NC STATE UNIVERSITY

A Linear Response Framework for Simulating Bosonic and Fermionic Correlation Functions Illustrated on Quantum Computers

Alexander (Lex) Kemper

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

ORNL QC Users Forum
07/19/2023

NSF DARPA

NC STATE UNIVERSITY

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

Alexander (Lex) Kemper

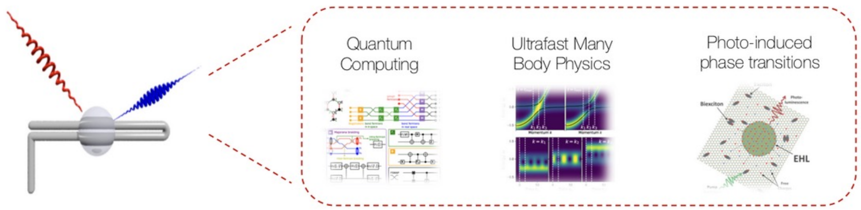
Department of Physics
North Carolina State University
https://go.ncsu.edu/kemper-lab

ORNL QC Users Forum
07/19/2023

NSF DARPA

NC STATE UNIVERSITY

Digital version of this talk



Kemper Lab

Quantum materials in and out of equilibrium.

Collaborations with:

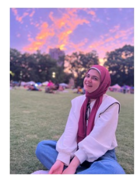
- Jim Freericks (Georgetown)
- Bert de Jong, Katie Klymko, Daan Camps, Roel van Beeumen, Akhil Francis (LBNL)
- Thomas Steckmann (UMD)

Current members


Alexander (Lex) Kemper
Principal investigator


Efekan Kökcü
Graduate Researcher


Anjali Agrawal
Graduate Researcher


Heba Labib
Graduate Researcher

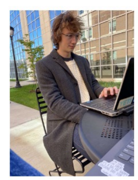

Jack Howard
Undergraduate Researcher


Natalia Wilson
Undergraduate Researcher


Daniel Brandon
Undergraduate Researcher


Sarah Klas
Undergraduate Researcher


Norman Hogan
Graduate Researcher

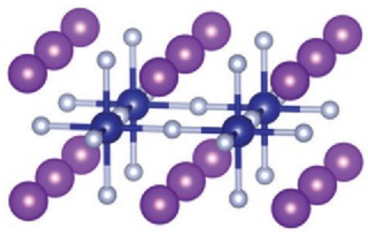

Ethan Blair
Undergraduate Researcher


Your Name
New lab member

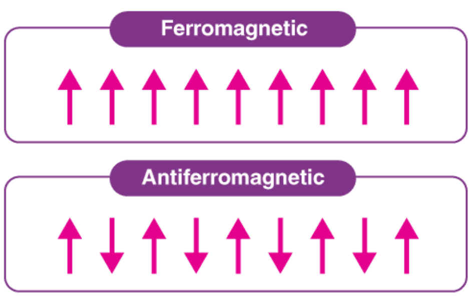
A Tale of Two Transitions

Ising Magnet

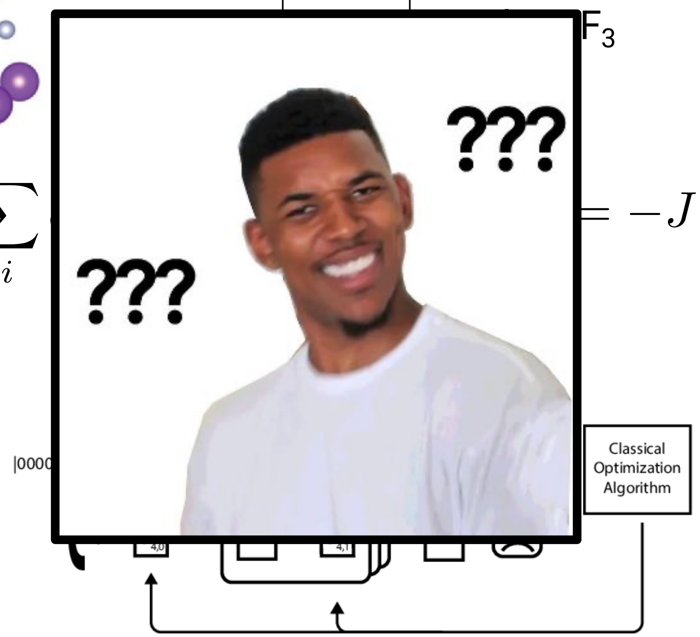
Rb_2CoF_4



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



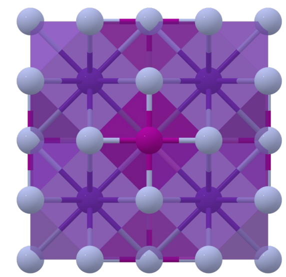
10.1039/c6cp02362b



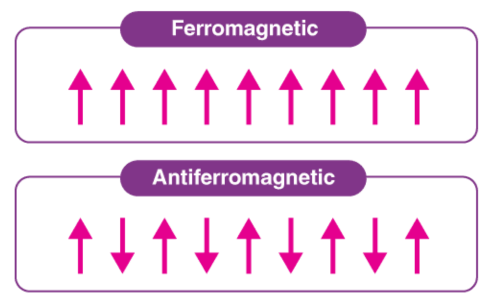
Optimization of the Variational Quantum Eigensolver for Quantum Chemistry Applications

Heisenberg Magnet

F_3



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



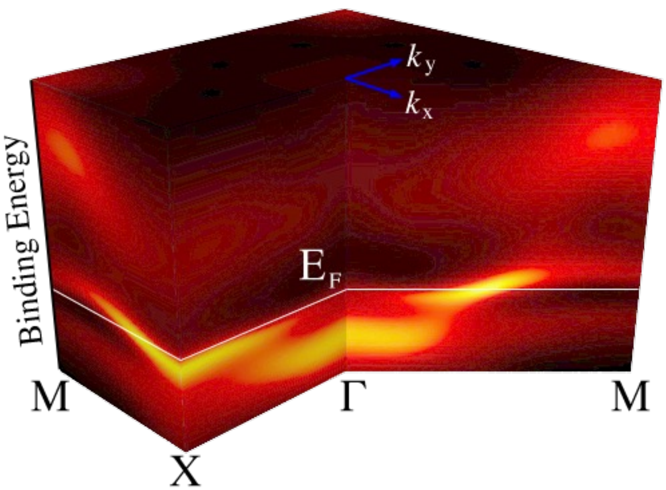
Materials project

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

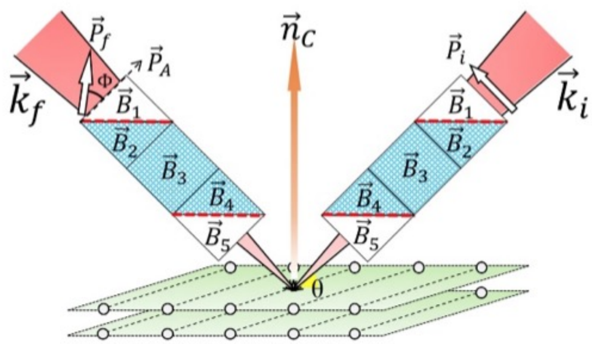
A: You measure its excitations.

Measuring Excitations

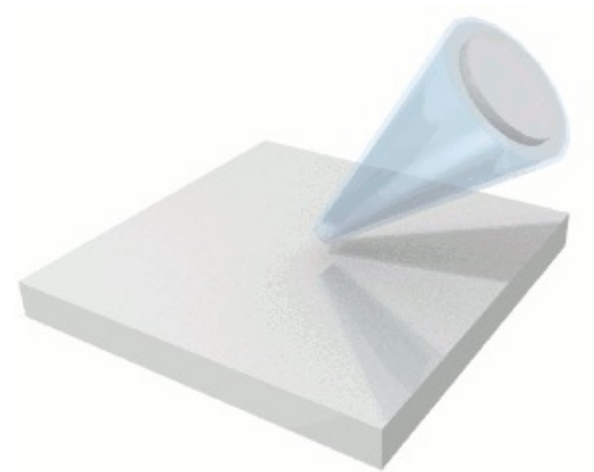
Figures courtesy of
Devereaux/Shen group
and ORNL



Angle-resolved Photoemission (ARPES)



Neutron Scattering

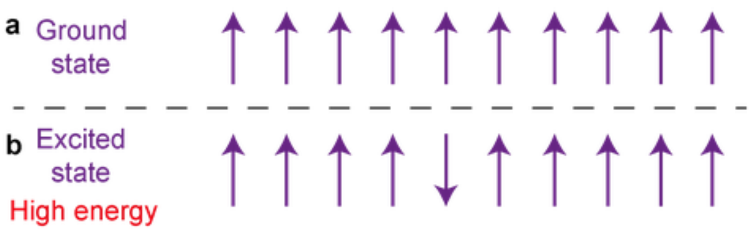


Time-resolved ARPES

Measuring Excitations

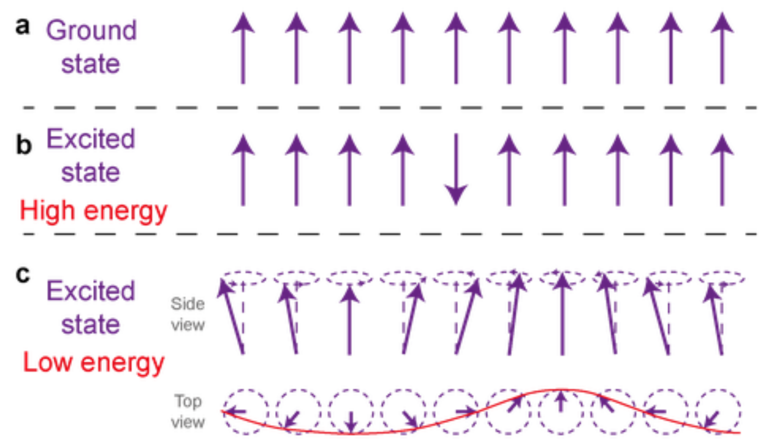
Ising Model

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

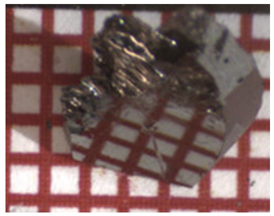


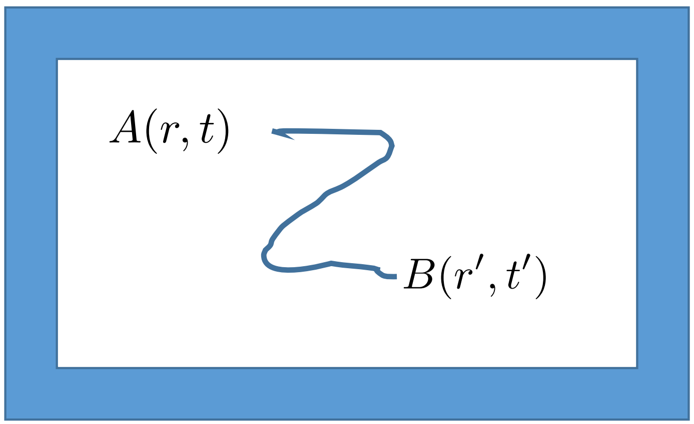
Heisenberg model

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



Correlation functions





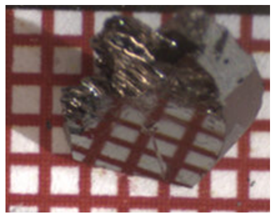
$$\langle A(r,t) B(r',t') \rangle$$

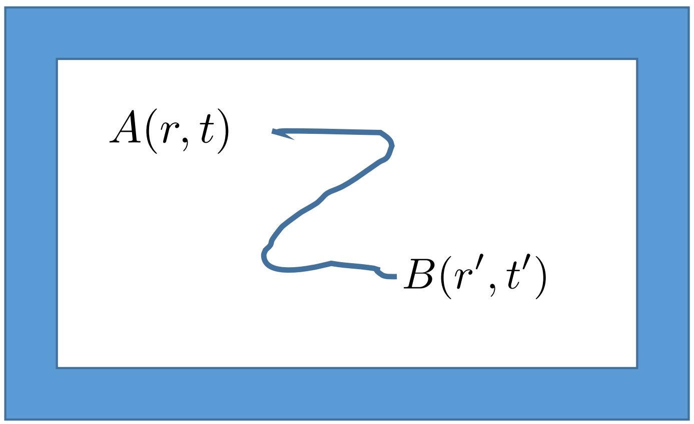
Given some (observable) operator B at (r',t'), what is the likelihood of some (observable) operator A at (r,t)?

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

NC STATE UNIVERSITY

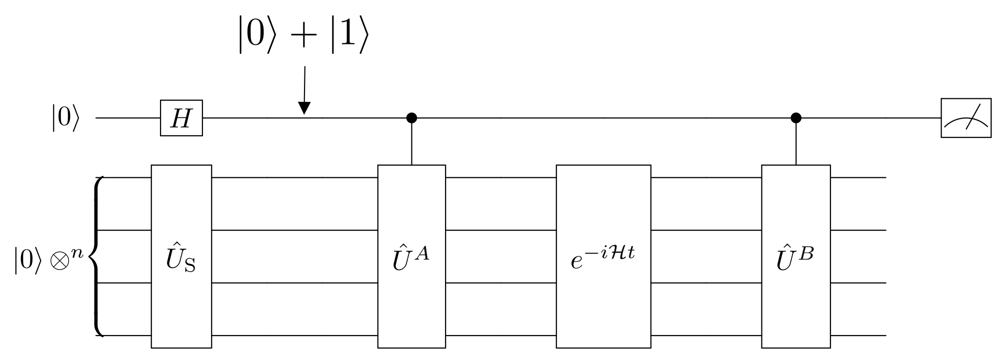
Correlation functions



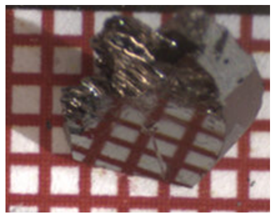


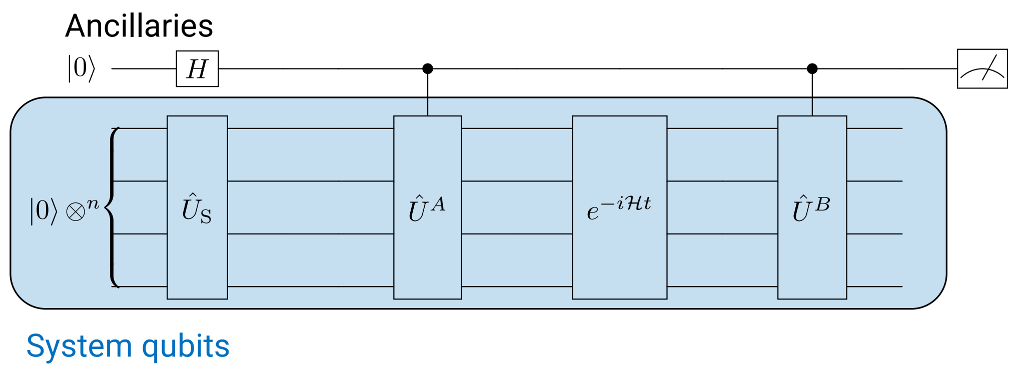
$$e^{iE_0 t}\langle\phi_0|Be^{-i\mathcal{H}t}A|\phi_0\rangle$$

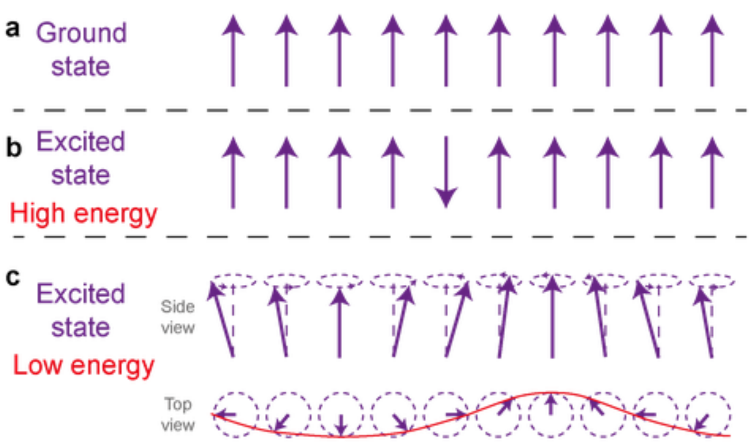
- $e^{iE_0 t}$: Interfere with ground state
- $\langle\phi_0|$: Complete expectation value
- B: Apply excitation B
- $e^{-i\mathcal{H}t}$: Time evolve
- A: Apply excitation A
- $|\phi_0\rangle$: Prepare state of interest



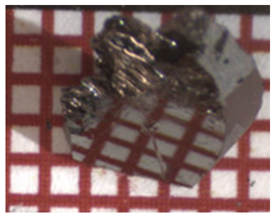
Correlation functions

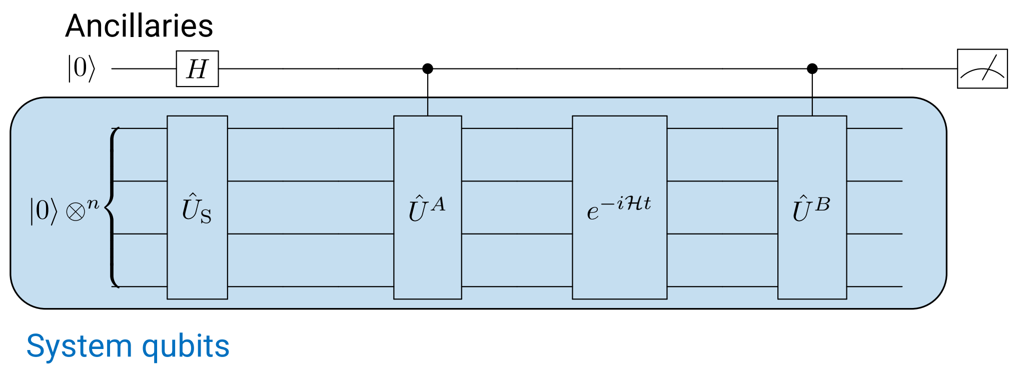






Correlation functions



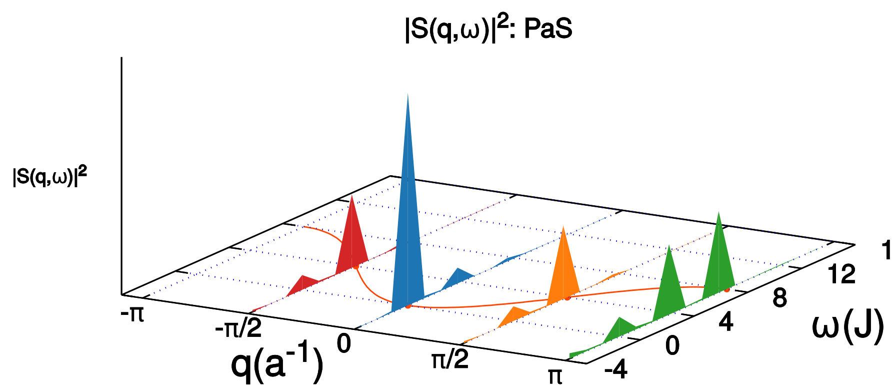


This works!

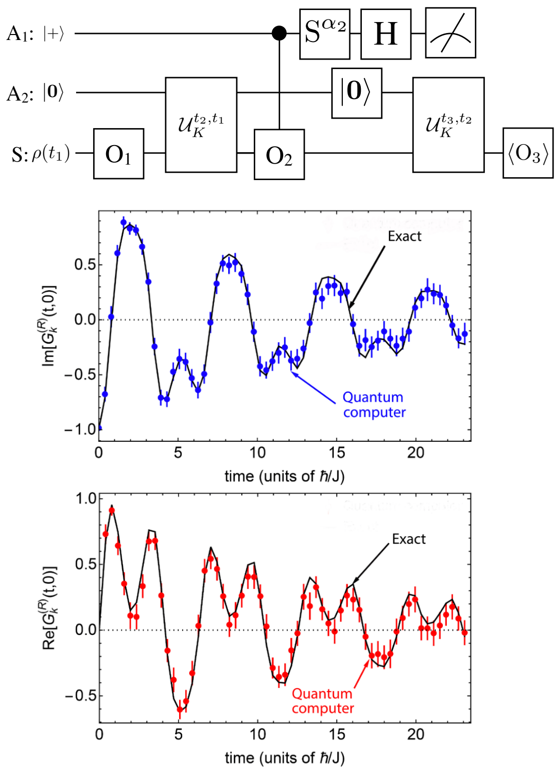
But:

- Need an ancilla with long coherence
- A and B need to be unitary & controlled
- More complex A,B need post-processing

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



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



(Anti-)Commutators, dissipative

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

PHYSICAL REVIEW A **96**, 022127 (2017)

Noninvasive measurement of dynamic correlation functions

Philipp Uhrich,[1,2] Salvatore Castrignano,[3] Hermann Uys,[2,4] and Michael Kastner[1,2,*]
[1]*National Institute for Theoretical Physics (NITheP), Stellenbosch 7600, South Africa*
[2]*Institute of Theoretical Physics, Department of Physics, University of Stellenbosch, Stellenbosch 7600, South Africa*
[3]*Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany*
[4]*Council for Scientific and Industrial Research, National Laser Centre, Pretoria, Brummeria, 0184, South Africa*

(Received 24 November 2016; revised manuscript received 16 January 2017; published 21 August 2017)

1. Initial state preparation
2. Time evolution until time t_1
3. Weak coupling of ancilla and system site i.
4. Measuring the ancilla
5. Time evolution until time t_2
6. Projective measurement at site j
7. Correlating the measured outcomes

Anti-commutators

10.1103/PhysRevA.96.022127

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)

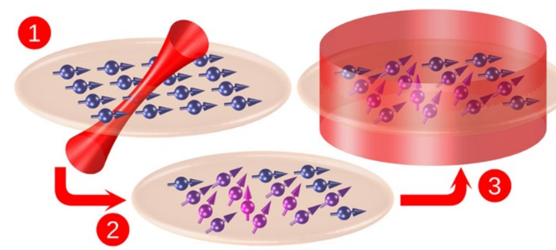


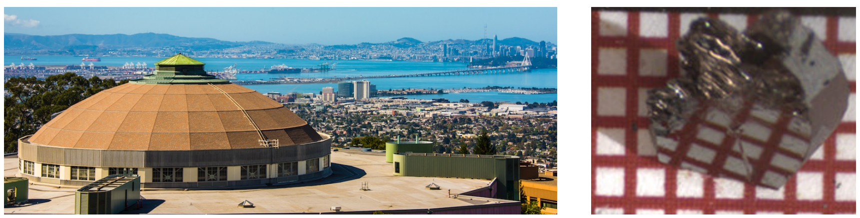
FIG. 1 (color online). Many-body Ramsey interferometry consists of the following steps: (1) A spin system prepared in its ground state is locally excited by $\pi/2$ rotation; (2) the system evolves in time; (3) a global $\pi/2$ rotation is applied, followed by the measurement of the spin state. This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

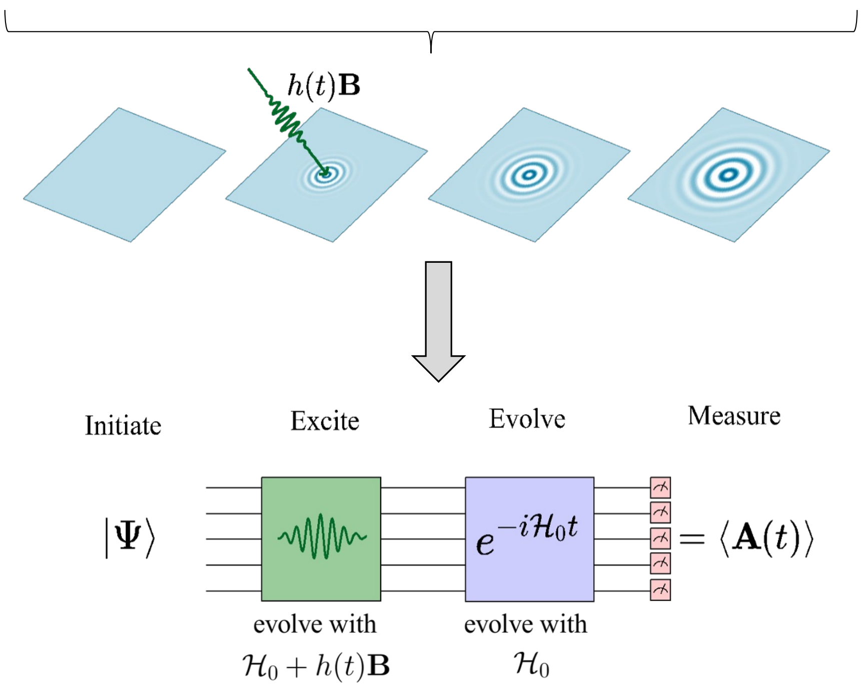
Commutators

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,*]

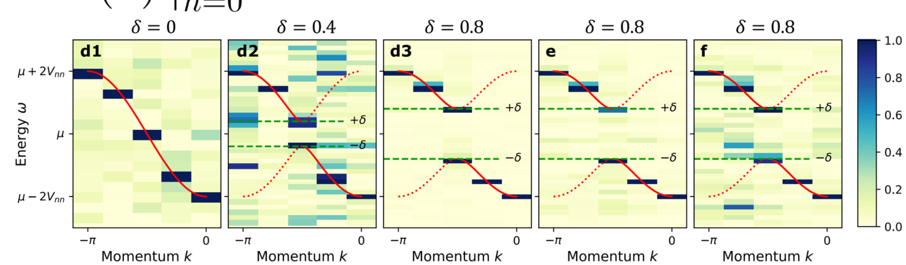
[1] *Department of Physics, North Carolina State University, Raleigh, North Carolina 27695, USA*
[2] *Department of Physics, Georgetown University, 37th and O Sts. NW, Washington, DC 20057 USA*

(Dated: February 22, 2023)

1. Make the excitation part of the quantum simulation

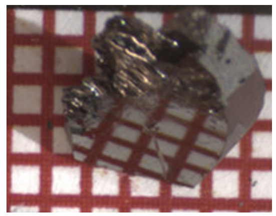
2. Post-process the data to get the response functions

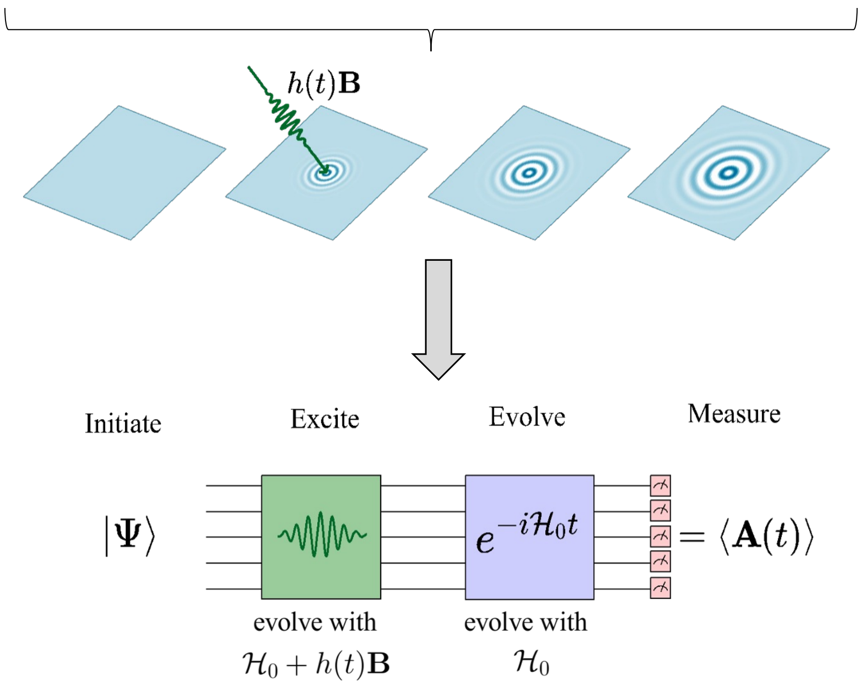
$$\left.\frac{\delta A(t)}{\delta h(t')}\right|_{h=0} = -i\theta(t-t')\langle\psi_0|[\mathbf{A}(t),\mathbf{B}(t')]|\psi_0\rangle$$



Linear Response

2302.10219





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

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)

Benefits

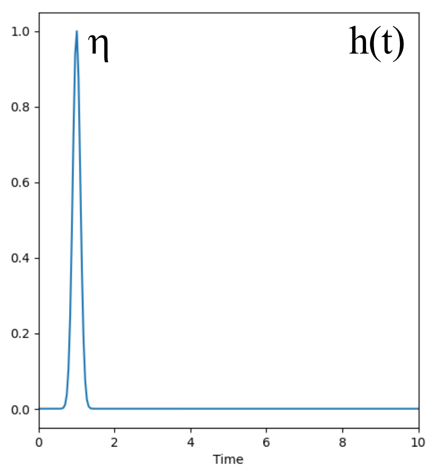
- Any operator A,B you desire (as long as it is Hermitian*)
- No ancillas/controlled operations needed
- Many correlation functions at the same time
- Less post-processing (less noise)
- Frequency/momentum selective

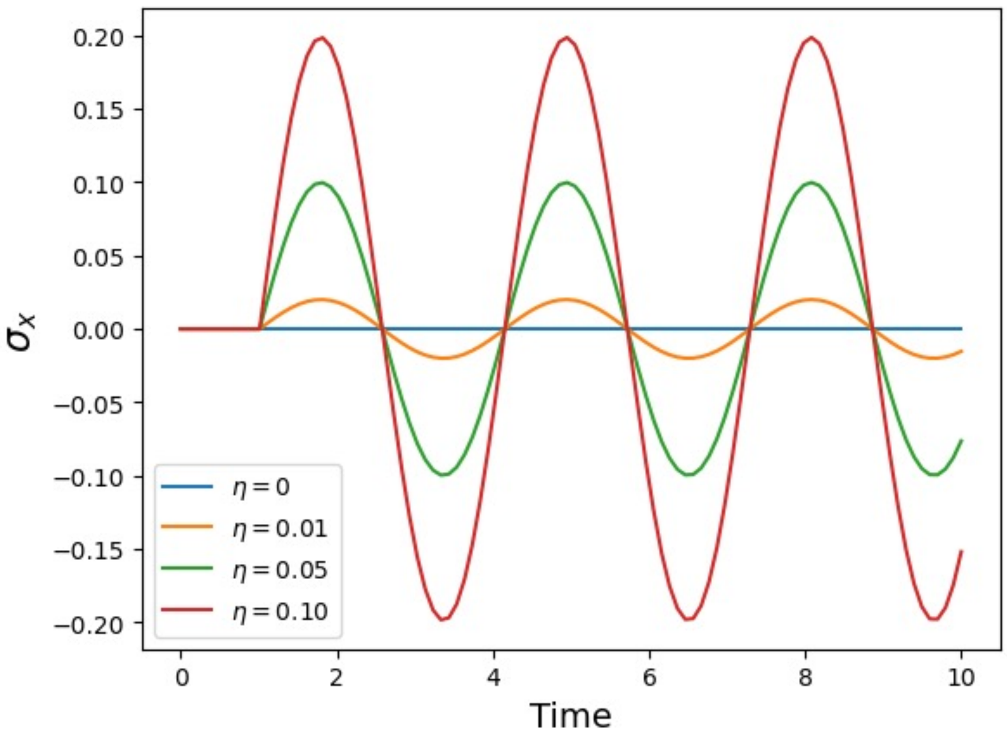
Linear Response

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

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

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



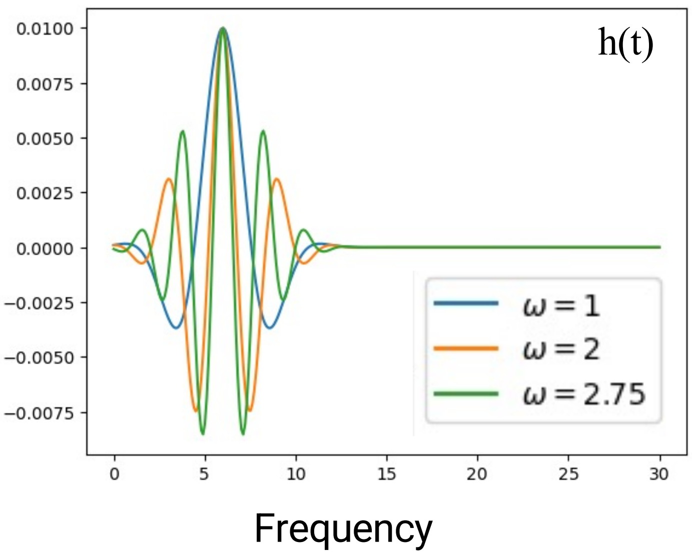


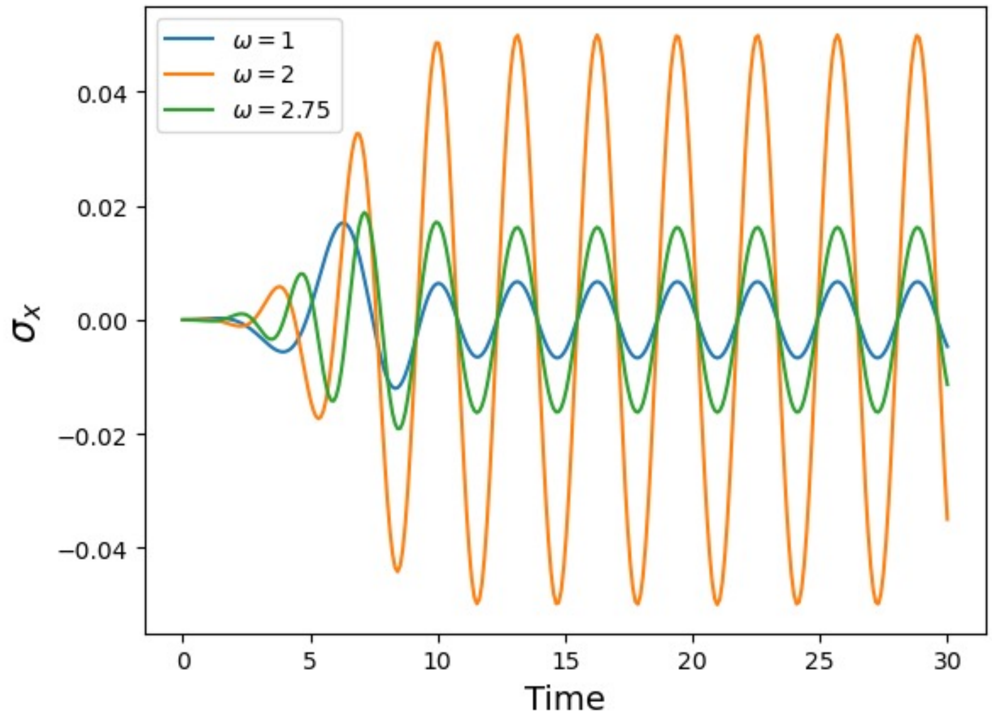
Linear Response

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

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

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



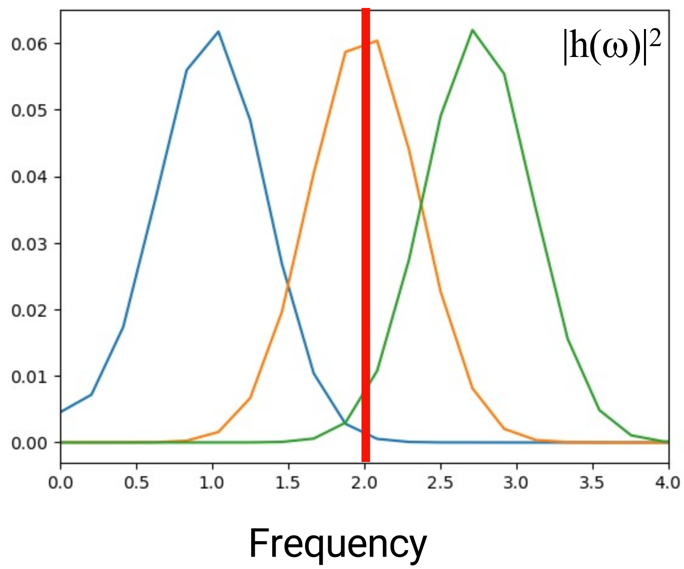


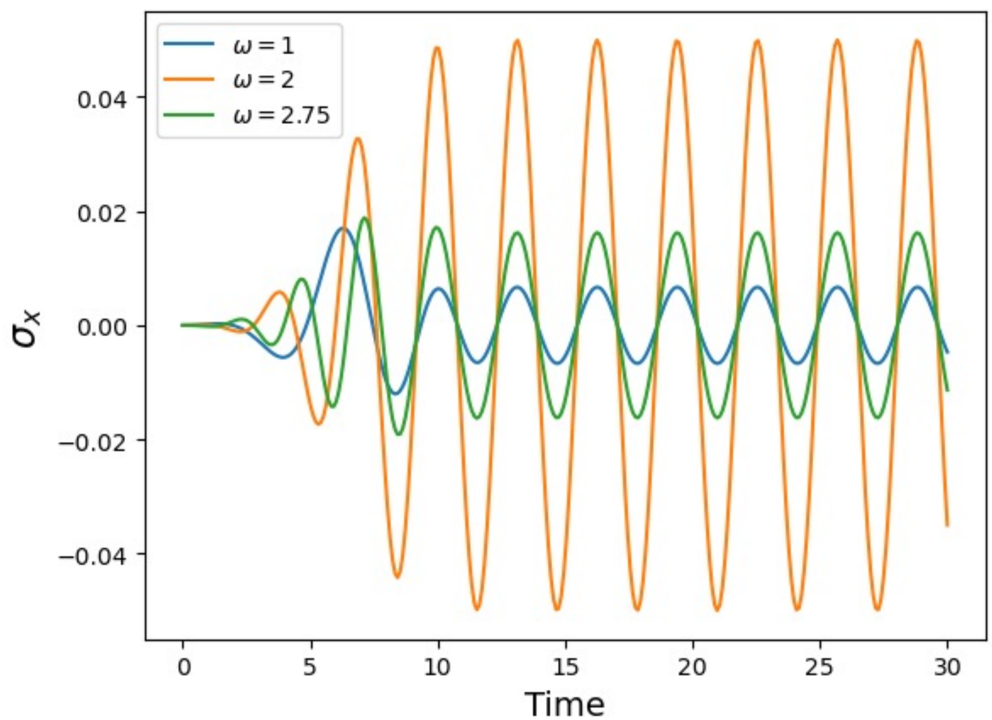
Linear Response

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

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

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

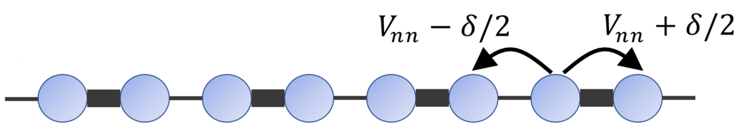




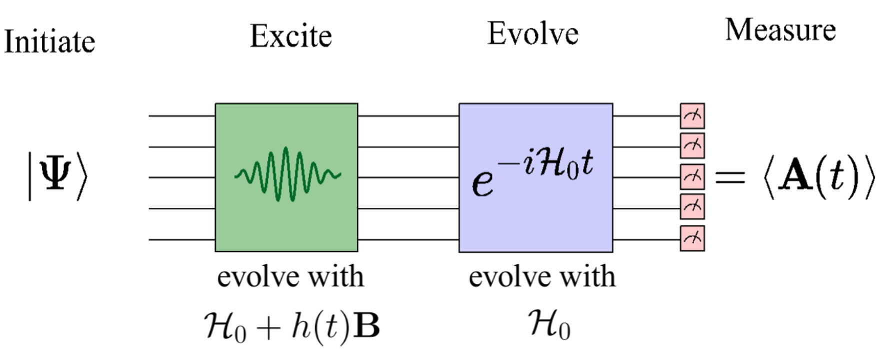
NC STATE UNIVERSITY

A Bosonic Correlation function: Polarizability

Su-Schrieffer-Heeger model for polyacetylene



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

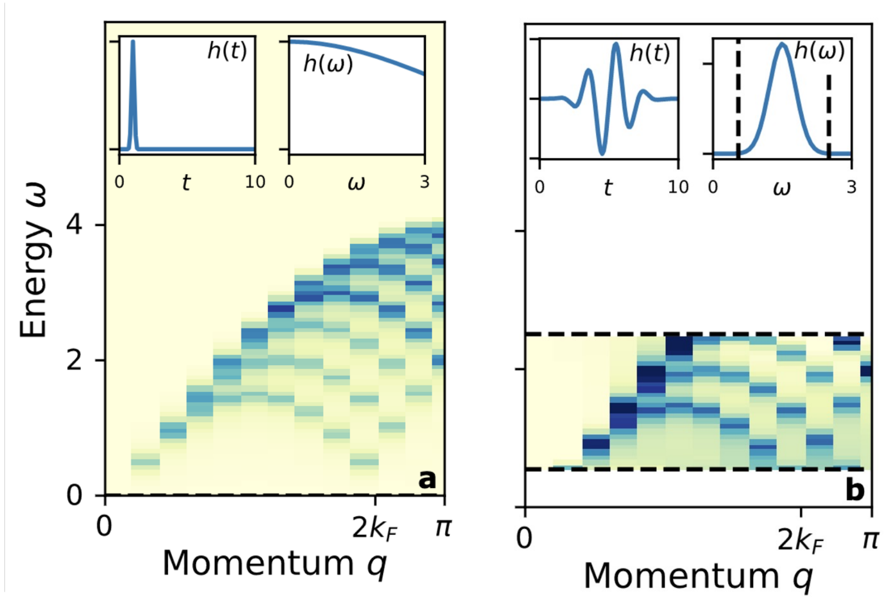


$$A(t) = \int dt' \chi^R(t - t') h(t') + \mathcal{O}(h^2)$$

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

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

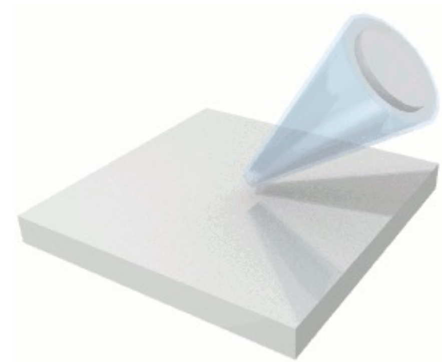
Wiggle potential on site 0 (**B**=n_0V_0)



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

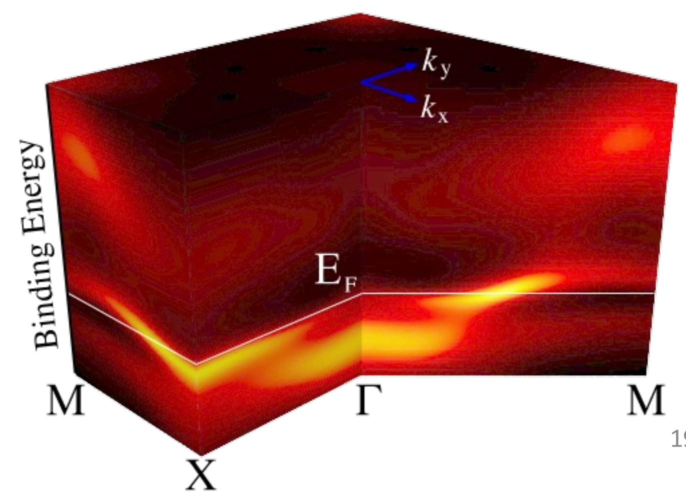


$$G(t,t') = -i\theta(t-t')\langle\psi_0|\{\mathbf{A}(t),\mathbf{B}(t')\}|\psi_0\rangle$$

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

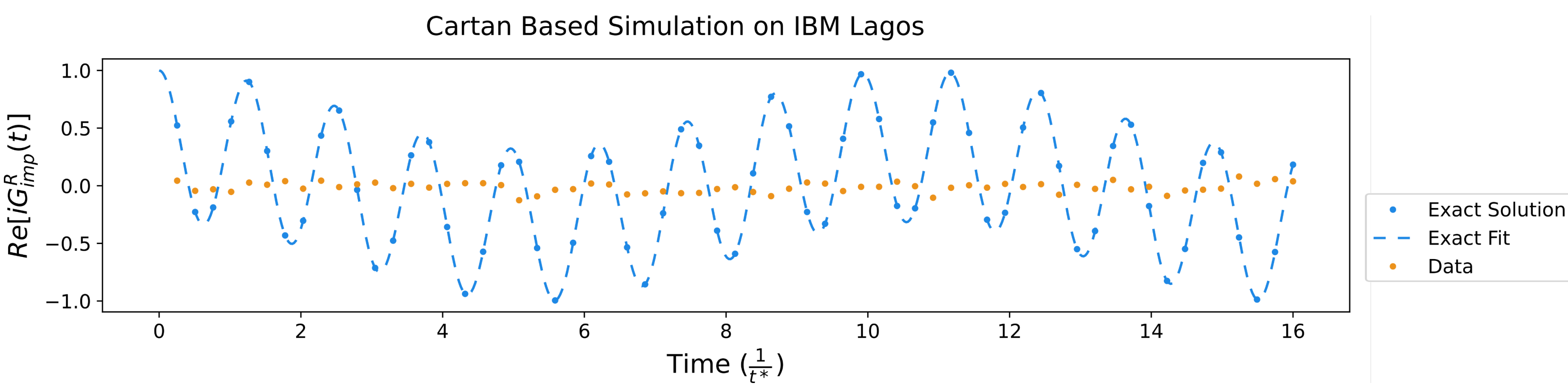


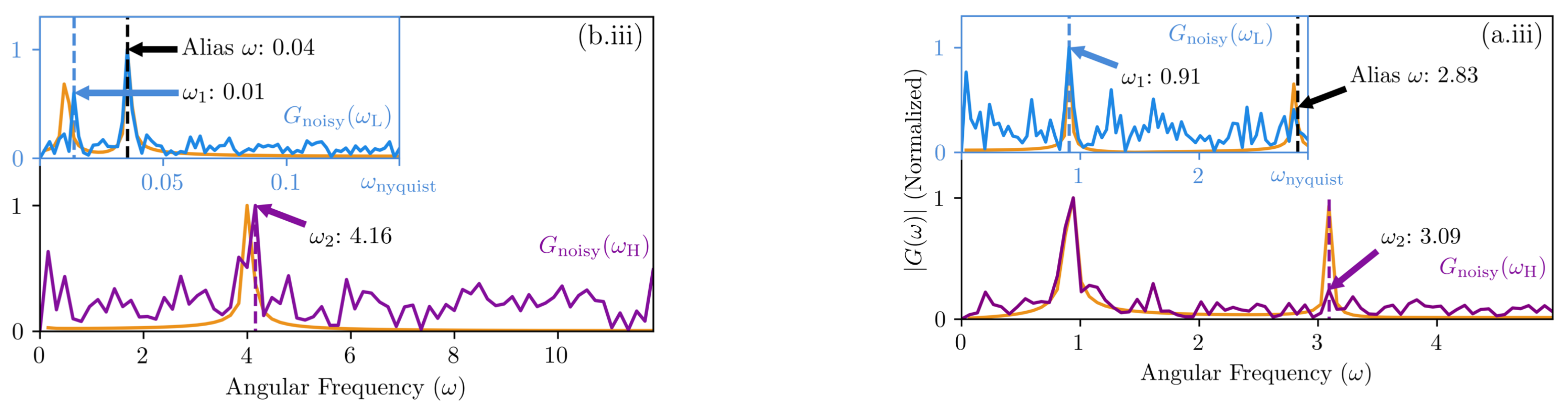
NC STATE UNIVERSITY

Application of Green's functions: DMFT

T. Steckmann et al., Phys. Rev. Research 5, 023198 (2023)

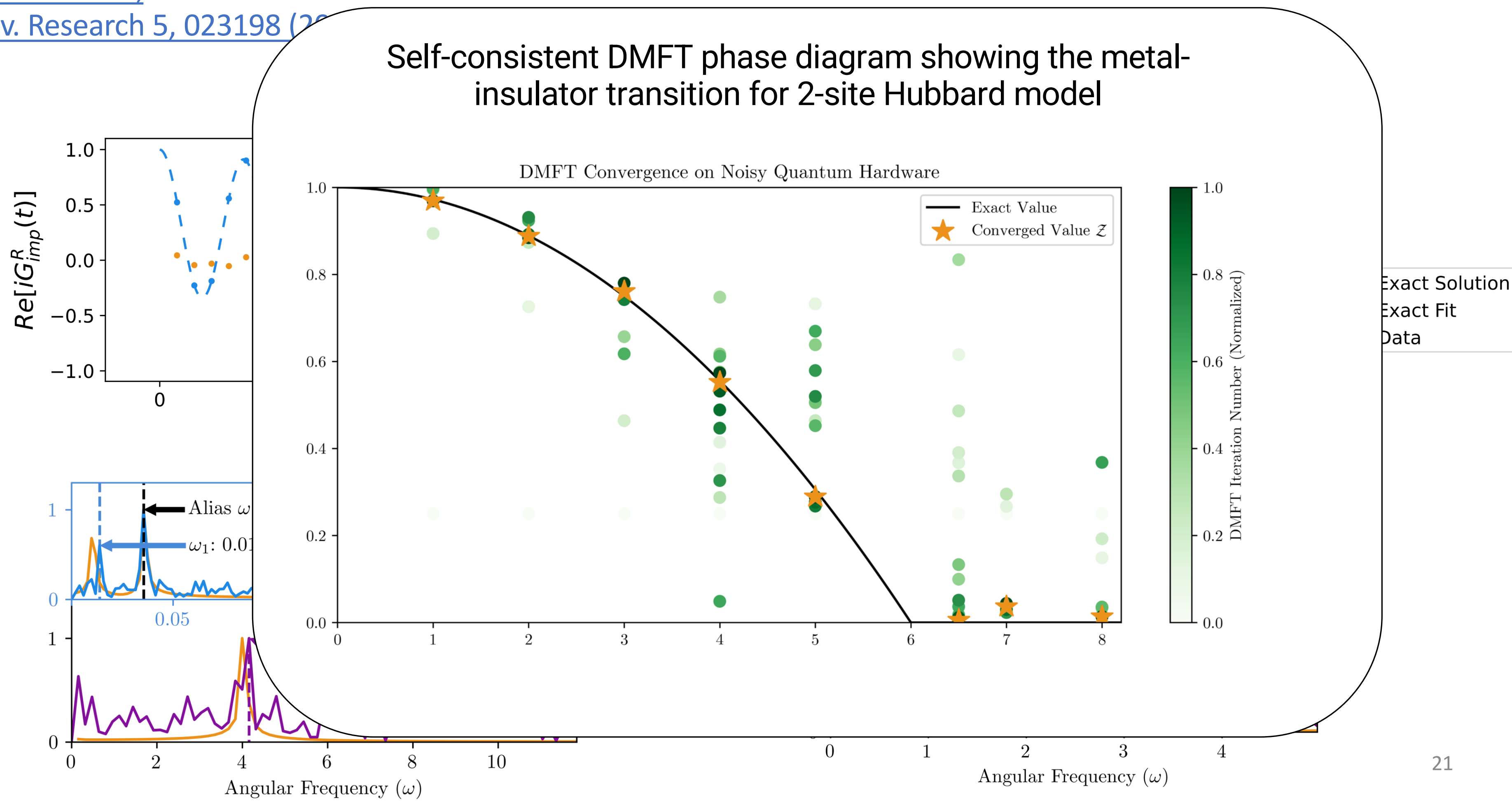
2-site Hubbard DMFT (5 qubits)





2-site Hubbard DMFT

T. Steckmann et al., Phys. Rev. Research 5, 023198 (2



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

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

Find an operator **P** such that:

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

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

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

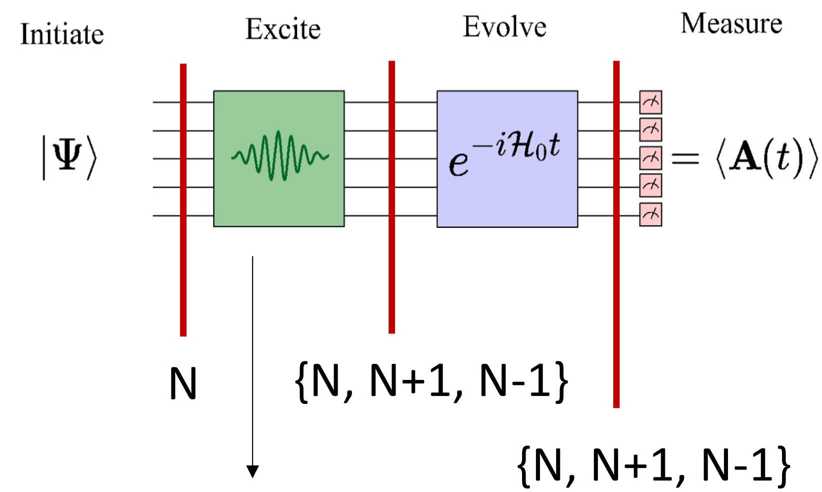
Then:

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

Example: parity

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

Option 2: Post-selection



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

Post-selection on particle number gives us

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

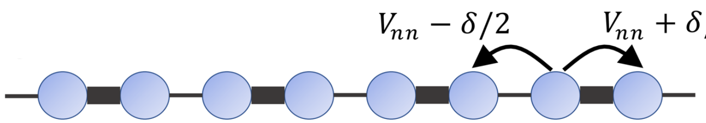
$$G^{>}_{ij}(t) = -i\,\langle\psi_0|c_i(t)c^\dagger_j(0)|\psi_0\rangle$$

NC STATE UNIVERSITY

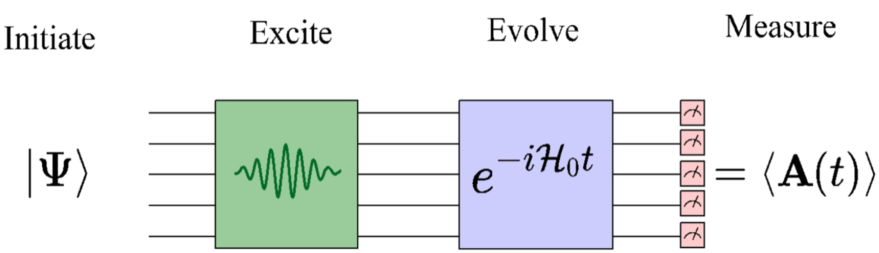
Linear Response -> Green's function

2302.10219

Su-Schrieffer-Heeger model for polyacetylene



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



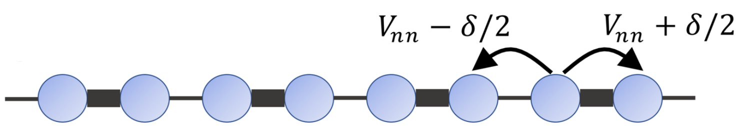
$$G^R(r_i, t; r_j, t') = -i\theta(t - t') \, \langle \psi_0 | \{ c_i(t), c_j^\dagger(t') \} | \psi_0 \rangle$$

NC STATE UNIVERSITY

Linear Response -> Green's function

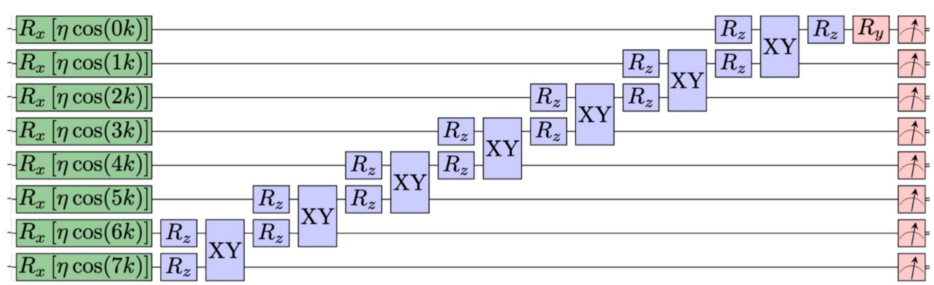
2302.10219

Su-Schrieffer-Heeger model for polyacetylene



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

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

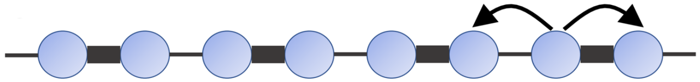
$$G_k^R(t) = -i\theta(t) \langle \psi_0 | \{ c_k(t), c_k^\dagger(0) \} | \psi_0 \rangle$$

NC STATE UNIVERSITY

Linear Response -> Green's function

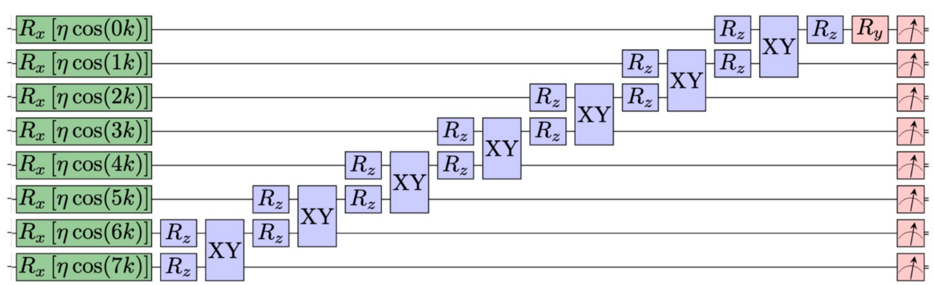
2302.10219

Su-Schrieffer-Heeger model for polyacetylene



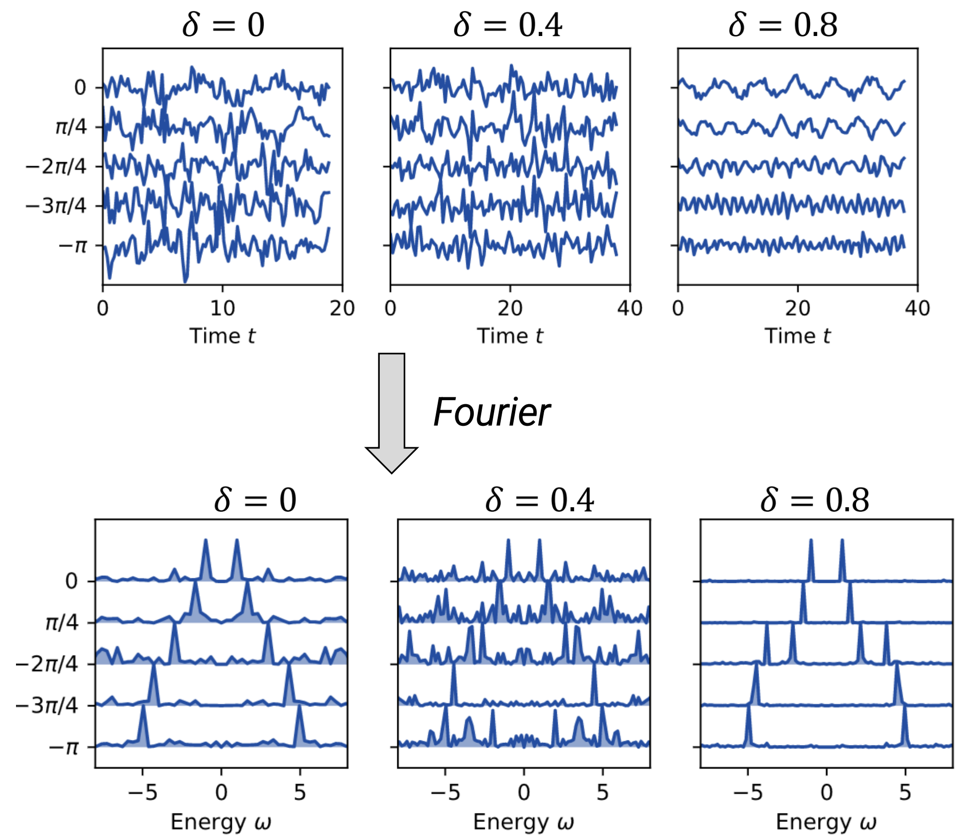
$$\mathcal{H}_0 = -\sum_{\langle i,j \rangle} \left[V_{nn} + (-1)^i \, \delta/2 \right] c_i^\dagger c_j - \mu \sum_i c_i^\dagger c_i$$

Compressed circuit run on *ibm_auckland*



Choose **B** to create a momentum eigenstate

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

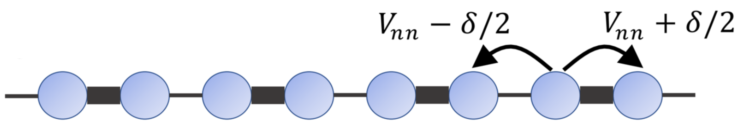


NC STATE UNIVERSITY

Linear Response -> Green's function

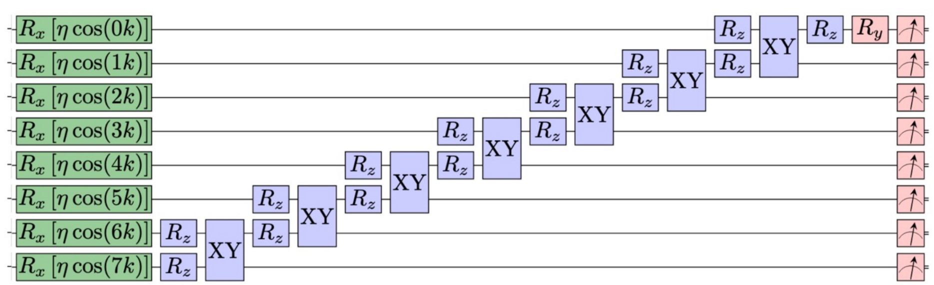
2302.10219

Su-Schrieffer-Heeger model for polyacetylene



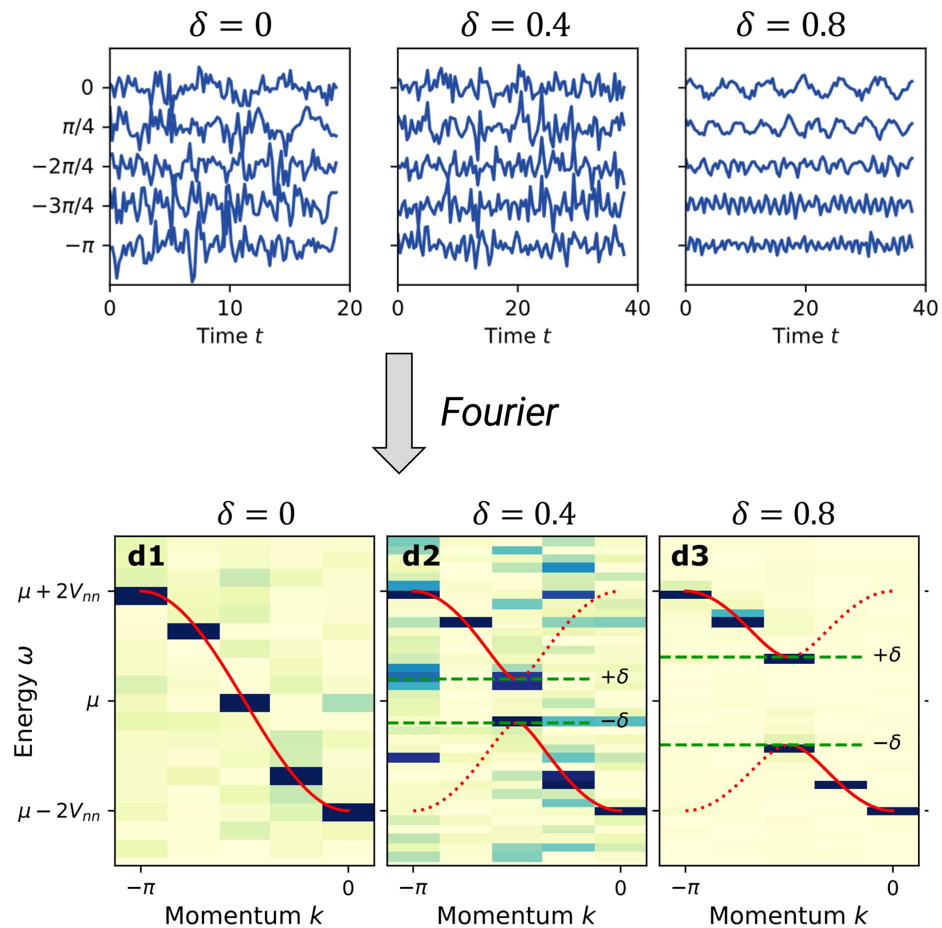
$$\mathcal{H}_0 = -\sum_{\langle i,j \rangle} \left[V_{nn} + (-1)^i \, \delta/2 \right] c_i^\dagger c_j - \mu \sum_i c_i^\dagger c_i$$

Compressed circuit run on *ibm_auckland*



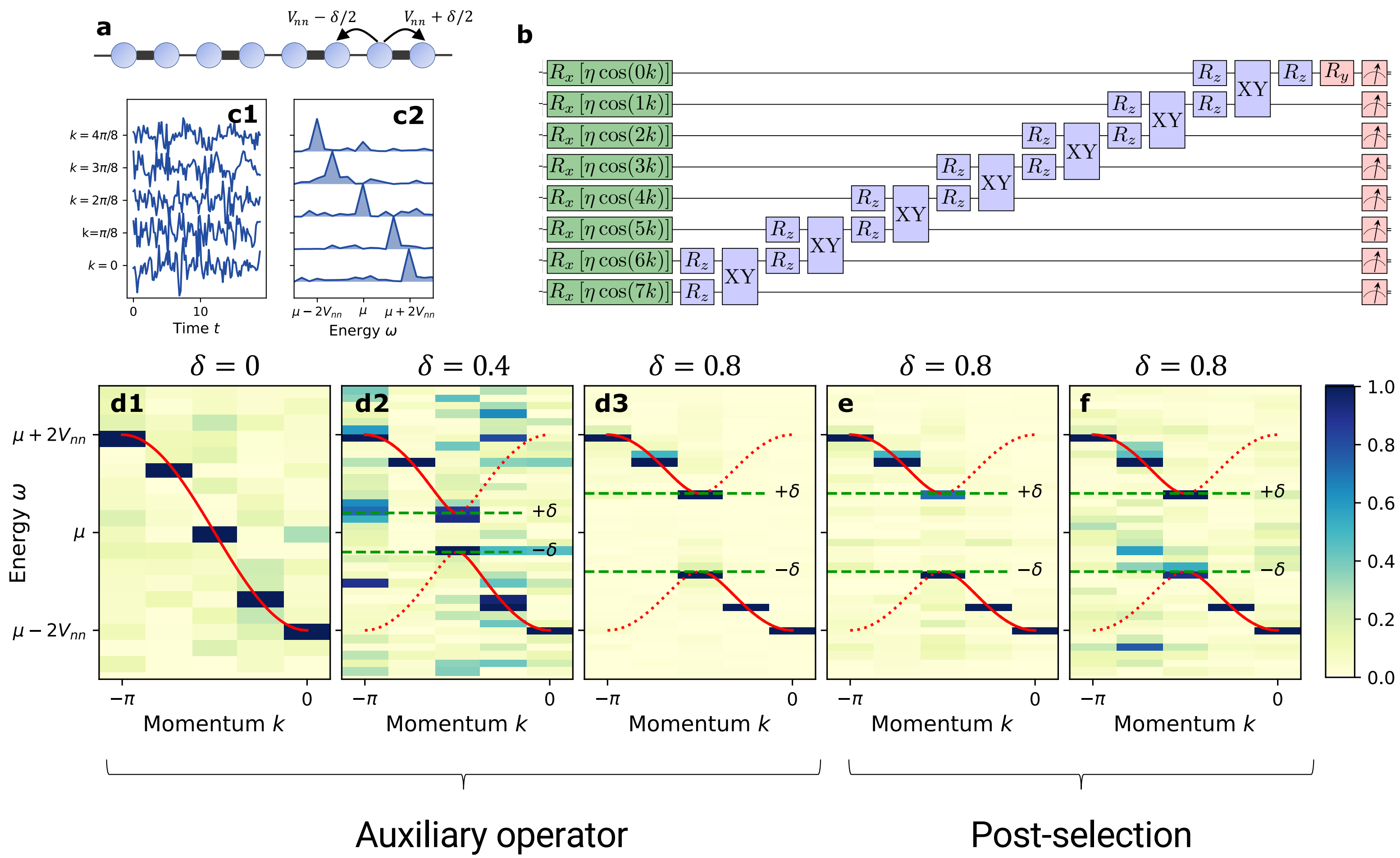
Choose **B** to create a momentum eigenstate

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



NC STATE UNIVERSITY

Linear Response -> Green's function

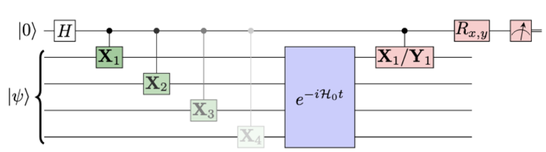


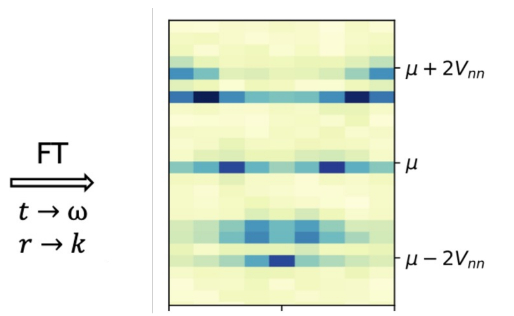
Linear Response -> Green's function

Why does this work so well?

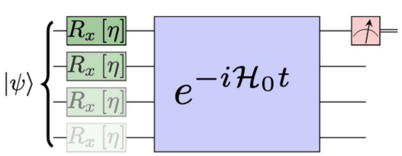
$$\mathbf{B} = \sum_i 2\cos(kr_i)\left[c_i + c_i^\dagger\right]$$

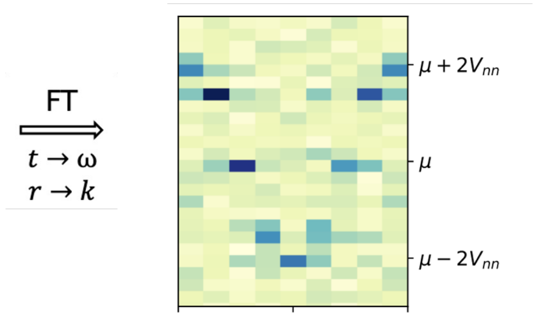
Hadamard test method



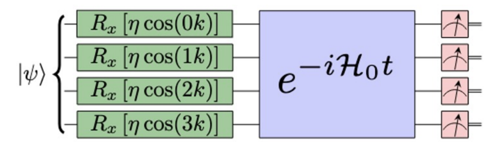


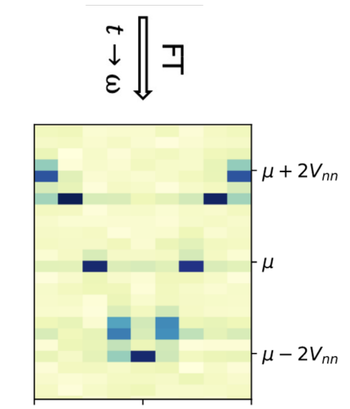
Position-selective linear response





Momentum-selective linear response

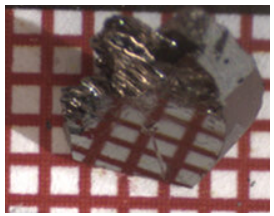


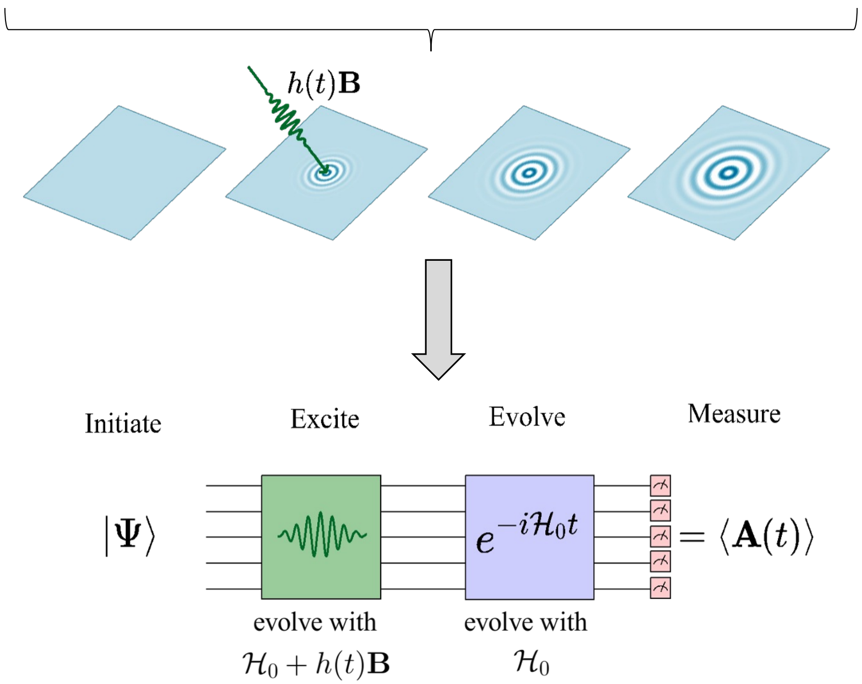


Data from noisy simulator with one/two qubit noise of 1% and 10%

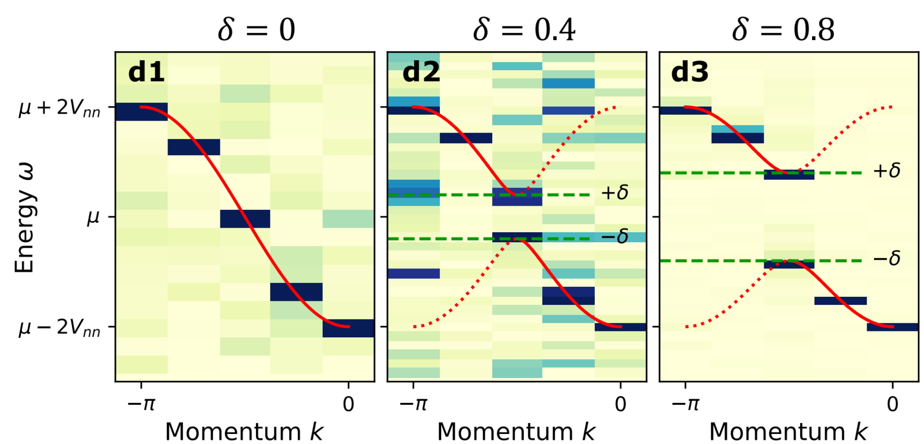
2302.10219

Linear Response





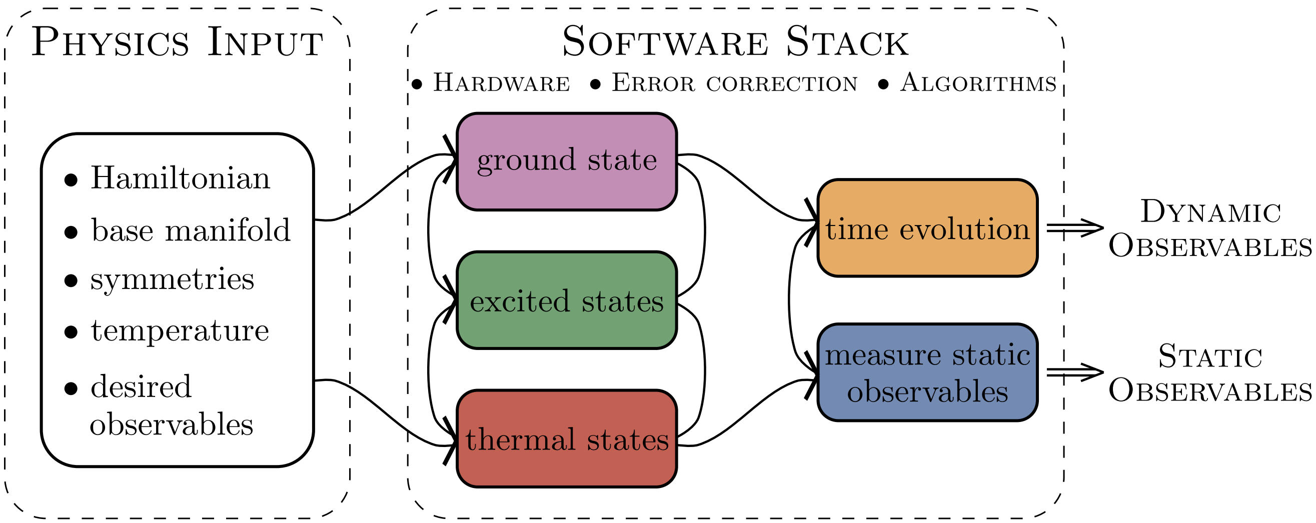
- Ancilla free
- Momentum and frequency selectivity
- Both bosonic and fermionic correlators
- More noise robust compared to existing methods



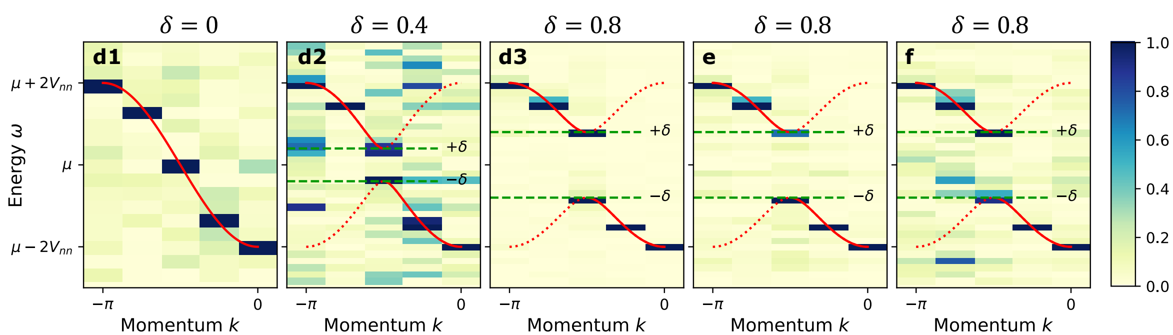
E. Kökcü, H.Labib, J.K. Freericks, AFK., arXiv:2302.10219

NC STATE UNIVERSITY

Quantum Matter meets Quantum Computing



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



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