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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

CECAM/QSE @ EPFL
Quantum Algorithms for Chemistry and Material Science Simulation
Lausanne, Switzerland
12/13/2023

Quantum Algorithms for Chemistry and Material Science Simulation: Bridging the Gap Between Classical and Quantum Approaches

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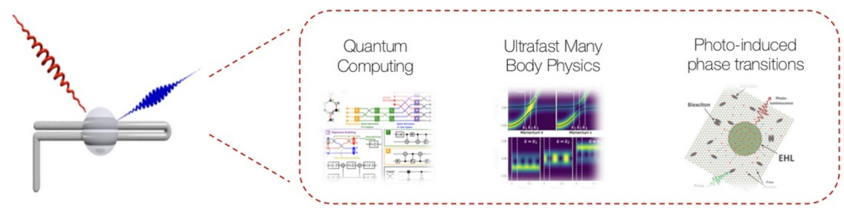


Kemper Lab

Quantum materials in and out of equilibrium.

Collaborations with:

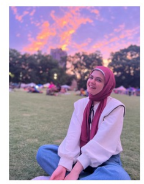
- Bojko Bakalov (NCSU)
- Marco Cerezo, Martin de la Rocca (LANL)
- Jim Freericks (Georgetown)
- Daan Camps, Roel van Beeumen, Bert de Jong, Akhil Francis (LBNL)
- Thomas Steckmann (UMD)
- Yan Wang, Eugene Dumitrescu (ORNL)

Current members

Alexander (Lex) Kemper
Principal investigator

Efekan Kökcü
Graduate Researcher

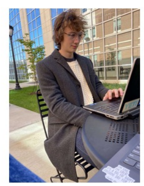
Anjali Agrawal
Graduate Researcher



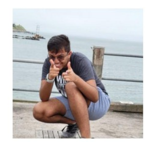
Heba Labib
Graduate Researcher

Jack Howard
Undergraduate Researcher

Norman Hogan
Graduate Researcher



Ethan Blair
Undergraduate Researcher



Arvin Kushwa a
Undergraduate Researcher

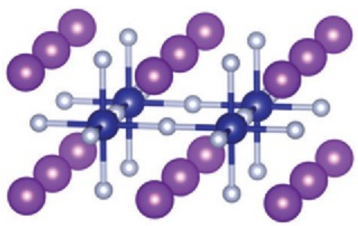
Your Na e
New lab memb

We're looking for postdocs to join our lab!

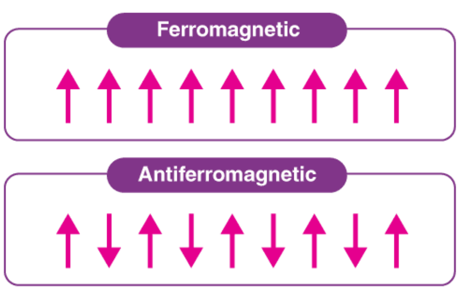
A Tale of Two Transitions

Ising Magnet

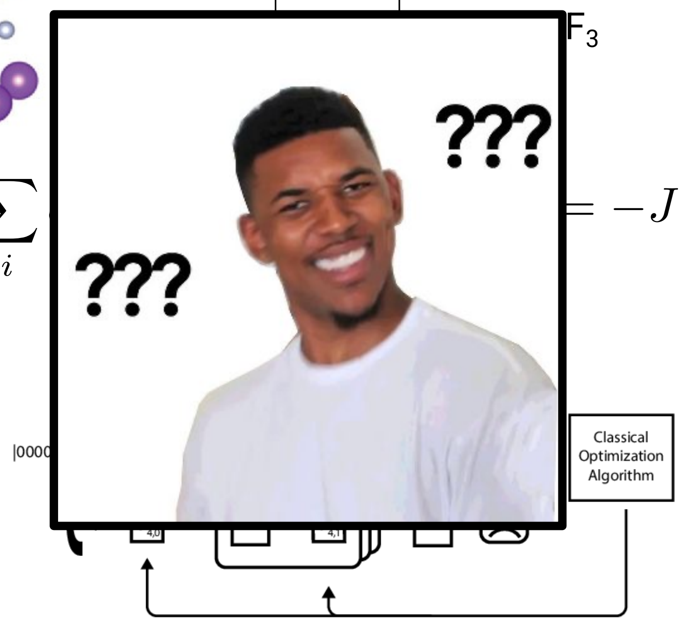
Rb_2CoF_4



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



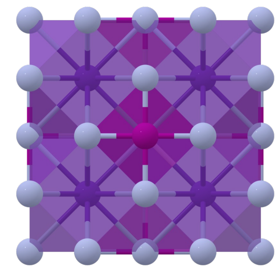
10.1039/c6cp02362b



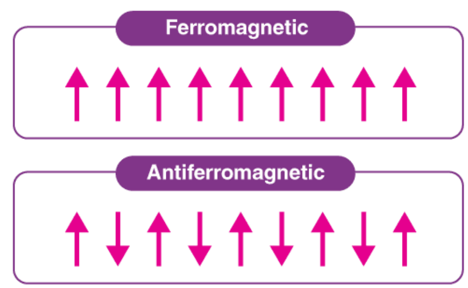
Optimization of the Variational Quantum Eigensolver for Quantum Chemistry Applications

Heisenberg Magnet

F_3



$$= -J\sum_i \vec{\sigma}_i \cdot \vec{\sigma}_{i+1} + h_x \sum_i \sigma_i^x$$



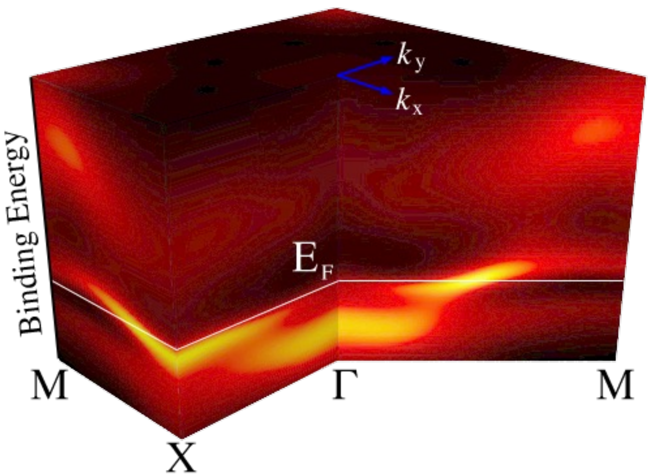
Materials project

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

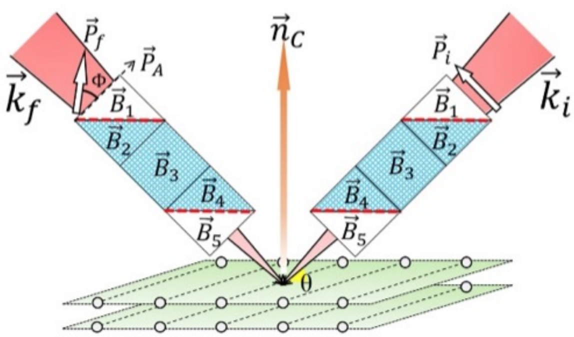
A: You measure its excitations.

Measuring Excitations

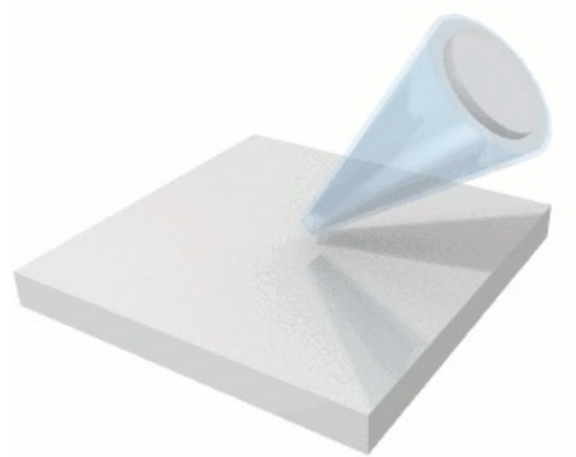
Figures courtesy of Devereaux/Shen group and ORNL



Angle-resolved Photoemission (ARPES)



Neutron Scattering



Time-resolved ARPES

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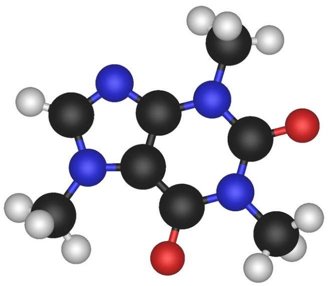
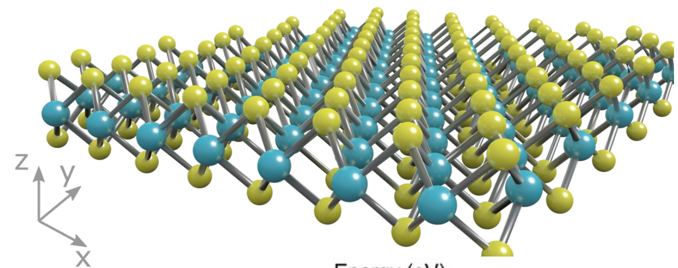
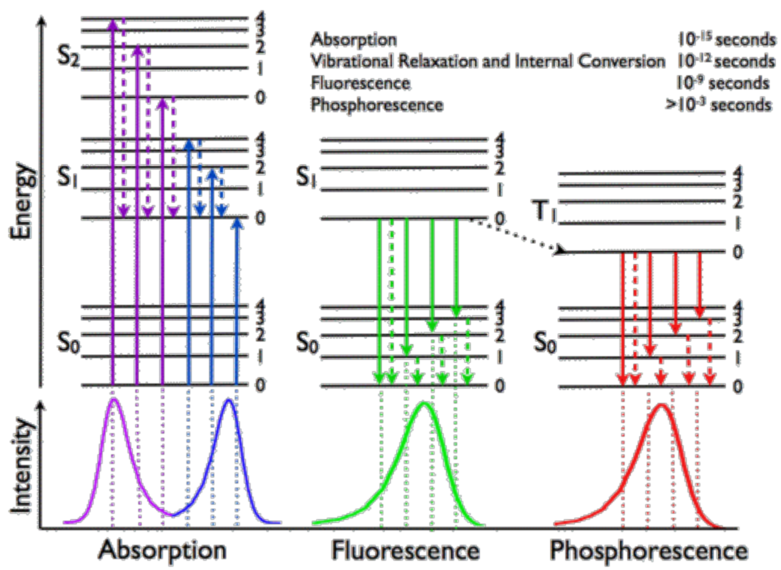
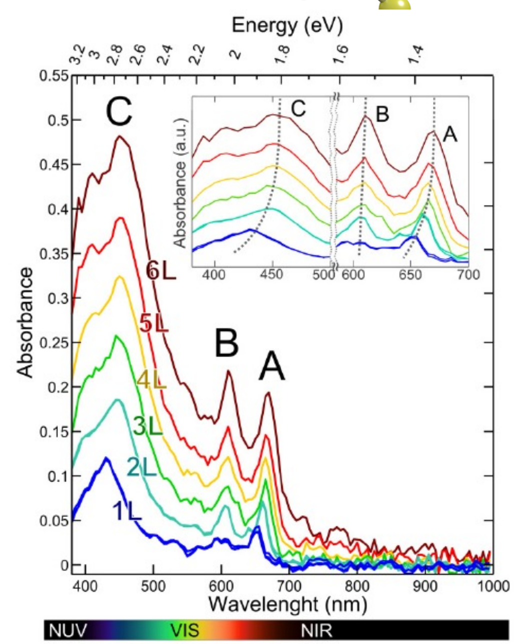
Measuring Excitations





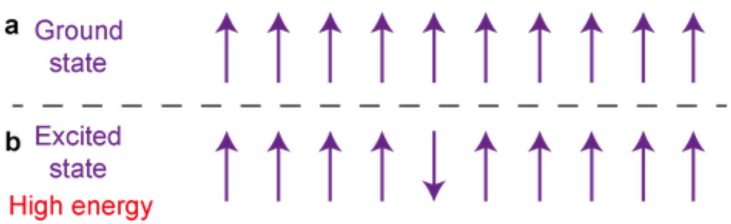




Measuring Excitations

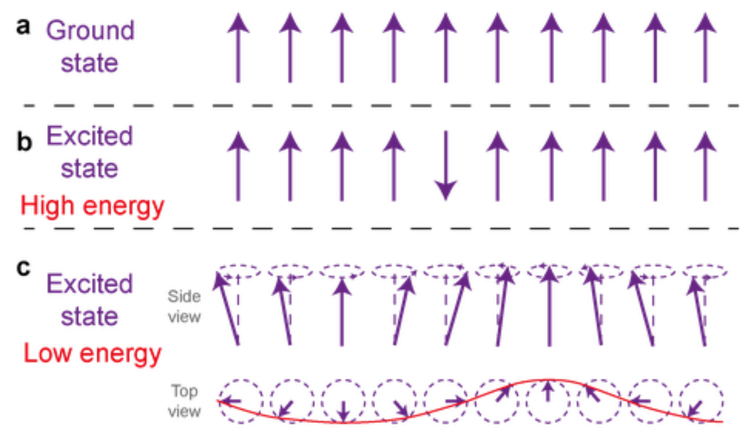
Ising Model

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

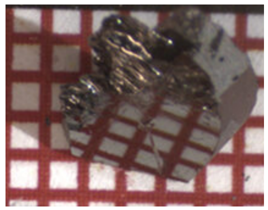


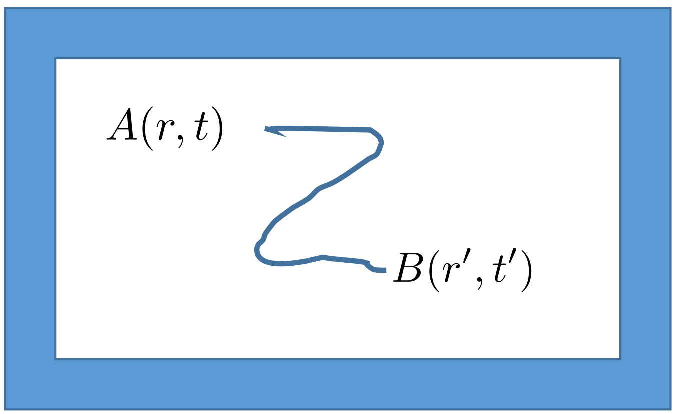
Heisenberg model

$$\mathcal{H} = -J \sum_i \vec{\sigma}_i \cdot \vec{\sigma}_{i+1} + h_x \sum_i \sigma_i^x$$



Correlation functions





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

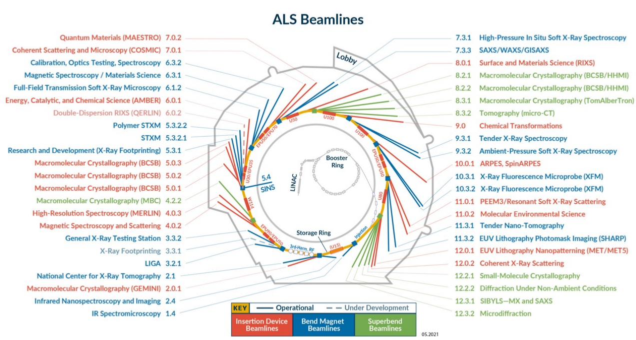
Given some (observable) operator B at (r',t'), what is the likelihood of some (observable) operator A at (r,t)?

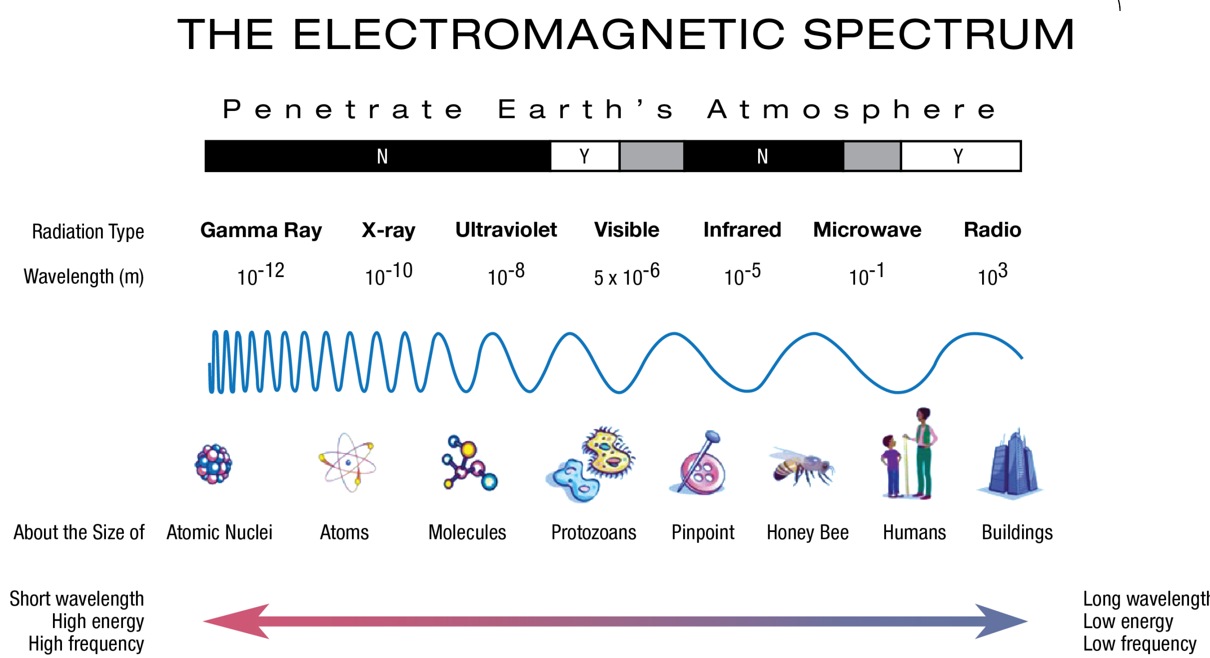
Optical conductivity, γ/X-ray scattering, photoemission, neutron scattering, Raman, IR absorption, etc.

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

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

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





The Electromagnetic Spectrum. Image Credit: NASA

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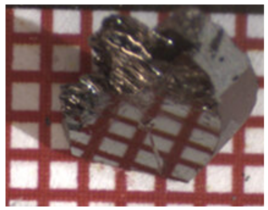
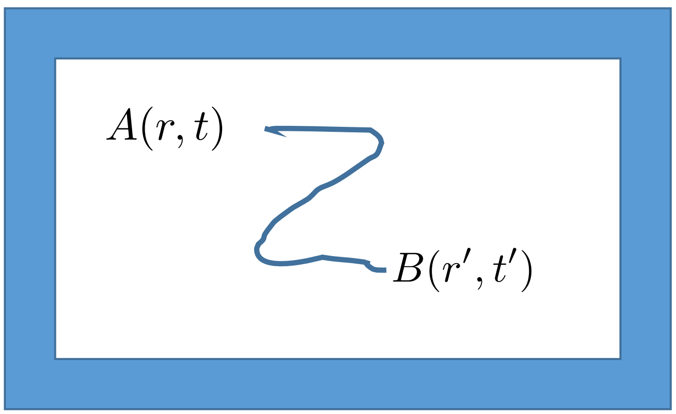
Correlation functions





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

Interfere with ground state

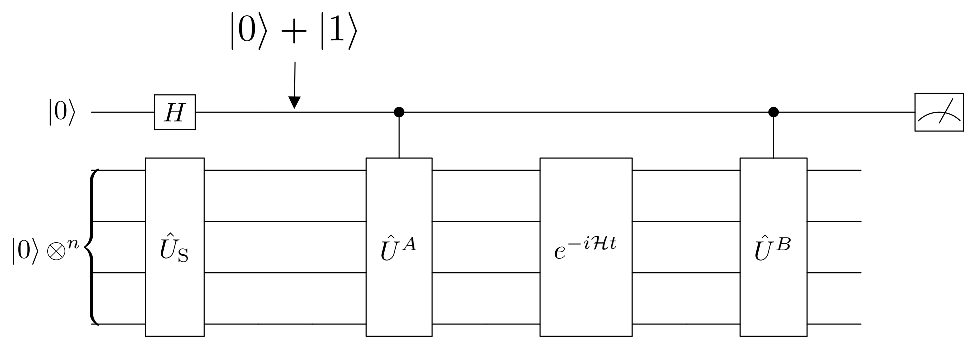
Complete expectation value

Apply excitation B

Time evolve

Apply excitation A

Prepare state of interest



Somma, Simulating physical phenomena by quantum networks (2002)

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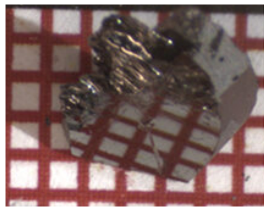
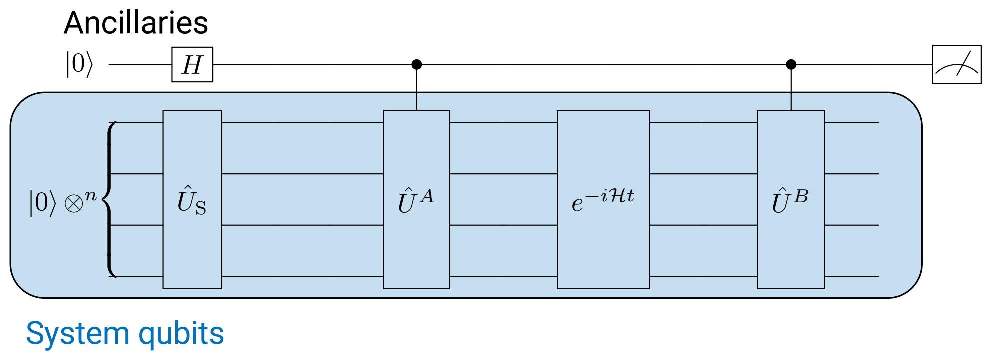
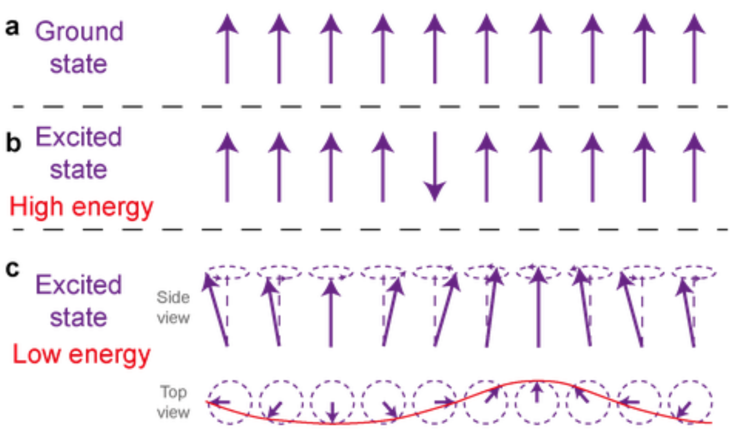
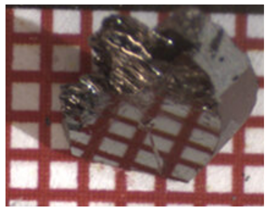
Correlation functions

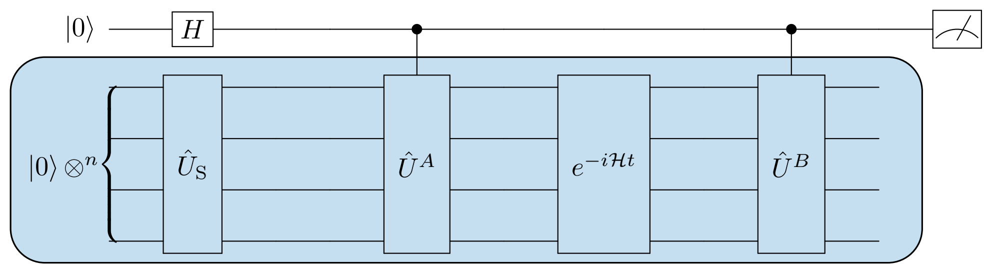






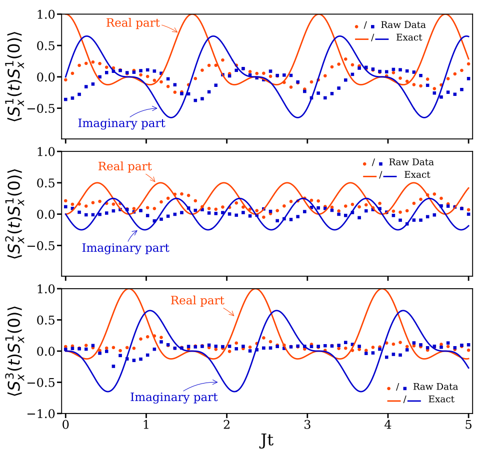
Correlation functions



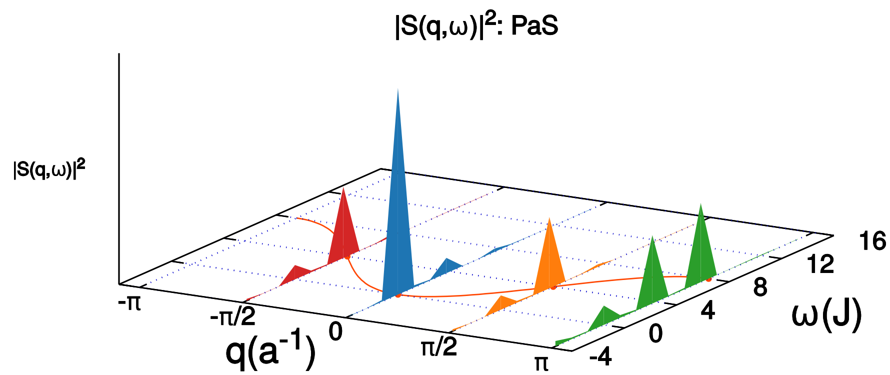


System qubits

Raw data (2019)



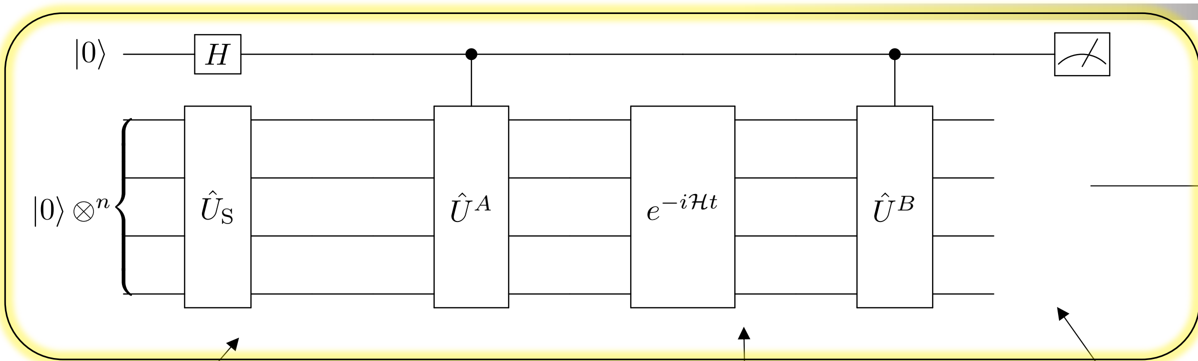
Error mitigation



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

A-Z quantum simulation

Digital version of this talk



Classical post-processing techniques

Prepare state of interest

Time evolve

Dynamical response functions

- *Physics-Informed Subspace Expansions*

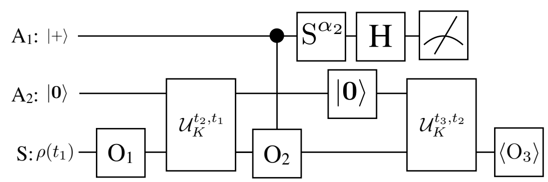
- *Lie-algebraic methods for time evolution*
- *Open quantum system evolution*

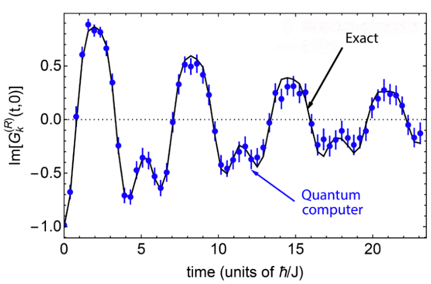
- *Neutron scattering (magnon) spectra*
- *Open quantum system Green's functions*
- *Dynamical Mean Field Theory*

(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

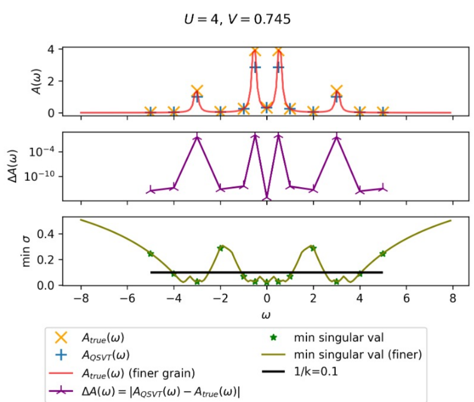
L. Del Re, B. Rost, M. Foss-Feig, AFK, J.K. Freericks
2204.12400

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)

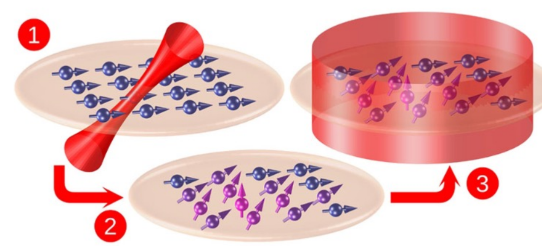


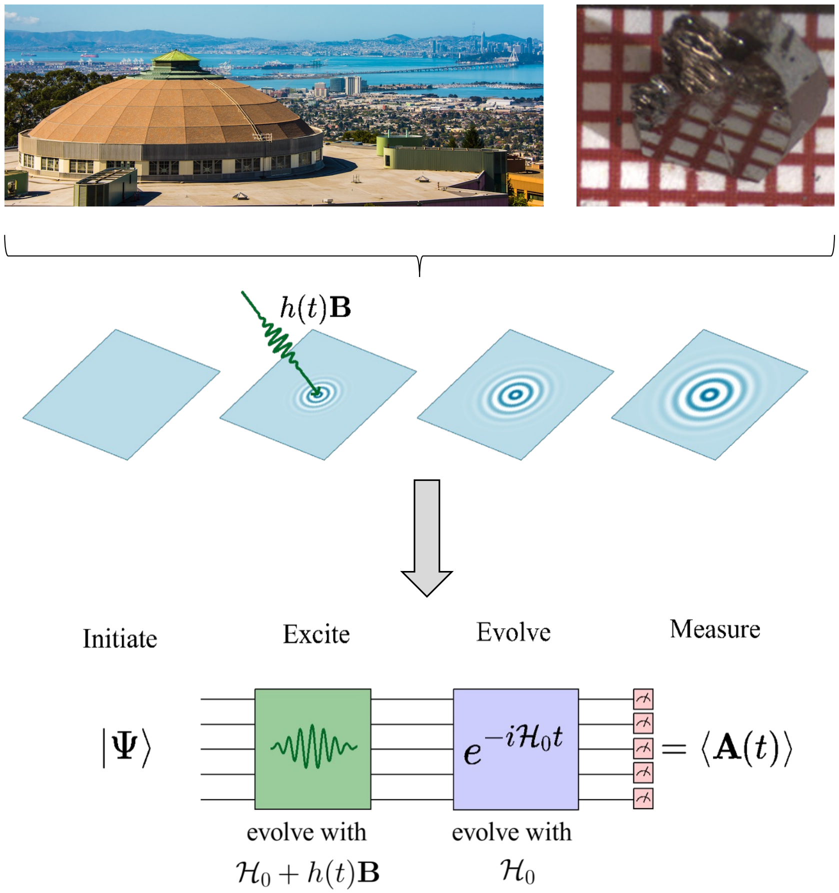
FIG. 1 (color online). Many-body Ramsey interferometry consists of the following steps: (1) A spin system prepared in its ground state is locally excited by $\pi/2$ rotation; (2) the system evolves in time; (3) a global $\pi/2$ rotation is applied, followed by the measurement of the spin state. This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

Commutators

10.1103/PhysRevLett.111.147205

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,*]

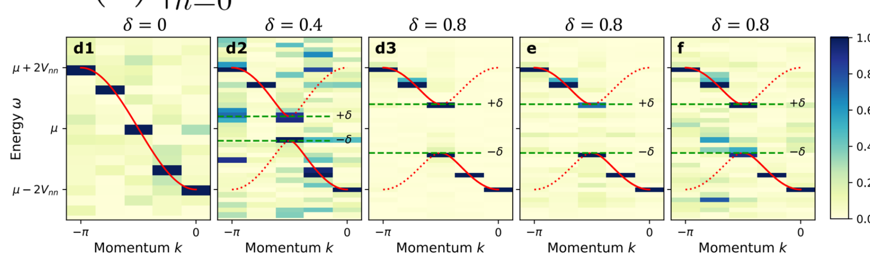
[1] Department of Physics, North Carolina State University, Raleigh, North Carolina 27695, USA
[2] Department of Physics, Georgetown University, 37th and O Sts. NW, Washington, DC 20057 USA

(Dated: February 22, 2023)

1. Make the excitation <u>part</u> of the quantum simulation

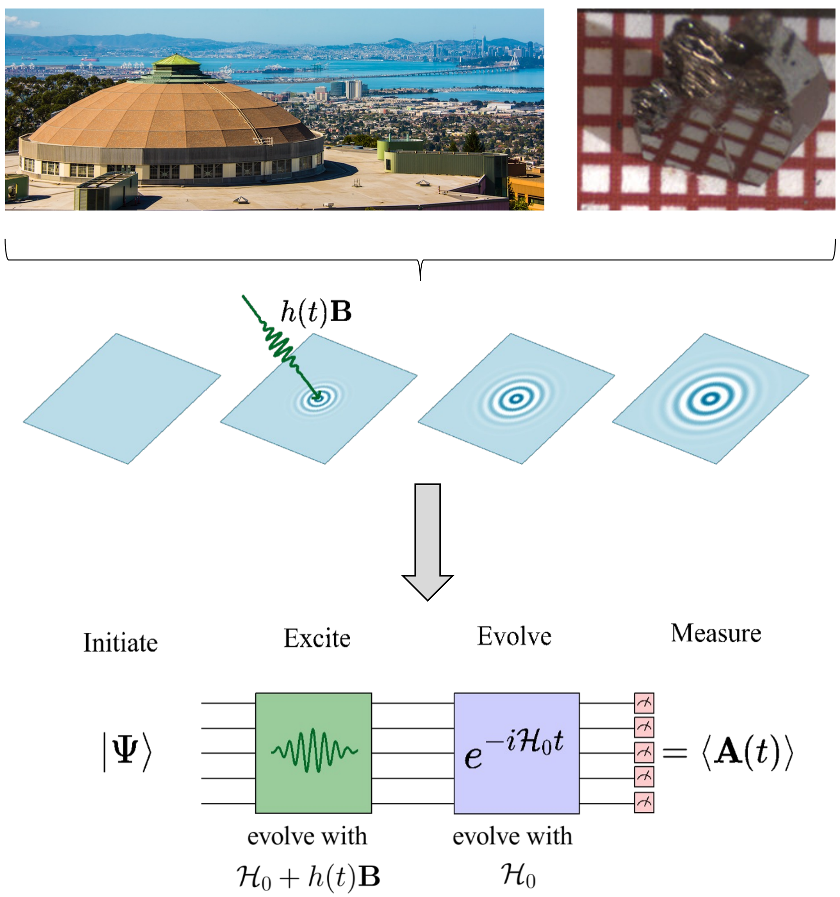
2. Post-process the data to get the response functions

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



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*
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(Dated: February 22, 2023)

Benefits

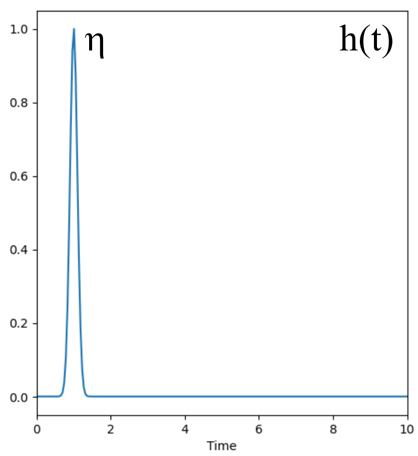
- Any operator A,B you desire (as long as it is Hermitian*)
- No ancillas/controlled operations needed
- Many correlation functions at the same time
- Less post-processing (less noise)
- Frequency/momentum selective

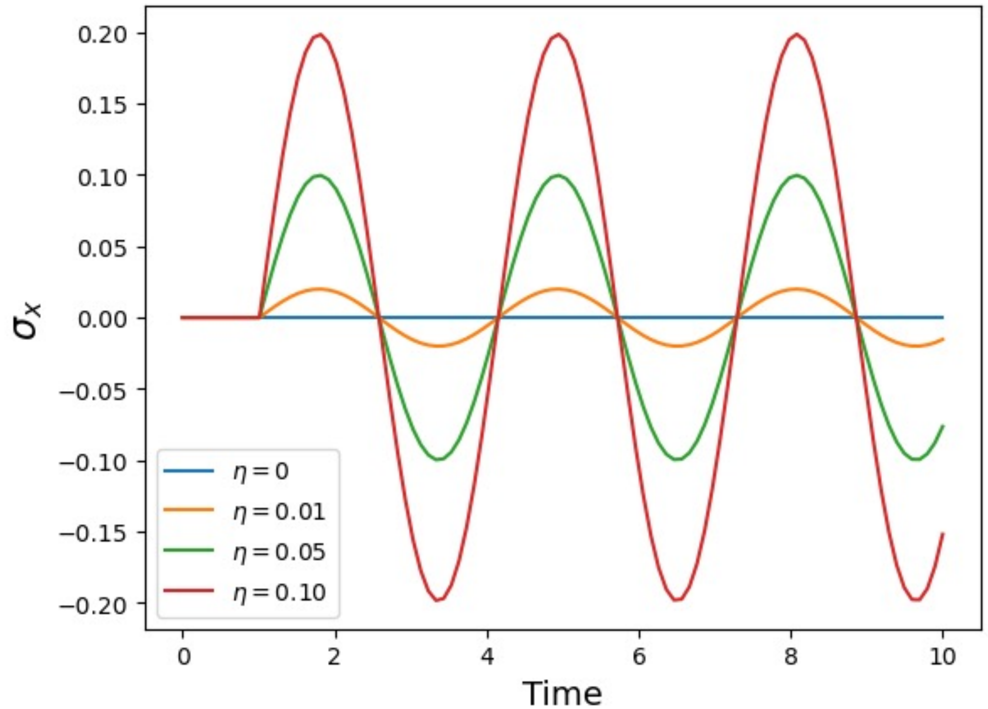
Linear Response

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

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

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





Linear Response

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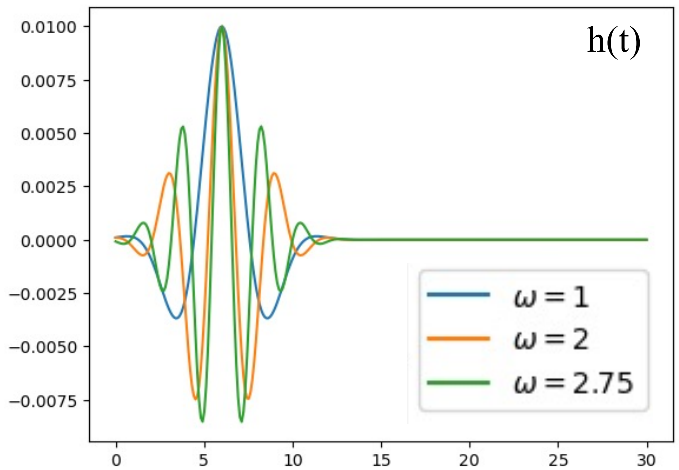
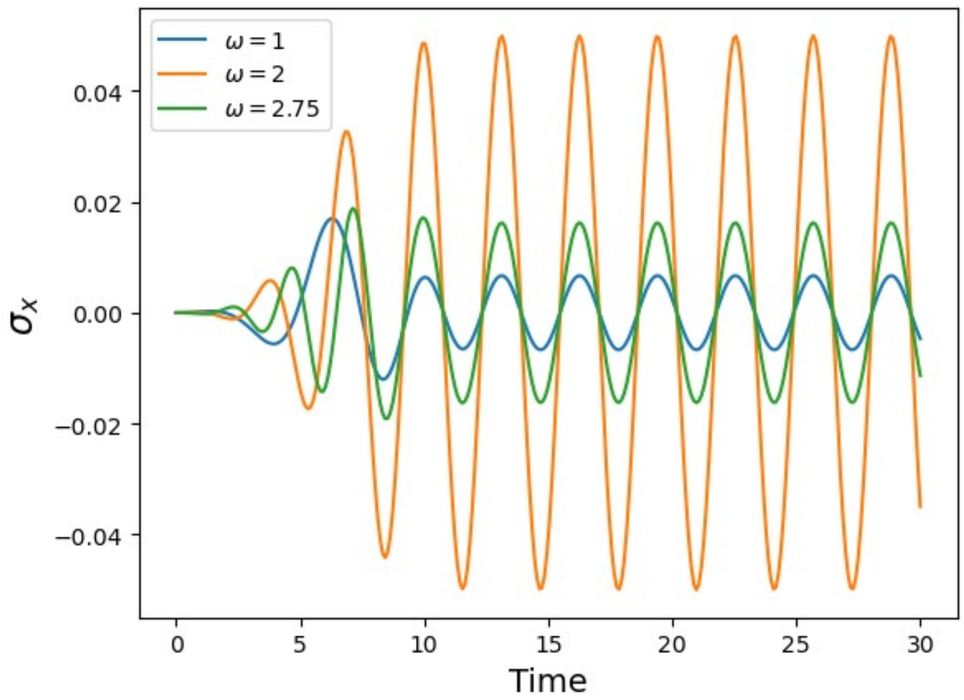


Frequency



Linear Response

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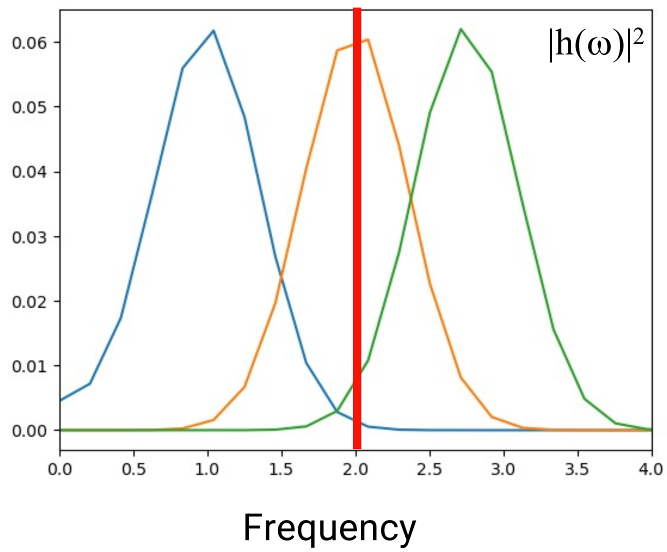

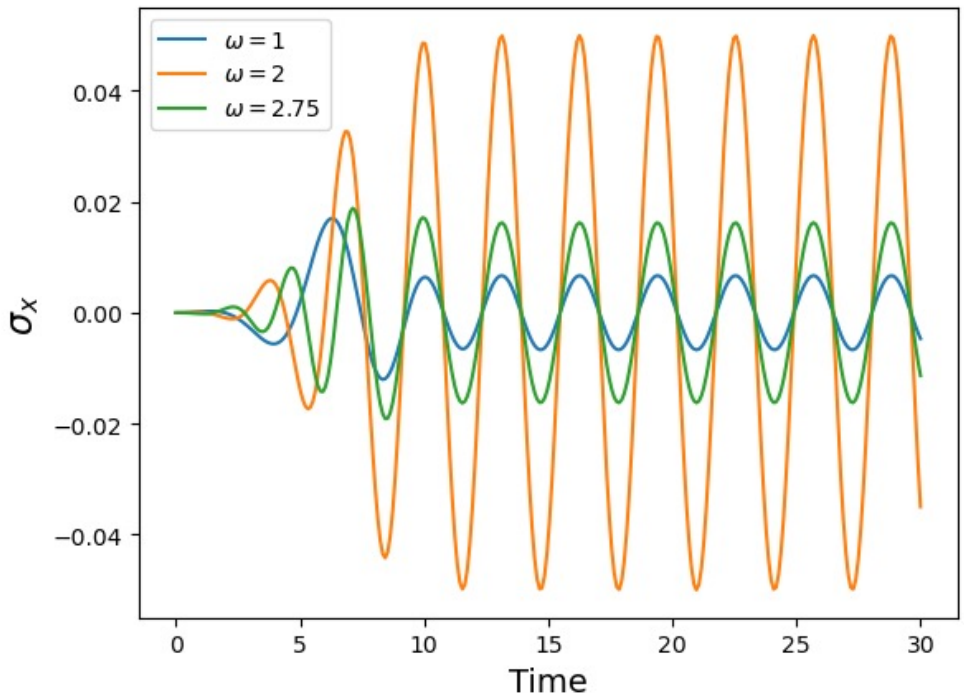

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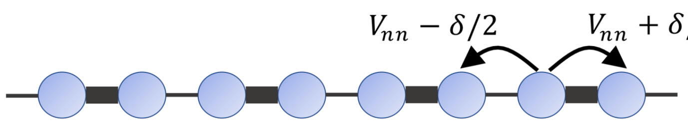
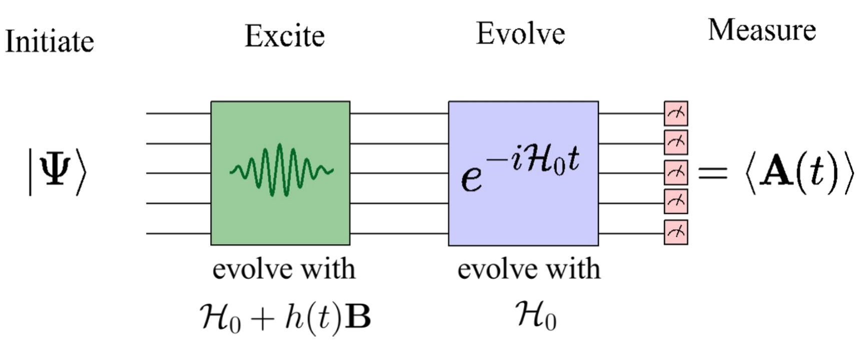
A Bosonic Correlation function: Polarizability

Su-Schrieffer-Heeger model for polyacetylene



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



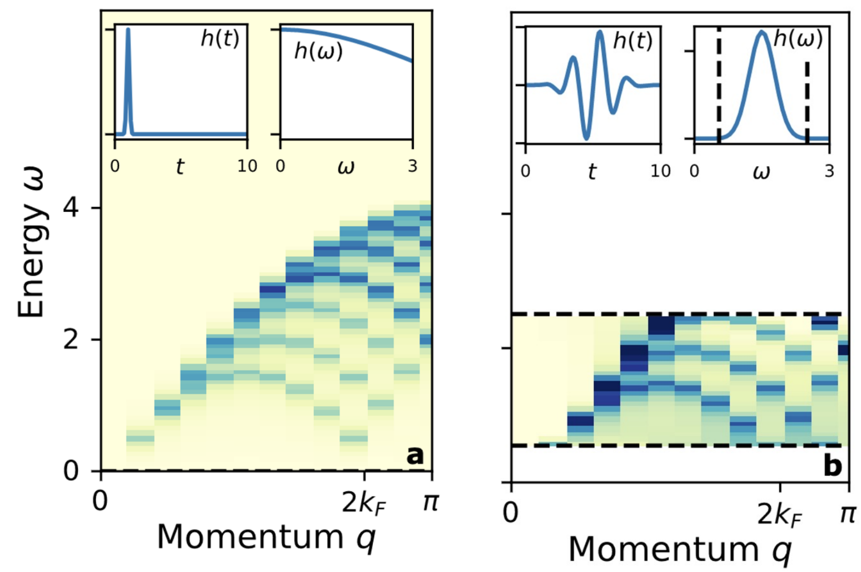
$$A(t) = \int dt' \chi^R(t-t') h(t') + \mathcal{O}(h^2)$$

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

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

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

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



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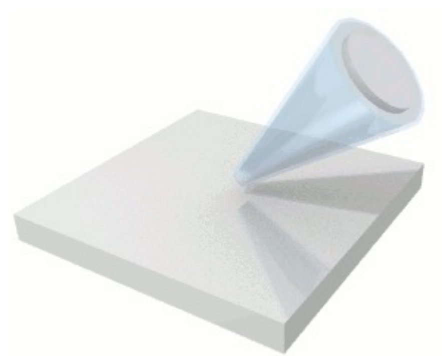
Fermionic Linear Response

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

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

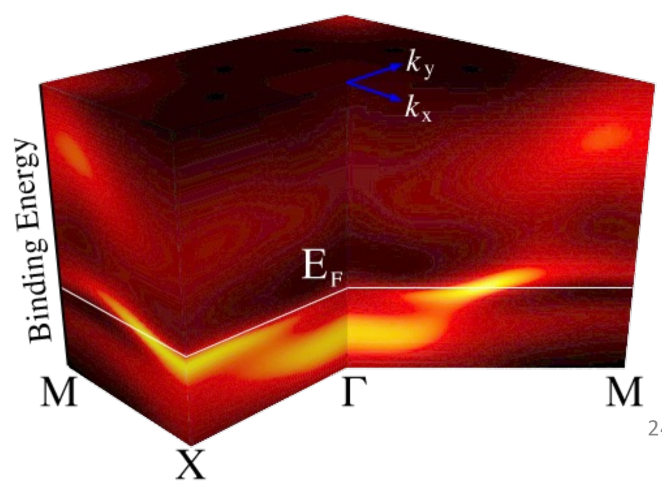
$$G(t,t') = -i\theta(t-t')\langle\psi_0|\{\mathbf{A}(t),\mathbf{B}(t')\}|\psi_0\rangle$$



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



Fermionic Linear Response

2302.10219

Option 1: Auxiliary operator

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

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:

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

Example: parity

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

Option 2: Post-selection

Fermionic Linear Response

2302.10219

Option 1: Auxiliary operator

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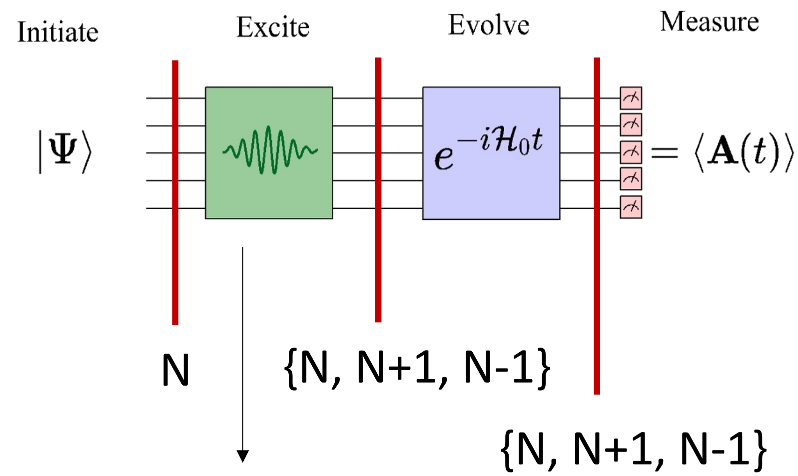
Option 2: Post-selection



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

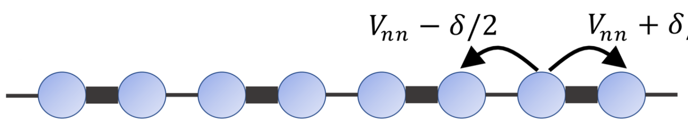
Post-selection on particle number gives us

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

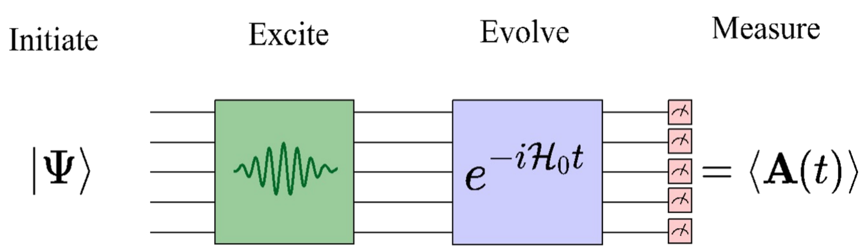
Linear Response -> Green's function

2302.10219

Su-Schrieffer-Heeger model for polyacetylene



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



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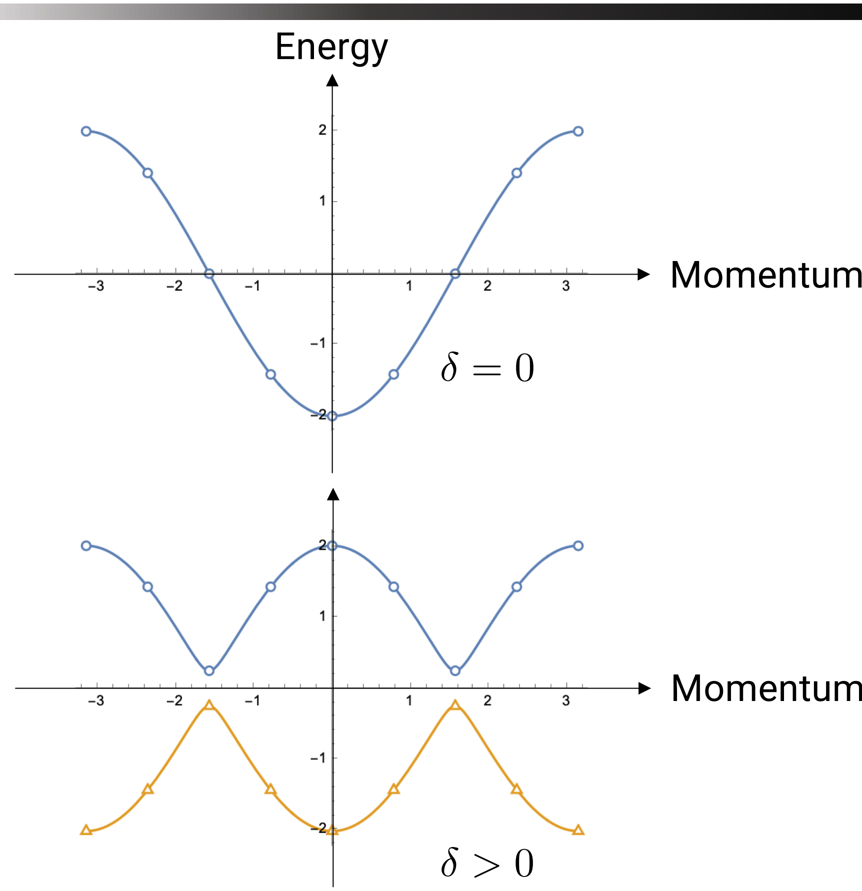

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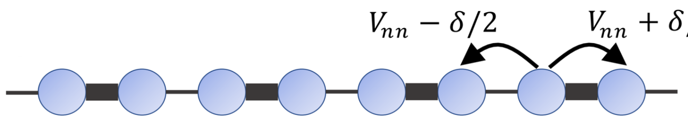

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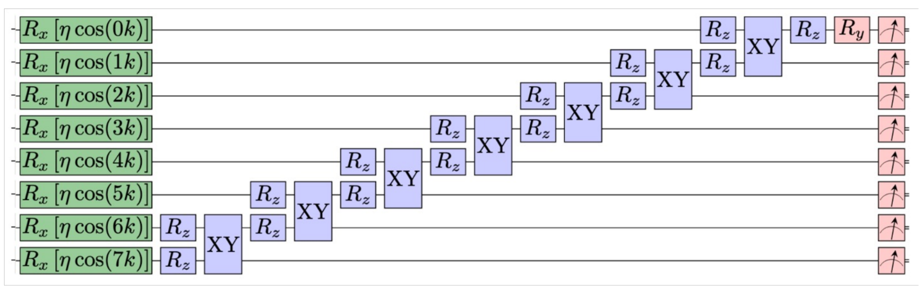
Compressed circuit run on *ibm_auckland*



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

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

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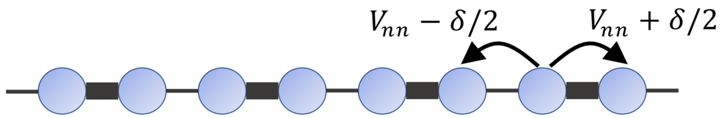

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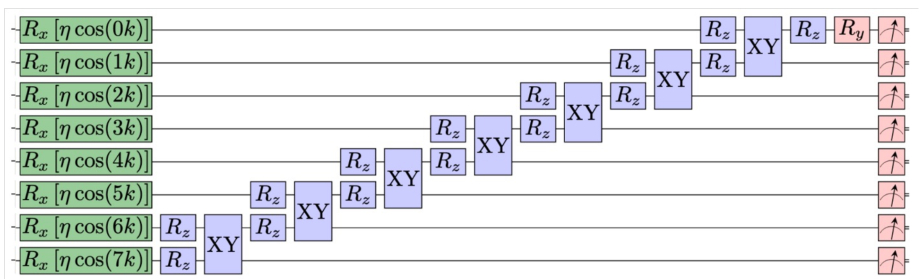

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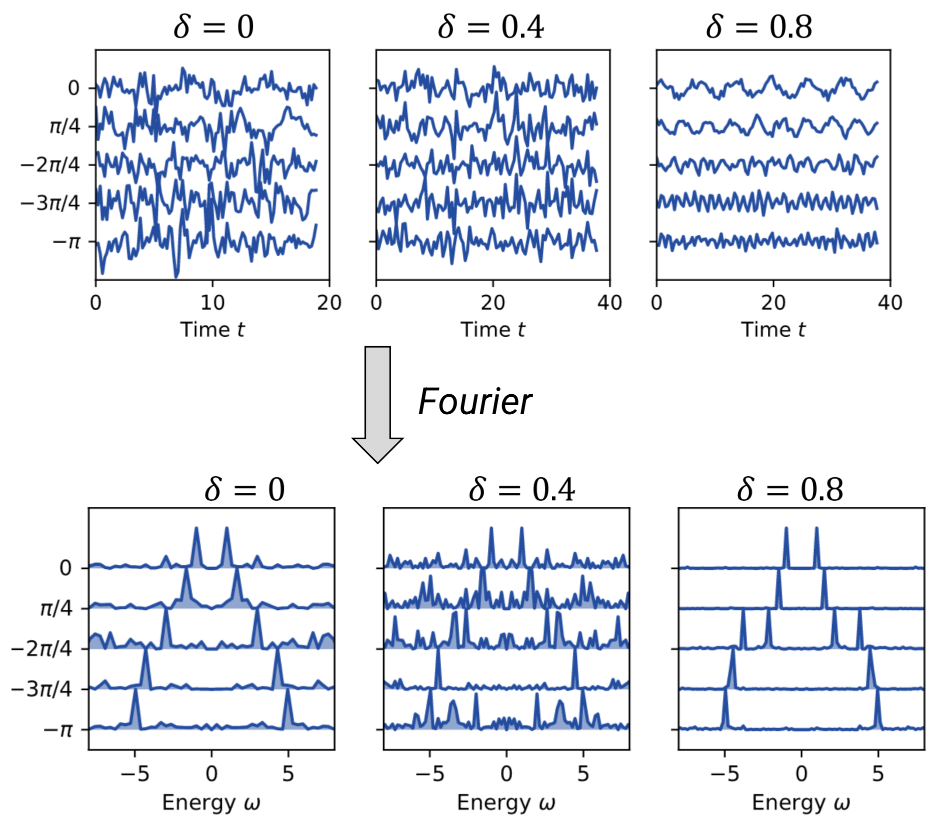

Linear Response -> Green's function

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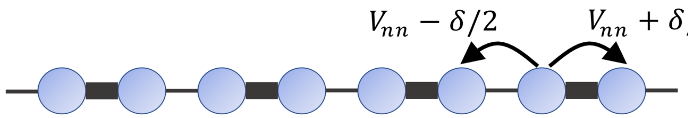

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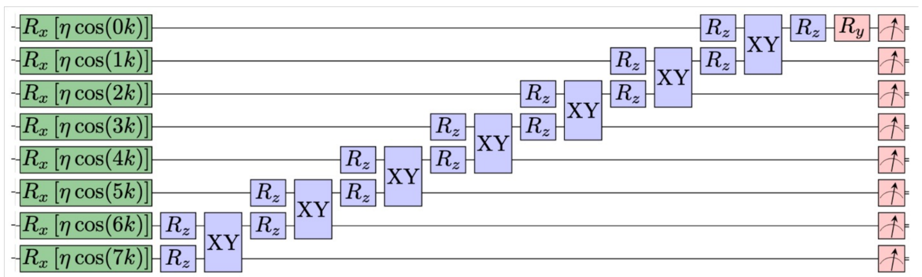

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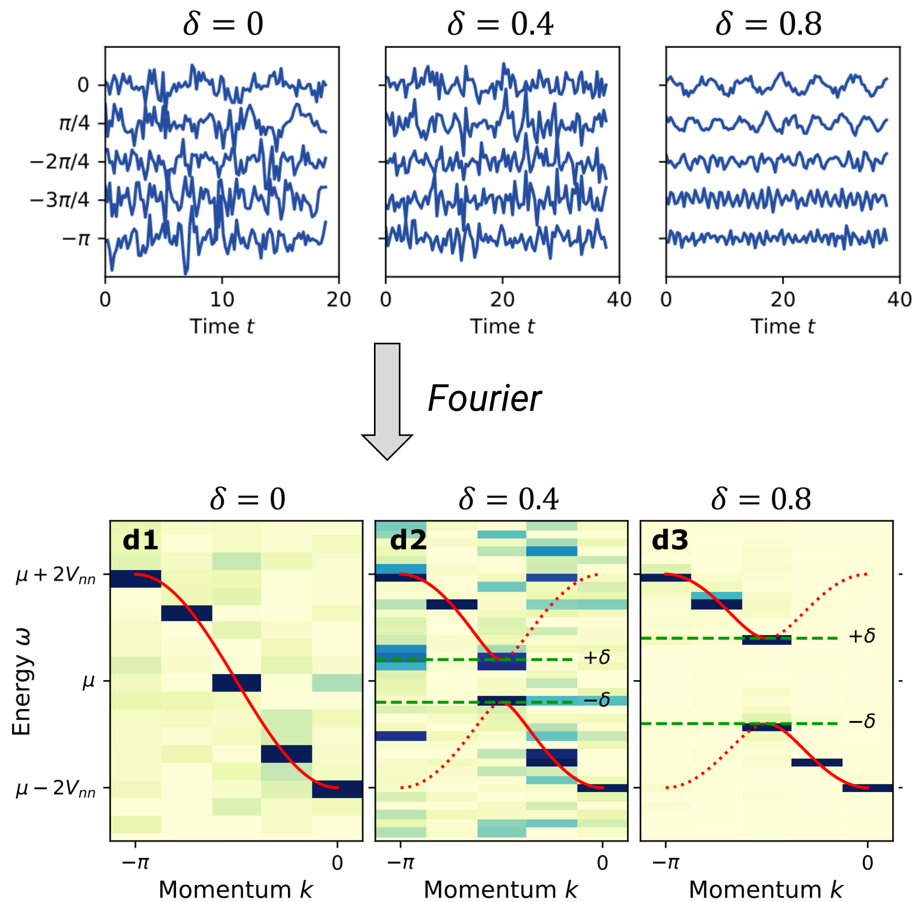
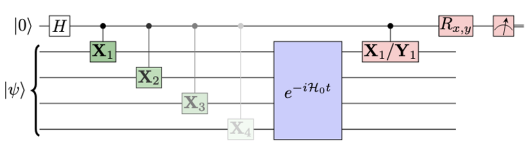


Linear Response -> Green's function

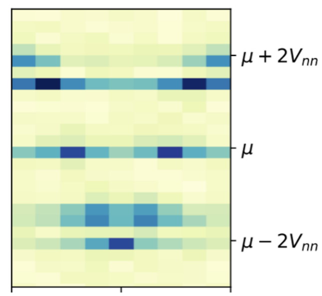
Why does this work so well?

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

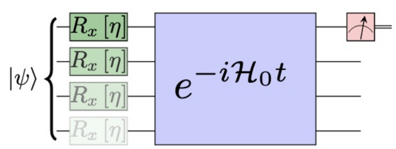
Hadamard test method



FT
$t \to \omega$
$r \to k$



Position-selective linear response



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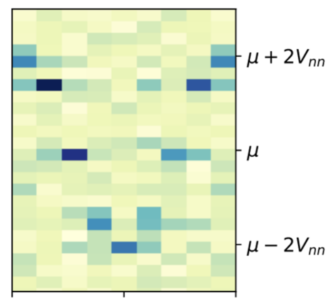
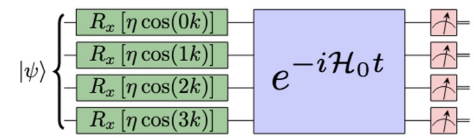
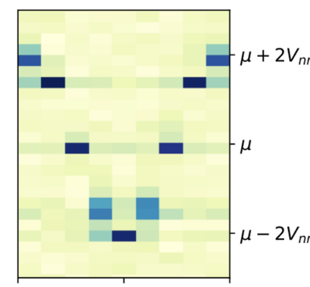


Momentum-selective linear response



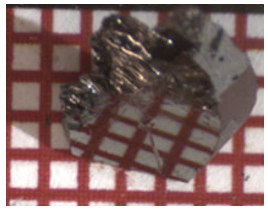
FT
$\omega \to t$

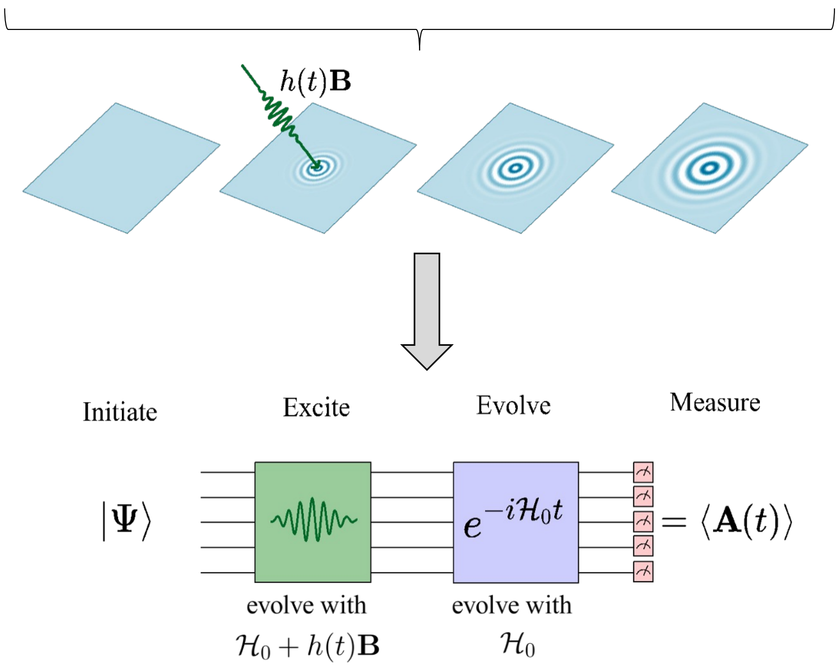


Data from noisy simulator with one/two qubit noise of 1% and 10%

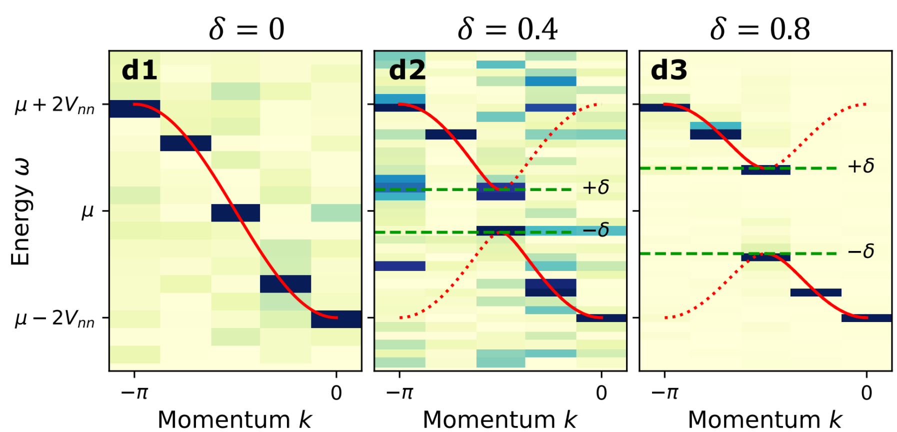
Digital version of this talk

Linear Response





- 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 (PSD) functions:

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

Kemper, Yang, Gull, arXiv:2309.02566

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

Kemper, Yang, Gull, arXiv:2309.02566

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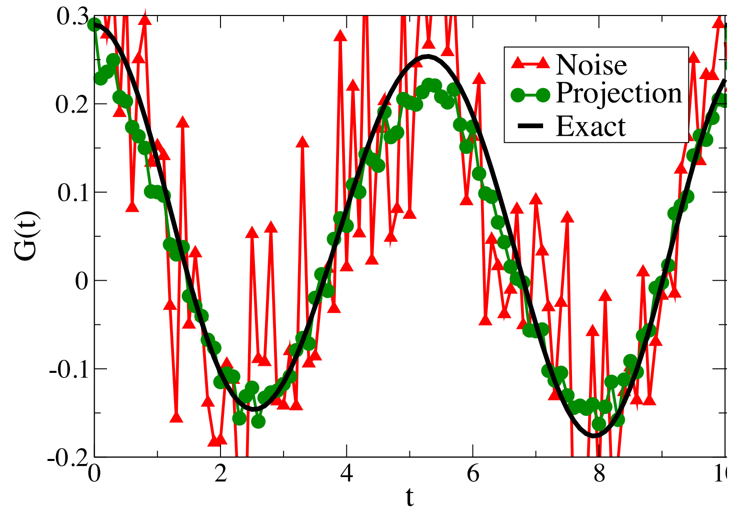
- What can I do with this?



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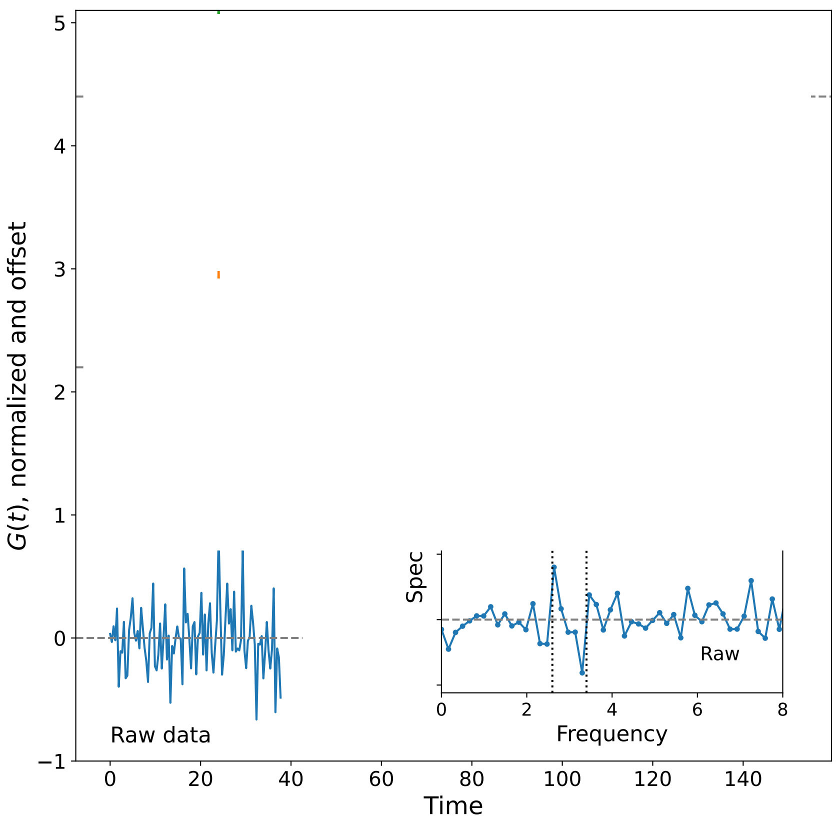

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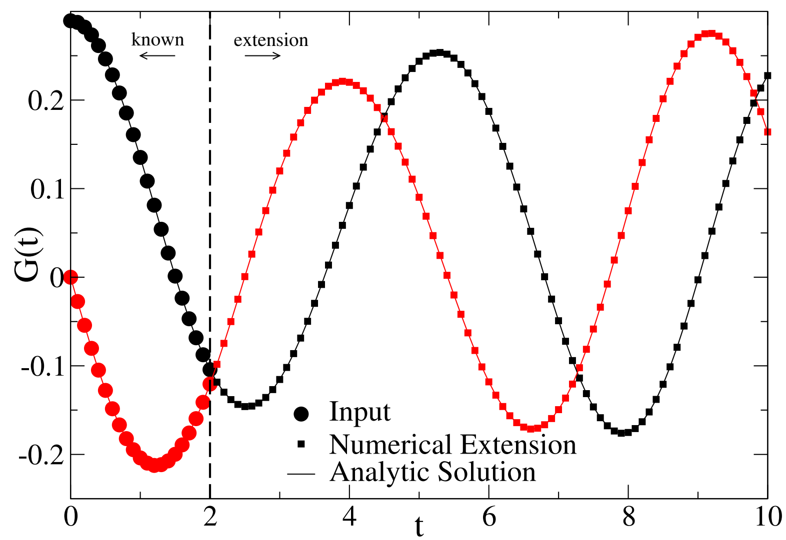
where $G_{AA}(t_i - t_j) \to f_{i-j}$

- What else can I do with this?



Kemper, Yang, Gull, arXiv:2309.02566

Further improvements via mathematics

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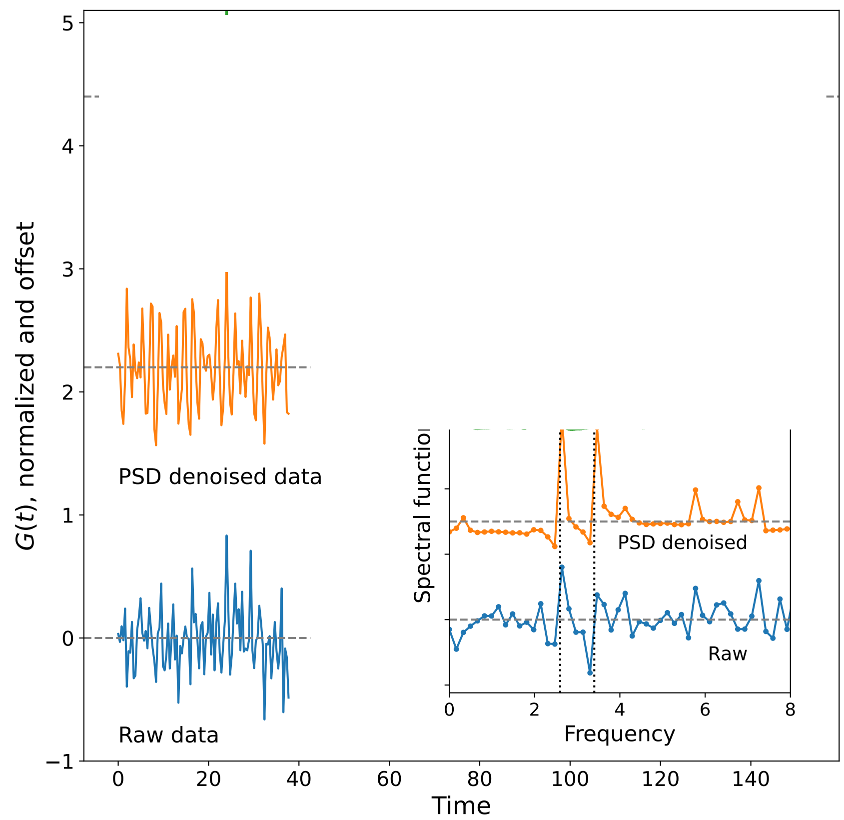

Kemper, Yang, Gull, arXiv:2309.02566

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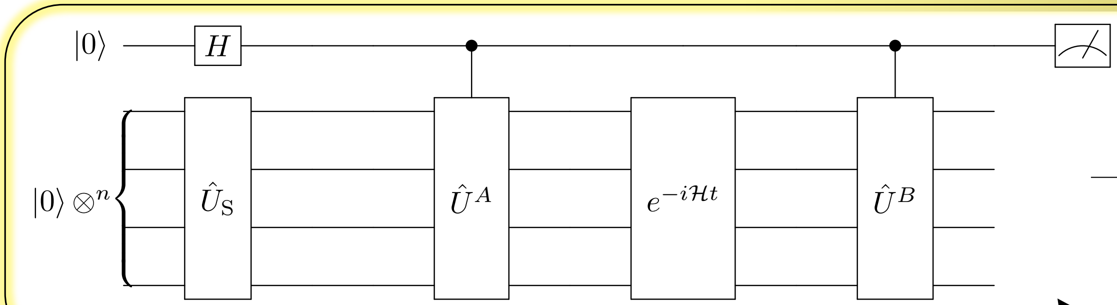
A-Z quantum simulation

Digital version of this talk



Classical post-processing techniques

Prepare state of interest

Time evolve

Dynamical response functions

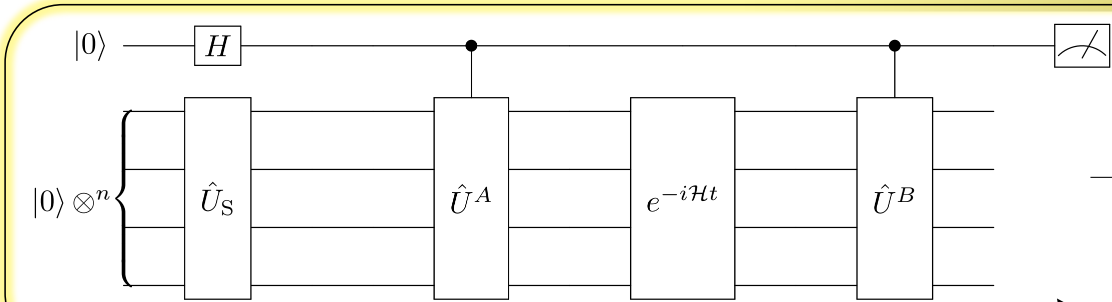
- *Physics-Informed Subspace Expansions*

- *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

Digital version of this talk



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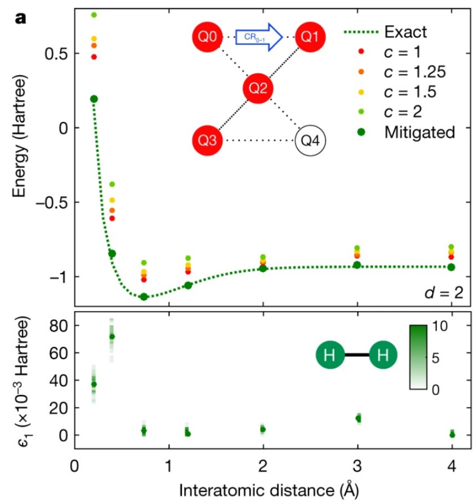
Preparing ground states

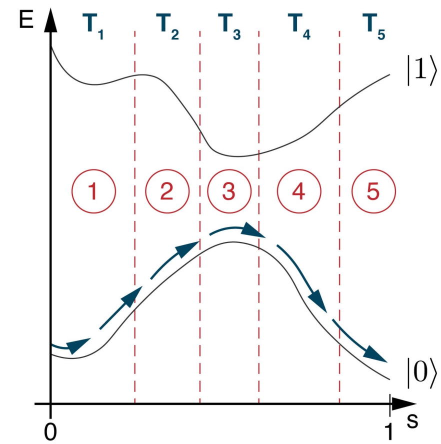
Variational Quantum Eigensolver



[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.

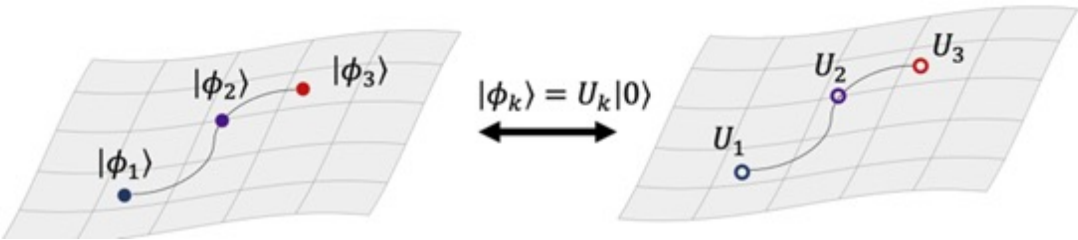
- Ground states
- Excited states
- Thermal states

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.

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



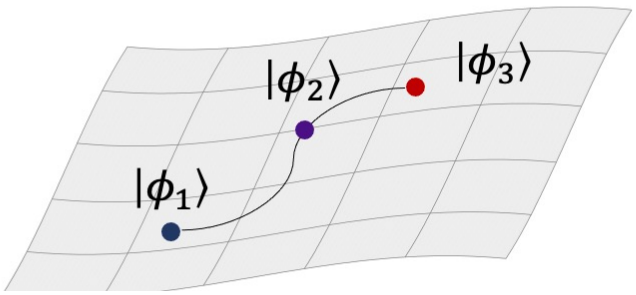
Using this:

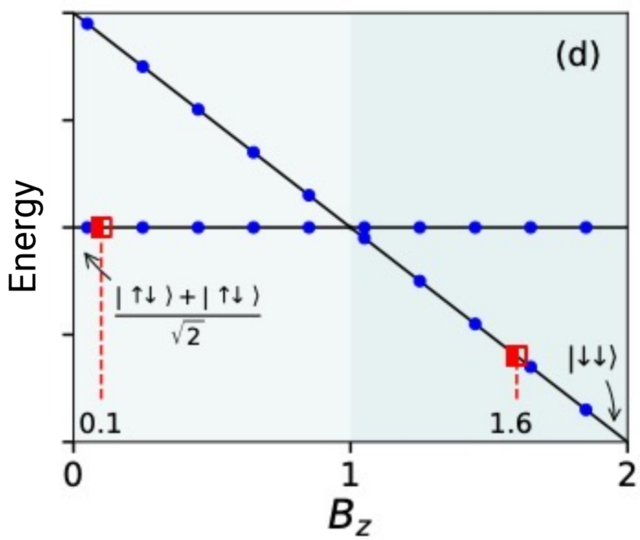
- Make a subspace using low energy states at different points in parameter space

- 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





$$\mathcal{H} = X_1 X_2 + Y_1 Y_2 + B_z (Z_1 + Z_2)$$

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

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

Choose k Hamiltonians at k parameter points

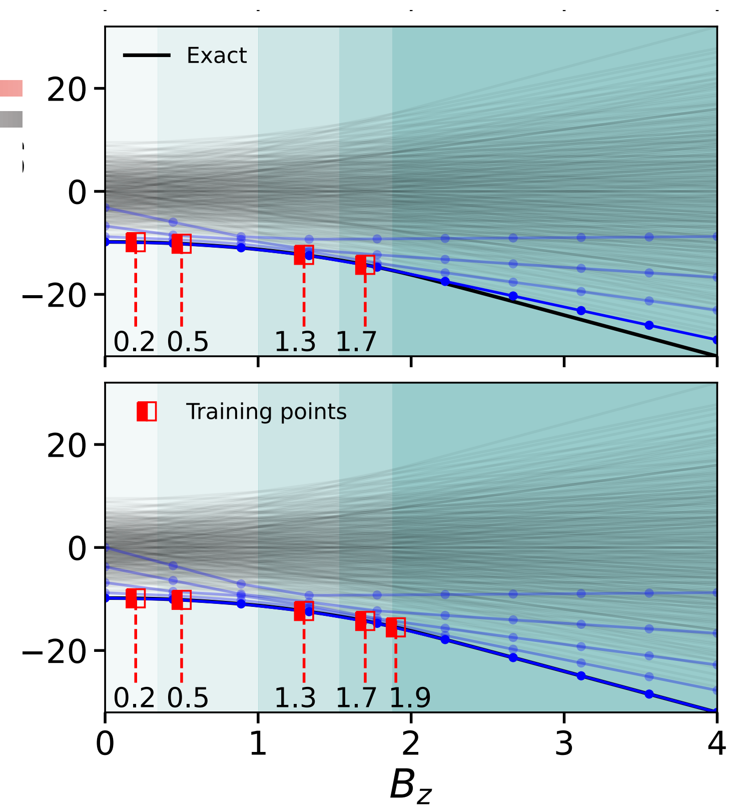
$$\{H(p_0), H(p_1), \ldots H(p_k)\}$$

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

Eigenvector Continuation

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

Choose k Hamiltonians at k parameter points

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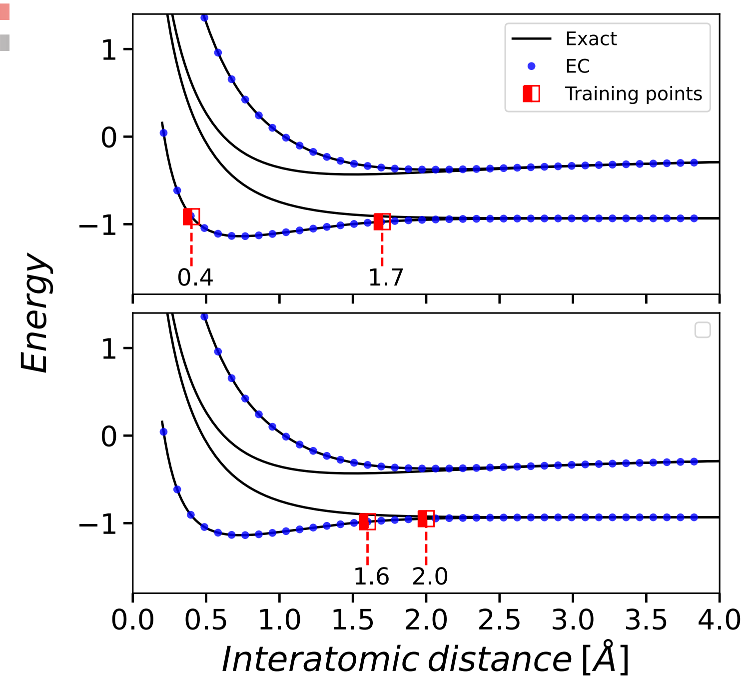
$$\{|\phi_0\rangle, |\phi_1\rangle, \dots |\phi_k\rangle\}$$

k Low energy state vectors

Subspace Diagonalization

Energy spectrum across the parameter range



A. Francis, AFK et al., 2209.10571

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Eigenvector Continuation

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

Choose k Hamiltonians at k parameter points

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

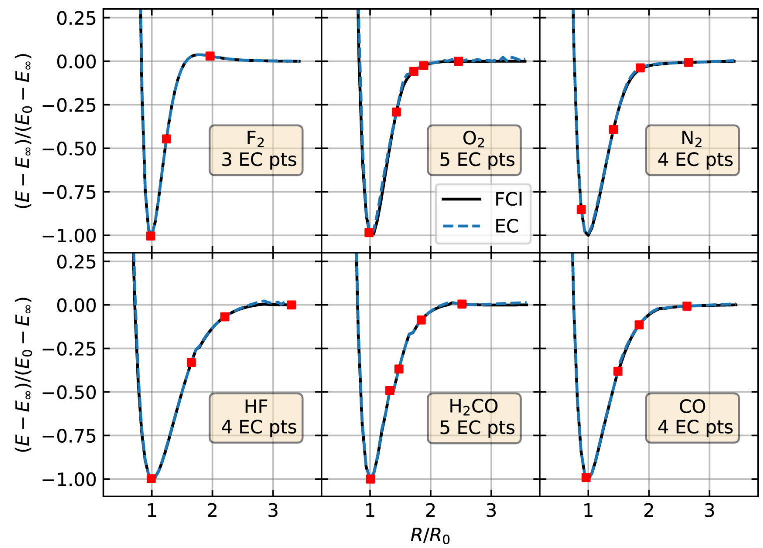
Solve for ground state vector

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

k Low energy state vectors

Subspace Diagonalization

Energy spectrum across the parameter range



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

Eigenvector Continuation

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

Choose k Hamiltonians at k parameter points

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

Solve for ground state vector

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

We can use any state preparation method

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

k low energy state vectors

Subspace Diagonalization

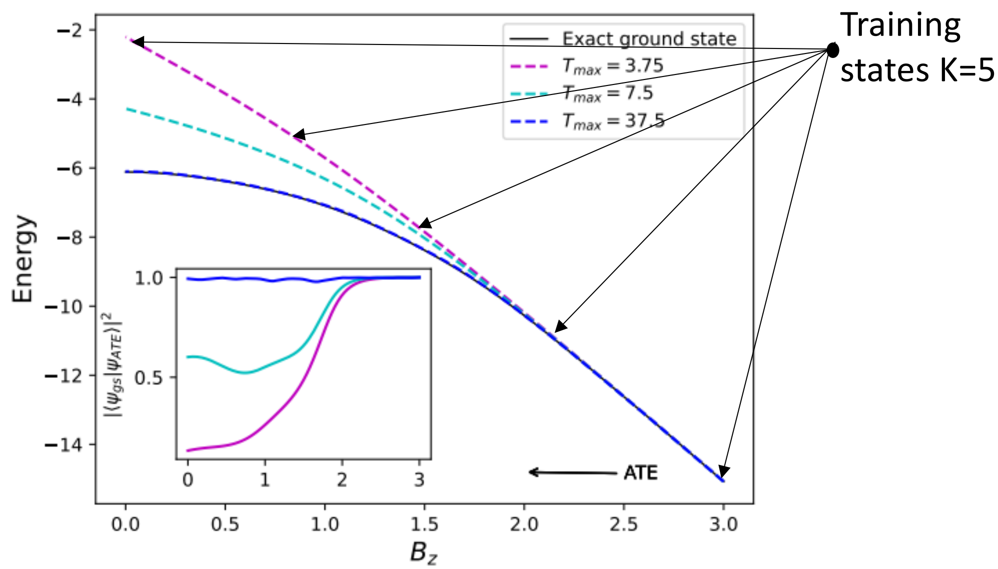
Energy spectrum across the parameter

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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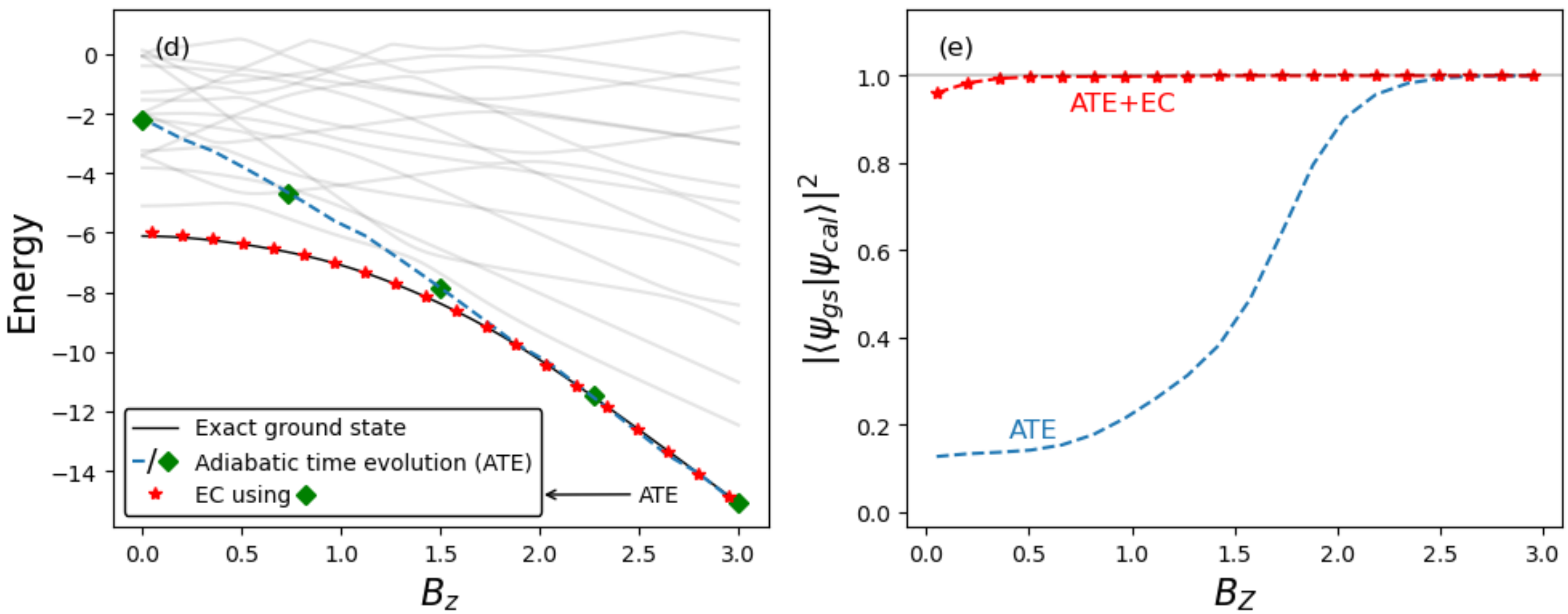

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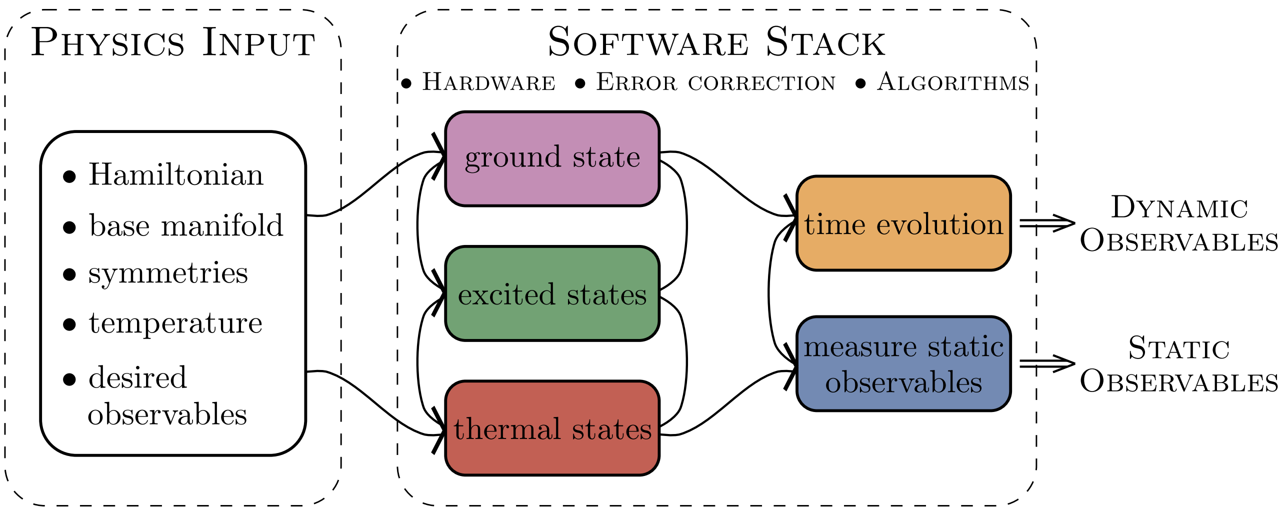
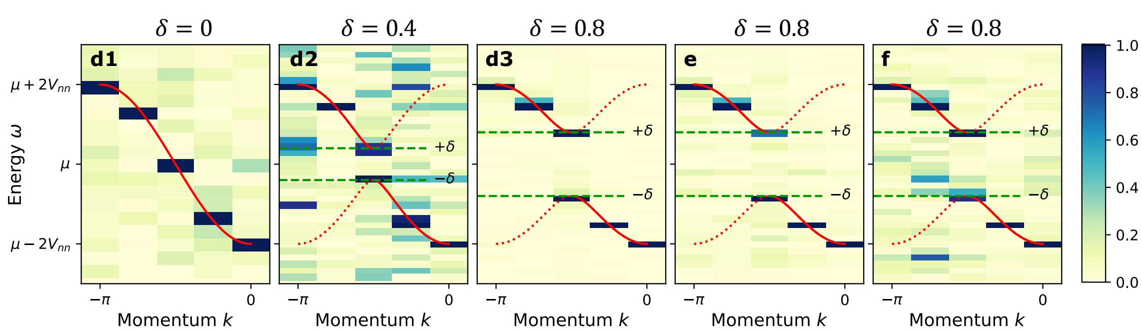
Quantum Matter meets Quantum Computing

Digital version of this talk



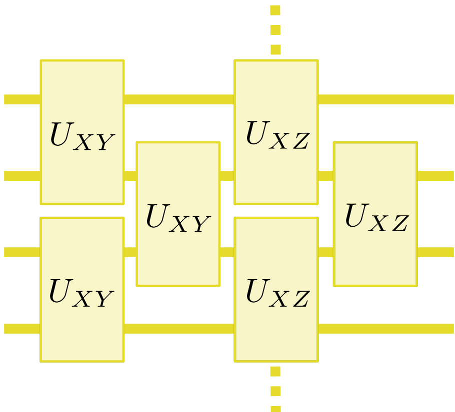
https://go.ncsu.edu/kemper-lab



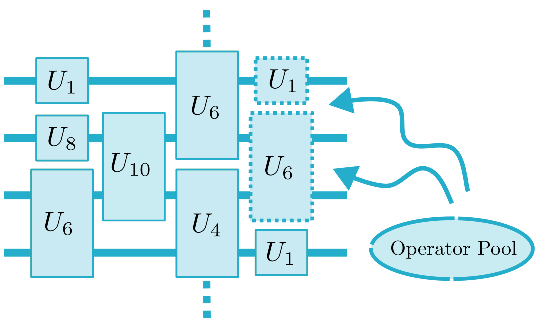
- Experimental relevance: Measuring correlation functions
- Measuring exact integer Chern numbers for topological states
- Open quantum evolution and fixed points (1000 Trotter steps)
- Time evolution via Lie algebraic decomposition and compression
- Thermodynamics via Lee-Yang Zeros
- Physics-Informed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

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

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

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

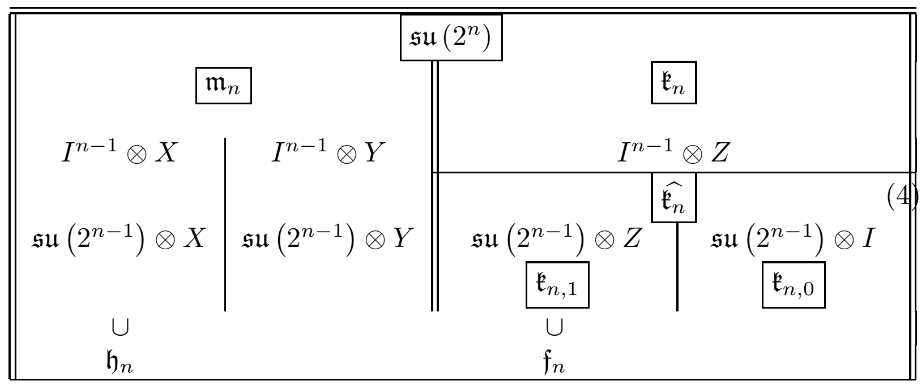
Wiersema, arXiv:2309.05690

Unitary Synthesis: Cartan Decomposition

- Cartan decomposition found its application in generic unitary synthesis for quantum circuits (*,**)

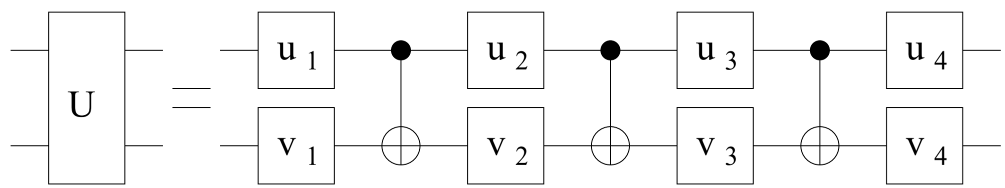
$$\mathfrak{g} = \mathfrak{m} \oplus \mathfrak{k}$$

$$\begin{aligned} [\mathfrak{k}, \mathfrak{k}] &\subset \mathfrak{k} \\ [\mathfrak{m}, \mathfrak{k}] &= \mathfrak{m} \\ [\mathfrak{m}, \mathfrak{m}] &\subset \mathfrak{k}. \end{aligned}$$



$$I^{n-1} = I^{\otimes(n-1)} = \underbrace{I \otimes .. \otimes I}_{n-1}$$

- It is optimal for SU(4) (2 qubits)! (***)



(*) N. Khaneja and S. J. Glaser, Chemical Physics 267, 11 (2001). (**) H. N. Sa Earp and J. K. Pachos, Journal of Mathematical Physics 46, 082108 (2005), doi.org/10.1063/1.2008210.

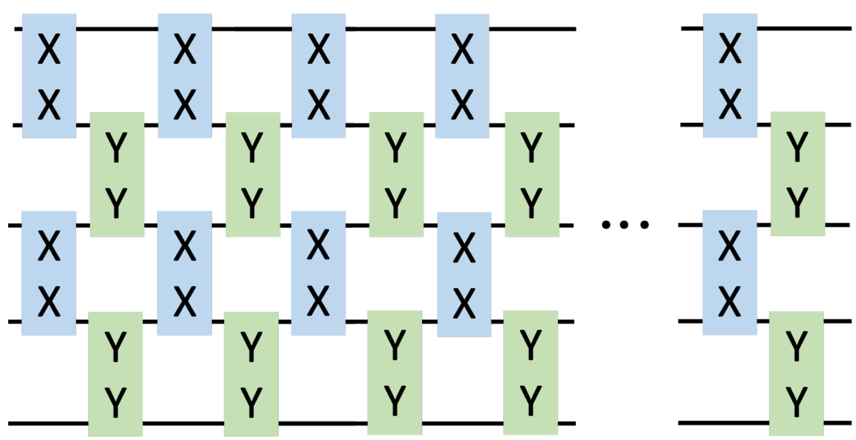
(***) G. Vidal and C. M. Dawson, Physical Review A 69, 010301 (2004).

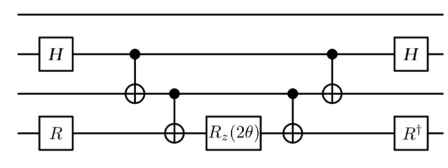
Main Problem

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

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

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

$U(t) =$ 

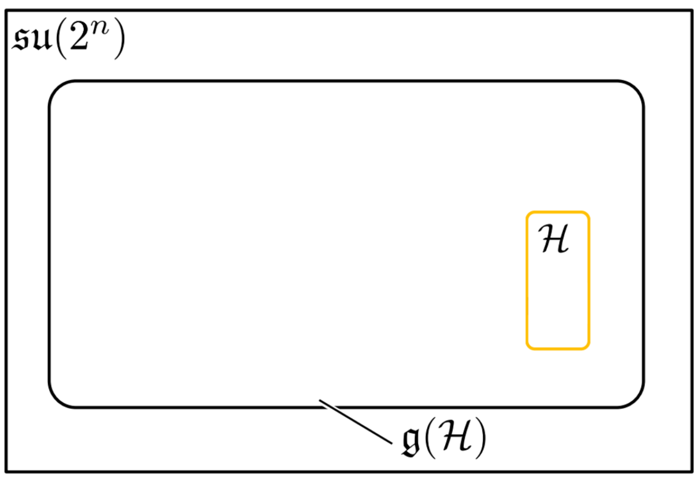
$e^{i\theta IXZYI} =$ 

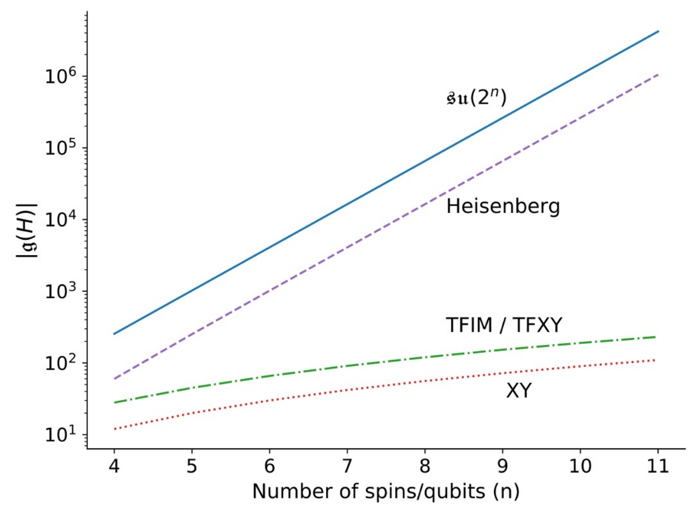
Main Problem

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

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

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





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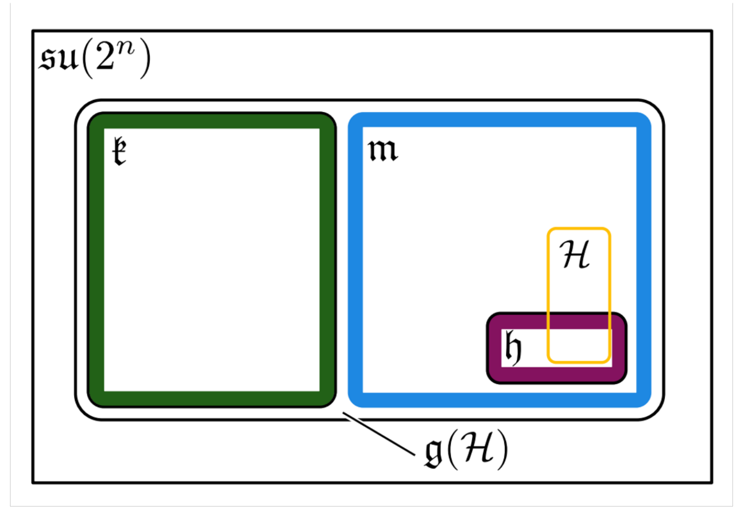
Cartan Decomposition and KHK Theorem

Definition 1 *Consider a compact semi-simple Lie subgroup* $\boldsymbol{G} \subset SU(2^n)$*, 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*

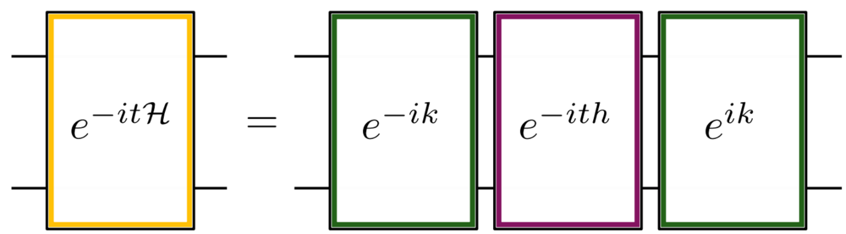
$$[\mathfrak{k}, \mathfrak{k}] \subset \mathfrak{k} \qquad [\mathfrak{m}, \mathfrak{m}] \subset \mathfrak{k} \qquad [\mathfrak{k}, \mathfrak{m}] = \mathfrak{m} \tag{4}$$

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*

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



Main Problem

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

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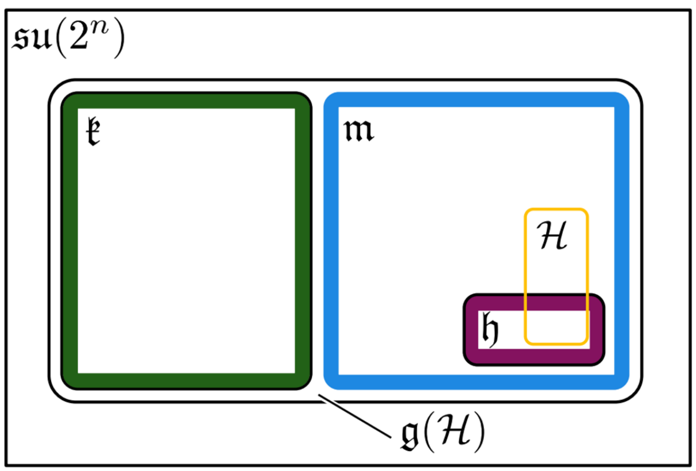
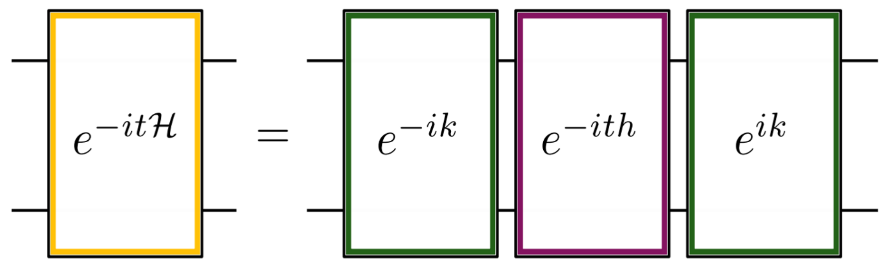
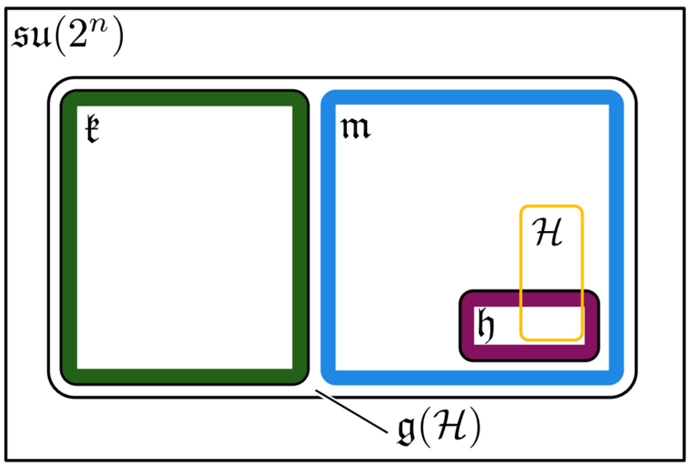
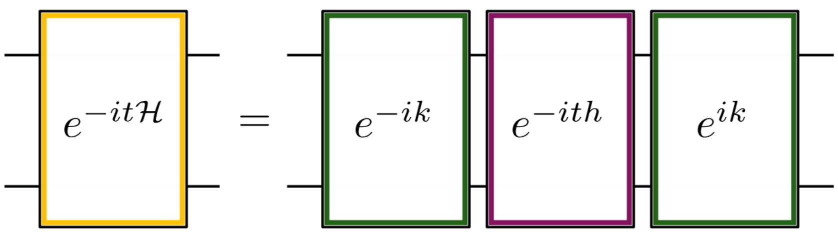




Cartan Decomposition and KHK Theorem





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

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

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

where

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

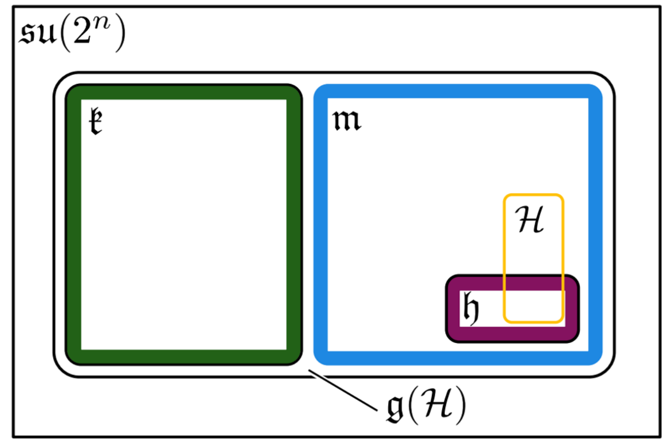
$$v = h_1 + \pi h_2 + \pi^2 h_3 + \ldots. + \pi^{n_h - 1} h_{n_h}$$

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

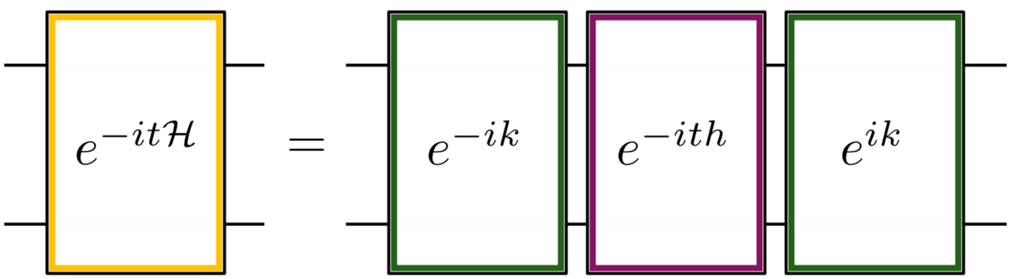
$$K_0^\dagger H K_0 \in \mathfrak{h}$$

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

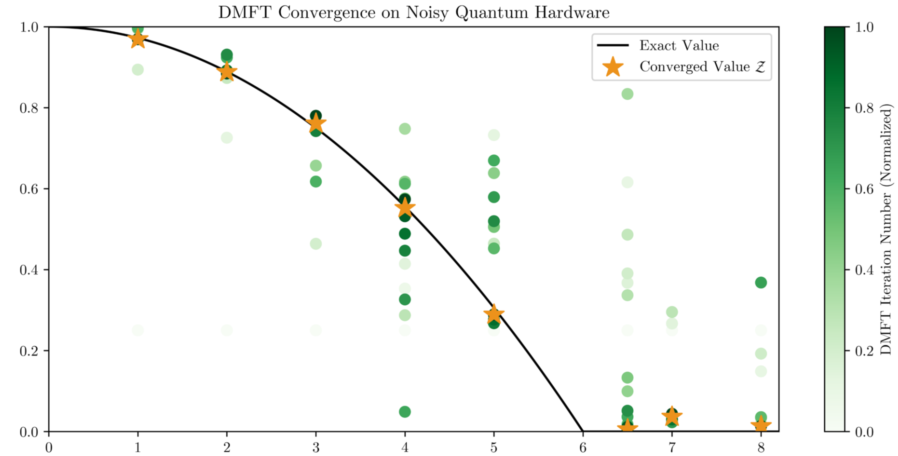


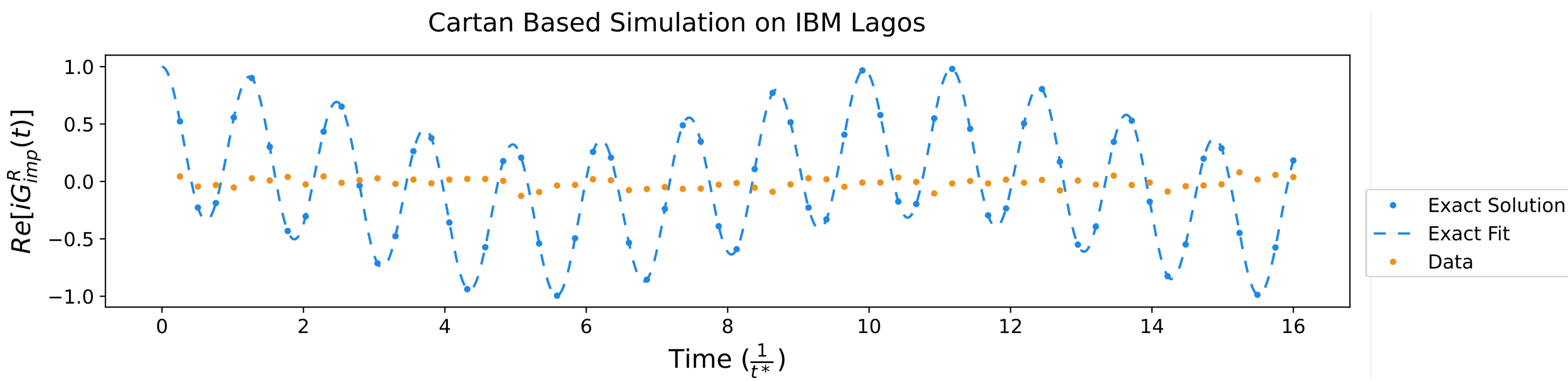
$$f(K) = \langle K v K^\dagger, \mathcal{H} \rangle$$



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.

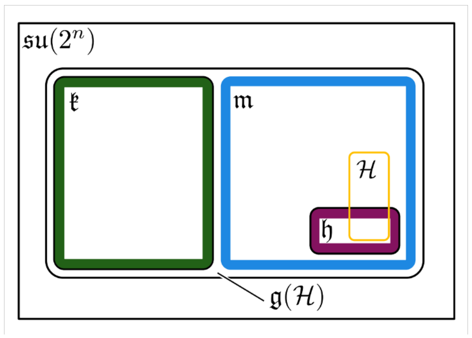


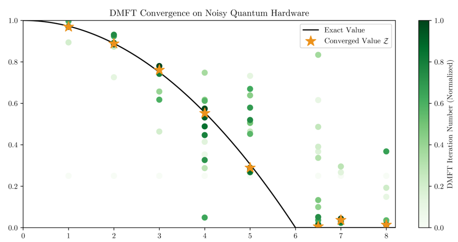


[T. Steckmann, Phys Rev Research (2023)]

2 Algebraic methods for circuit compression

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

2 Algebraic methods for circuit generation

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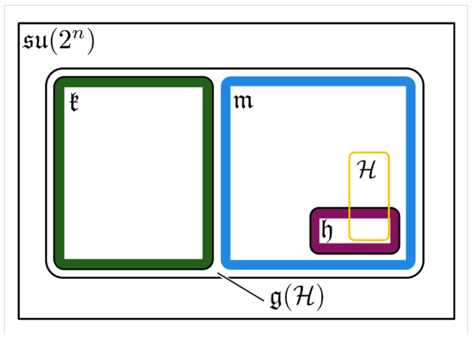

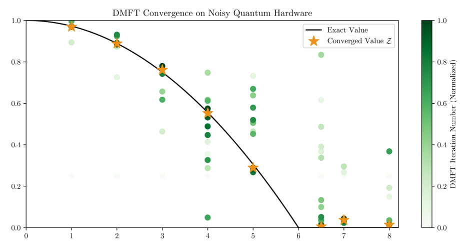

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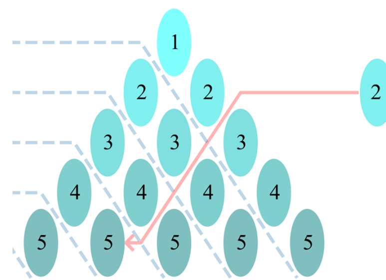

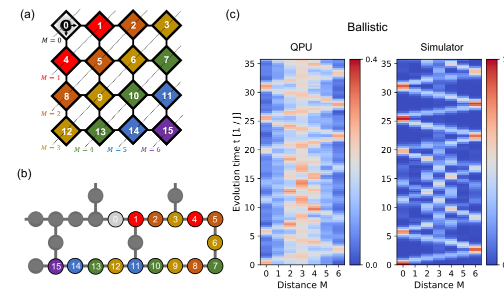

- Compressed Trotter circuits down to a shallow fixed depth circuit for 1-D nearest neighbor TFXY, TFIM, XY and Kitaev models.
- Based on 3 easy to check, local properties.
- We have code available! Check F3C, F3C++ and F3Cpy at https://github.com/QuantumComputingLab

Kökcü PRL (2022) , Steckmann PRR (2023)

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

Quantum Matter meets Quantum Computing

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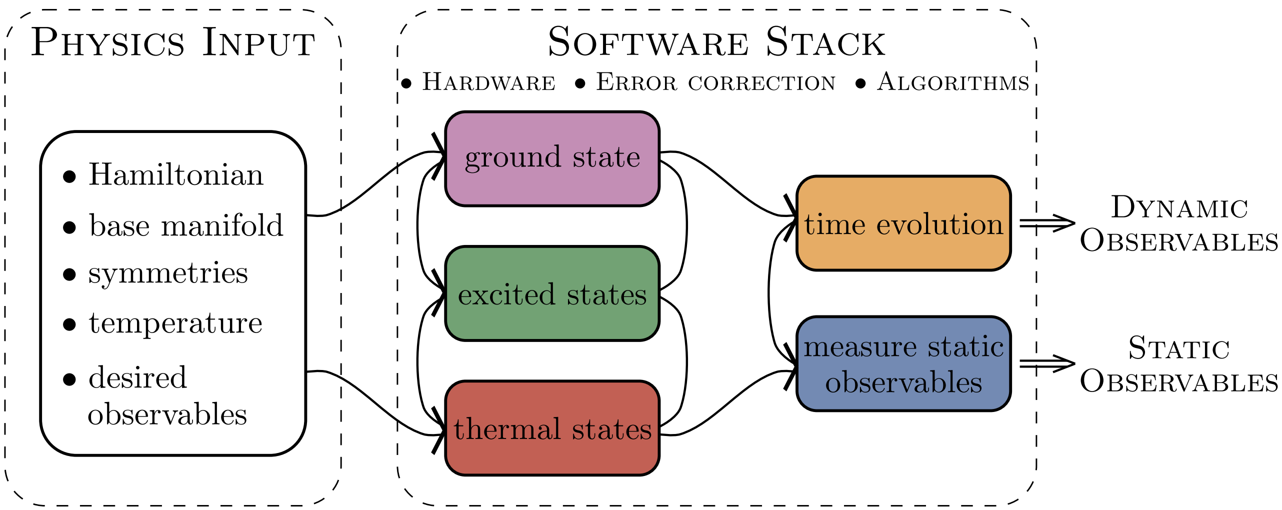

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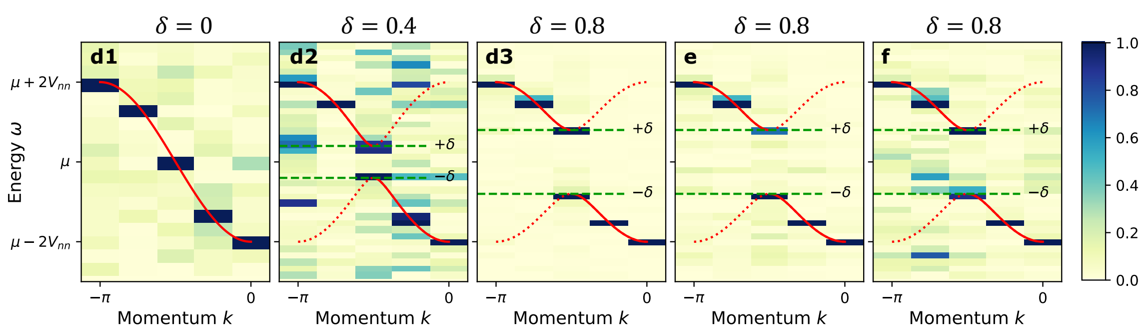

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