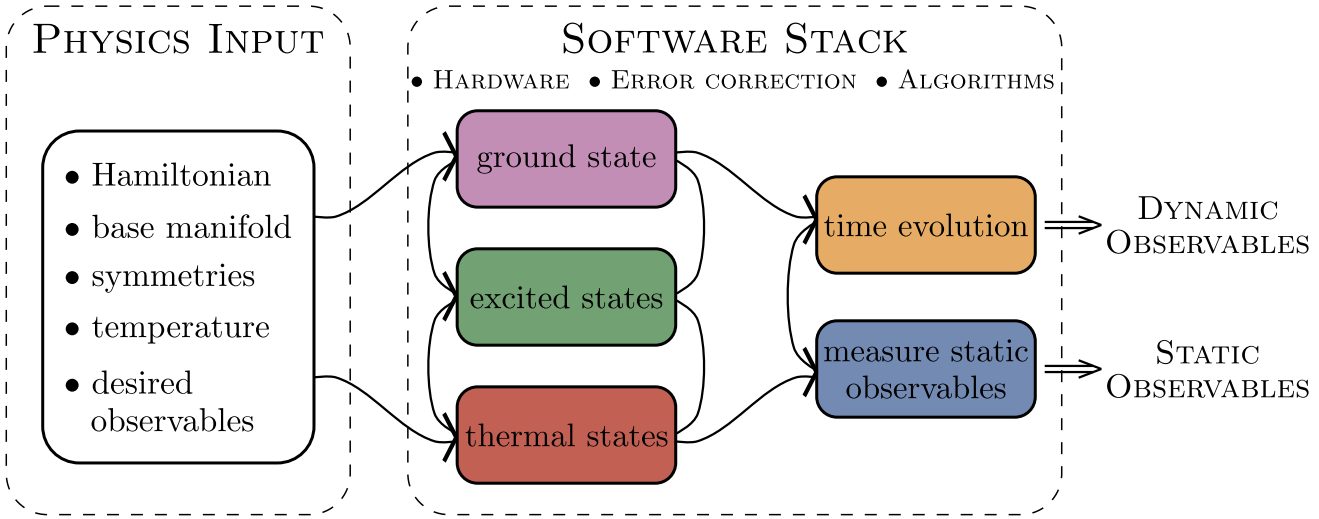
A-Z quantum simulation



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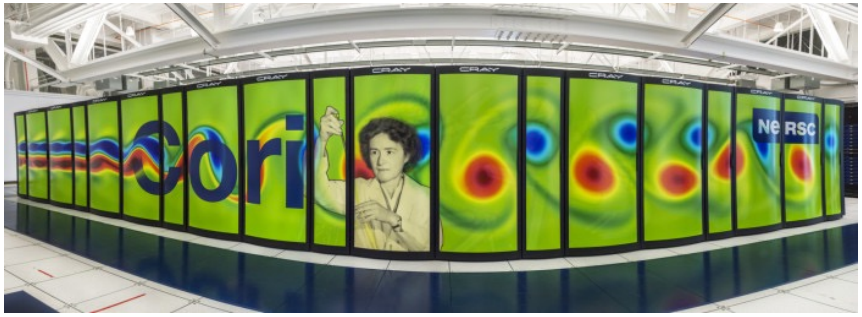
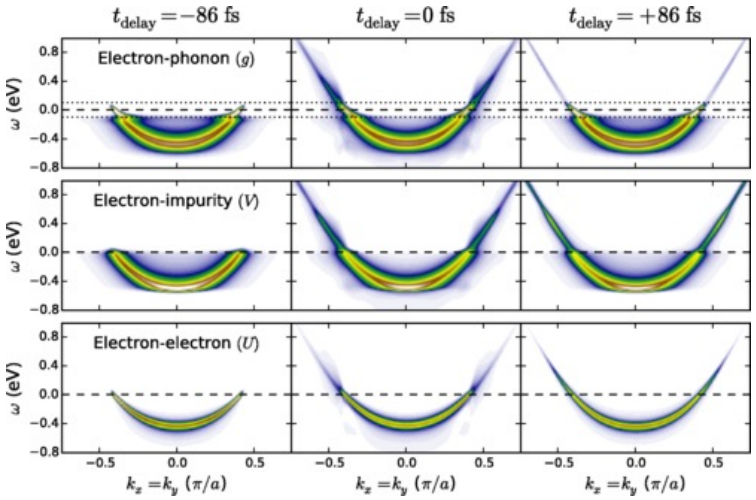
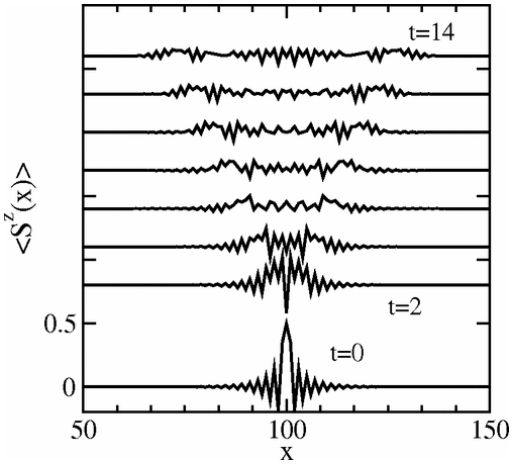




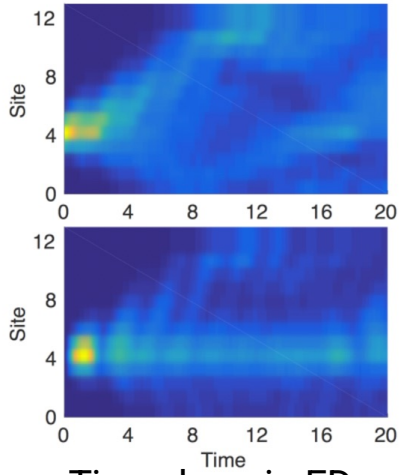
Non-Equilibrium Green's functions

Phys. Rev. X 8, 041009 (2018)



Time domain DMRG

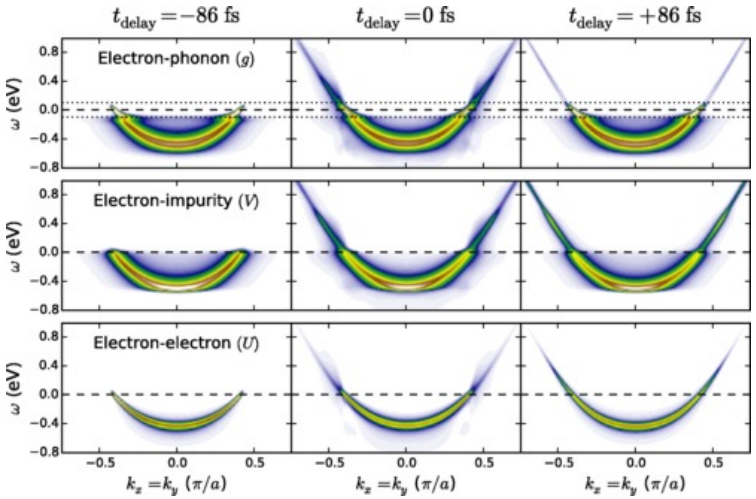
Phys. Rev. Lett. 93, 076401 (2004)



Time domain ED

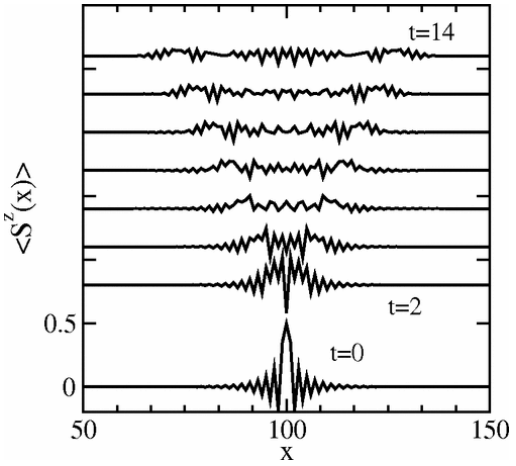
Johnston & Kemper, unpublished

All these techniques eventually reach a barrier.



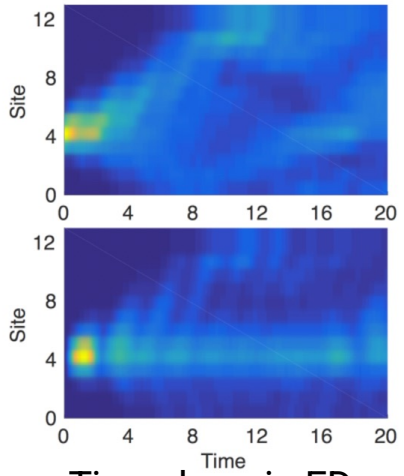
Non-Equilibrium Green's functions

Phys. Rev. X 8, 041009 (2018)



Time domain DMRG

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



Time domain ED

Johnston & Kemper, unpublished

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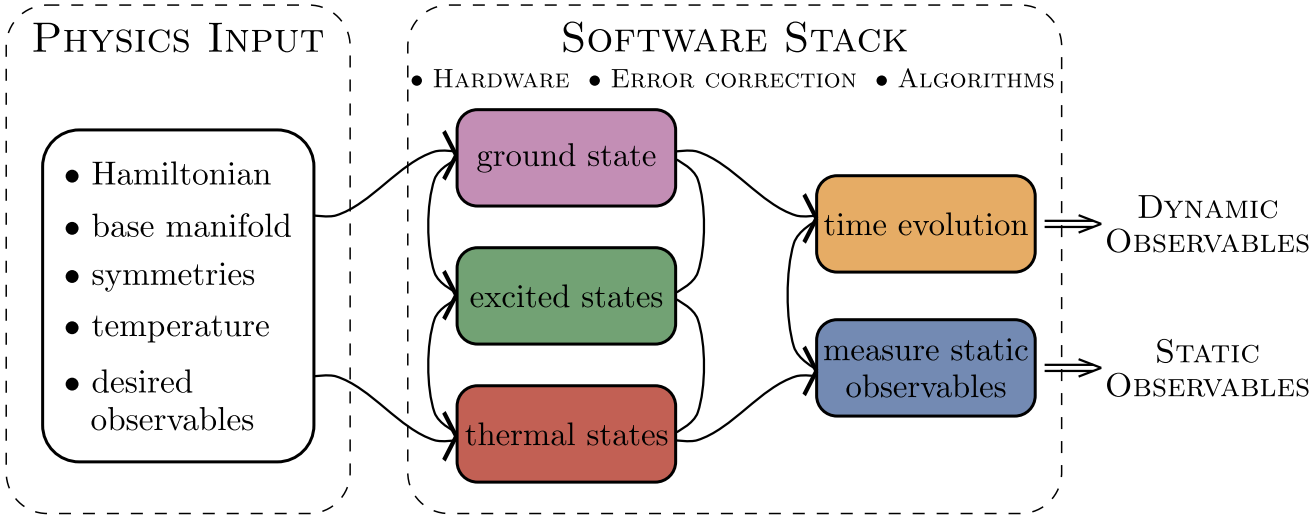
A-Z quantum simulation



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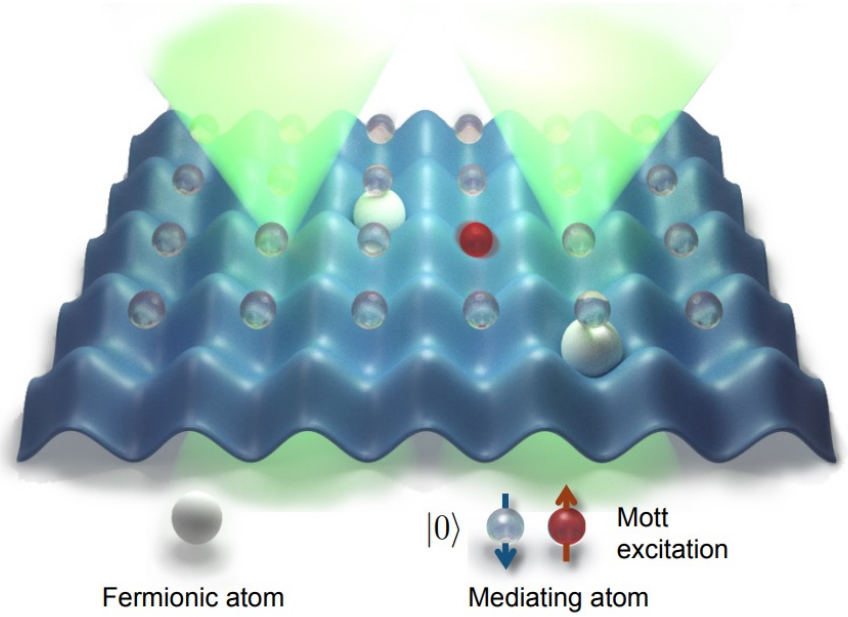
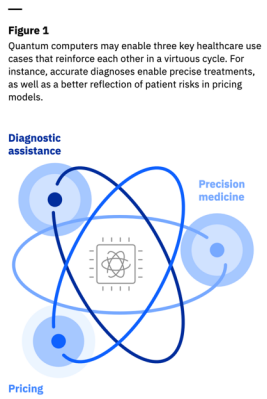
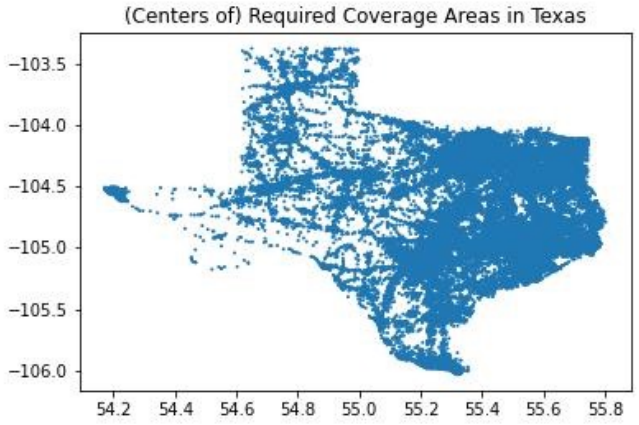
Bespoke quantum simulator

Digital algorithms







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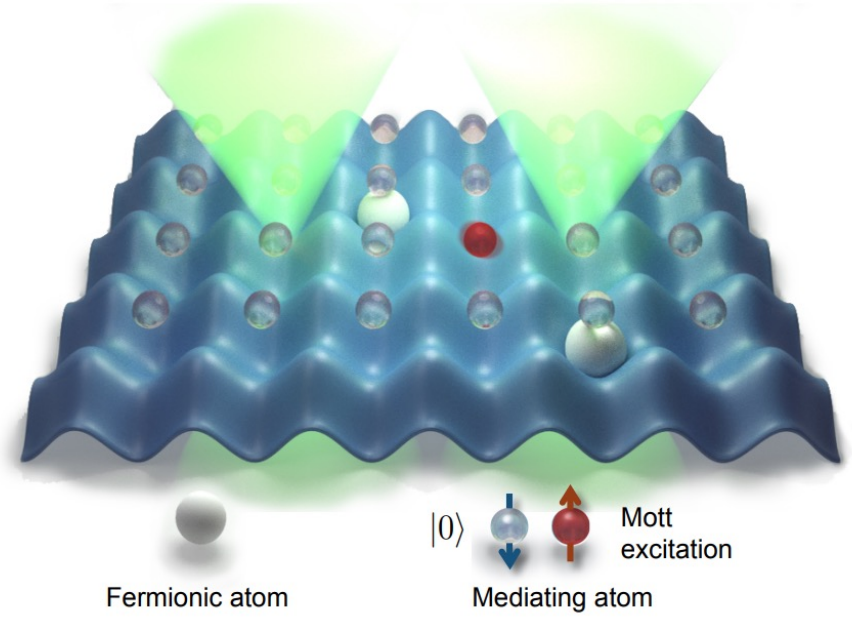
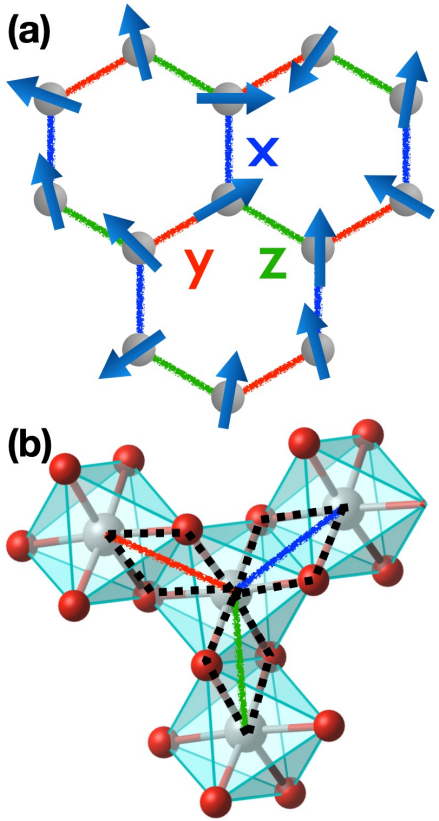
Bespoke quantum simulator — *Digital algorithms*





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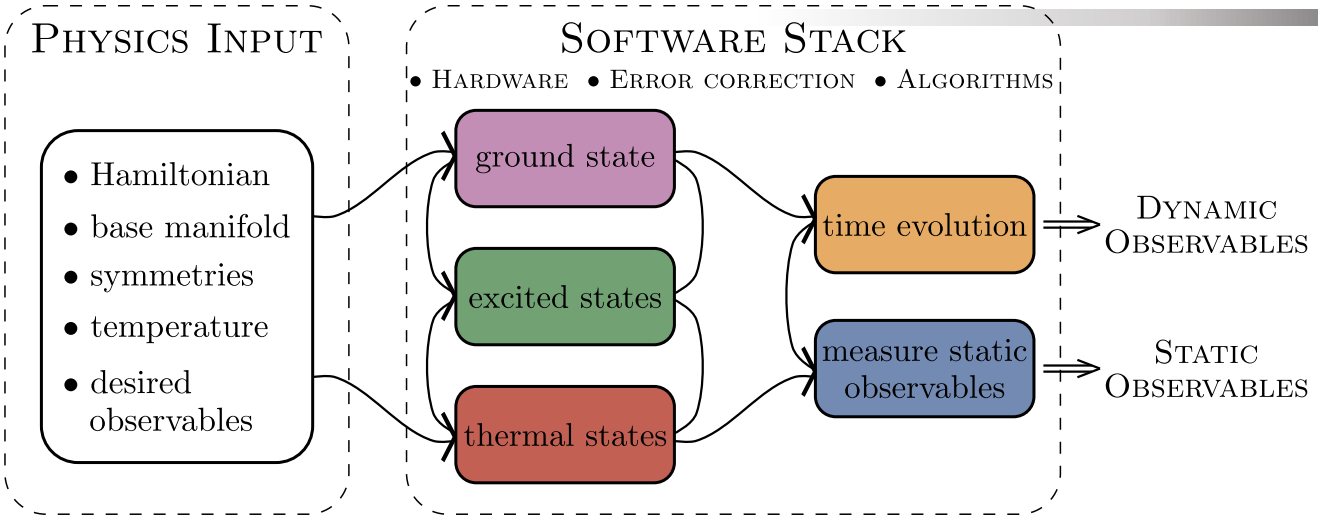
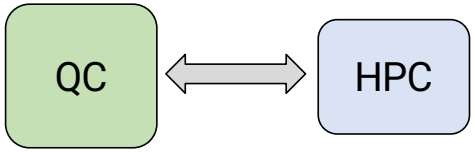
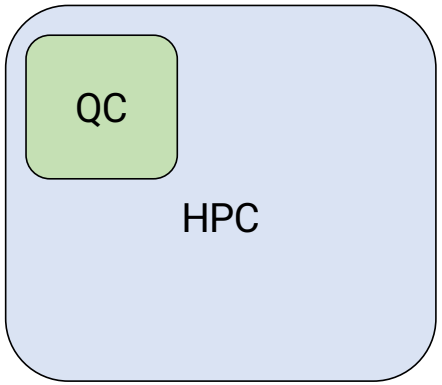
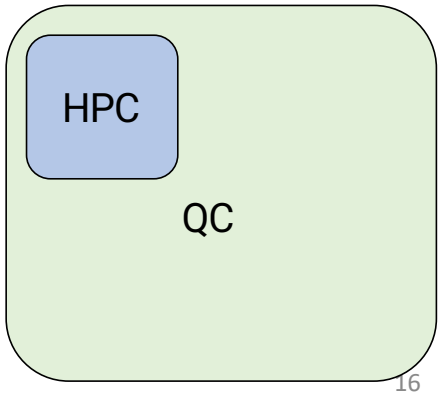
A-Z quantum simulation

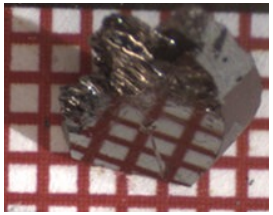


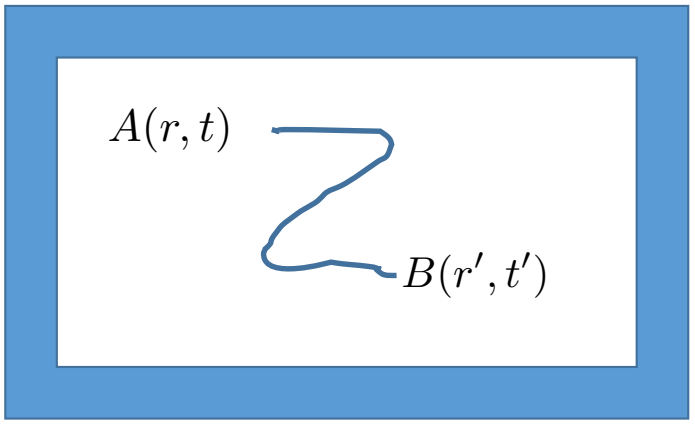






Correlation functions



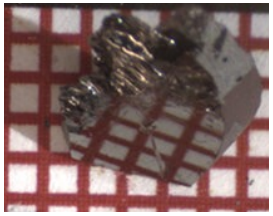


$$\langle A(r,t)B(r',t')\rangle$$

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

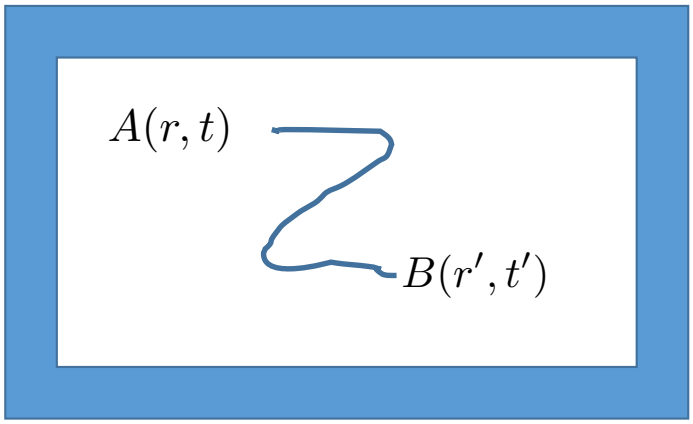
Optical conductivity, γ/X-ray scattering, photoemission, neutron scattering, Raman, IR absorption, etc.

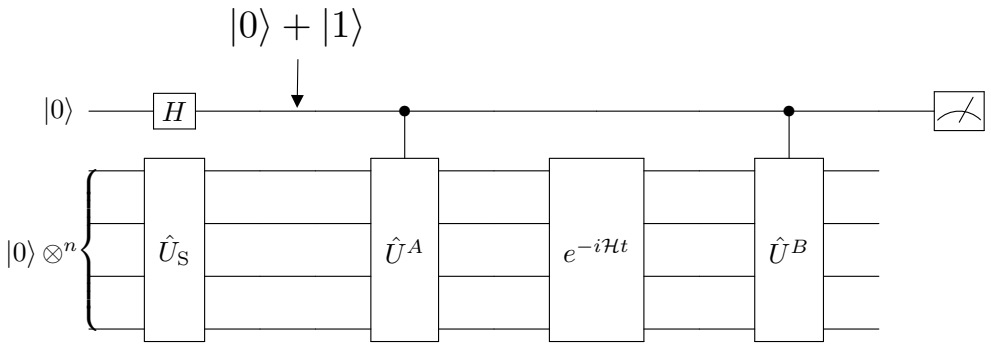
Correlation functions



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

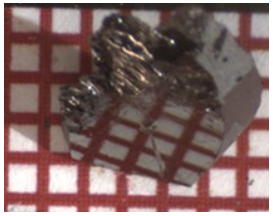
- Interfere with ground state
- Complete expectation value
- Apply excitation B
- Time evolve
- Apply excitation A
- Prepare state of interest

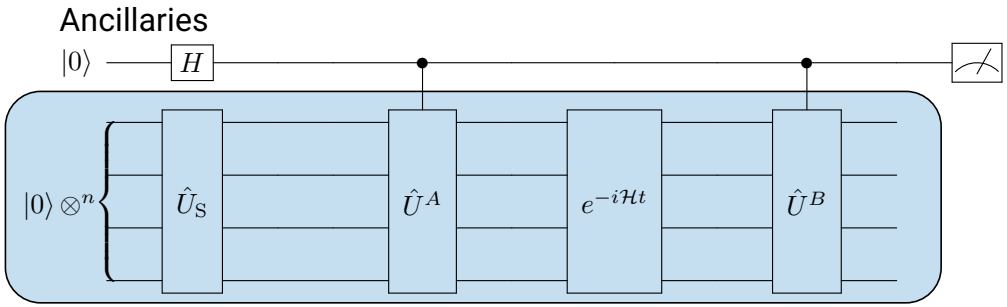


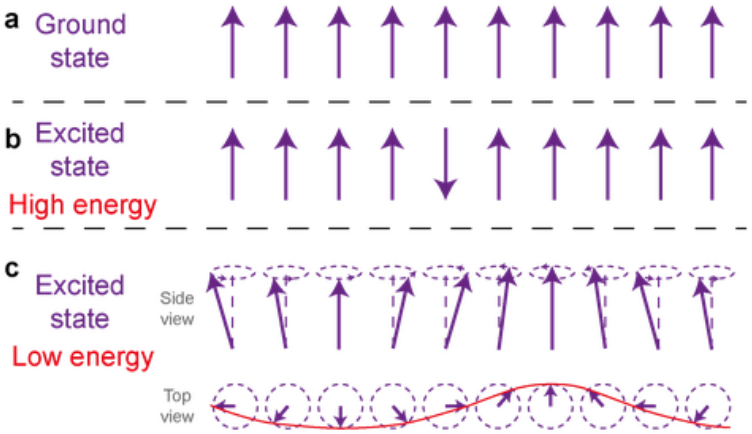


Somma, Simulating physical phenomena by quantum networks (2002)

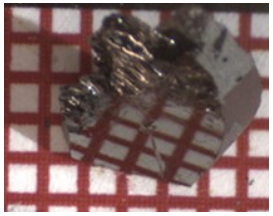
Correlation functions

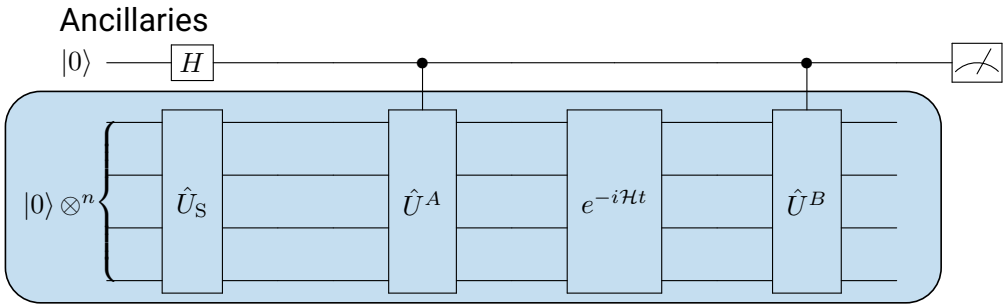




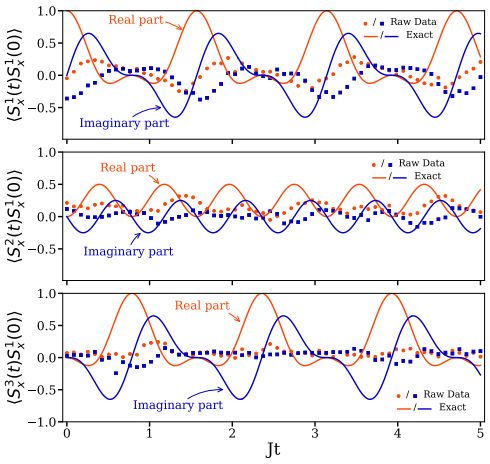


Correlation functions

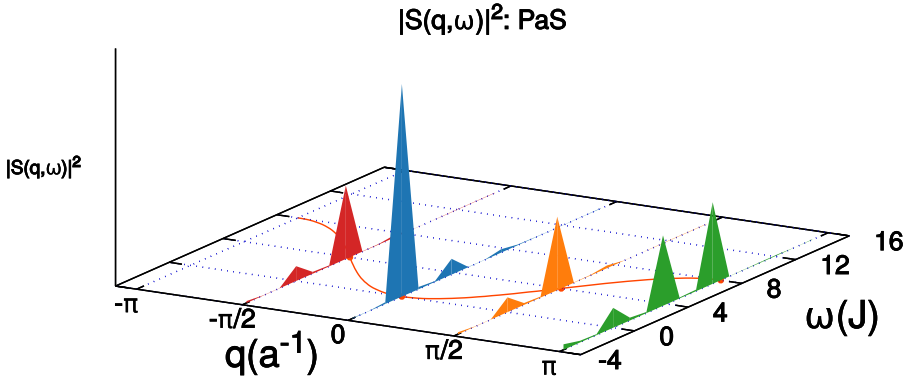




Raw data (2019)



Error mitigation



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

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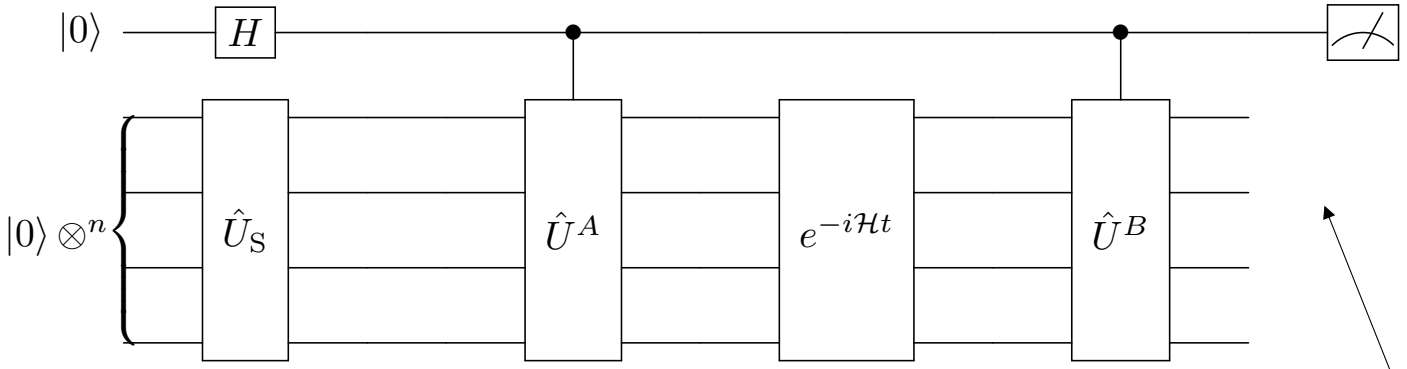
A-Z quantum simulation



Classical post-processing techniques

Prepare state of interest

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

Time evolve

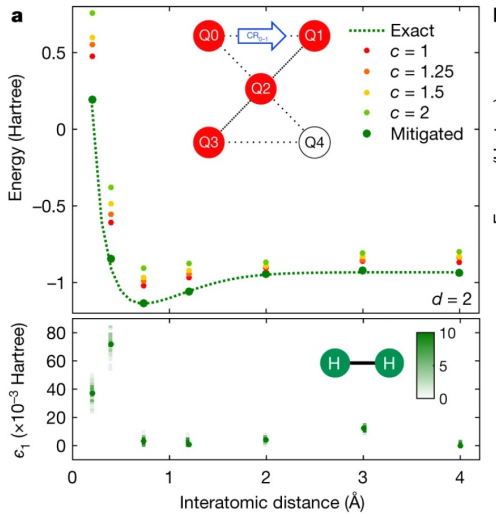
- *Lie-algebraic methods for time evolution*
- *Open quantum system evolution*

Dynamical response functions

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

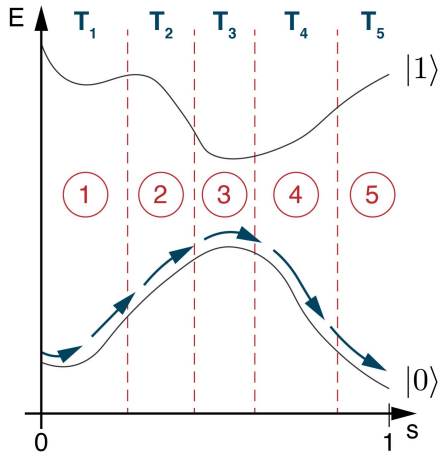
A-Z quantum simulation

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]

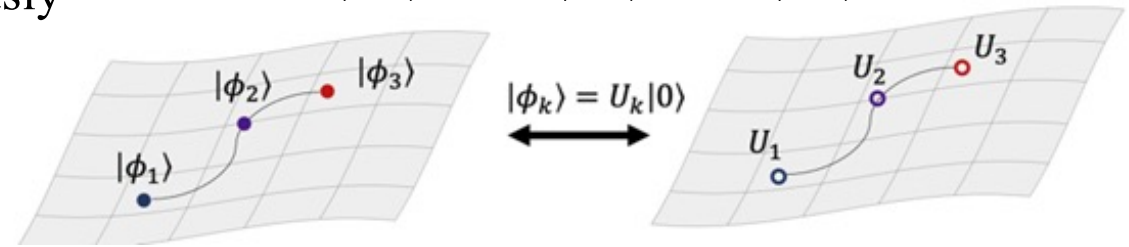
Barren Plateau

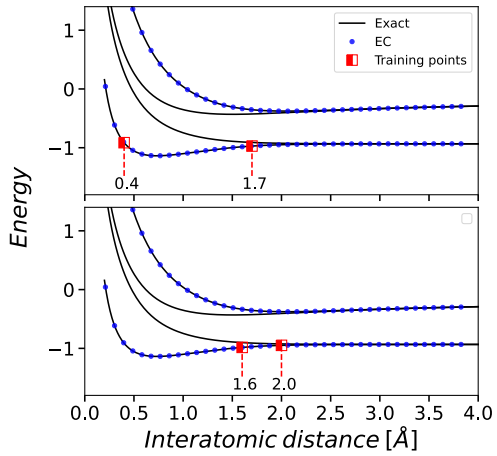
Larger depth circuits

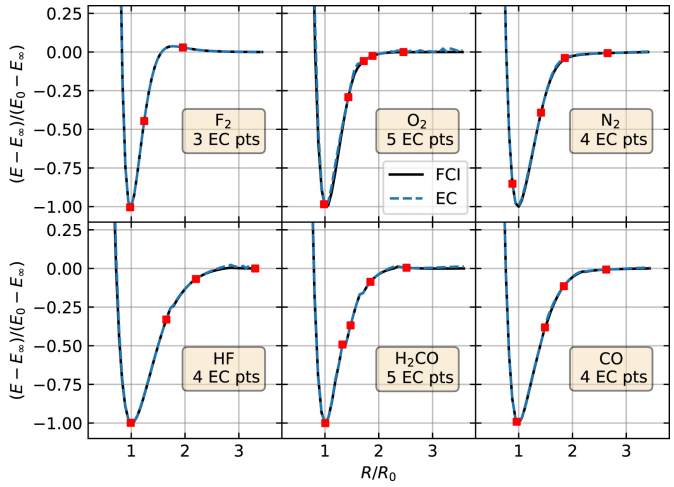
A-Z quantum simulation

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

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







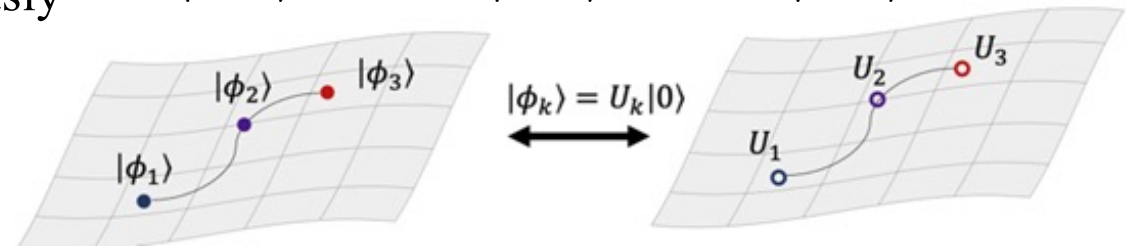
arXiv:2209.10571

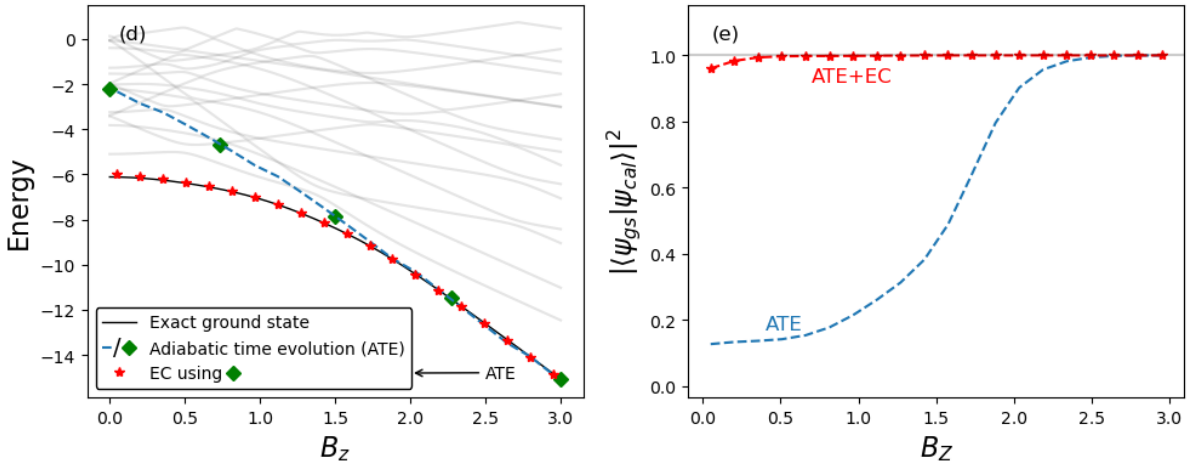
C. Mejuto-Zaera et al., Electron. Struct. 2023

A-Z quantum simulation

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

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





Agrawal, arXiv:2406.17037

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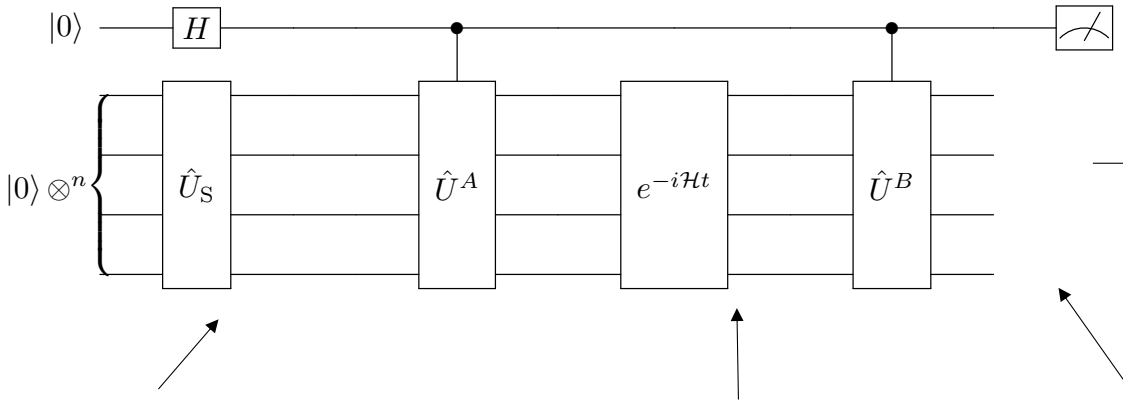
A-Z quantum simulation



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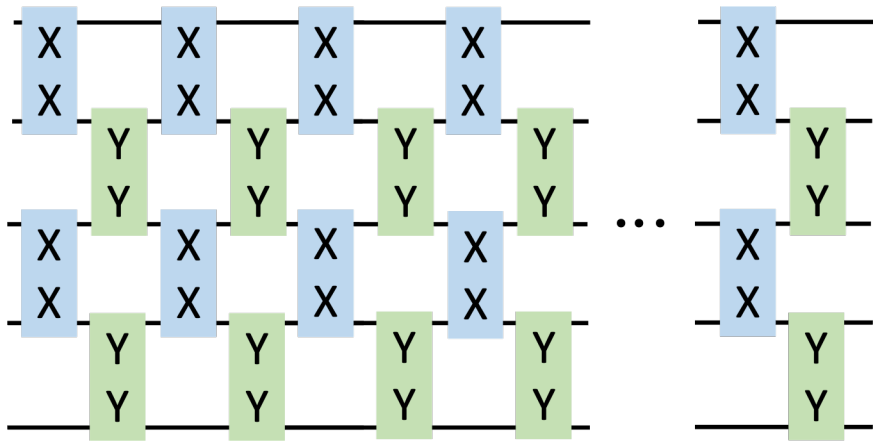
A-Z quantum simulation

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

$U(t) =$ 

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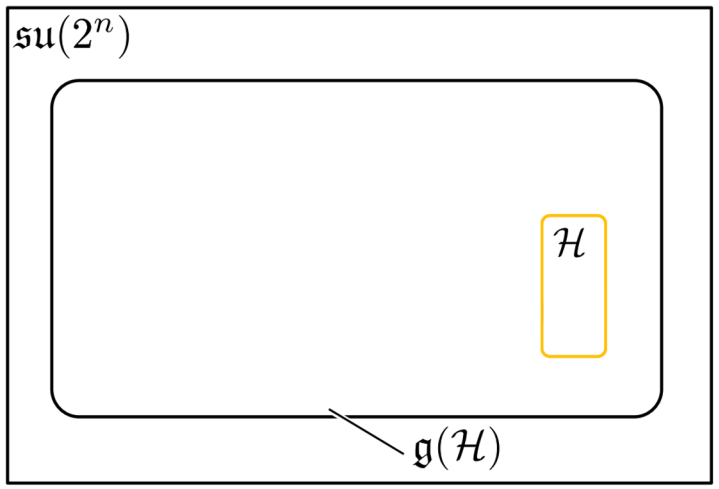
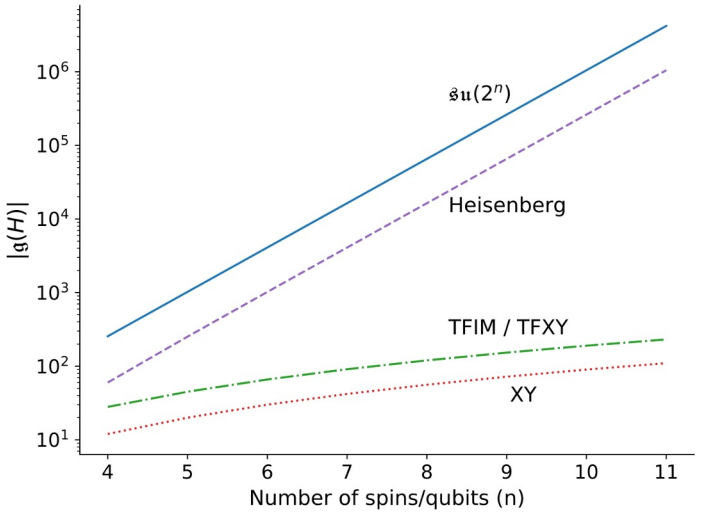
$$U(t) = e^{-it\mathcal{H}} = \prod_{\bar{\sigma}^i \in \mathfrak{su}(2^n)} e^{i\kappa_i \bar{\sigma}^i}$$

$$\bar{\sigma}^i \in \mathfrak{g}(\mathcal{H})$$

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





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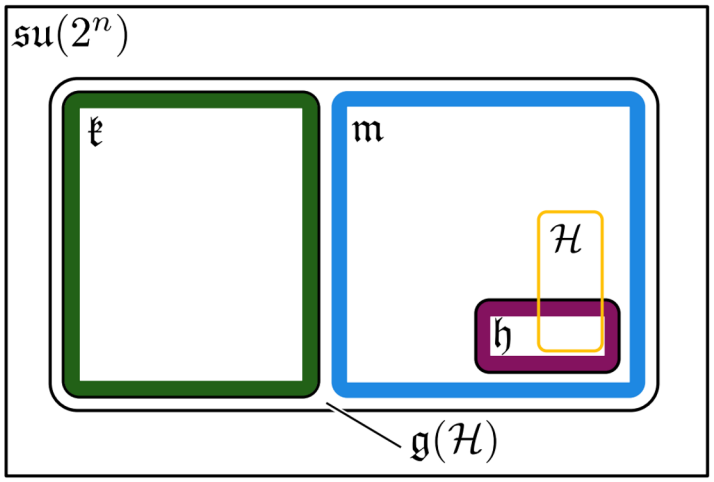

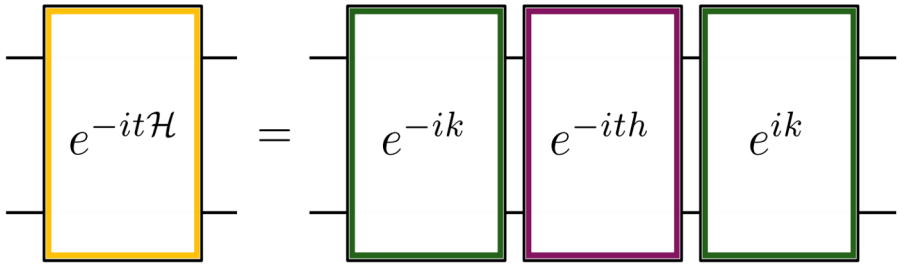

E. Kökcü et al., Phys. Rev. Lett. (2022)

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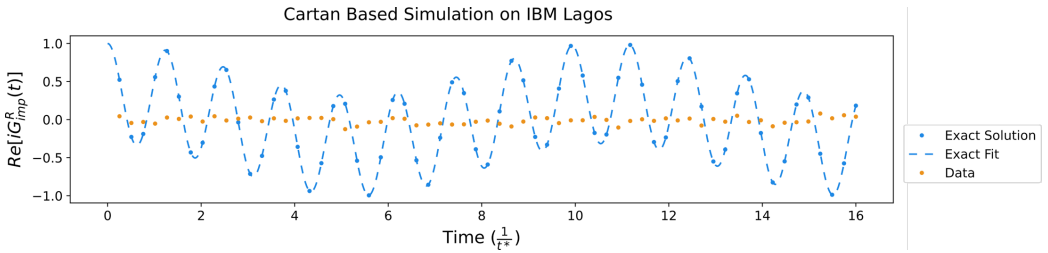

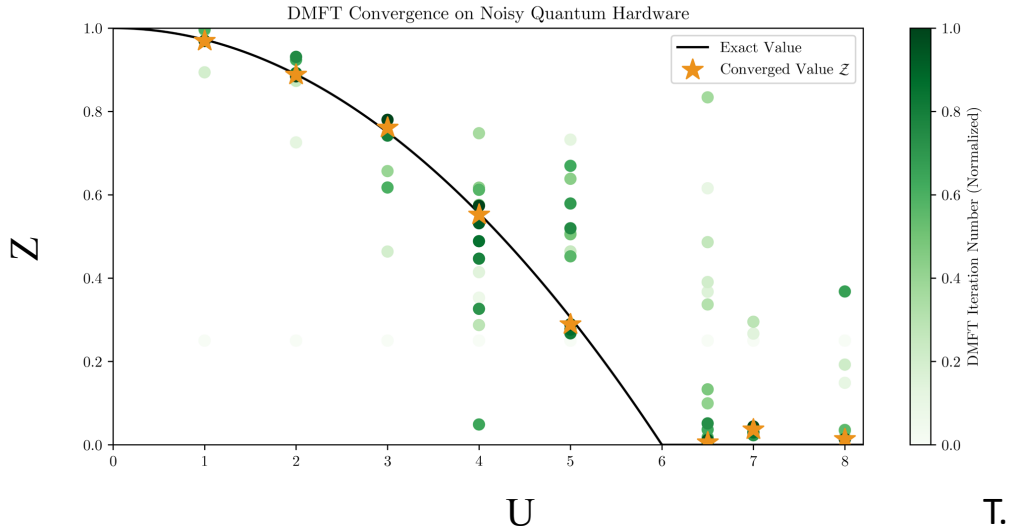

T. Steckmann et al., PRR (2023)

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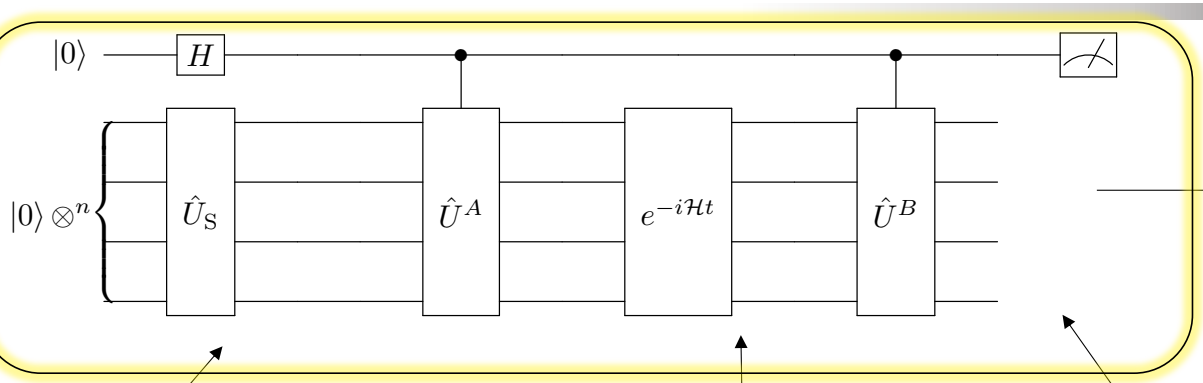

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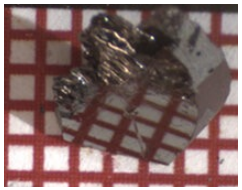
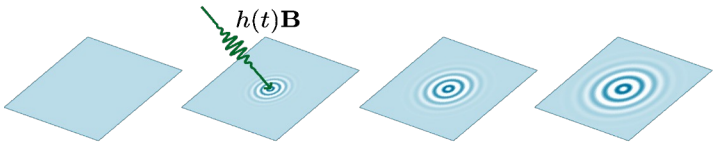
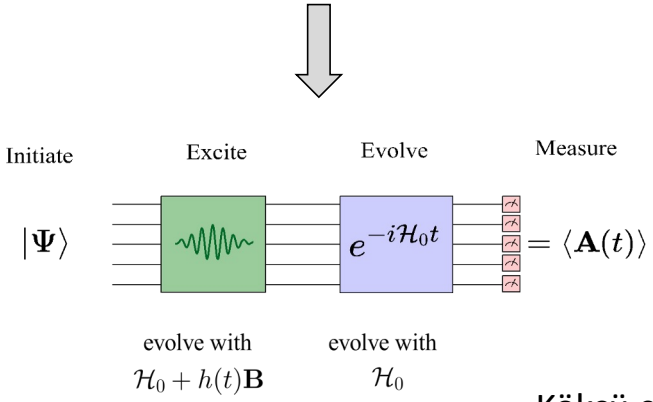






A linear response framework for simulating bosonic and fermionic correlation functions illustrated on quantum computers

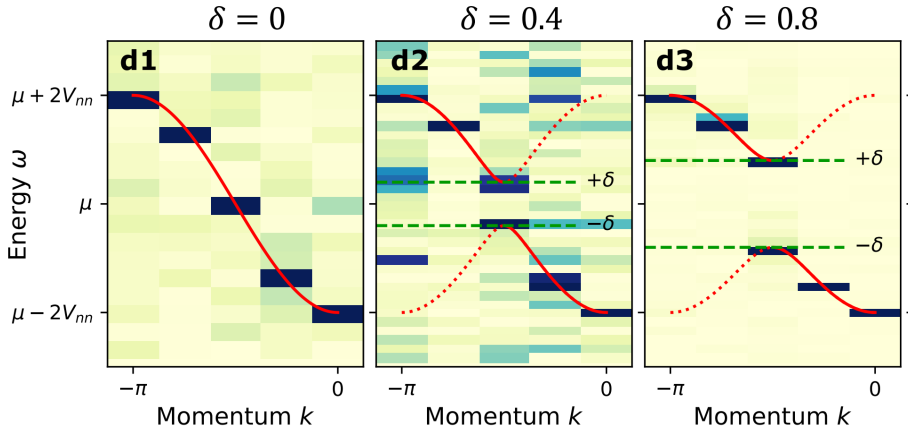
Efekan Kökcü [1], Heba A. Labib [1], J. K. Freericks [2], and A. F. Kemper [1,*]

[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)

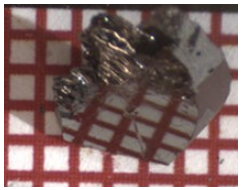
1. Make the excitation part of the quantum simulation

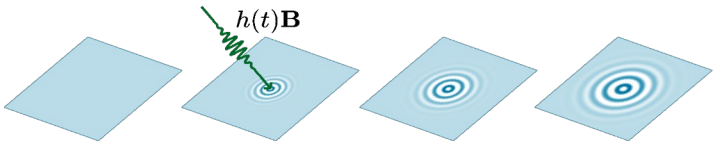
2. Post-process the data to get the response functions

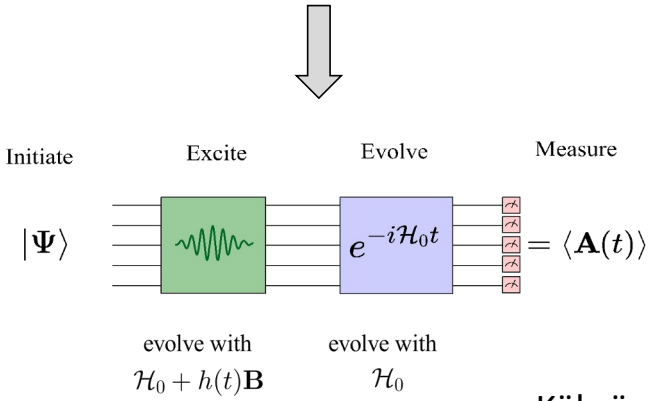


Kökcü et al., Nat. Comm. 2024

A-Z quantum simulation







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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

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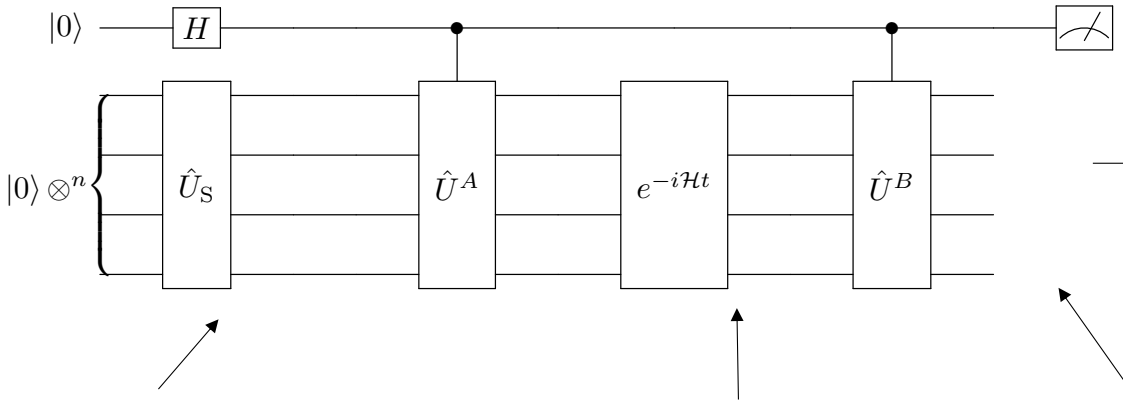
A-Z quantum simulation



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A-Z quantum simulation

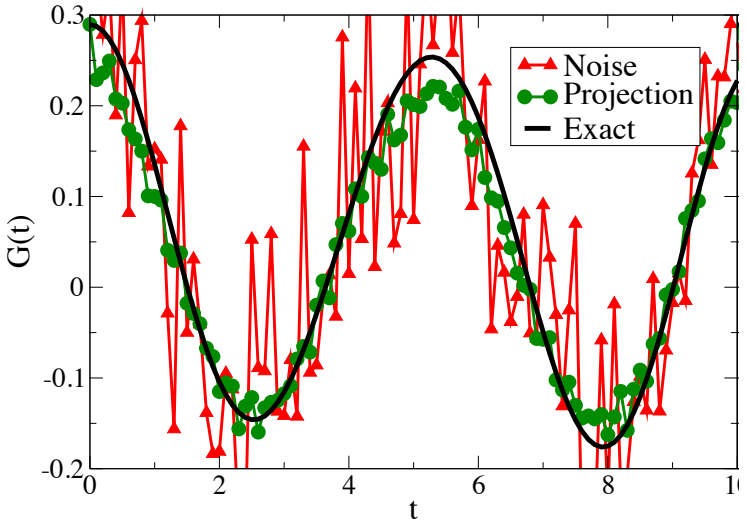
- It turns out that these are positive semi-definite (PSD) functions:

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

- 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 et al., PRL (2024)

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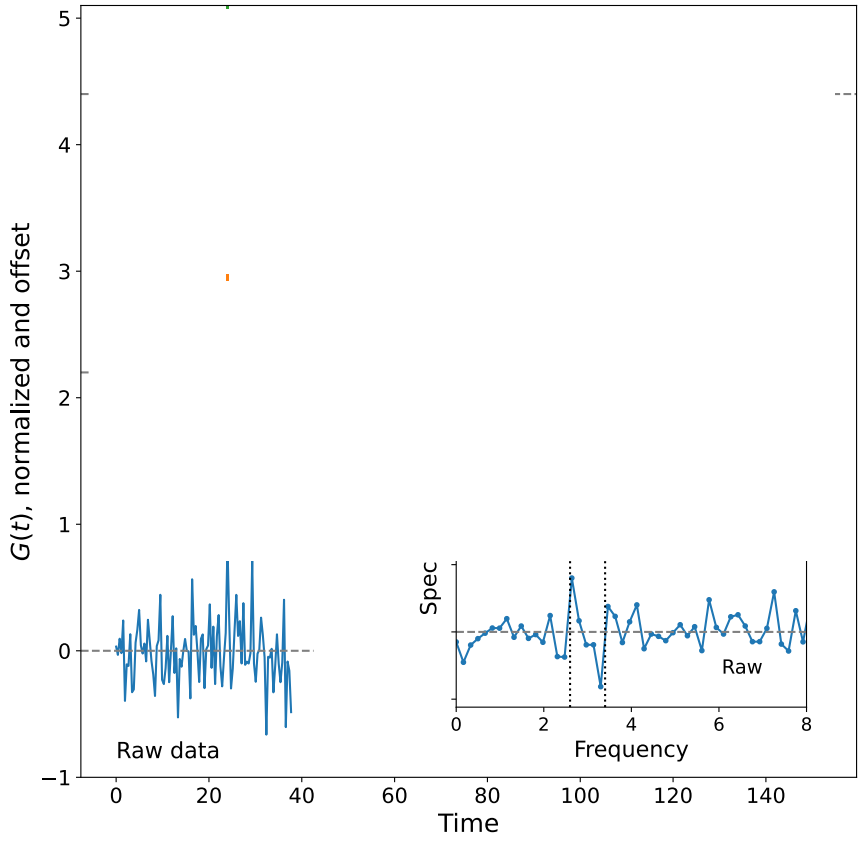

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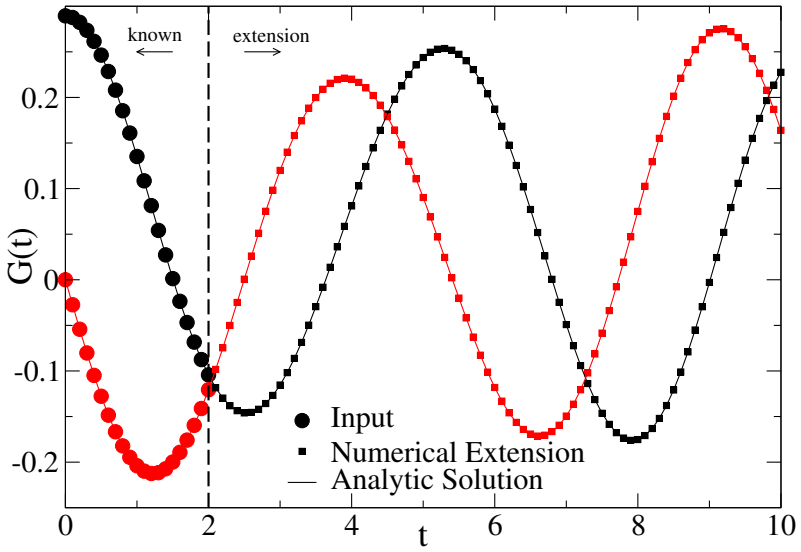

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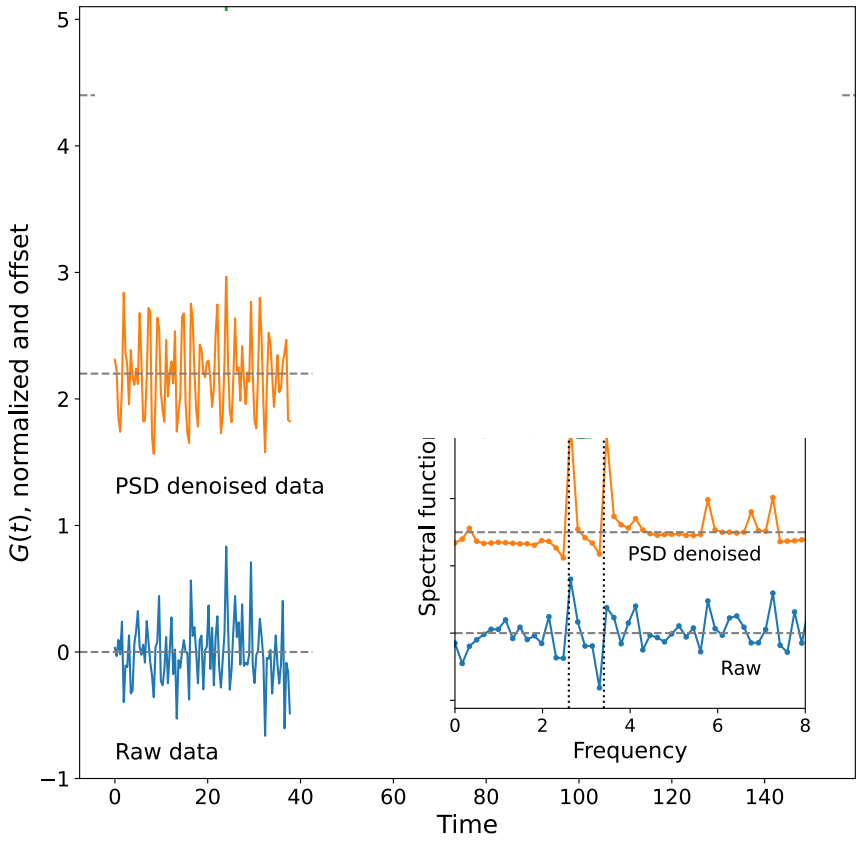

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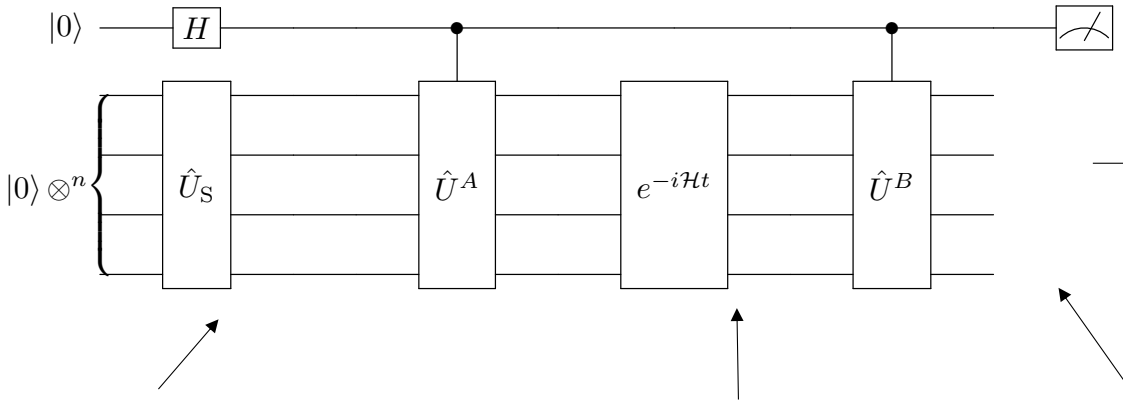

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