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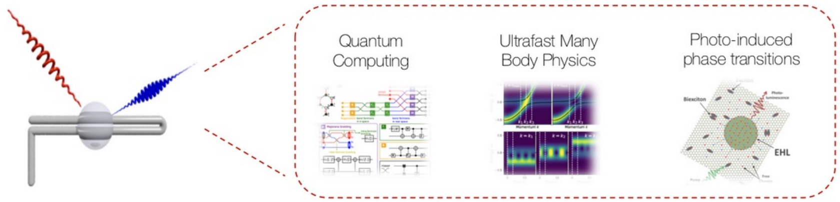
Quantum algorithms for dynamics and dynamical observables

Alexander (Lex) Kemper

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

Virginia Tech
11/16/2023



Kemper Lab

Quantum materials in and out of equilibrium.

Collaborations with:

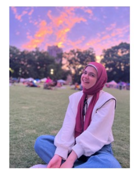
- Bojko Bakalov (NCSU)
- Marco Cerezo, Martin de la Rocca (LANL)
- Jim Freericks (Georgetown)
- Daan Camps, Roel van Beeumen, Bert de Jong, Akhil Francis (LBNL)
- Thomas Steckmann (UMD)
- Yan Wang, Eugene Dumitrescu (ORNL)

Current members

Alexander (Lex) Kemper
Principal investigator

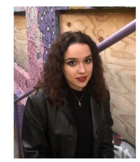
Efekan Kökcü
Graduate Researcher

Anjali Agrawal
Graduate Researcher



Heba Labib
Graduate Researcher

Jack Howard
Undergraduate Researcher

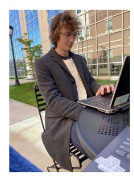


Natalia Wilson
Undergraduate Researcher

Daniel Brandon
Undergraduate Researcher

Sarah Klas
Undergraduate Researcher

Norman Hogan
Graduate Researcher



Ethan Blair
Undergraduate Researcher

Your Name
New lab member

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Brief outline

- Quantum Matter meets Quantum Computing
- Response functions
  - Why we care
  - How do find them
- A different paradigm: Making the experiment part of the simulation via linear response
- Lie algebras for fun and profit (and quantum computing)

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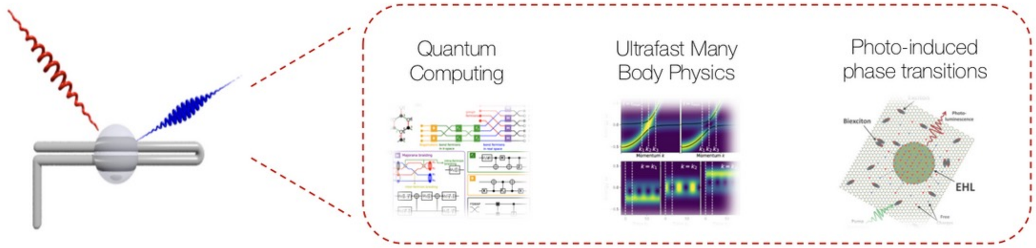
Why quantum computing for condensed matter?



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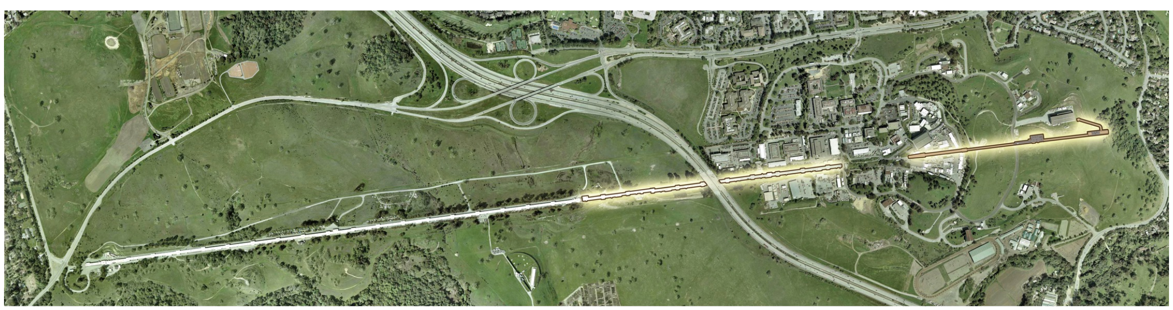
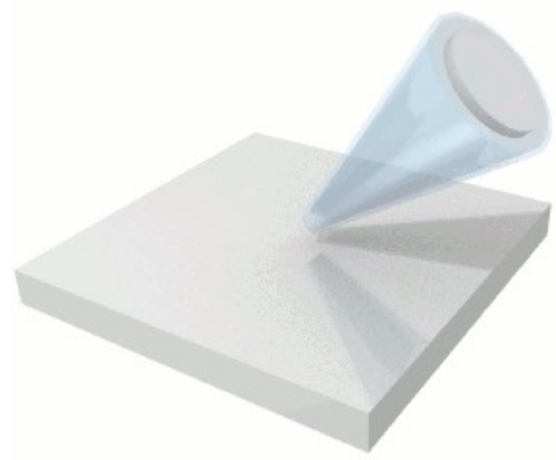
Quantum materials in and out of equilibrium.

Time-resolved experiments





Shen group (Stanford)

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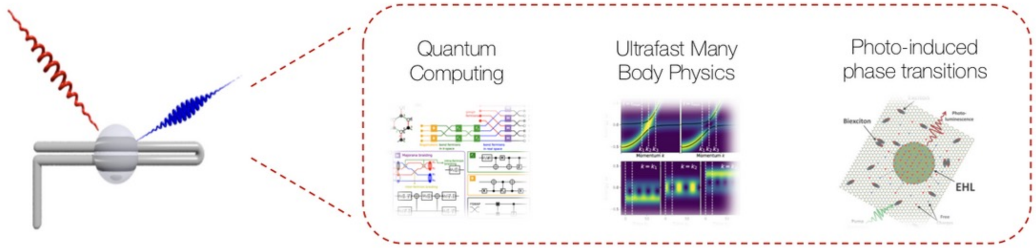

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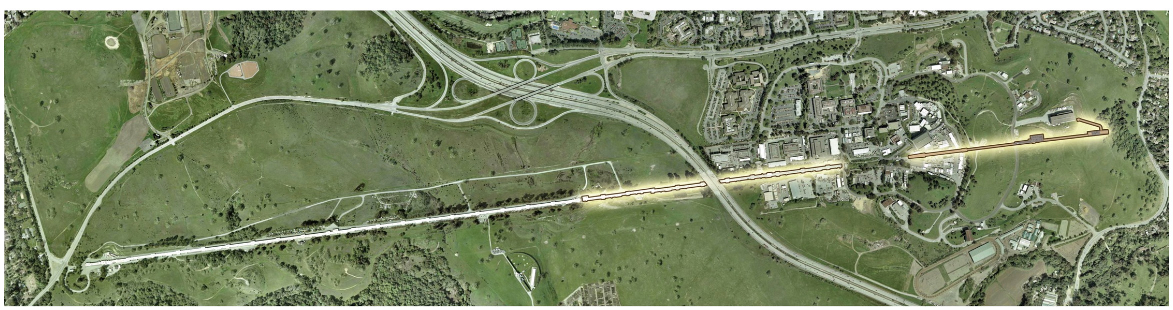
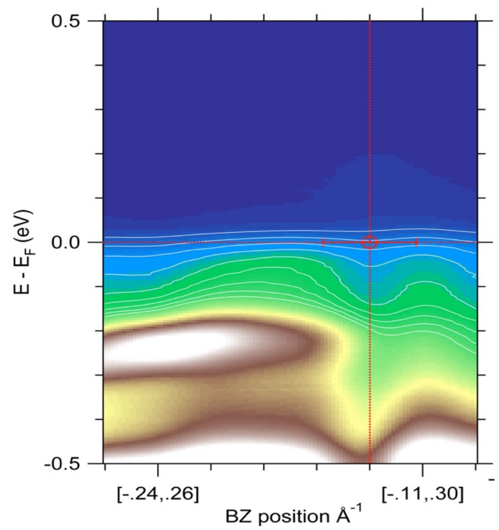


$ErTe_3$



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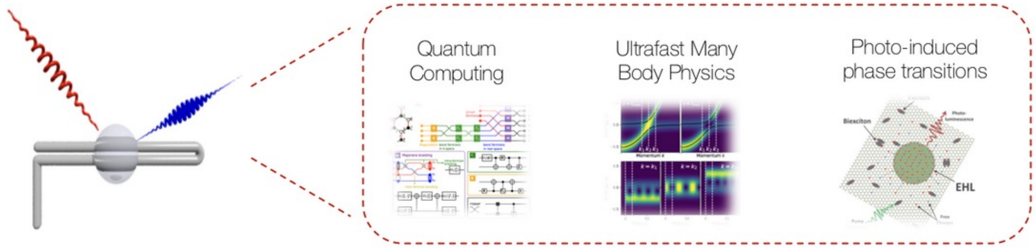

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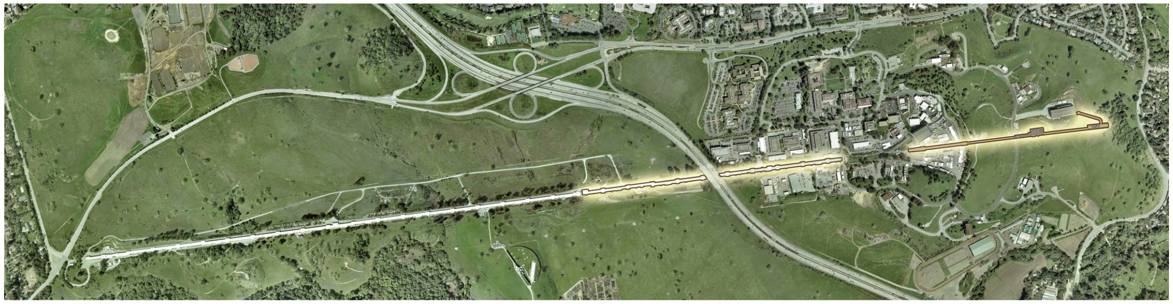

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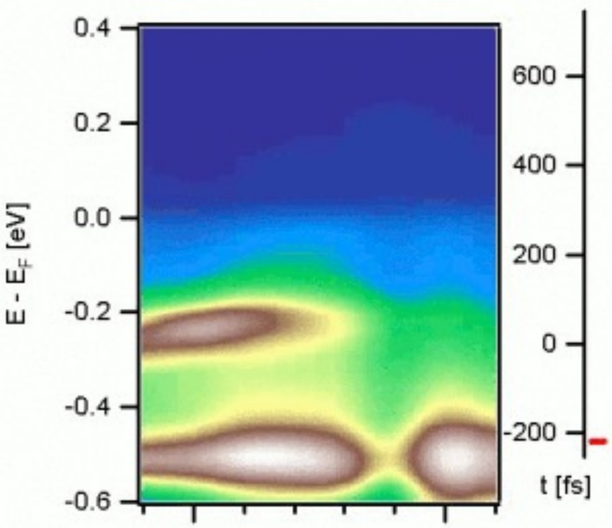

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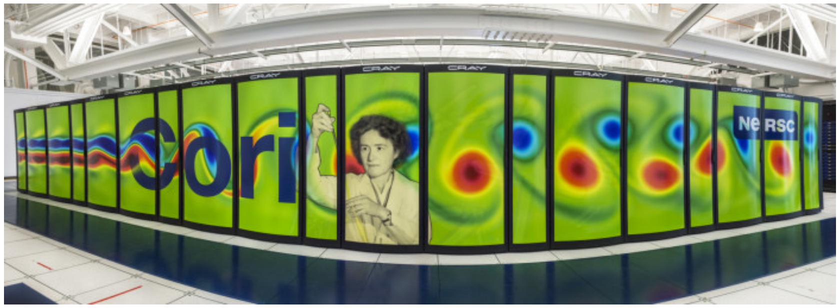
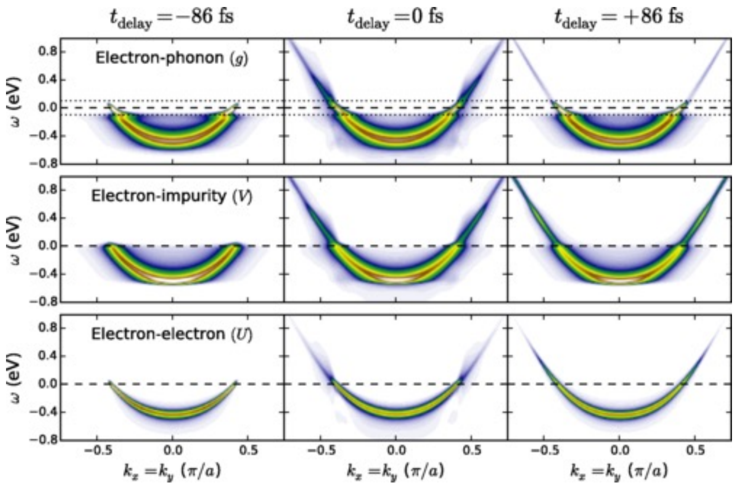
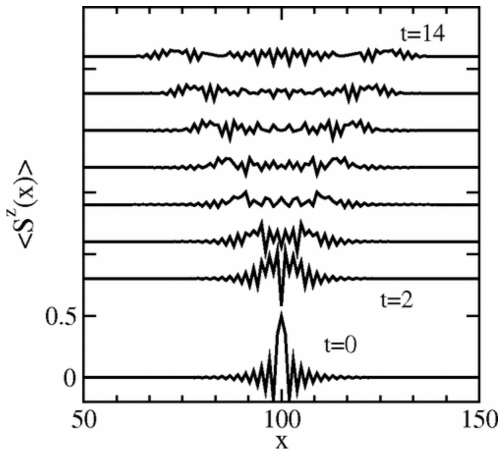




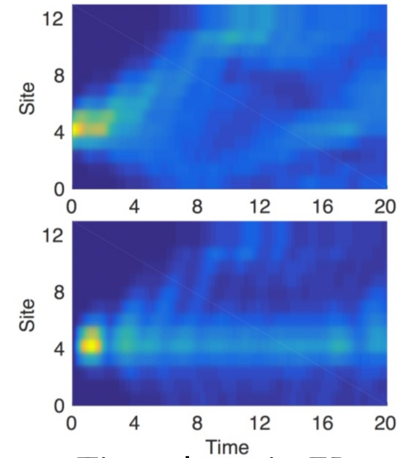
Non-Equilibrium Green's functions

Phys. Rev. X 8, 041009 (2018)



Time domain DMRG

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

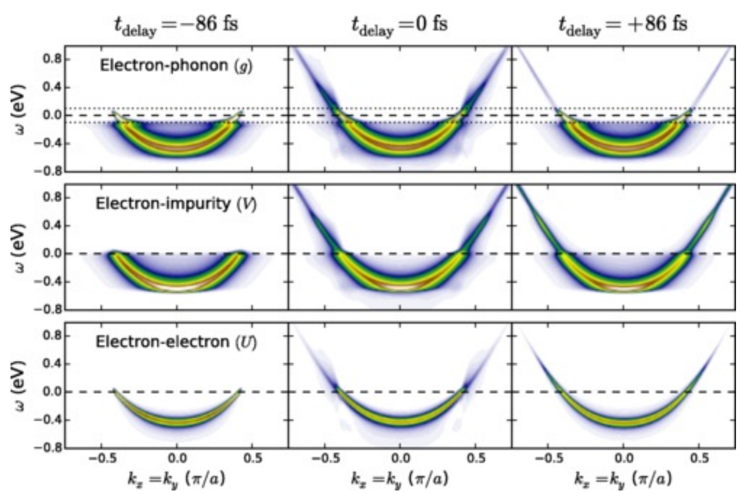


Time domain ED

Johnston & Kemper, unpublished

Why quantum computing for condensed matter?

All these techniques eventually reach a barrier.



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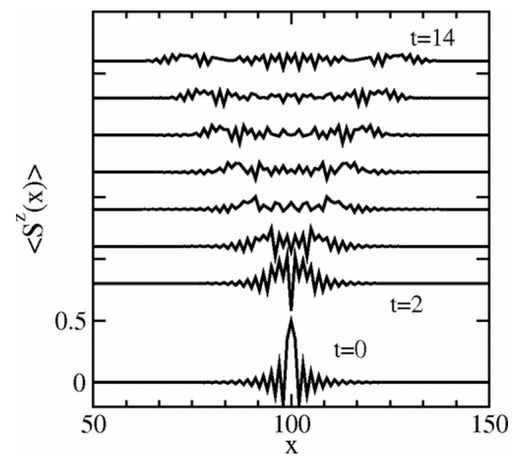

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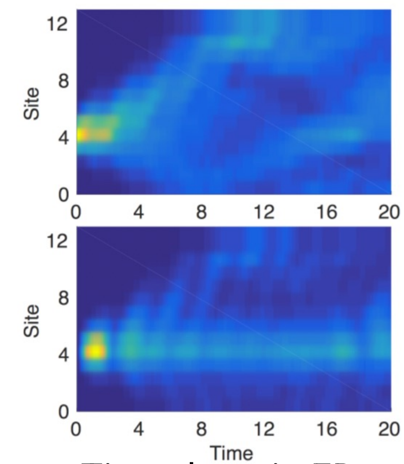

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Quantum Matter meets Quantum Computing

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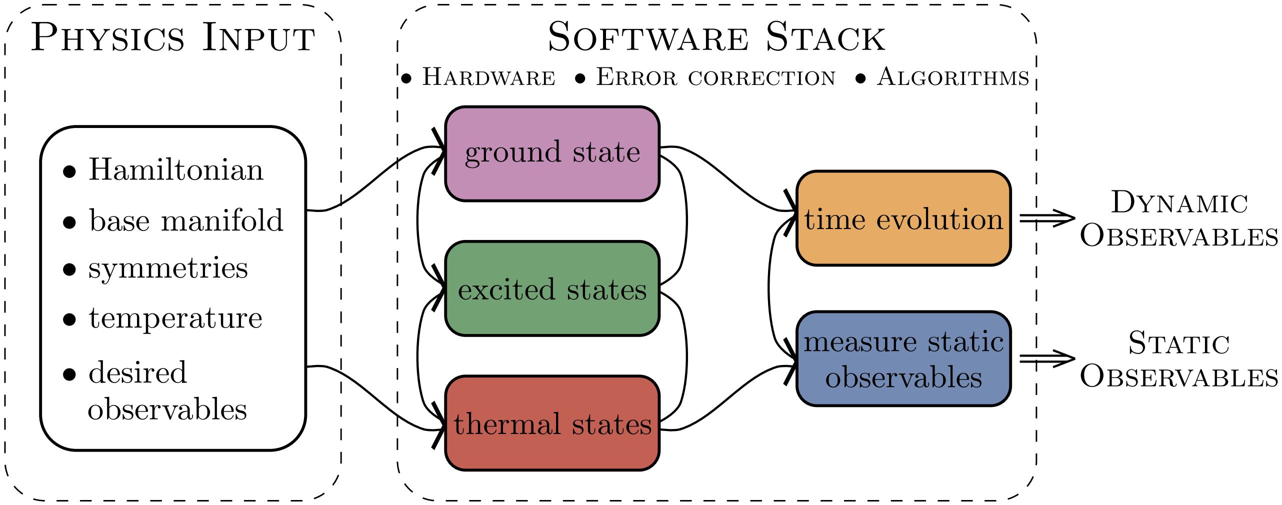
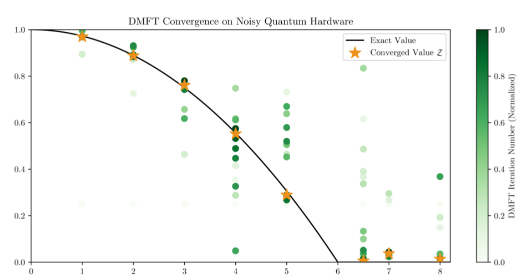
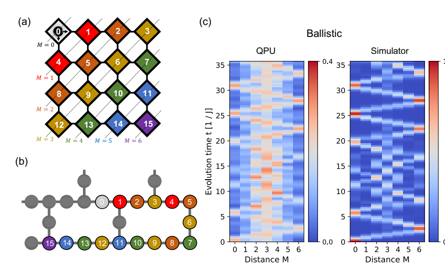


Self-consistent DMFT phase diagram for 2-site Hubbard model on IBM hardware



Free fermionic evolution on a 4x4 lattice on IBM hardware



- Experimental relevance: Measuring correlation functions
- Measuring exact integer Chern numbers for topological states
- Driven/dissipative systems and fixed points (1000 Trotter steps)
- Exact time evolution via Lie algebraic decomposition and compression
- Thermodynamics via Lee-Yang Zeros
- Physics-Informed Subspace Expansions

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

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Ising Model

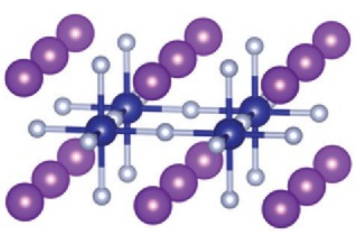
794 Brazilian Journal of Physics, vol. 30, no. 4, December, 2000

The Ising Model and Real Magnetic Materials

W. P. Wolf
Yale University, Department of Applied Physics,
P.O. Box 208284, New Haven, Connecticut 06520-8284, U.S.A.

Received on 3 August, 2000

The factors that make certain magnetic materials behave similarly to corresponding Ising models are reviewed. Examples of extensively studied materials include $Dy(C_2H_5SO_4)_3.9H_2)$ (DyES), $Dy_3Al_5O_{12}$ (DyAlG), $DyPO_4$, $Dy_2Ti_2O_7$, $LiTbF_4$, K_2CoF_4, and Rb_2CoF_4. Various comparisons between theory and experiment for these materials are examined. The agreement is found to be generally very good, even when there are clear differences between the ideal Ising model and the real materials. In a number of experiments behavior has been observed that requires extensions of the usual Ising model. These include the effects of long range magnetic dipole interactions, competing interaction effects in field-induced phase transitions, induced staggered field effects and frustration effects, and dynamic effects. The results show that the Ising model and real magnetic materials have provided an unusually rich and productive field for the interaction between theory and experiment over the past 40 years.



10.1039/c6cp02362b

Heisenberg model

PHYSICAL REVIEW B
covering condensed matter and materials physics

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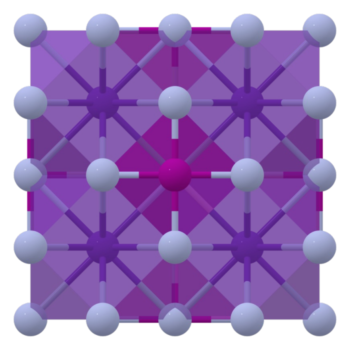
Critical behavior of the three-dimensional Heisenberg antiferromagnet $RbMnF_3$

R. Coldea, R. A. Cowley, T. G. Perring, D. F. McMorrow, and B. Roessli
Phys. Rev. B **57**, 5281 – Published 1 March 1998



Materials project

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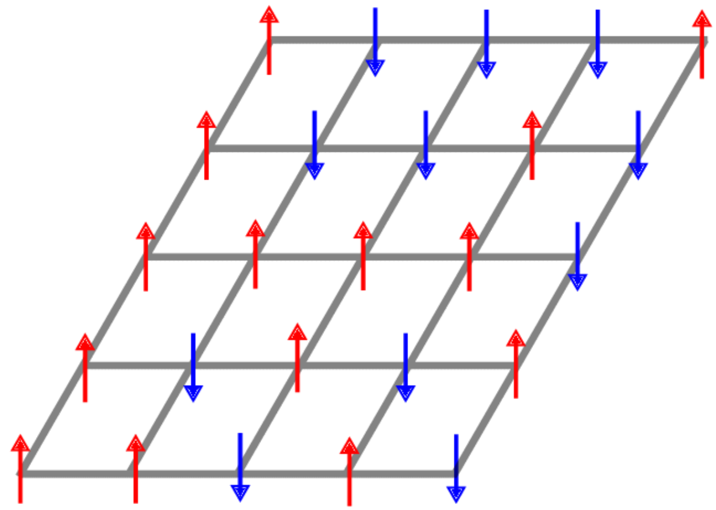
Ising Model

$$\mathcal{H} = -J\sum_i \sigma_i^z \sigma_{i+1}^z + h_x \sum_i \sigma_i^x$$



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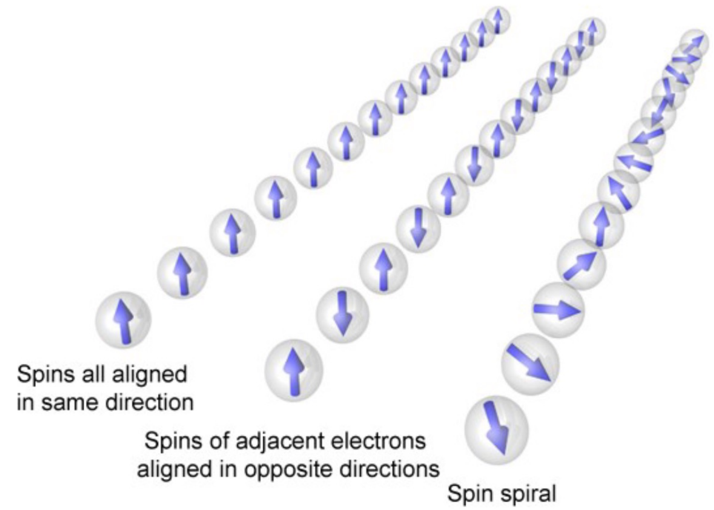

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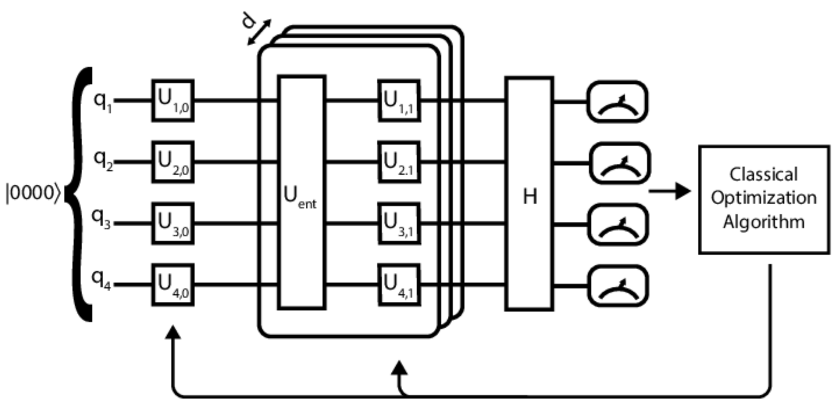

[Optimization of the Variational Quantum Eigensolver for Quantum Chemistry Applications]()

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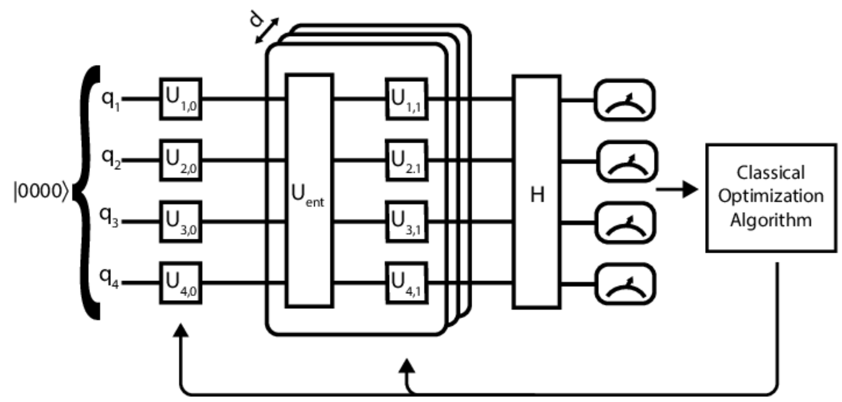

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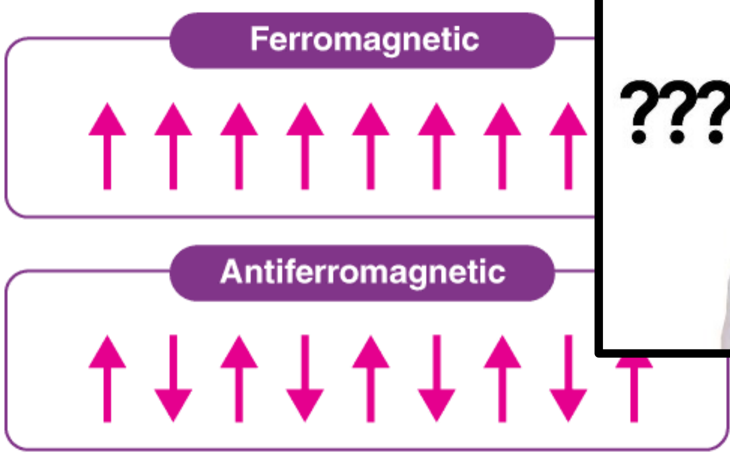

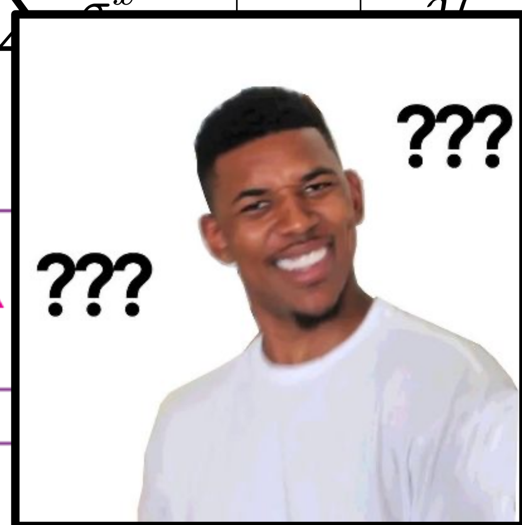

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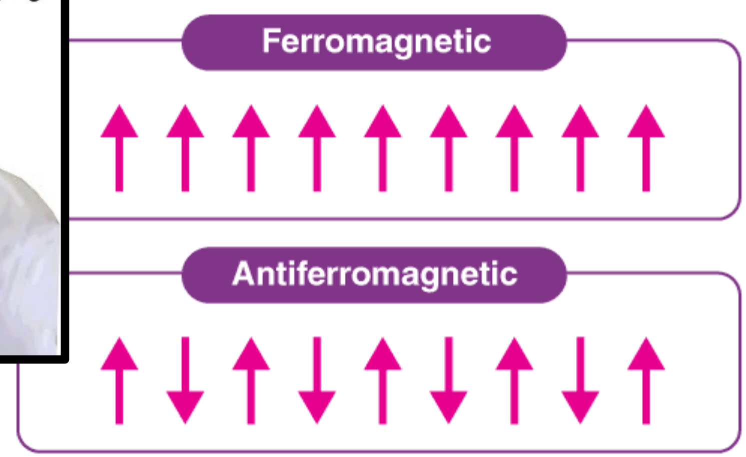
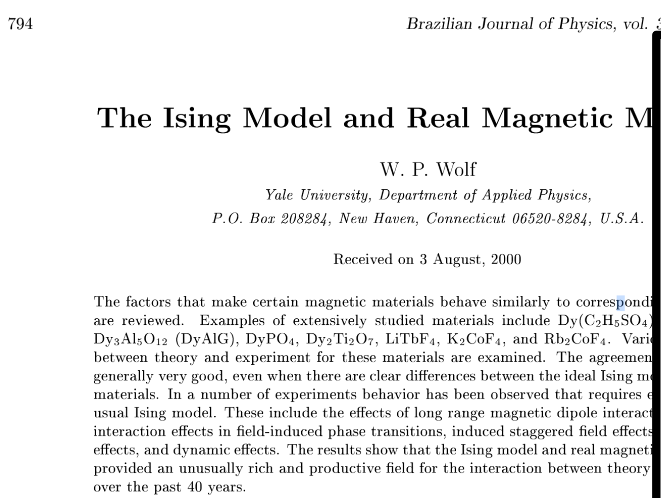


Ising Model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The Ising Model and Real Magnetic M

W. P. Wolf

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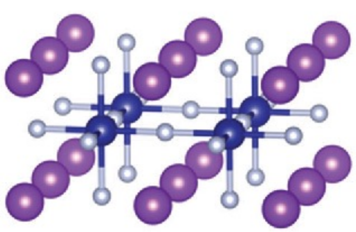

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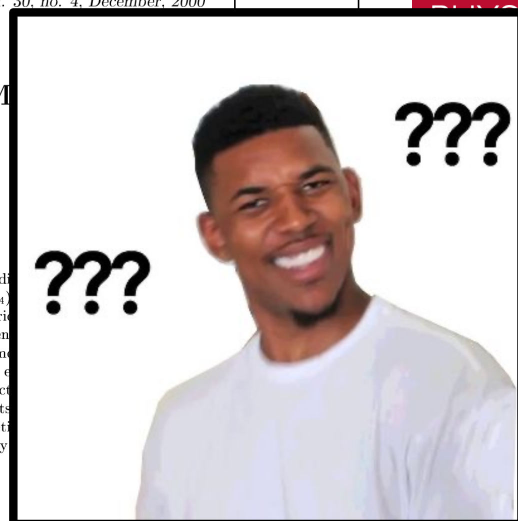

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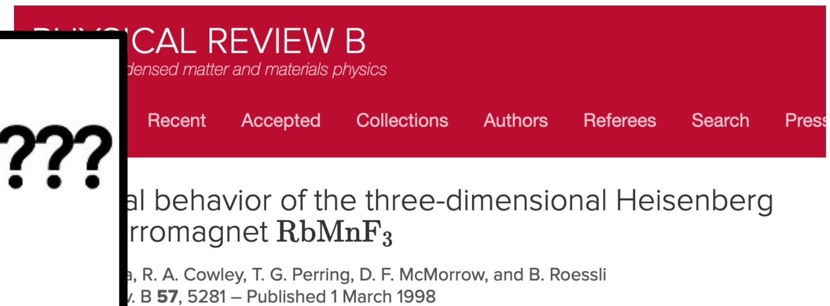
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densed matter and materials physics

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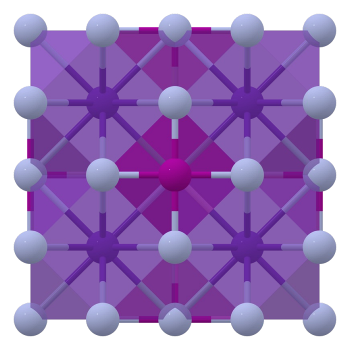


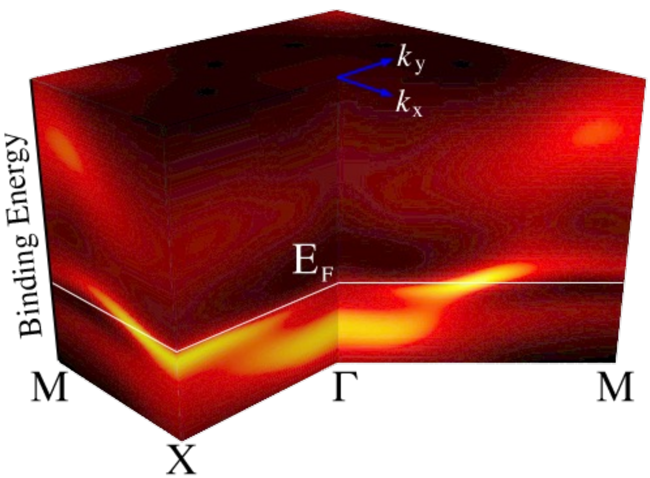
Materials project

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

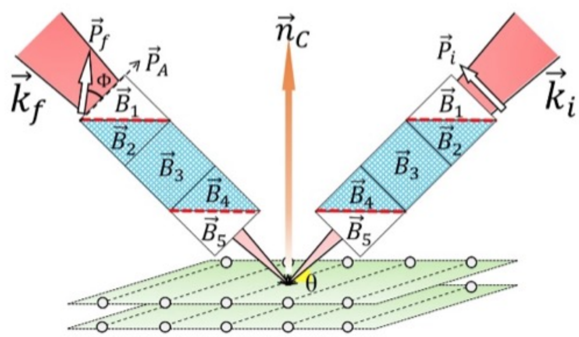
A: You measure its excitations.

Measuring Excitations

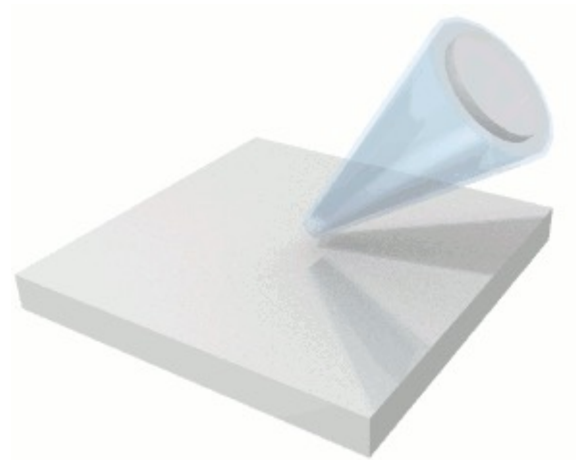
Figures courtesy of Devereaux/Shen group and ORNL



Angle-resolved Photoemission (ARPES)



Neutron Scattering



Time-resolved ARPES

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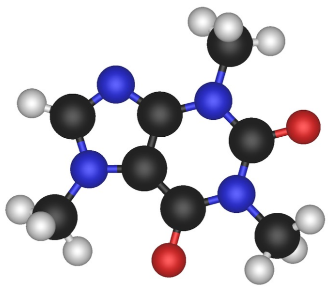
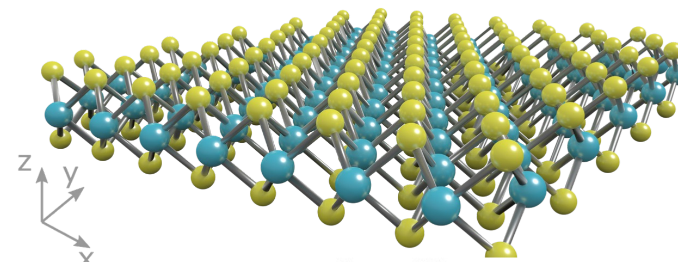
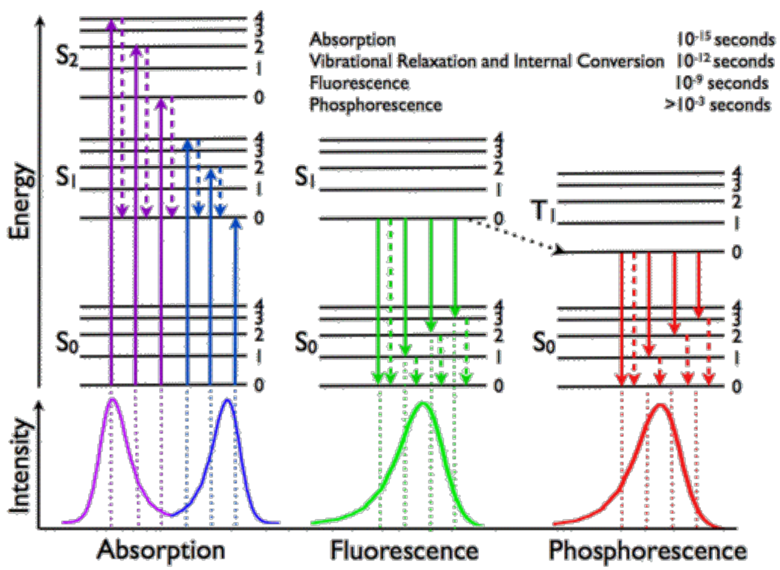
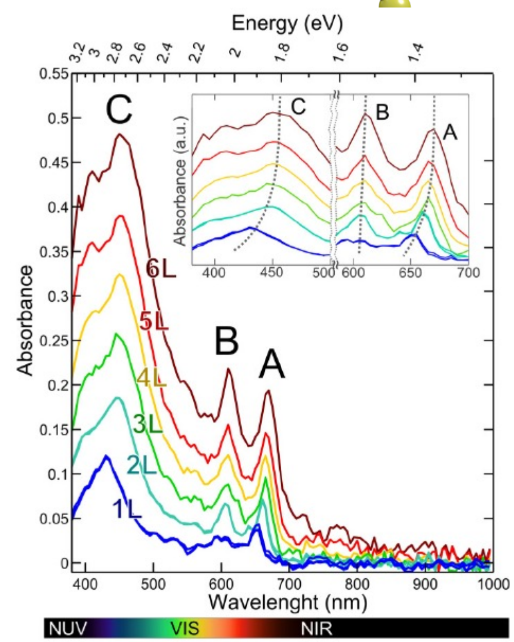
Measuring Excitations









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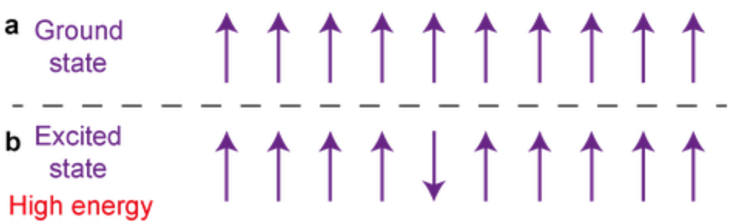

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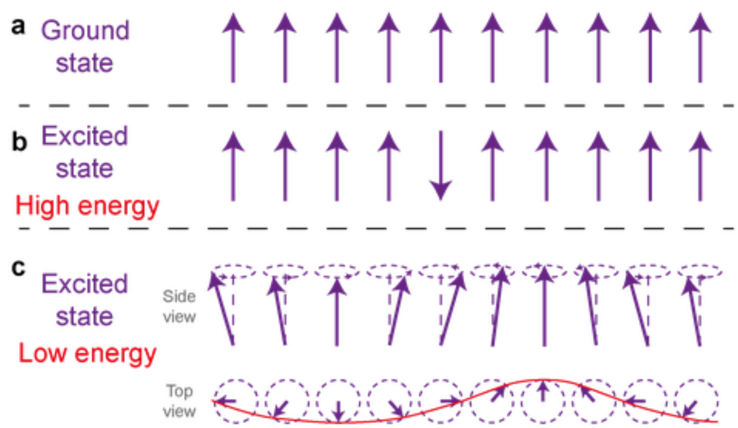
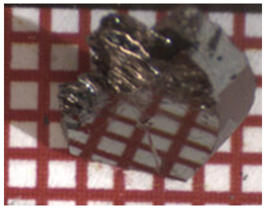
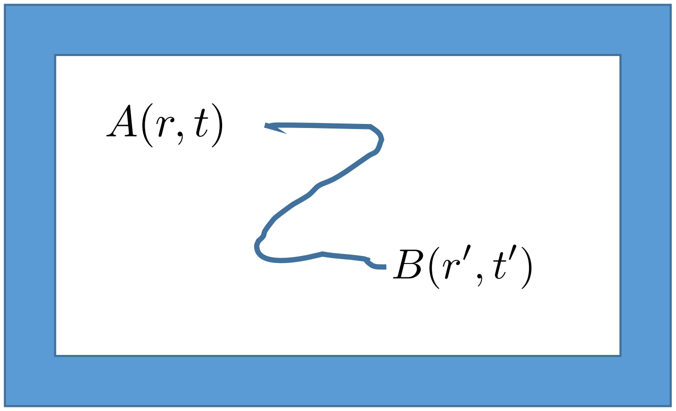


Correlation functions





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

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.

$$\delta A(t) = -i \int_{-\infty}^{t} \langle [\mathbf{A}(t), \mathbf{B}] \rangle h(\bar{t}) d\bar{t} = \int_{\infty}^{\infty} \chi^{R}(t, \bar{t}) h(\bar{t}) d\bar{t}$$

Experiment	Applied field B	Measured operator A	Correlation function
AC Conductivity	Electric field	Current	[j,j]
Neutron Scattering	Spin flip	Spin flip/Z	[Sx,Sx] etc
Magnetic Susceptibility	Magnetic	Spin	[Sz,Sz], [S+,S-]
Photoemission spectroscopy	Particle removal	Particles at detector	$[c^{+},c]$
Light absorption	p.A	j	A.[p, j]
Light scattering	p.A	p.A	A1.[p1, p2].A2

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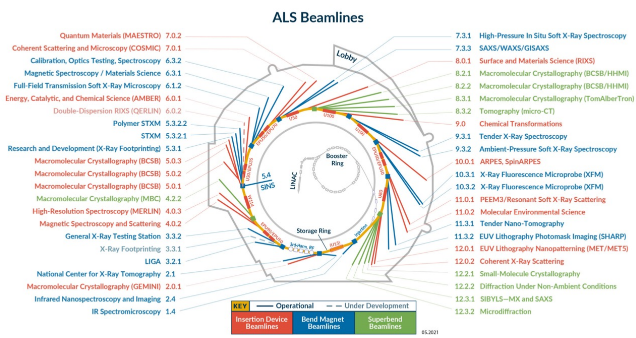
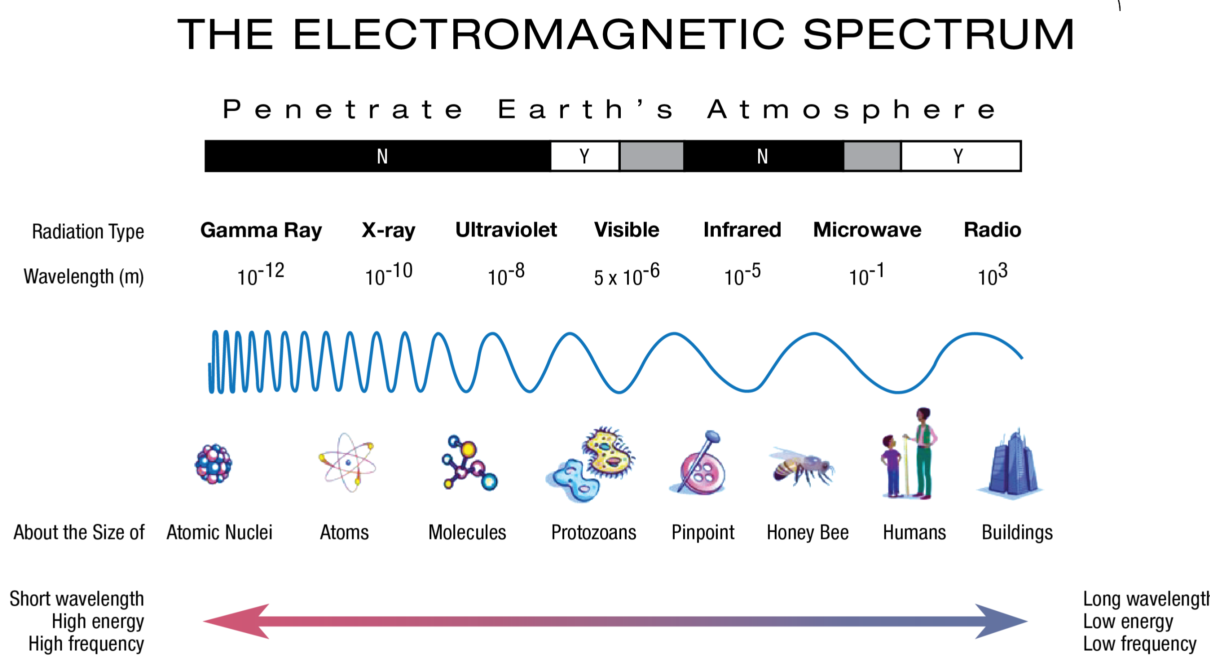
$$\delta A(t) = -i\int_{-\infty}^{t} \langle [\mathbf{A}(t), \mathbf{B}] \rangle h(\bar{t})d\bar{t} = \int_{\infty}^{\infty} \chi^{R}(t,\bar{t})h(\bar{t})d\bar{t}$$





The Electromagnetic Spectrum. Image Credit: NASA

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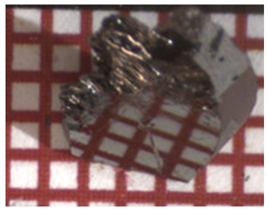
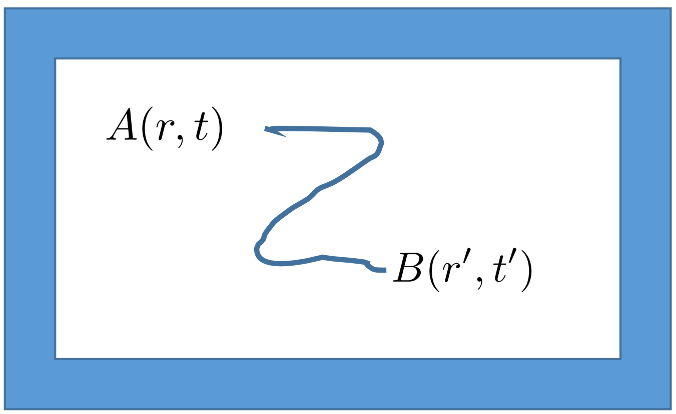
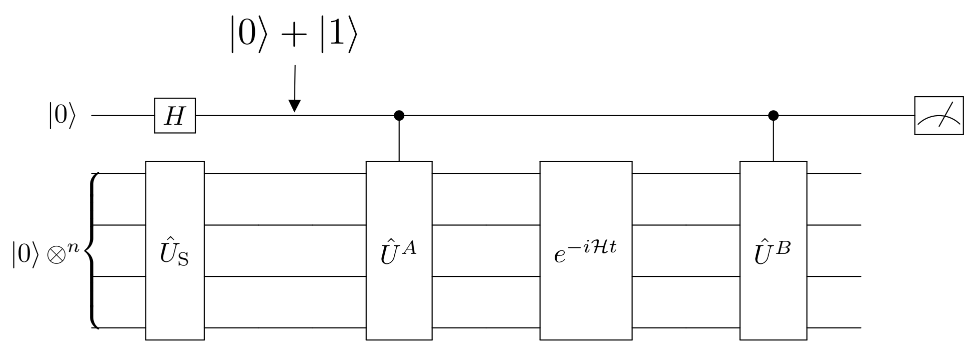
Correlation functions





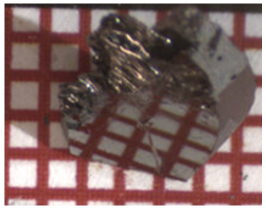
$$e^{iE_0 t}\langle\phi_0|Be^{-i\mathcal{H}t}A|\phi_0\rangle$$

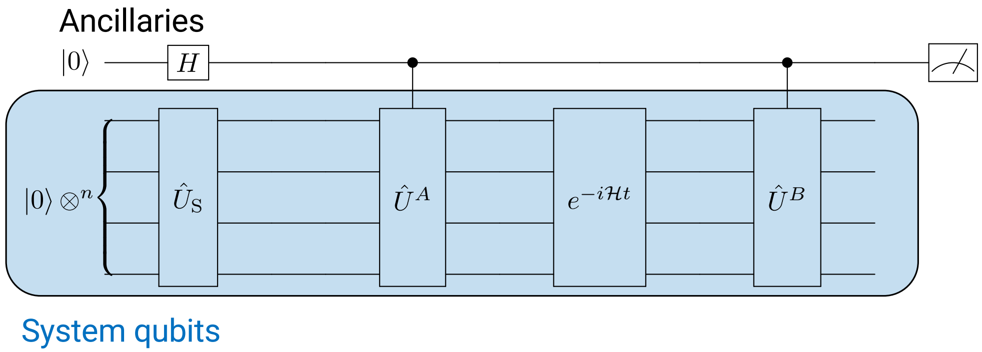
- $e^{iE_0 t}$: Interfere with ground state
- $\langle\phi_0|$: Complete expectation value
- B: Apply excitation B
- $e^{-i\mathcal{H}t}$: Time evolve
- A: Apply excitation A
- $|\phi_0\rangle$: Prepare state of interest

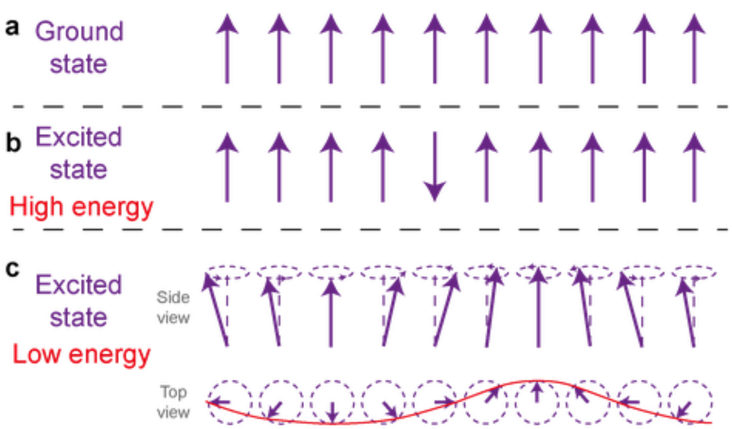


Somma, Simulating physical phenomena by quantum networks (2002)

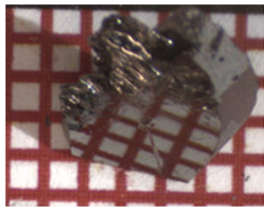
Correlation functions



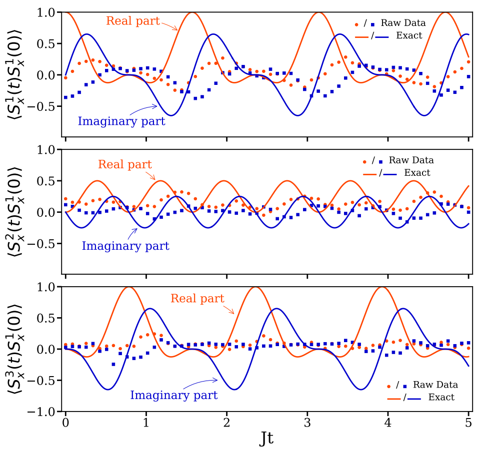




Correlation functions



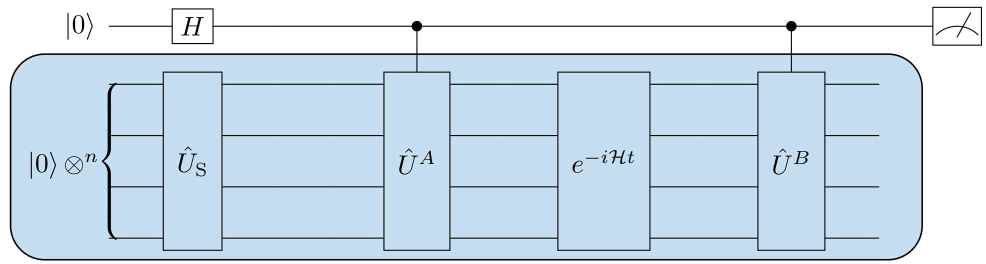
Raw data (2019)



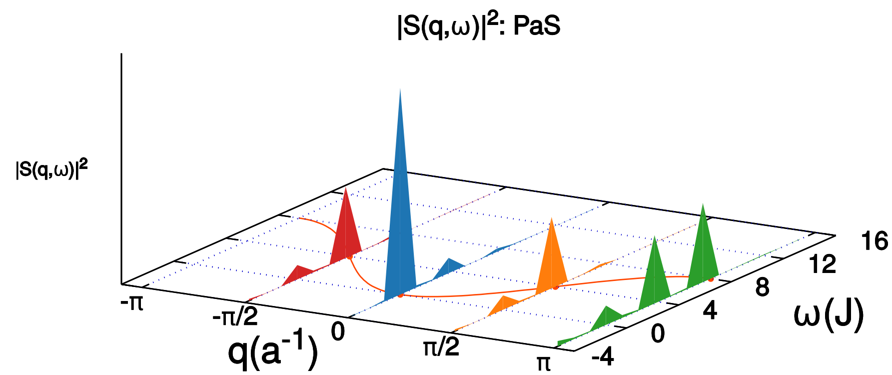
$$\langle A(r,t)B(r',t')\rangle$$

Error mitigation

Ancillaries



System qubits



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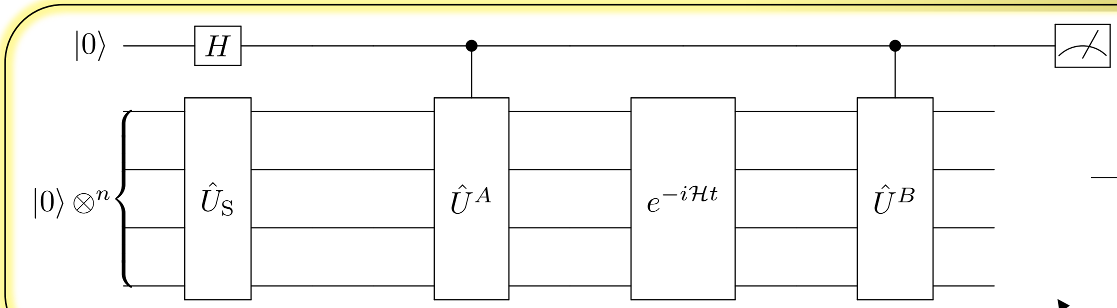
A-Z quantum simulation



Classical post-processing techniques

Prepare state of interest

Time evolve

Dynamical response functions

- *Physics-Informed Subspace Expansions*

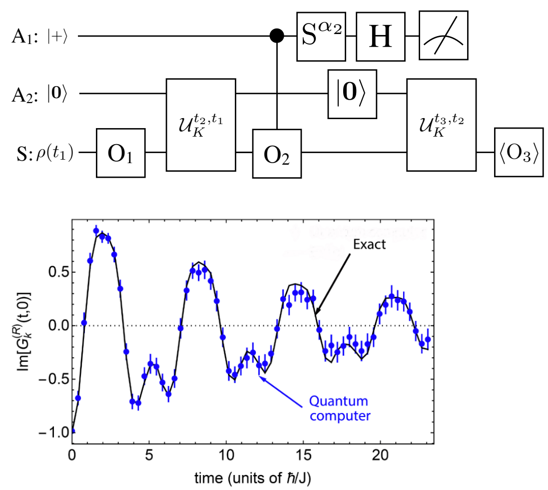
- *Lie-algebraic methods for time evolution*
- *Open quantum system evolution*

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

(A 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

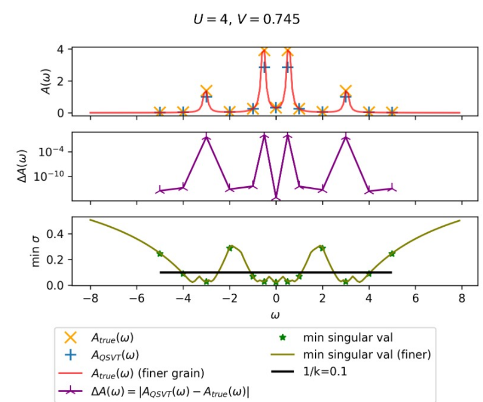
L. Del Re, B. Rost, M. Foss-Feig, AFK, J.K. Freericks
2204.12400

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)

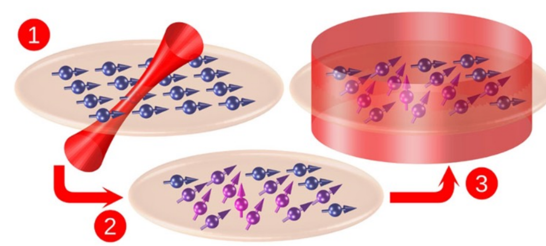


FIG. 1 (color online). Many-body Ramsey interferometry consists of the following steps: (1) A spin system prepared in its ground state is locally excited by $\pi/2$ rotation; (2) the system evolves in time; (3) a global $\pi/2$ rotation is applied, followed by the measurement of the spin state. This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

Commutators

10.1103/PhysRevLett.111.147205

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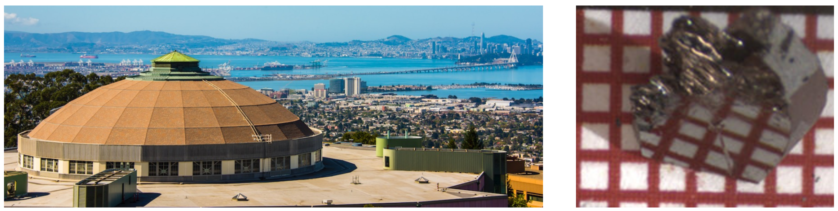
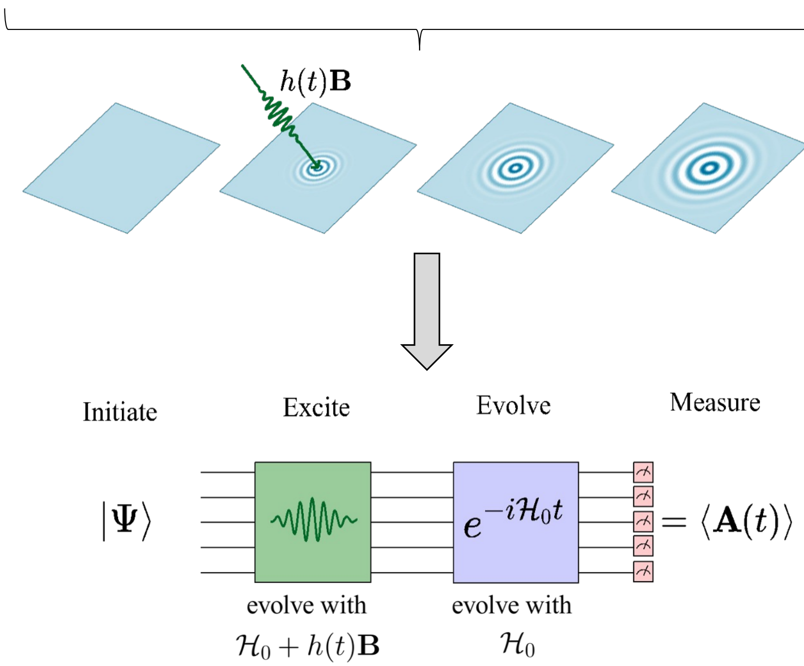
Linear Response

2302.10219





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,*]

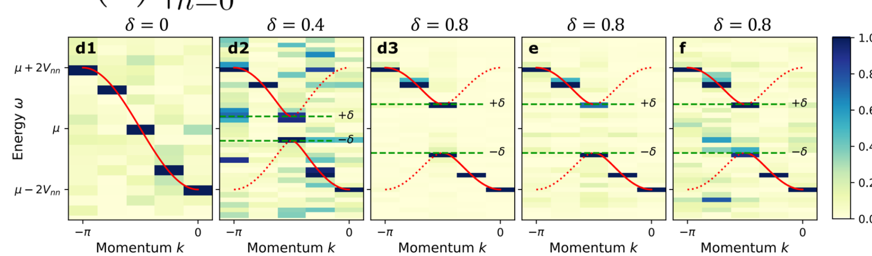
[1] *Department of Physics, North Carolina State University, Raleigh, North Carolina 27695, USA*
[2] *Department of Physics, Georgetown University, 37th and O Sts. NW, Washington, DC 20057 USA*

(Dated: February 22, 2023)

1. Make the excitation part of the quantum simulation

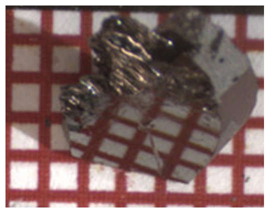
2. Post-process the data to get the response functions

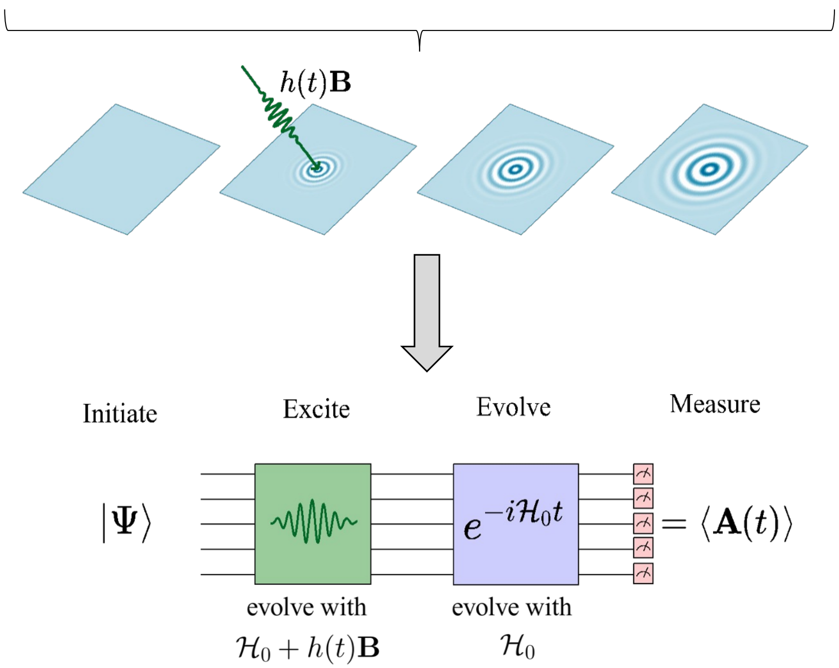
$$\left.\frac{\delta A(t)}{\delta h(t')}\right|_{h=0} = -i\theta(t-t')\langle\psi_0|[\mathbf{A}(t),\mathbf{B}(t')]|\psi_0\rangle$$



Linear Response

2302.10219





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

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[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)

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

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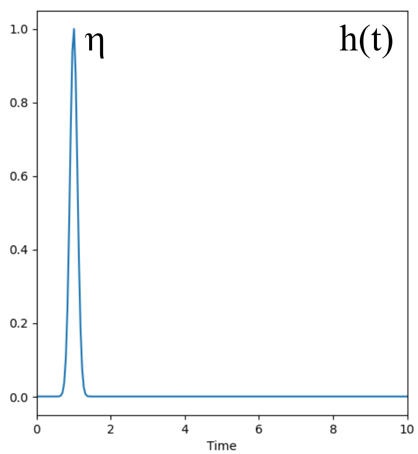
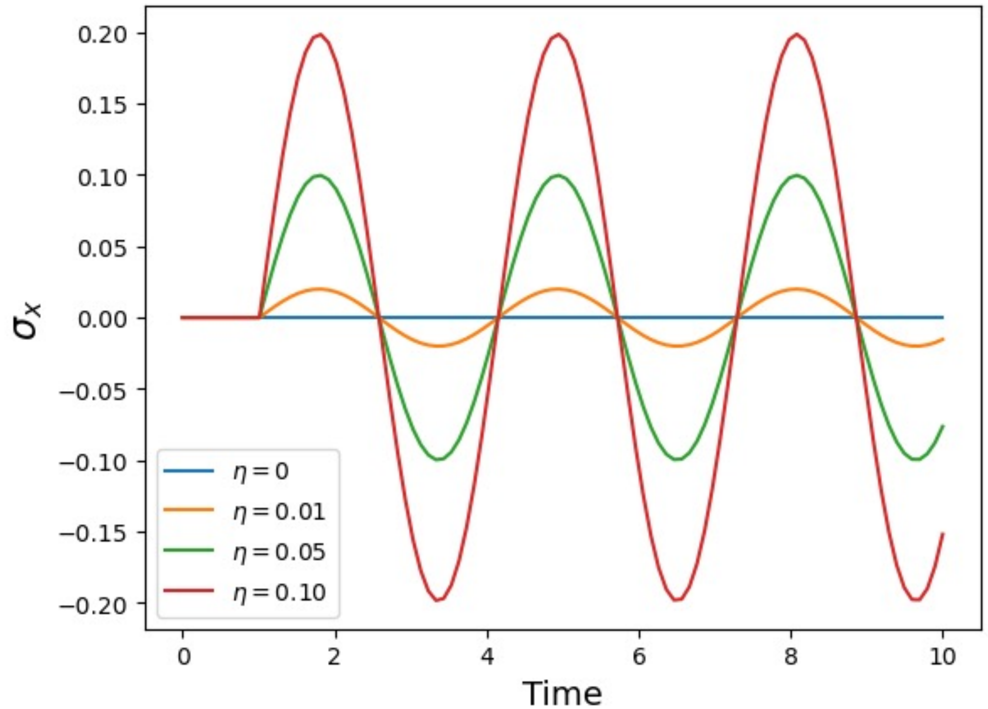
Linear Response

A simple example: single spin with energy level difference = 2

$$\mathbf{H}_0 = \sigma^z$$

$$\mathbf{A} = \mathbf{B} = \sigma^x$$





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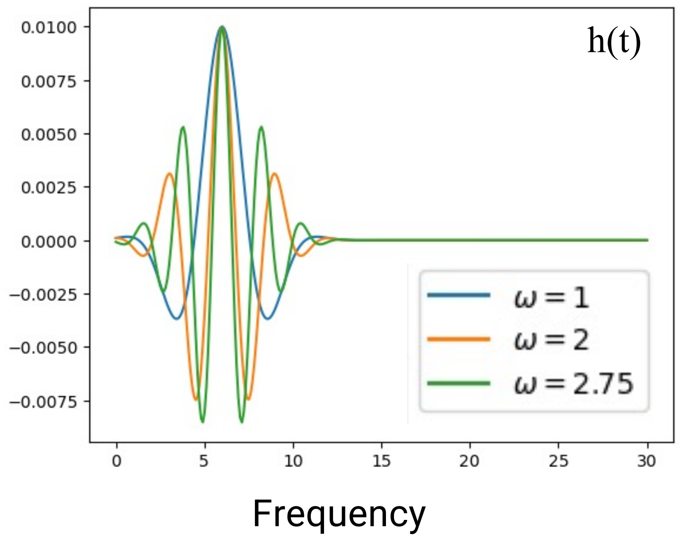

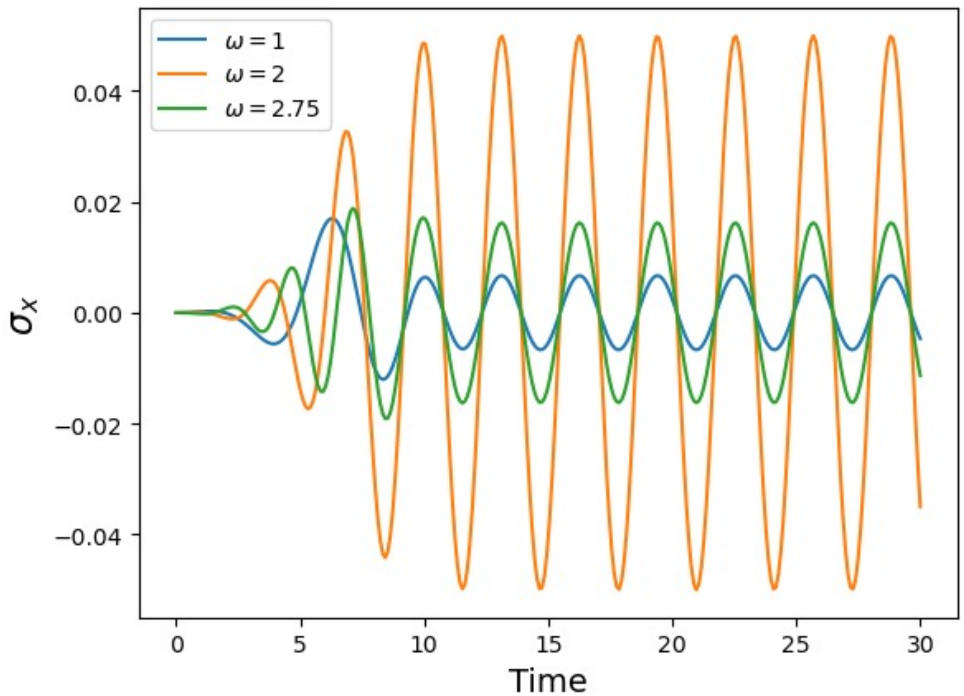

Linear Response

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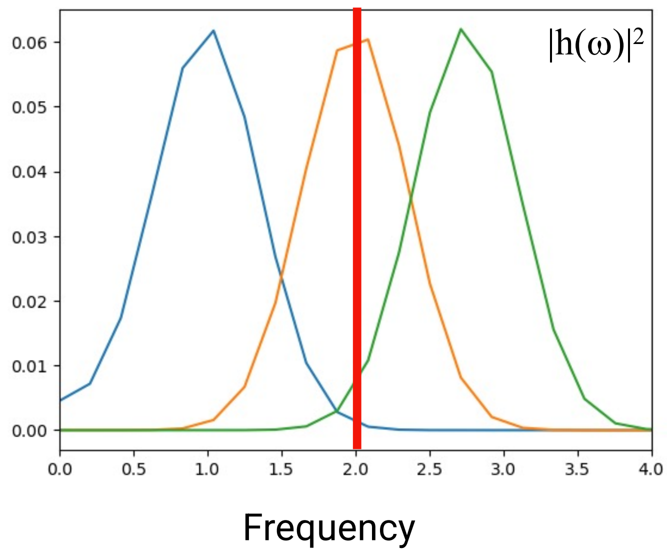

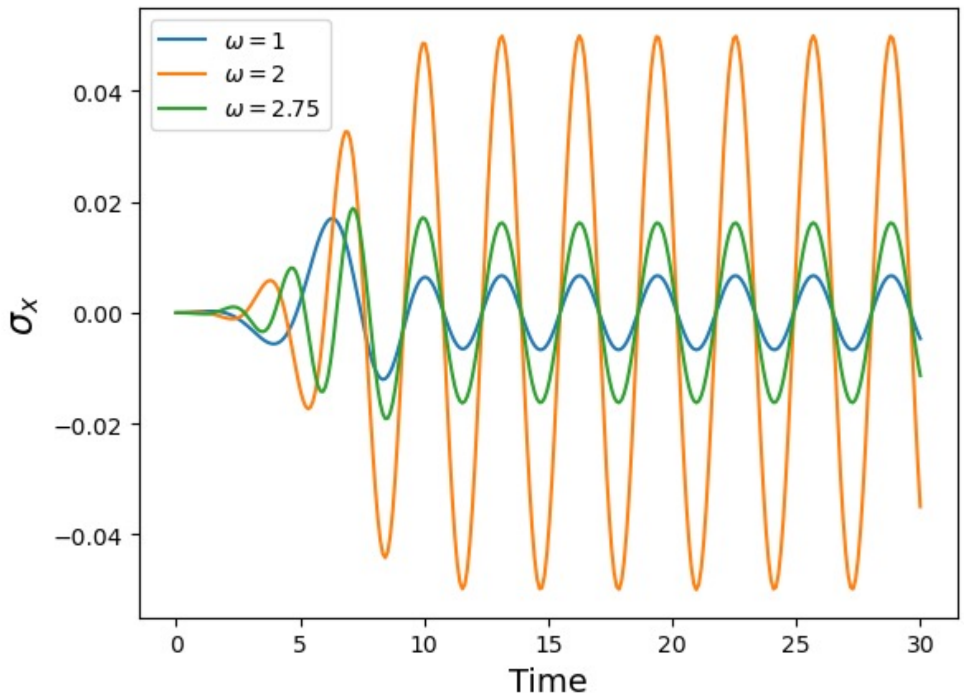

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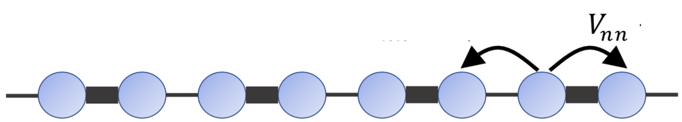
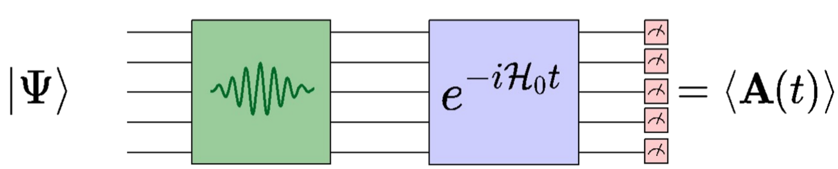
A Bosonic Correlation function: Polarizability

1D fermion chain



$$\mathcal{H}_0 = -\sum_i V_{nn} c_i^\dagger c_{i+1} + \text{h.c.}$$

Initiate | Excite | Evolve | Measure



evolve with $\mathcal{H}_0 + h(t)\mathbf{B}$ | evolve with $\mathcal{H}_0$

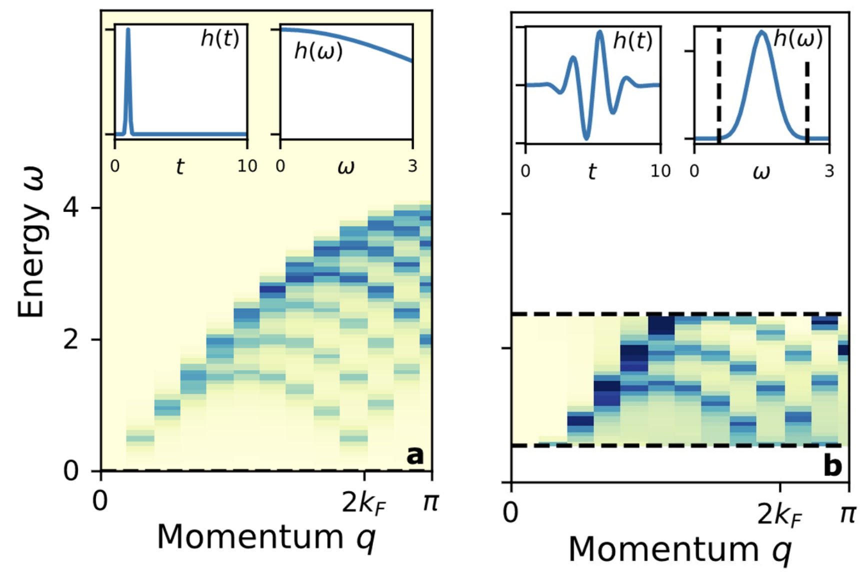
$$A(t) = \int dt' \chi^R(t-t') h(t') + \mathcal{O}(h^2)$$

$$A(\omega) = \chi^R(\omega) h(\omega)$$

$$\chi(r,t) = -i \langle \psi_0 | \delta n(r,t) \delta n(r=0, t=0) | \psi_0 \rangle$$

Measure density on all sites (**A**=n_i)

Wiggle potential on site 0 (**B**=$n_0 V_0$)



Fermionic Linear Response

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

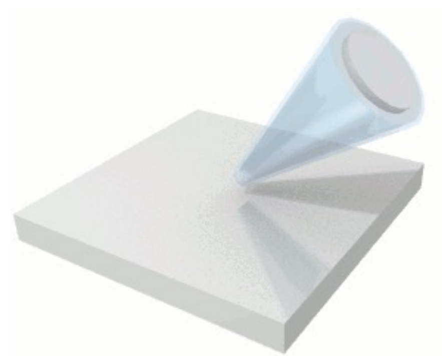
Notice this is a commutator…
… we might also want to have an anti-commutator

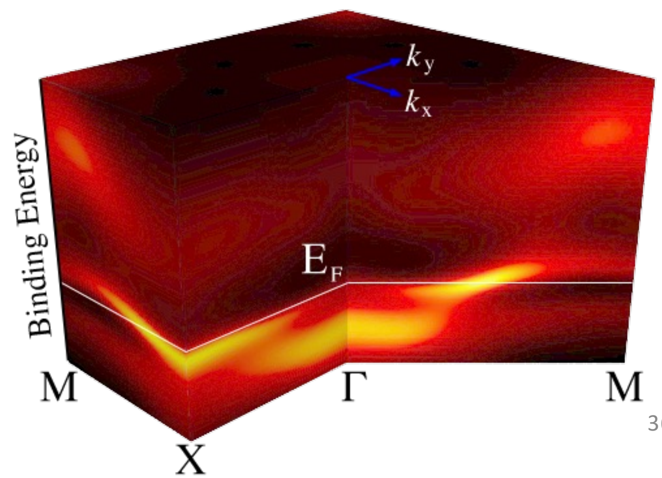
$$G(t,t') = -i\theta(t-t')\langle\psi_0|\{\mathbf{A}(t),\mathbf{B}(t')\}|\psi_0\rangle$$

Why?

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

Fermionic creation/
annihilation operators

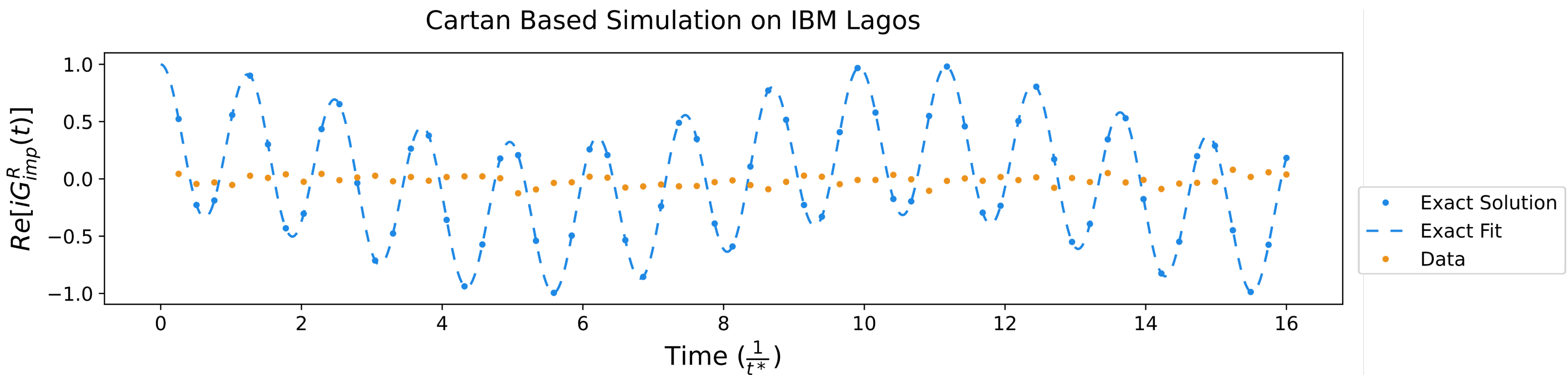


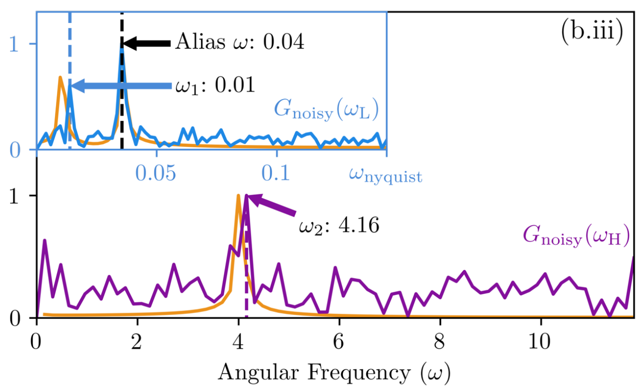


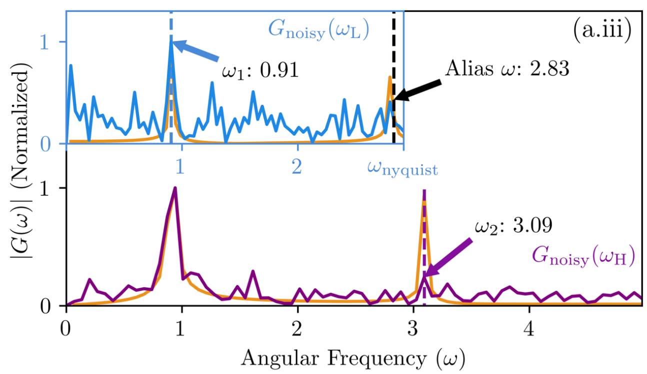
Application of Green's functions: DMFT

T. Steckmann et al., arXiv:2112.05688

2-site Hubbard DMFT (5 qubits)



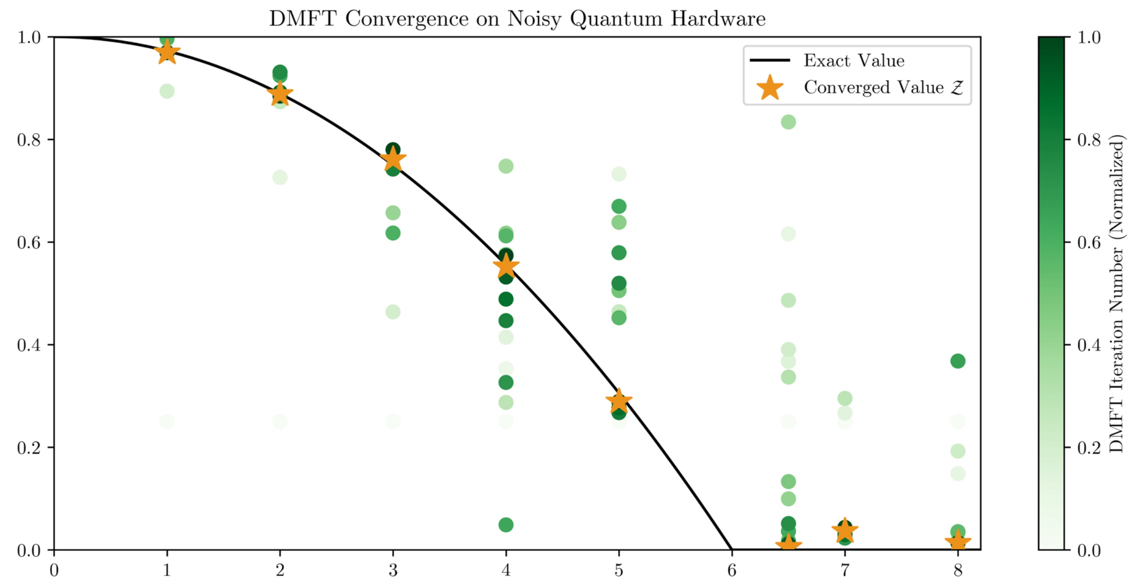


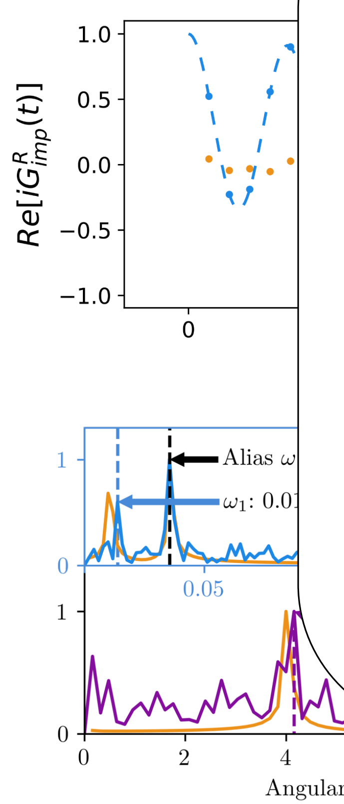


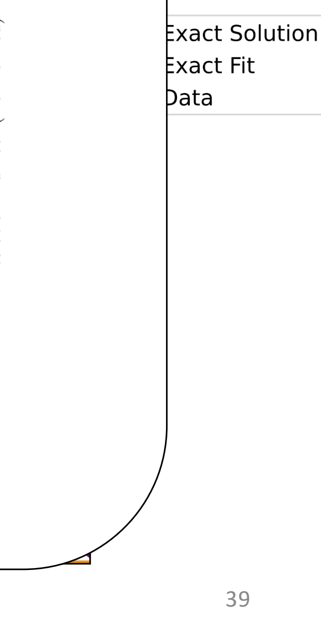
2-site Hubbard DMFT

[T. Steckmann et al., arXiv:2112.05688](https://arxiv.org/abs/2112.05688)

Self-consistent DMFT phase diagram showing the metal-insulator transition for 2-site Hubbard model







Fermionic Linear Response

2302.10219

Option 1: Auxiliary operator

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

Find an operator **P** such that:

$$\{\mathbf{B}(t),\mathbf{P}\} = 0$$

$$[\mathcal{H}_0,\mathbf{P}] = 0$$

$$\mathbf{P}|\psi_0\rangle = s|\psi_0\rangle$$

Then:

$$G(t,t') = -i\theta(t-t')\langle\psi_0|\{\mathbf{A}(t),\mathbf{B}(t')\}|\psi_0\rangle$$
$$= \frac{i}{s}\theta(t-t')\langle\psi_0|[\mathbf{A}(t)\mathbf{P}(t),\mathbf{B}(t')]|\psi_0\rangle$$

Example: parity

$$\mathbf{P} = Z_1 Z_2 \ldots Z_n$$

Option 2: Post-selection

Fermionic Linear Response

Option 1: Auxiliary operator

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$$\begin{aligned} G(t,t') &= -i\theta(t-t')\langle\psi_0|\{\mathbf{A}(t),\mathbf{B}(t')\}|\psi_0\rangle \\ &= \frac{i}{s}\theta(t-t')\langle\psi_0|[\mathbf{A}(t)\mathbf{P}(t),\mathbf{B}(t')]|\psi_0\rangle \end{aligned}$$

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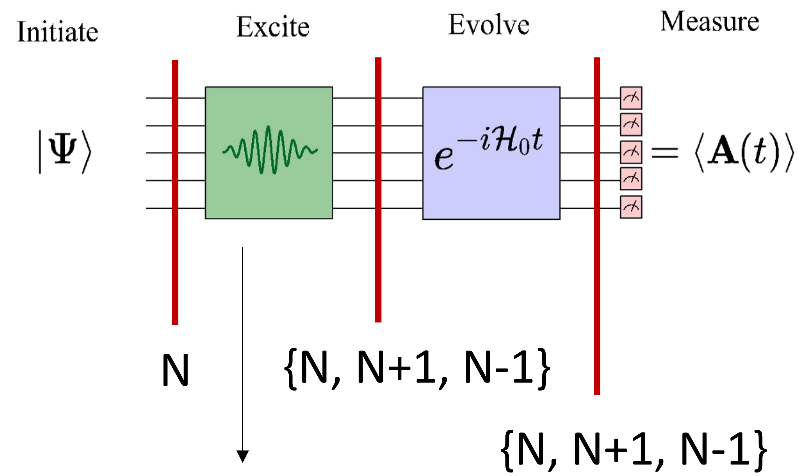


$$\mathbf{B} = \eta\left(c + c^\dagger\right)$$

Post-selection on particle number gives us

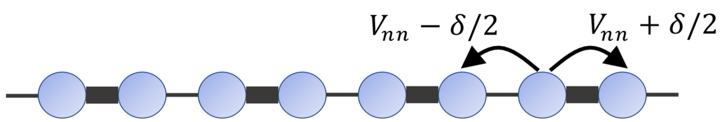
$$G^<_{ij}(t) = i\,\langle\psi_0|c^\dagger_j(0)c_i(t)|\psi_0\rangle$$

$$G^>_{ij}(t) = -i\,\langle\psi_0|c_i(t)c^\dagger_j(0)|\psi_0\rangle$$

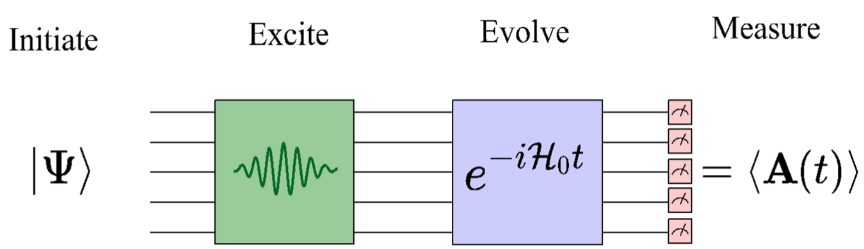
Linear Response -> Green's function

2302.10219

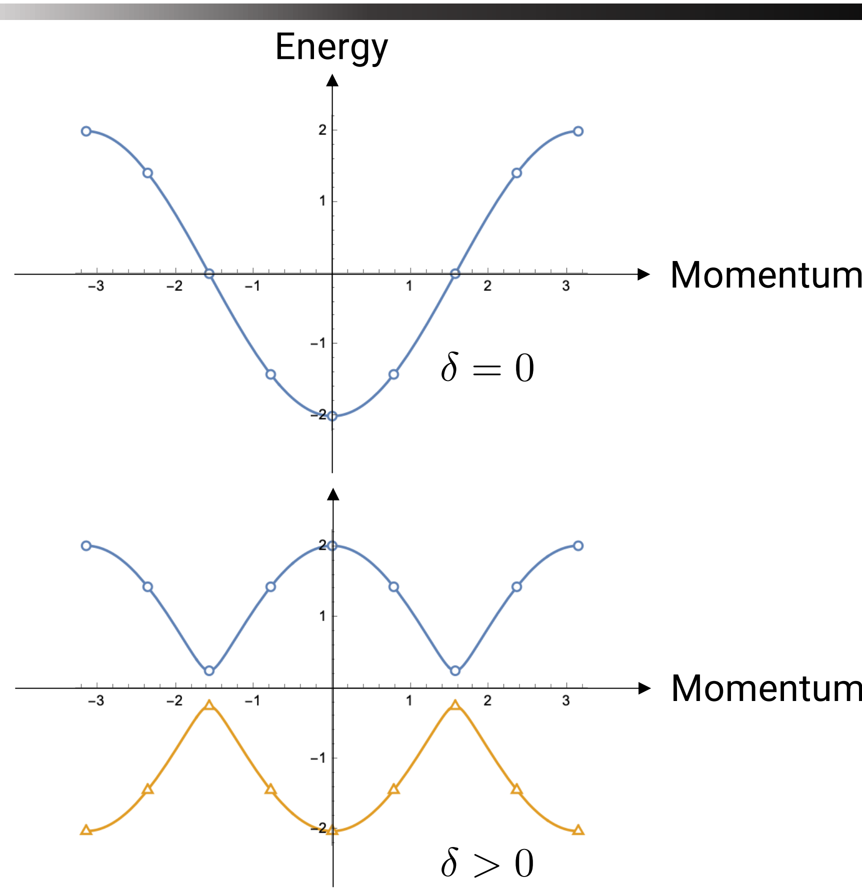
Su-Schrieffer-Heeger model for polyacetylene



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



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



Linear Response -> Green's function

2302.10219

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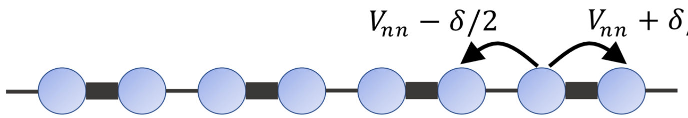

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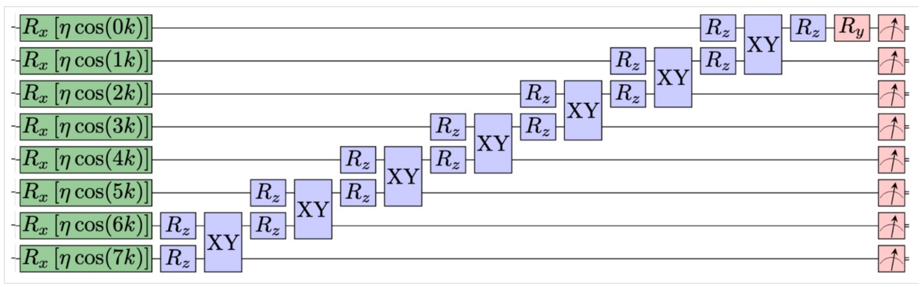
Compressed circuit run on *ibm_auckland*



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

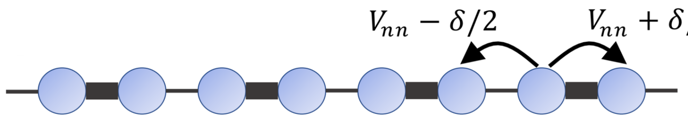
Choose **B** to create a momentum eigenstate

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

Linear Response -> Green's function

2302.10219

Su-Schrieffer-Heeger model for polyacetylene



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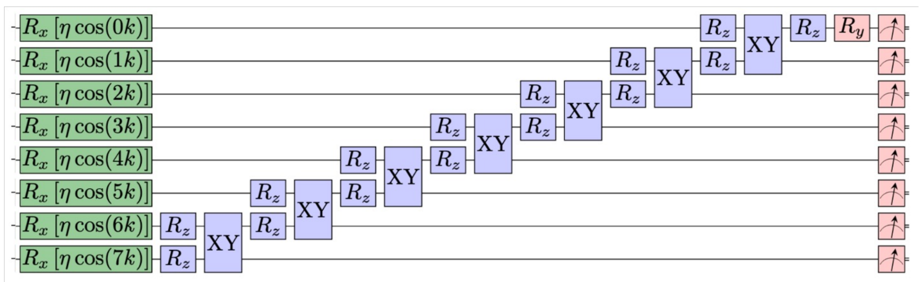

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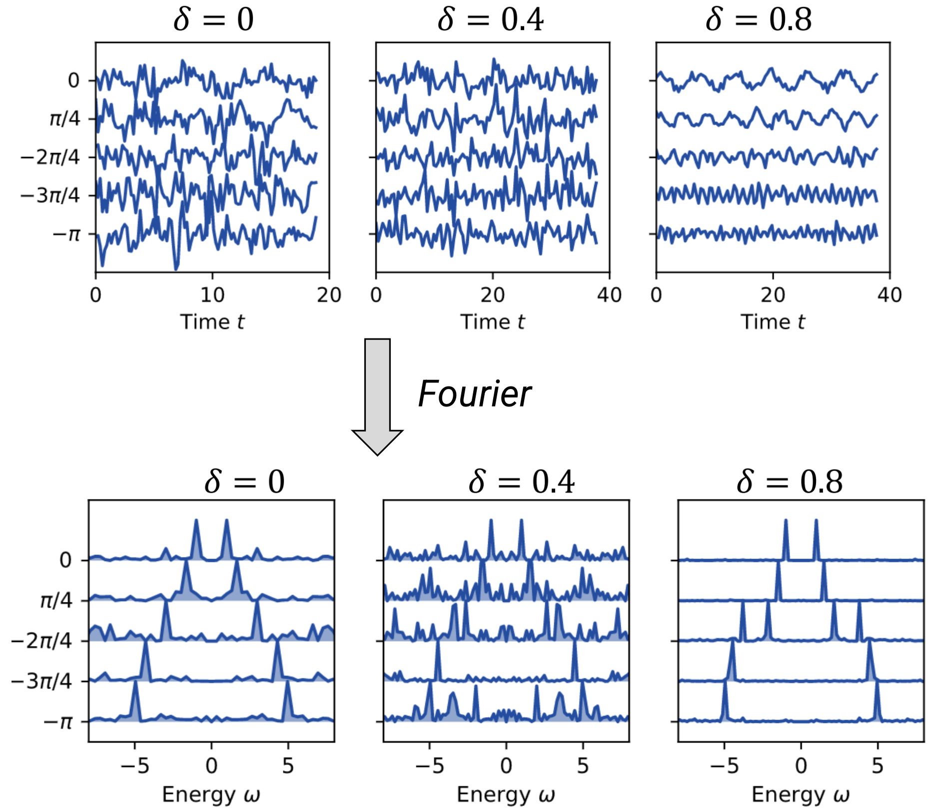

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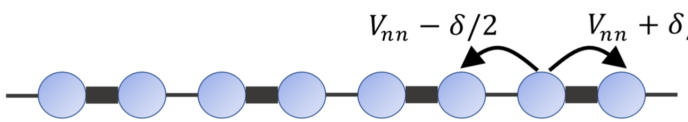
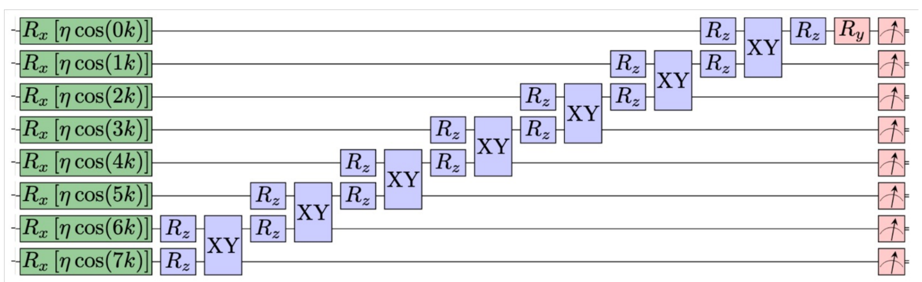
Su-Schrieffer-Heeger model for polyacetylene



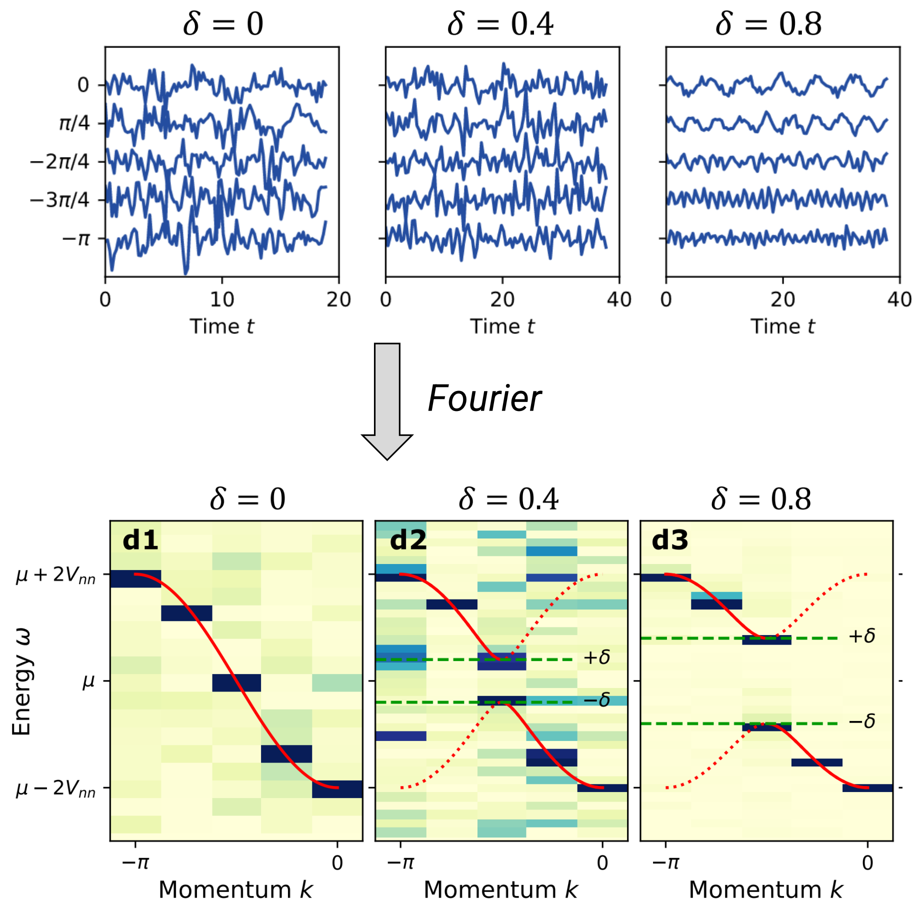
$$\mathcal{H}_0 = -\sum_{\langle i,j\rangle}\left[V_{nn} + (-1)^i\,\delta/2\right] c_i^\dagger c_j - \mu \sum_i c_i^\dagger c_i$$

Compressed circuit run on *ibm_auckland*



Choose **B** to create a momentum eigenstate

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



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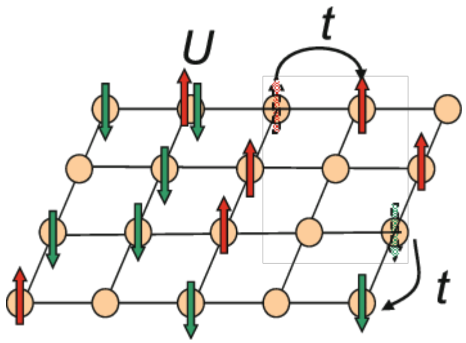
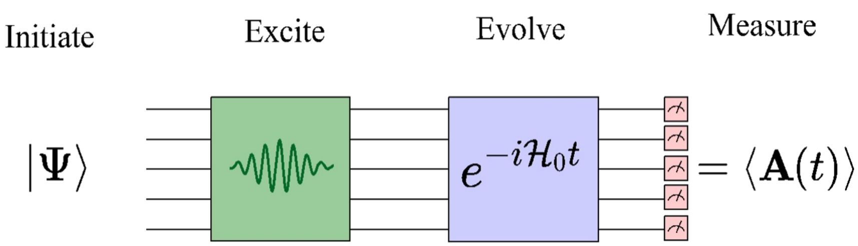
Linear Response -> Green's function

2302.10219





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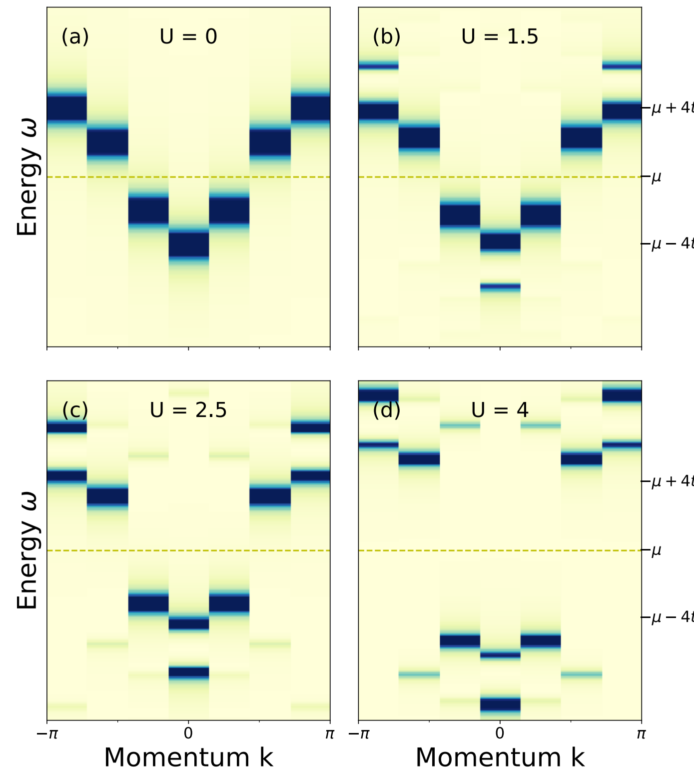
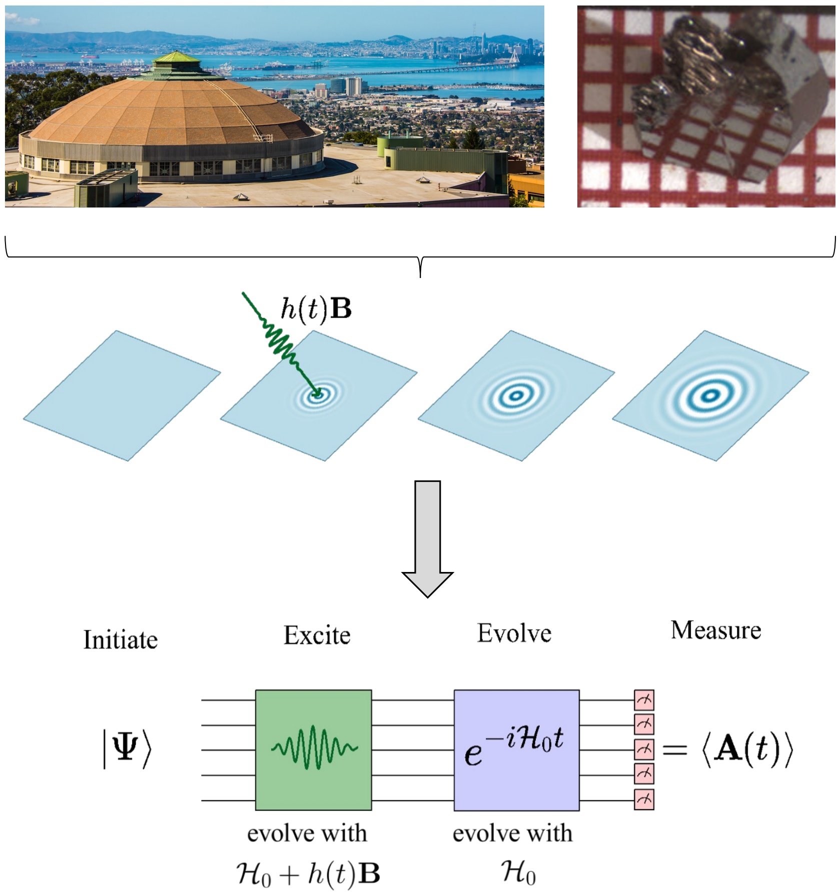
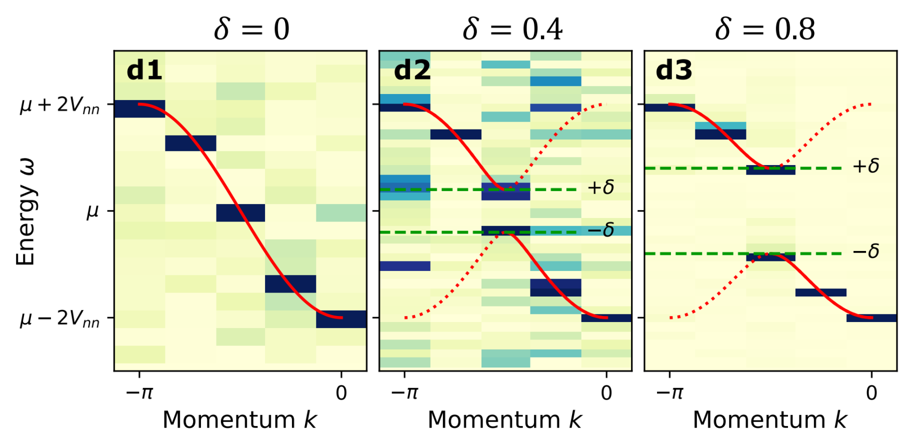


Linear Response

Digital version of this talk



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

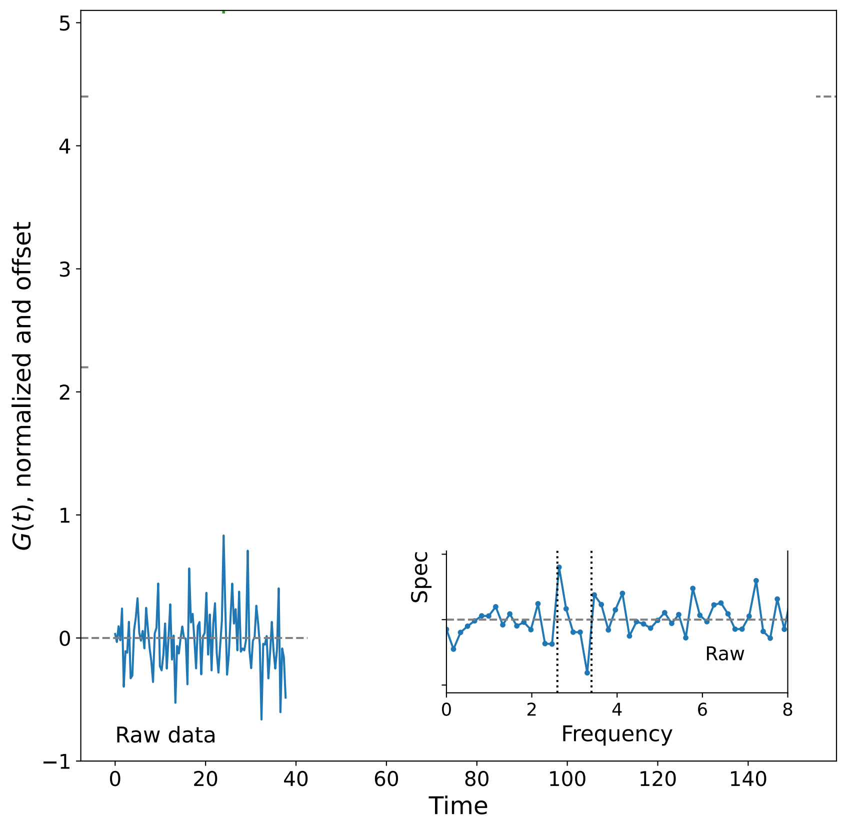


E. Kökcü, H.Labib, J.K. Freericks, AFK., arXiv:2302.10219

Further improvements via mathematics

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

$$\langle A^\dagger(t) A(t') \rangle$$



Kemper, Yang, Gull, arXiv:2309.02566

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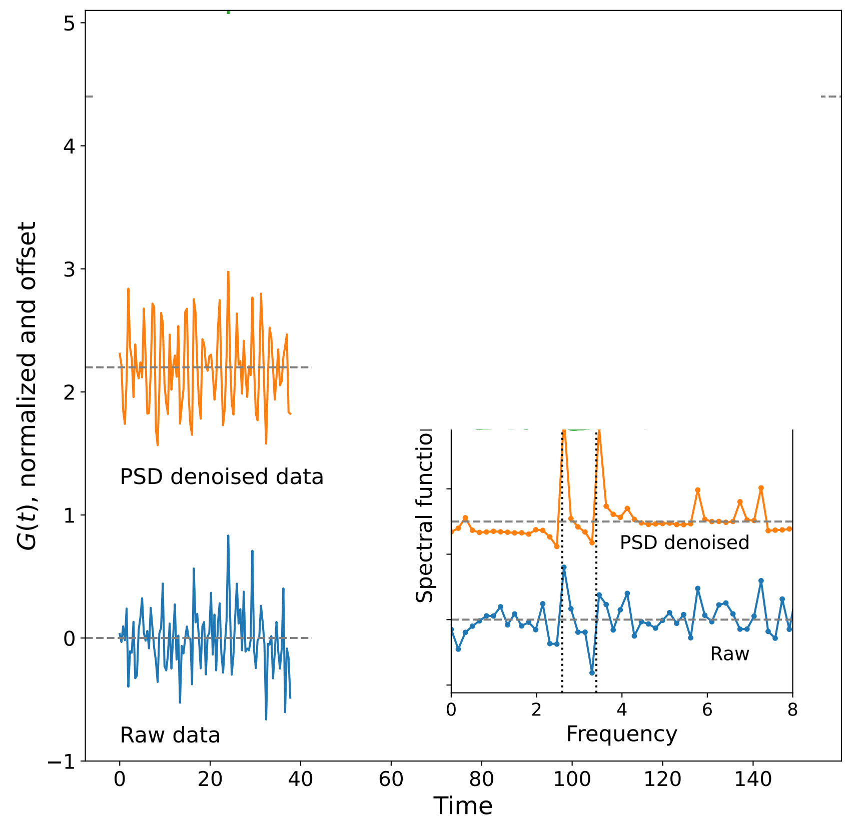


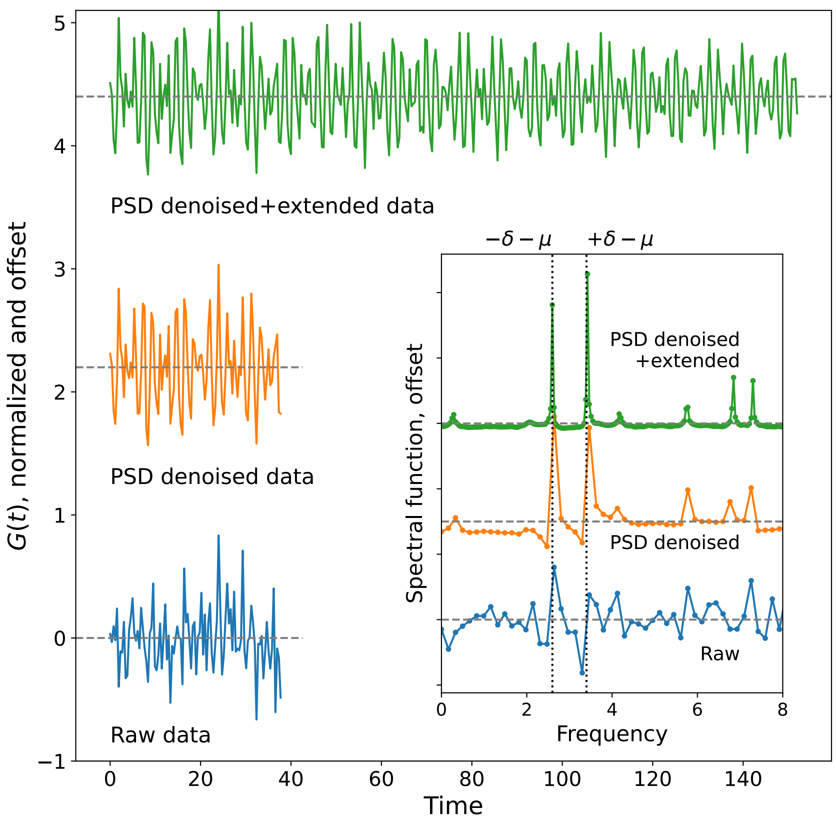
Kemper, Yang, Gull, arXiv:2309.02566

Further improvements via mathematics

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

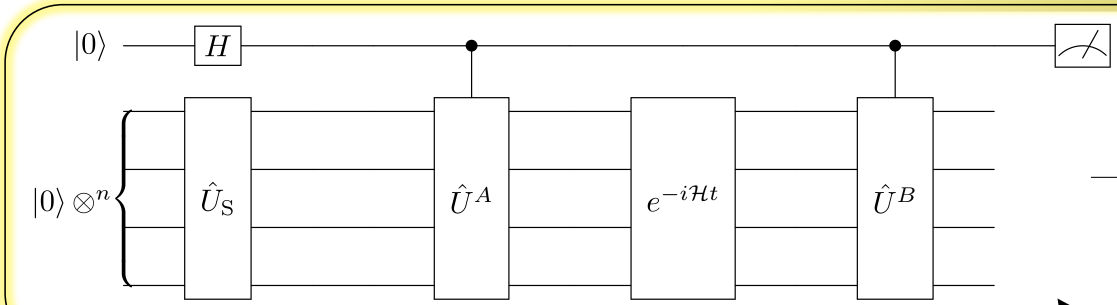
$$\langle A^\dagger(t) A(t') \rangle$$

- We can project the noisy data onto the nearest PSD function
- Given sufficiently dense data, a unique extension exists* and we can extend the data to longer times



Kemper, Yang, Gull, arXiv:2309.02566

A-Z quantum simulation



Classical post-processing techniques

Prepare state of interest

Time evolve

Dynamical response functions

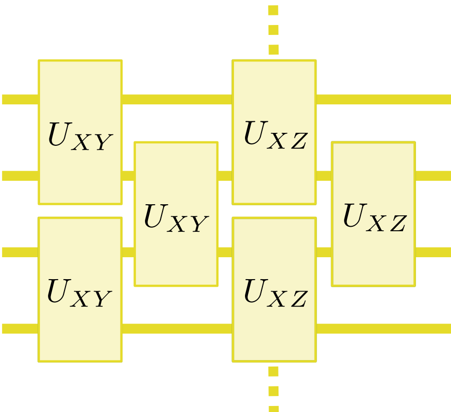
- *Physics-Informed Subspace Expansions*

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

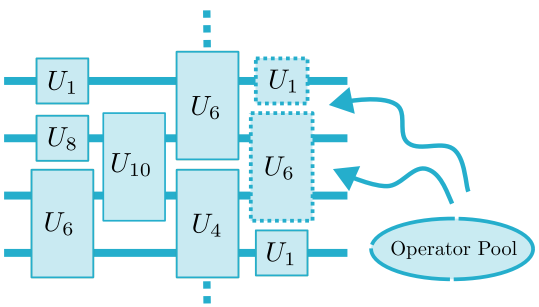
- *Neutron scattering (magnon) spectra*
- *Open quantum system Green's functions*
- *Dynamical Mean Field Theory*

Lie algebraic methods for quantum computing

Time evolution



Variational ansätze

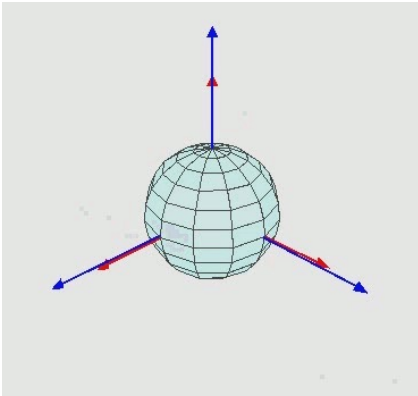


Dynamical Lie algebras

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

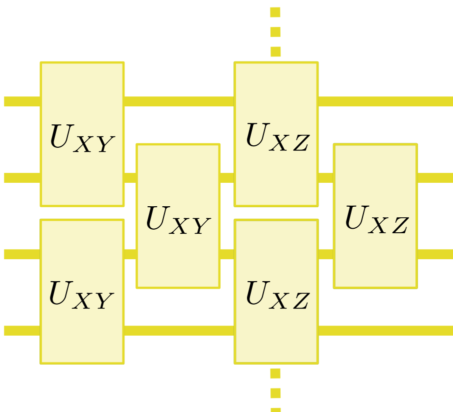
Their Dynamical Lie Algebra expresses all the operators that can be generated by this set

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



Lie algebraic methods for quantum computing

Time evolution



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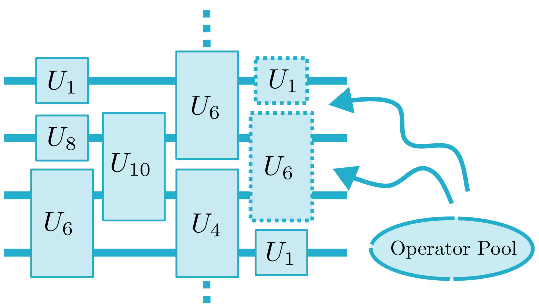

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Cartan decomposition for exact time evolution

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

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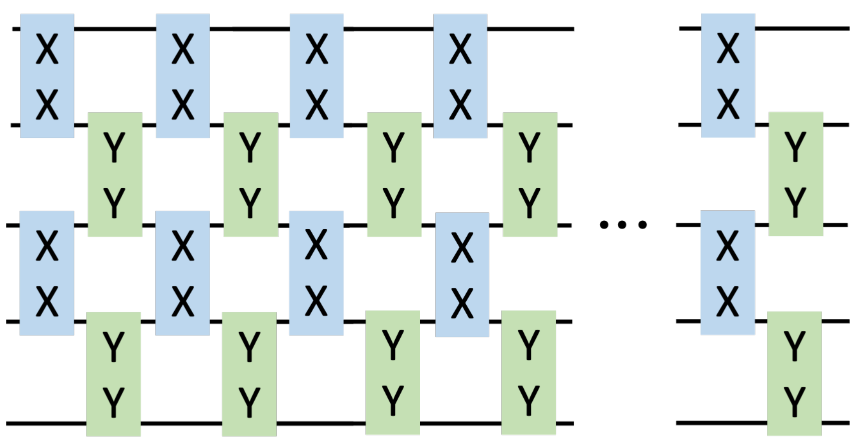
Main Problem

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

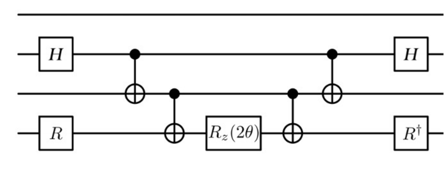
$$\mathcal{H} = a\,XXIII + b\,IYYII + c\,IIXXI + d\,IIIYY$$

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

$U(t) =$



$e^{i\theta IXZYI} =$



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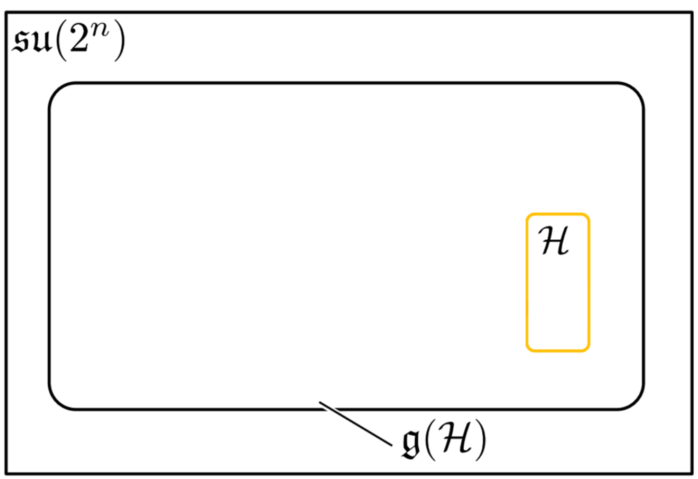
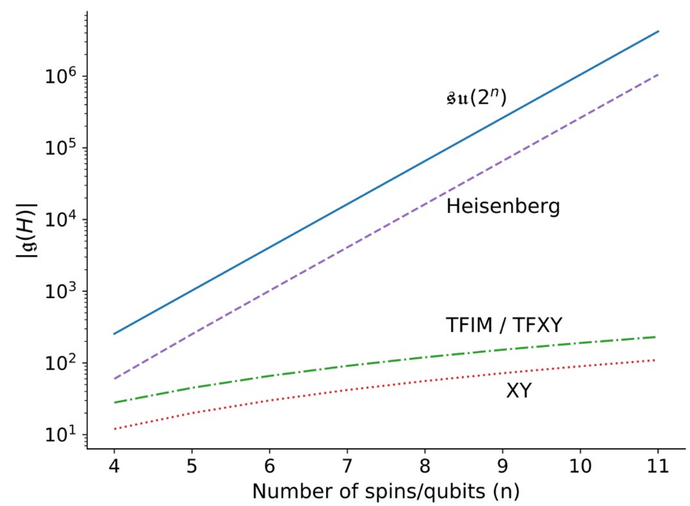
$$U(t) = e^{-it\mathcal{H}} = \prod_{\substack{\cancel{\sigma^i \in \mathfrak{su}(2^n)} \\ \bar{\sigma}^i \in \mathfrak{g}(\mathcal{H})}} e^{i\kappa_i \bar{\sigma}^i}$$

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





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

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

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

$$\mathfrak{a}_3(n) \cong \begin{cases} \mathfrak{so}(2^{n-2})^{\oplus 4}, & \dim = 2^{n-1}(2^{n-2}-1), \quad n\equiv 0 \mod 8, \\ \mathfrak{so}(2^{n-1}), & \dim = 2^{n-2}(2^{n-1}-1), \quad n\equiv \pm1 \mod 8, \\ \mathfrak{su}(2^{n-2})^{\oplus 2}, & \dim = 2^{2n-3}-2, \quad n\equiv \pm2 \mod 8, \\ \mathfrak{sp}(2^{n-2}), & \dim = 2^{n-2}(2^{n-1}+1), \quad n\equiv \pm3 \mod 8, \\ \mathfrak{sp}(2^{n-3})^{\oplus 4}, & \dim = 2^{n-1}(2^{n-2}+1), \quad n\equiv 4 \mod 8, \end{cases}$$

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

$$\mathfrak{a}_5(n) \cong \begin{cases} \mathfrak{so}(2^{n-2})^{\oplus 4}, & \dim = 2^{n-1}(2^{n-2}-1), \quad n\equiv 0 \mod 6, \\ \mathfrak{so}(2^{n-1}), & \dim = 2^{n-2}(2^{n-1}-1), \quad n\equiv \pm1 \mod 6, \\ \mathfrak{su}(2^{n-2})^{\oplus 2}, & \dim = 2^{2n-3}-2, \quad n\equiv \pm2 \mod 6, \\ \mathfrak{sp}(2^{n-2}), & \dim = 2^{n-2}(2^{n-1}+1), \quad n\equiv 3 \mod 6, \end{cases}$$

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

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

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

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

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

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

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

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

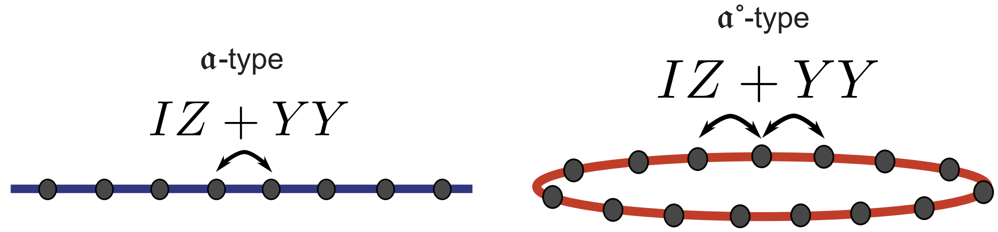
$$\mathfrak{b}_1(n) = \mathrm{span}\{X_i, X_jX_{j+1}\}_{1\le i\le n,\ 1\le j\le n-1} \cong \mathfrak{u}(1)^{\oplus(2n-1)}, \quad \dim = 2n-1,$$

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

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

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

List of unique dynamical Lie algebras



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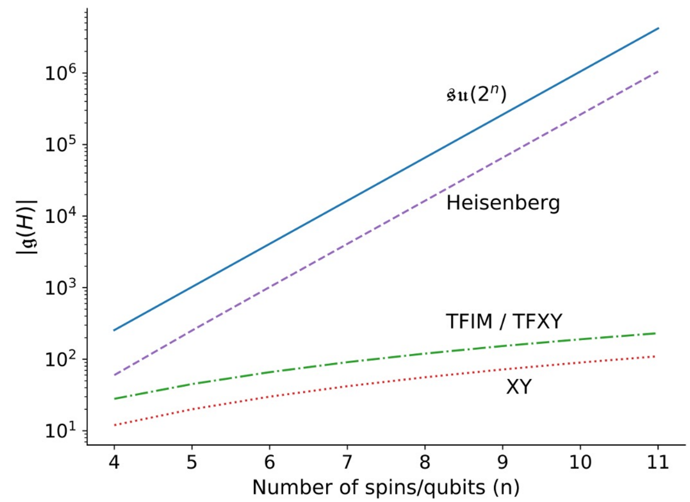

Wiersema, Roeland, et al. , arXiv preprint arXiv:2309.05690 (2023).

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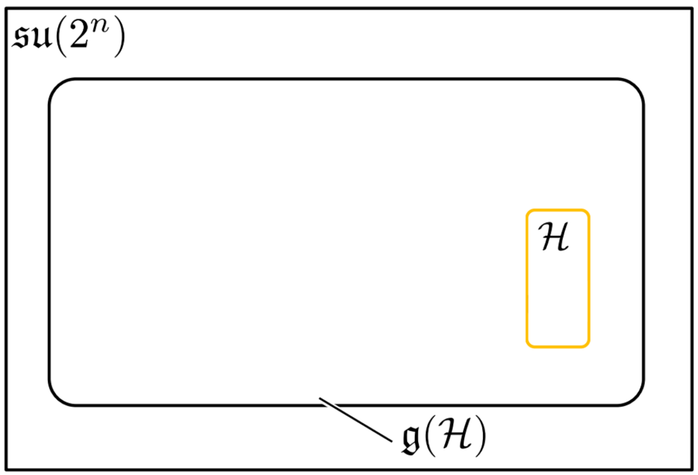
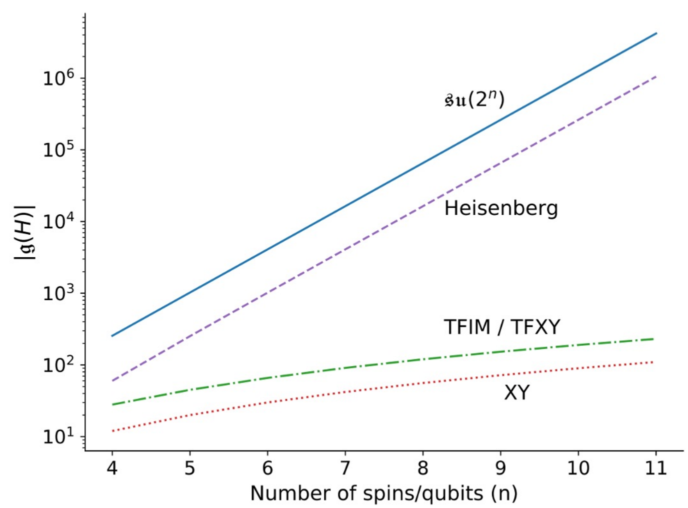


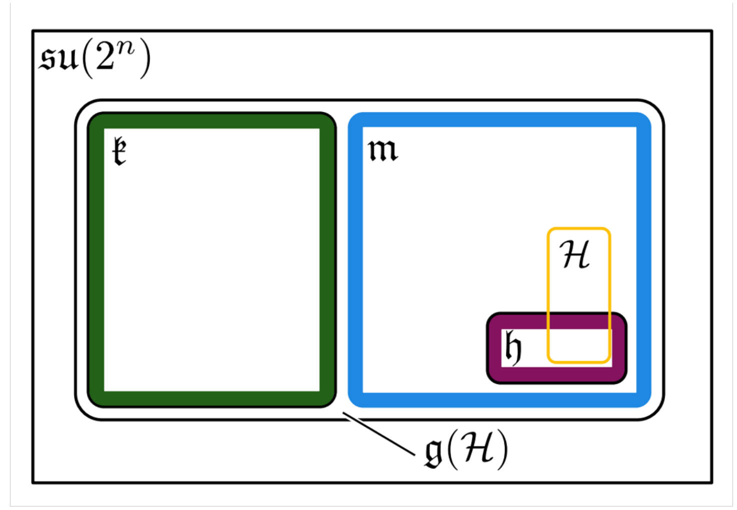


Cartan Decomposition and KHK Theorem

Definition 1 *Consider a compact semi-simple Lie subgroup* $G \subset SU(2^n)$*, which has a corresponding Lie subalgebra* $\mathfrak{g}$*. A* ***Cartan decomposition*** *on* $\mathfrak{g}$ *is defined as an orthogonal split* $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{m}$ *satisfying*

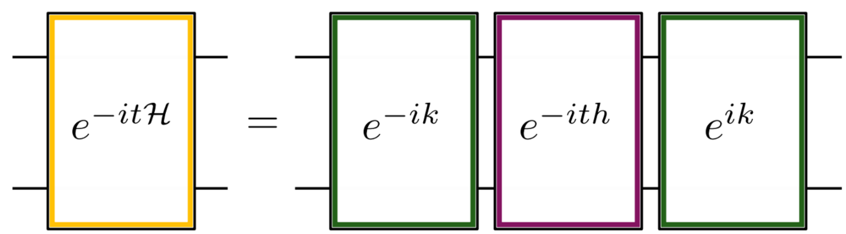
$$[\mathfrak{k}, \mathfrak{k}] \subset \mathfrak{k} \qquad [\mathfrak{m}, \mathfrak{m}] \subset \mathfrak{k} \qquad [\mathfrak{k}, \mathfrak{m}] = \mathfrak{m} \tag{4}$$

and is referred as $(\mathfrak{g}, \mathfrak{k})$*.* ***Cartan subalgebra*** *of this decomposition is defined as one of the maximal Abelian subalgebras of* $\mathfrak{m}$*, and denoted as* $\mathfrak{h}$*.*



Theorem 1 *Given a Cartan decomposition* $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{m}$*, for any element* $\mathcal{H} \in \mathfrak{m}$ *there exist a* $K \in e^{\mathfrak{k}}$ *and* $h \in \mathfrak{h}$ *such that*

$$\mathcal{H} = K h K^{\dagger} \tag{5}$$



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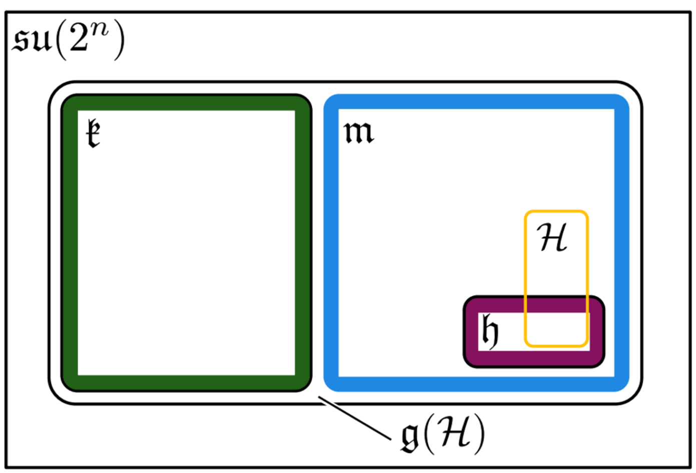

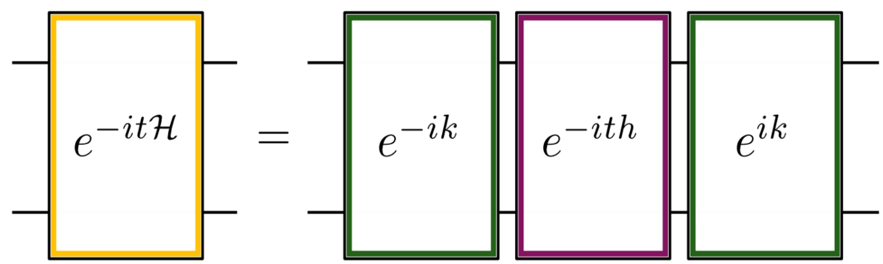

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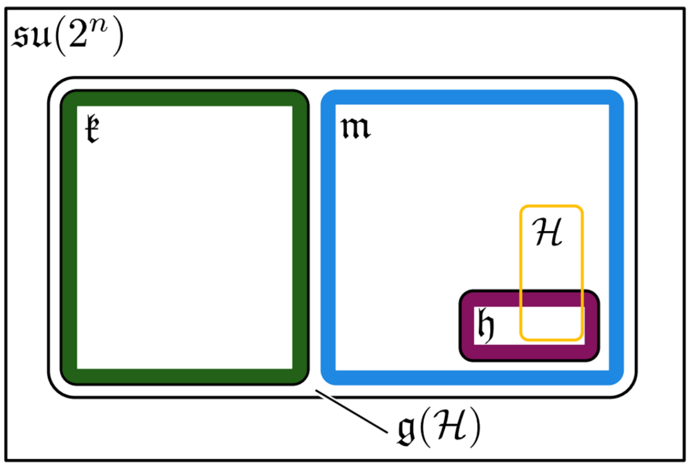
Cartan Decomposition and KHK Theorem



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

Have $H \in \mathfrak{m}$, and consider the following function

$$\boxed{f(K) = \langle K v K^\dagger H \rangle}$$

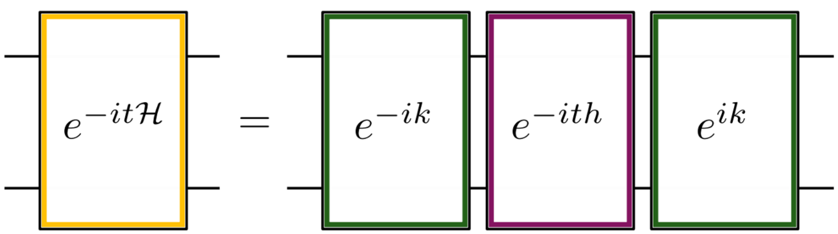
where

$$K = e^{\theta_1 k_1} e^{\theta_2 k_2} ... e^{\theta_{n_k} k_{n_k}}$$

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

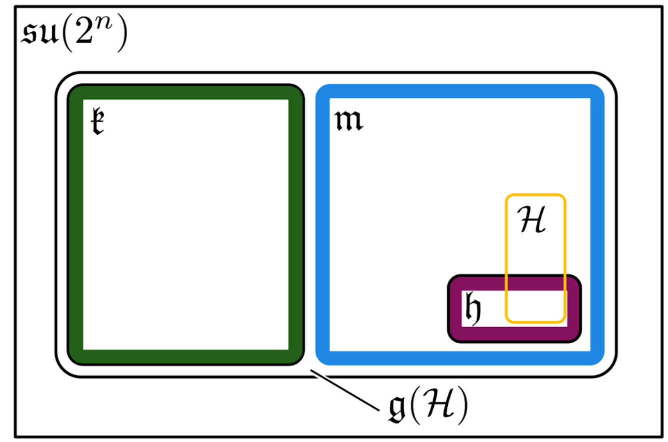
Then for any local minimum or maximum of the function f denoted by K_0 will satisfy

$$K_0^\dagger H K_0 \in \mathfrak{h}$$

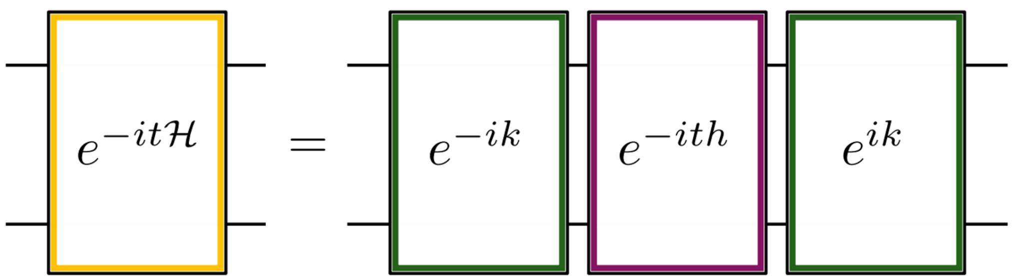


Algorithm

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

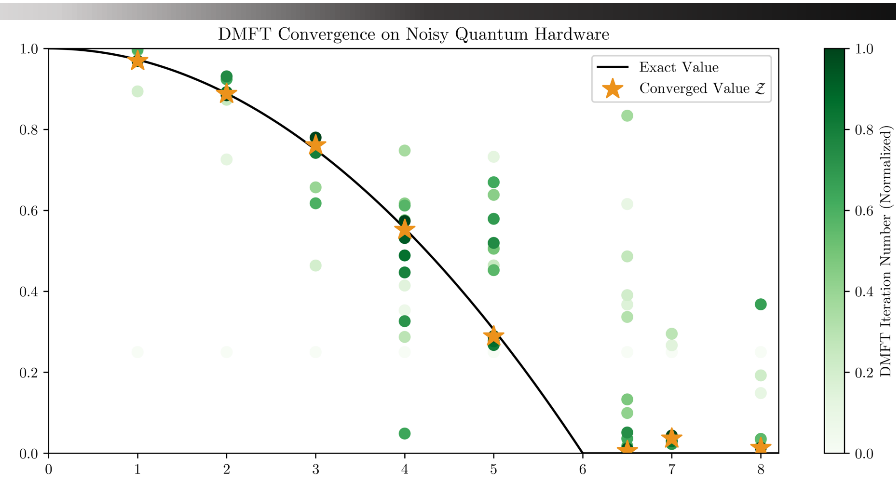


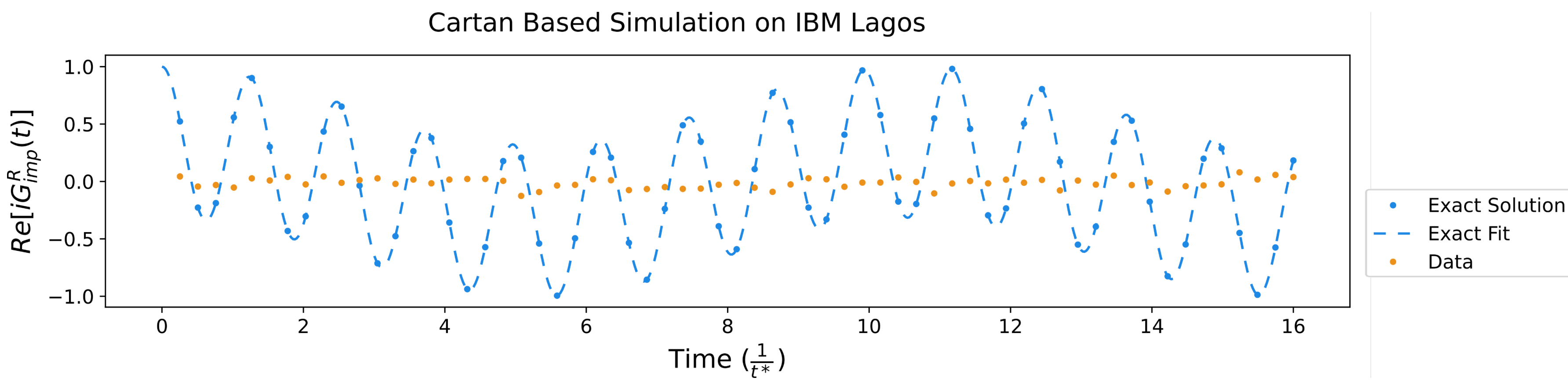
$$f(K) = \langle K v K^{\dagger}, \mathcal{H} \rangle$$



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)

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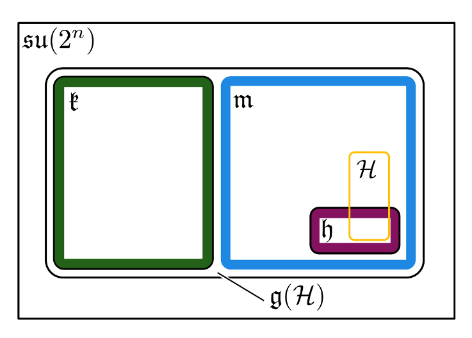
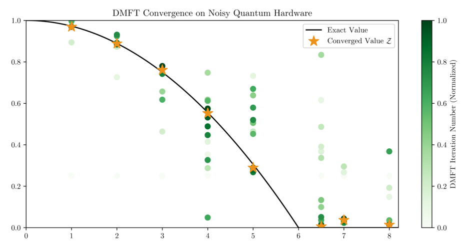
2 Algebraic methods for circuit generation

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

Kökcü PRL (2022) , Steckmann PRR (2023)

Algebraic Compression

Kökcü PRA (2021), Camp SIMAX 2022, Kökcü arXiv:2303.09538

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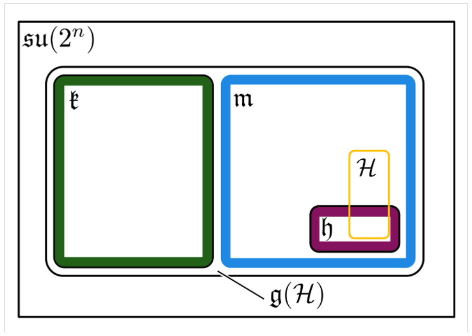
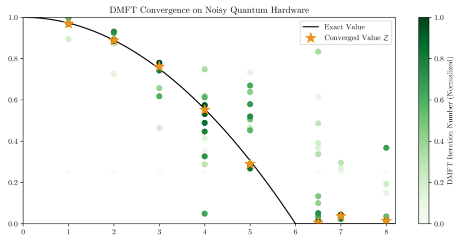
2 Algebraic methods for circuit generation

Cartan Decomposition





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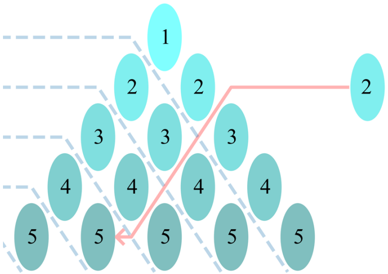
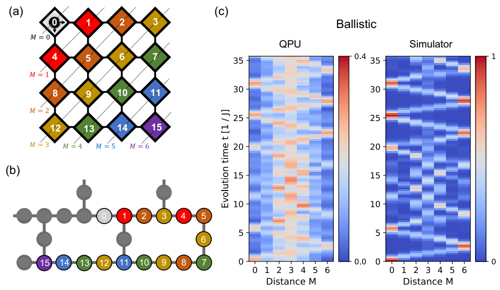
- We have code available! https://github.com/kemperlab/cartan-quantum-synthesizer

Algebraic Compression





- Compressed Trotter circuits down to a shallow fixed depth circuit for 1-D nearest neighbor TFXY, TFIM, XY and Kitaev models.
- Based on 3 easy to check, local properties.
- We have code available! Check F3C, F3C++ and F3Cpy at https://github.com/QuantumComputingLab

Kökcü PRL (2022) , Steckmann PRR (2023)

Kökcü PRA (2021), Camp SIMAX 2022, Kökcü arXiv:2303.09538

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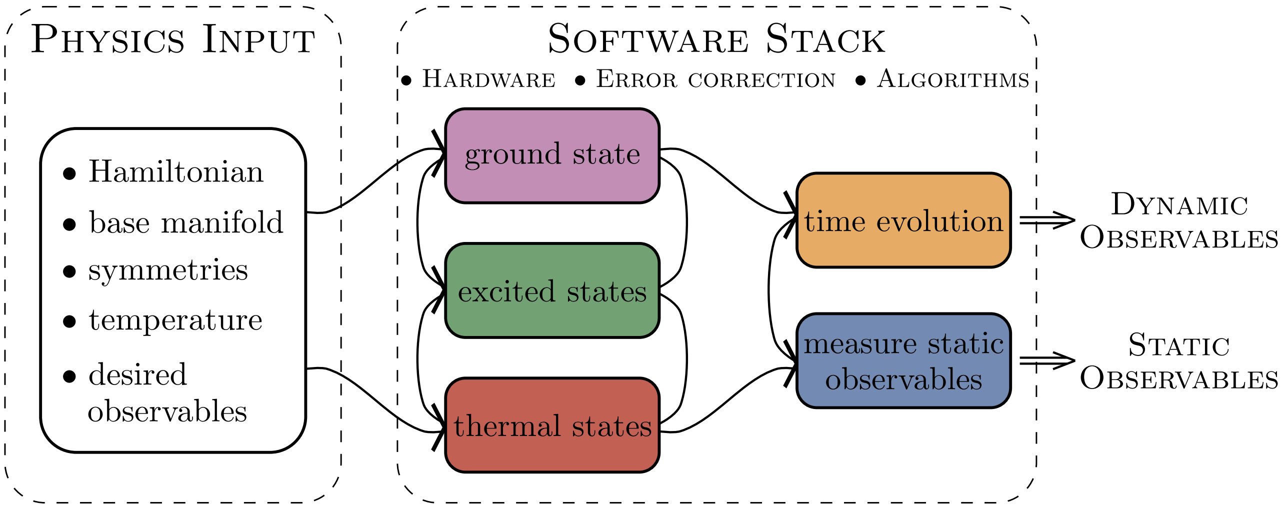
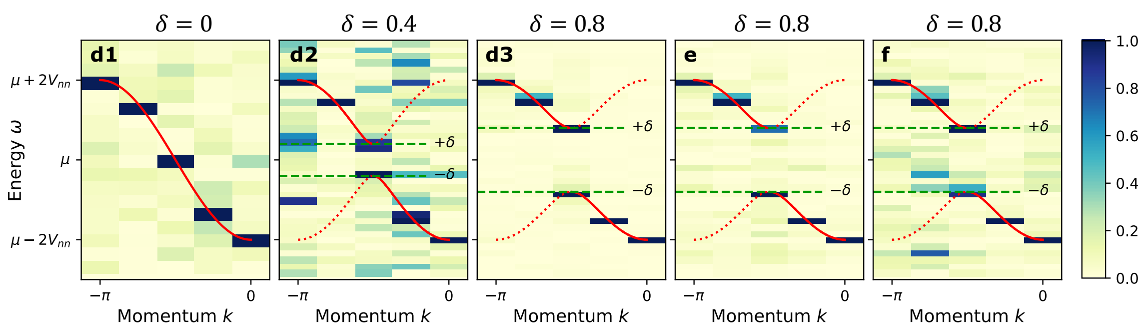
Quantum Matter meets Quantum Computing



https://go.ncsu.edu/kemper-lab



- Experimental relevance: Measuring correlation functions
- Measuring exact integer Chern numbers for topological states
- Open quantum evolution and fixed points (1000 Trotter steps)
- Time evolution via Lie algebraic decomposition and compression
- Thermodynamics via Lee-Yang Zeros
- Physics-Informed Subspace Expansions