NC STATE UNIVERSITY

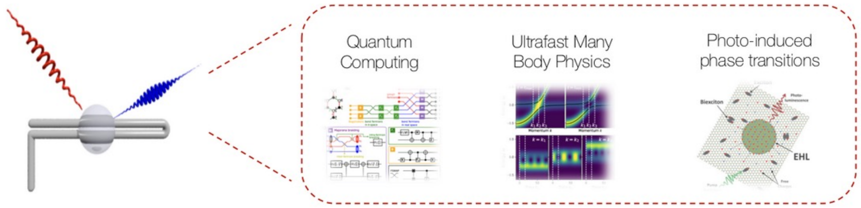
What do you do with a quantum state once you've prepared one?

Alexander (Lex) Kemper

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

LANL QC Summer School
06/27/2023

NC STATE UNIVERSITY



Kemper Lab

Quantum materials in and out of equilibrium.

Collaborations with:

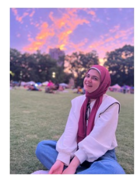
- Jim Freericks (Georgetown)
- Bert de Jong, Katie Klymko, Daan Camps, Roel van Beeument, Akhil Francis (LBNL)
- Thomas Steckmann (UMD)

Current members


Alexander (Lex) Kemper
Principal investigator


Efekan Kökcü
Graduate Researcher


Anjali Agrawal
Graduate Researcher


Heba Labib
Graduate Researcher

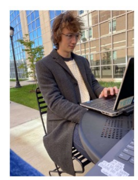

Jack Howard
Undergraduate Researcher


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

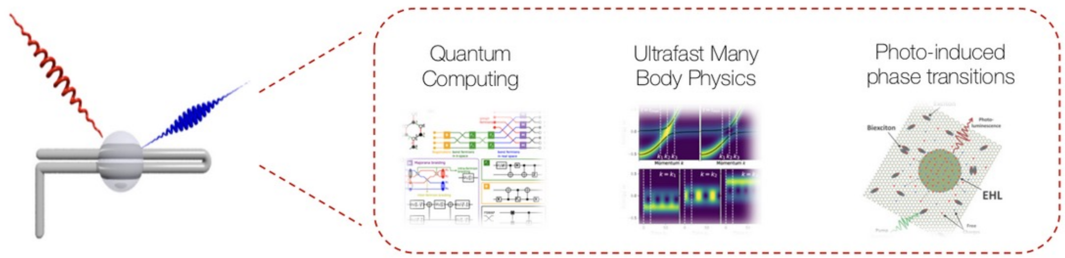
NC STATE UNIVERSITY

Brief outline

- Quantum Matter meets Quantum Computing
- Response functions
  - Why we care
  - How do find them
- A new paradigm: Making the experiment part of the simulation via linear response

NC STATE UNIVERSITY

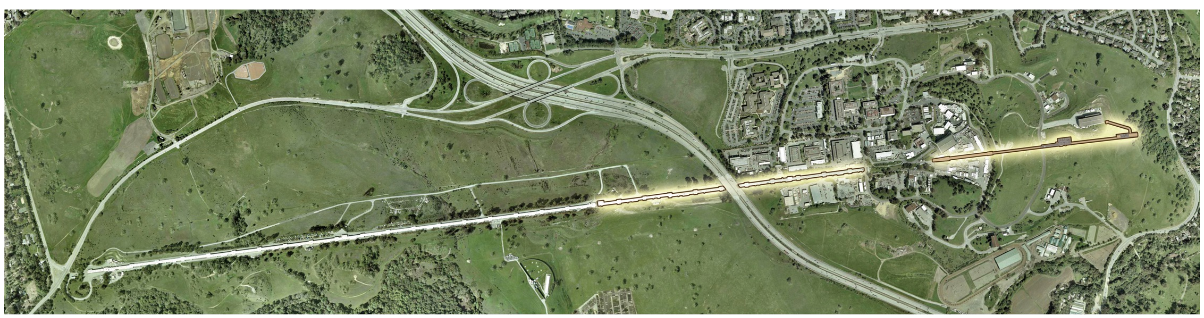
Why quantum computing for condensed matter?

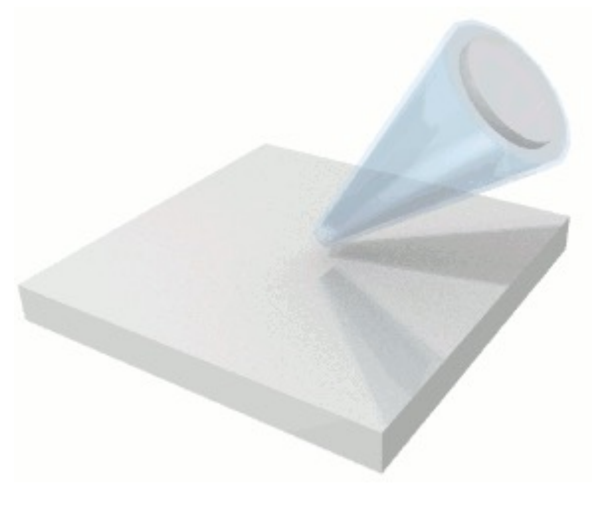


Kemper Lab

Quantum materials in and out of equilibrium.

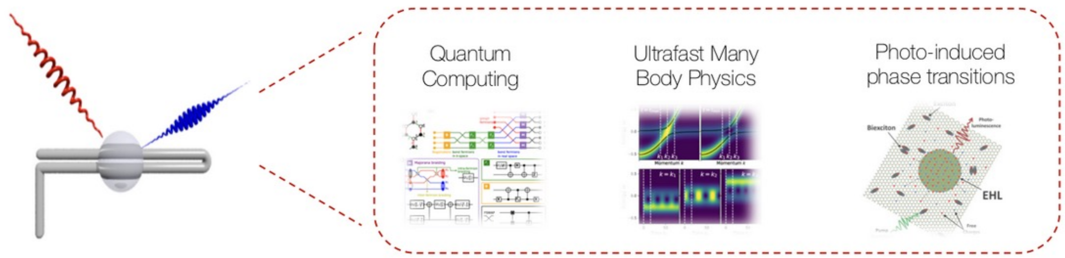
Time-resolved experiments





Shen group (Stanford)

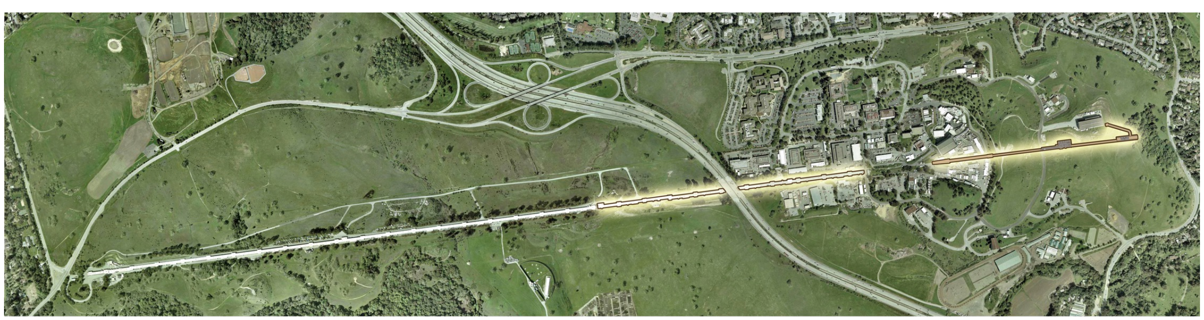
Why quantum computing for condensed matter?



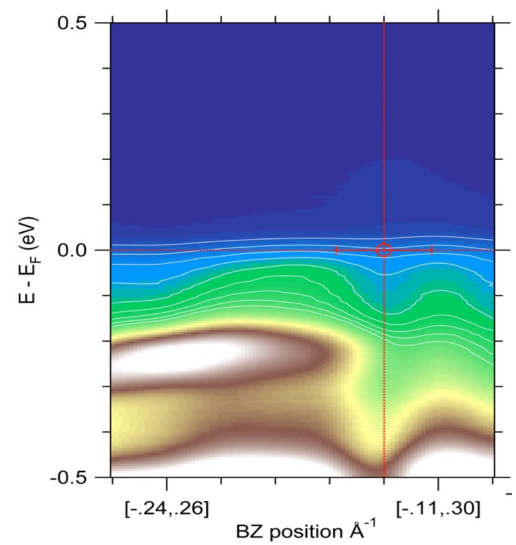
Kemper Lab

Quantum materials in and out of equilibrium.

Time-resolved experiments

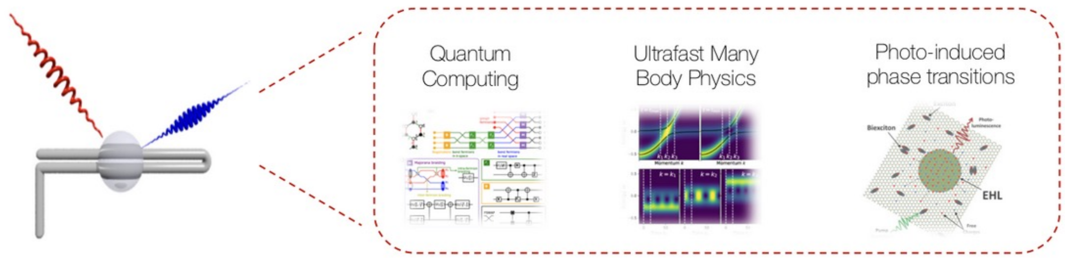


$ErTe_3$



Shen group (Stanford)

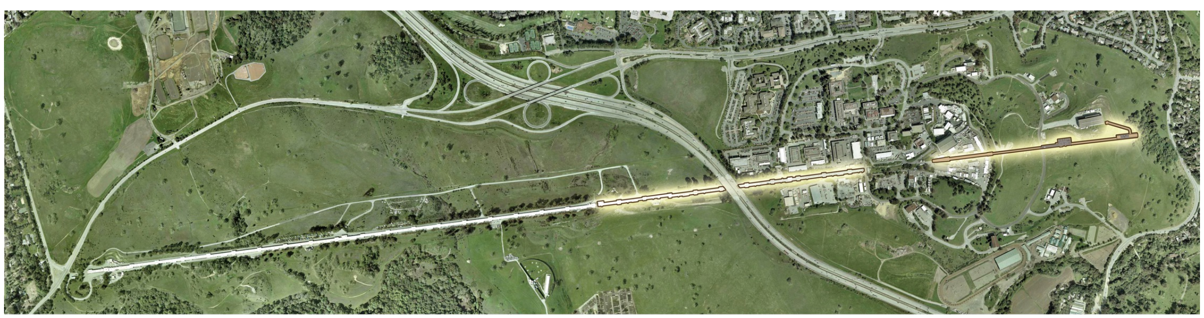
Why quantum computing for condensed matter?



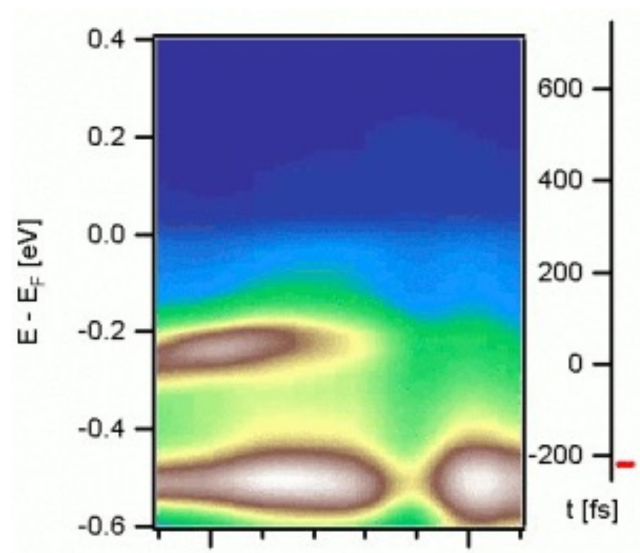
Kemper Lab

Quantum materials in and out of equilibrium.

Time-resolved experiments

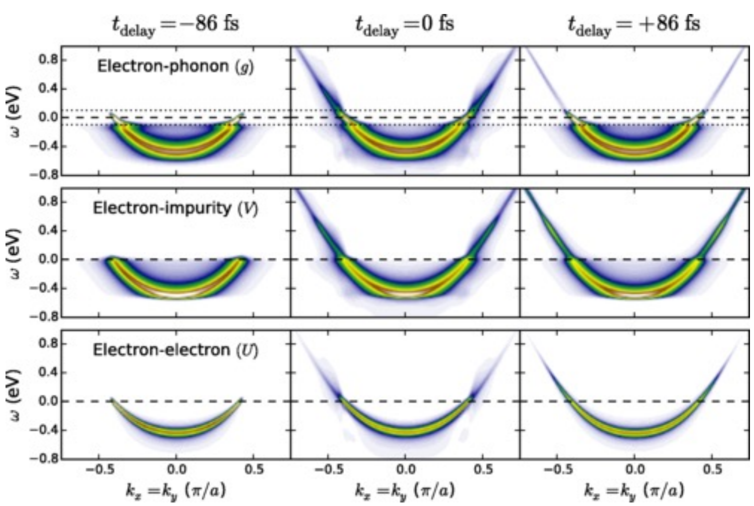


$ErTe_3$



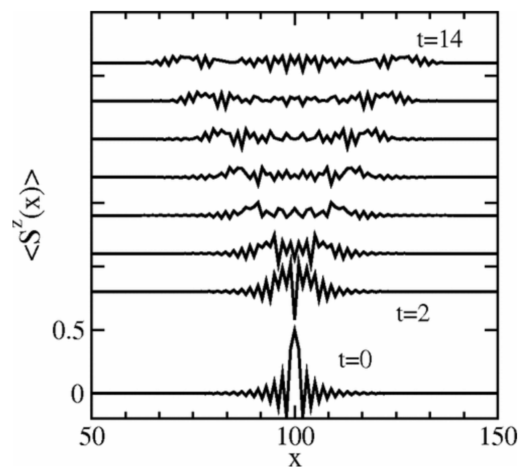
Shen group (Stanford)

Why quantum computing for condensed matter?



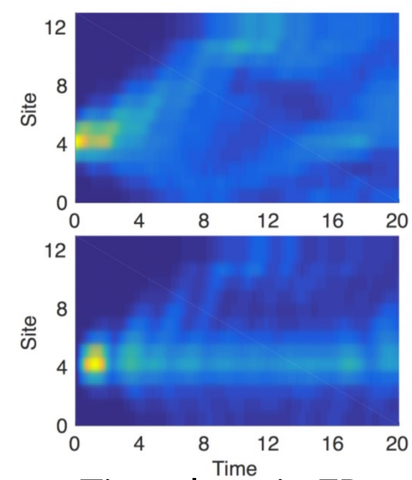
Non-Equilibrium Green's functions

Phys. Rev. X 8, 041009 (2018)



Time domain DMRG

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



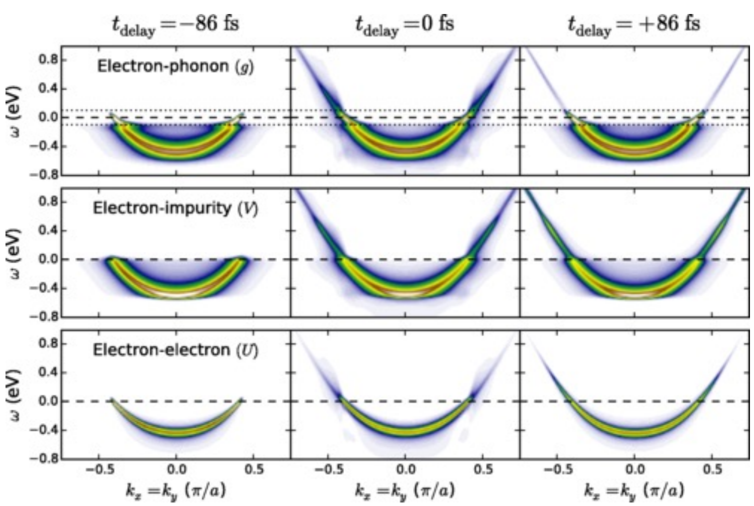
Time domain ED

Johnston & Kemper, unpublished

NC STATE UNIVERSITY

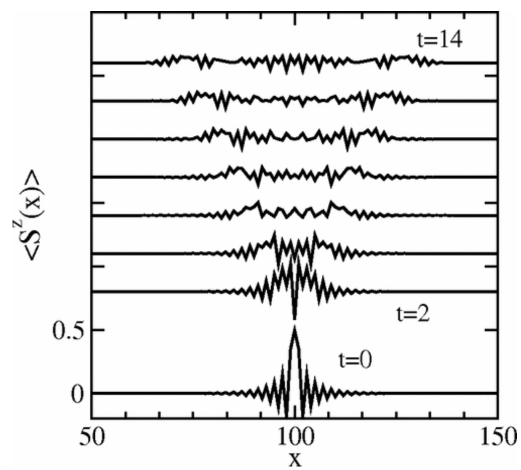
Why quantum computing for condensed matter?

All these techniques eventually reach a barrier.



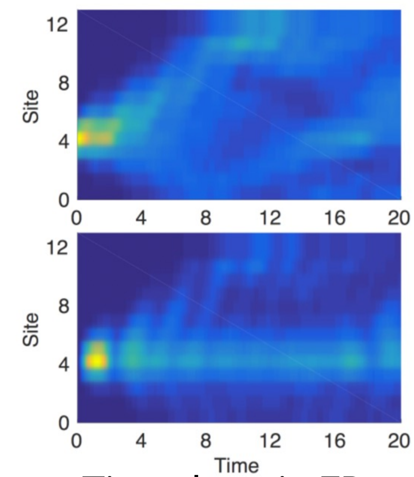
Non-Equilibrium Green's functions

Phys. Rev. X 8, 041009 (2018)



Time domain DMRG

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

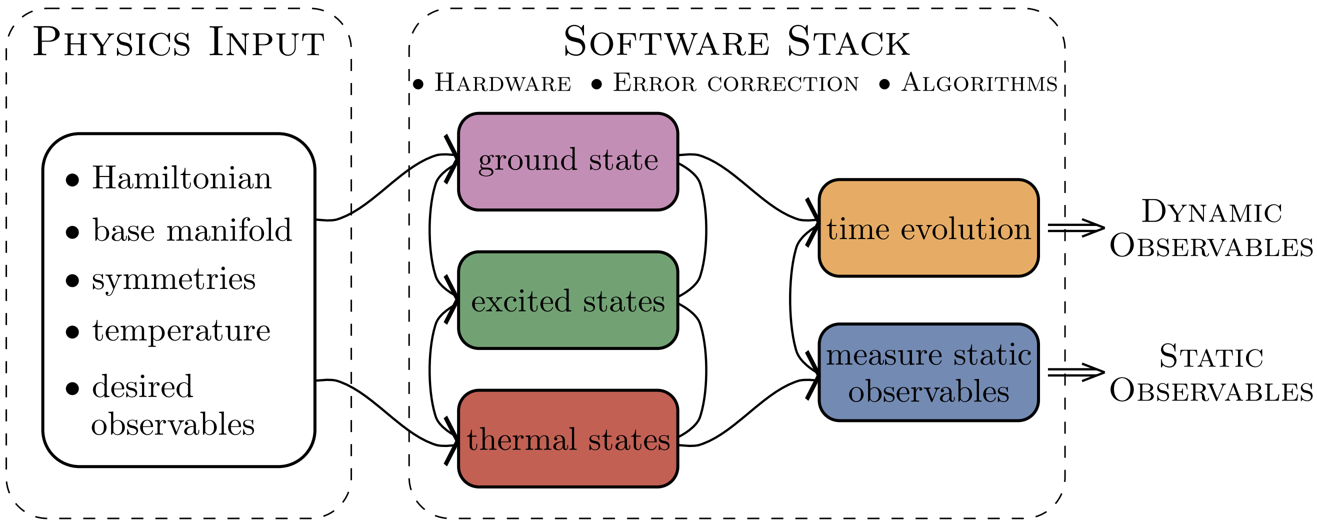


Time domain ED

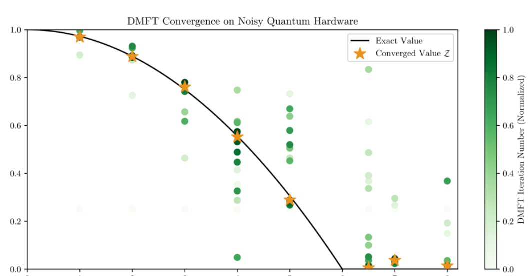
Johnston & Kemper, unpublished

Quantum Matter meets Quantum Computing

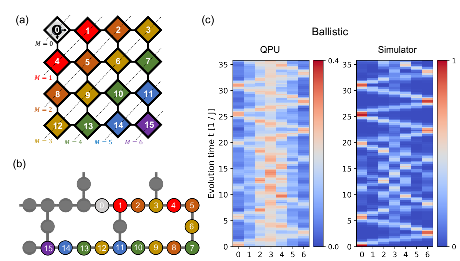
https://go.ncsu.edu/kemper-lab



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

NC STATE UNIVERSITY

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

NC STATE UNIVERSITY

Ising Model

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

The Ising Model and Real Magnetic Materials

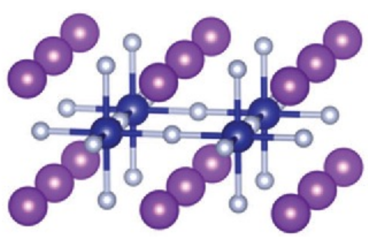
W. P. Wolf

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

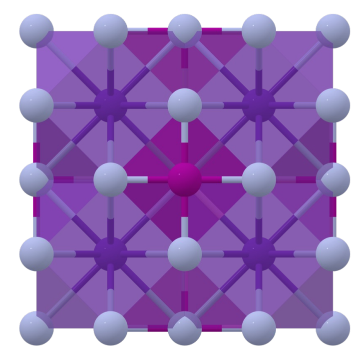
covering condensed matter and materials physics

Highlights Recent Accepted Collections Authors Referees Search Press

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

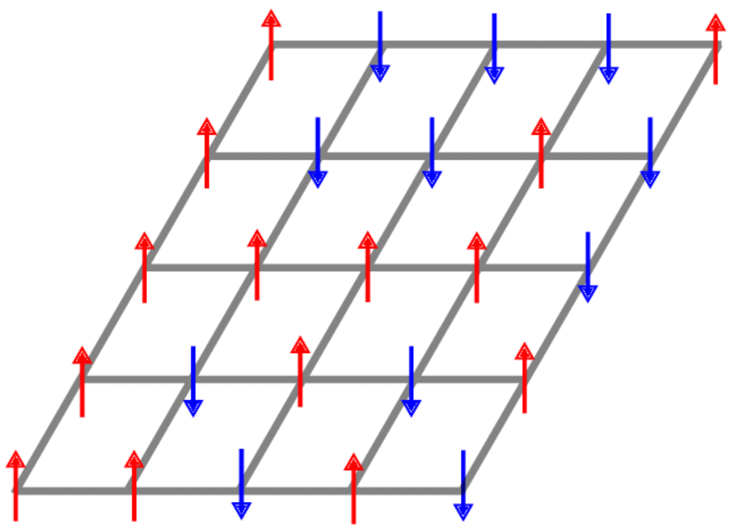


Materials project

NC STATE UNIVERSITY

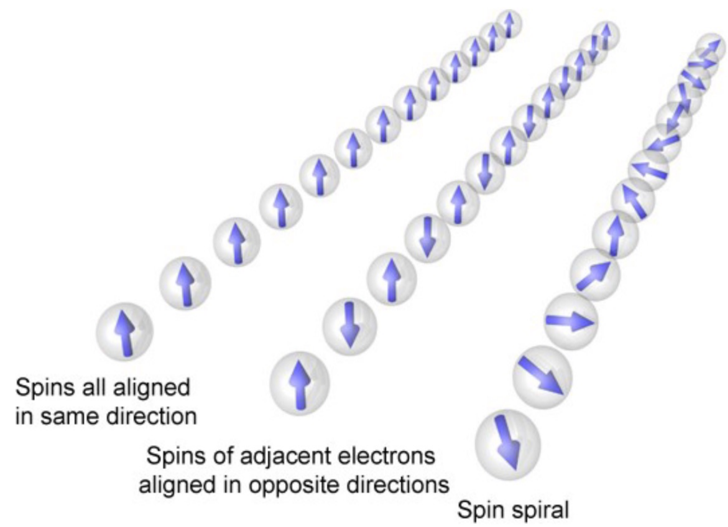
Ising Model

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



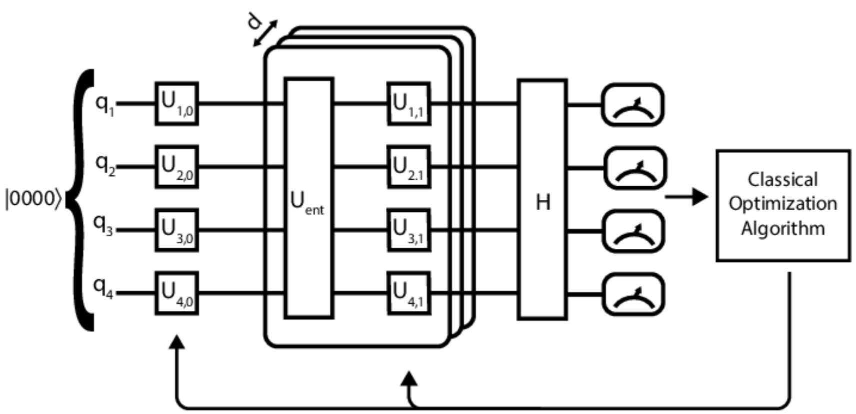
Heisenberg model

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



Ising Model

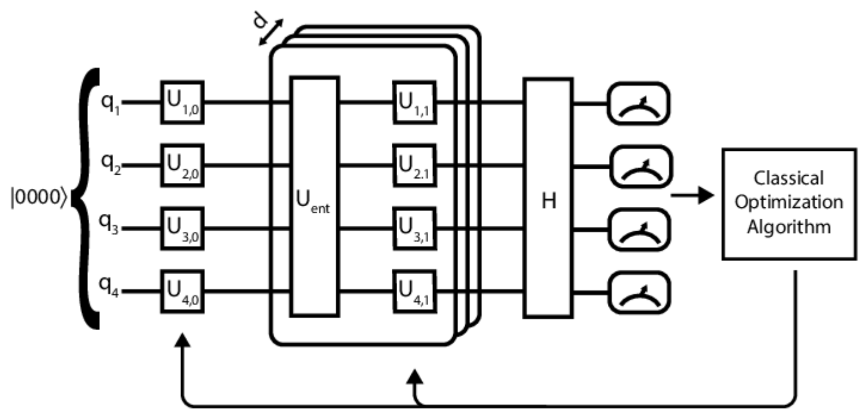
$$\mathcal{H} = -J \sum_i \sigma_i^z \sigma_{i+1}^z + h_x \sum_i \sigma_i^x$$



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

Heisenberg model

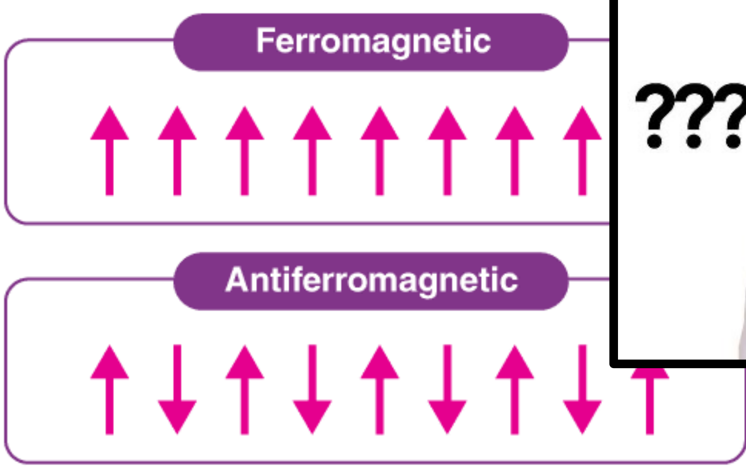
$$\mathcal{H} = -J \sum_i \vec{\sigma}_i \cdot \vec{\sigma}_{i+1} + h_x \sum_i \sigma_i^x$$

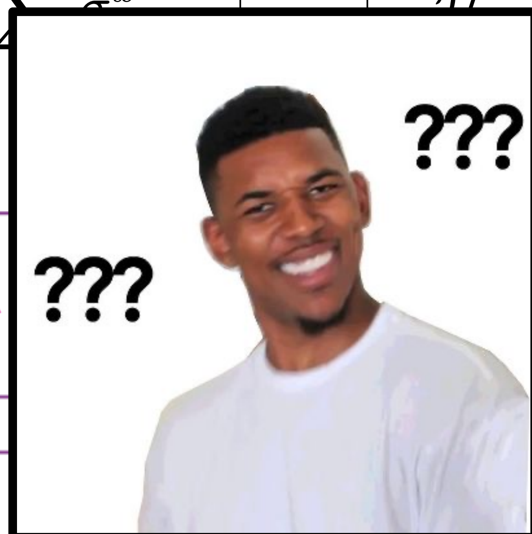


NC STATE UNIVERSITY

Ising Model

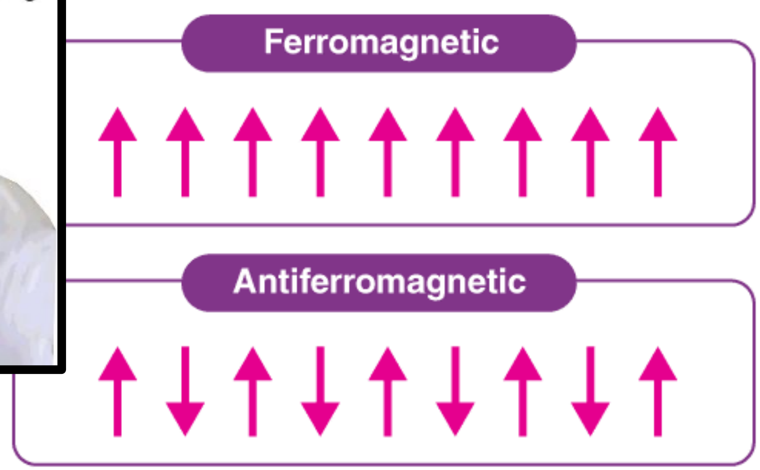
$$\mathcal{H} = -J\sum_i \sigma_i^z \sigma_{i+1}^z + h_x \sum \sigma^x$$





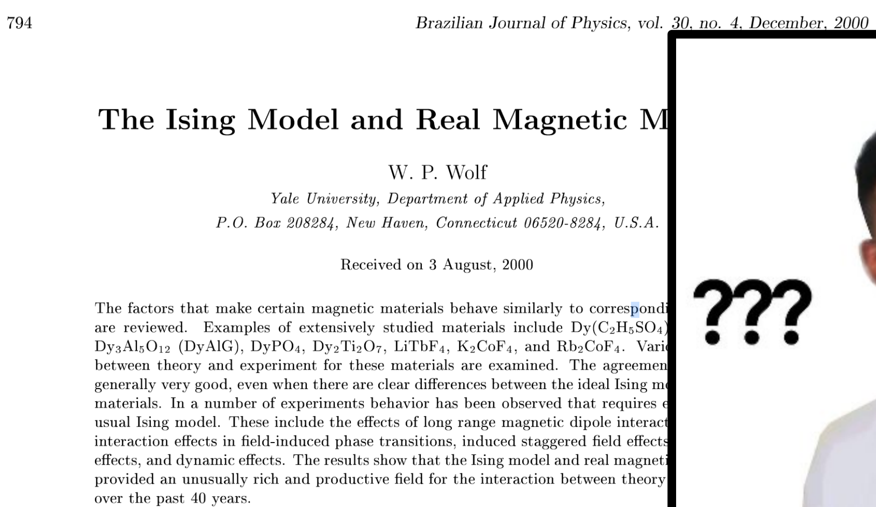
Heisenberg model

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



NC STATE UNIVERSITY

Ising Model


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

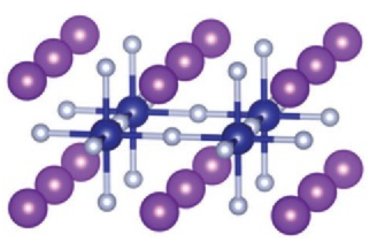
The Ising Model and Real Magnetic M

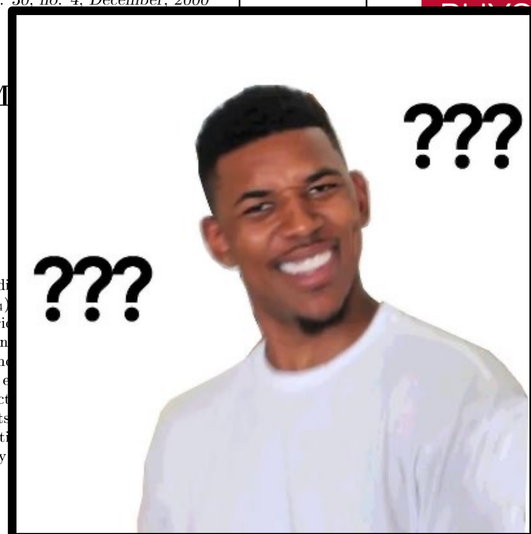
W. P. Wolf

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

Received on 3 August, 2000

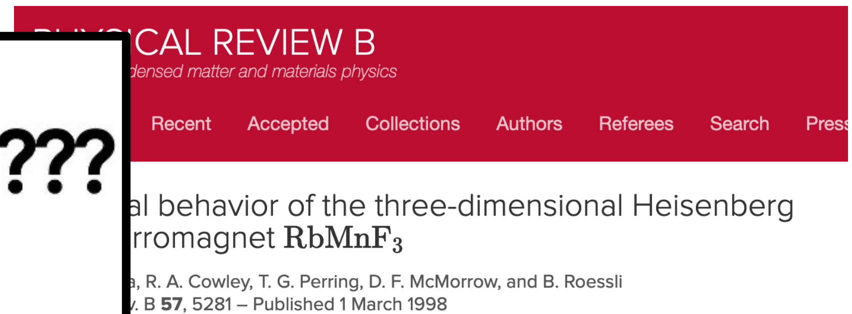
The factors that make certain magnetic materials behave similarly to correspondi
are reviewed. Examples of extensively studied materials include $Dy(C_2H_5SO_4)$
$Dy_3Al_5O_{12}$ (DyAlG), $DyPO_4$, $Dy_2Ti_2O_7$, $LiTbF_4$, K_2CoF_4, and Rb_2CoF_4. Vari
between theory and experiment for these materials are examined. The agreemen
generally very good, even when there are clear differences between the ideal Ising m
materials. In a number of experiments behavior has been observed that requires e
usual Ising model. These include the effects of long range magnetic dipole interact
interaction effects in field-induced phase transitions, induced staggered field effects
effects, and dynamic effects. The results show that the Ising model and real magneti
provided an unusually rich and productive field for the interaction between theory
over the past 40 years.

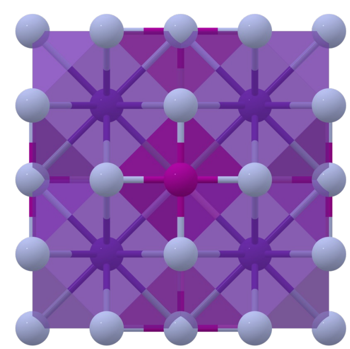




10.1039/c6cp02362b

Heisenberg model





Materials project

NC STATE UNIVERSITY

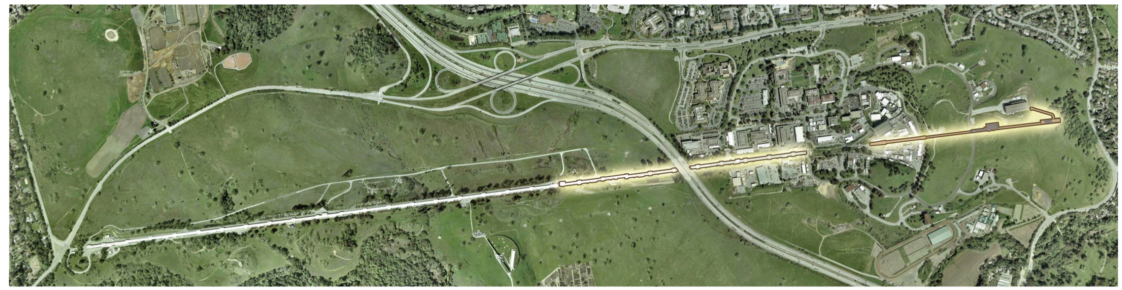
Q: What do you do with a quantum state once you've prepared one?

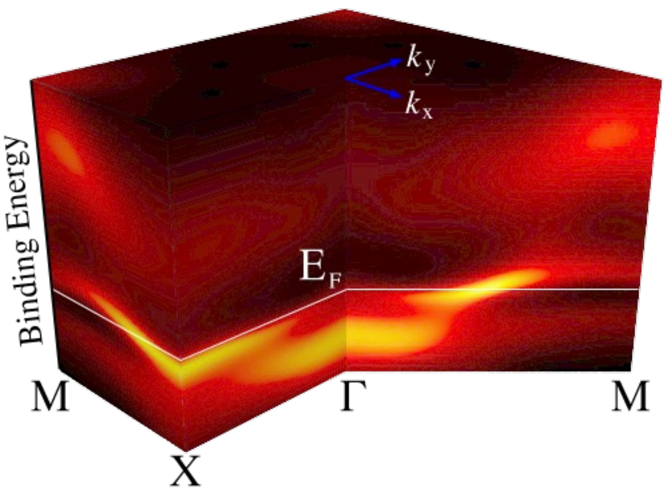
A: You measure its excitations.

NC STATE UNIVERSITY

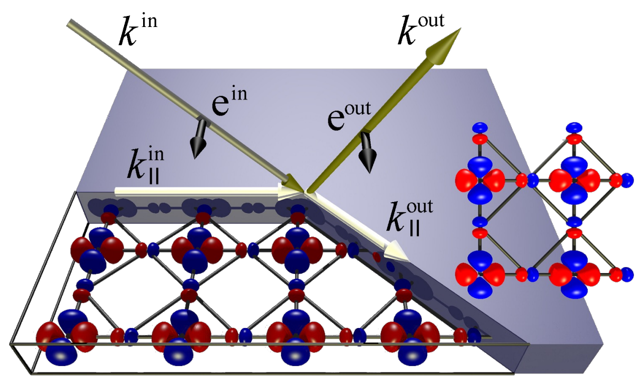
Measuring Excitations

Figures courtesy of Devereaux group

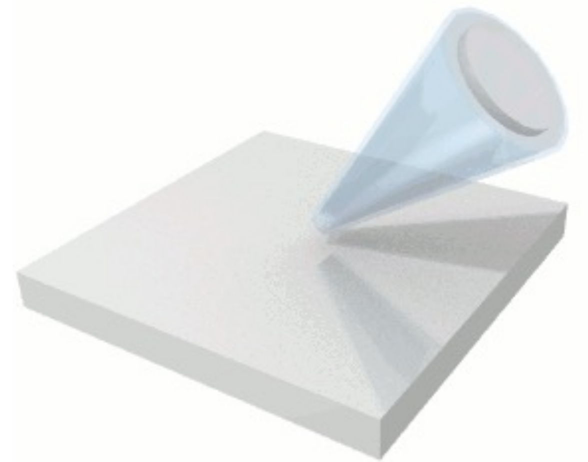




Angle-resolved Photoemission (ARPES)

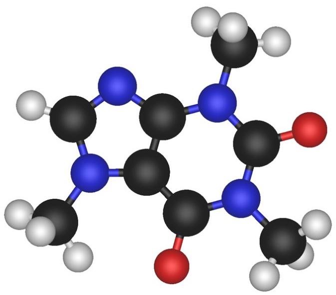


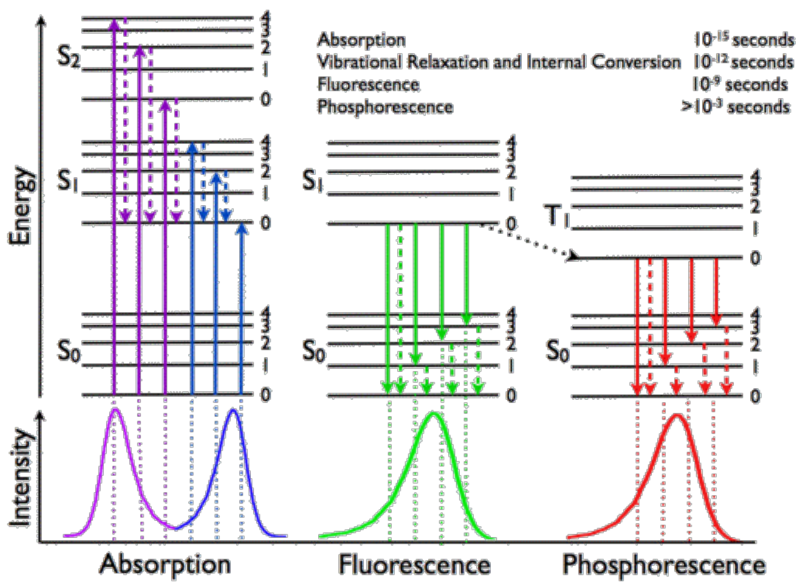
Resonant Inelastic X-Ray Scattering

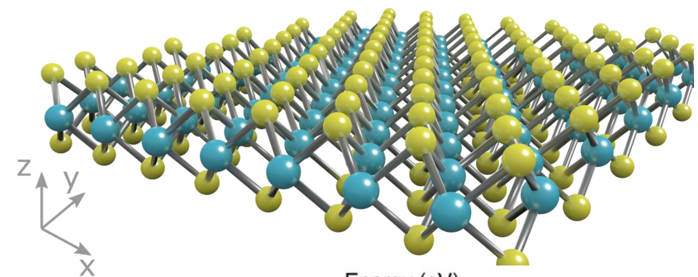


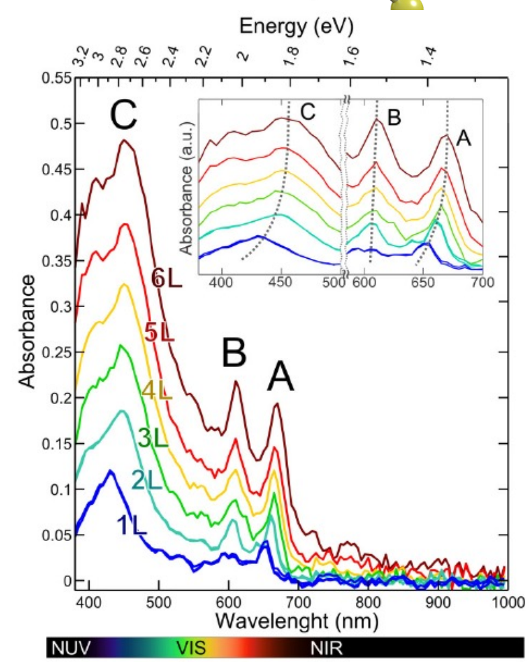
Time-resolved ARPES

Measuring Excitations





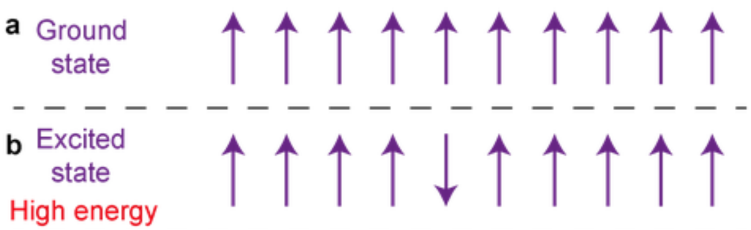




Measuring Excitations

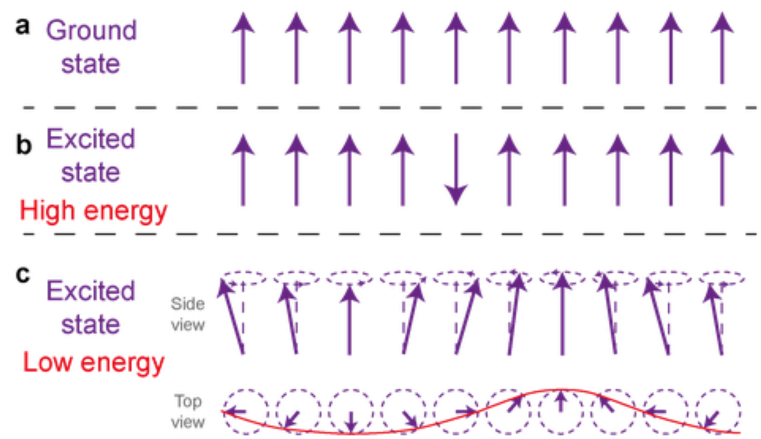
Ising Model

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



Heisenberg model

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



NC STATE UNIVERSITY

Measuring Excitations – Response functions

Schrödinger Picture $$i\partial_t|\psi(t)\rangle = H|\psi(t)\rangle$$

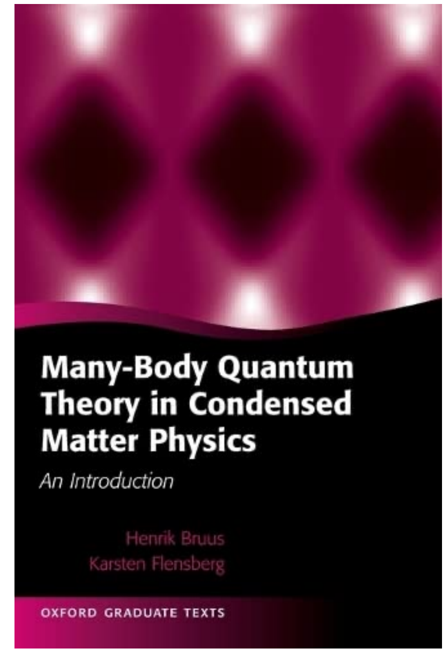
Heisenberg Picture $$i\partial_t\mathcal{O}(t) = [\mathcal{O}(t), H(t)]$$

Interaction Picture

$$H = H_0 + V(t)$$

$$i\partial_t|\psi(t)\rangle = V(t)|\psi(t)\rangle$$

$$i\partial_t\mathcal{O}(t) = [\mathcal{O}(t), H_0]$$



NC STATE UNIVERSITY

Some Mathematics…

The time evolution operator satisfies

$$i\partial_t U(t) = V(t)U(t)$$

Which is formally solved by

$$U(t) = \mathcal{T}exp\left(-i\int_{-\infty}^{t} V(\bar{t})d\bar{t}\right)$$

Or approximately(for small V) by

$$U(t) \approx 1 - i\int_{-\infty}^{t} V(\bar{t})d\bar{t}$$

Thus the wave function is given by

$$|\psi(t)\rangle \approx |\psi_0\rangle - i\int_{-\infty}^{t} V(\bar{t})|\psi_0\rangle d\bar{t}$$

We now pick an operator **A** to evaluate

$$\langle\psi(t)|\mathbf{A}(t)|\psi(t)\rangle = \ \langle\psi_0|\mathbf{A}(t)|\psi_0\rangle =$$

$$-i\int_{-\infty}^{t}\langle\psi_0|\left[\mathbf{A}(t), \mathbf{V}(\bar{t})\right]|\psi_0\rangle d\bar{t}$$

Putting the time dependence outside via $\mathbf{V}(t) = h(t)\mathbf{B}$

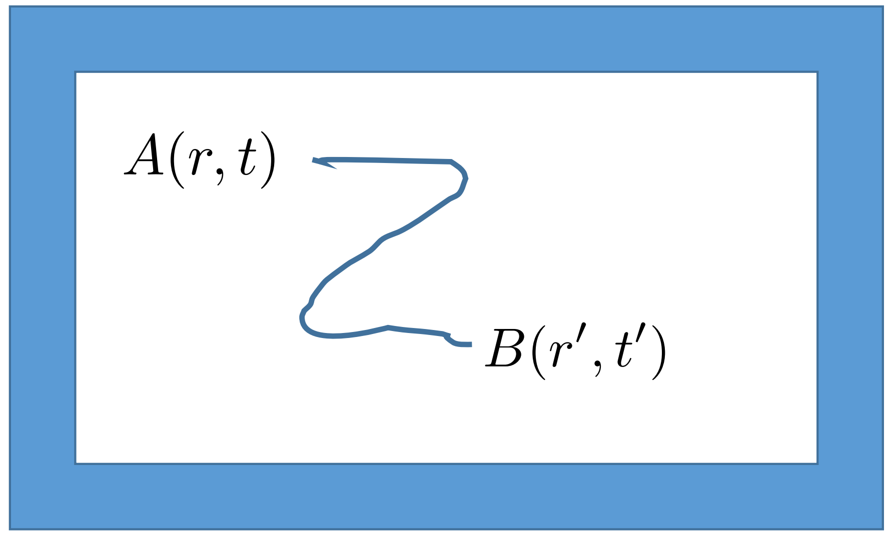
$$\delta A(t) = -i\int_{-\infty}^{t}\langle[\mathbf{A}(t), \mathbf{B}]\rangle h(\bar{t})d\bar{t}$$

$$\delta A(t) = \int_{\infty}^{\infty}\chi^R(t,\bar{t})h(\bar{t})d\bar{t}$$

Low-energy excitations: correlation functions

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

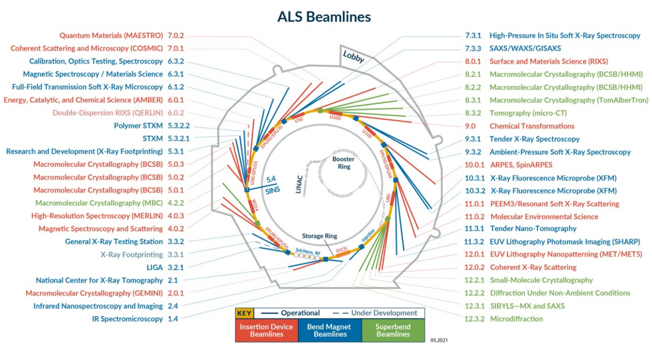
Given some (observable) operator B at (r',t'), what is the likelihood of some (observable) operator A at (r,t)?

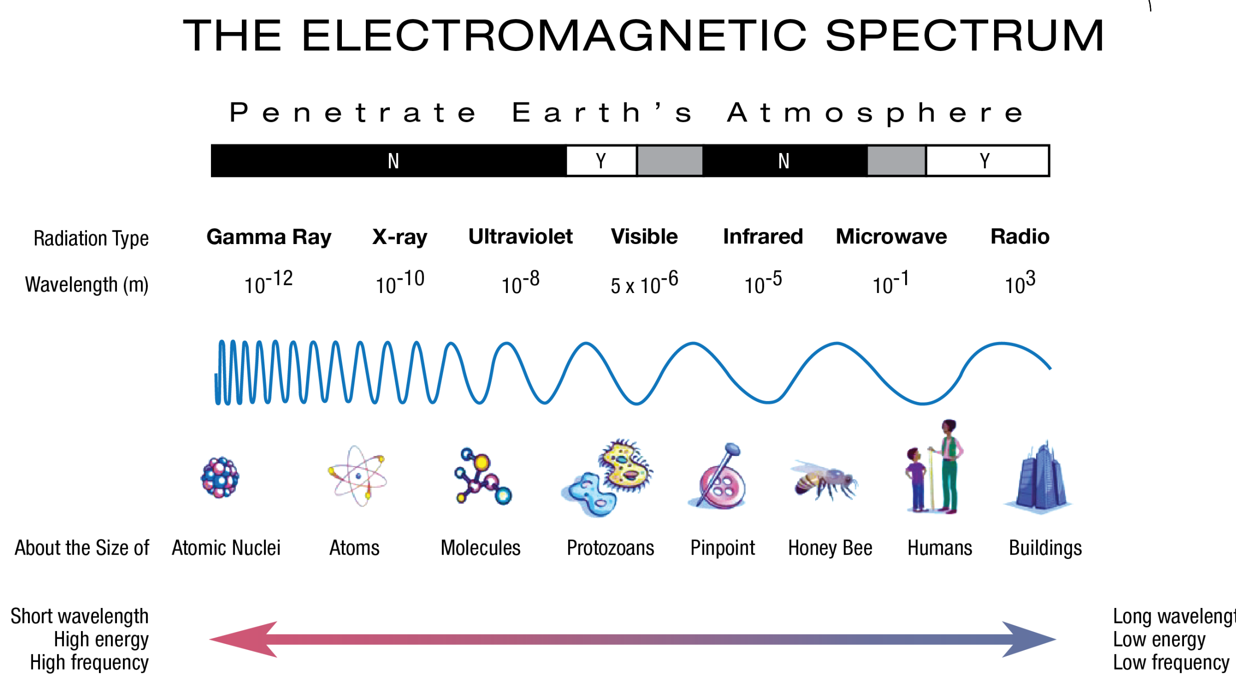


$$\delta A(t) = -i \int_{-\infty}^{t} \langle [\mathbf{A}(t), \mathbf{B}] \rangle h(\bar{t}) d\bar{t} = \int_{\infty}^{\infty} \chi^{R}(t, \bar{t}) h(\bar{t}) d\bar{t}$$

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

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

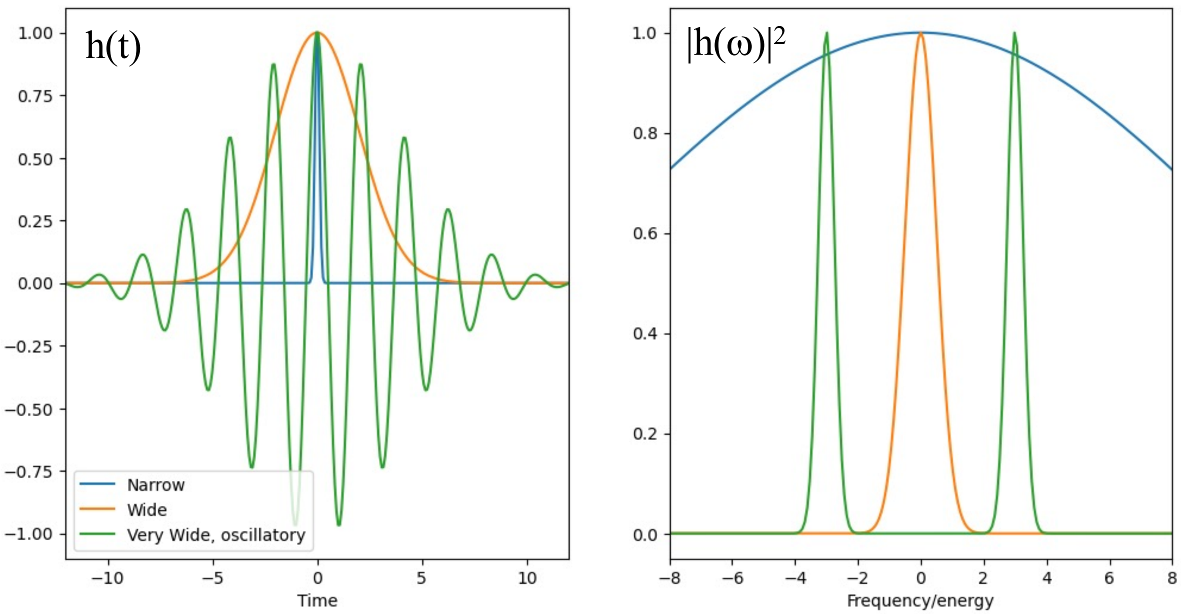




The Electromagnetic Spectrum. Image Credit: NASA

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

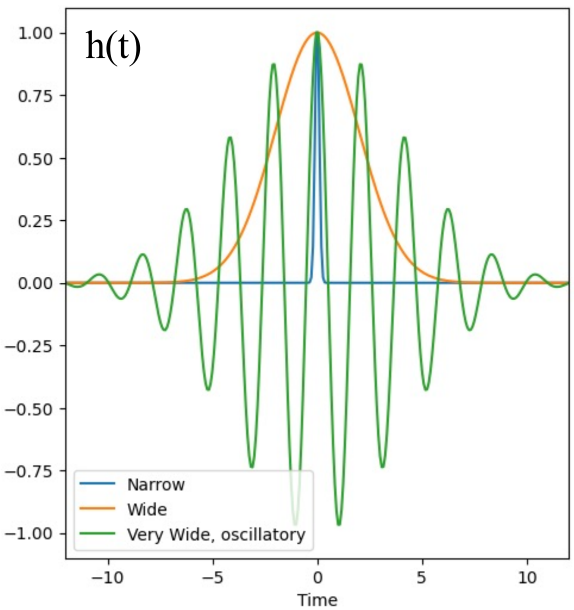
h(t) encodes the energy range/resolution

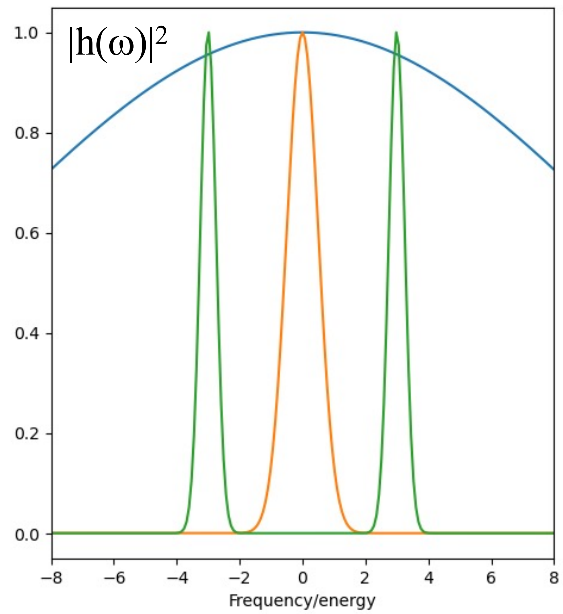


NC STATE UNIVERSITY

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

h(t) encodes the energy range/resolution





B can be used for spatial encoding

$$\mathbf{B} = \frac{1}{N} \sum_i \sigma_i^z$$

vs

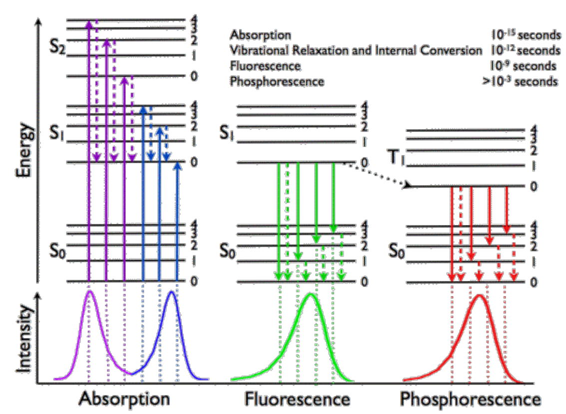
$$\mathbf{B} = \frac{1}{N} \sum_i (-1)^i \sigma_i^z$$

Some More Mathematics…

The task is to calculate

$$\chi(t) := -i\theta(t)\langle\psi_0|\mathbf{A}(t)\mathbf{B}|\psi_0\rangle$$

$$\chi(\omega) = \sum_j \frac{\langle\psi_0|\mathbf{A}|j\rangle\langle j|\mathbf{B}|\psi_0\rangle}{\omega - E_j + E_0 + i\varepsilon}$$

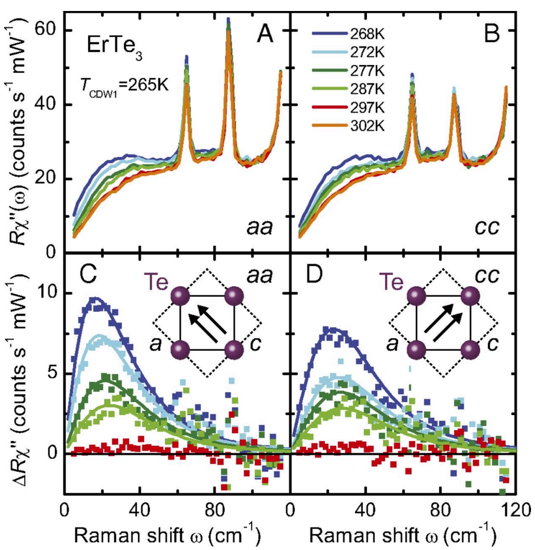


Some More Mathematics…

The task is to calculate

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

$$\chi(q,\omega) = \int d(r-r')e^{-iq(r-r')}\frac{\langle\psi_0|\mathbf{A}(r)|j\rangle\langle j|\mathbf{B}(r')|\psi_0\rangle}{\omega - E_j + E_0 + i\varepsilon}$$



RESEARCH ARTICLE | PHYSICAL SCIENCES

Alternative route to charge density wave formation in multiband systems

Hans-Martin Eiter, Michela Lavagnini, Rudi Hackl, +6, and Leonardo Degiorgi Authors Info & Affiliations

Edited by M. Brian Maple, University of California at San Diego, La Jolla, CA, and approved November 15, 2012 (received for review August 24, 2012)

December 17, 2012 | 110 (1) 64-69 | https://doi.org/10.1073/pnas.1214745110

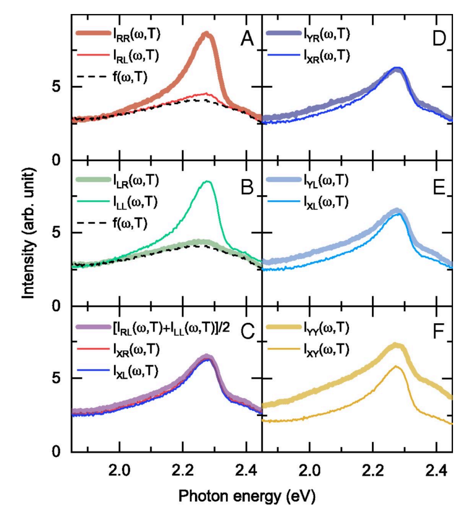
RESEARCH ARTICLE | APPLIED PHYSICAL SCIENCES

Observation of chiral surface excitons in a topological insulator Bi_2Se_3

H.-H. Kung, A. P. Goyal, D. L. Maslov, +4, and G. Blumberg Authors Info & Affiliations

Edited by Angel Rubio, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany, and approved January 22, 2019 (received for review August 5, 2018)

February 20, 2019 | 116 (10) 4006-4011 | https://doi.org/10.1073/pnas.1813514116



NC STATE UNIVERSITY

Quantum Algorithm(s) for χ

NC STATE UNIVERSITY

Quantum Algorithm(s) for χ

APPROACH 1: Stick with the many—body textbook

$$\chi(\omega) = \sum_j \frac{\langle\psi_0|\mathbf{A}|j\rangle\langle j|\mathbf{B}|\psi_0\rangle}{\omega - E_j + E_0 + i\varepsilon}$$

$$\chi(\omega) = \langle\psi_0|\mathbf{A}\frac{1}{\omega - \mathbf{H} + E_0 + i\varepsilon}\mathbf{B}|\psi_0\rangle$$

APPROACH 2: Go back to our roots

$$\chi(t) = e^{iE_0 t}\langle\psi_0|\mathbf{A}e^{-i\mathbf{H}_0 t}\mathbf{B}|\psi_0\rangle$$

NC STATE UNIVERSITY

Quantum Algorithm(s) for χ

$$\chi(t) = e^{iE_0 t}\langle\psi_0|\mathbf{A}e^{-i\mathbf{H}_0 t}\mathbf{B}|\psi_0\rangle$$

Interfere with ground state

Complete expectation value

Apply excitation B

Time evolve

Apply excitation A

Prepare state of interest

PHYSICAL REVIEW A, VOLUME 65, 042323

Simulating physical phenomena by quantum networks

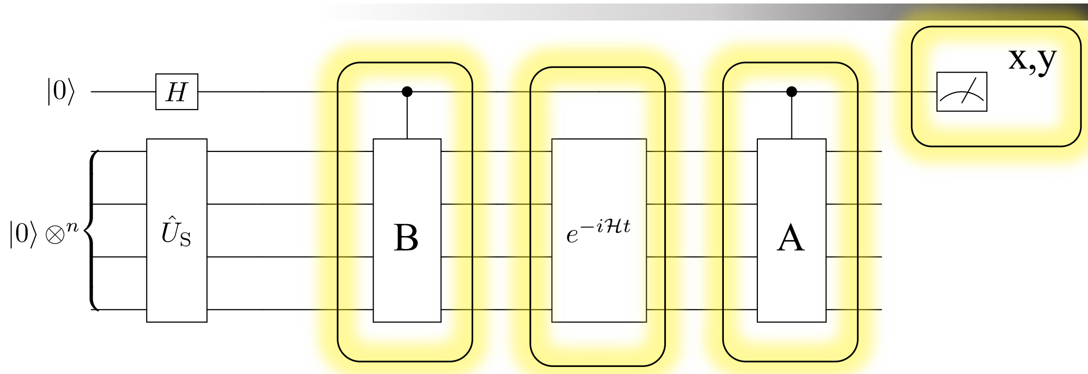
R. Somma, G. Ortiz, J. E. Gubernatis, E. Knill, and R. Laflamme
Los Alamos National Laboratory, Los Alamos, New Mexico 87545
(Received 12 September 2001; published 9 April 2002)

PRL **113,** 020505 (2014) PHYSICAL REVIEW LETTERS week ending 11 JULY 2014

Efficient Quantum Algorithm for Computing *n*-time Correlation Functions

J. S. Pedernales,[1] R. Di Candia,[1] I. L. Egusquiza,[2] J. Casanova,[1] and E. Solano[1,3]
[1]*Department of Physical Chemistry, University of the Basque Country UPV/EHU, Apartado 644, 48080 Bilbao, Spain*
[2]*Department of Theoretical Physics and History of Science, University of the Basque Country UPV/EHU, Apartado 644, 48080 Bilbao, Spain*
[3]*IKERBASQUE, Basque Foundation for Science, Alameda Urquijo 36, 48011 Bilbao, Spain*
(Received 20 January 2014; revised manuscript received 30 April 2014; published 10 July 2014)

Quantum Algorithm(s) for χ

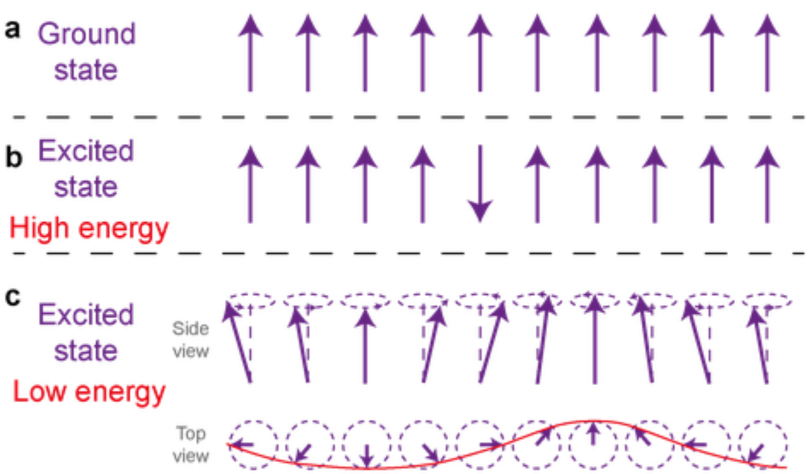


$$(|0\rangle + |1\rangle)\,|\psi_0\rangle$$

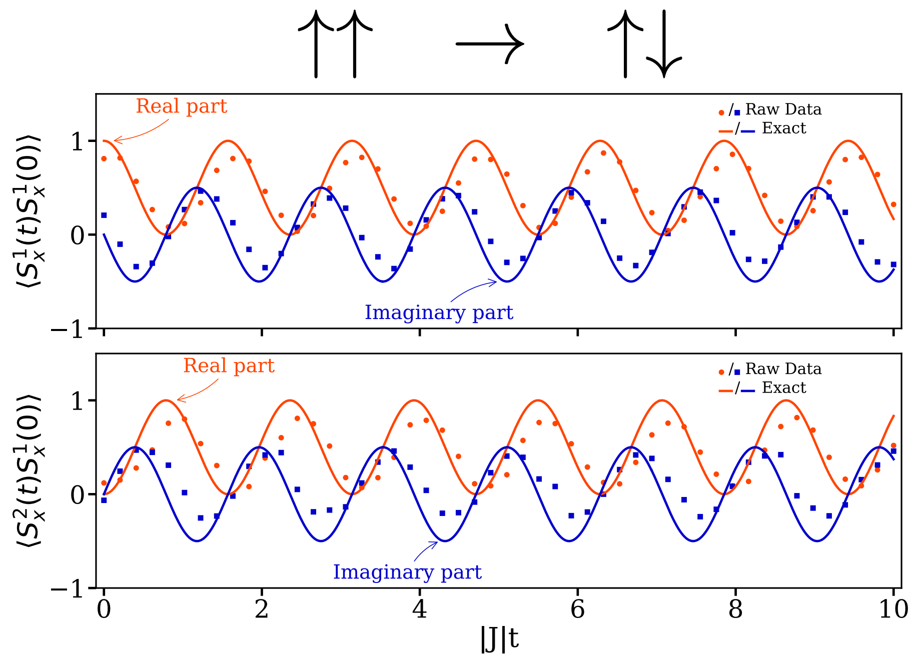
$$\mathrm{P}(0) = \frac{1}{2}\left[1 + \mathrm{Re}\, e^{iE_0 t}\langle\psi_0|\mathbf{A}e^{-i\mathbf{H}_0 t}\mathbf{B}|\psi_0\rangle\right]$$

Low-energy excitations: 2-site magnons

Spin-spin correlation function for periodic Heisenberg model: Magnons!



$$\hat{H} = 2SJ\sum_k (1-\cos(k))\hat{c}_k^\dagger \hat{c}_k$$

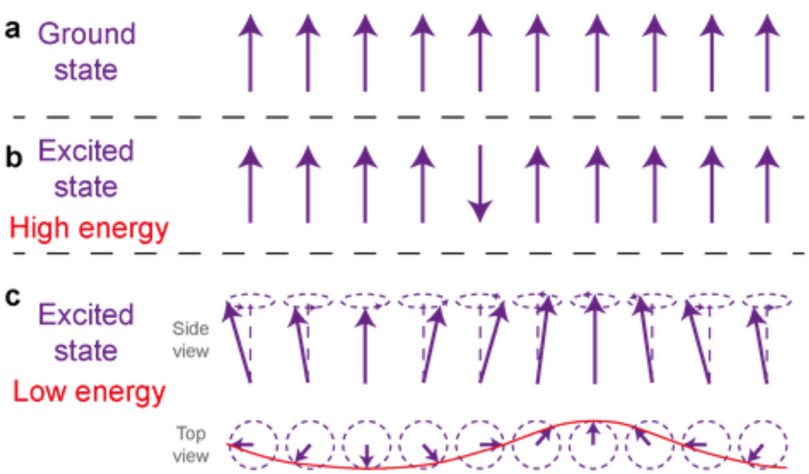


Data from *ibmq_tokyo*

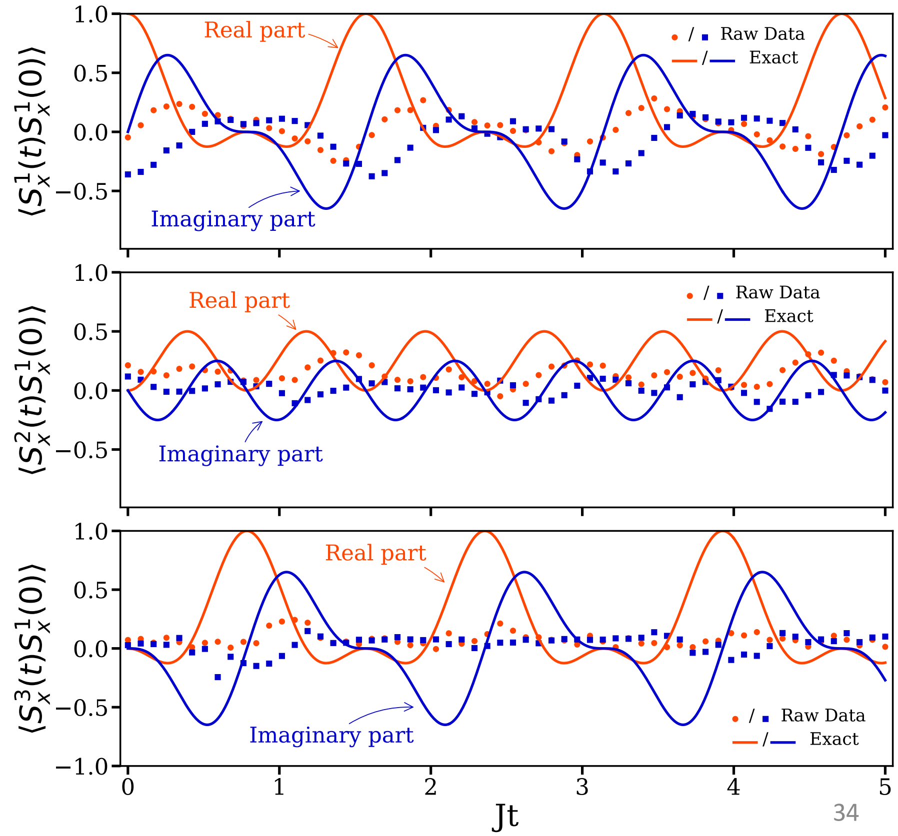
10.1103/PhysRevB.101.014411

Low-energy excitations: 4-site magnons

Spin-spin correlation function for periodic Heisenberg model $\uparrow\uparrow\uparrow\uparrow \;\rightarrow\; \uparrow\uparrow\uparrow\downarrow$

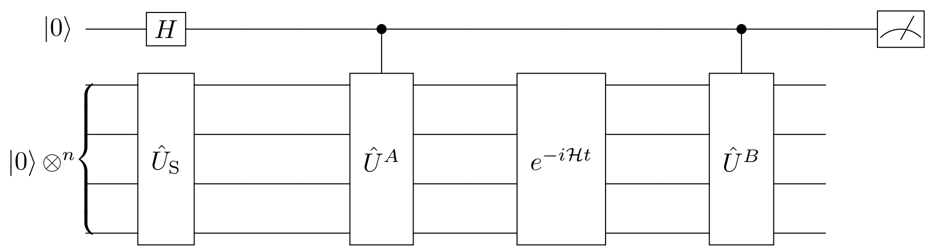


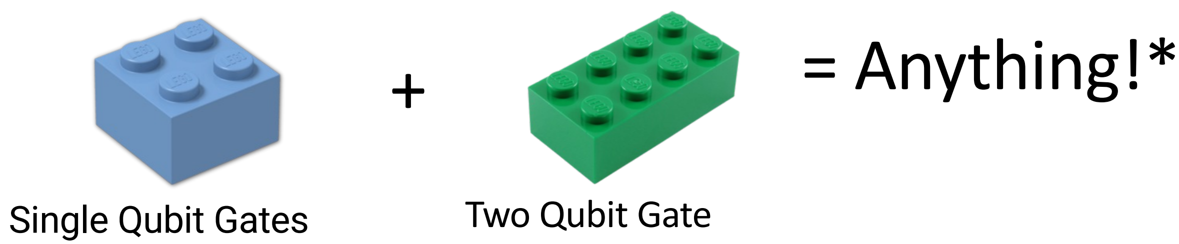
$$\hat{H} = 2SJ\sum_k (1-\cos(k))\hat{c}_k^\dagger \hat{c}_k$$



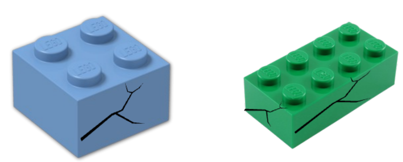
Data from *ibmq_tokyo*

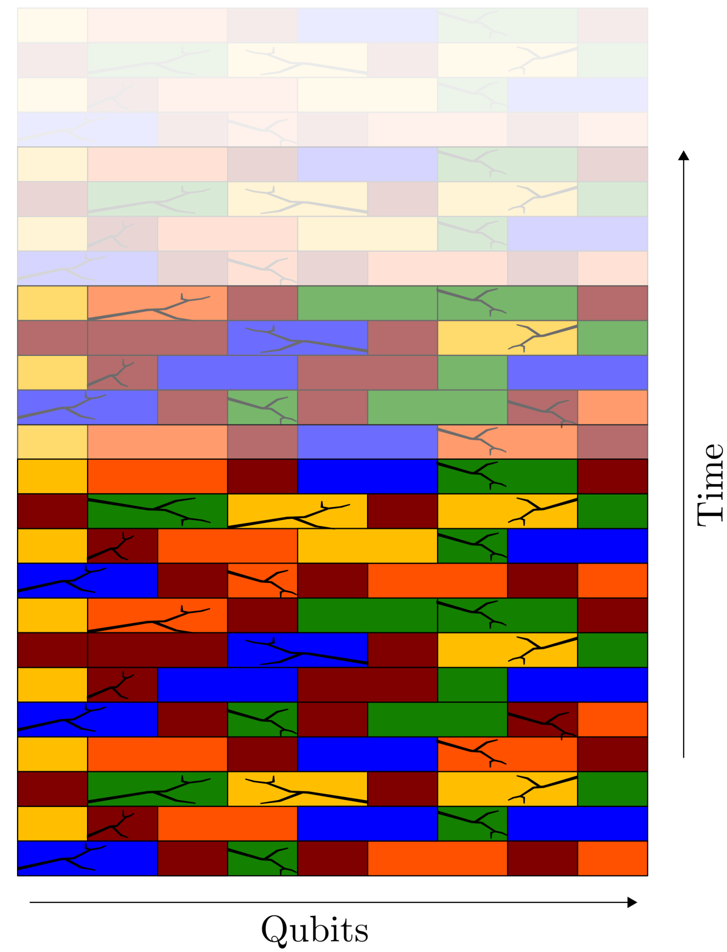
Quantum Compiling





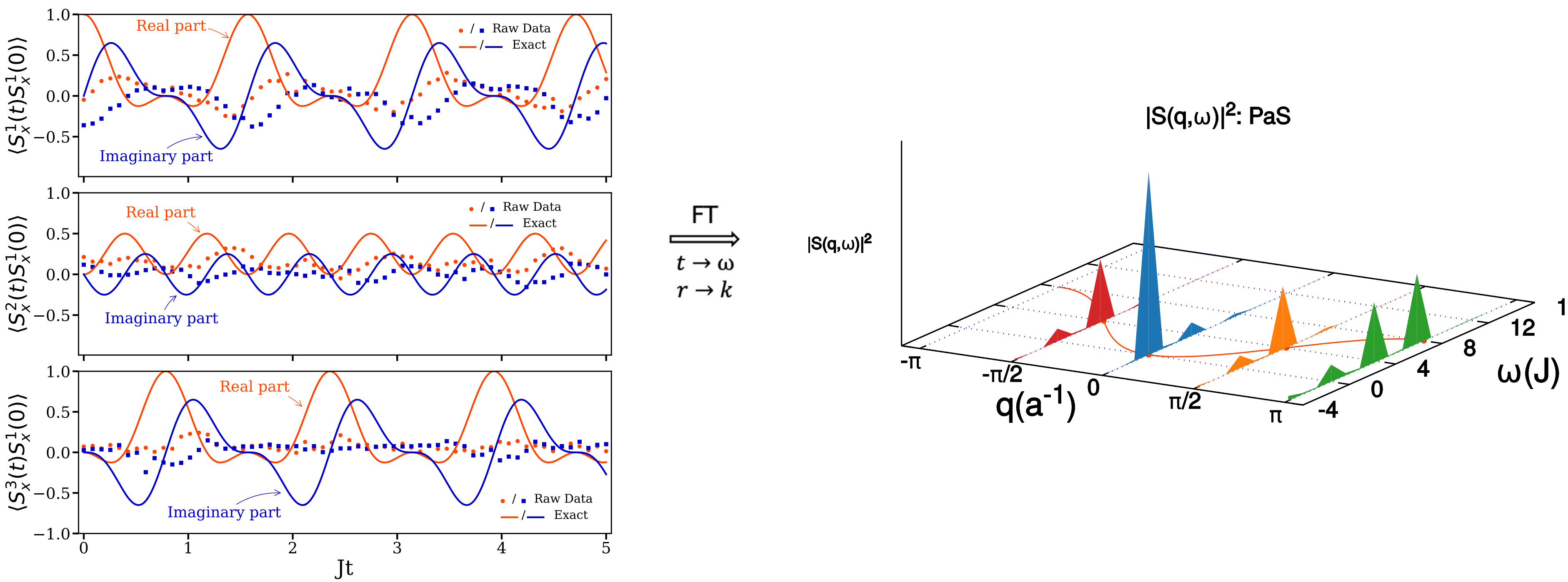
*Actual Gates





Low-energy excitations: 4-site magnons

Spin-spin correlation function for periodic Heisenberg model: Magnons!

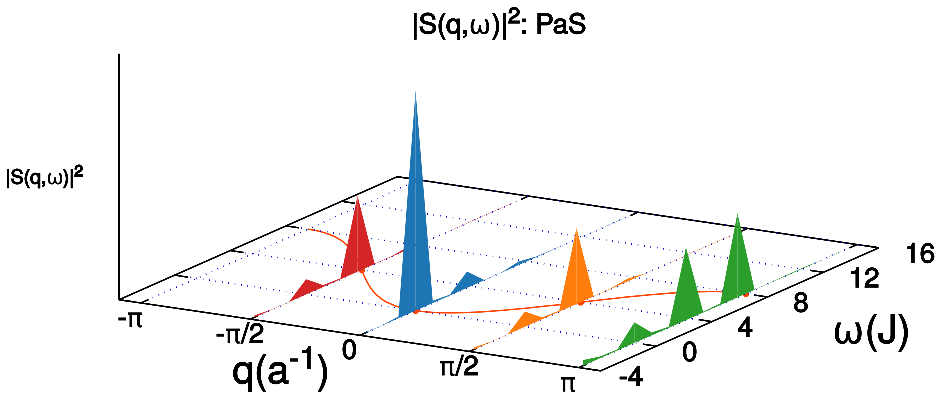


10.1103/PhysRevB.101.014411

NC STATE UNIVERSITY

Low-energy excitations: 4-site magnons

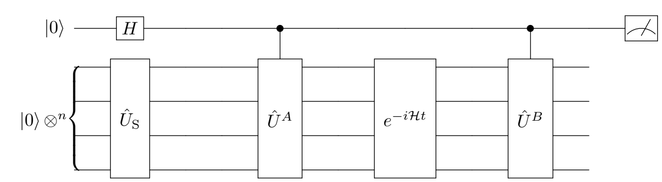
Spin-spin correlation function for periodic Heisenberg model: Magnons!



This works!

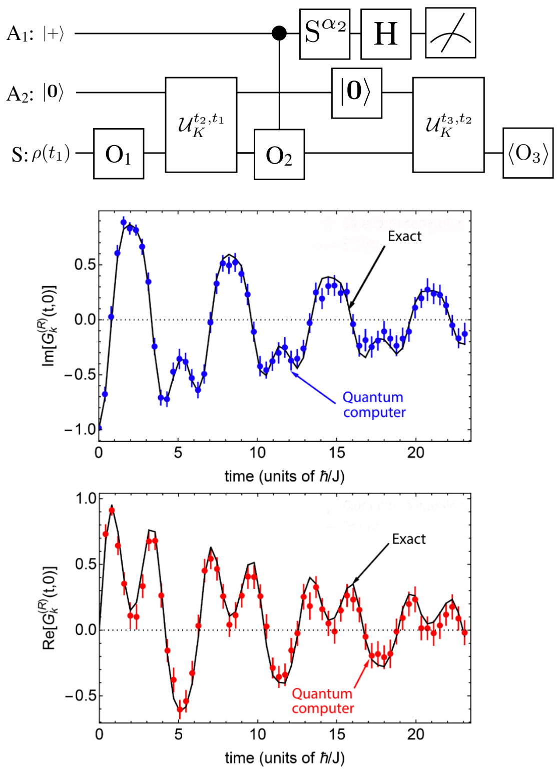
But:

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



[10.1103/PhysRevB.101.014411](https://doi.org/10.1103/PhysRevB.101.014411)

(A few) Quantum Algorithm(s) for χ



(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)

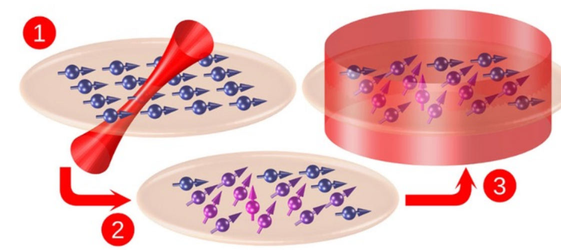


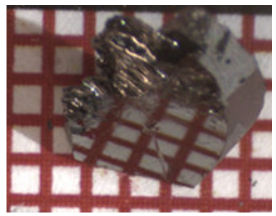
FIG. 1 (color online). Many-body Ramsey interferometry consists of the following steps: (1) A spin system prepared in its ground state is locally excited by $\pi/2$ rotation; (2) the system evolves in time; (3) a global $\pi/2$ rotation is applied, followed by the measurement of the spin state. This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

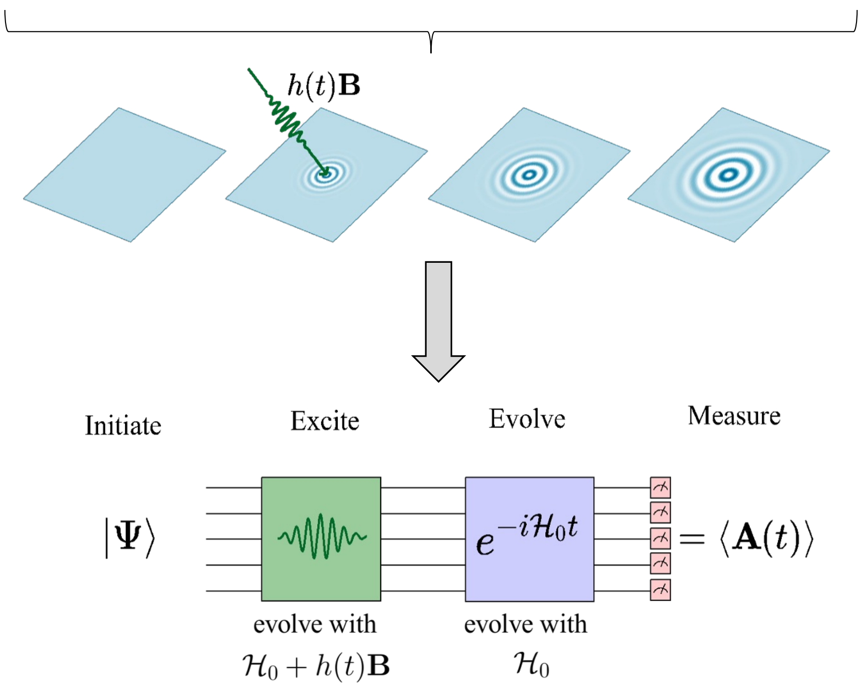
Commutators

10.1103/PhysRevLett.111.147205

Linear Response

2302.10219





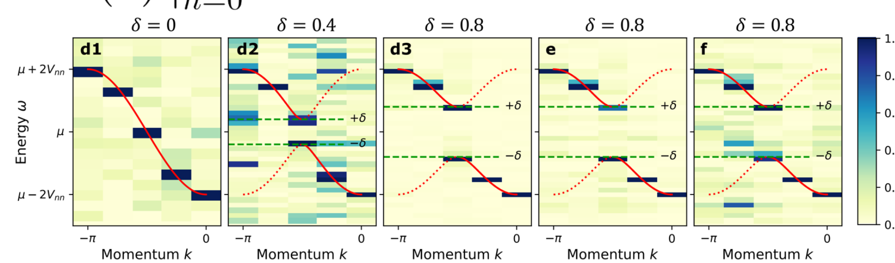
A linear response framework for simulating bosonic and fermionic correlation functions illustrated on quantum computers

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

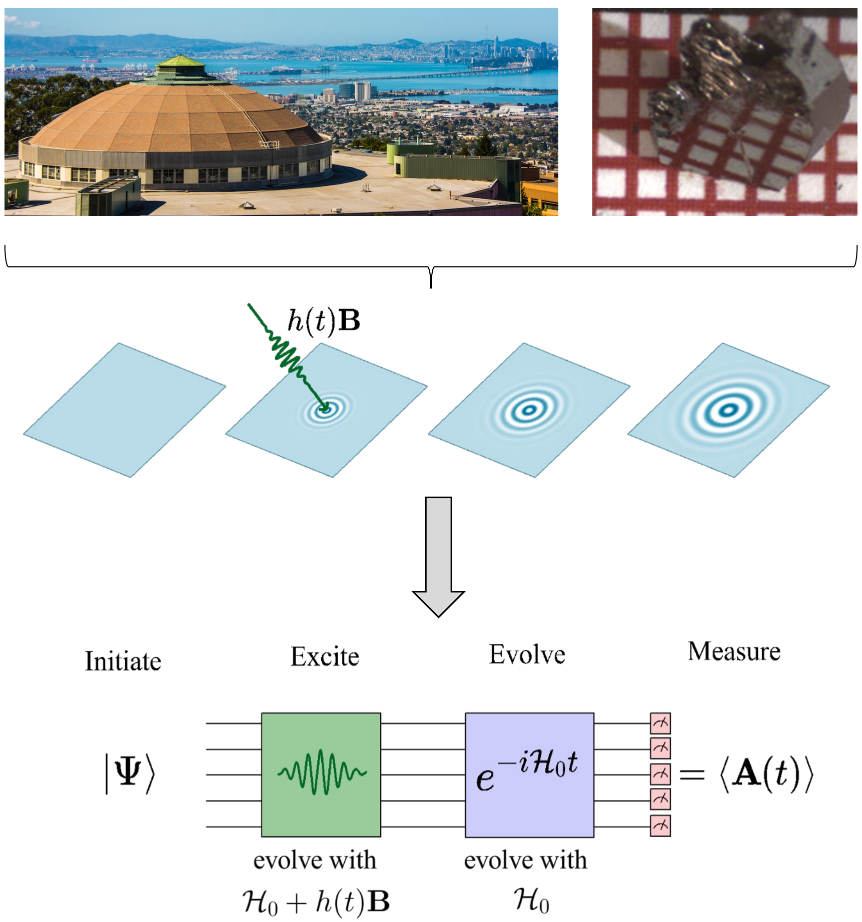
$$\left.\frac{\delta A(t)}{\delta h(t')}\right|_{h=0} = -i\theta(t-t')\langle\psi_0|[\mathbf{A}(t),\mathbf{B}(t')]|\psi_0\rangle$$



NC STATE UNIVERSITY

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,*]

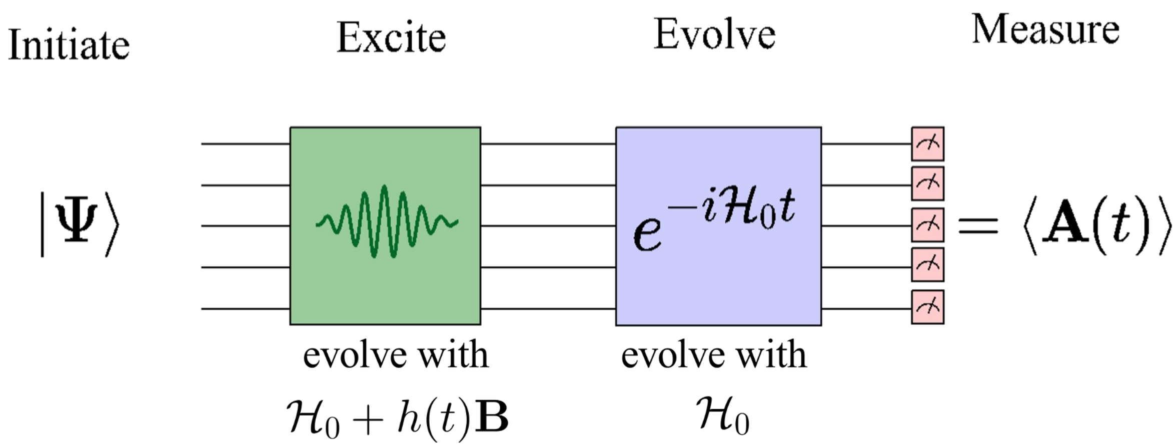
[1] *Department of Physics, North Carolina State University, Raleigh, North Carolina 27695, USA*
[2] *Department of Physics, Georgetown University, 37th and O Sts. NW, Washington, DC 20057 USA*

(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

Even More Mathematics…



Even More Mathematics…

$$
\begin{aligned}
\langle \mathbf{A}(t) \rangle &= \langle \psi_0 | U(t)^\dagger \mathbf{A} U(t) | \psi_0 \rangle \\
&= \langle \psi_0 | \mathcal{T} e^{i \int_{-\infty}^{t} [\mathbf{H}_0 + \mathbf{B} h(\bar{t})] d\bar{t}} \mathbf{A} \mathcal{T} e^{-i \int_{-\infty}^{t} [\mathbf{H}_0 + \mathbf{B} h(\bar{t})] d\bar{t}} | \psi_0 \rangle
\end{aligned}
$$

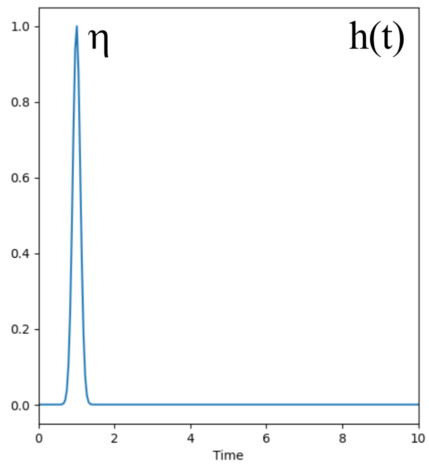
$$\Downarrow$$

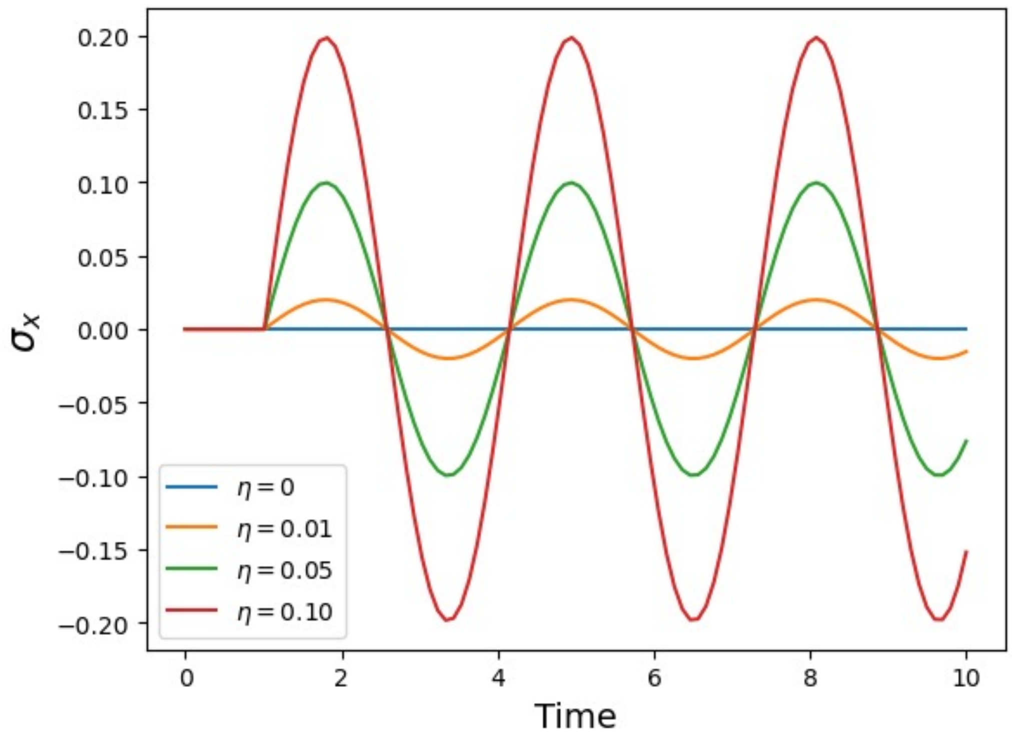
Linear Response

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

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

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



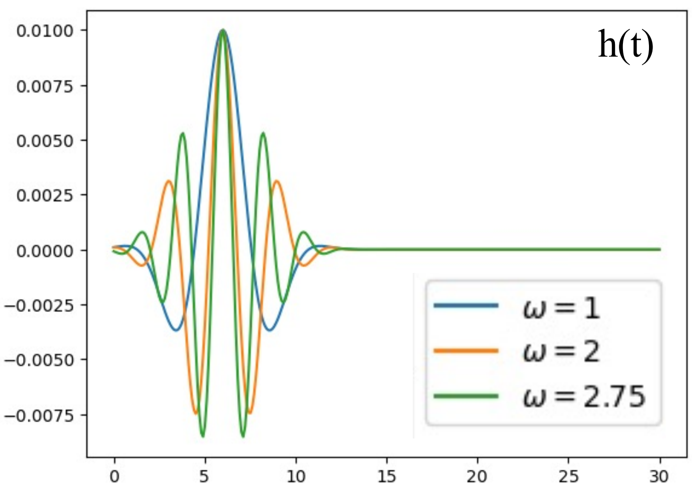


Linear Response

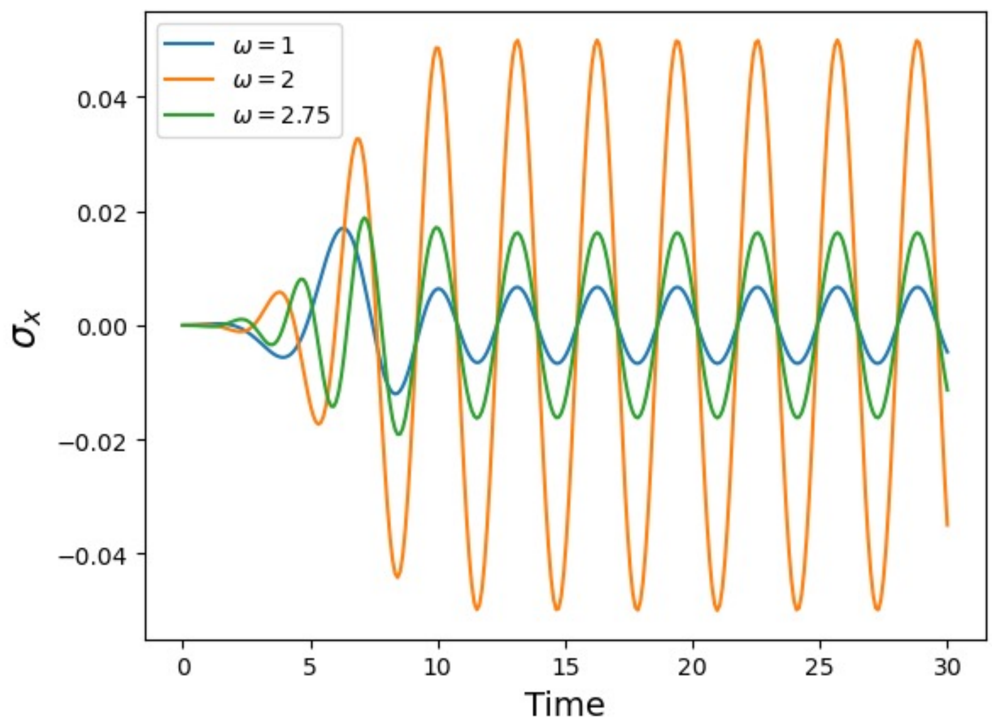
A simple example: single spin with energy level difference = 2

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

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



Frequency

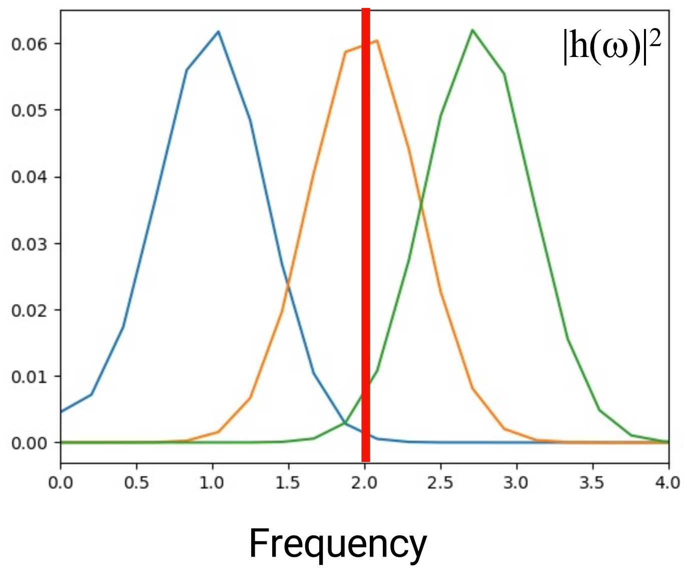


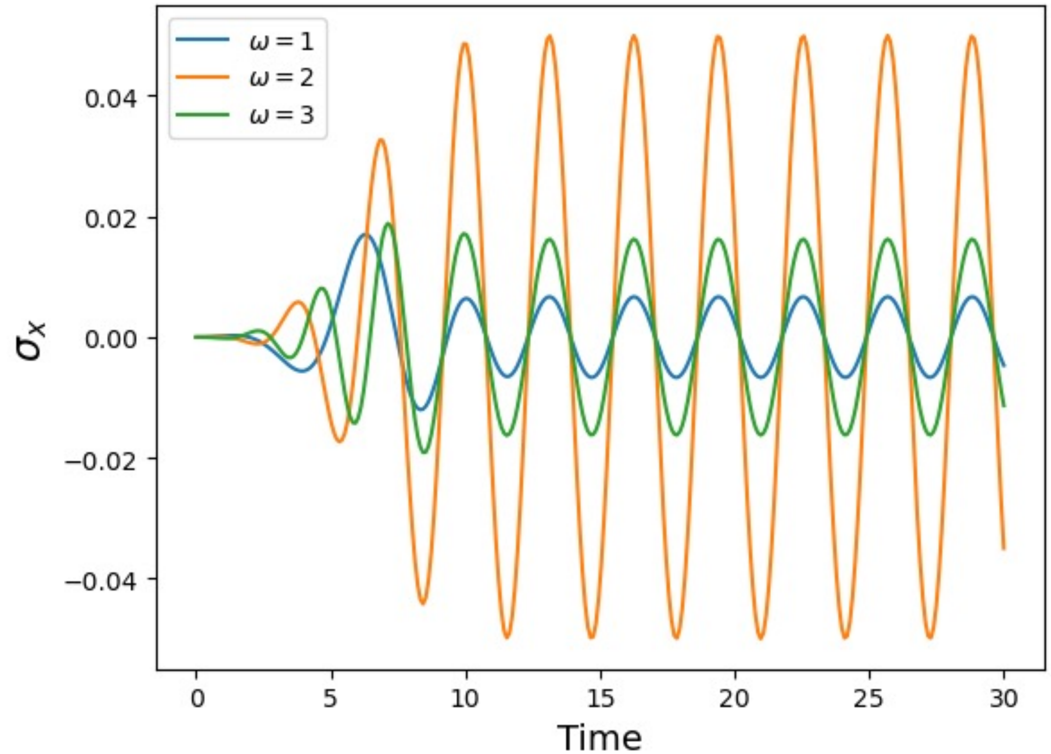
Linear Response

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

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

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





NC STATE UNIVERSITY

Bosonic (commutator) response functions:

- We calculate the functional derivative in the following way. For small values of $h(t)$:

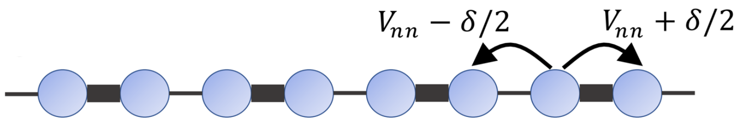
$$A(t) = \int dt' \chi^R(t-t')h(t') + \mathcal{O}(h^2)$$

- Fourier transformation leads to

$$A(\omega) = \chi^R(\omega)h(\omega) + \mathcal{O}(h^2)$$

A Bosonic Correlation function: Polarizability

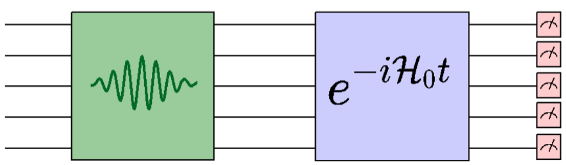
Su-Schrieffer-Heeger model for polyacetylene



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

Initiate | Excite | Evolve | Measure

$|\Psi\rangle$



$= \langle \mathbf{A}(t) \rangle$

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

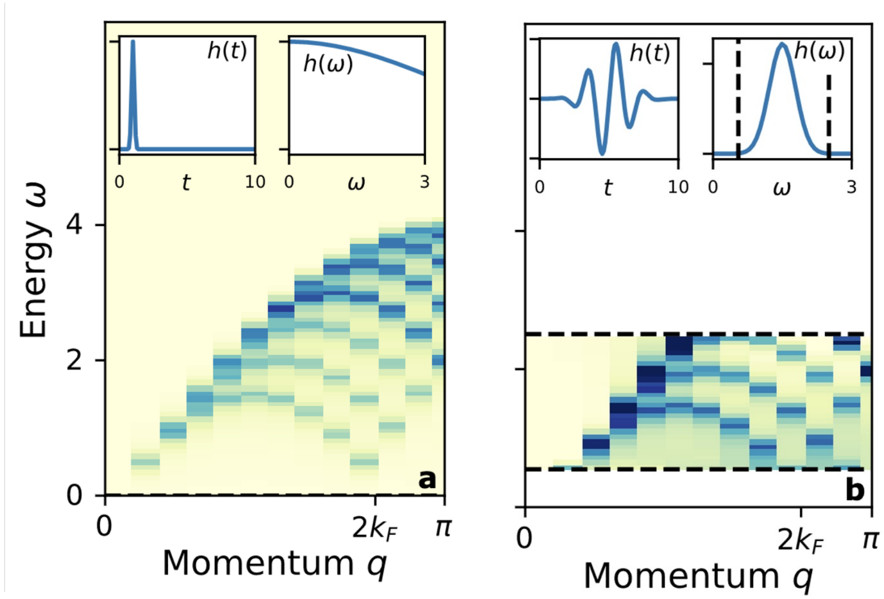
evolve with $\mathcal{H}_0$

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

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

Measure density on all sites

Wiggle potential on site 0



Fermionic Linear Response

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

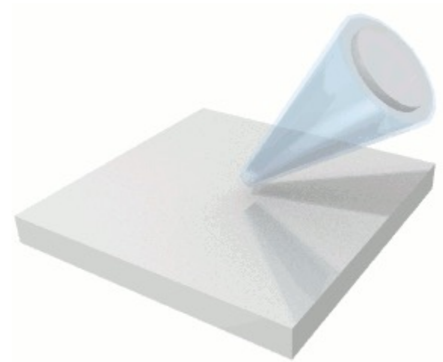
Notice this is a commutator…
… we might also want to have an anti-commutator

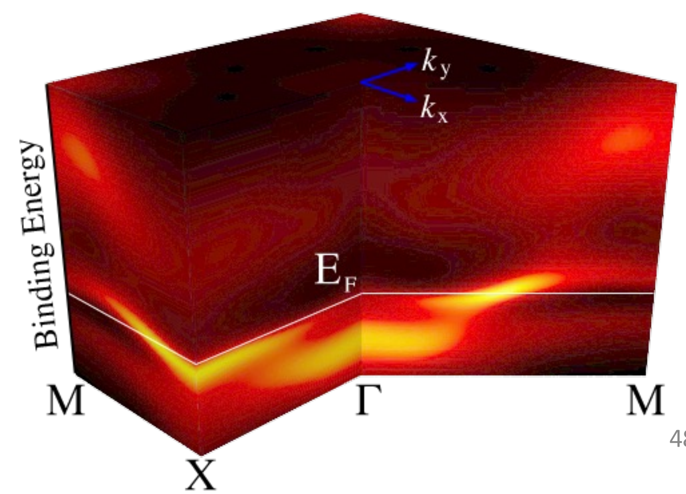
$$G(t,t') = -i\theta(t-t')\langle\psi_0|\{\mathbf{A}(t),\mathbf{B}(t')\}|\psi_0\rangle$$

Why?

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

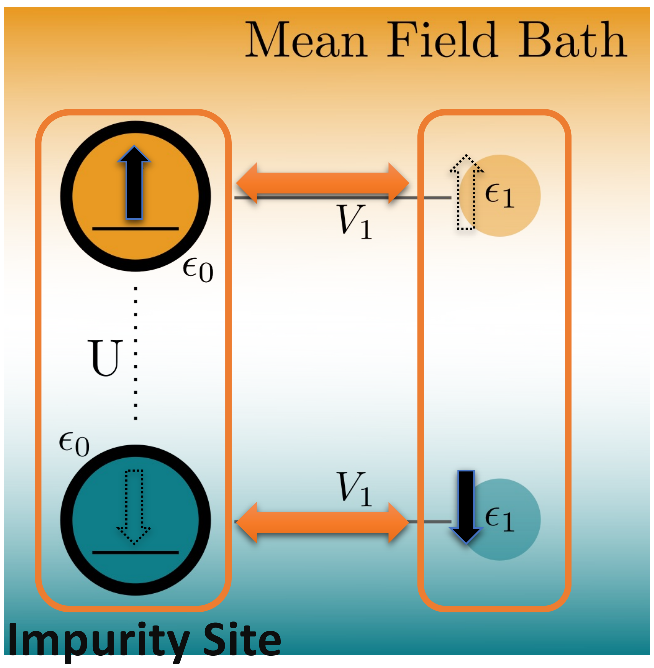
Fermionic creation/
annihilation operators



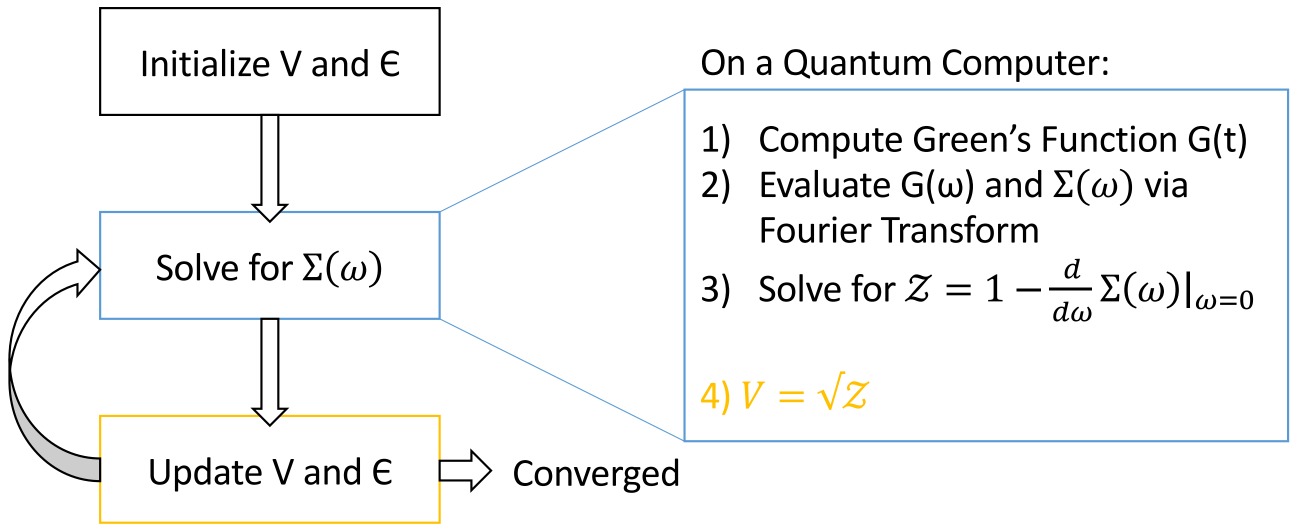


Application of Green's functions: DMFT

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



Simplified DMFT Loop

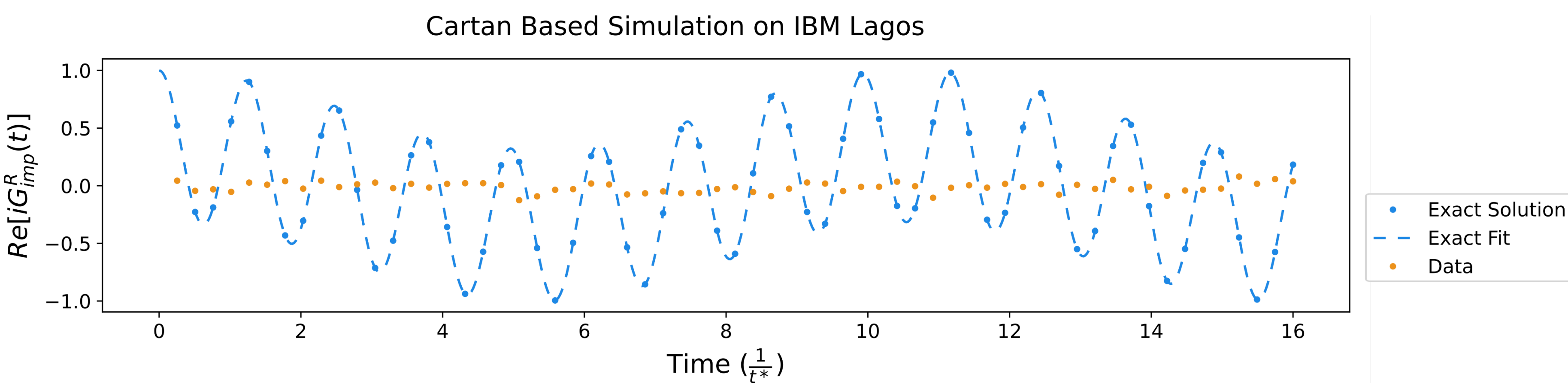


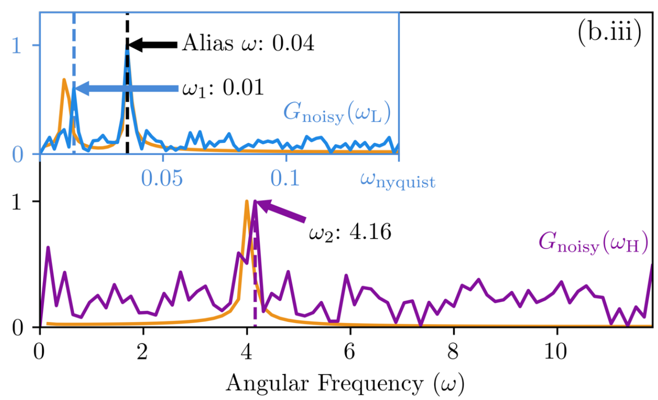
NC STATE UNIVERSITY

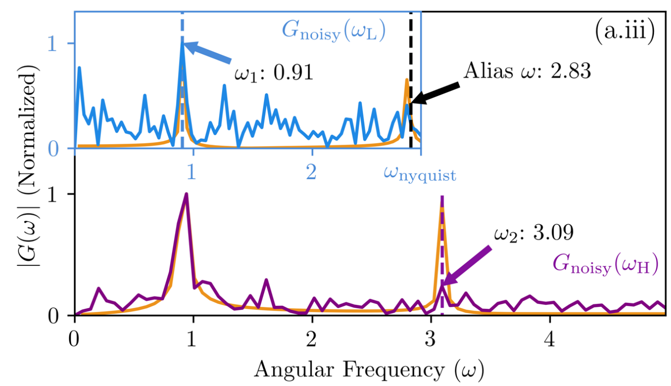
Application of Green's functions: DMFT

T. Steckmann et al., arXiv:2112.05688

2-site Hubbard DMFT (5 qubits)



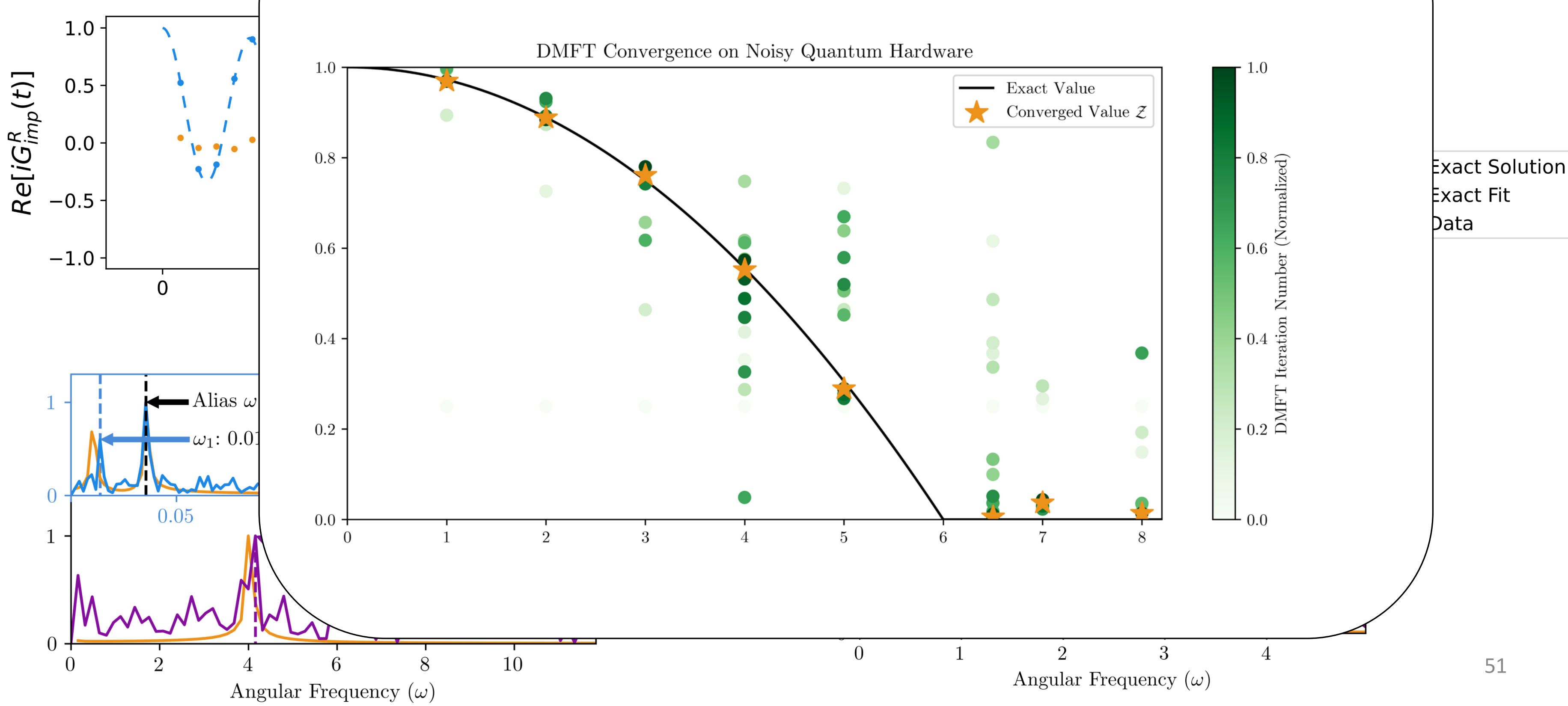




2-site Hubbard DMFT

T. Steckmann et al., arXiv:2112.05688

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



Even More Mathematics… Are we done yet?

Option 1: Auxiliary operator method:

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

Even More Mathematics… Are we done yet?

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

- The method relies on the following identity:

$$[\mathbf{A}(t)\mathbf{P},\mathbf{B}(t')] = \mathbf{A}(t)\{\mathbf{P},\mathbf{B}(t')\} - \{\mathbf{A}(t),\mathbf{B}(t')\}\mathbf{P}$$

- If $\mathbf{P}$ satisfies $\{\mathbf{B}(t),\mathbf{P}\}=0, \quad \mathbf{P}|\psi_0\rangle = s|\psi_0\rangle$ with $s \neq 0$

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

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

Even More Mathematics… Are we done yet?

- Finally, if $\mathbf{P}$ satisfies $[\mathcal{H}_0, \mathbf{P}] = 0$, we have $\mathbf{P} = \mathbf{P}(t)$, which leads to

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

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

- This allows us to measure anti-commutators via the previous method

Example: retarded Green's function

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

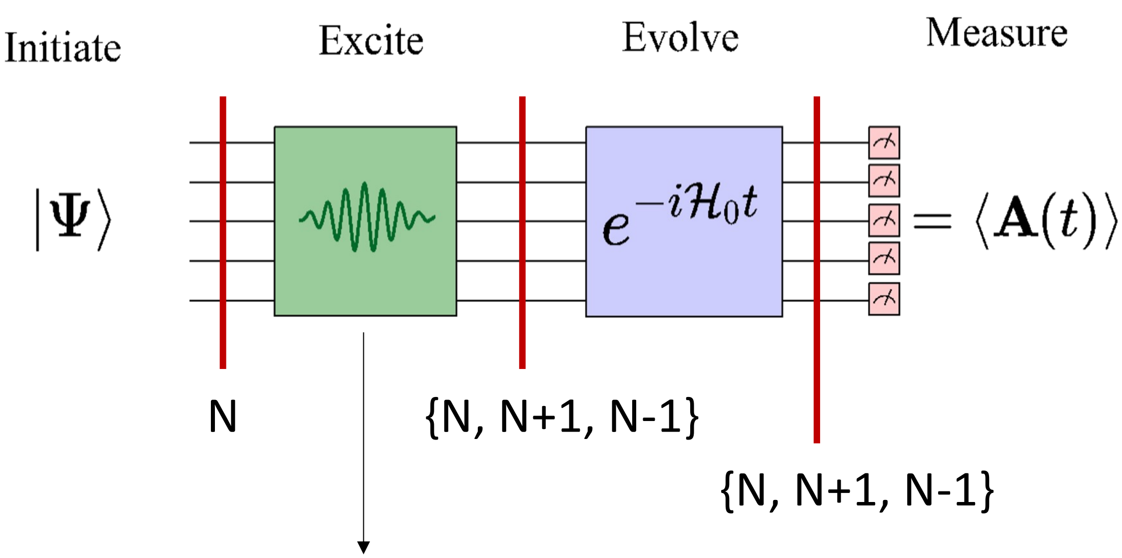
- The operator $\mathbf{P} = Z_1 Z_2 ... Z_n$ satisfies $\{\mathbf{B}(t), \mathbf{P}\} = 0$
- For systems that preserves particle number parity: $[\mathcal{H}_0, \mathbf{P}] = 0$
- If state $|\psi_0\rangle$ has definite parity (even or odd particle number), then

  $\mathbf{P}|\psi_0\rangle = s|\psi_0\rangle$ with s = +1 or -1
- This works both for particle conserving and superconducting systems

Option 2: Post selection method:

Option 2: Post selection method:

- Assume that the Hamiltonian is particle conserving, and the ground state has a definite number of particles (which we denote with N).



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

Post-selection on particle number gives us

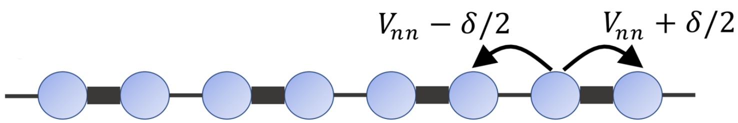
$$G^{<}_{ij}(t) = i\,\langle\psi_0|c^\dagger_j(0)c_i(t)|\psi_0\rangle$$

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

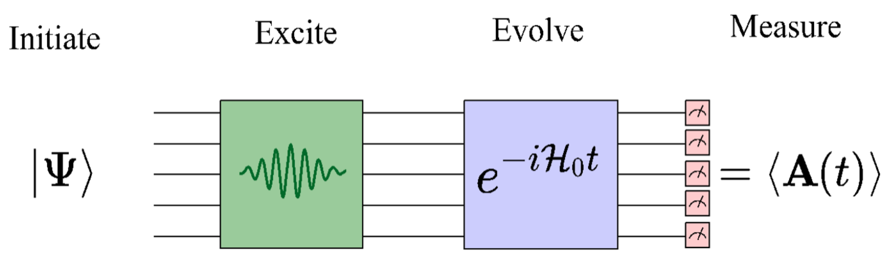
Which we can combine to the desired anti-correlation function.

Linear Response -> Green's function

Su-Schrieffer-Heeger model for polyacetylene



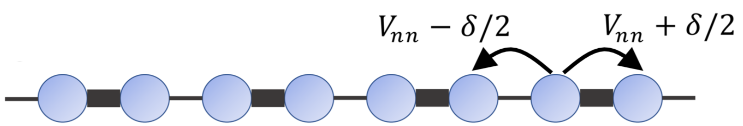
$$\mathcal{H}_0 = -\sum_{\langle i,j \rangle} \left[V_{nn} + (-1)^i \, \delta/2 \right] c_i^\dagger c_j - \mu \sum_i c_i^\dagger c_i$$



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

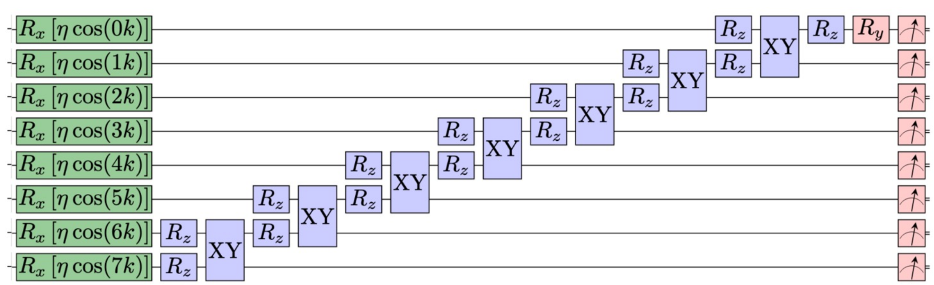
Linear Response -> Green's function

Su-Schrieffer-Heeger model for polyacetylene



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

Compressed circuit run on *ibm_auckland*



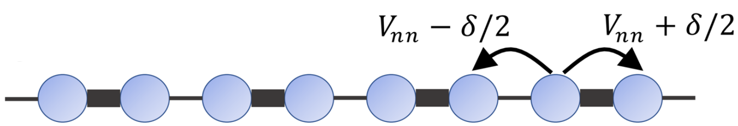
$$\mathbf{B} = \sum_i 2\cos(kr_i) \left[c_i + c_i^\dagger \right]$$

Choose **B** to create a momentum eigenstate

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

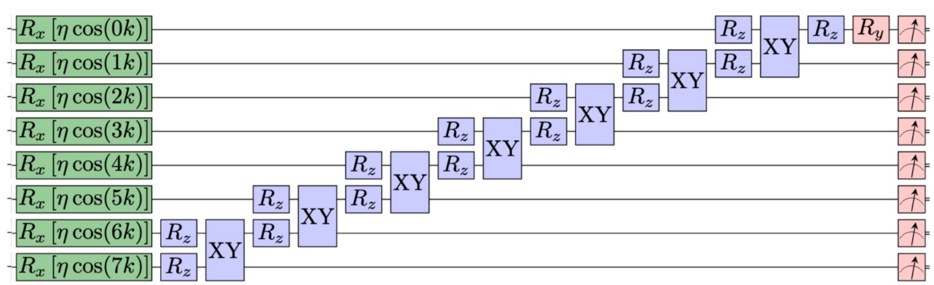
Linear Response -> Green's function

Su-Schrieffer-Heeger model for polyacetylene



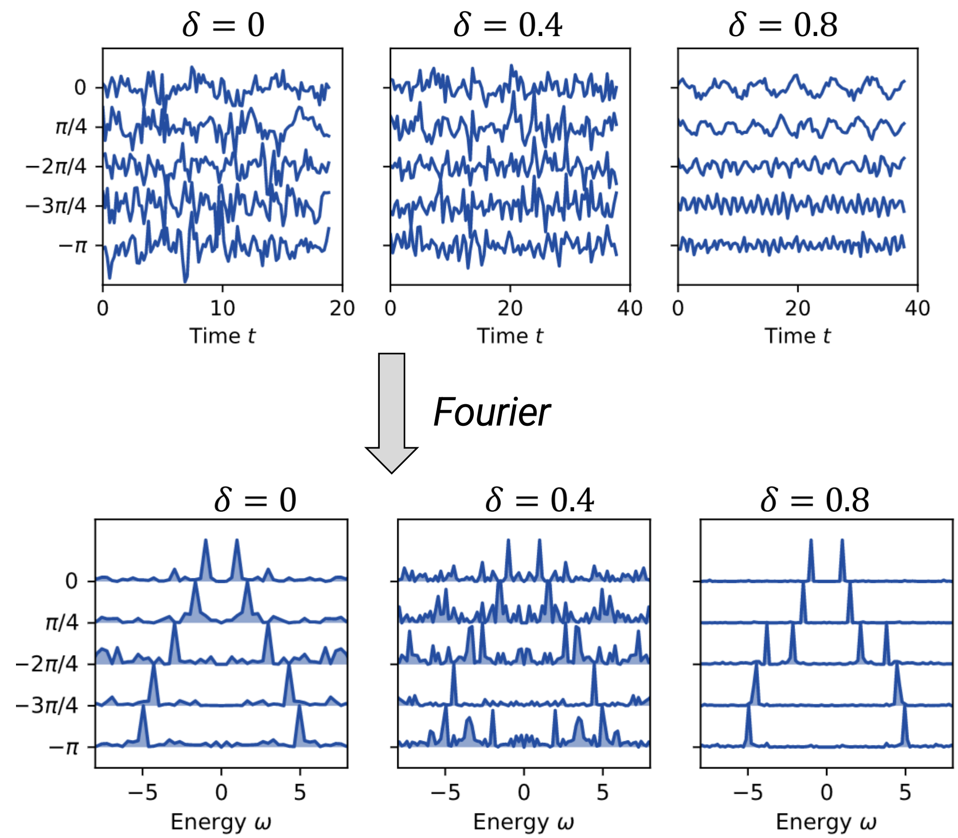
$$\mathcal{H}_0 = -\sum_{\langle i,j \rangle} \left[V_{nn} + (-1)^i \, \delta/2 \right] c_i^\dagger c_j - \mu \sum_i c_i^\dagger c_i$$

Compressed circuit run on *ibm_auckland*



Choose **B** to create a momentum eigenstate

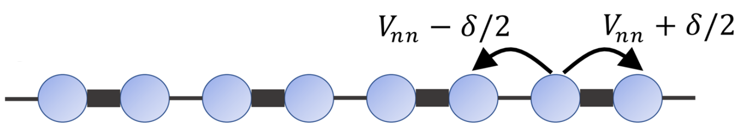
$$G_k^R(t) = -i\theta(t)\langle\psi_0|\{c_k(t), c_k^\dagger(0)\}|\psi_0\rangle$$



Linear Response -> Green's function

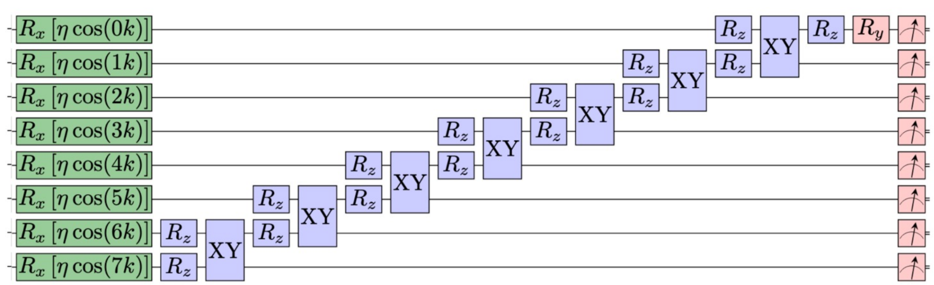
2302.10219

Su-Schrieffer-Heeger model for polyacetylene



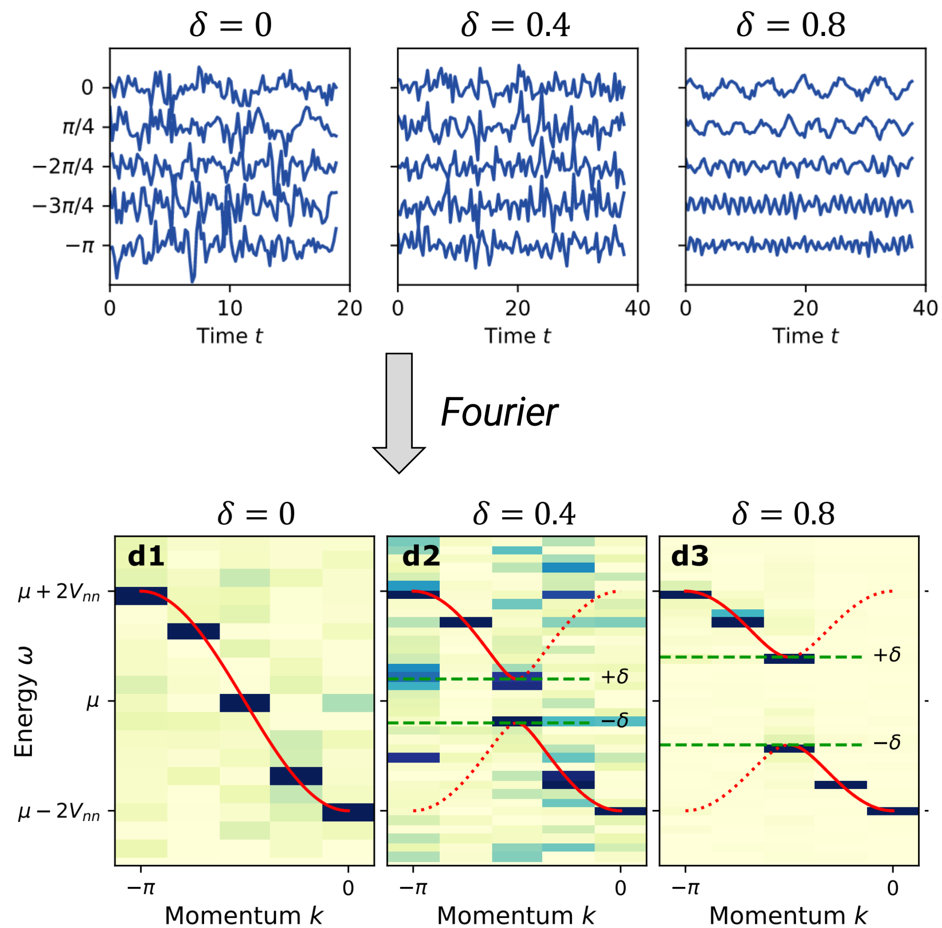
$$\mathcal{H}_0 = -\sum_{\langle i,j \rangle} \left[V_{nn} + (-1)^i \, \delta/2 \right] c_i^\dagger c_j - \mu \sum_i c_i^\dagger c_i$$

Compressed circuit run on *ibm_auckland*

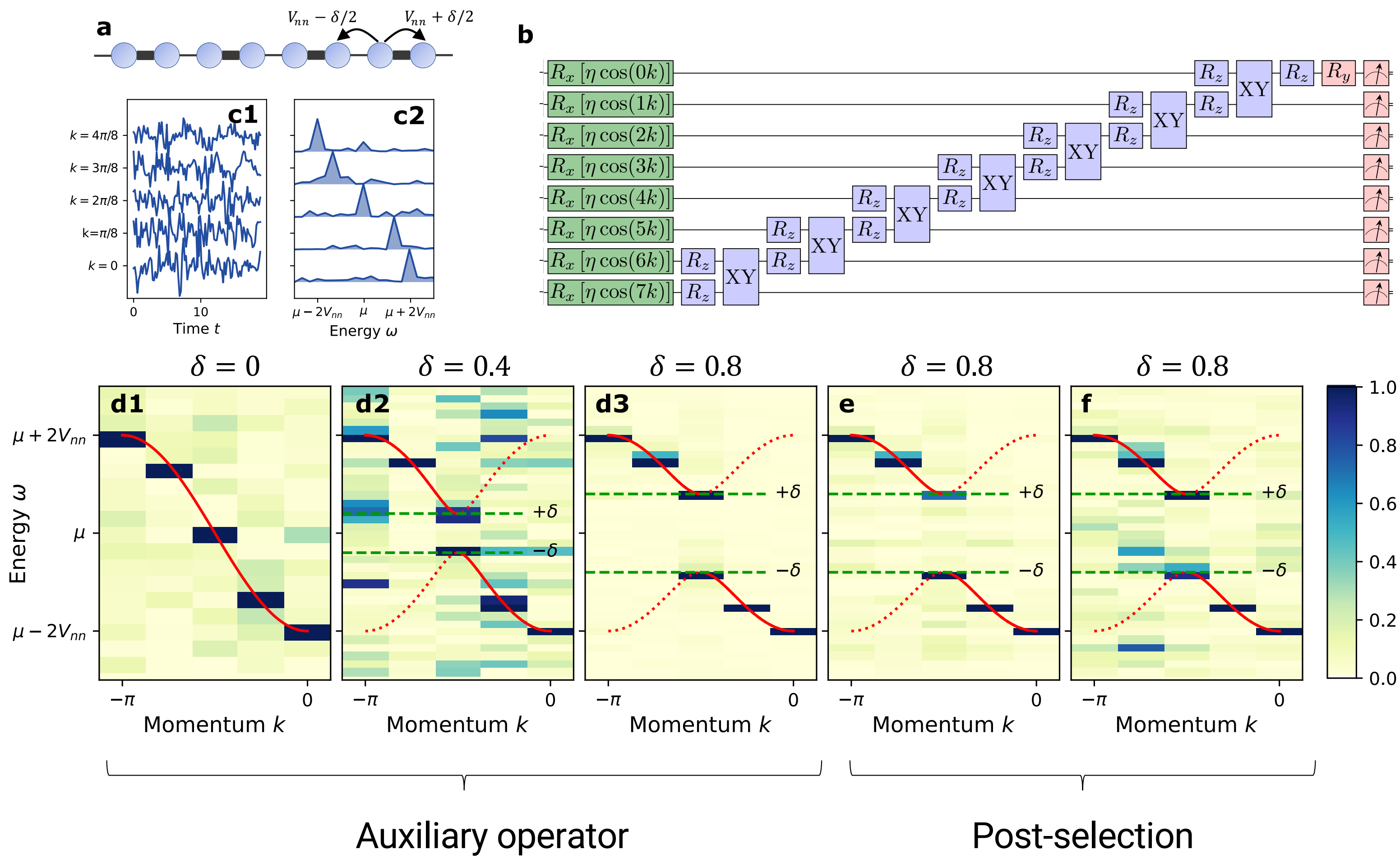


Choose **B** to create a momentum eigenstate

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



Linear Response -> Green's function

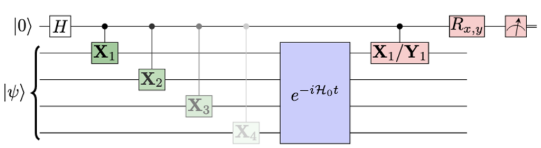


Linear Response -> Green's function

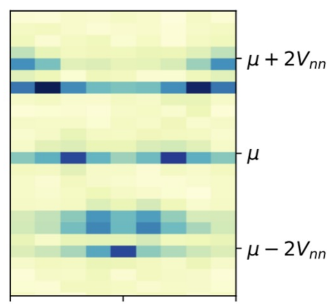
Why does this work so well?

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

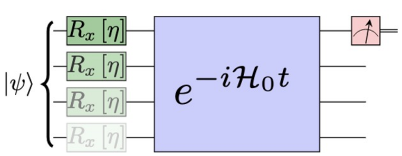
Hadamard test method



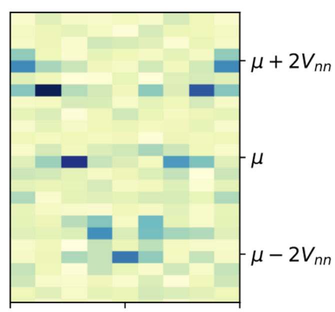
FT
$t \to \omega$
$r \to k$



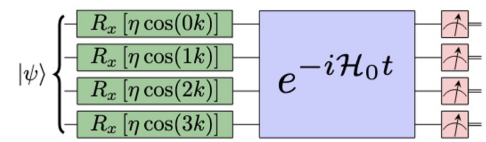
Position-selective linear response



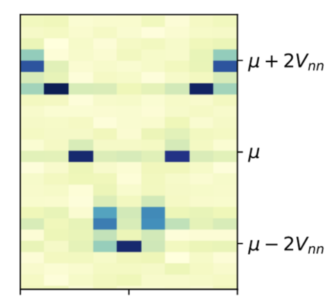
FT
$t \to \omega$
$r \to k$



Momentum-selective linear response



FT
$t \to \omega$

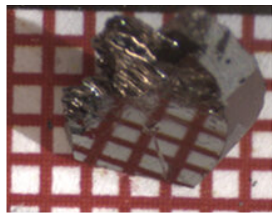


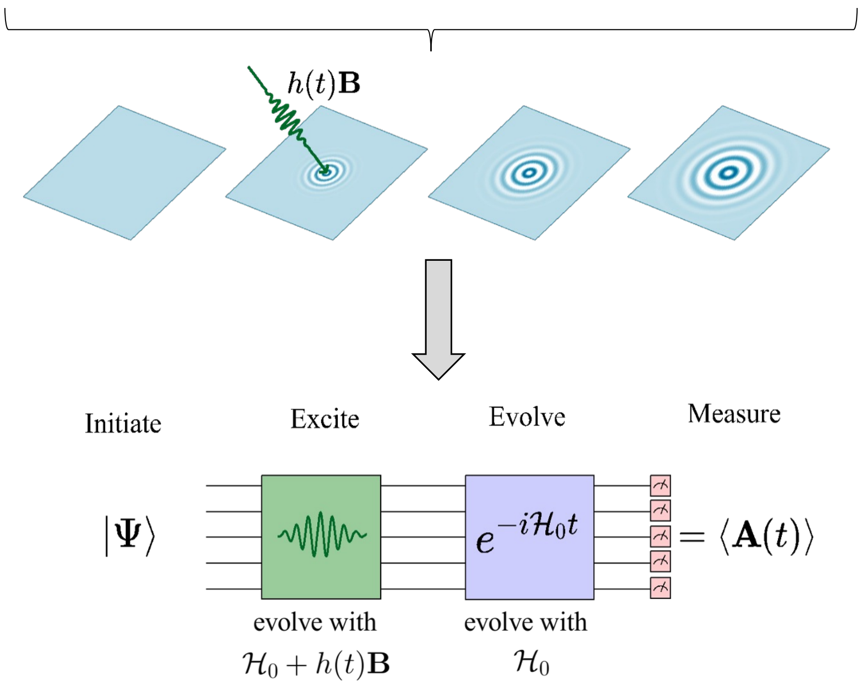
Data from noisy simulator with one/two qubit noise of 1% and 10%

NC STATE UNIVERSITY

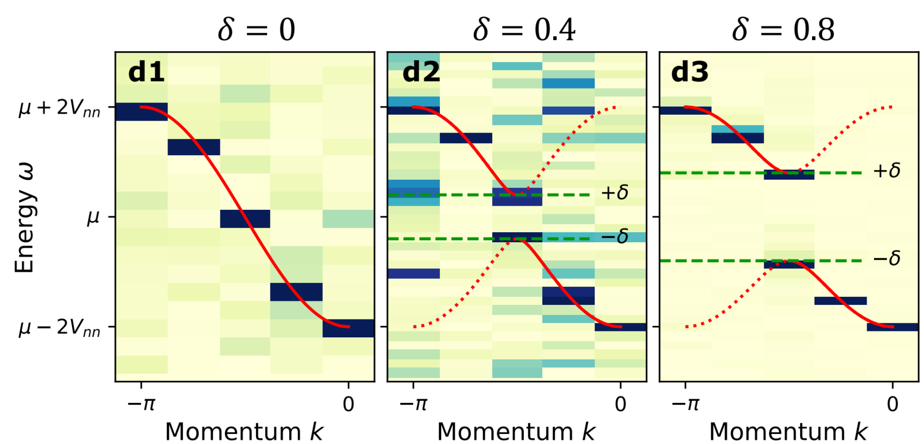
Linear Response

2302.10219





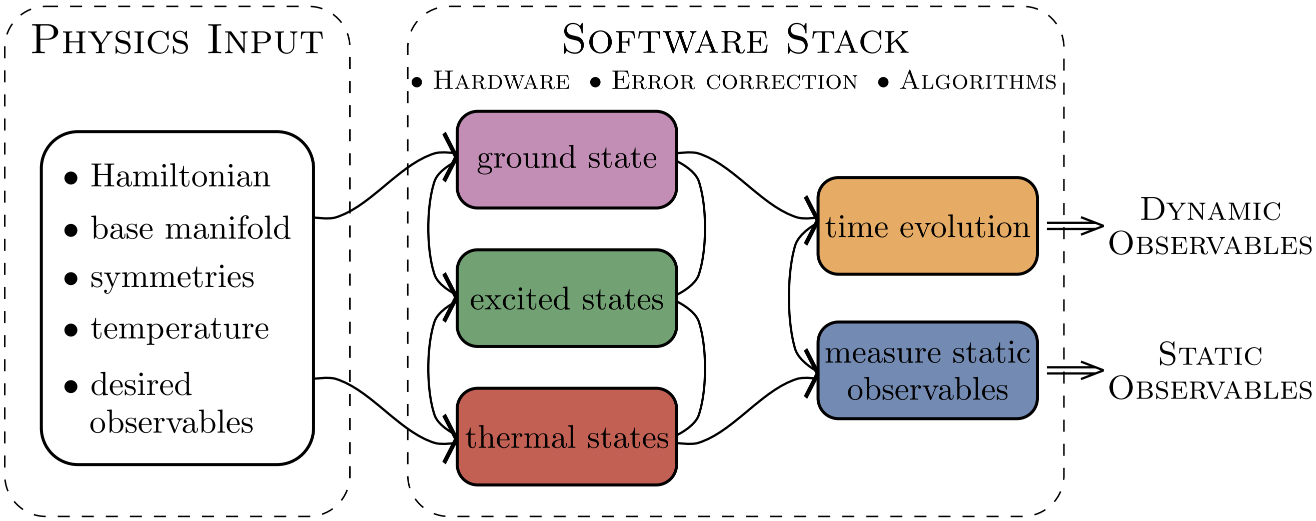
- Ancilla free
- Momentum and frequency selectivity
- Both bosonic and fermionic correlators
- More noise robust compared to existing methods



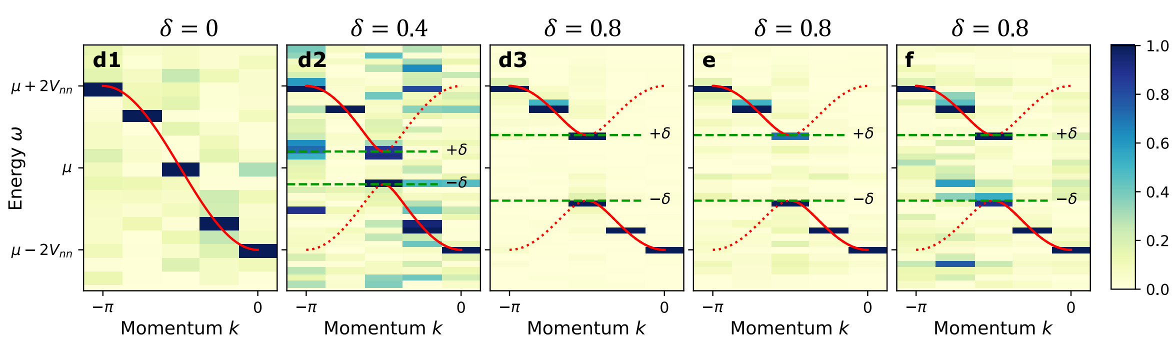
E. Kökcü, H.Labib, J.K. Freericks, AFK., arXiv:2302.10219

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