Quantum Materials Meet Quantum Computing

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

Alvarez Workshop @ LBNL
06/15/2023

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Why quantum computing for quantum materials?

Why quantum computing?

Problems with an unreasonably large solution space

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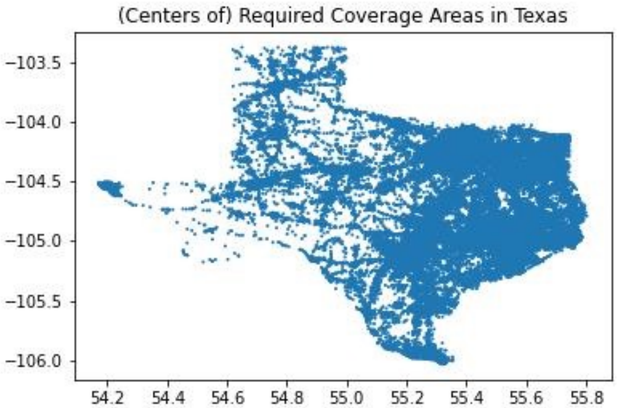

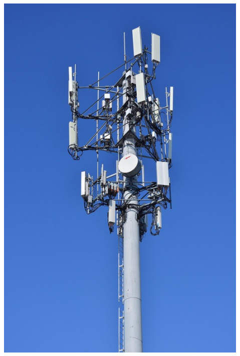

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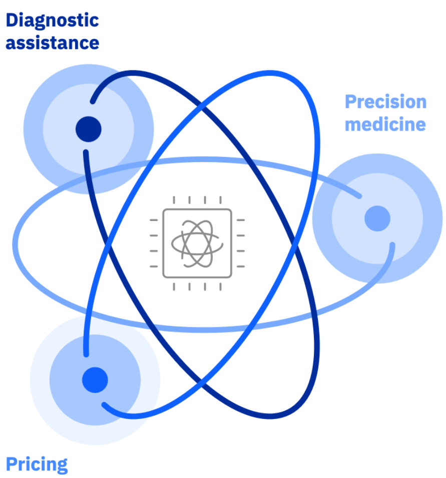
Figure 1
Quantum computers may enable three key healthcare use cases that reinforce each other in a virtuous cycle. For instance, accurate diagnoses enable precise treatments, as well as a better reflection of patient risks in pricing models.



https://www.ibm.com/downloads/cas/8QDGKDZJ

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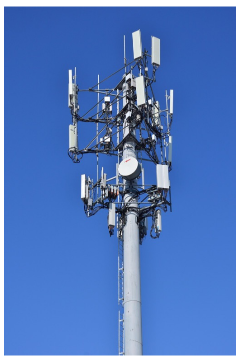

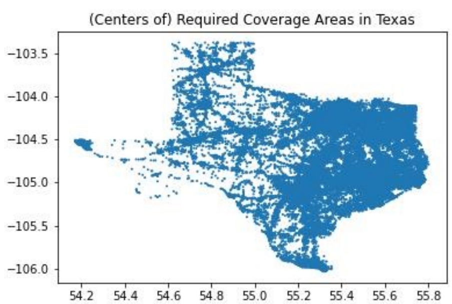

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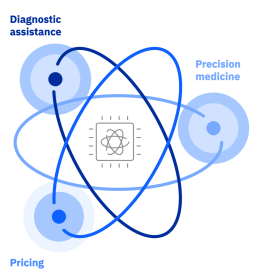

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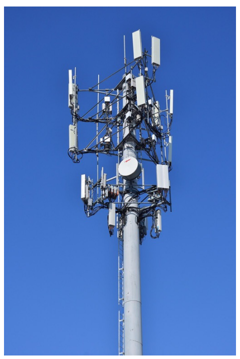

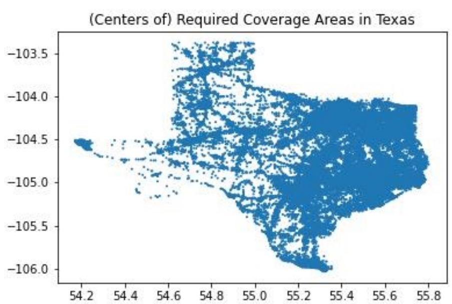

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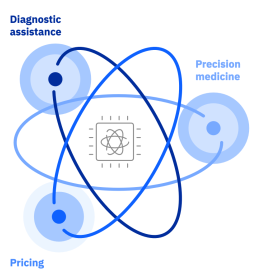
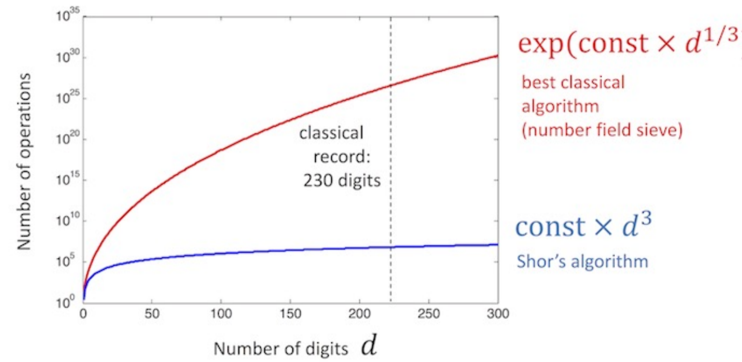
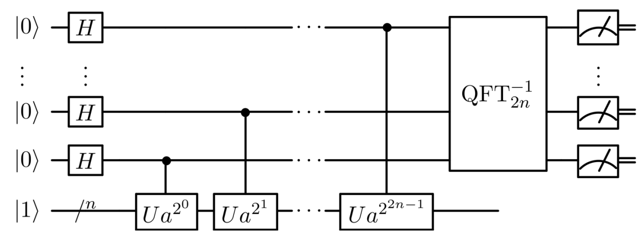


Efficient algorithms





https://quantum-computing.ibm.com/

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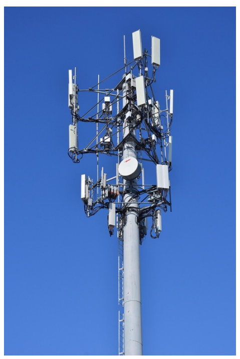

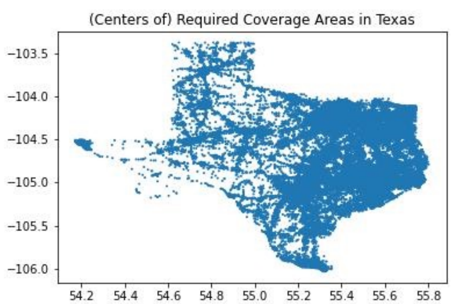

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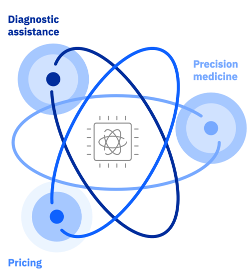
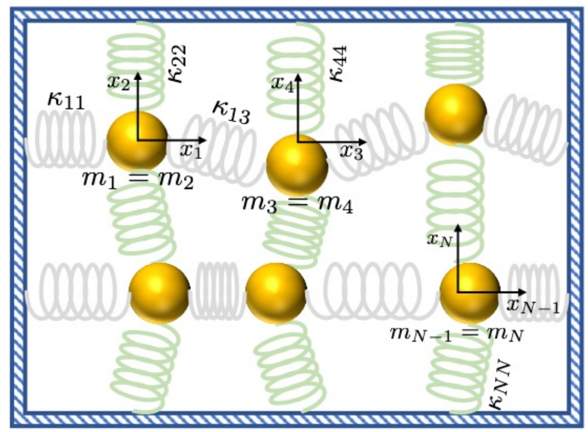


Efficient algorithms

Exponential quantum speedup in simulating coupled classical oscillators

Ryan Babbush,[1] Dominic W. Berry,[2] Robin Kothari,[1] Rolando D. Somma,[1] and Nathan Wiebe[3,4,5]



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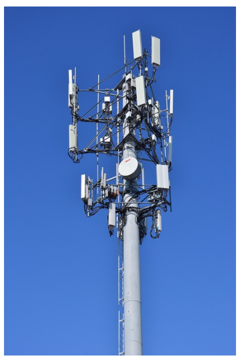
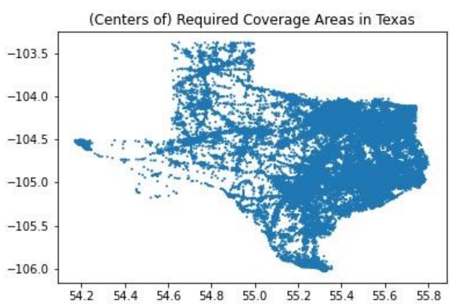
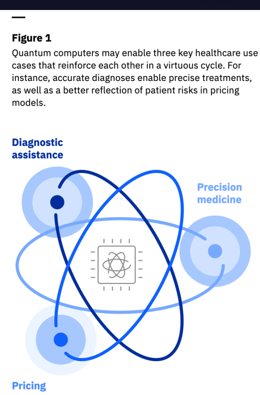
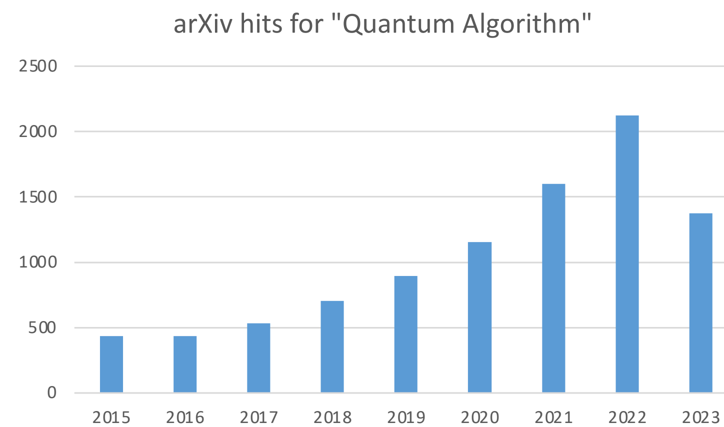


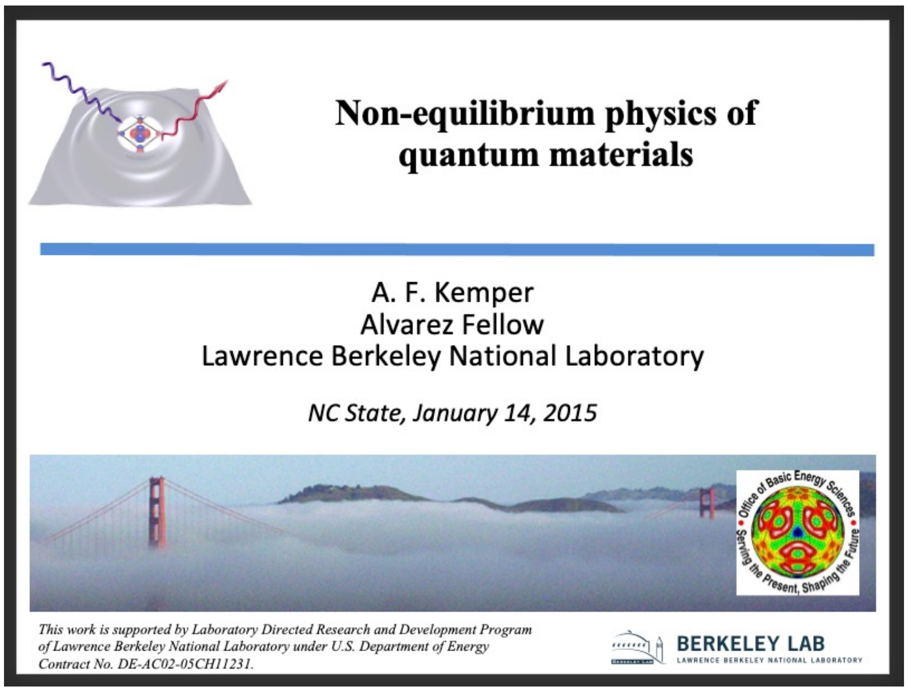


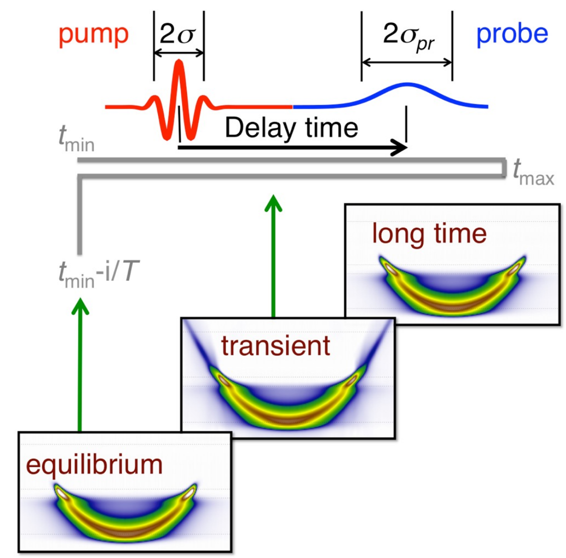


Efficient algorithms



Why quantum computing for quantum materials?





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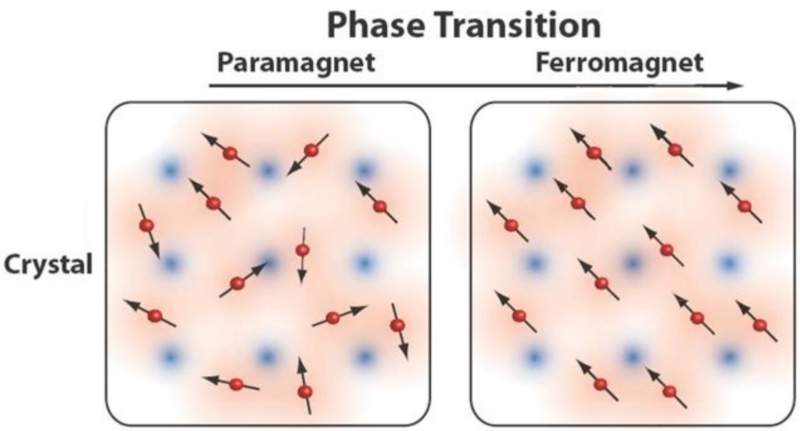

50 spins = 1,125,899,906,842,624 states

Efficient algorithms

Good scientists!

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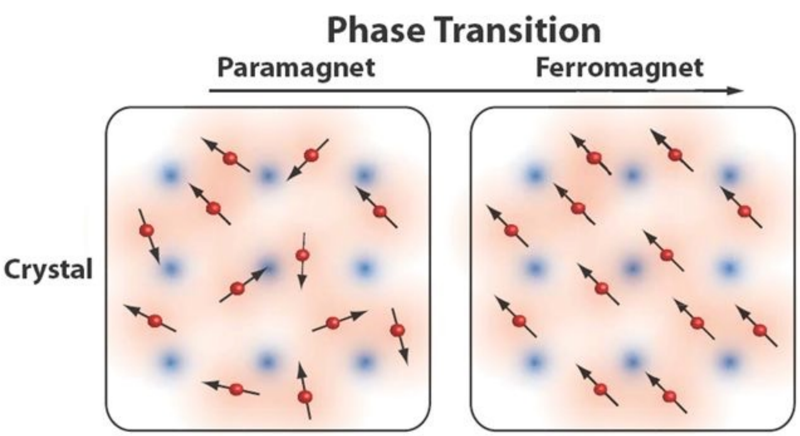

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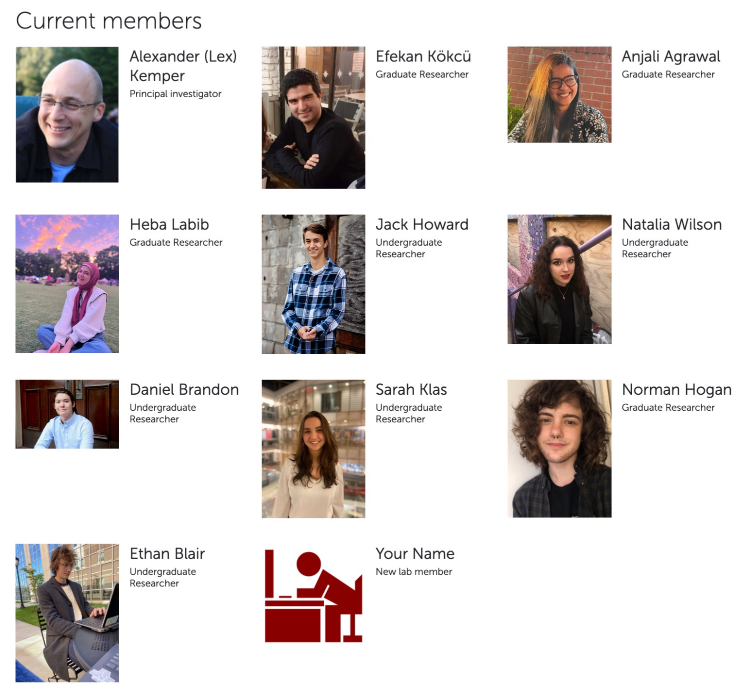
Efficient algorithms



Good scientists!

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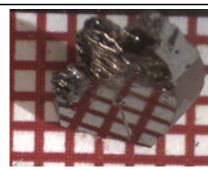
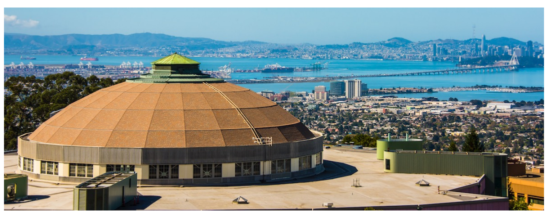
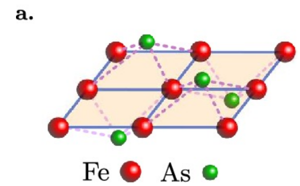
Quantum Computer = Quantum Simulator

- Theory
- Numerical Experiments
- Experiment

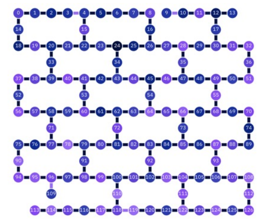


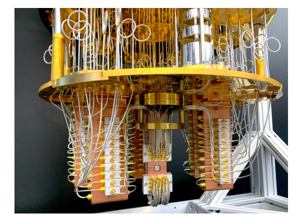


Model? →



- Theory + experiment





New/better experiments and algorithms

SCIENCE

APPLICATIONS

New/better hardware and algorithms

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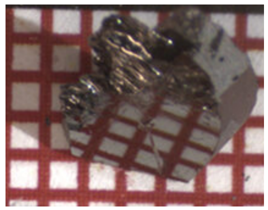
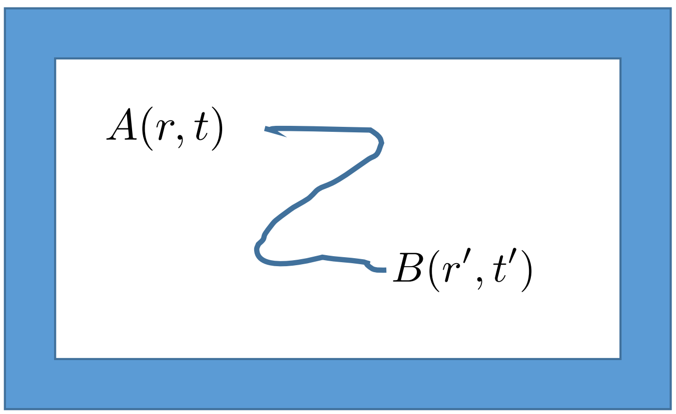
Quantum Computer = Quantum Simulator



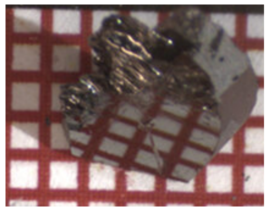


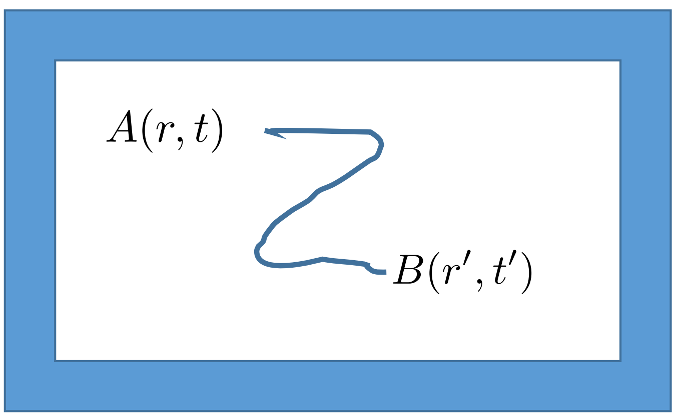
$$\langle A(r,t)B(r',t')\rangle$$

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

Optical conductivity, X-ray scattering, photoemission, etc.

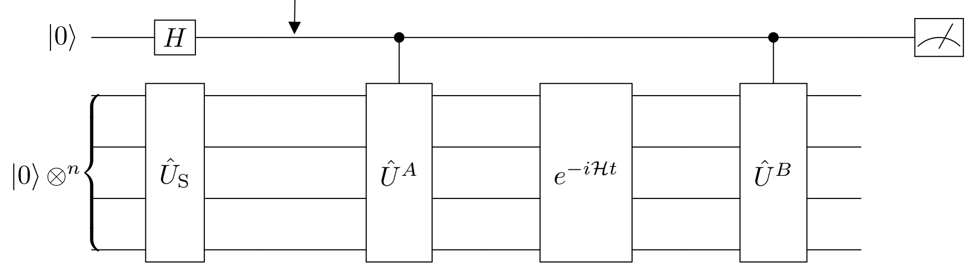
Quantum Computer = Quantum Simulator



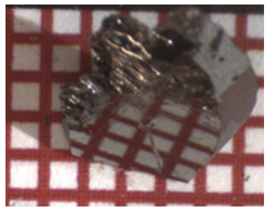


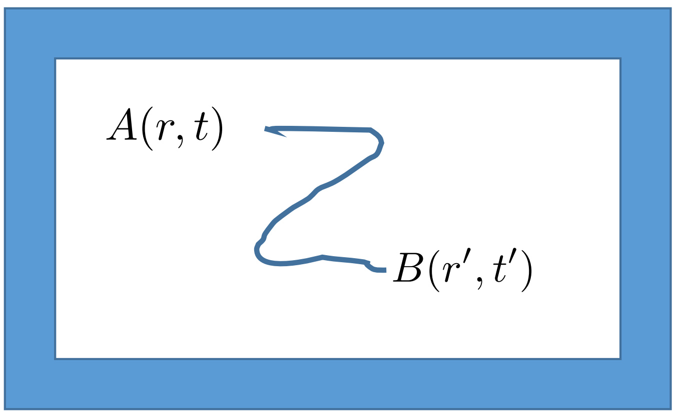
$$e^{iE_0 t}\langle\phi_0|Be^{-i\mathcal{H}t}A|\phi_0\rangle$$

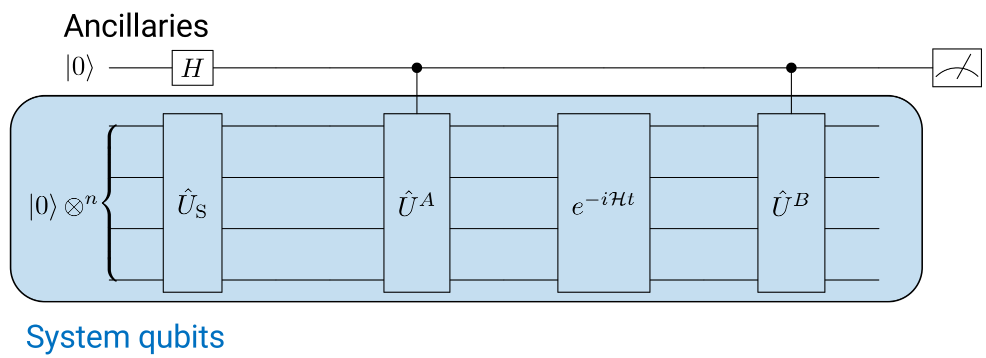
- $e^{iE_0 t}$: Interfere with ground state
- $\langle\phi_0|$: Complete expectation value
- B: Apply excitation B
- $e^{-i\mathcal{H}t}$: Time evolve
- A: Apply excitation A
- $|\phi_0\rangle$: Prepare state of interest

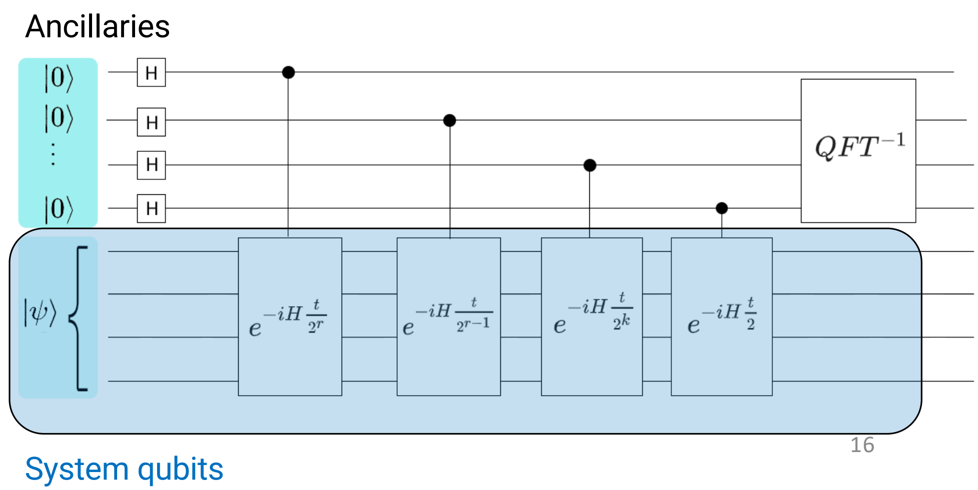


Quantum Computer = Quantum Simulator









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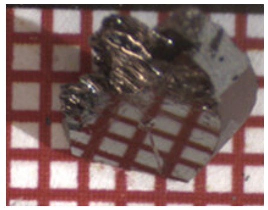
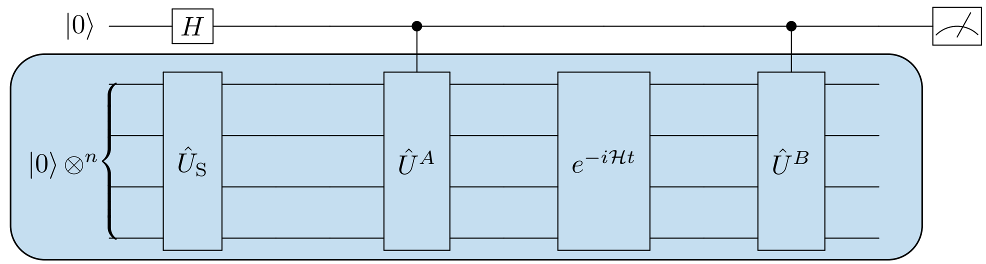
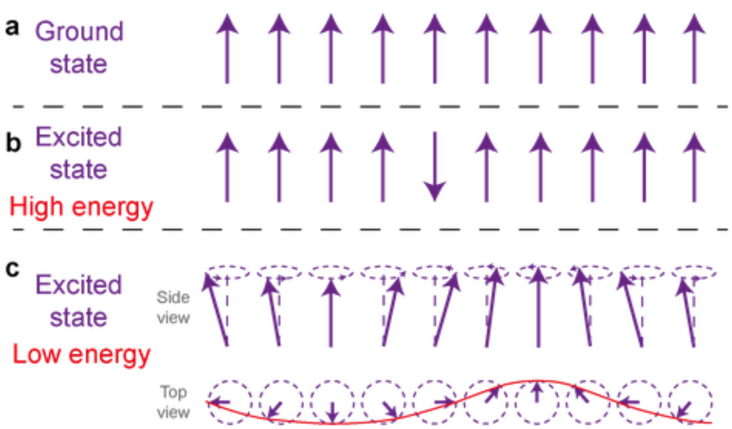


Ancillaries



System qubits



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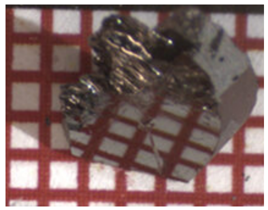
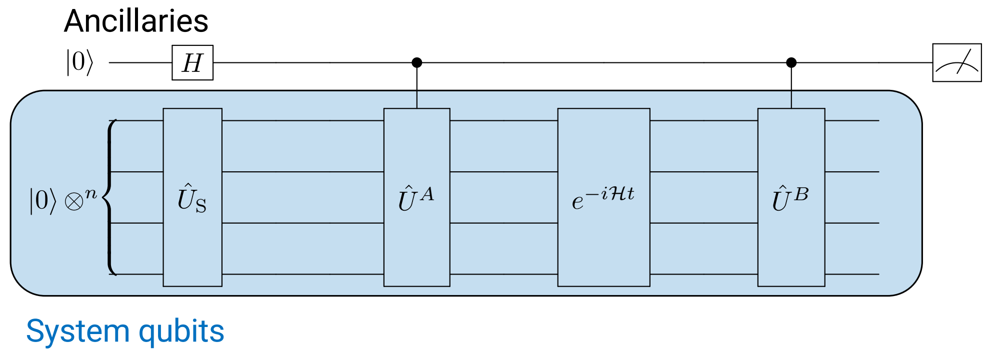
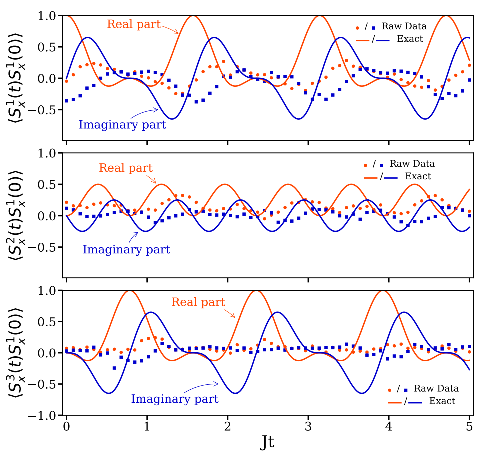
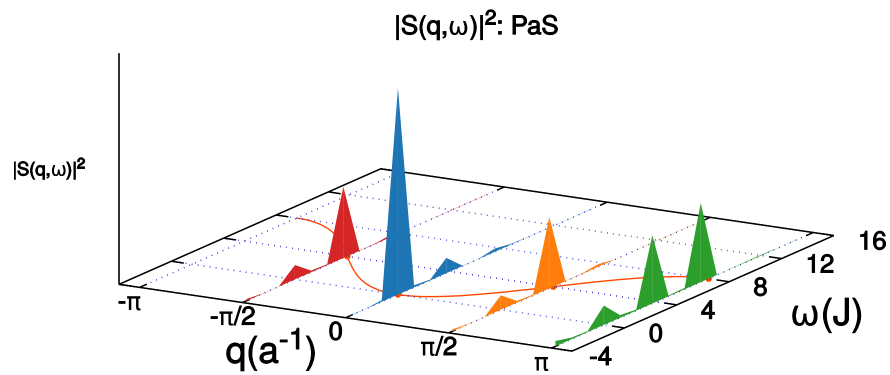




Raw data (2019)



Error mitigation



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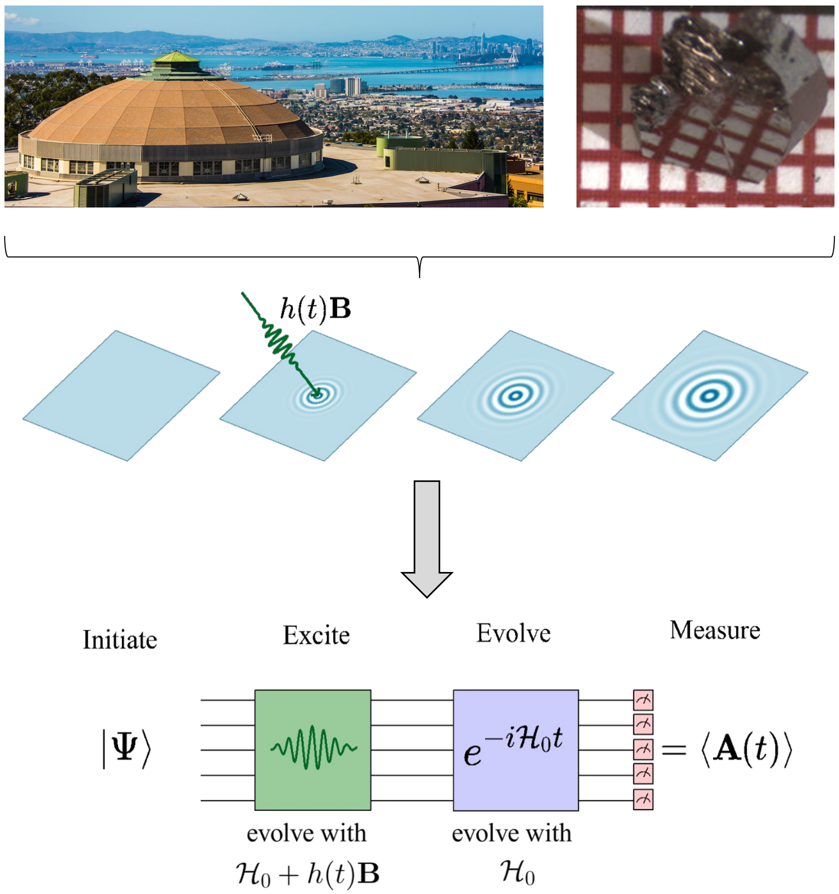
Linear Response

2302.10219



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

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

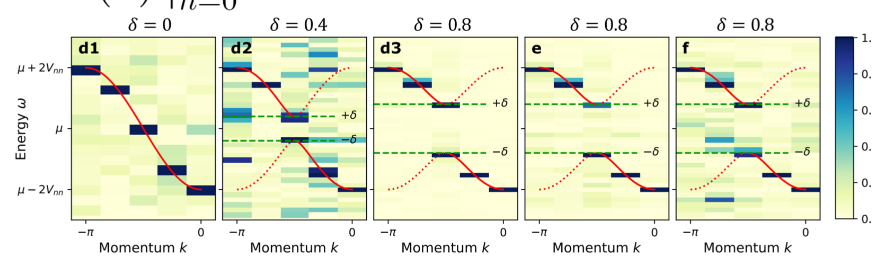
[1] Department of Physics, North Carolina State University, Raleigh, North Carolina 27695, USA
[2] Department of Physics, Georgetown University, 37th and O Sts. NW, Washington, DC 20057 USA

(Dated: February 22, 2023)

1. Make the excitation part of the quantum simulation

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

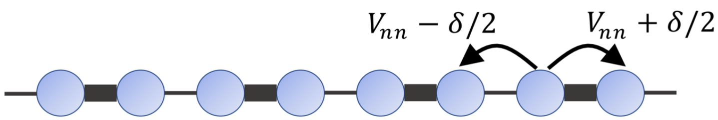
$$\left.\frac{\delta A(t)}{\delta h(t')}\right|_{h=0} = -i\theta(t-t')\langle\psi_0|[\mathbf{A}(t),\mathbf{B}(t')]|\psi_0\rangle$$



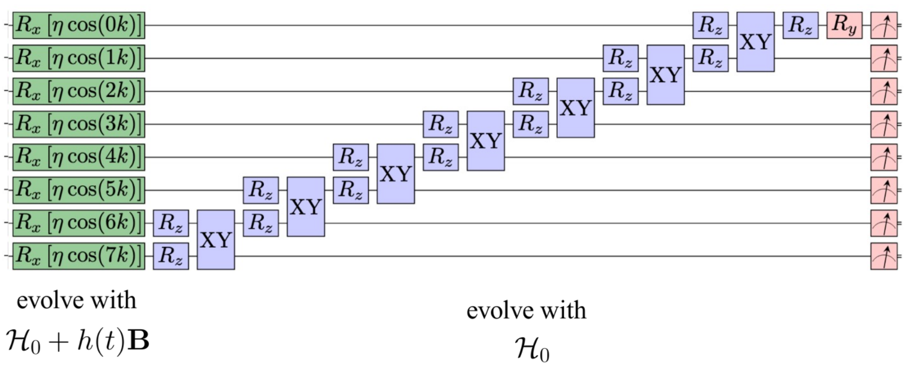
Linear Response -> Green's function

2302.10219

Su-Schrieffer-Heeger model for polyacetylene

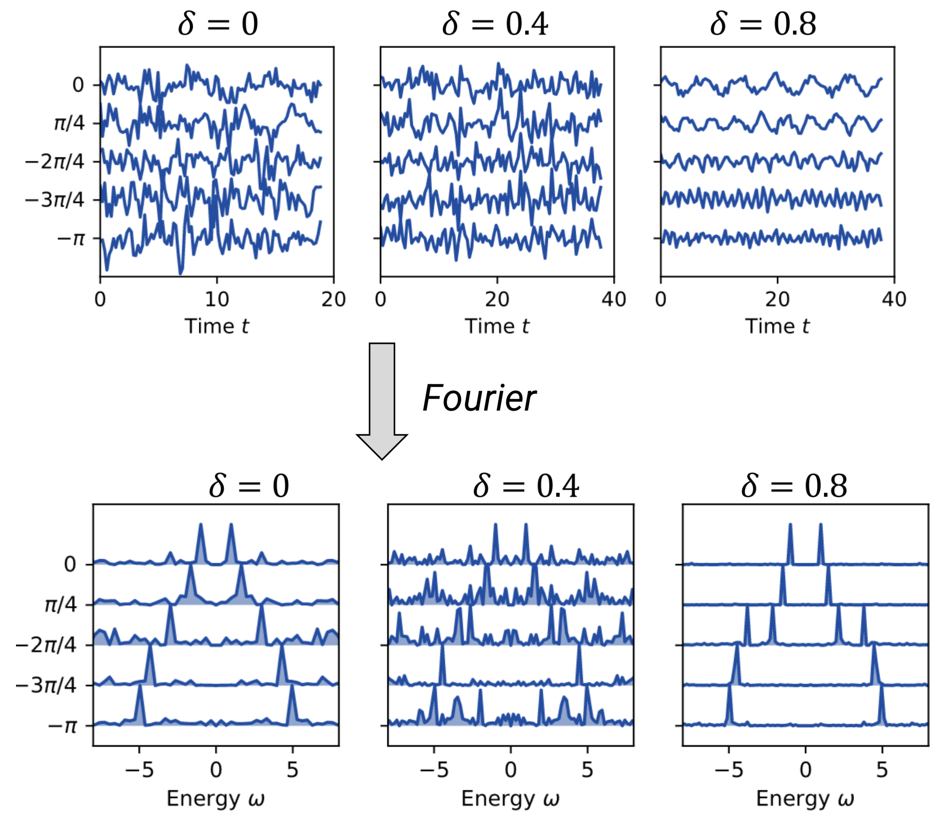


Compressed circuit run on *ibm_auckland*



Choose **B** to create a momentum eigenstate

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



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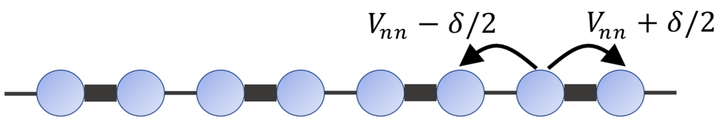

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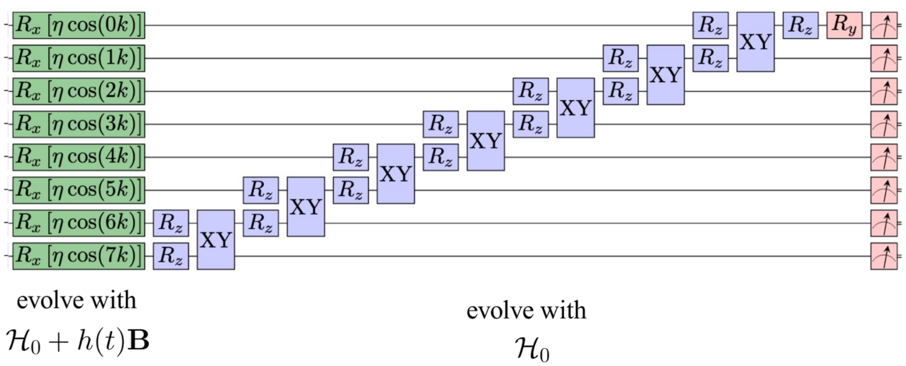

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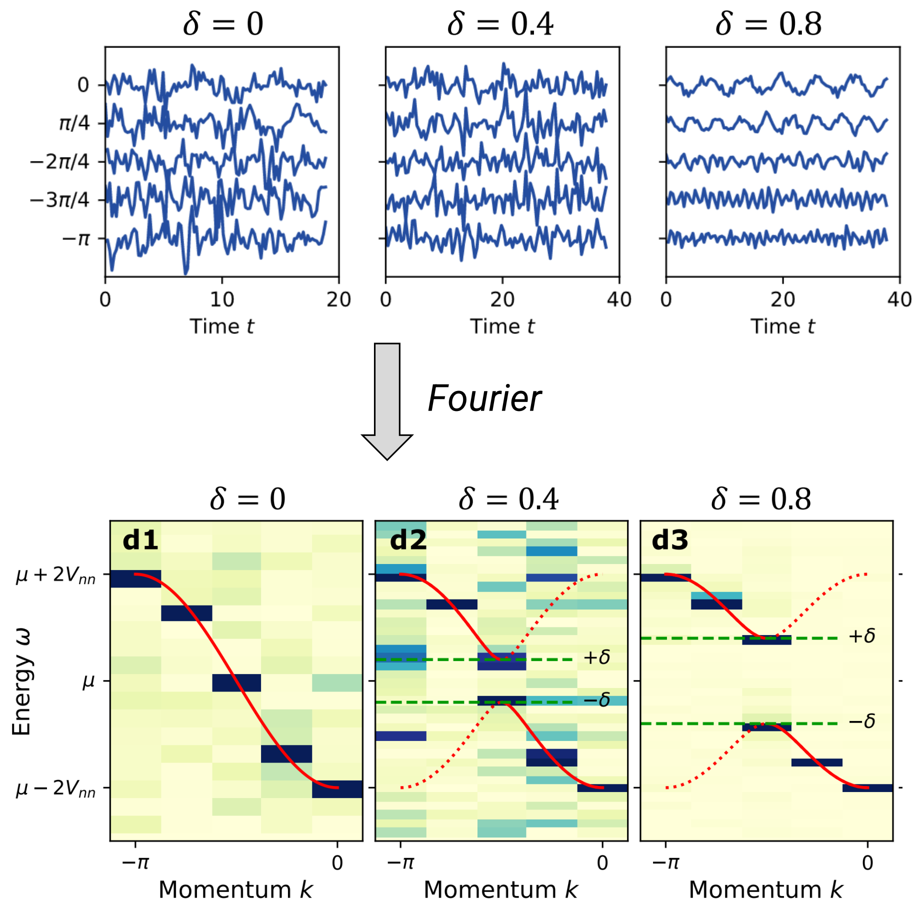

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Linear Response -> Green’s function

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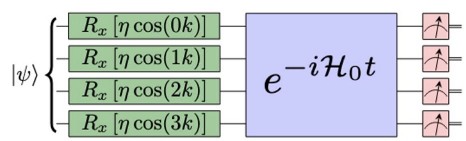
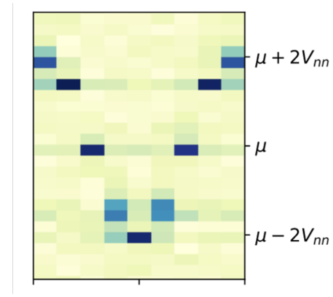
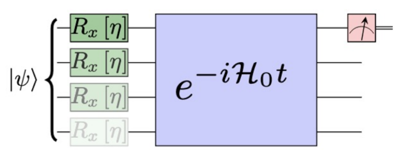
Momentum-selective linear response



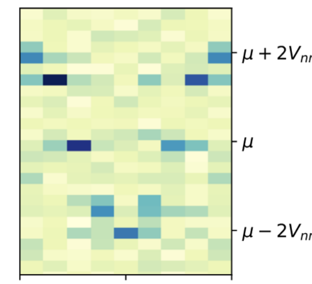
FT
$t \to \omega$



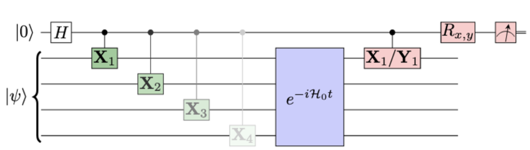
Position-selective linear response



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



Hadamard test method



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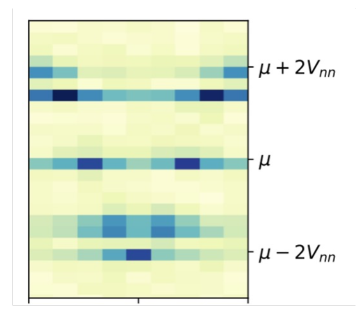
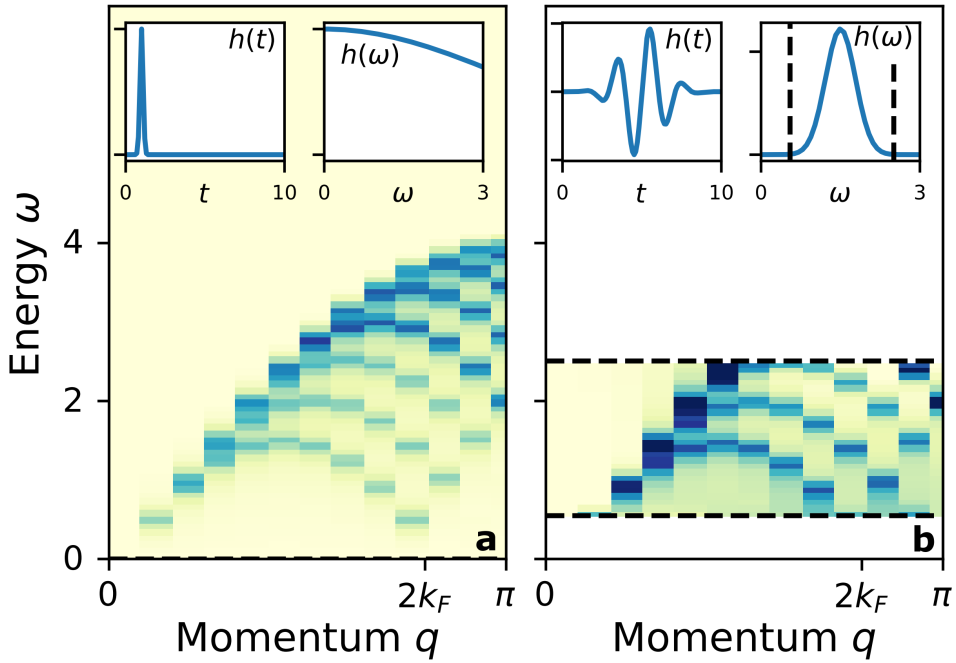


Data from noisy simulator with one/two qubit noise of 1% and 10%

Linear Response -> Polarizability

2302.10219



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

Data from statevector simulator

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Linear Response

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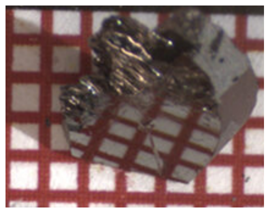
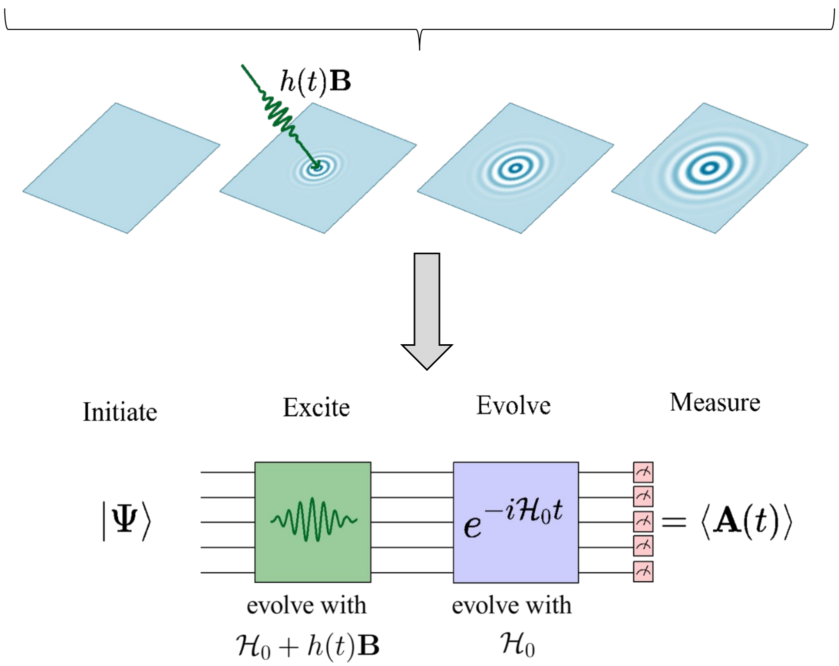
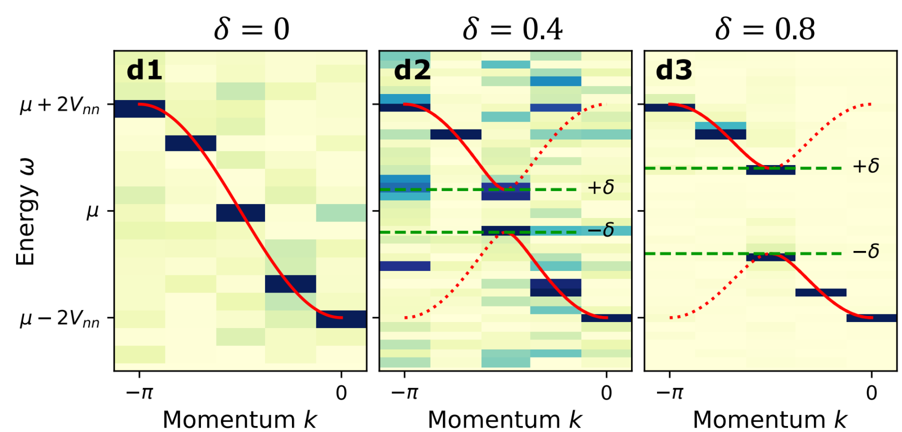




- Ancilla free
- Momentum and frequency selectivity
- Both bosonic and fermionic correlators
- More noise robust compared to existing methods



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

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HPC + QC

All is not well in QC…

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HPC + QC

All is not well in QC…

- ☹️ Barren Plateaus

$$\mathrm{Var}[\partial C] \sim \frac{1}{2^n}$$

HPC + QC

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All is not well in QC…

☹️ Barren Plateaus

☹️ No quantum advantage for chemistry

Is there evidence for exponential quantum advantage in quantum chemistry?

Seunghoon Lee, Joonho Lee, Huanchen Zhai, Yu Tong, Alexander M. Dalzell, Ashutosh Kumar, Phillip Helms, Johnnie Gray, Zhi-Hao Cui, Wenyuan Liu, Michael Kastoryano, Ryan Babbush, John Preskill, David R. Reichman, Earl T. Campbell, Edward F. Valeev, Lin Lin, Garnet Kin-Lic Chan

The idea to use quantum mechanical devices to simulate other quantum systems is commonly ascribed to Feynman. Since the original suggestion, concrete proposals have appeared for simulating molecular and materials chemistry through quantum computation, as a potential ``killer application". Indications of potential exponential quantum advantage in artificial tasks have increased interest in this application, thus, it is critical to understand the basis for potential exponential quantum advantage in quantum chemistry. Here we gather the evidence for this case in the most common task in quantum chemistry, namely, ground-state energy estimation. We conclude that evidence for such an exponential advantage across chemical space has yet to be found. While quantum computers may still prove useful for quantum chemistry, it may be prudent to assume exponential speedups are not generically available for this problem.

According to the authors: No.

HPC + QC

All is not well in QC…

- ☹️ Barren Plateaus
- ☹️ No quantum advantage for chemistry
- ☹️ Need at least n^3 speedup to overcome Quantum Error Correction overhead

Perspective Open Access

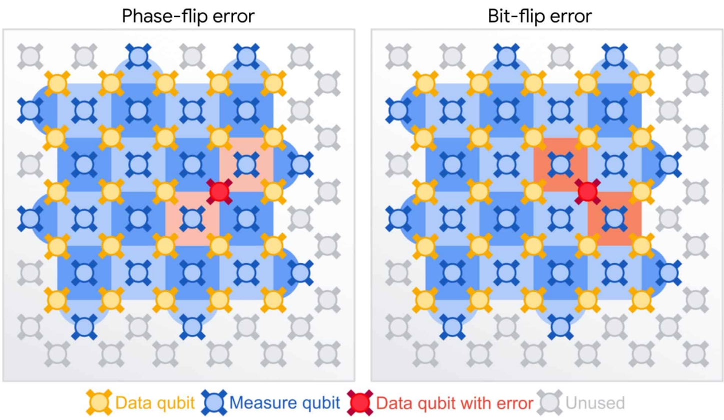
Focus beyond Quadratic Speedups for Error-Corrected Quantum Advantage

Ryan Babbush, Jarrod R. McClean, Michael Newman, Craig Gidney, Sergio Boixo, and Hartmut Neven
PRX Quantum **2**, 010103 – Published 29 March 2021

HPC + QC

All is not well in QC…

- ☹️ Barren Plateaus
- ☹️ No quantum advantage for chemistry
- ☹️ Need at least n^3 speedup to overcome Quantum Error Correction overhead
- ☹️ Quantum Error Correction can require heavy classical compute resources



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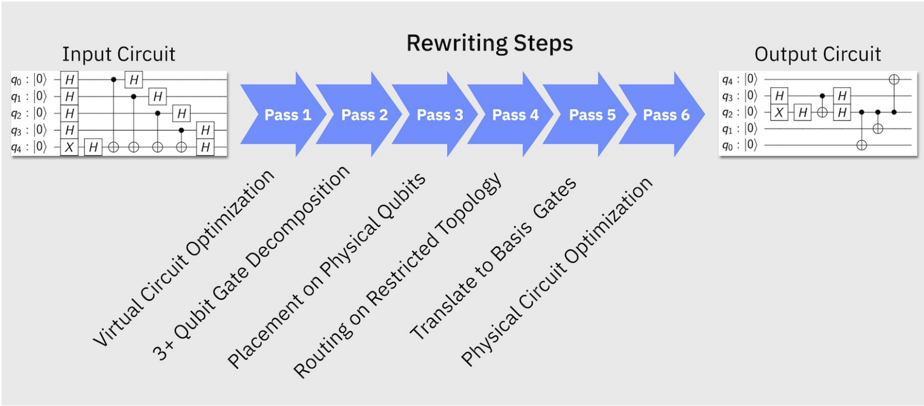
HPC + QC

All is not well in QC…

- 🙁 Barren Plateaus
- 🙁 No quantum advantage for chemistry
- 🙁 Need at least n^3 speedup to overcome Quantum Error Correction overhead
- 🙁 Quantum Error Correction can require heavy classical compute resources
- 🙁 Compiling Quantum Circuits is (NP-) hard



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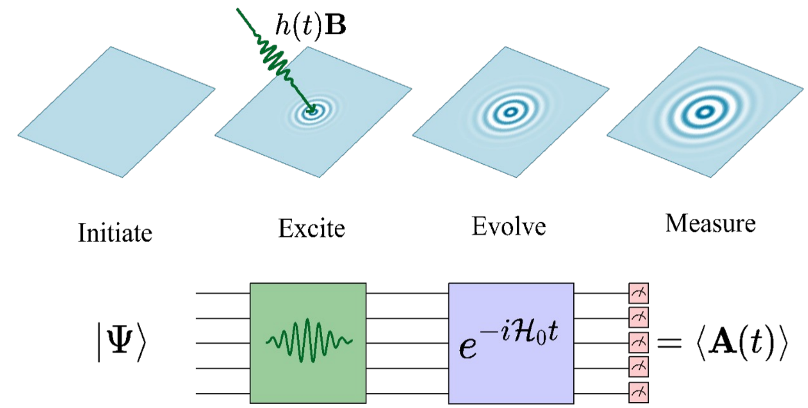
HPC + QC

All is not well in QC…

- ☹️ Barren Plateaus *(optimization, pure math, statistics, error mitigation)*
- ☹️ No quantum advantage for chemistry *(quantum chemistry)*
- ☹️ Need at least n^3 speedup to overcome Quantum Error Correction overhead
- ☹️ Quantum Error Correction can require heavy classical compute resources *(algorithm optimization)*
- ☹️ Compiling Quantum Circuits is (NP-) hard *(compilers, graphical calculi)*

Quantum Materials Meet Quantum Computing



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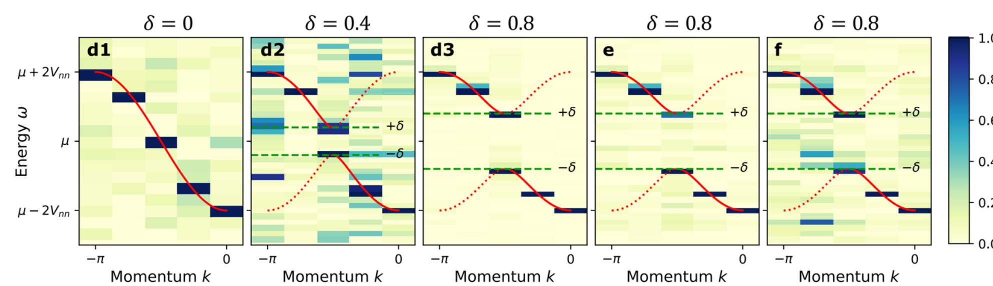

Alvarez Workshop
06/15/2023

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