

# Quantum Computational Science

---

---

Aiichiro Nakano

*Collaboratory for Advanced Computing & Simulations*

*Department of Computer Science*

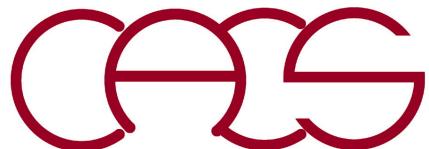
*Department of Physics & Astronomy*

*Department of Quantitative & Computational Biology*

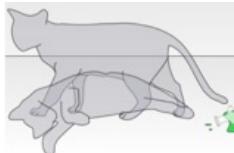
*University of Southern California*

Email: [anakano@usc.edu](mailto:anakano@usc.edu)

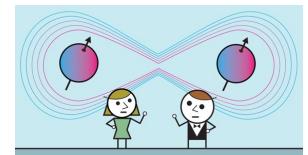
Goal: Quantum dynamics simulation on quantum circuits



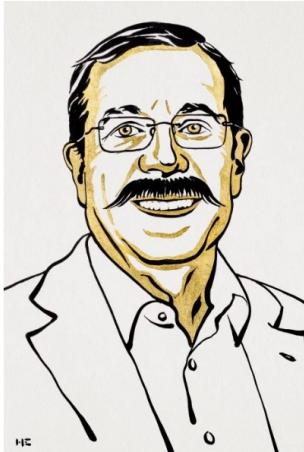
# Quantum Computing Is Hot



Quantum computing utilizes quantum properties such as superposition & entanglement for computation



## The Nobel Prize in Physics 2022



III. Niklas Elmehed © Nobel Prize Outreach

Alain Aspect

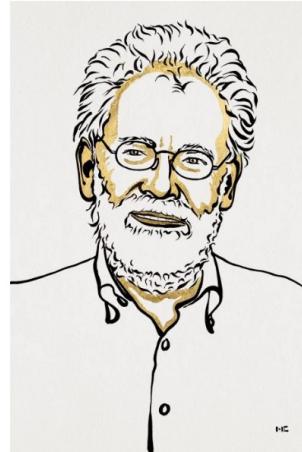
Prize share: 1/3



III. Niklas Elmehed © Nobel Prize Outreach

John F. Clauser

Prize share: 1/3

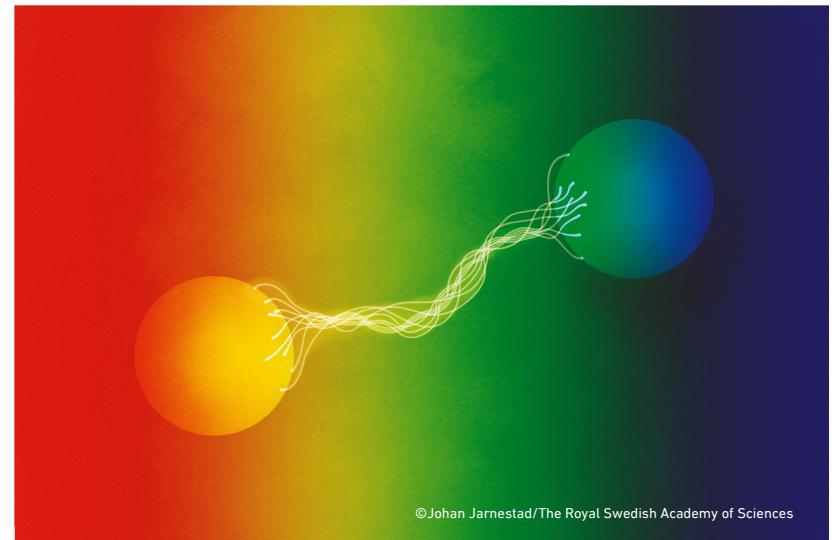


III. Niklas Elmehed © Nobel Prize Outreach

Anton Zeilinger

Prize share: 1/3

*It's entanglement!*



© Johan Jarnestad/The Royal Swedish Academy of Sciences

The Nobel Prize in Physics 2022 was awarded jointly to Alain Aspect, John F. Clauser and Anton Zeilinger "for experiments with entangled photons, establishing the violation of Bell inequalities and pioneering quantum information science"

*cf.* Microsoft Majorana 1 chip (Feb. 19, '25)  
<https://news.microsoft.com/azure-quantum/>

# Quantum Computing Is Now

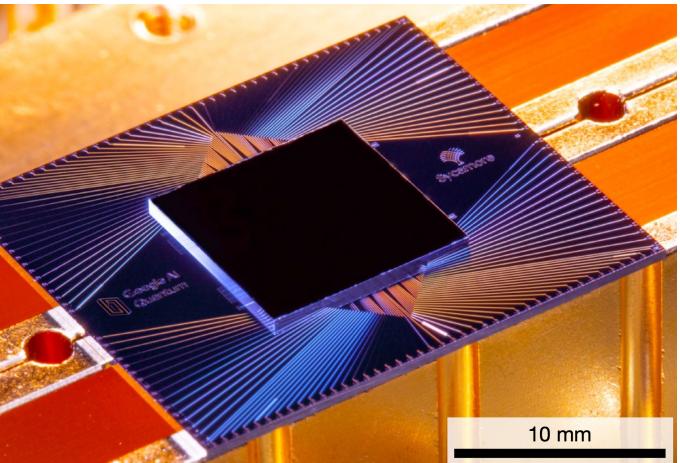
- U.S. Congress (Dec. 21, '18) signed National Quantum Initiative Act to ensure leadership in quantum computing & its applications
- Quantum supremacy (*i.e.*, quantum computer is faster than the fastest supercomputer) was demonstrated by Google  
F. Arute, J. Martinis, et al., *Nature* 574, 505 ('19)
- Google's Sycamore quantum computer consumed 26 kilowatts of power to outperform the 13 megawatts Summit supercomputer at Oak Ridge National Lab, *i.e.*, 500 times more energy efficient



9,216-CPU & 27,648-GPU Summit



*Fast  
&  
frugal*



53-qubit Google Sycamore

# Quantum Computing Gets Hotter

## Nobel Prize in Physics 2025



Ill. Niklas Elmehed © Nobel Prize Outreach

John Clarke

Prize share: 1/3



Ill. Niklas Elmehed © Nobel Prize Outreach

Michel H. Devoret

Prize share: 1/3

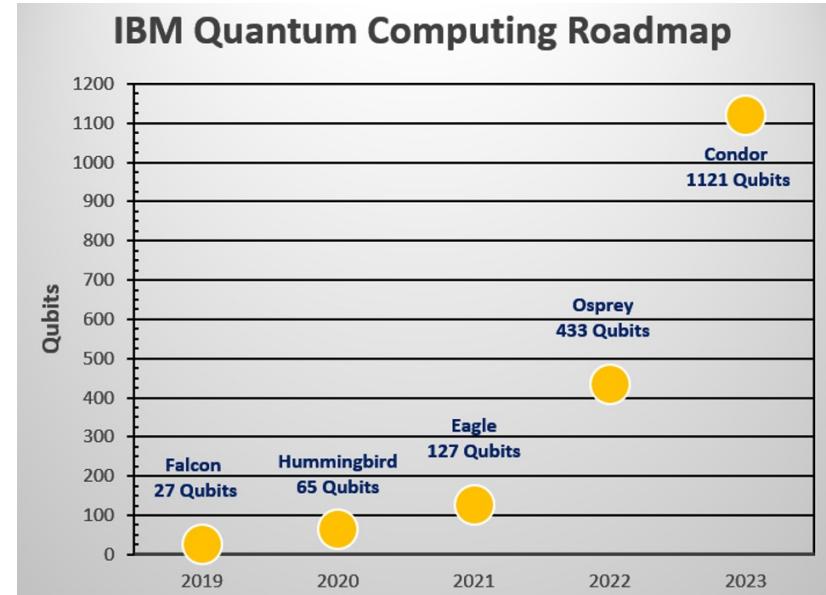
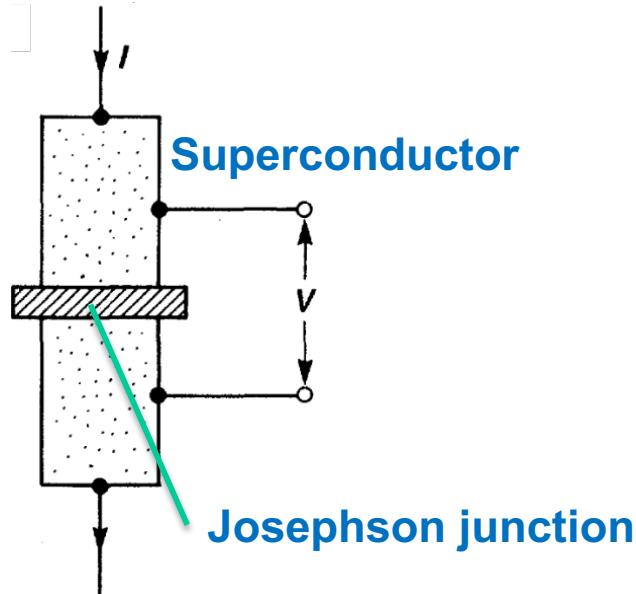


Ill. Niklas Elmehed © Nobel Prize Outreach

John M. Martinis

Prize share: 1/3

The Nobel Prize in Physics 2025 was awarded jointly to John Clarke, Michel H. Devoret and John M. Martinis "for the discovery of macroscopic quantum mechanical tunnelling and energy quantisation in an electric circuit"



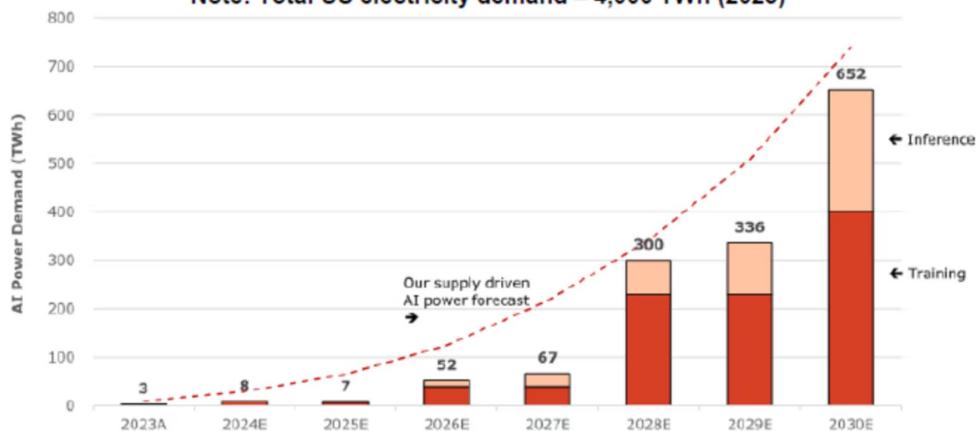
*Foundation of superconducting quantum circuits*

# Why Care?

## Summary of GenAI demand forecast

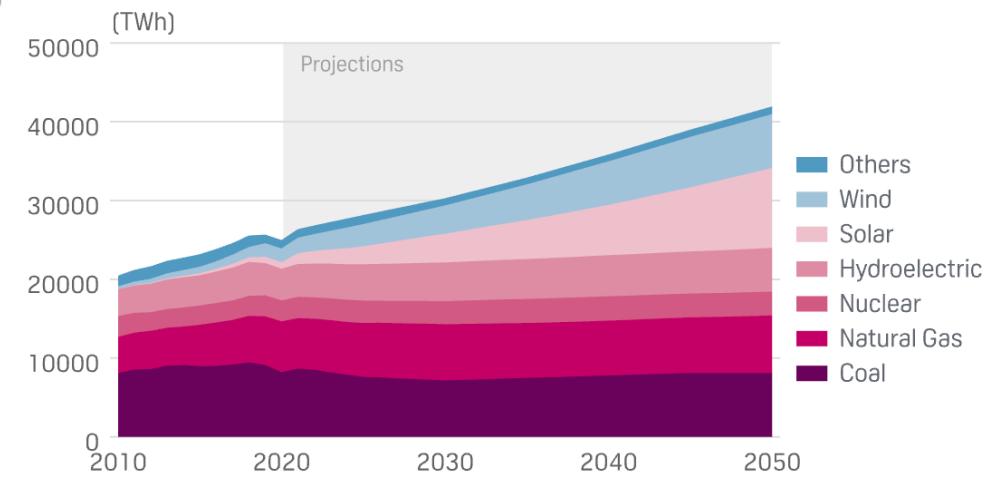
Source: Wells Fargo

Note: Total US electricity demand – 4,000 TWh (2023)



- Exponential growth of energy demand for AI-computing

## GLOBAL NET ELECTRICITY GENERATION BY SOURCE

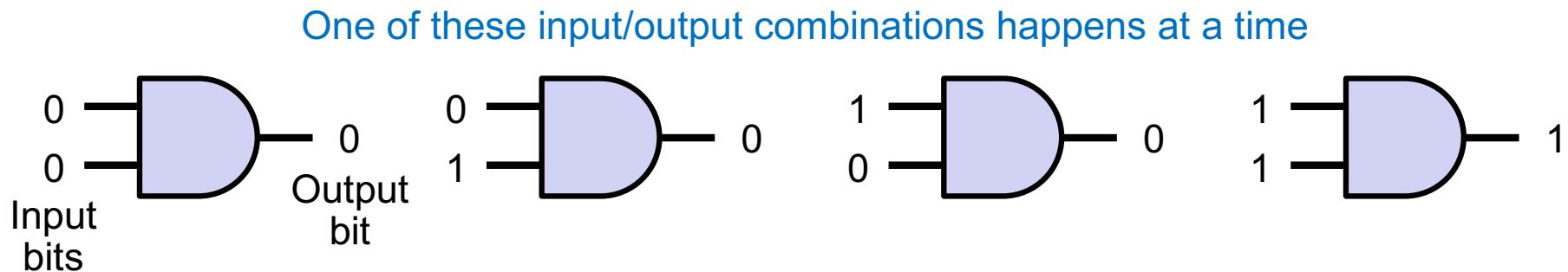


Source: EIA's International Energy Outlook 2021

- Who will power your future AI-computing without burning out the Earth?
- Quantum computing may be the answer!

# What Is Computing?

- Information is stored as a string of bits (0 or 1, e.g., low or high voltage)
- Computer performs arithmetic (add, multiply, subtract, divide) & logical (and, or, not) operations on bit strings
- Example: logical AND gate



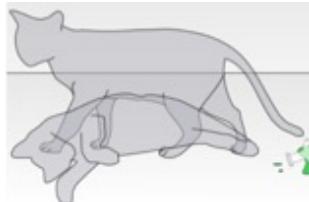
von Neumann computer architecture (1944)



# What Is Quantum Mechanics?

- State of matter (e.g., electron) is described by a complex-number wave function; its square is the probability to find the matter in a particular state
- Qubit: Superposition of 0 & 1 states with complex-number prefactors

$$|\psi_{\text{qubit}}\rangle = a|0\rangle + b|1\rangle$$

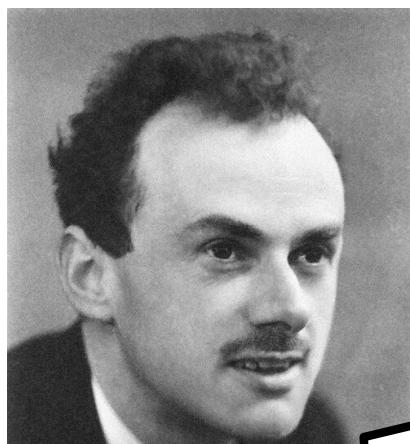


$$|\text{cat}\rangle = a|\text{alive}\rangle + b|\text{dead}\rangle$$

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] \psi(\vec{r}, t)$$
$$P(\vec{r}, t) = |\psi(\vec{r}, t)|^2 \sim \text{probability}$$
$$\psi(\vec{r}, t) = \text{Re}\psi(\vec{r}, t) + i\text{Im}\psi(\vec{r}, t)$$
$$i = \sqrt{-1}$$



Erwin Schrödinger  
1933 Nobel physics prize

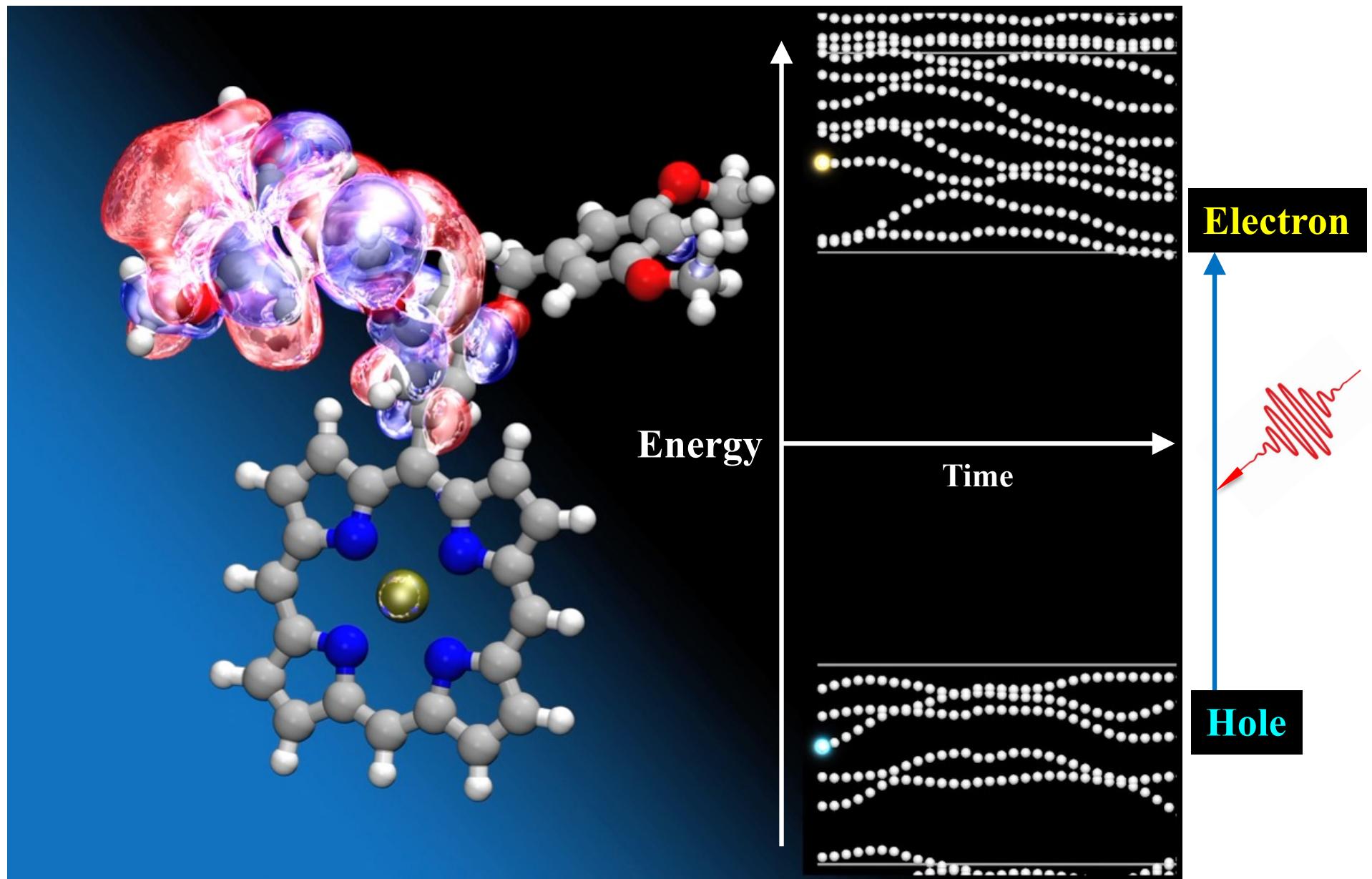


Paul Dirac  
1933 Nobel  
physics prize

- Quantum mechanics is exponentially hard — just describing  $n$ -qubit quantum state requires  $2^n$  coefficients (e.g.,  $2^{100} \sim 10^{30}$ )

The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are completely known, and the difficulty is only that the exact application of these laws leads to equations **much too complicated to be soluble**.

# Quantum Mechanics on Supercomputers



*That's what we do*

# In the Beginning ...



*Journey of Electrons and Atoms: Personal Story of Quantum Mechanics & Supercomputing (Nov. 16 & 17, '24, Culver City, CA)*



<https://magazine.viterbi.usc.edu/spring-2025/engineering/just-dance/>

# Now the Problem ... and Solution

- Quantum mechanics is exponentially hard — just describing  $n$ -qubit quantum state requires  $2^n$  coefficients (e.g.,  $2^{100} \sim 10^{30}$ )
- But, the memory size of the world's largest supercomputer, El Capitan at Lawrence Livermore National Lab, is merely  $7 \times 10^5$  double-precision words



*Nature isn't classical,  
dammit, and if you want to  
make a simulation of nature,  
you'd better make it quantum  
mechanical.*



- Feynman to the rescue: Let quantum mechanics compute itself, i.e., quantum computing!

Int. J. Theor. Phys. 21, 467 ('82)

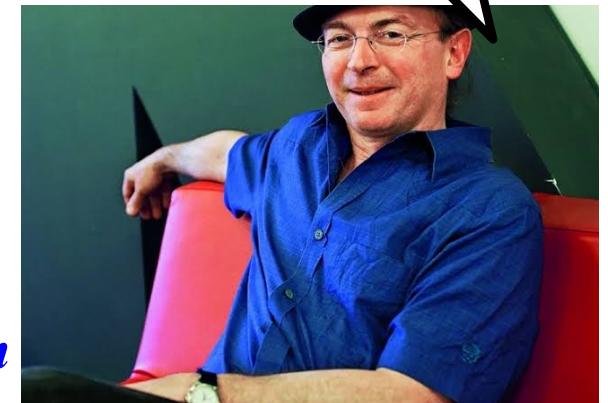
Richard Feynman  
1965 Nobel physics prize

# Quantum Computational Science

- An exciting scientific application of quantum computers is as a universal simulator of quantum many-body dynamics, as envisioned by Richard Feynman *Int. J. Theor. Phys.* **21**, 467 ('82)
- Seth Lloyd provided concrete algorithms and analysis *Science* **273**, 1073 ('96)  
Watch Seth's movie: <https://www.youtube.com/watch?v=EMzKshc6x2M>

<https://www.amazon.com/Programming-Universe-Quantum-Computer-Scientist-ebook/dp/B000GCFBP6>

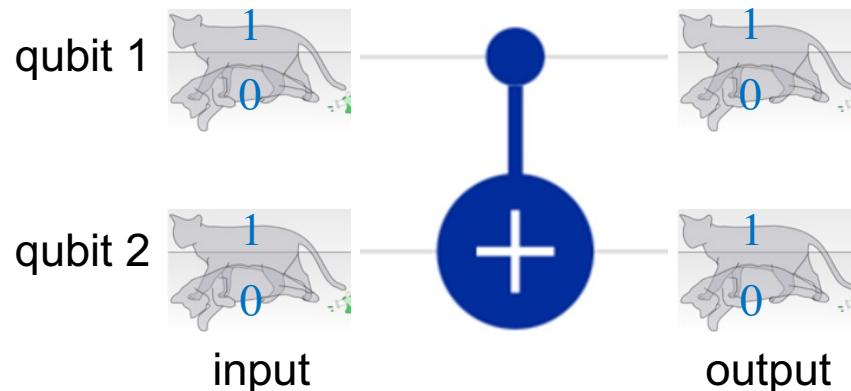
*Is the universe actually a giant quantum computer? According to Seth Lloyd, the answer is yes.*
- Success in simulating *static* properties of quantum systems (*i.e.*, ground-state energy of small molecules)  
Aspuru-Guzik *et al.*, *Science* **309**, 1704 ('05)
- Challenge: Simulate quantum many-body *dynamics* on current-to-near-future noisy intermediate-scale quantum (**NISQ**) computers  
J. Preskill, *Quantum* **2**, 79 ('18)
- Second edition of *Feynman Lectures on Computation* (2023) added a section on “Simulating quantum dynamics” by John Preskill [arXiv:2106.10522 \('21\)](https://arxiv.org/abs/2106.10522)



<https://www.amazon.com/Feynman-Lectures-Computation-Anniversary-Frontiers/dp/0367857332>

# How Quantum Computing Works

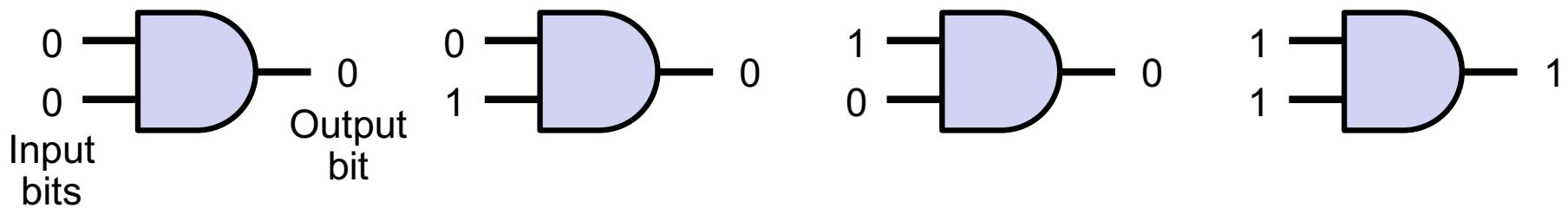
- **Quantum parallelism:** *Quantum gate acting on  $n$ -qubit computes all  $2^n$  case works all at once*, thus achieving exponential speedup
- Example: Quantum CNOT (conditional not) gate



Mathematically, CNOT gate multiplies a  $4 \times 4$  matrix to a  $4 (= 2^2)$ -element input vector

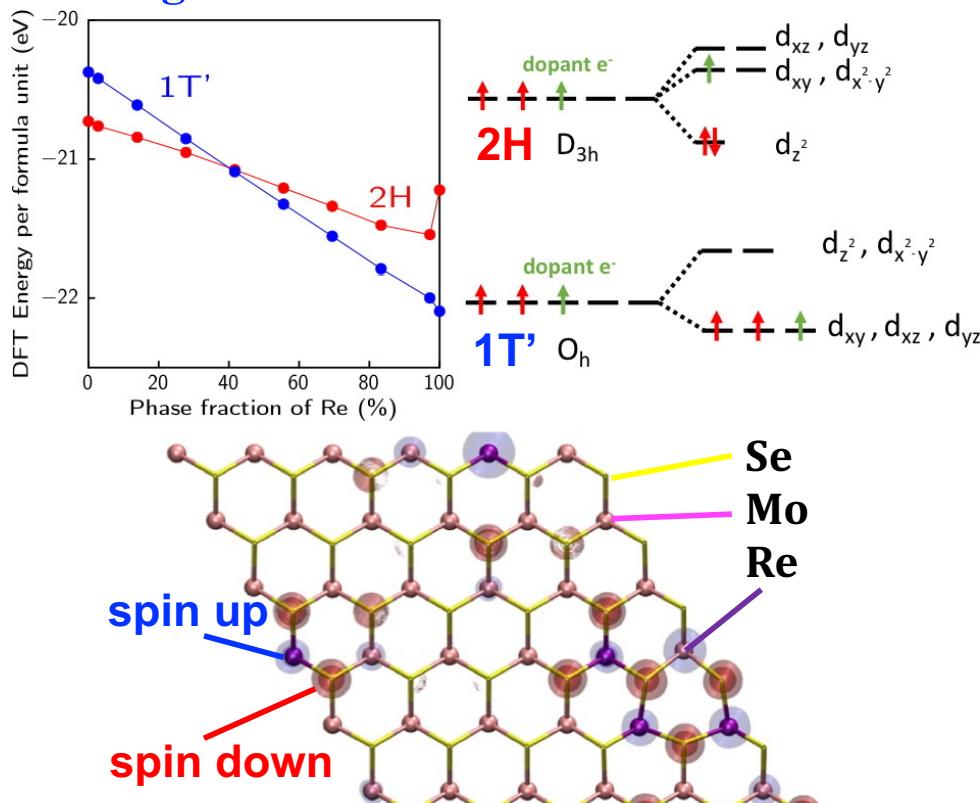
$$U_{\text{CNOT}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{matrix} \text{input} \\ 00 \\ 01 \\ 10 \\ 11 \end{matrix} \begin{matrix} \text{output} \\ 00 \\ 01 \\ 10 \\ 11 \end{matrix}$$

*cf. Classical gate computes only one case at a time*

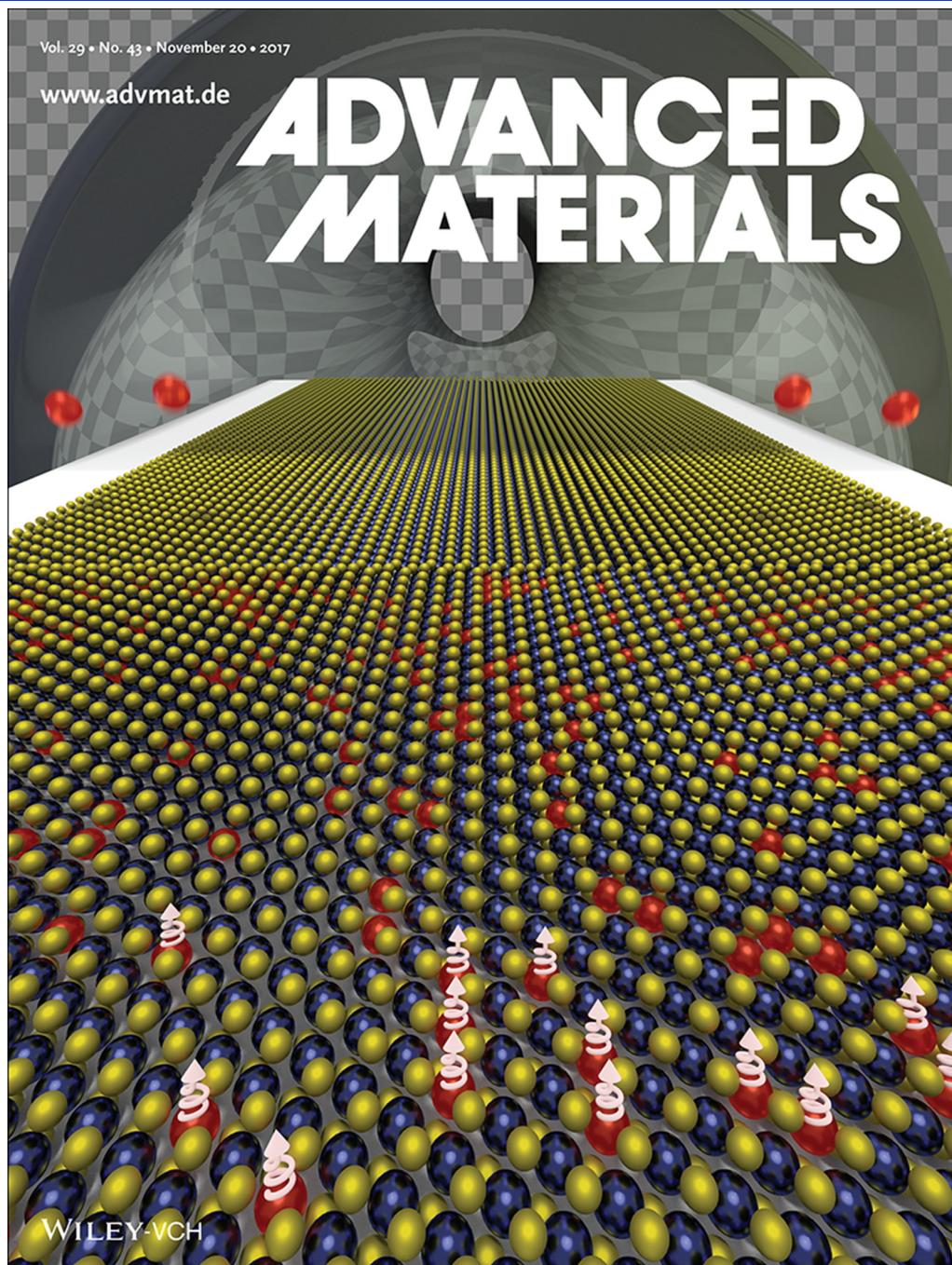


# Emergent Magnetism: Structural Transition via Doping

- Experiment at Rice showed 2H-to-1T' phase transformation by alloying MoSe<sub>2</sub> with Re
- Simulations at USC elucidated its electronic origin
- Simulation & experiment showed novel magnetism centered at Re atoms



V. Kochat et al., Adv. Mater. 29, 1703754 ('17)



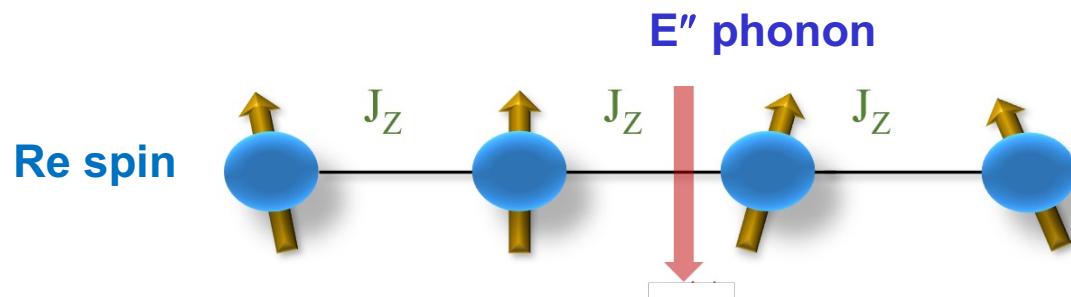
# Transverse Field Ising Model

- Electromagnetic-field control of quantum states in a chain of rhenium-magnets in  $\text{MoSe}_2$  monolayer to realize desired material properties on demand, thereby pushing the envelope of “quantum materials science”

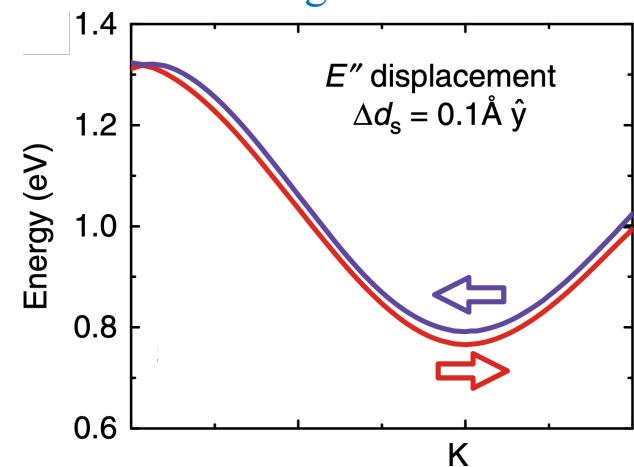
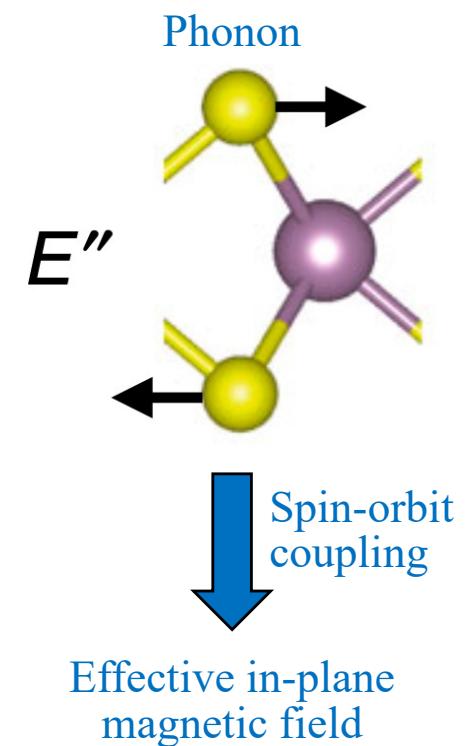
$$\begin{aligned}
 H(t) &= -J_z \sum_{j=1}^{N-1} \sigma_z^j \sigma_z^{j+1} - \varepsilon_{ph} \sin(\omega_{ph} t) \sum_{j=1}^N \sigma_x^j \\
 &= H_z + H_x(t)
 \end{aligned}$$

Phonon frequency  
Phonon-induced energy split

$$\sigma_z^j = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad \sigma_x^j = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} // \text{Act on } j\text{-th qubit}$$



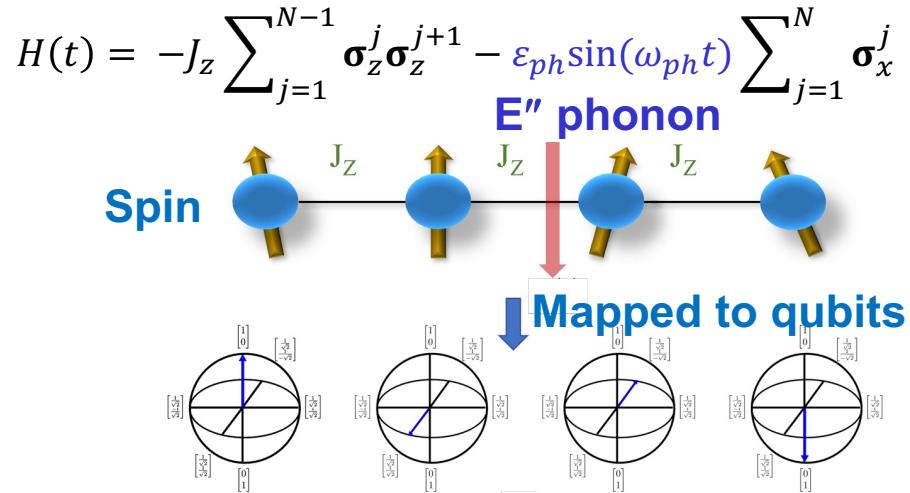
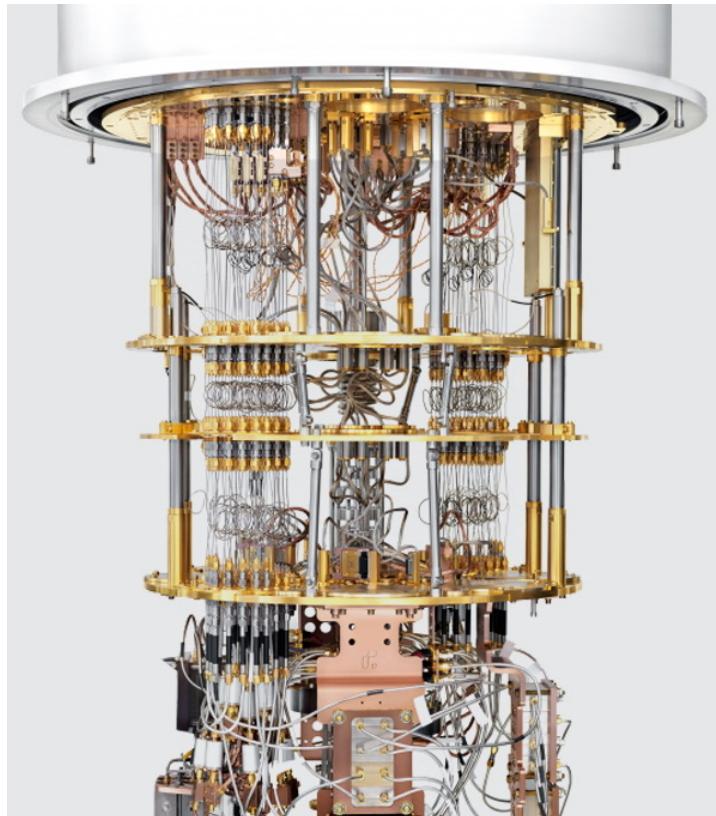
D. Shin et al., Nat. Commun. 9, 638 ('18)



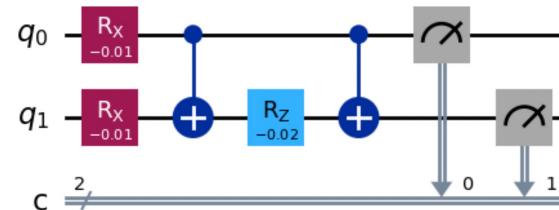
# Quantum Computing of Magnetism

- Simulated quantum many-body dynamics of magnetic spins on IBM's Q16 Melbourne & Rigetti's Aspen quantum processors

L. Bassman *et al.*, Phys. Rev. 101, 184305 ('20)



Quantum circuit:  $U(\Delta t) = \exp(-iH\Delta t)$



Quantum (Python) program

```
circ.rx(-2*dt*B, 0)
circ.rx(-2*dt*B, 1)
circ.cx(0, 1)
circ.rz(-2*dt*B, 1)
circ.cx(0, 1)
```

# Quantum Dynamics on NISQ Computers

---

- Time-evolution operator for wave function  $|\Psi(t)\rangle$  for small time interval  $\Delta t$  (atomic unit,  $\hbar = 1$ )

$$|\Psi(\Delta t)\rangle = U(\Delta t)|\Psi(t=0)\rangle$$
$$U(\Delta t) = \exp(-iH\Delta t)$$

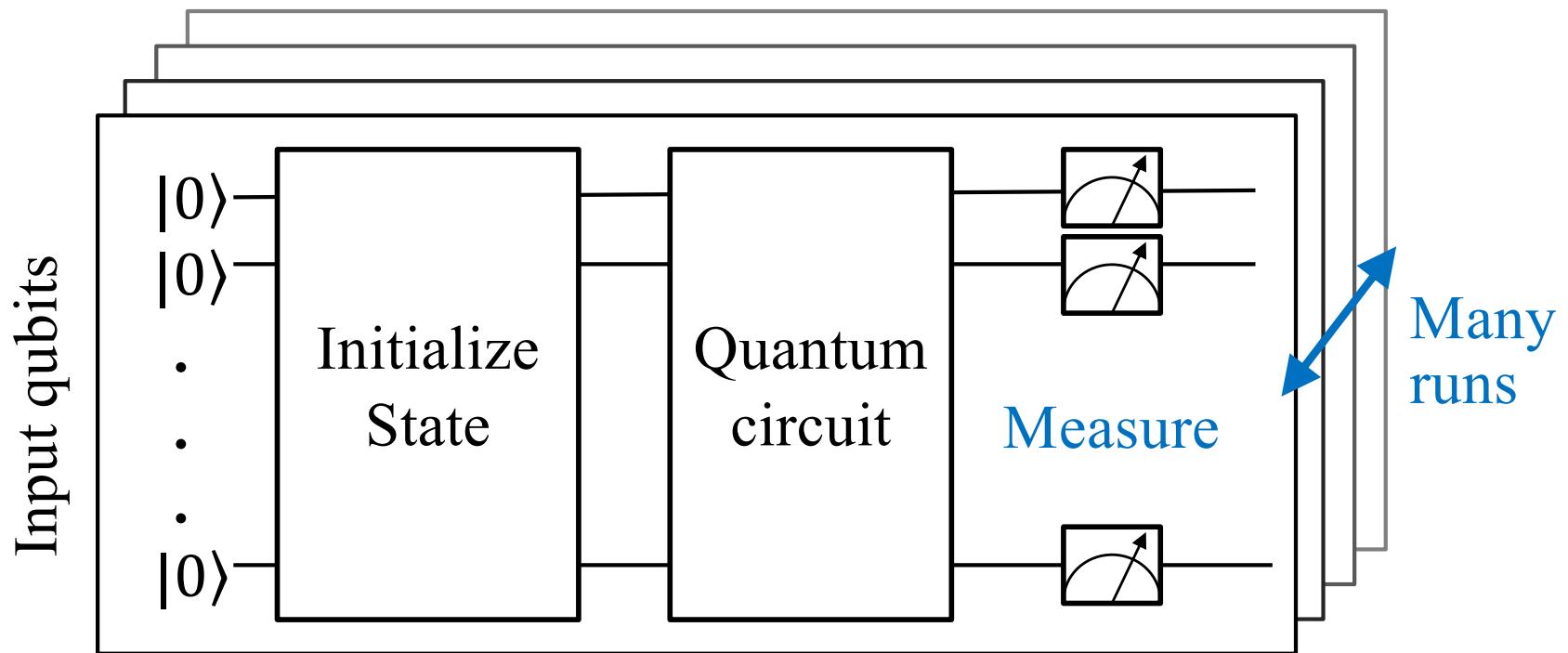
- Time discretization with time-step  $\Delta t$  and Trotter expansion

$$U(n\Delta t) \approx \prod_{k=0}^{n-1} \exp(-iH_z\Delta t) \exp(-iH_x((k + 1/2)\Delta t)\Delta t)$$

- One simulation run provides measurement for only one time instance ( $t = n\Delta t$ ) — if you can see intermediate time steps, it's not quantum computing

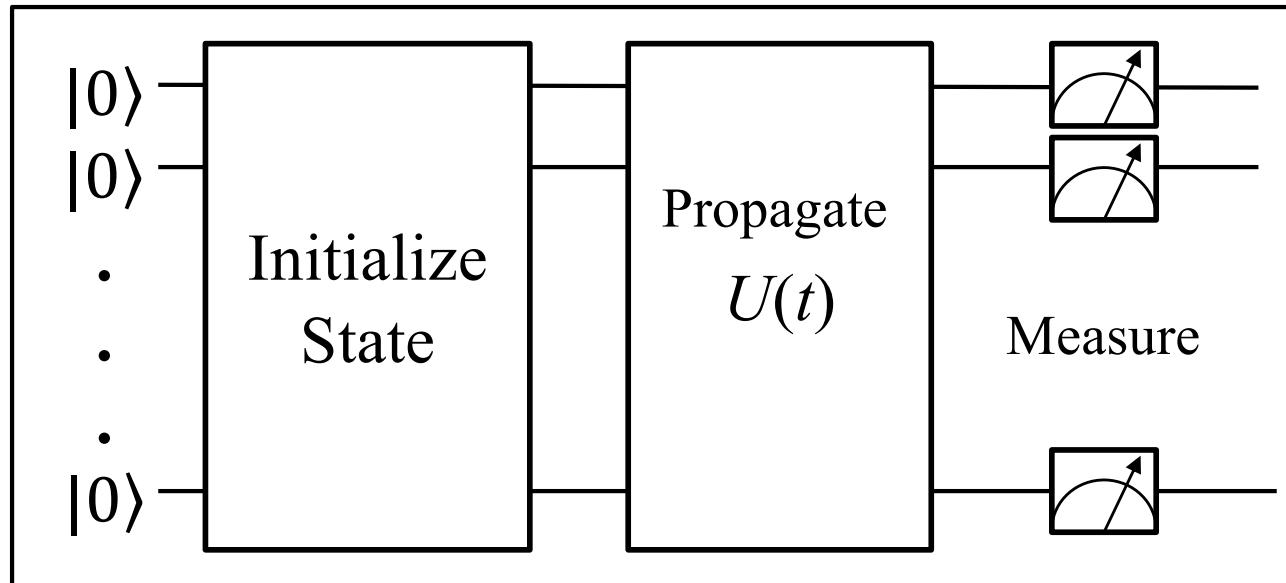
# Quantum Computing Runs & Measurements

- While a qubit stored in a quantum register is a superposition of 0 & 1 states, once it is measured, the measured value is either 0 or 1, with the probability according to its quantum wave function

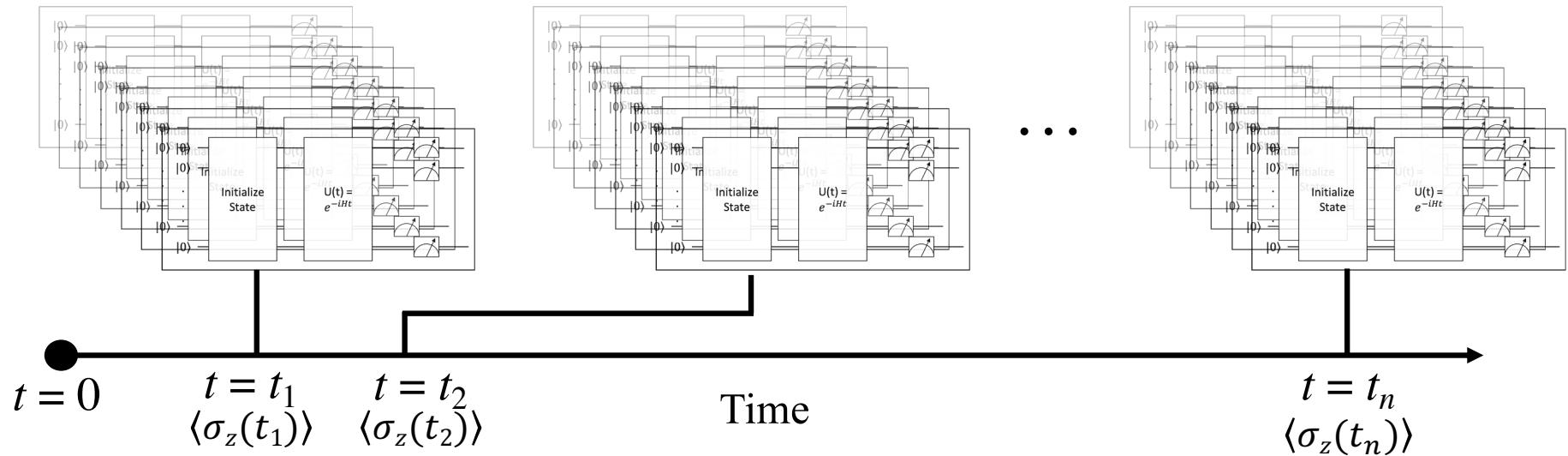


- For each program, thousands of runs need be performed on a quantum computer to obtain statistics

# More Runs for Quantum Dynamics



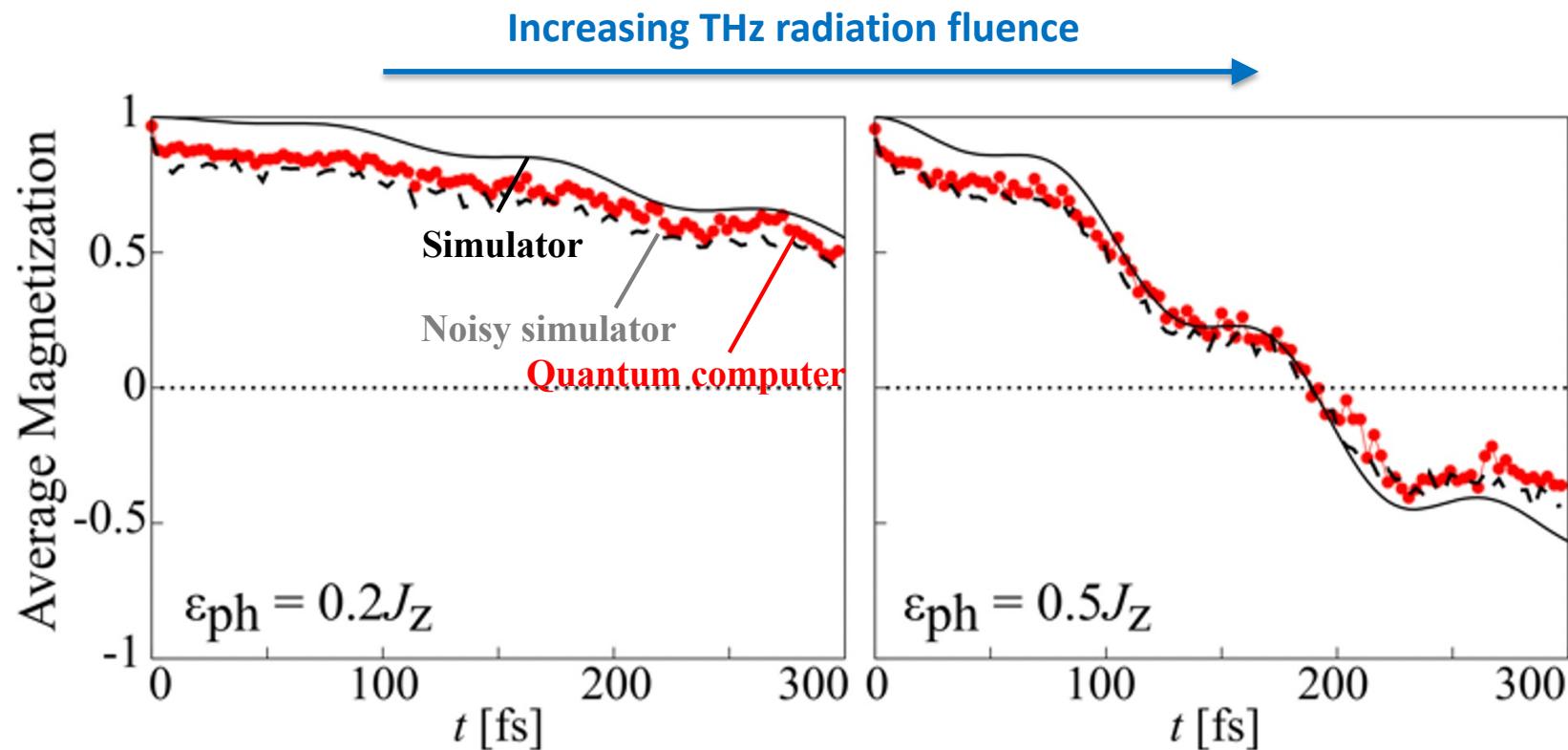
For each of many time instances, many runs to obtain statistics



Note measurement destroys a quantum state  
—can't peek into intermediate time steps

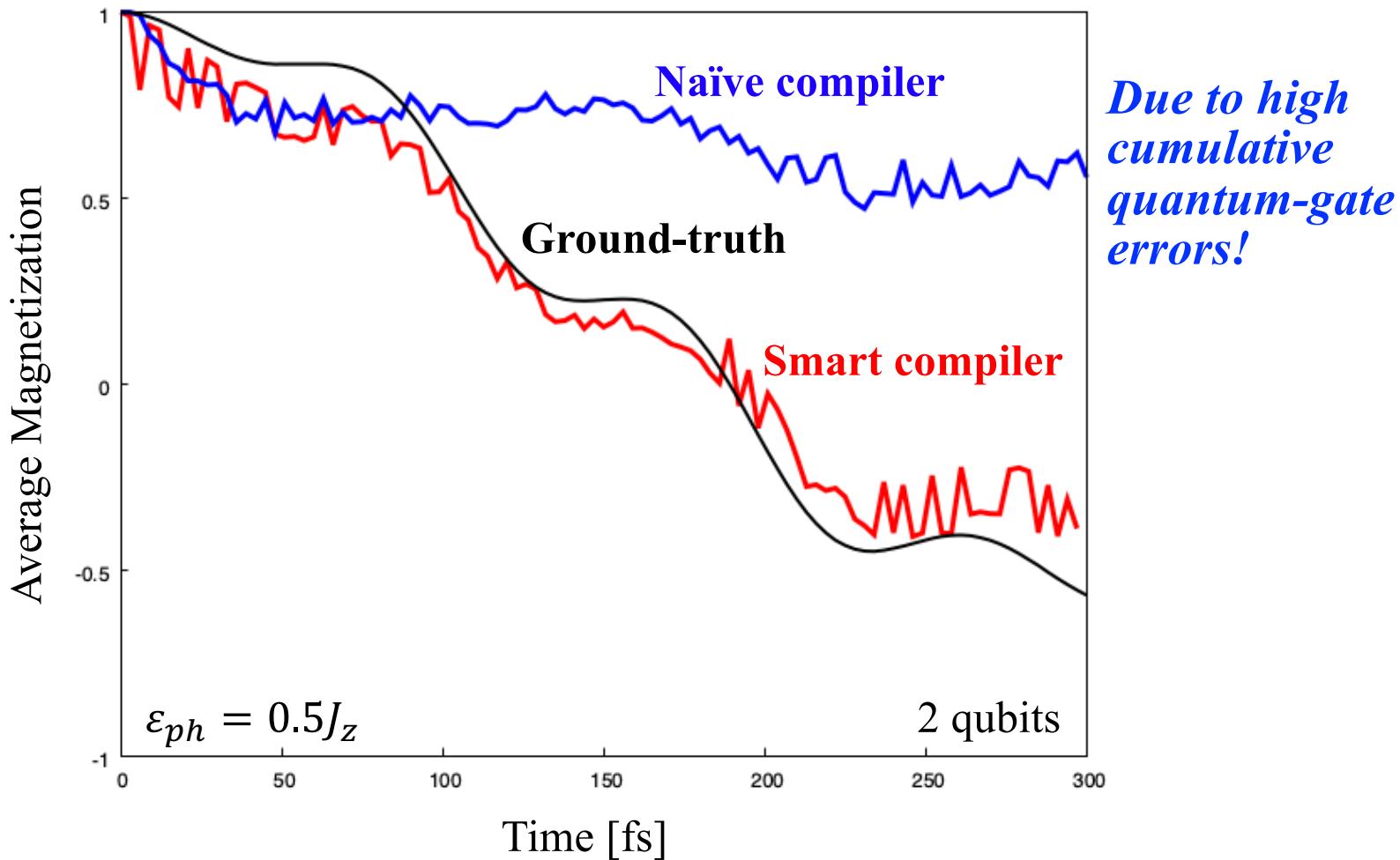
# Quantum Computing Results

- Quantum-dynamics simulations on NISQ computers show dynamic suppression of magnetization by THz radiation



# Circuit Size vs. Simulation Fidelity

- Reduced circuit size improves the fidelity of simulation



Naïve compiler: circuit size  $\propto$  time

Smart compile: Constant circuit size w.r.t. time

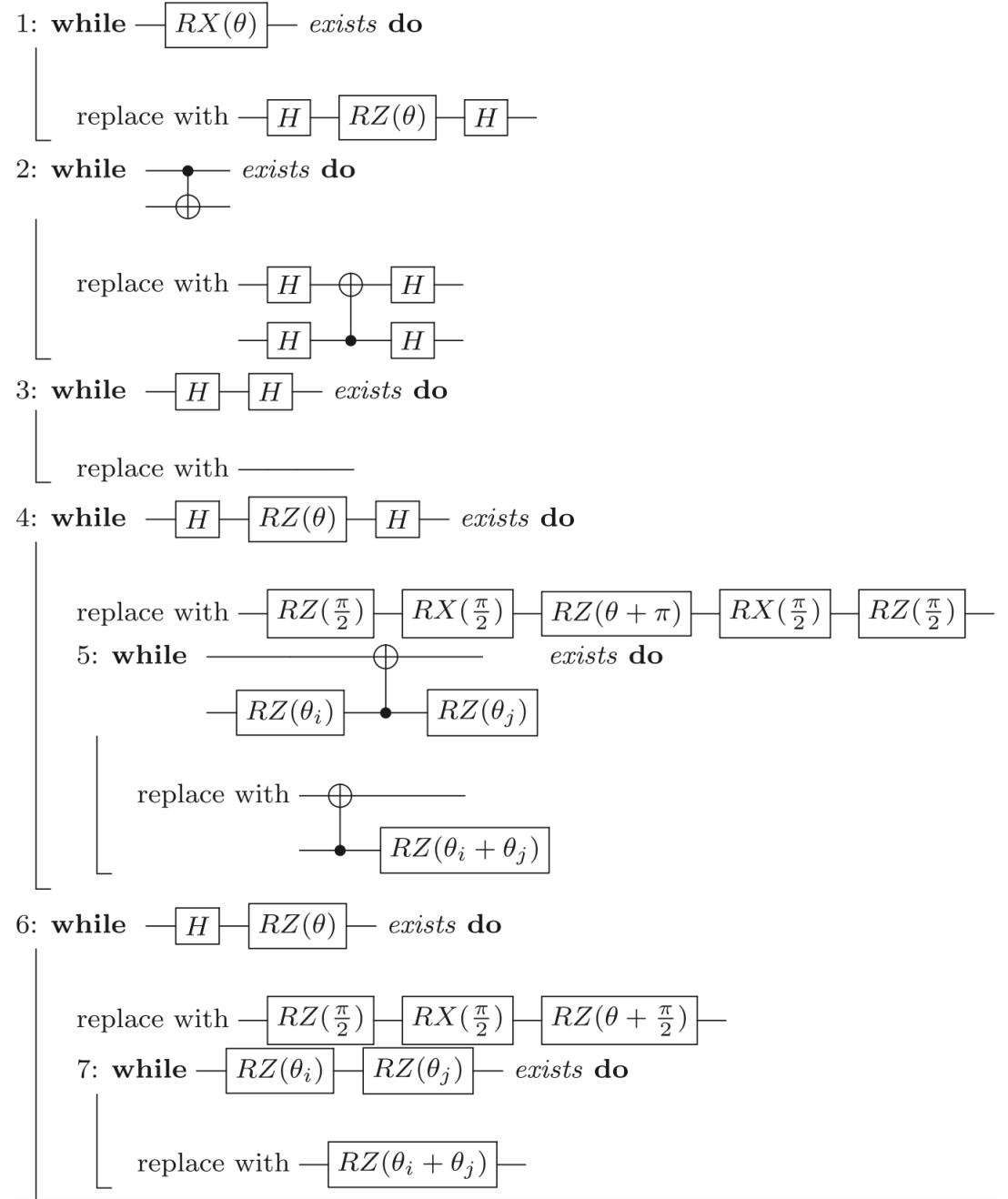
# Quantum Compiler: Math

- **Problem:** High gate errors make long-time simulations impractical
- **Solution:** Domain-specific compiler = use algebraic identities to derive an equivalent circuit with reduced circuit size

No.	Common gate set in TFIM circuits	Equivalent
1		
2		
3		
4		
5		
6		
7		—
8		
9		
10		
11		

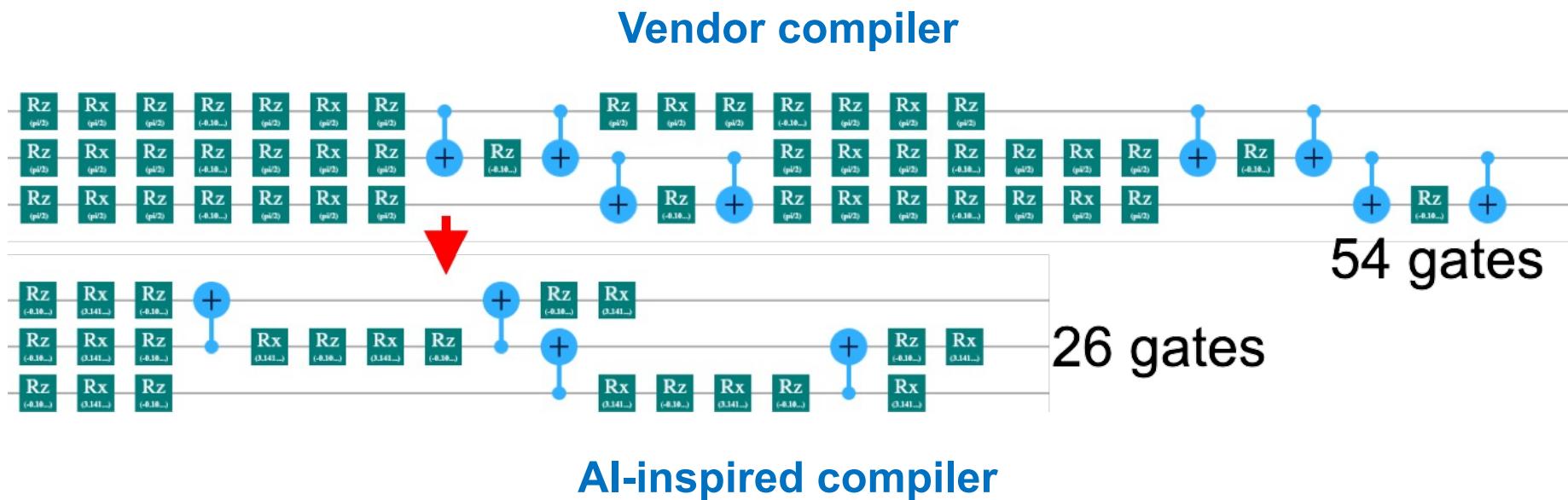
# Algorithm for IBM Native Gates

- Heuristic algorithm similar to unit propagation in artificial intelligence (AI)
- The heuristic order & types of identities applied are specific to the particular quantum dynamics we simulated



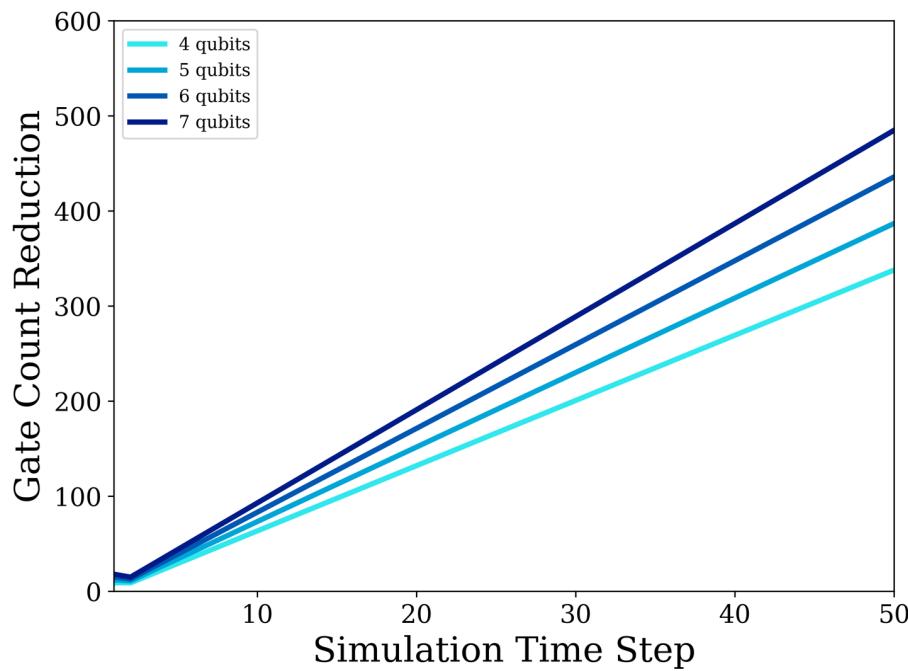
# Domain-Specific Quantum Compiler

- Take advantage of specific problem structure
- AI-inspired quantum compiler reduced the circuit size by 30% to mitigate environmental noise

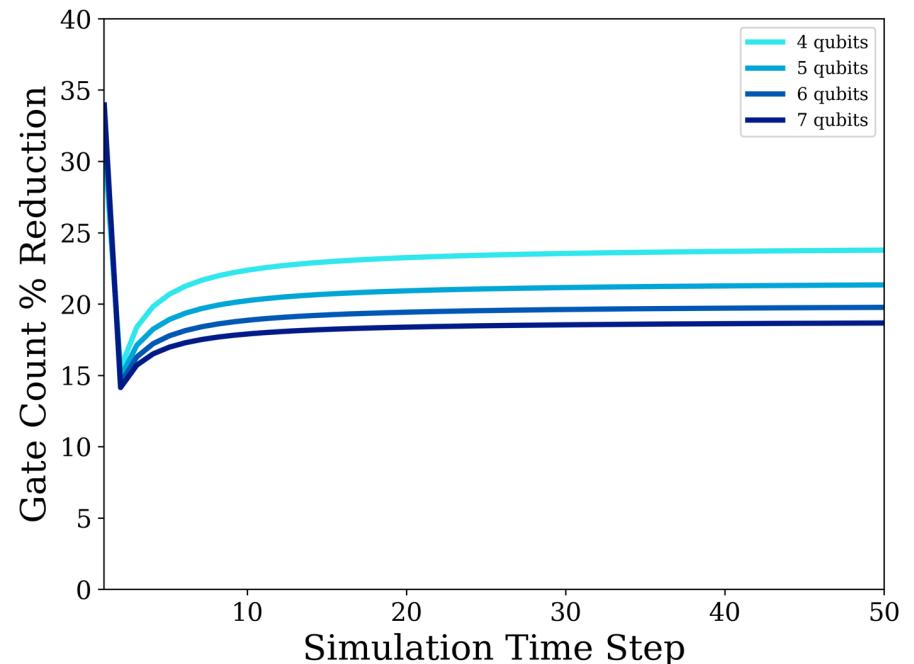


# Performance of Domain-Specific Compiler

**Absolute gate count difference**  
*(IBM Compiler - DS Compiler)*

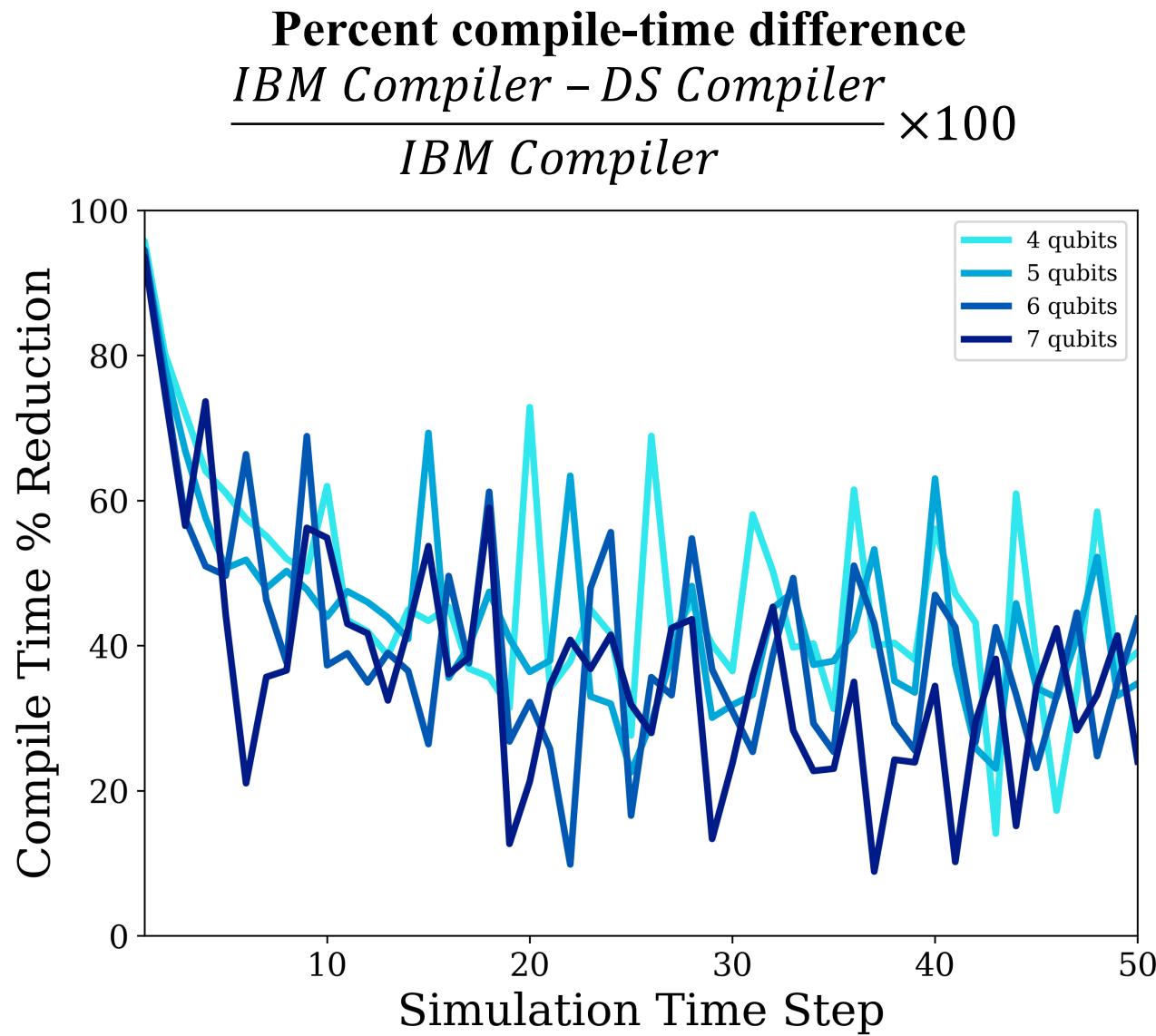


**Percent gate count difference**  
$$\frac{IBM\ Compiler - DS\ Compiler}{IBM\ Compiler} \times 100$$



Domain-specific compiler reduces gate count compared to IBM compiler

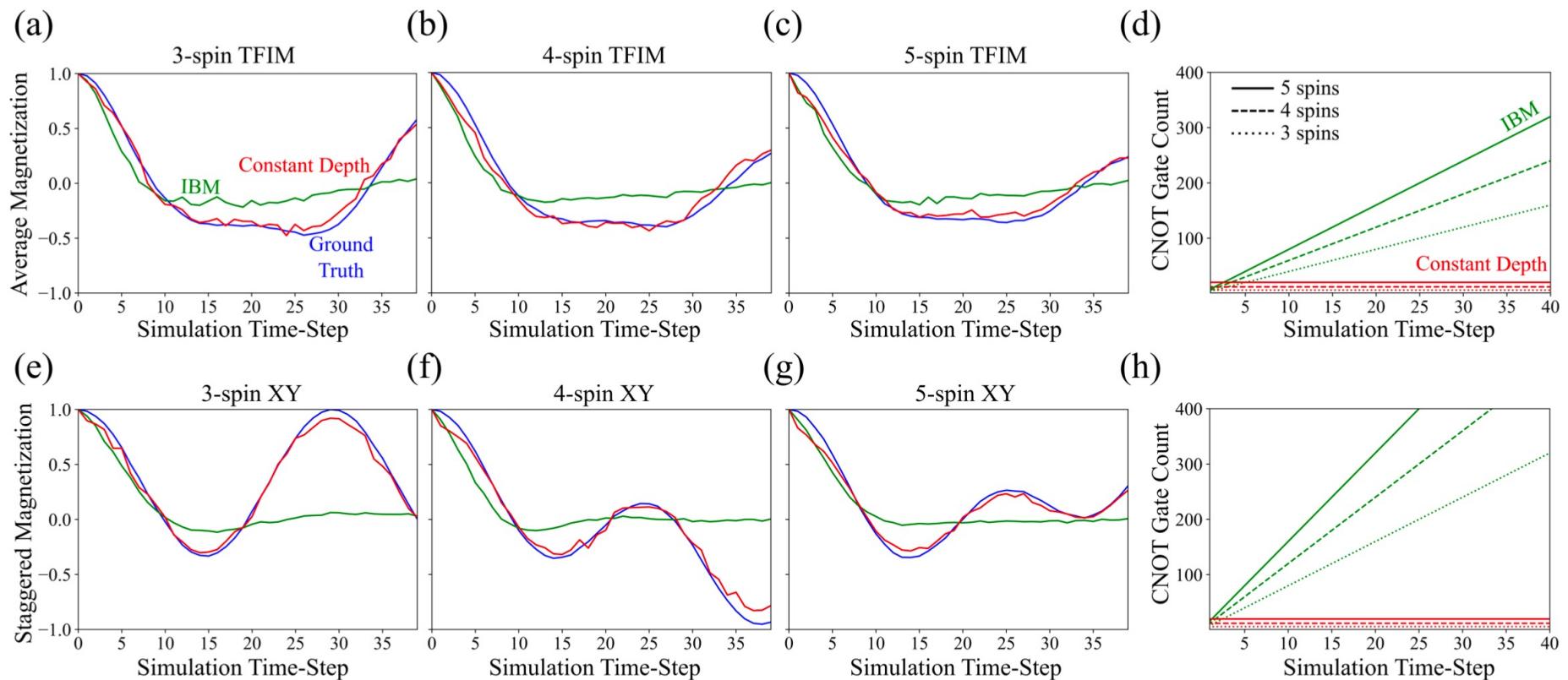
# Speed of Domain-Specific Compiler



... and does it faster

# Extension: Constant Circuit-Depth Algorithm

- Mathematical identities allow constant circuit depth independent of the number of time steps  $n$  for arbitrary number of spins  $N$  in a linear spin chain

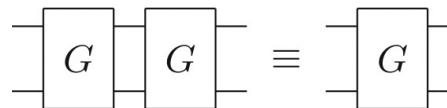


Exception for the “no-fast-forwarding theorem”

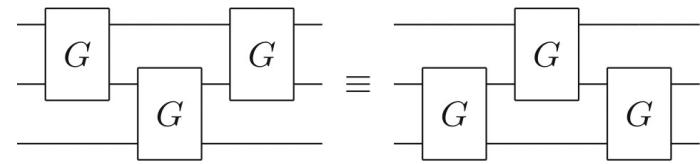
# Constant Circuit-Depth: How It is Done

- Matchgate (shifted  $2 \times 2$  block diagonal)

$$G(A, B) = \begin{bmatrix} p & q \\ w & x \\ y & z \\ r & s \end{bmatrix}$$



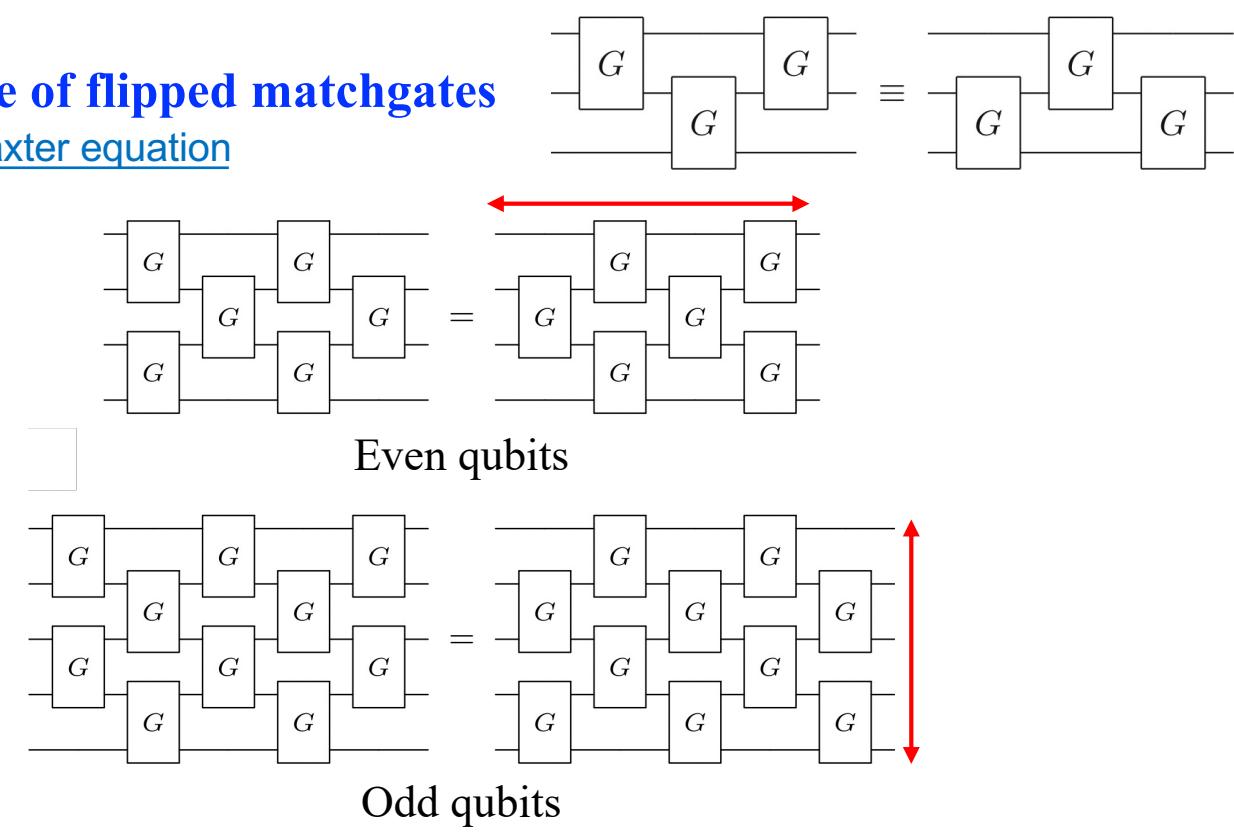
- Contraction: product of matchgates is a matchgates



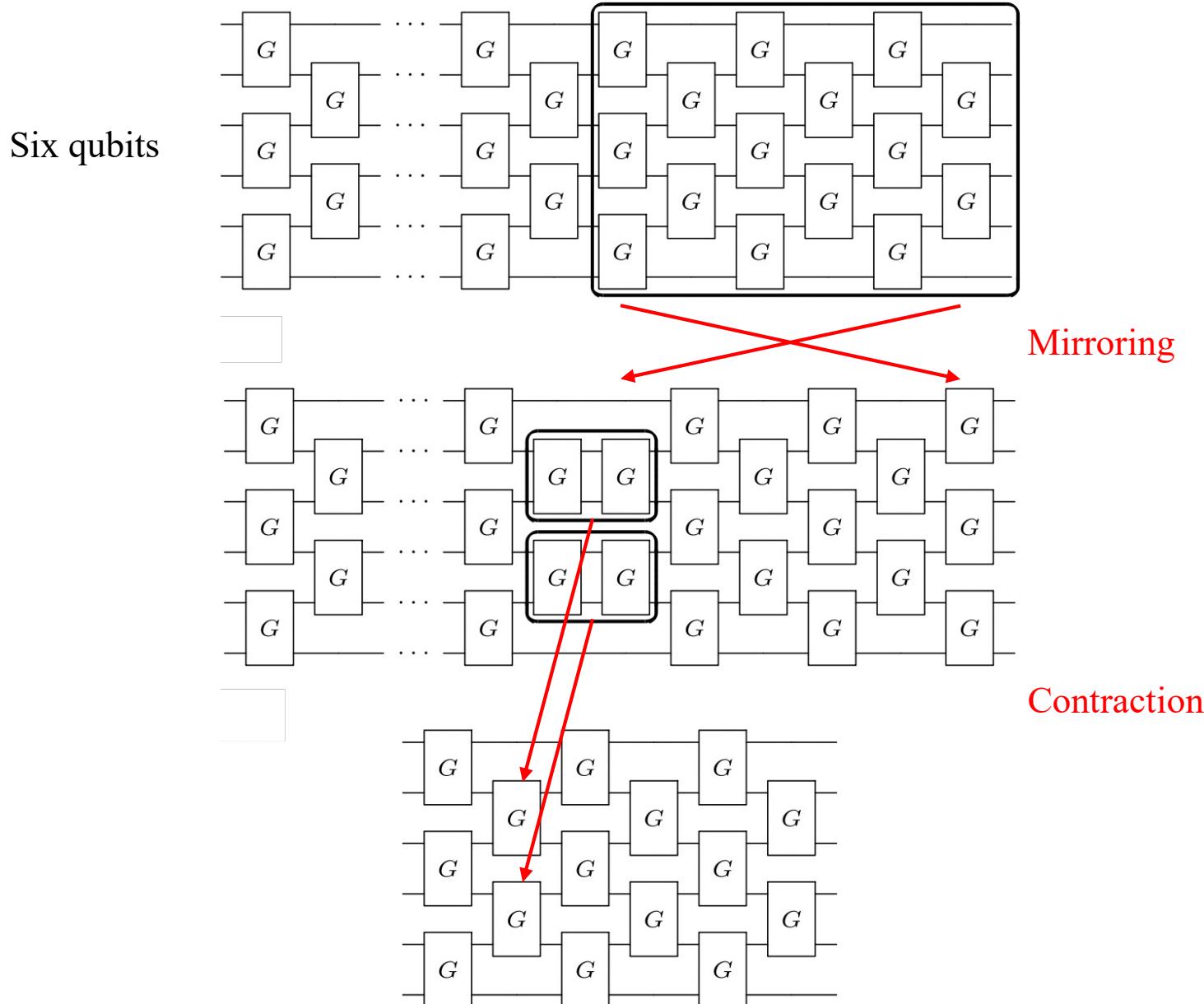
- Conjecture: existence of flipped matchgates

*cf. Yang-Baxter equation*

- Mirroring identities



# Downfolding to Constant-Depth



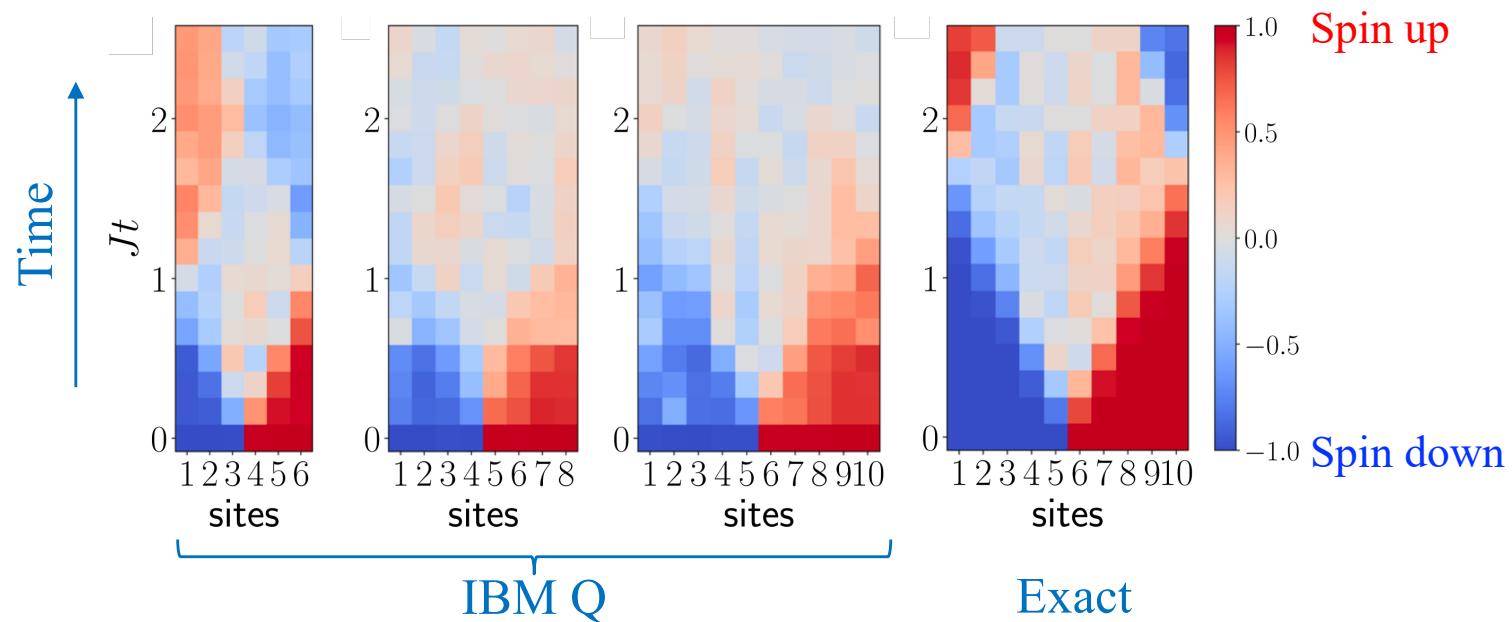
# Richer Physics: Heisenberg Model

$$H = - \underbrace{\sum_{j=1}^{N-1} (J_x \sigma_x^j \sigma_x^{j+1} + J_y \sigma_y^j \sigma_y^{j+1} + J_z \sigma_z^j \sigma_z^{j+1})}_{\text{Exchange coupling}} - h \underbrace{\sum_{j=1}^N \sigma_z^j}_{\text{Magnetic field}}$$

Pauli spin-1/2 matrices

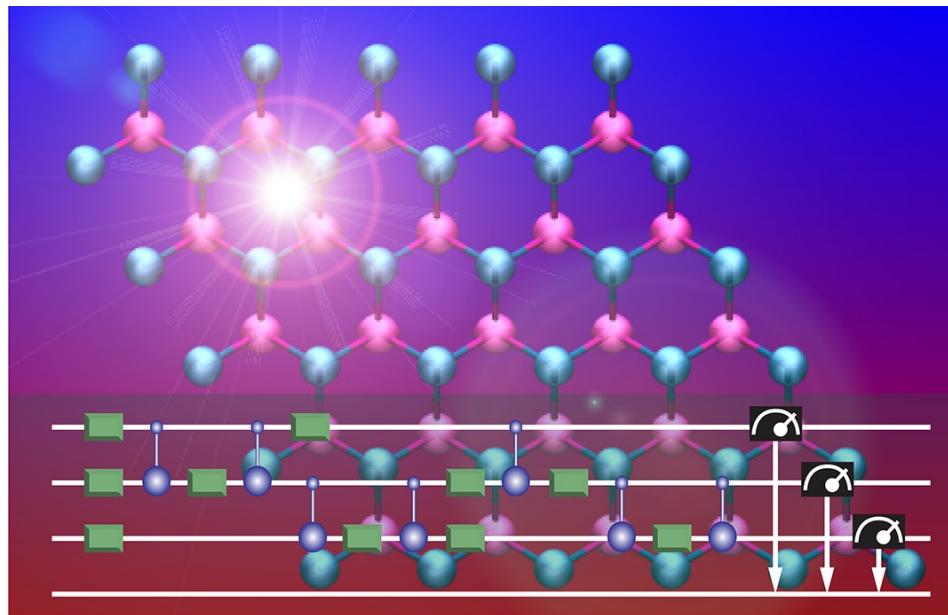
$$\sigma_x^j = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \sigma_y^j = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \sigma_z^j = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} // \text{Act on } j\text{-th qubit}$$

Domain-wall dynamics (6-, 8- & 10-site spin chains)



# Open-Source Quantum Software

- Full-stack, cross-platform software for quantum dynamics simulations on NISQ computers was made available open-source



MISTIQS

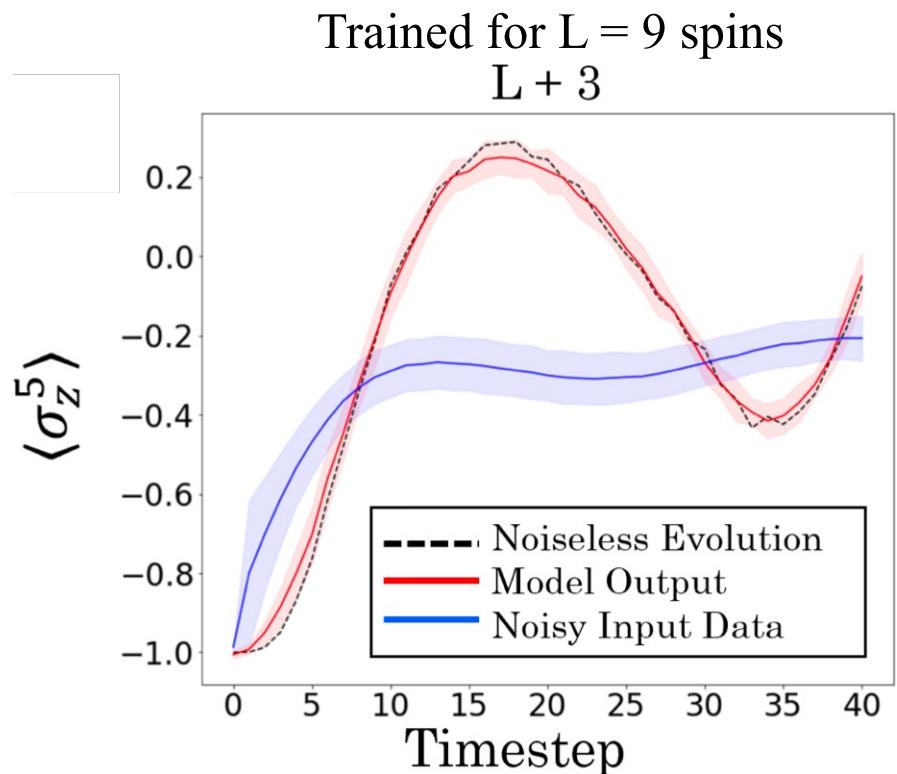
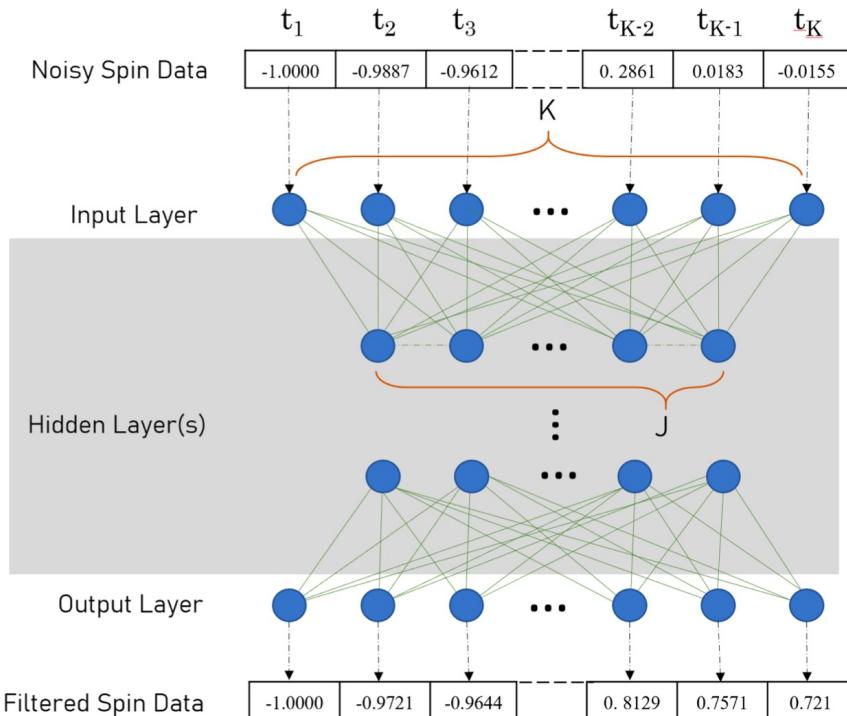
**M**ultiplatform  
**S**oftware for  
**T**ime-dependent  
**Q**uantum  
**S**imulation

Paper: C. Powers et al., SoftwareX 14, 100696 ('21)

Software: <https://github.com/USCCACS/MISTIQS>

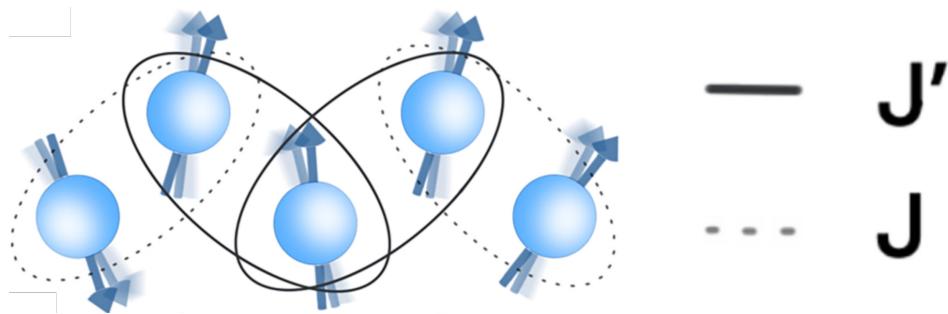
# Extension: Machine Learning

- Alternative noise mitigation using machine learning:  
Autoencoder, trained with quantum simulations of small systems, is capable of filtering noise from dynamic simulations of larger systems run on quantum computers

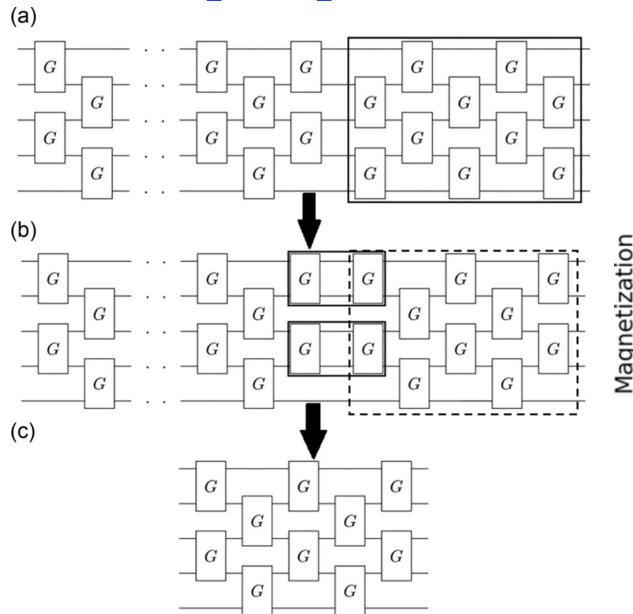


# Topological Quantum Dynamics

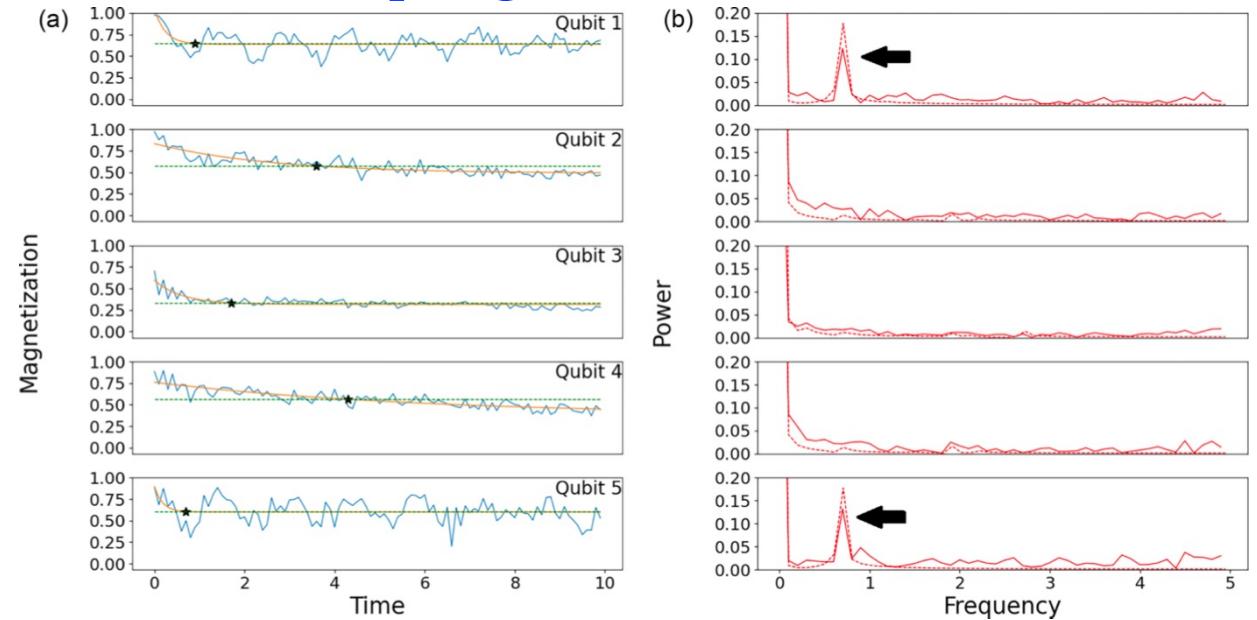
## Quantum spin chain



## Constant-depth quantum circuit



## Topological surface mode



M. Mercado *et al.*, Phys. Rev. B **110**, 075116 ('24)

New: Periodically-driven Floquet topology simulated

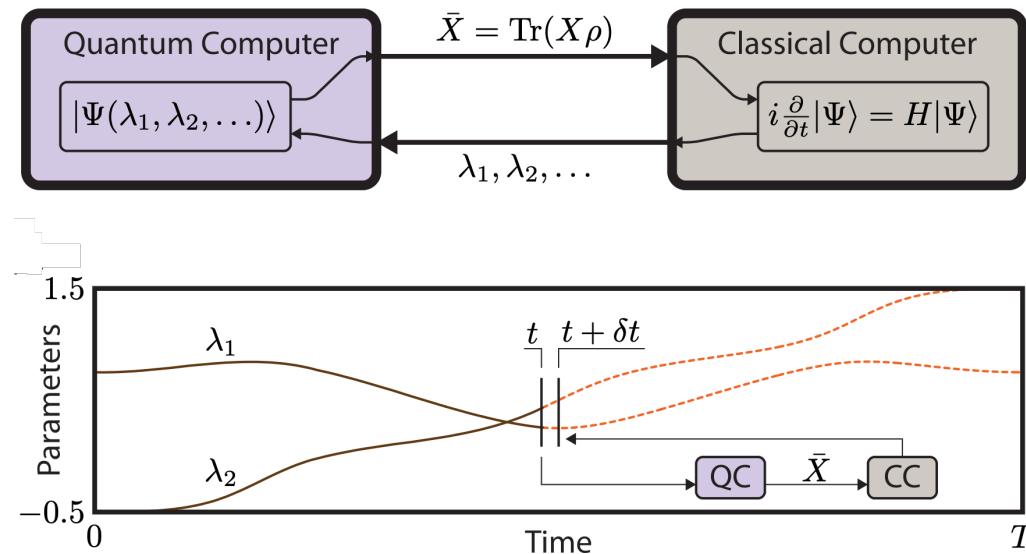
# Variational Quantum Simulator

**Hybrid quantum/classical approach:** Boost the power of a classical supercomputer using a quantum co-processor

- A variational approach similar to variational quantum eigensolver (VQE) can be applied to quantum dynamics

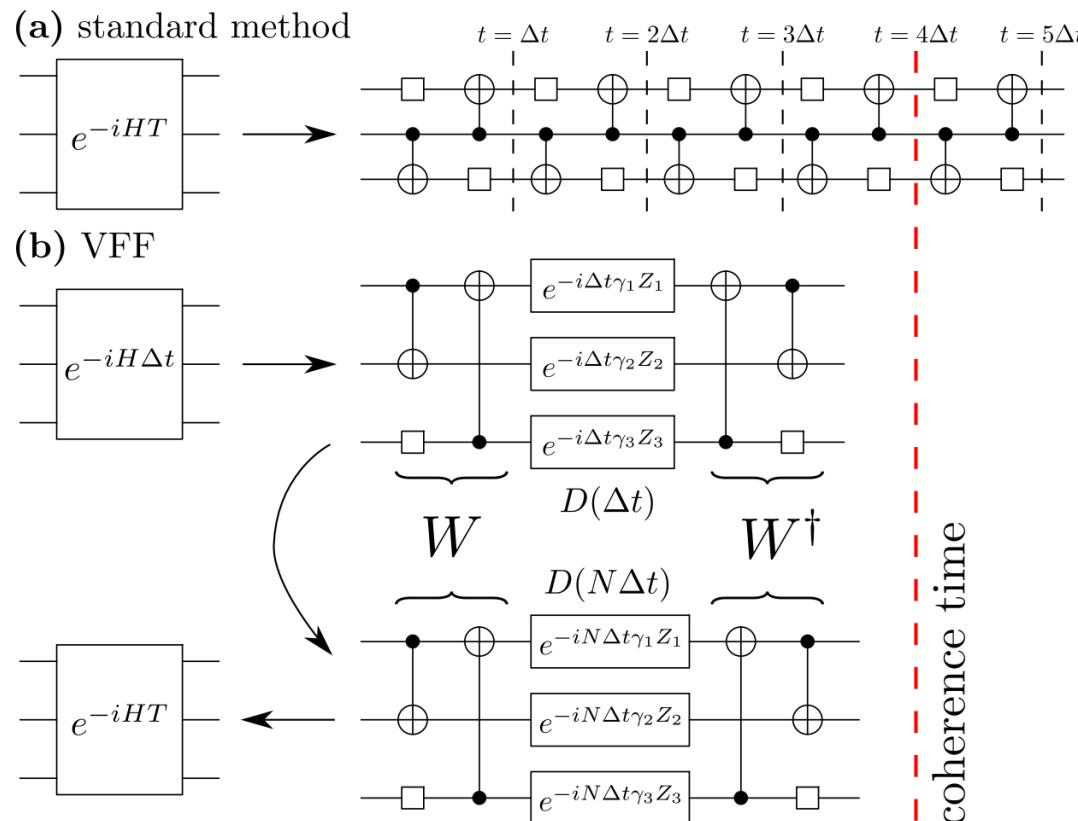
$$\delta \int_{t_i}^{t_f} dt \left\langle \psi(t) \right| \left( i \frac{\partial}{\partial t} - H \right) \left| \psi(t) \right\rangle = 0$$

- Short-time propagation of a many-body wave function on a quantum computer is mapped back to a parameterized variational wave function,  $|\Psi(t)\rangle = |\Psi(\lambda_1(t), \dots, \lambda_p(t))\rangle$ , which is tractable on a classical computer



# Variational Fast Forwarding

- A variational approximation of the diagonalization of a Trotterized time evolution
- The optimal equivalent circuit with a fixed number of gates is obtained by quantum-assisted quantum compiling



C. Cirstoiu et al., *npjQI* 6, 82 ('20)

See B. Fauseweh, *Nat. Commun.* 15, 2133 ('24) for a review

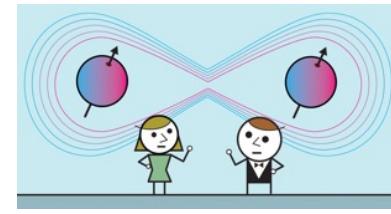
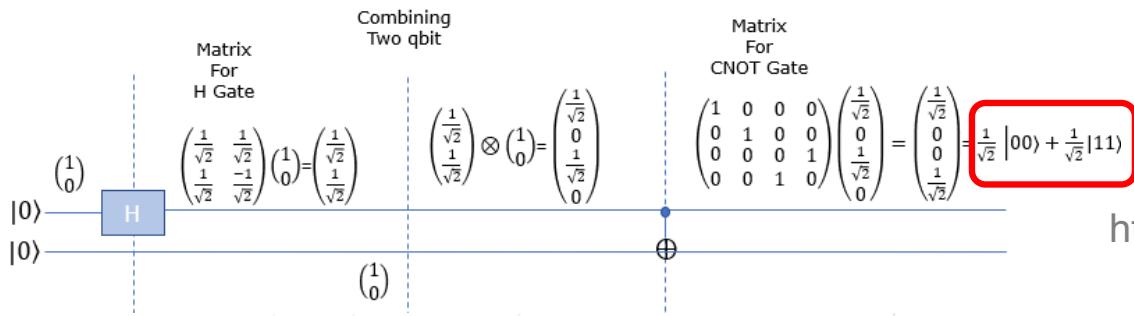
# Do-It-Yourself Quantum Computing

- Sign up & sign in to IBM Quantum cloud

<https://quantum.cloud.ibm.com>

- Open Composer (GUI-based quantum programming platform) 

- Build a quantum circuit to prepare an *entangled Bell's state*, which has played an essential role in quantum information science (2022 Nobel physics prize), using Hadamard & CNOT gates



[https://en.wikipedia.org/wiki/Bell\\_state](https://en.wikipedia.org/wiki/Bell_state)

Operations

Search

H  $\oplus$   $\otimes$   $\oplus$   $\otimes$   $\times$   $\text{I}$   
T S Z  $T^\dagger$   $S^\dagger$  P  
RZ  $\text{rz}$   $|0\rangle$   $|1\rangle$   $\bullet$  if  
 $\sqrt{X}$   $\sqrt{X}^\dagger$  Y RX RY RXX  
RZZ U RCCX RC3X

Probabilities

Computational basis states

Q-sphere

Qsphere

Probabilities (%)

0 00 01 10 11

100  
80  
60  
40  
20  
0

00 01 10 11

Phase 0  $\pi/2$   $3\pi/2$  0

State Phase angle

```
from qiskit import QuantumRegister, ClassicalRegister, QuantumCircuit
from numpy import pi

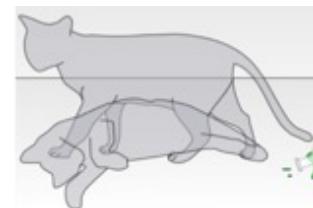
qreg_q = QuantumRegister(2, 'q')
creg_c = ClassicalRegister(4, 'c')
circuit = QuantumCircuit(qreg_q, creg_c)

circuit.h(qreg_q[0])
circuit.cx(qreg_q[0], qreg_q[1])
```

**Hadamard gate transforms a pure qubit ( $|0\rangle$  or  $|1\rangle$ ) into a superposition of  $|0\rangle$  &  $|1\rangle$ :**

$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

$$H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$



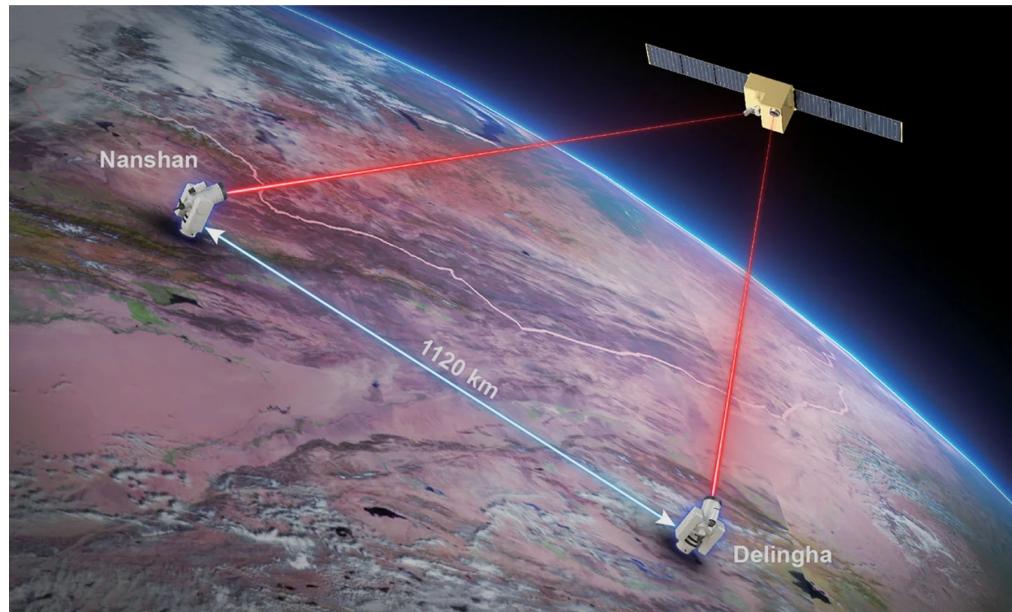
# Entanglement: What's the Big Deal?

---

China's quantum satellite achieves 'spooky action' at record distance:  
Result paves way for hack-proof quantum communications

*Science Journal* (June 15, '17)

**Quantum entanglement**—physics at its strangest—has moved out of this world and into space. In a study that shows China's growing mastery of both the quantum world and space science, a team of physicists reports that it sent eerily intertwined quantum particles from a satellite to ground stations **separated by 1200 kilometers**, smashing the previous world record. The result is a stepping-stone to **ultrasecure communication networks and, eventually, a space-based quantum internet.**



<https://www.science.org/content/article/china-s-quantum-satellite-achieves-spooky-action-record-distance>

# Where to Go from Here

---

- New MS degree in Quantum Information Science ([MSQIS](#)) started in 2021
- Required foundational courses
  - 1. EE 520: Introduction to Quantum Information Processing
  - 2. EE 514: Quantum Error Correction
  - 3. Phys 513: Applications of Quantum Computing
- Core — at least two courses from
  - 1. EE 589: Quantum Information Theory
  - 2. Phys 550: Open Quantum Systems
  - 3. Phys 559: Quantum Devices
  - 4. Phys 660: Quantum Information Science & Many-Body Physics
- Phys 513: Application of Quantum Computing (co-taught with Prof. Rosa Di Felice) — quantum simulations on quantum circuits & adiabatic quantum annealer ([syllabus](#))
- Phys 516, CSCI 596, CSCI 653: Elective for MSQIS

Go through hands on exercise on  
(1) [qubits & quantum circuits](#) and (2) [quantum dynamics simulation](#)