Quantum Information meets Quantum Matter

Alexander (Lex) Kemper

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

UNC Chapel Hill Colloquium
11/20/2023

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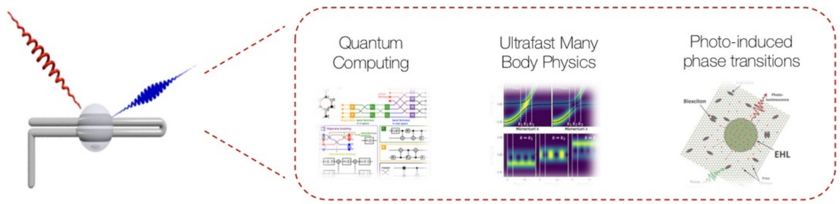


Kemper Lab

Quantum materials in and out of equilibrium.

Collaborations with:

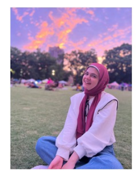
- Bojko Bakalov (NCSU)
- Marco Cerezo, Martin de la Rocca (LANL)
- Jim Freericks (Georgetown)
- Daan Camps, Roel van Beeumen, Bert de Jong, Akhil Francis (LBNL)
- Thomas Steckmann (UMD)
- Yan Wang, Eugene Dumitrescu (ORNL)

Current members

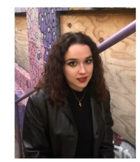

Alexander (Lex) Kemper
Principal investigator


Efekan Kökcü
Graduate Researcher


Anjali Agrawal
Graduate Researcher


Heba Labib
Graduate Researcher

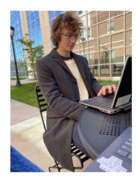

Jack Howard
Undergraduate Researcher


Natalia Wilson
Undergraduate Researcher


Daniel Brandon
Undergraduate Researcher


Sarah Klas
Undergraduate Researcher


Norman Hogan
Graduate Researcher


Ethan Blair
Undergraduate Researcher


Your Name
New lab member

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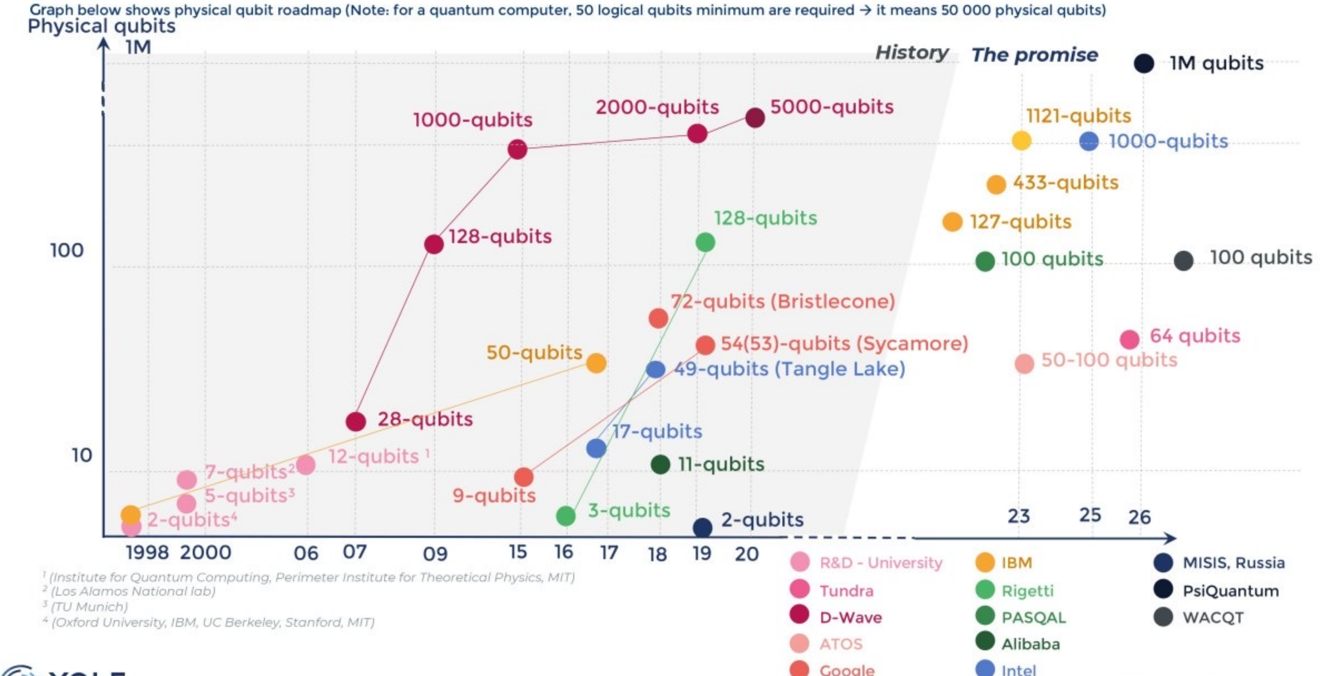
Brief outline

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

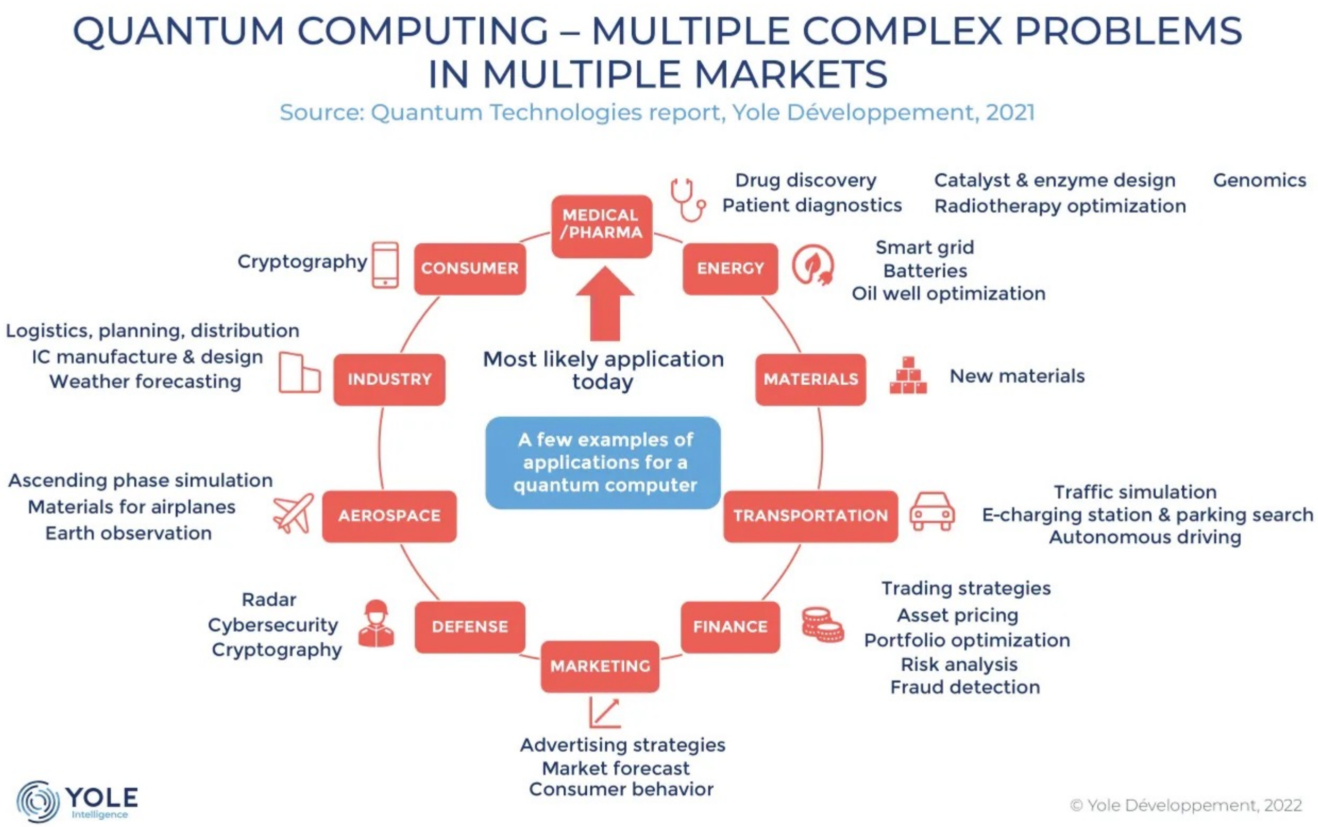
PHYSICAL QUBIT ROADMAP FOR QUANTUM COMPUTER – HISTORY AND FUTURE

Source: Quantum Technologies report, Yole Développement, 2021

Graph below shows physical qubit roadmap (Note: for a quantum computer, 50 logical qubits minimum are required → it means 50 000 physical qubits)



YOLE Intelligence


QUANTUM COMPUTING – MULTIPLE COMPLEX PROBLEMS IN MULTIPLE MARKETS
Source: Quantum Technologies report, Yole Développement, 2021
MEDICAL /PHARMA
Drug discovery
Patient diagnostics
Catalyst & enzyme design
Radiotherapy optimization
Genomics
ENERGY
Smart grid
Batteries
Oil well optimization
MATERIALS
New materials
TRANSPORTATION
Traffic simulation
E-charging station & parking search
Autonomous driving
FINANCE
Trading strategies
Asset pricing
Portfolio optimization
Risk analysis
Fraud detection
MARKETING
Advertising strategies
Market forecast
Consumer behavior
DEFENSE
Radar
Cybersecurity
Cryptography
AEROSPACE
Ascending phase simulation
Materials for airplanes
Earth observation
INDUSTRY
Logistics, planning, distribution
IC manufacture & design
Weather forecasting
CONSUMER
Cryptography
Most likely application today
A few examples of applications for a quantum computer
YOLE Intelligence
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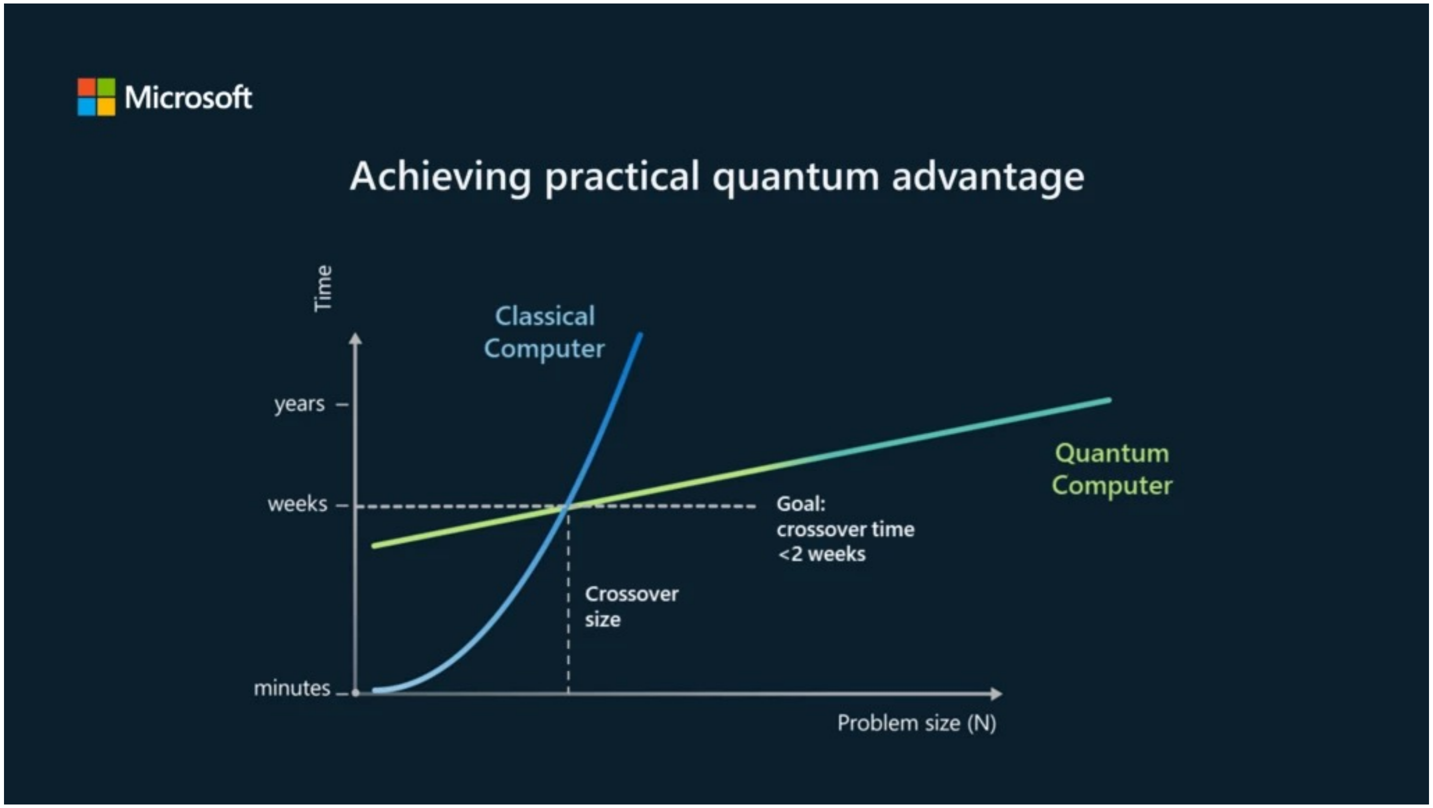
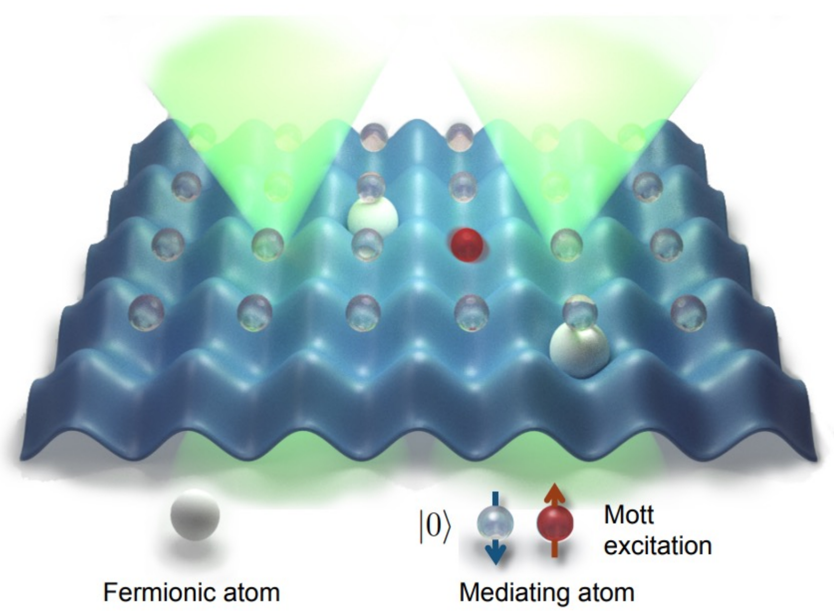
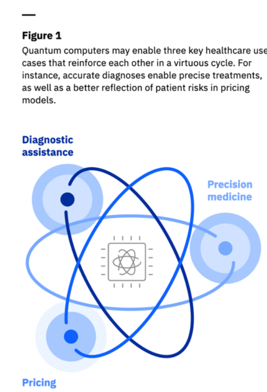
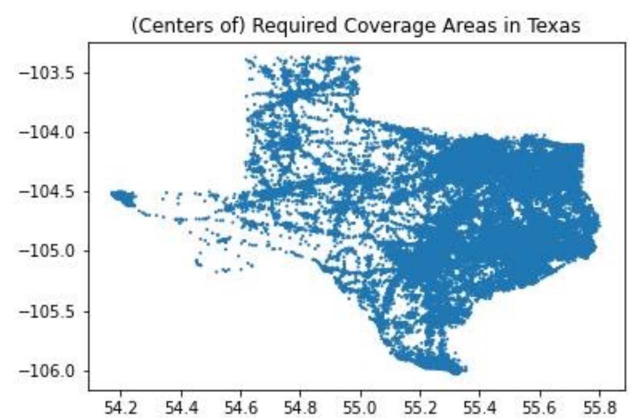


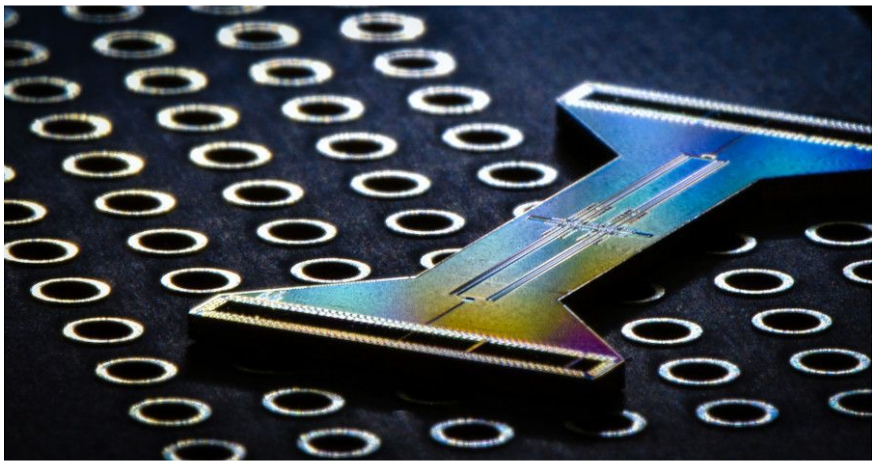
Bespoke quantum simulator — Digital algorithms

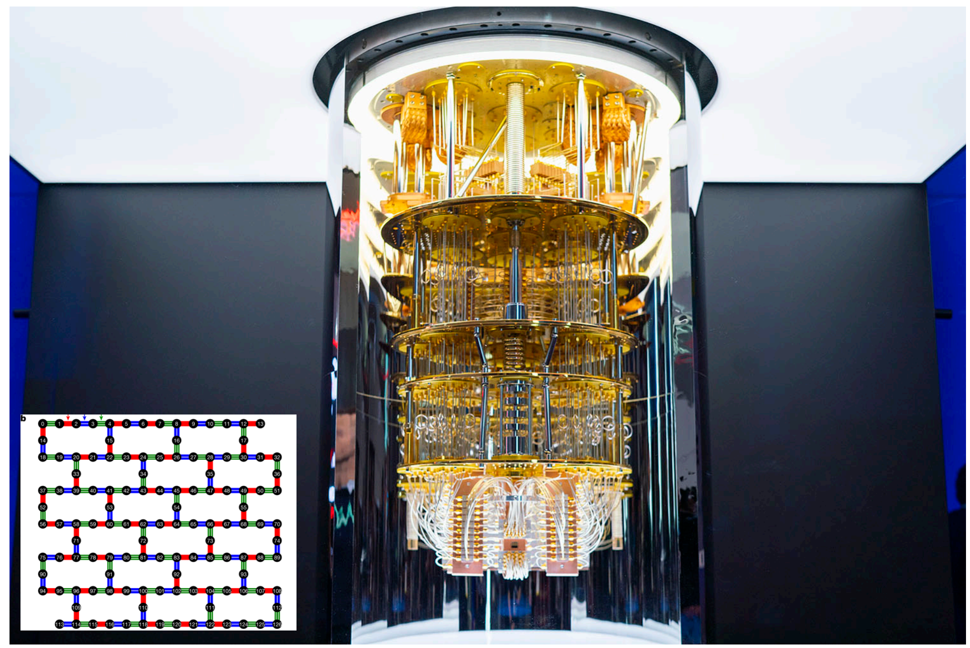






Bespoke quantum simulator *Digital algorithms*





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Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981

1. Can classical physics be simulated by a classical computer?
2. Can quantum physics be simulated by a classical computer?
3. Can physics be simulated by a quantum computer?
4. Can a quantum simulation be universal?

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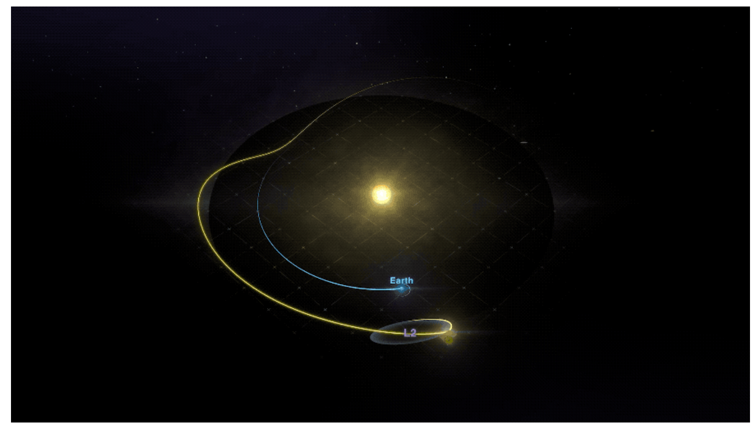

NASA

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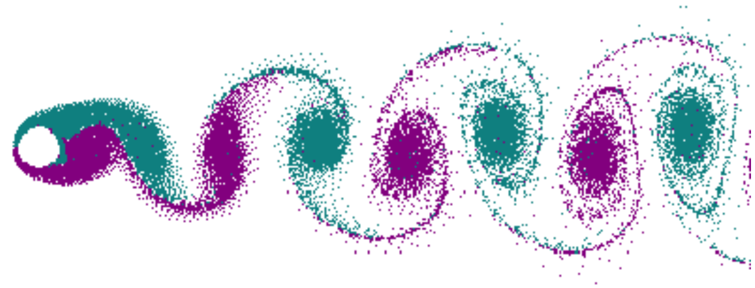

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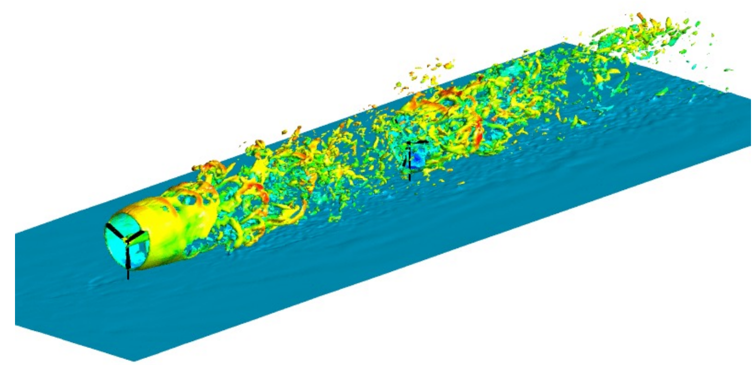

Wikipedia, https://fluids.eng.sydney.edu.au/computer-codes/

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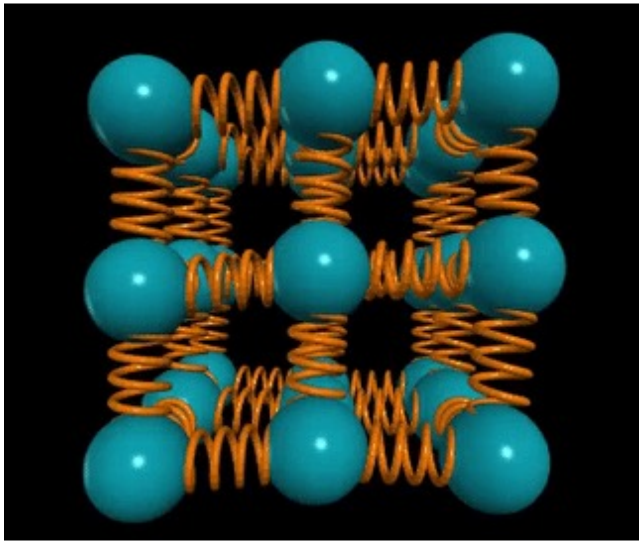

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RESEARCH

TOPOLOGICAL MATTER

Observation of chiral phonons

Hanyu Zhu,[1,2] Jun Yi,[1] Ming-Yang Li,[3] Jun Xiao,[1] Lifa Zhang,[4] Chih-Wen Yang,[3] Robert A. Kaindl,[2] Lain-Jong Li,[3] Yuan Wang,[1,2*] Xiang Zhang[1,2*]

DOI: 10.1126/science.aar2711

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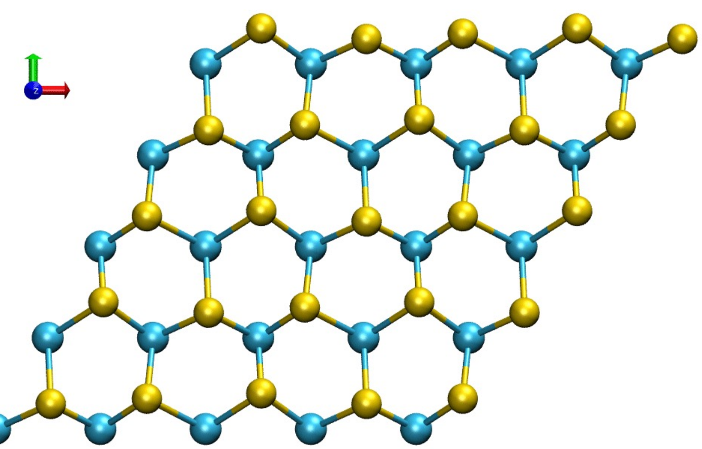

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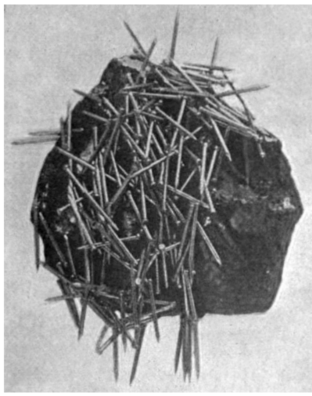
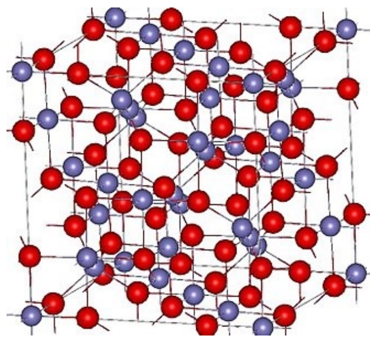
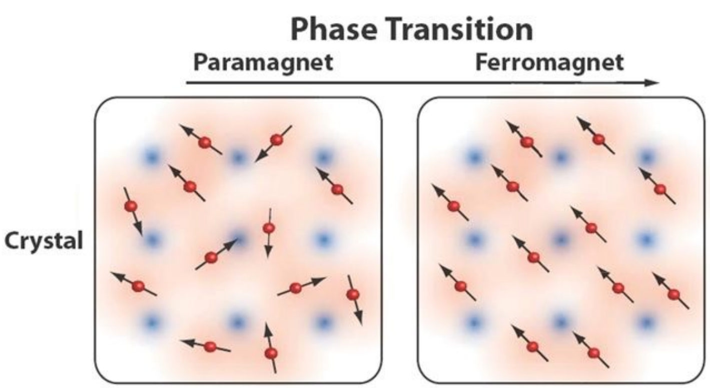
Magnetite [$Fe^{2+}(Fe^{3+})_2(O^{2-})_4$]





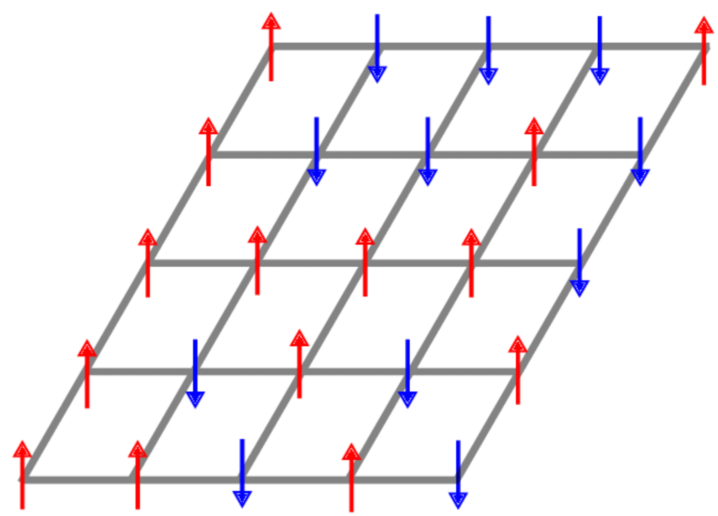


Published: February 1925

Beitrag zur Theorie des Ferromagnetismus

Ernst Ising

Zeitschrift für Physik **31**, 253–258 (1925) | Cite this article



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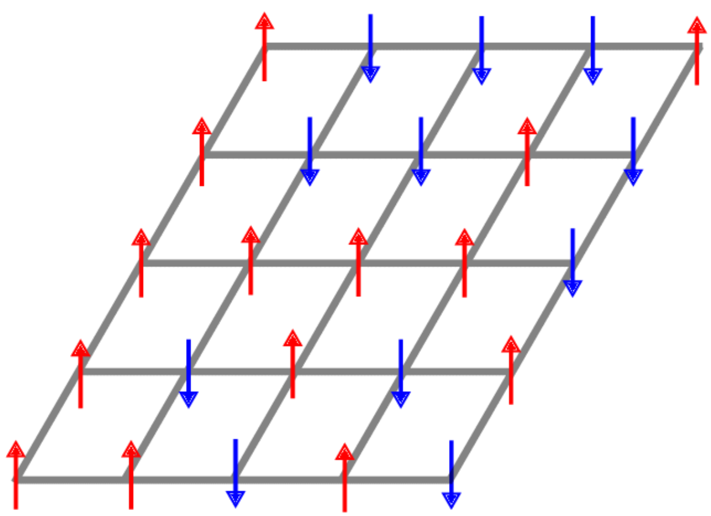

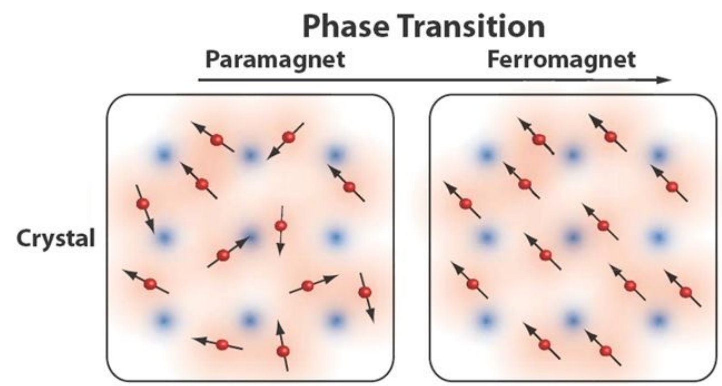

50 spins = ? states

a) 1,000 – 10,000
b) 10,000 – 1,000,000
c) 1,000,000 – 1,000,000,000
d) More than 1,000,000,000

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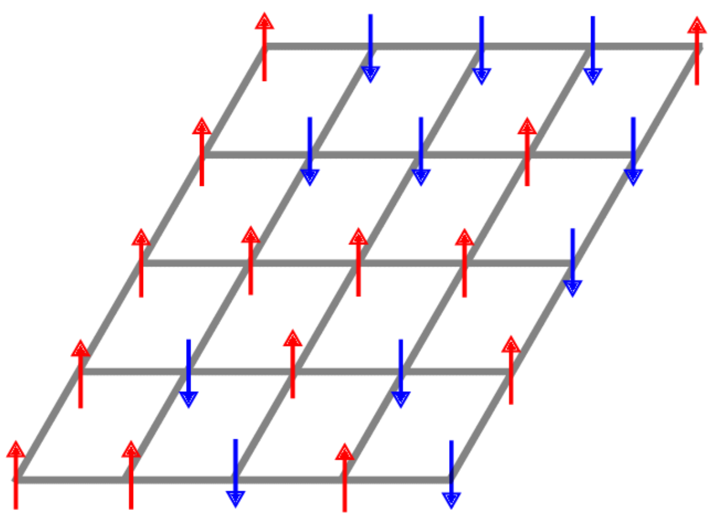
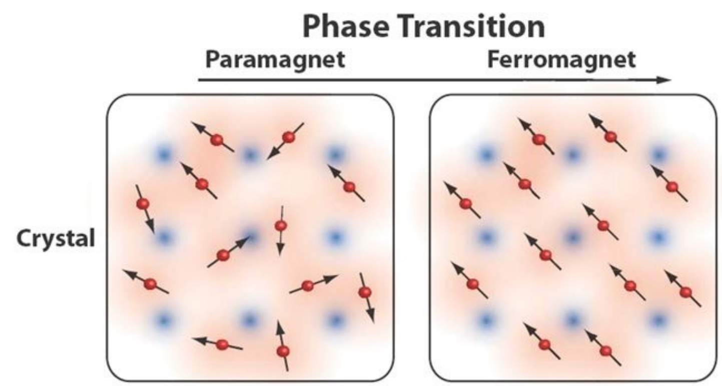
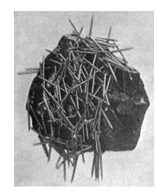




50 spins = 1,125,899,906,842,624 states

18 Petabytes of memory

10^{23} atoms



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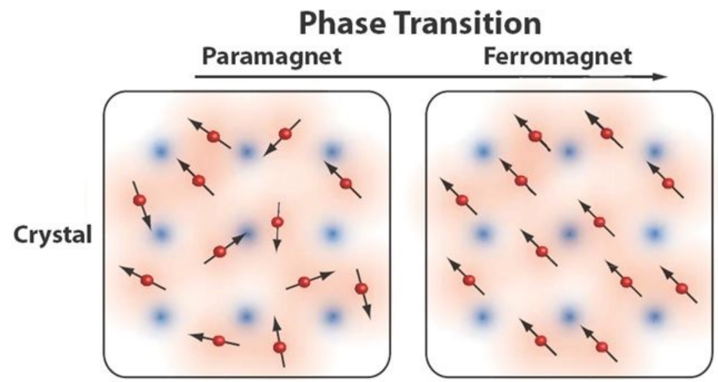

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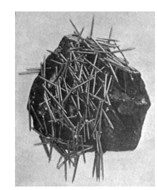

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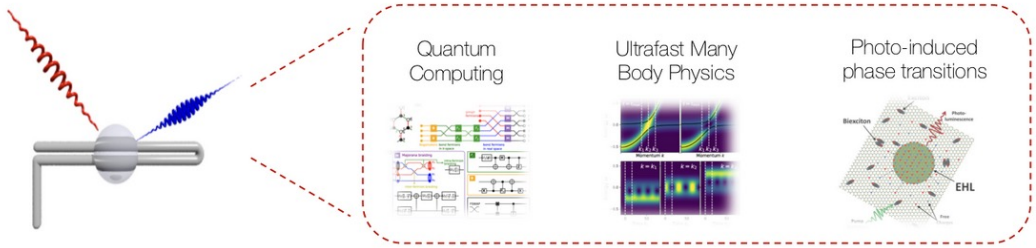

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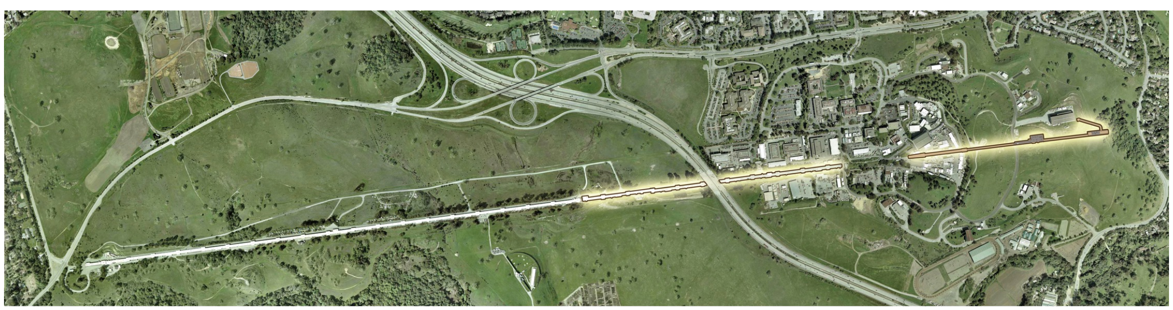
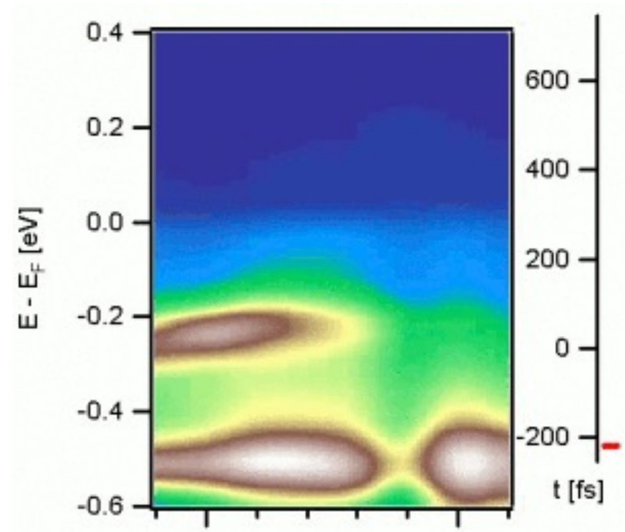
Quantum materials in and out of equilibrium.

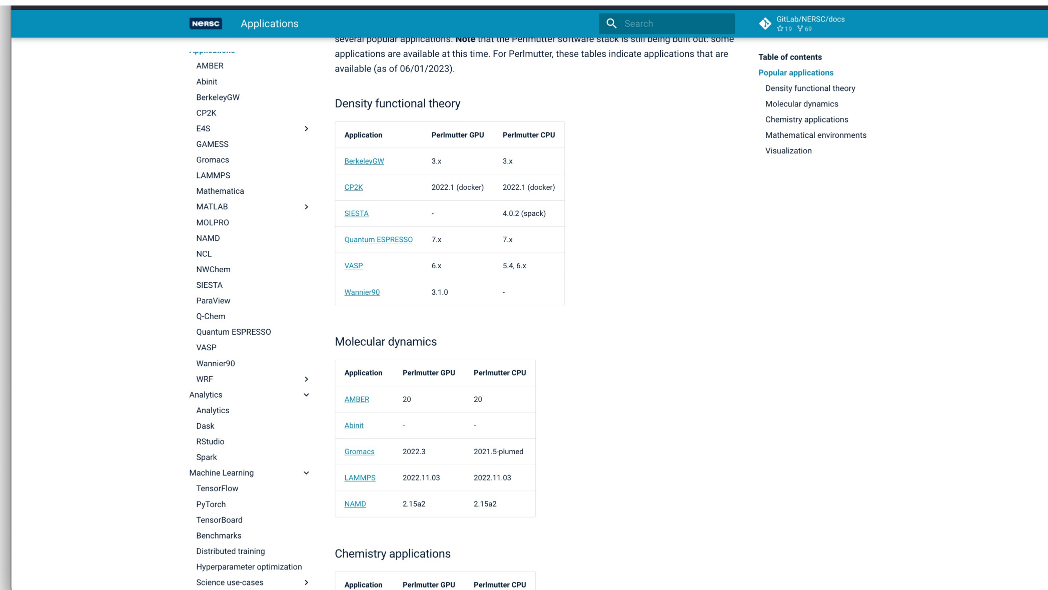
Time-resolved experiments





Shen group (Stanford)

2. Can quantum physics be simulated by a classical computer?


NERSC Applications
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19 69

AMBER
Abinit
BerkeleyGW
CP2K
E4S
GAMESS
Gromacs
LAMMPS
Mathematica
MATLAB
MOLPRO
NAMD
NCL
NWChem
SIESTA
ParaView
Q-Chem
Quantum ESPRESSO
VASP
Wannier90
WRF
Analytics
Analytics
Dask
RStudio
Spark
Machine Learning
TensorFlow
PyTorch
TensorBoard
Benchmarks
Distributed training
Hyperparameter optimization
Science use-cases

several popular applications. **Note** that the Perlmutter software stack is still being built out: some applications are available at this time. For Perlmutter, these tables indicate applications that are available (as of 06/01/2023).

Density functional theory

Application	Perlmutter GPU	Perlmutter CPU
BerkeleyGW	3.x	3.x
CP2K	2022.1 (docker)	2022.1 (docker)
SIESTA	-	4.0.2 (spack)
Quantum ESPRESSO	7.x	7.x
VASP	6.x	5.4, 6.x
Wannier90	3.1.0	-

Molecular dynamics

Application	Perlmutter GPU	Perlmutter CPU
AMBER	20	20
Abinit	-	-
Gromacs	2022.3	2021.5-plumed
LAMMPS	2022.11.03	2022.11.03
NAMD	2.15a2	2.15a2

Chemistry applications

Application	Perlmutter GPU	Perlmutter CPU

Table of contents
Popular applications
Density functional theory
Molecular dynamics
Chemistry applications
Mathematical environments
Visualization

Density functional theory/GW
Exact diagonalization
Quantum Monte Carlo
Non-equilibrium Green’s functions
Matrix Product States
Tensor Networks

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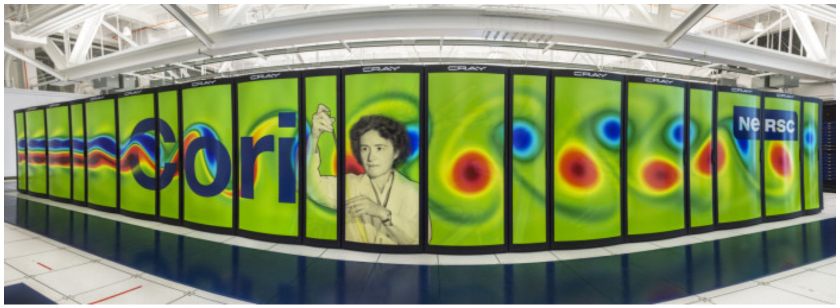
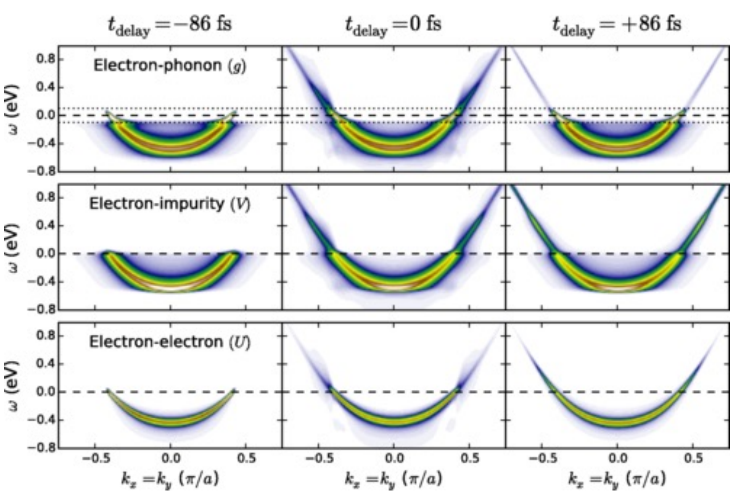
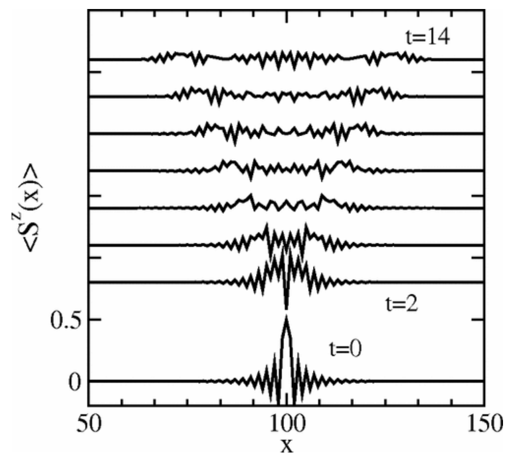
2. Can quantum physics be simulated by a classical computer?





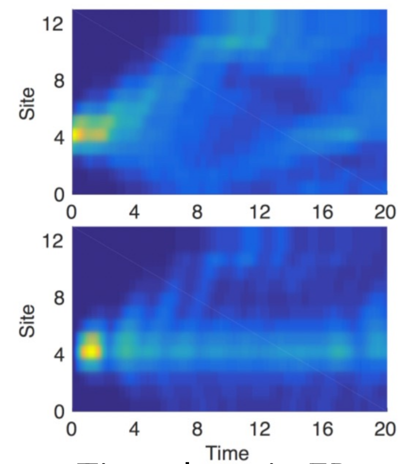
Non-Equilibrium Green's functions

Phys. Rev. X 8, 041009 (2018)



Time domain DMRG

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

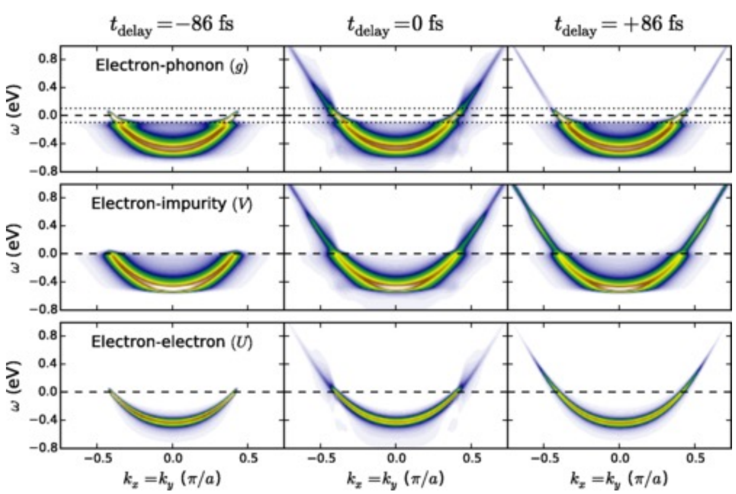


Time domain ED

Johnston & Kemper, unpublished

2. Can quantum physics be simulated by a classical computer?

All these techniques eventually reach a barrier.



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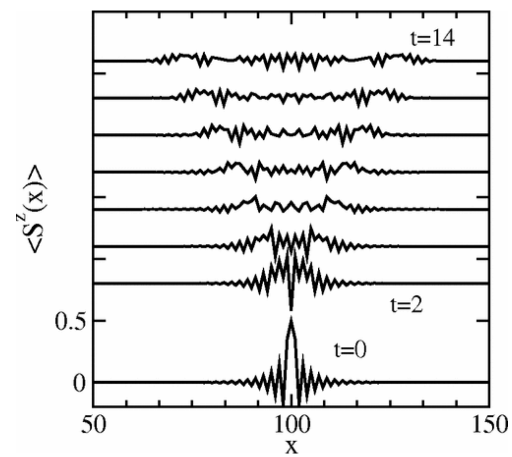
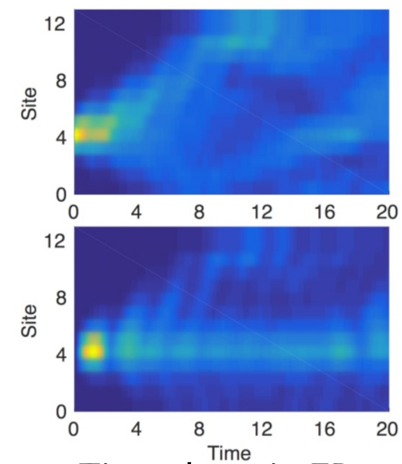
Phys. Rev. X 8, 041009 (2018)



Time domain DMRG

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



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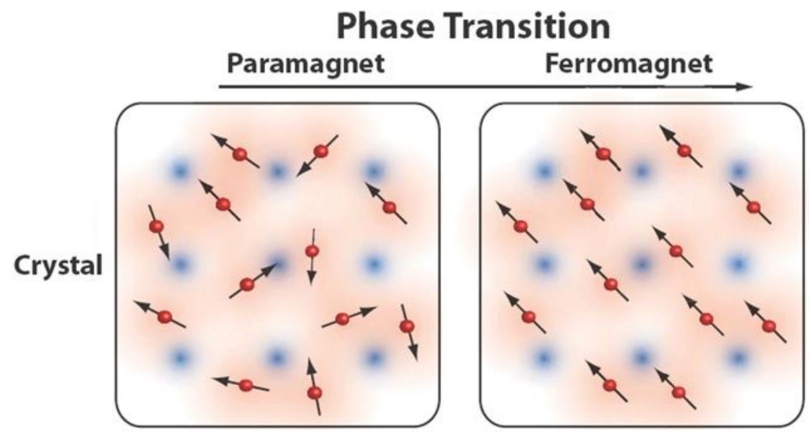

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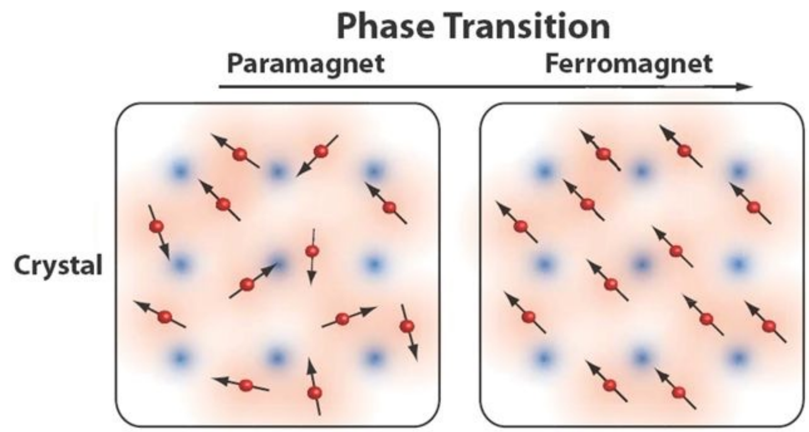
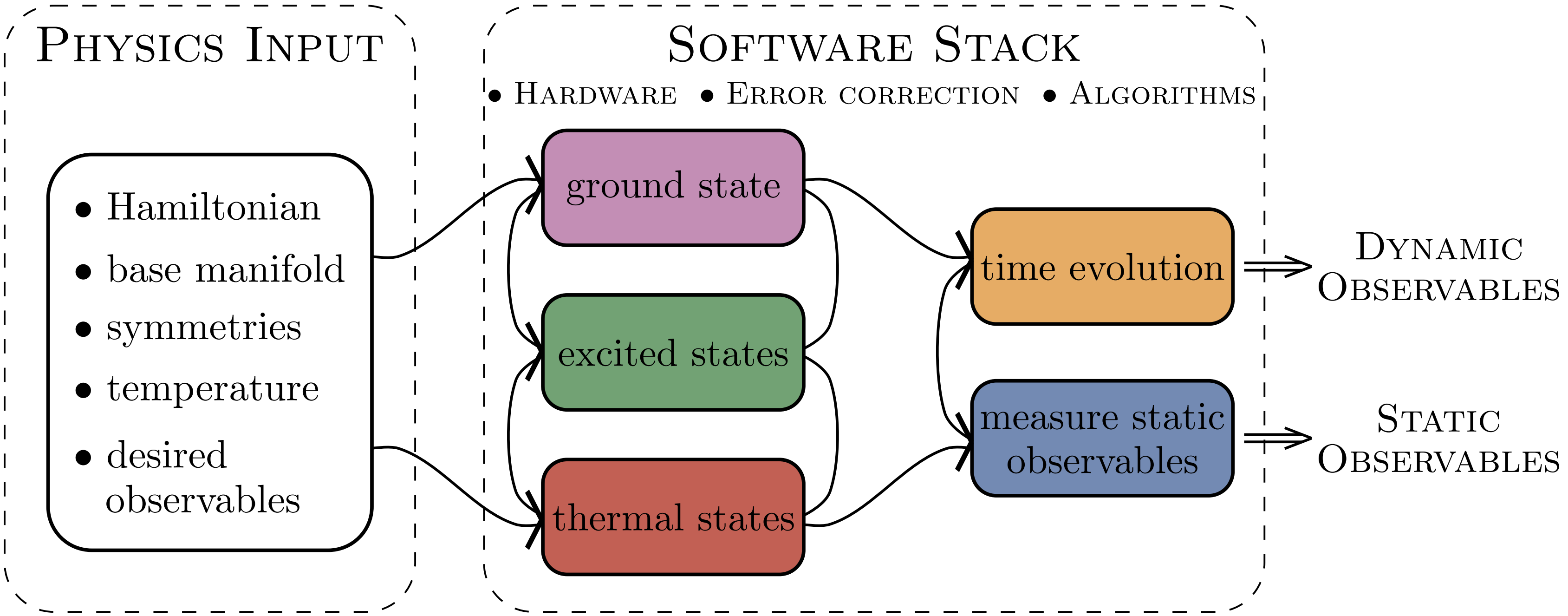


50 spins = 50 qubits

Quantum Matter meets Quantum Computing



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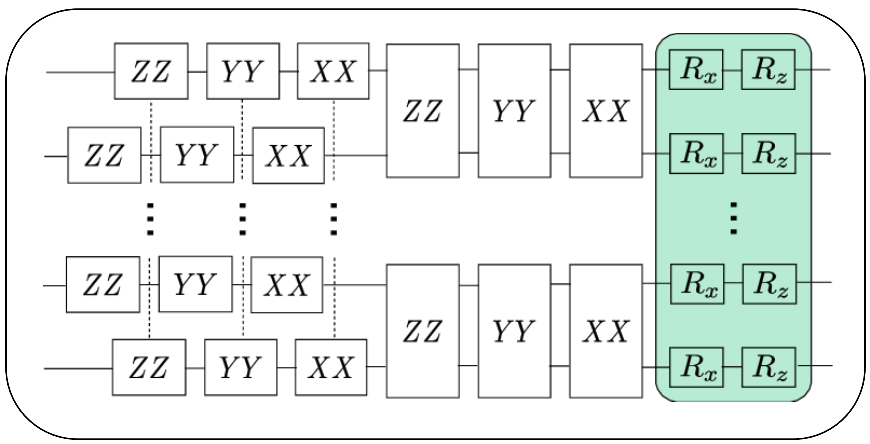
3. Can quantum physics be simulated by a quantum computer?

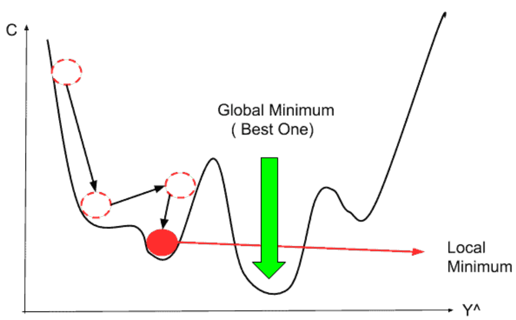
Variational Principle: $$E_{\text{ground}} \leq \langle\phi|\, H \,|\phi\rangle$$

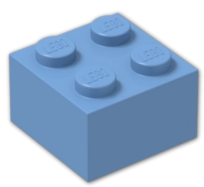
Wave function guess:

$$\{\theta_i\} \longrightarrow$$



$$\longrightarrow |\phi\rangle$$





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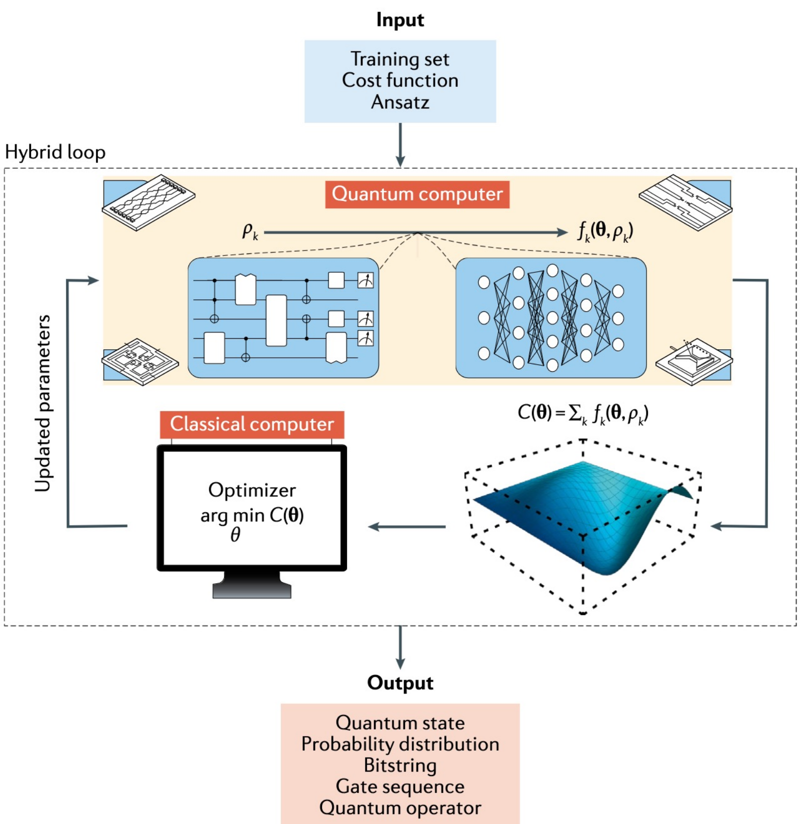
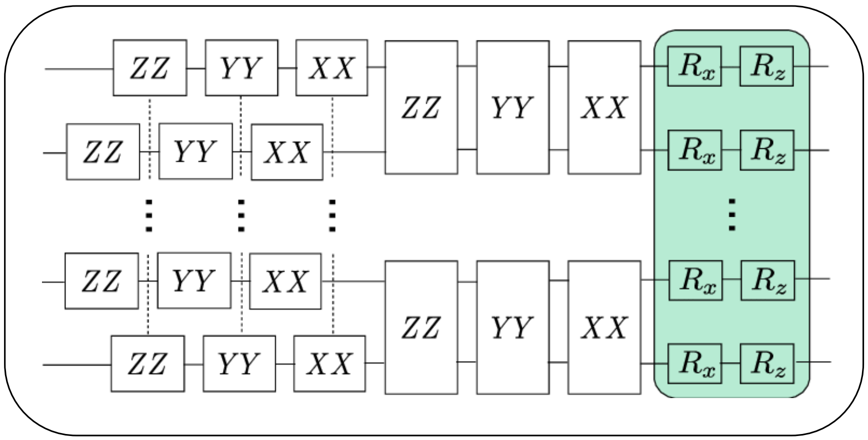
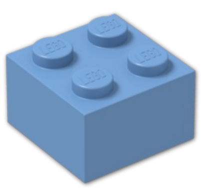


Cost function: Energy of the molecular configuration

10.1038/nature23879

Wave function guess:





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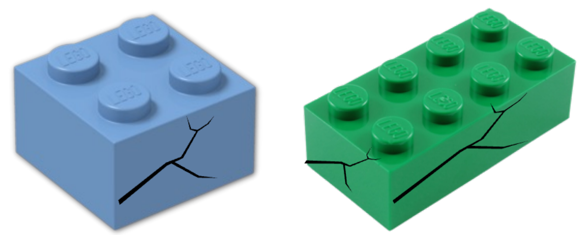
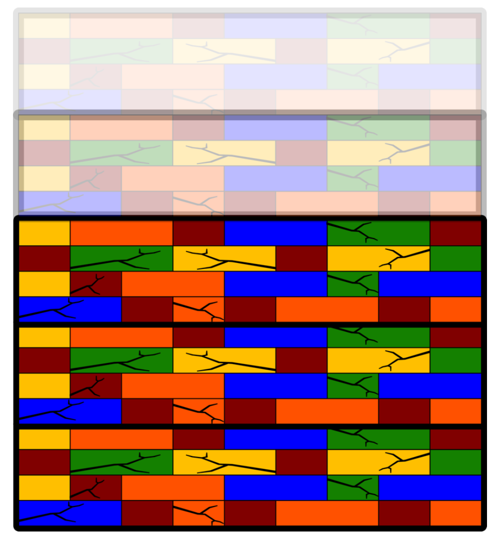
Single Qubit Gates

Two Qubit Gate

*Actual Gates





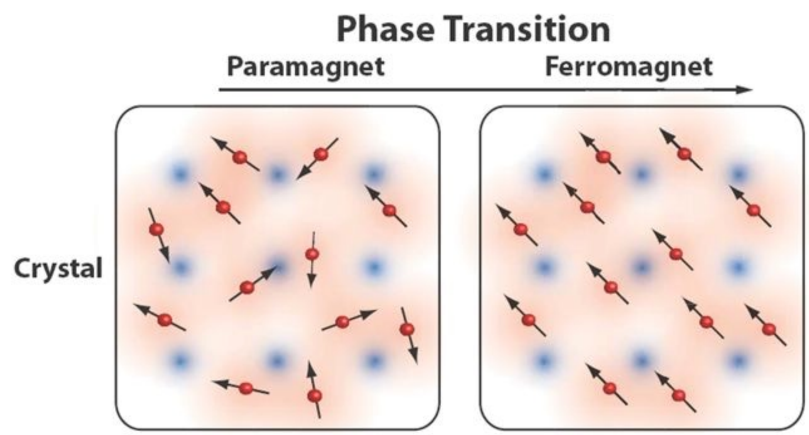
Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

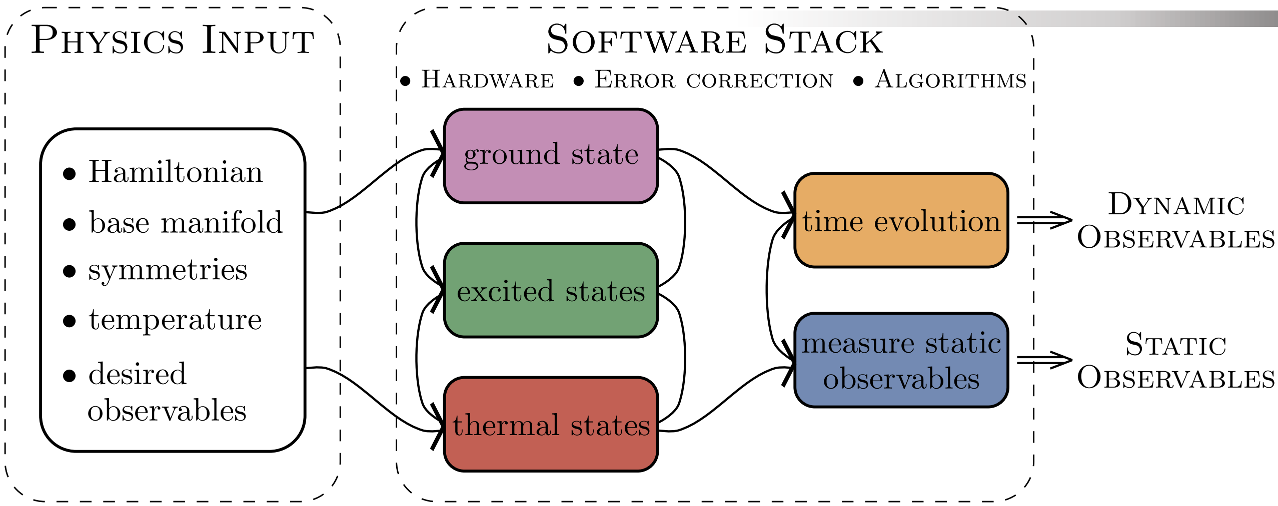
Received May 7, 1981

1. Can classical physics be simulated by a classical computer? ✓
2. Can quantum physics be simulated by a classical computer? ?
3. Can physics be simulated by a quantum computer? ✓



50 spins = 50 qubits

A-Z quantum simulation



Classical post-processing techniques

Prepare state of interest

Time evolve

Dynamical response functions

- *Physics-Informed Subspace Expansions*

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

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

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

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Ising Model

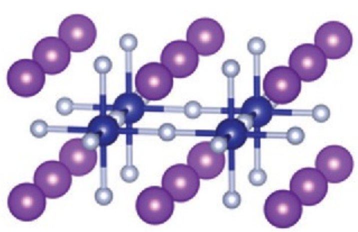
794 Brazilian Journal of Physics, vol. 30, no. 4, December, 2000

The Ising Model and Real Magnetic Materials

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

Received on 3 August, 2000

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



10.1039/c6cp02362b

Heisenberg model

PHYSICAL REVIEW B
covering condensed matter and materials physics

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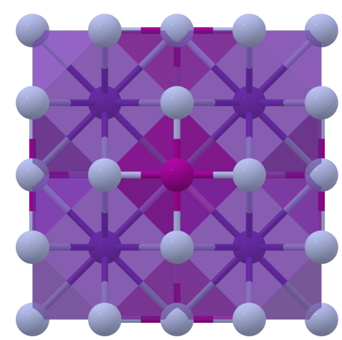
Critical behavior of the three-dimensional Heisenberg antiferromagnet $RbMnF_3$

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



Materials project

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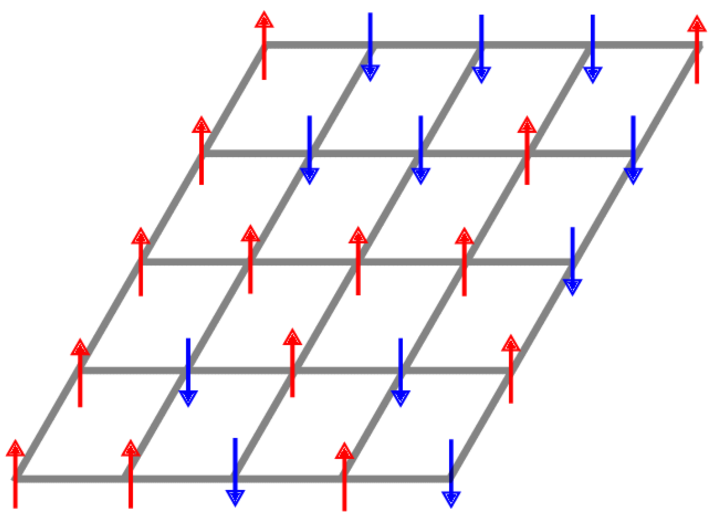
Ising Model

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



Heisenberg model

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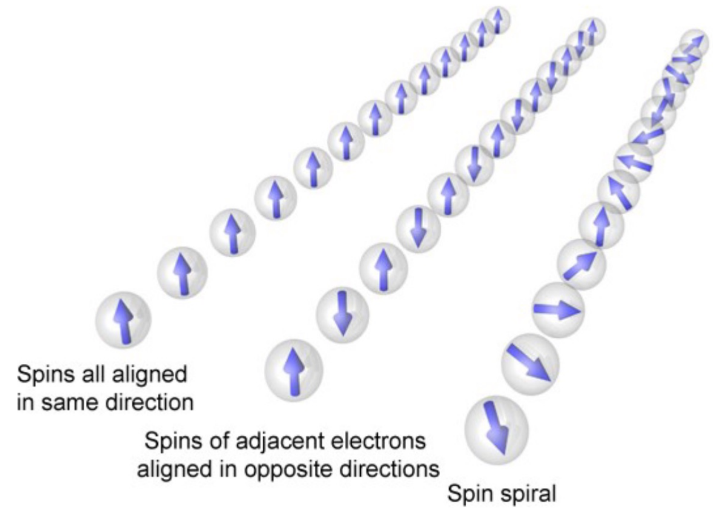

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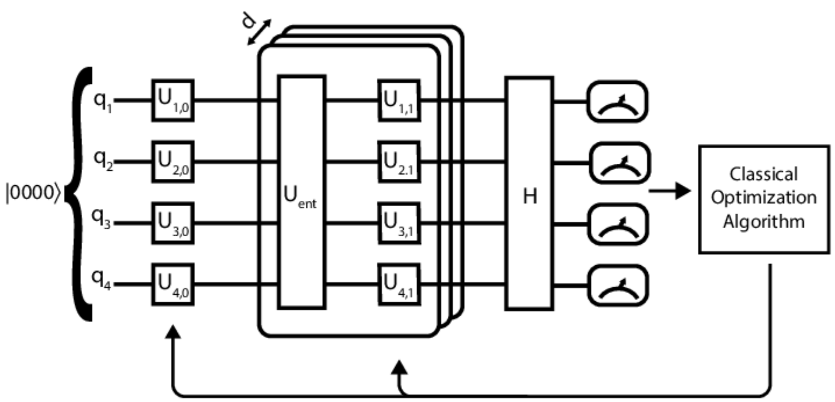

[Optimization of the Variational Quantum Eigensolver for Quantum Chemistry Applications]

Heisenberg model

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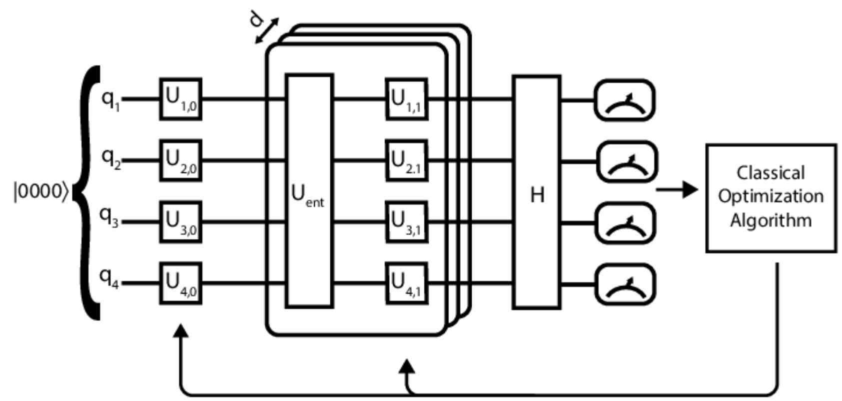

Ising Model

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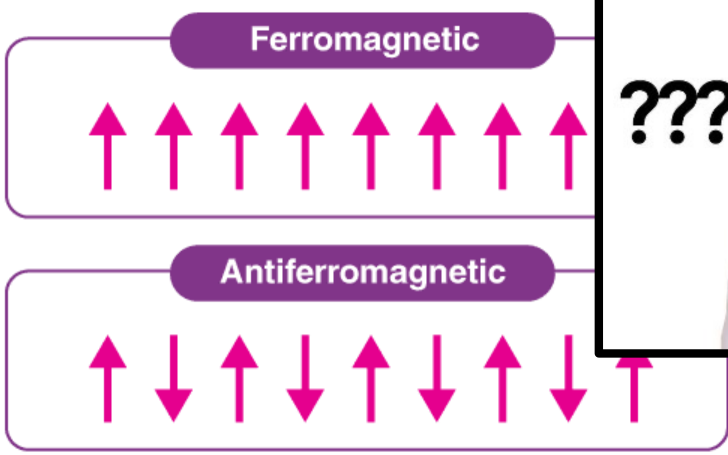

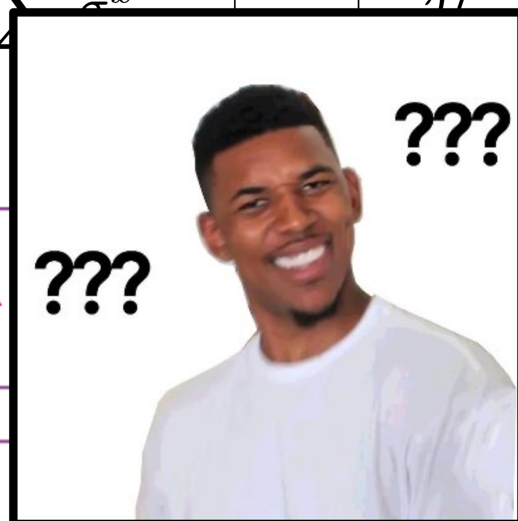

Heisenberg model

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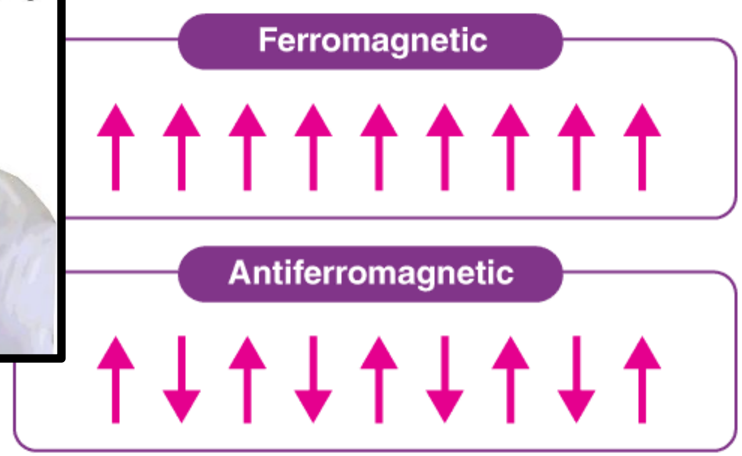

Ising Model

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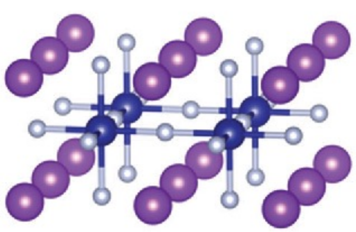

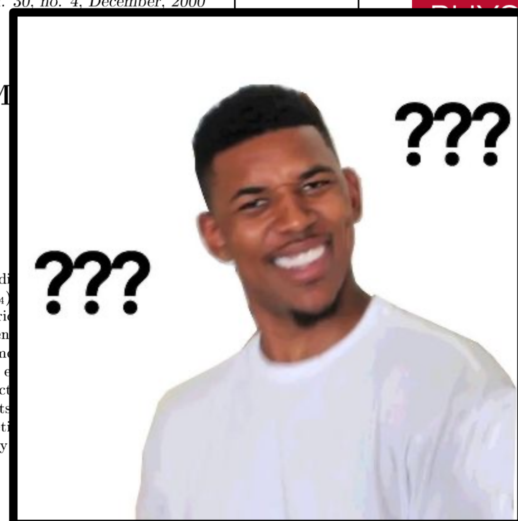

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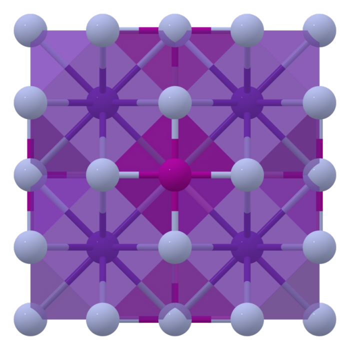

Materials project

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

A: You measure its excitations.

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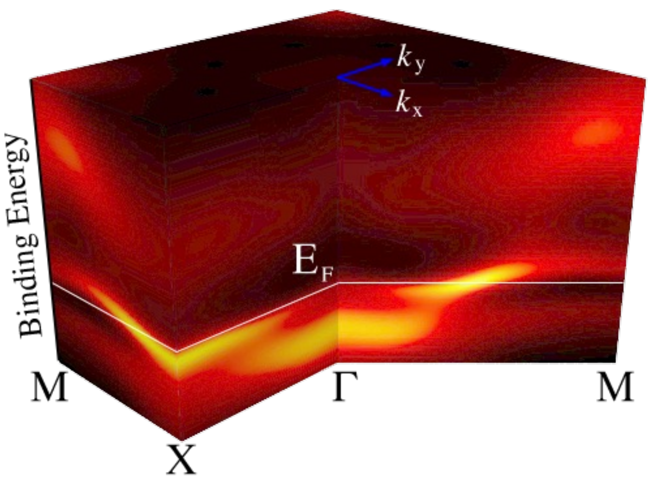
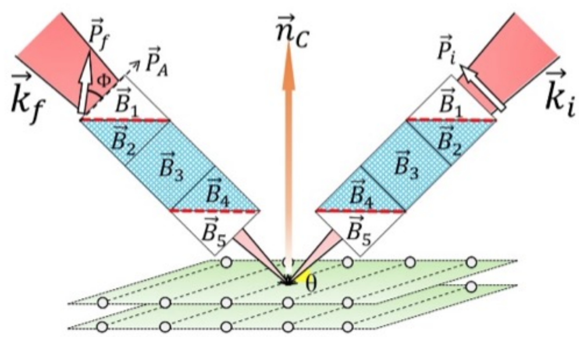
Measuring Excitations

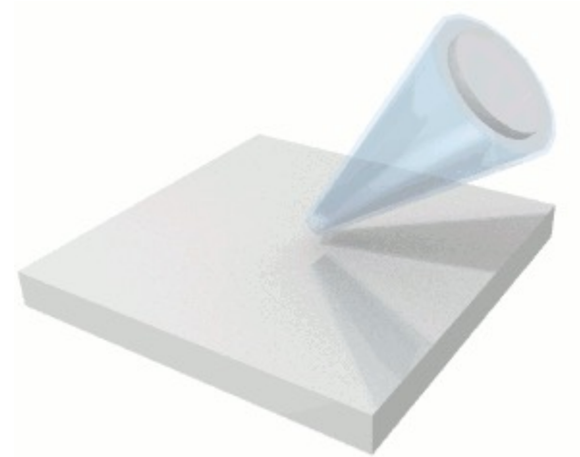
Figures courtesy of Devereaux/Shen group and ORNL



Angle-resolved Photoemission (ARPES)

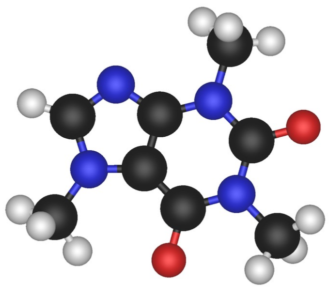


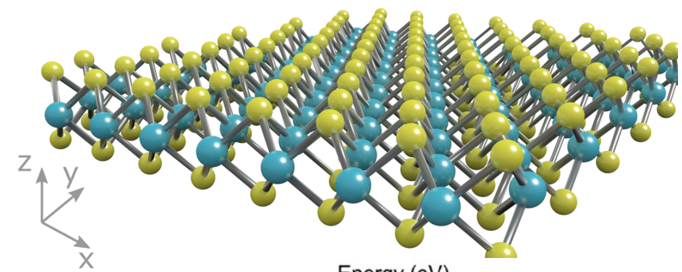
Neutron Scattering

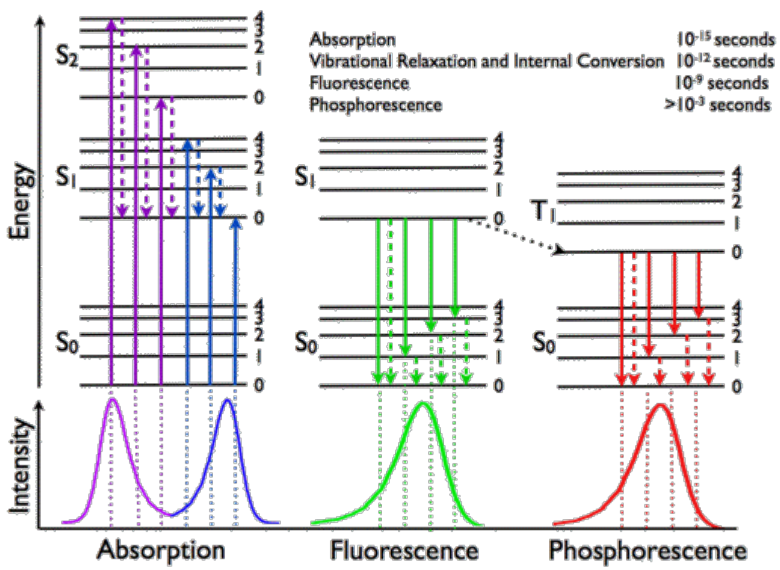


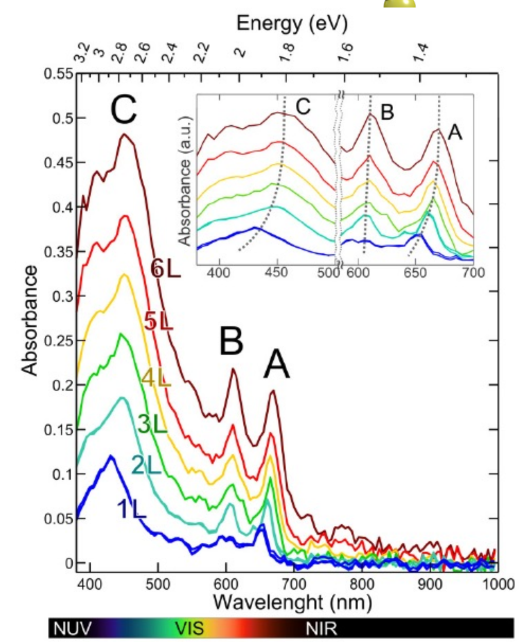
Time-resolved ARPES

Measuring Excitations









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Measuring Excitations

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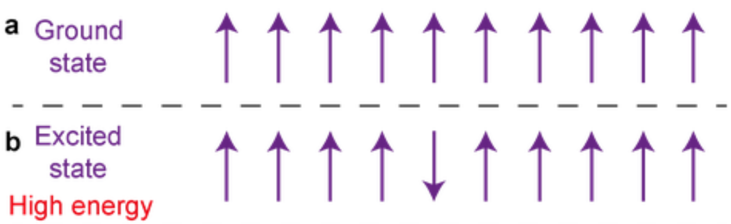

Heisenberg model

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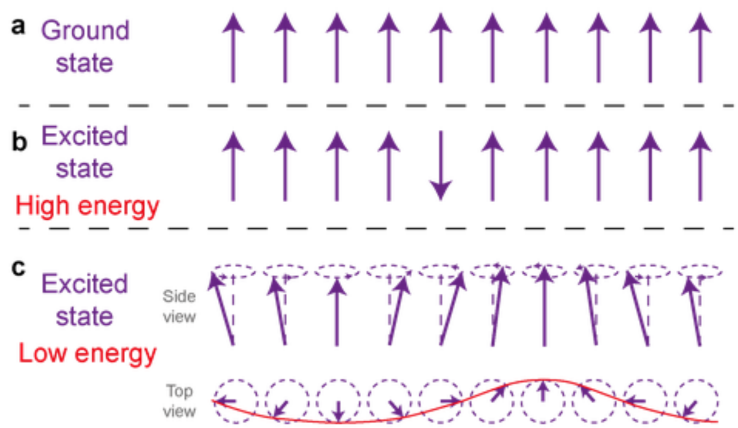
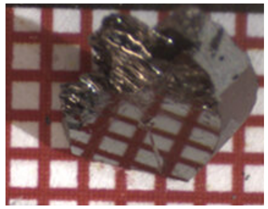
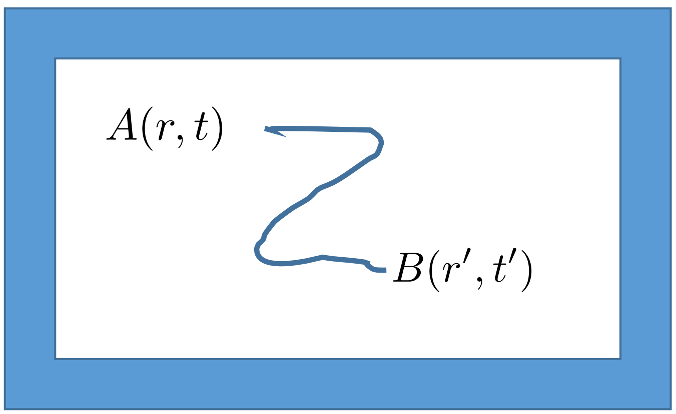


Quantum Computer = Quantum Simulator





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

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.

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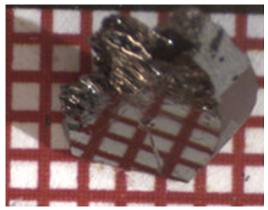
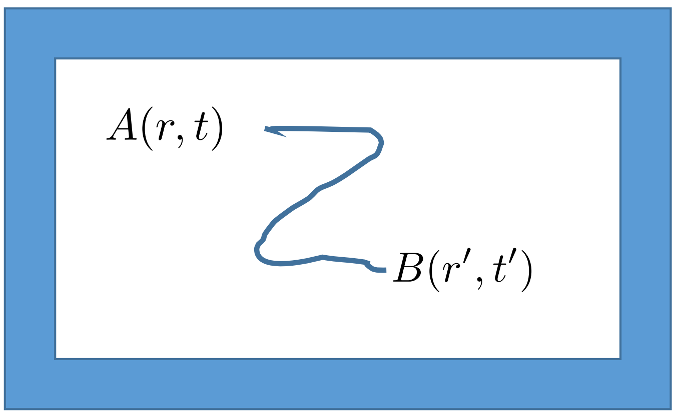
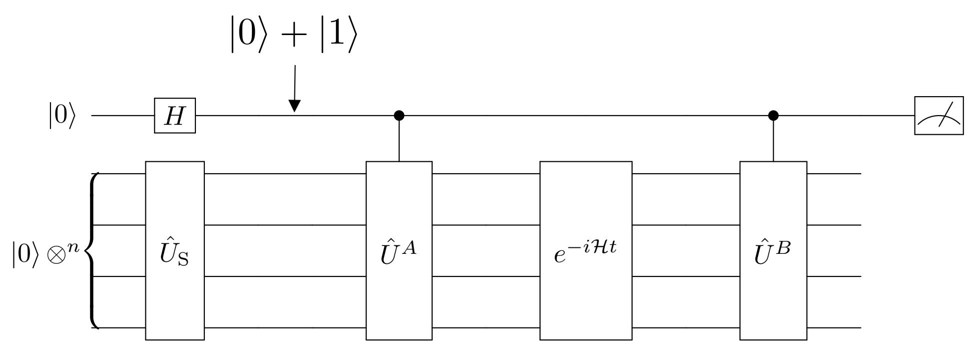
Quantum Computer = Quantum Simulator



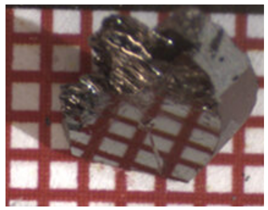


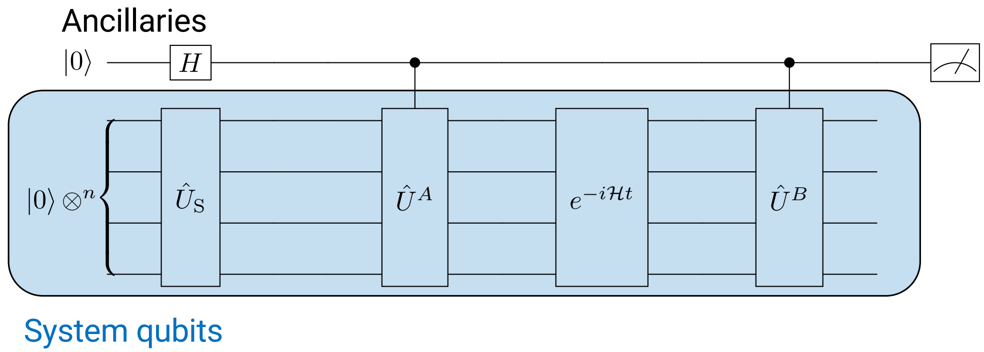
$$e^{iE_0 t}\langle\phi_0|Be^{-i\mathcal{H}t}A|\phi_0\rangle$$

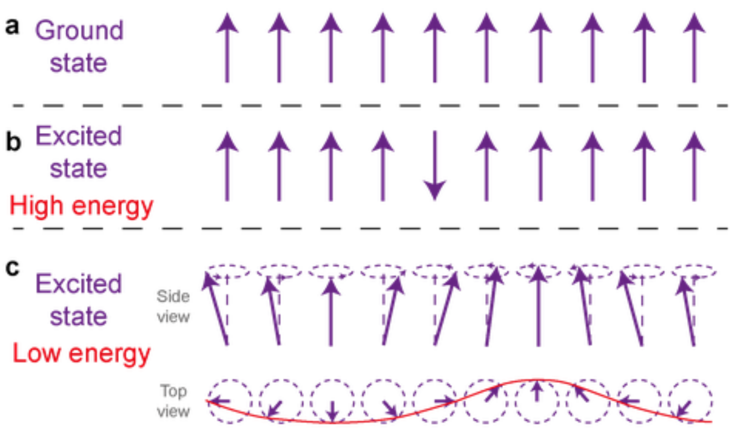
- Interfere with ground state
- Complete expectation value
- Apply excitation B
- Time evolve
- Apply excitation A
- Prepare state of interest



Correlation functions







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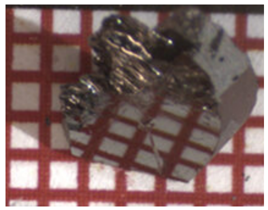
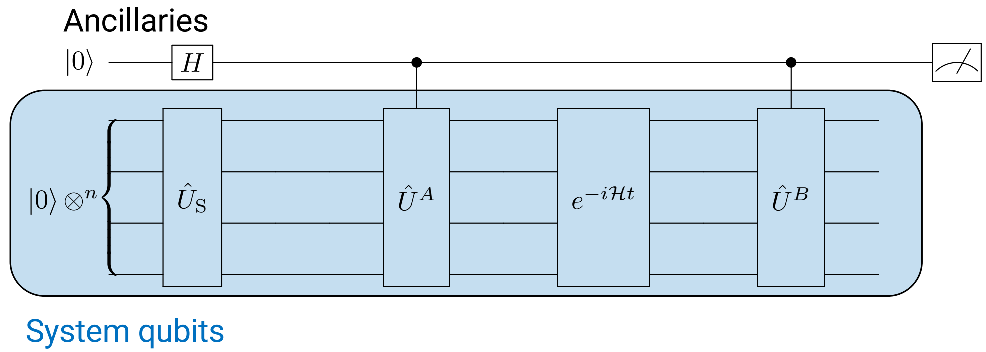
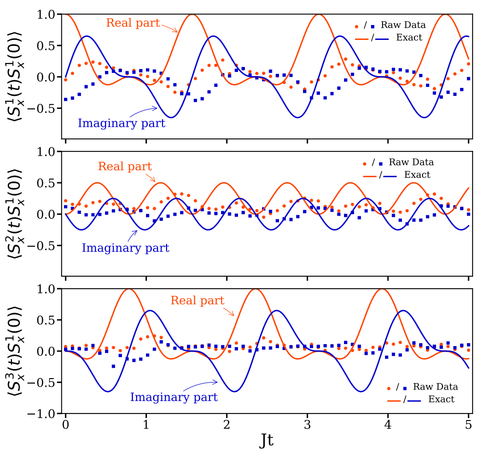


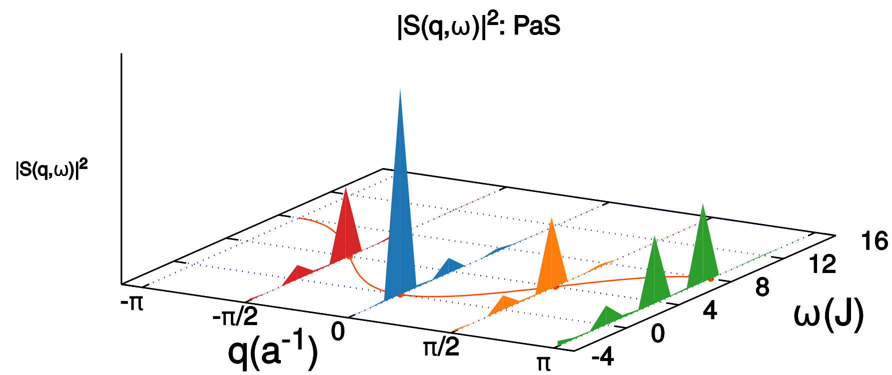


Raw data (2019)



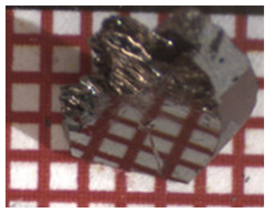
$$\langle A(r,t)B(r',t')\rangle$$

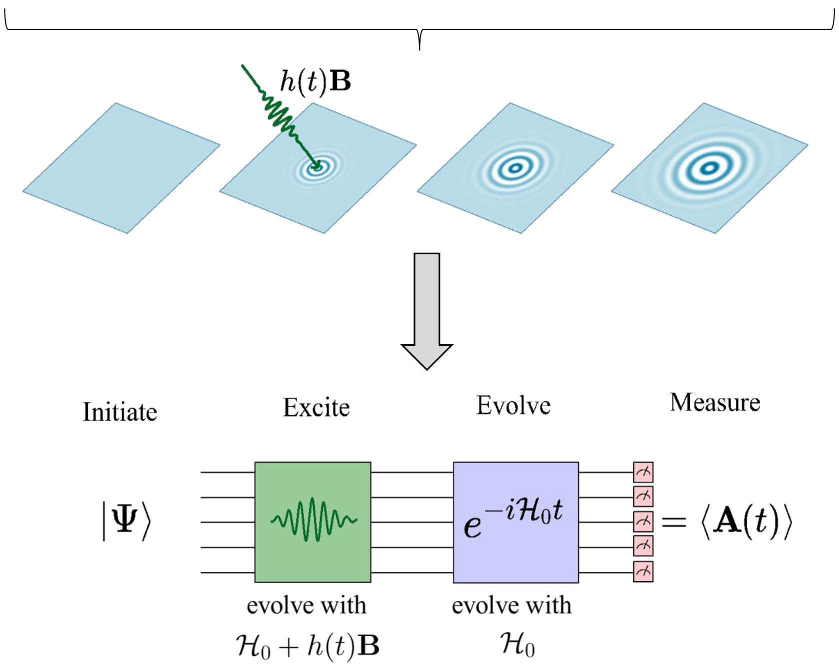
Error mitigation



Linear Response

2302.10219





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

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

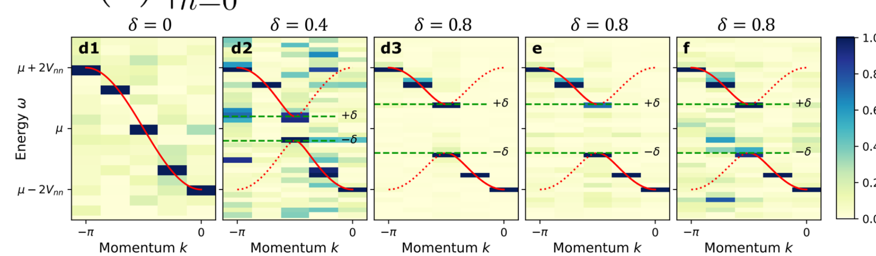
[1] *Department of Physics, North Carolina State University, Raleigh, North Carolina 27695, USA*
[2] *Department of Physics, Georgetown University, 37th and O Sts. NW, Washington, DC 20057 USA*

(Dated: February 22, 2023)

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

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

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

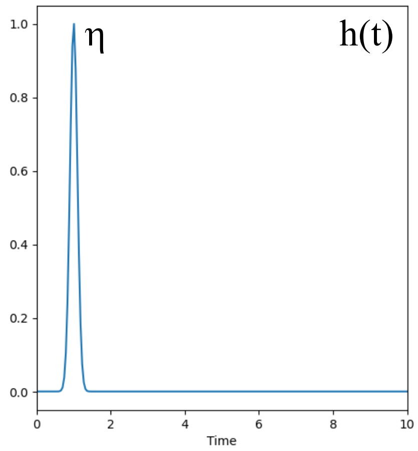


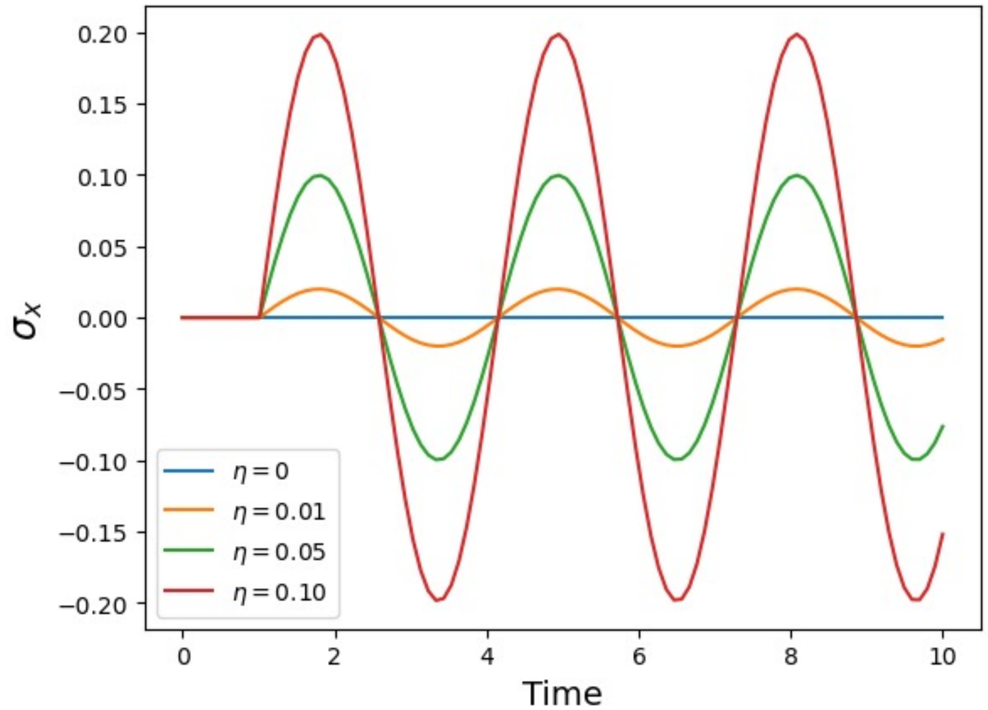
Linear Response

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

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

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





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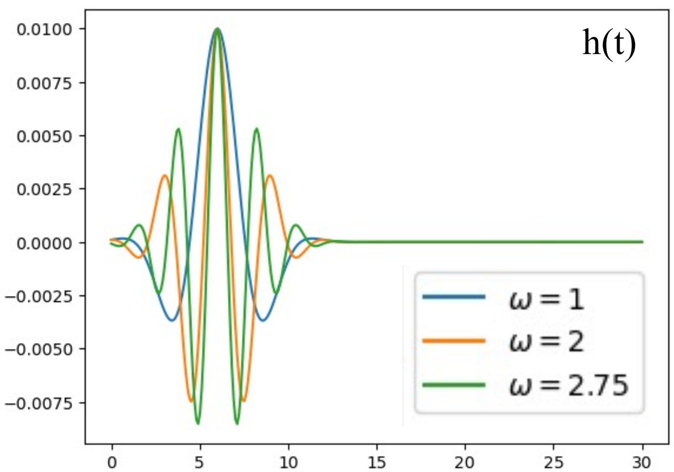
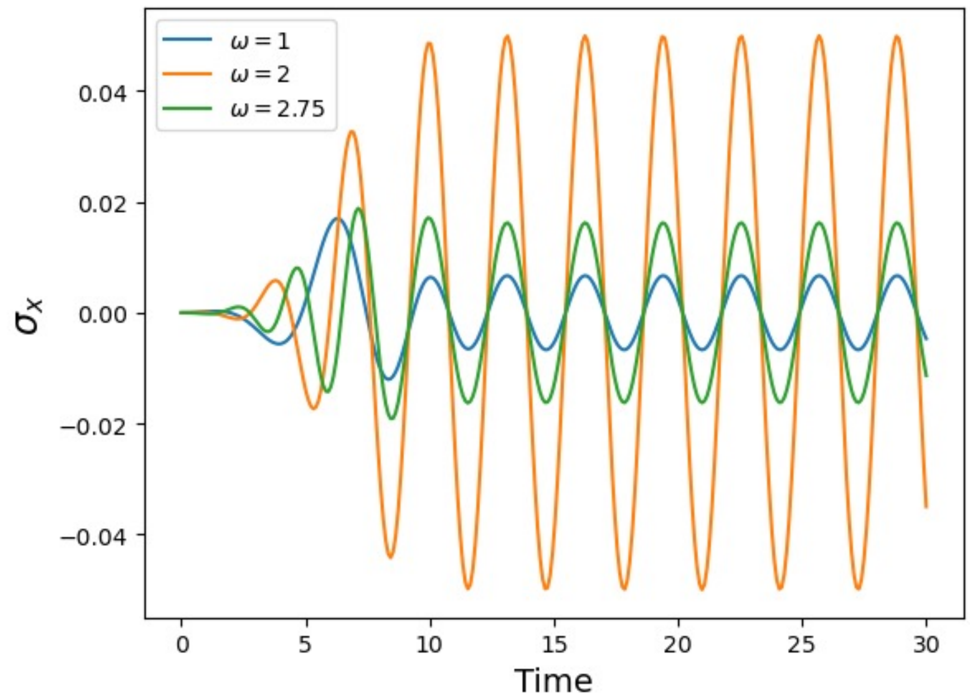


Frequency



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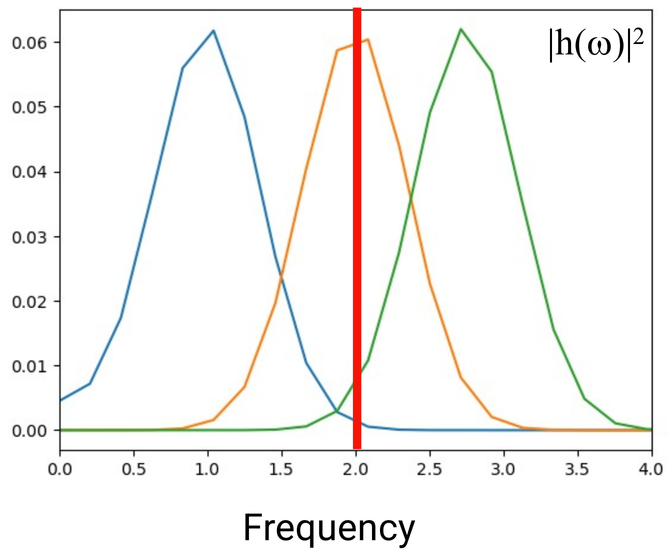
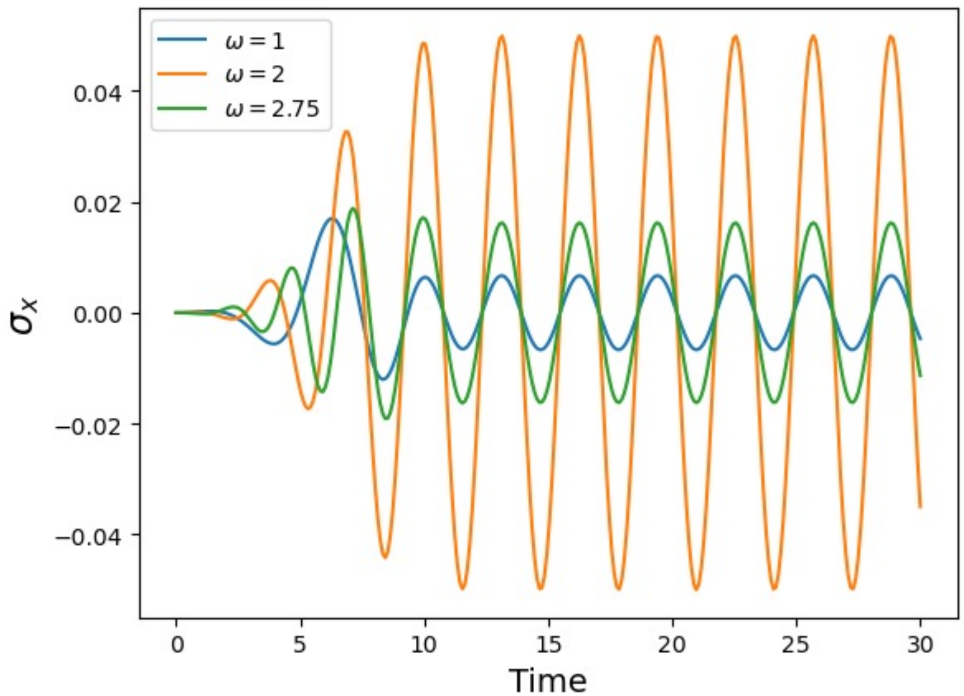
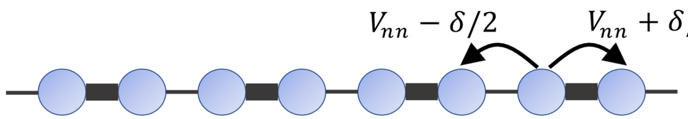




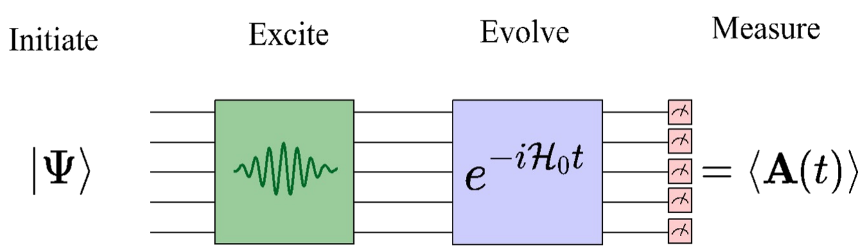
Linear Response -> Green's function

2302.10219

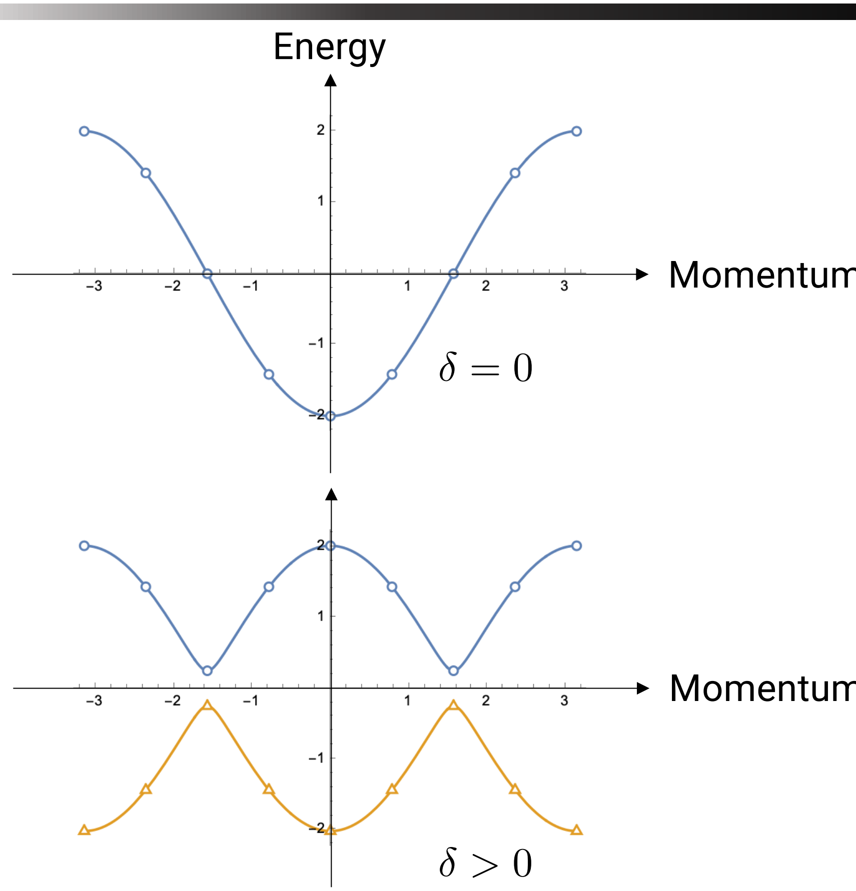
Su-Schrieffer-Heeger model for polyacetylene



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



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



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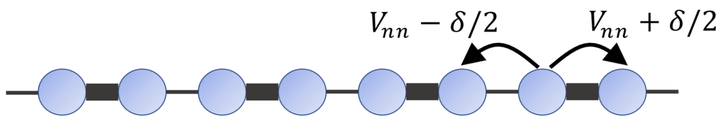

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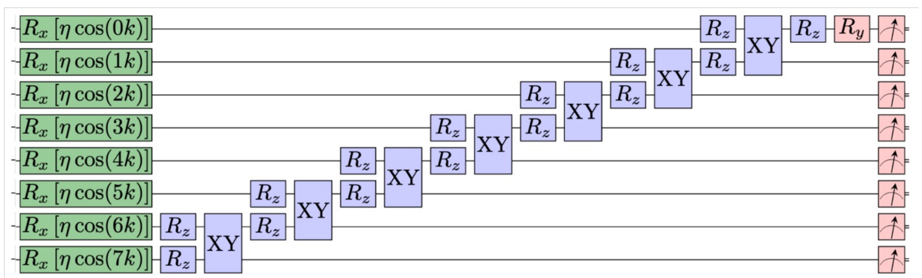
Compressed circuit run on *ibm_auckland*



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

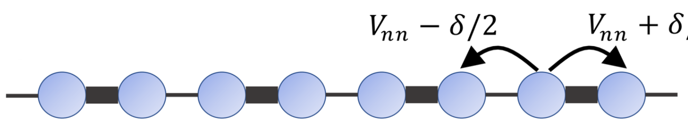
Choose **B** to create a momentum eigenstate

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

Linear Response -> Green's function

2302.10219

Su-Schrieffer-Heeger model for polyacetylene



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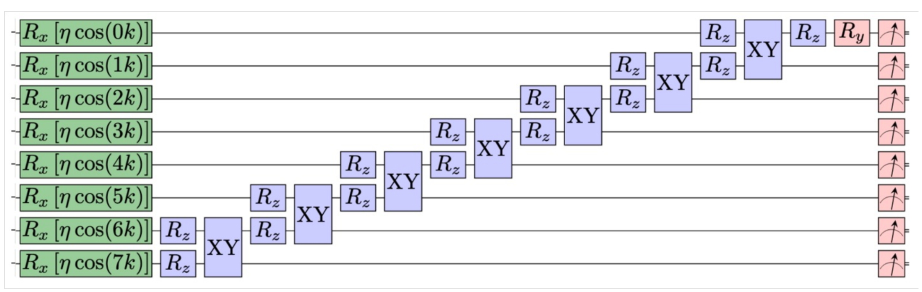
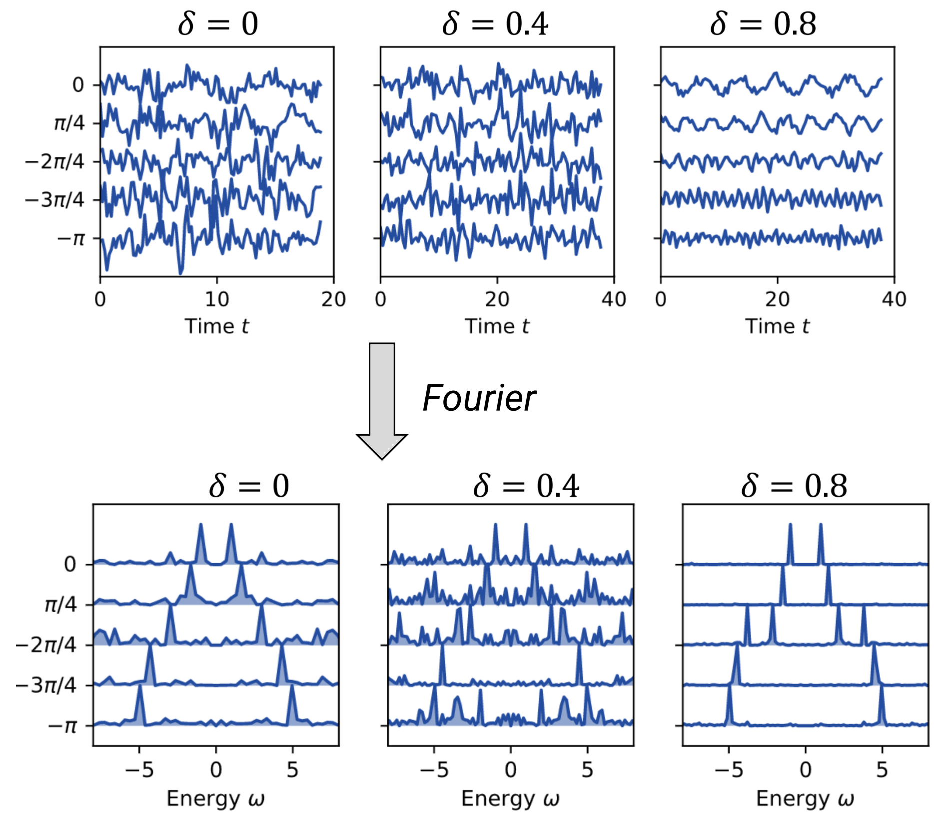
Compressed circuit run on *ibm_auckland*



Choose **B** to create a momentum eigenstate

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



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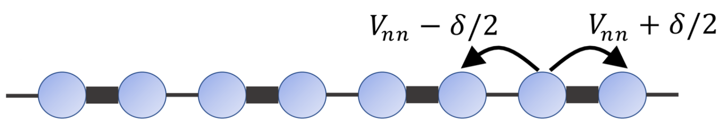
Linear Response -> Green's function

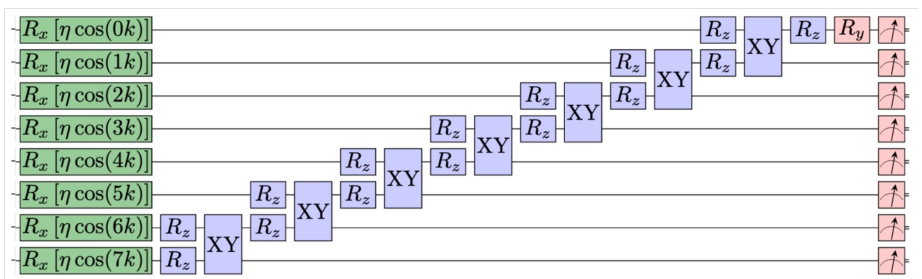
2302.10219

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*



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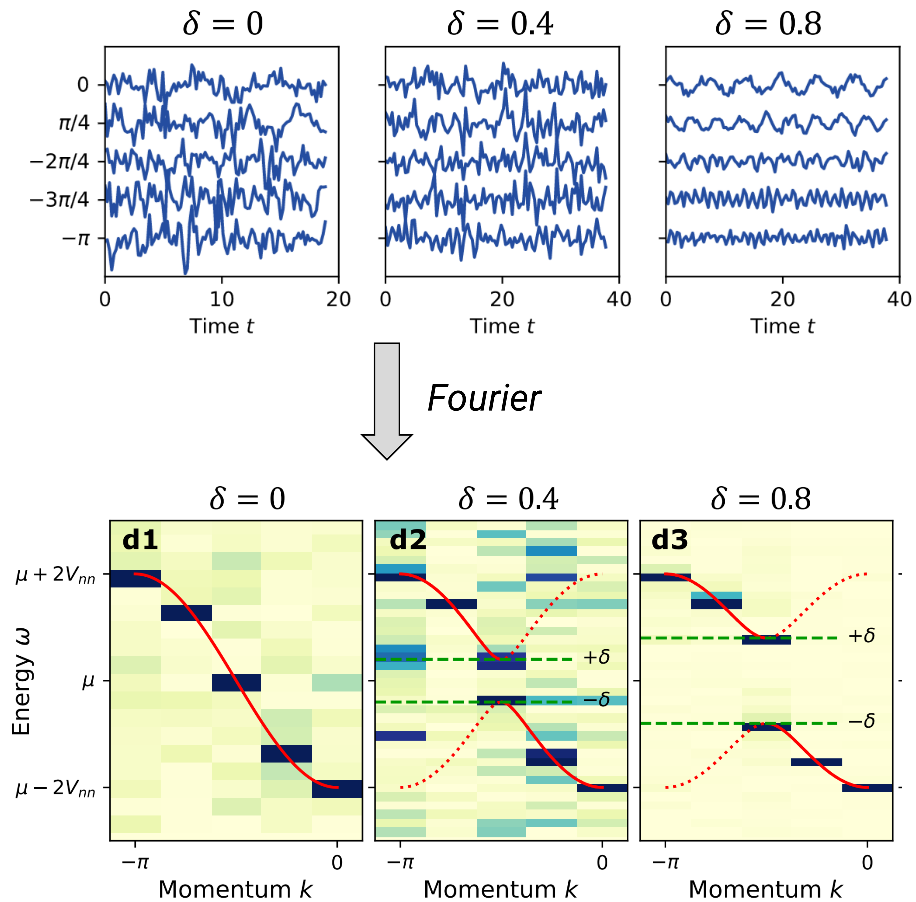

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Linear Response -> Green's function

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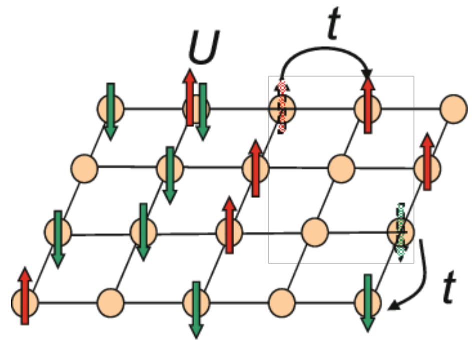

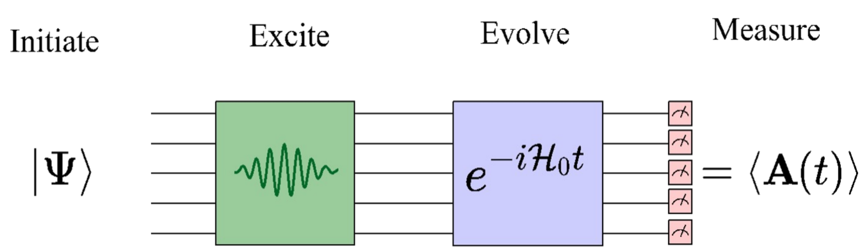

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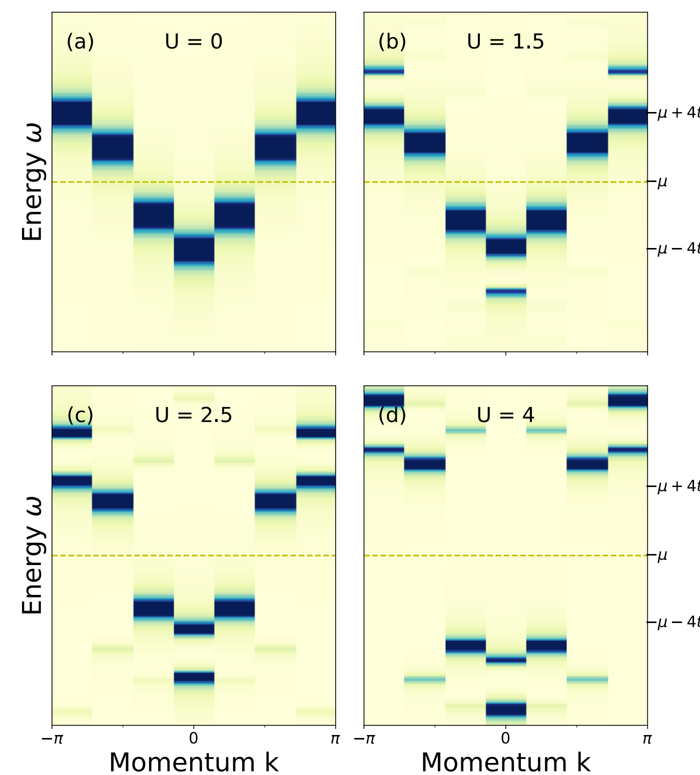

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Simulating Physics with Computers

Richard P. Feynman

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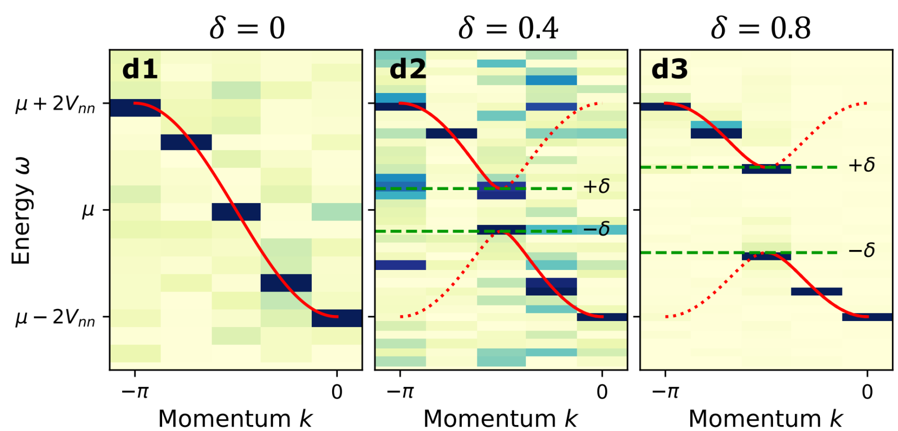
Received May 7, 1981



1. Can classical physics be simulated by a classical computer? ✓
2. Can quantum physics be simulated by a classical computer? ?
3. Can physics be simulated by a quantum computer? ✓

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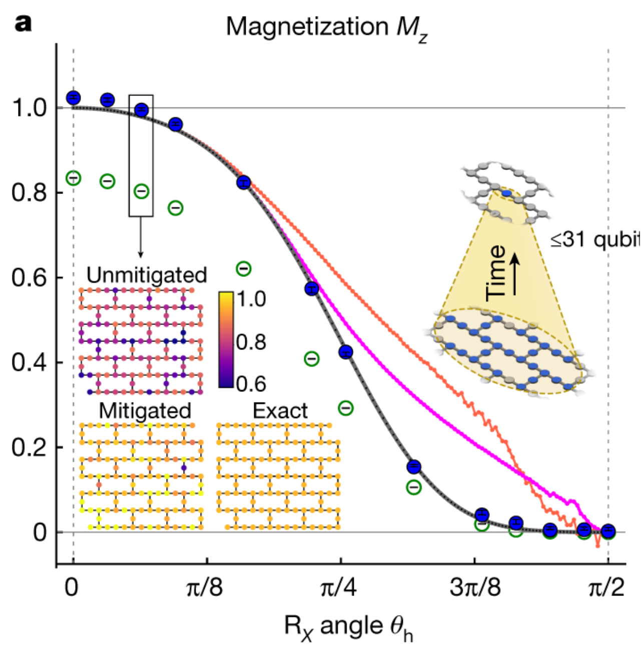
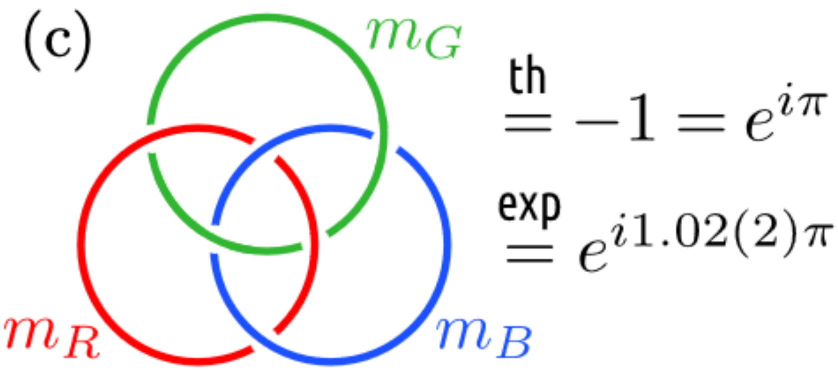
Bespoke quantum simulator — *Digital algorithms*



“Evidence for the utility of quantum computing before fault tolerance”
10.1038/s41586-023-06096-3



“Creation of Non-Abelian Topological Order and Anyons on a Trapped-Ion Processor,” arXiv:2305.03766.

Bespoke quantum simulator *Digital algorithms*

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Schor's algorithm
Integer factorization
Linear solvers (HHL)
Quantum Adiabatic Optimization
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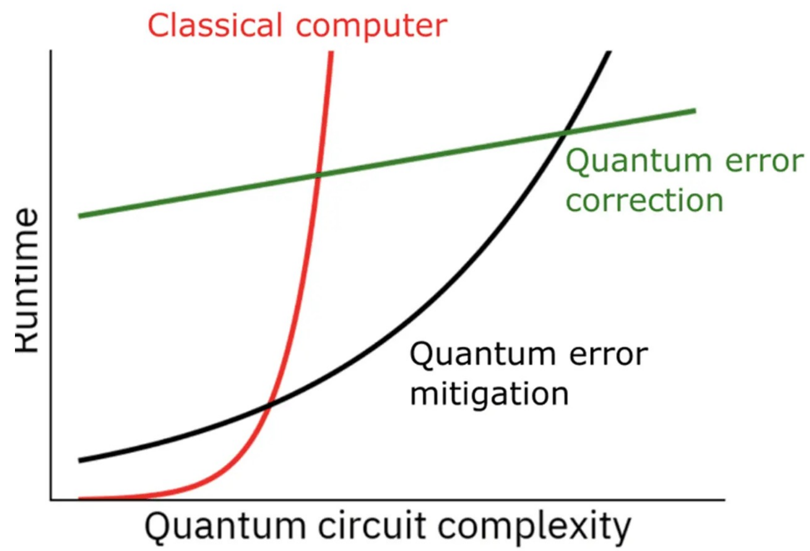

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Bespoke quantum simulator — *Digital algorithms*

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Schor's algorithm
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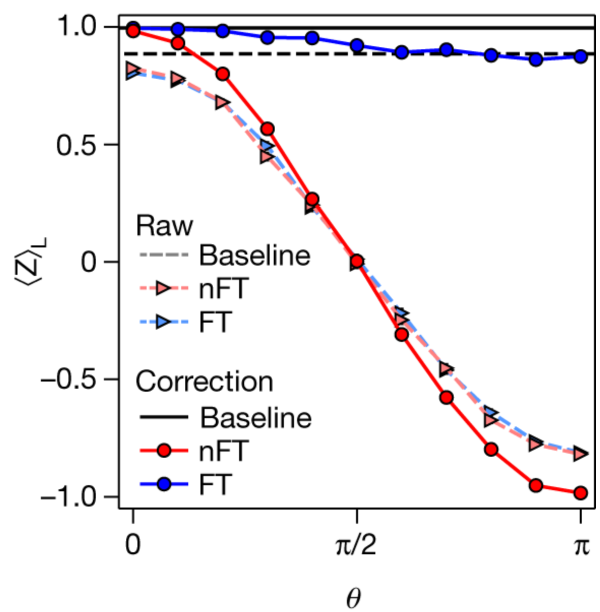

"Fault-tolerant control of an error-corrected qubit"
10.1038/s41586-021-03928-y

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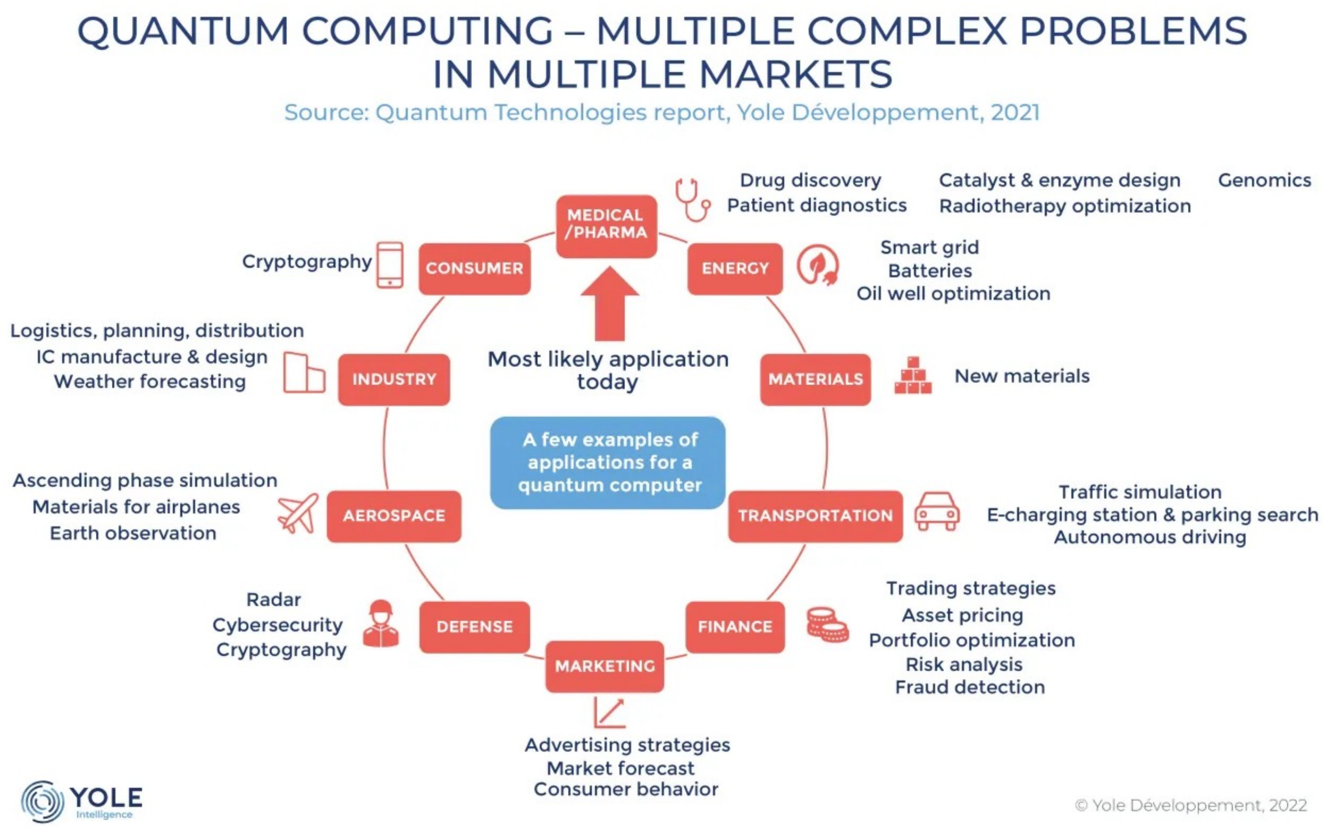

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frontiers in PHYSICS

REVIEW ARTICLE
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Ising formulations of many NP problems

Andrew Lucas*

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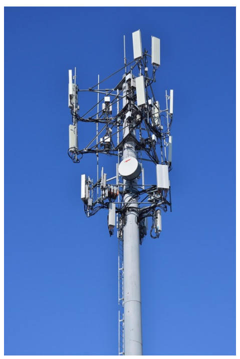
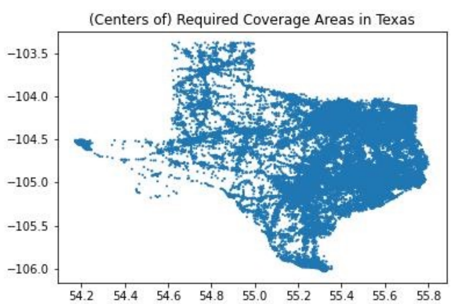
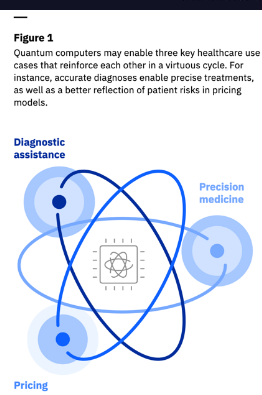
We provide Ising formulations for many NP-complete and NP-hard problems, including all of Karp's 21 NP-complete problems. This collects and extends mappings to the Ising model from partitioning, covering, and satisfiability. In each case, the required number of spins is at most cubic in the size of the problem. This work may be useful in designing adiabatic quantum optimization algorithms.

Keywords: spin glasses, complexity theory, adiabatic quantum computation, NP, algorithms

Problems with an unreasonably large solution space

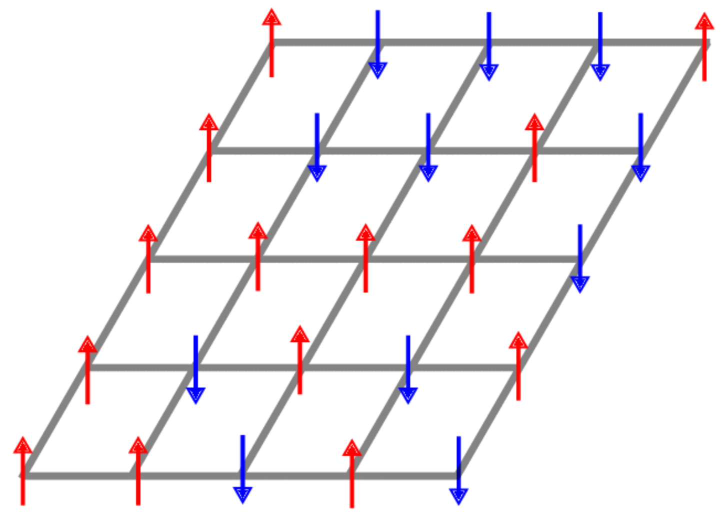






Ising Model

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



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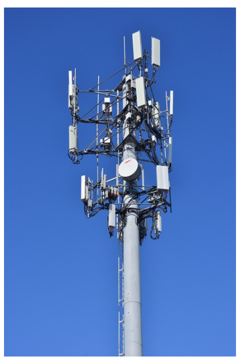

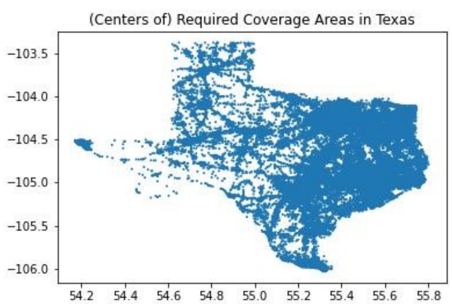

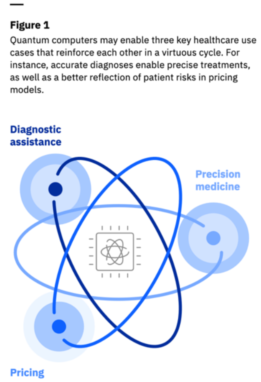

Variational algorithms

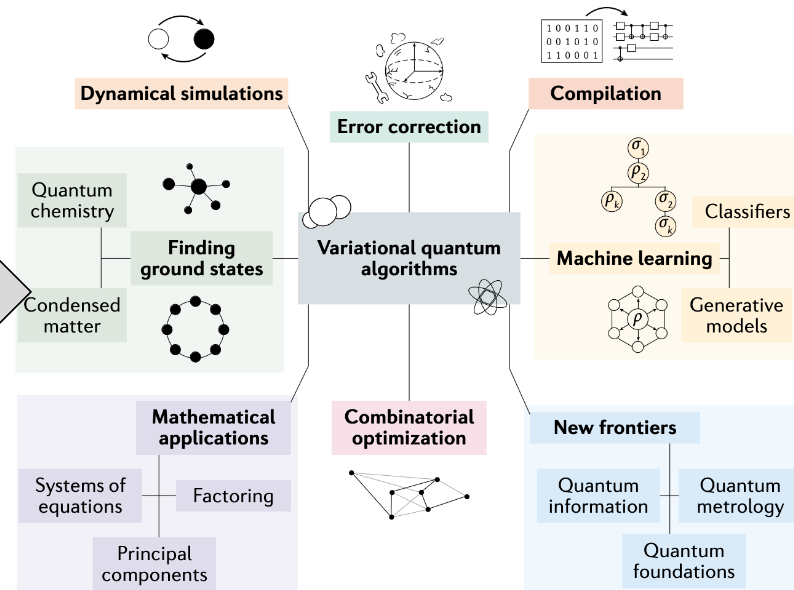

Fig. 1 | **Applications of variational quantum algorithms.** Many applications have been envisaged for variational quantum algorithms. Here we show some of the key applications that are discussed in this Review.

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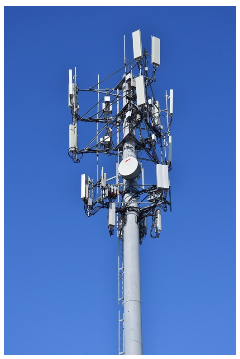
Problems with an unreasonably large solution space



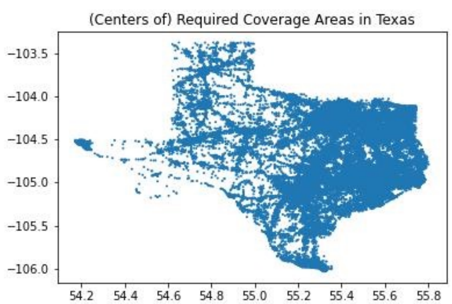
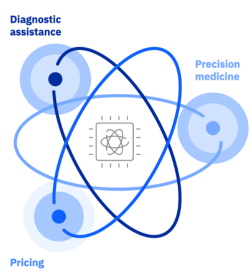


Figure 1
Quantum computers may enable three key healthcare use cases that reinforce each other in a virtuous cycle. For instance, accurate diagnoses enable precise treatments, as well as a better reflection of patient risks in pricing models.

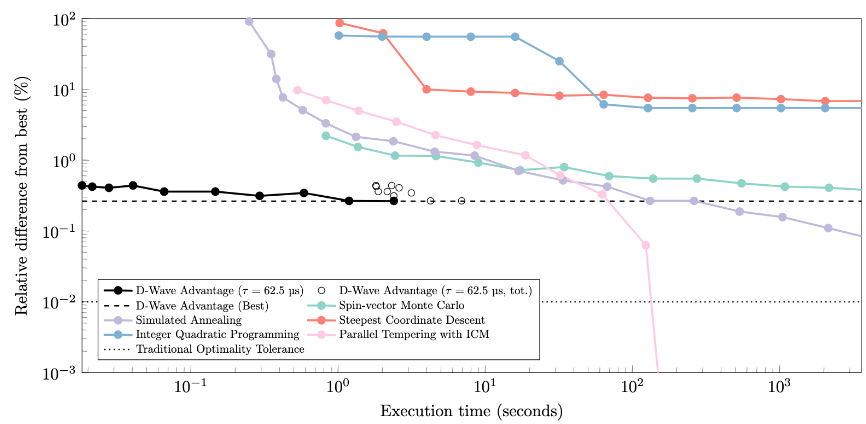


On the Emerging Potential of Quantum Annealing Hardware for Combinatorial Optimization

Byron Tasseff
Los Alamos National Laboratory, Los Alamos, NM 87545

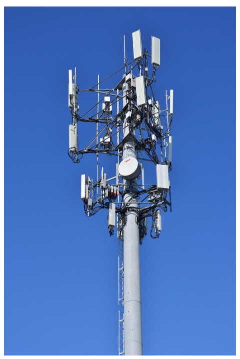
Tameem Albash
University of New Mexico, Albuquerque, NM 87131

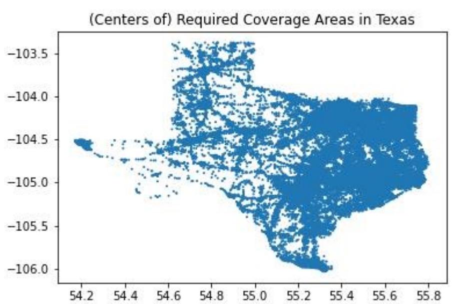
Zachary Morrell, Marc Vuffray, Andrey Y. Lokhov, Sidhant Misra, Carleton Coffrin*
Los Alamos National Laboratory, Los Alamos, NM 87545

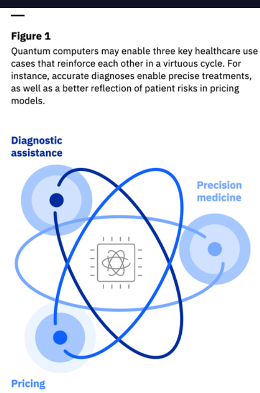


Why quantum computing?

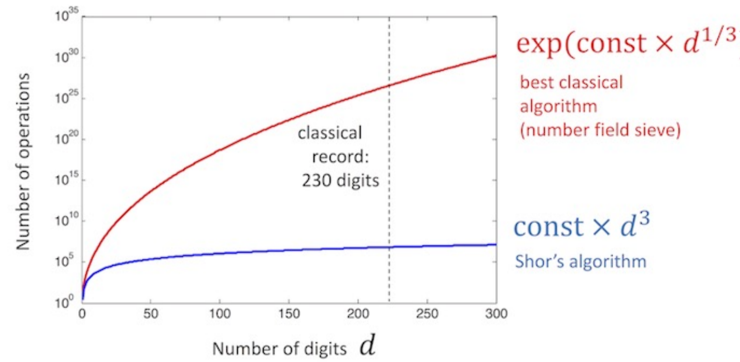
Problems with an unreasonably large solution space

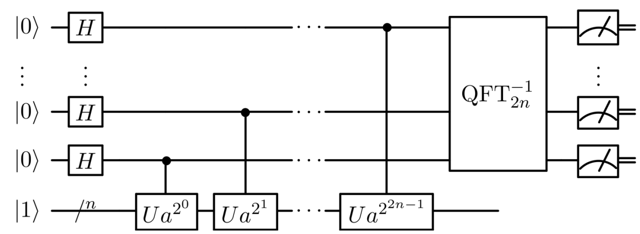






Efficient algorithms

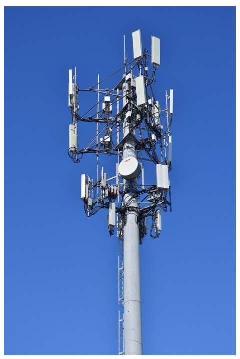


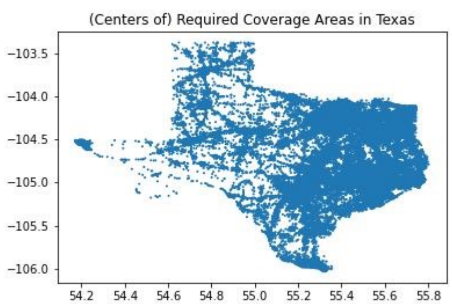


https://quantum-computing.ibm.com/

Why quantum computing?

Problems with an unreasonably large solution space





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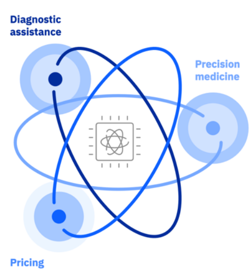
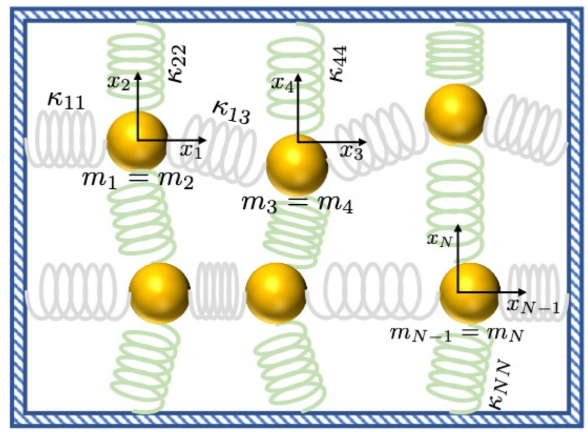


Efficient algorithms

Exponential quantum speedup in simulating coupled classical oscillators

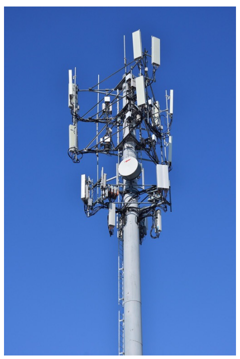
Ryan Babbush,[1] Dominic W. Berry,[2] Robin Kothari,[1] Rolando D. Somma,[1] and Nathan Wiebe[3,4,5]

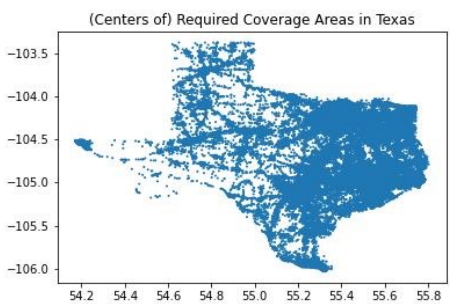


2303.13012

Why quantum computing?

Problems with an unreasonably large solution space





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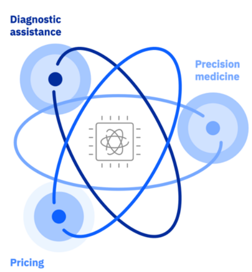


Efficient algorithms

A quantum algorithm for the linear Vlasov equation with collisions

Abtin Ameri
Plasma Science and Fusion Center, Massachusetts Institute of Technology, Cambridge, MA 02139

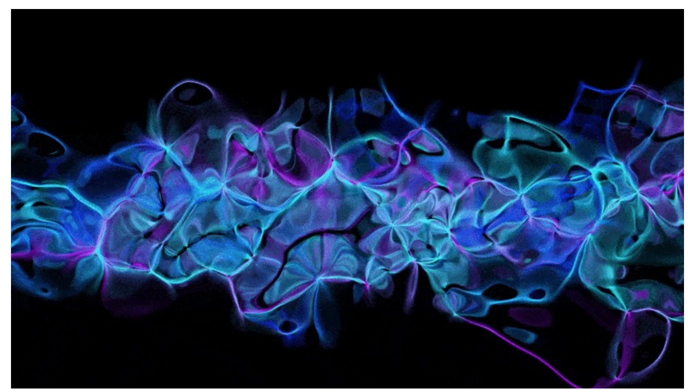
Paola Cappellaro
Research Laboratory of Electronics and Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139

Hari Krovi
Riverlane Research, Cambridge, MA 02142

Nuno F. Loureiro
Plasma Science and Fusion Center, Massachusetts Institute of Technology, Cambridge, MA 02139

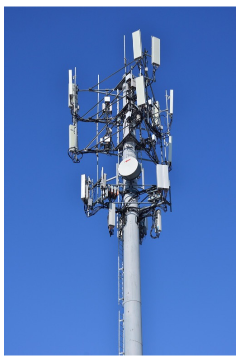
Erika Ye
Plasma Science and Fusion Center, Massachusetts Institute of Technology, Cambridge, MA 02139

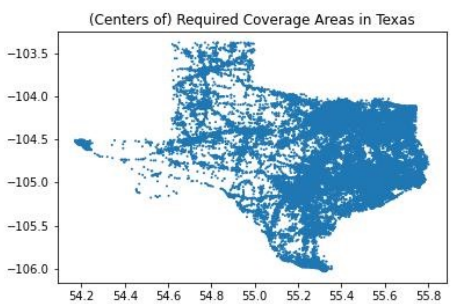
(Dated: March 8, 2023)



Why quantum computing?

Problems with an unreasonably large solution space





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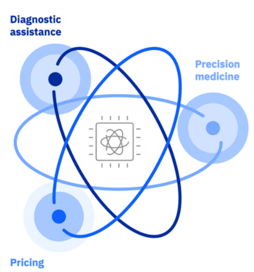
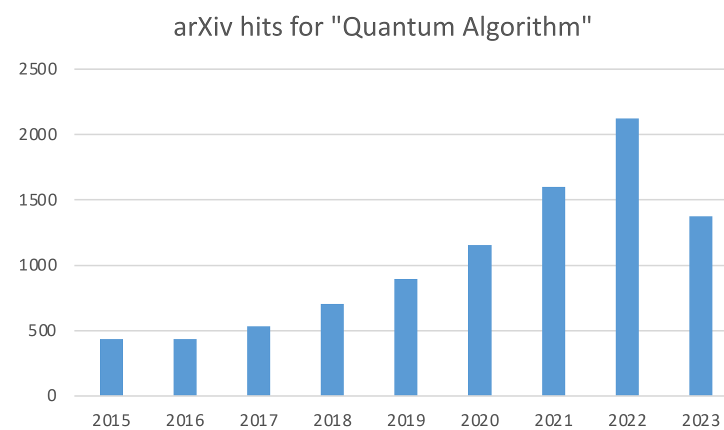


Efficient algorithms



(data from June 2023)

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Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981

1. Can classical physics be simulated by a classical computer?
2. Can quantum physics be simulated by a classical computer?
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Quantum Matter meets Quantum Computing

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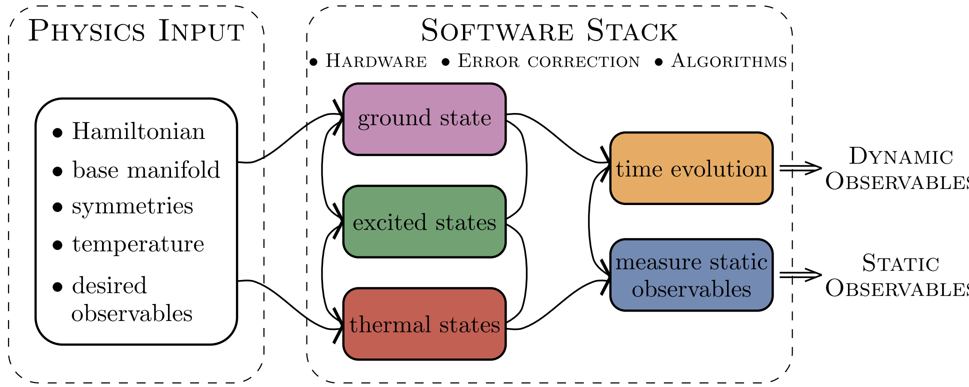

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