Quantum Computational Science

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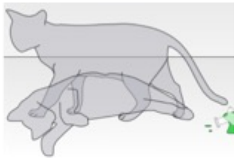
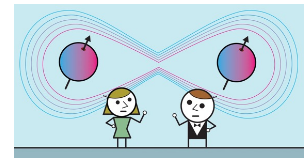
Goal: Quantum dynamics simulation on quantum circuits

Quantum Computing Is Hot



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



The Nobel Prize in Physics 2022

Ill. Niklas Elmehed © Nobel Prize Outreach

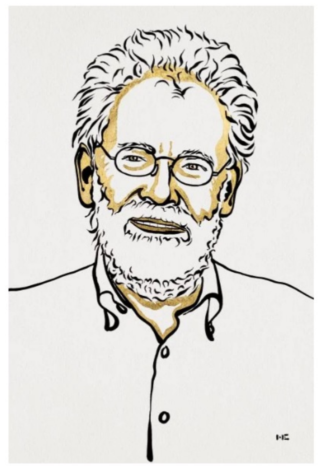
Alain Aspect

Prize share: 1/3

Ill. Niklas Elmehed © Nobel Prize Outreach

John F. Clauser

Prize share: 1/3



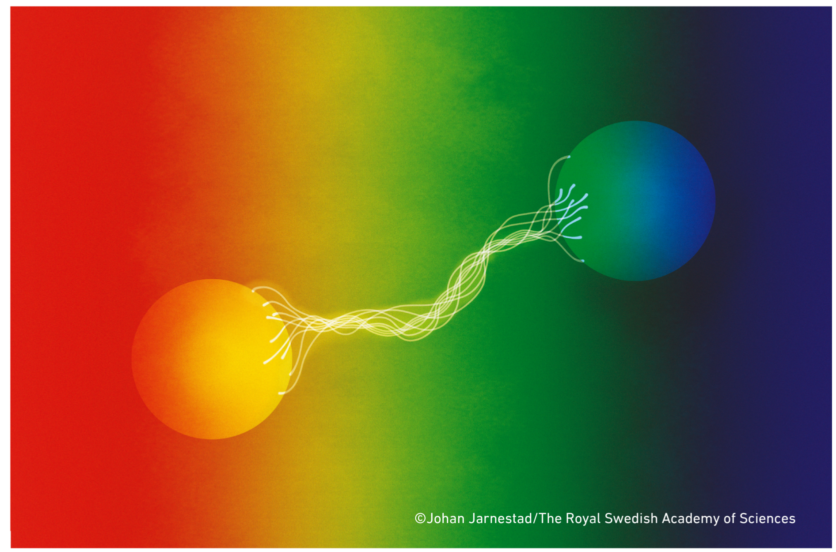
Ill. Niklas Elmehed © Nobel Prize Outreach

Anton Zeilinger

Prize share: 1/3

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"

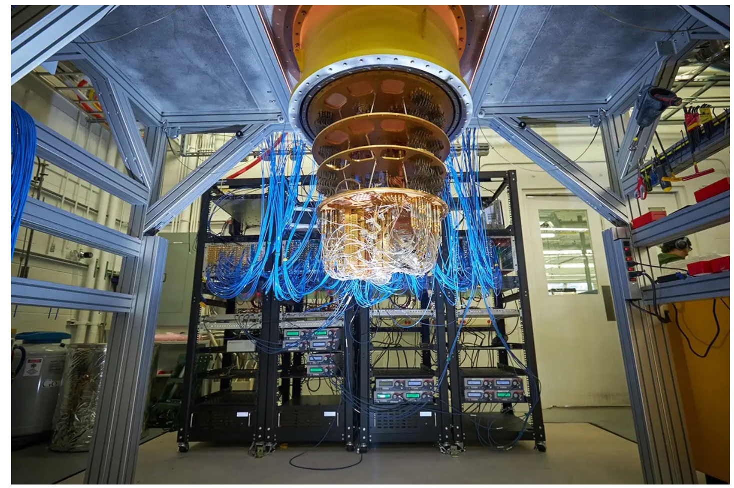
It's entanglement!

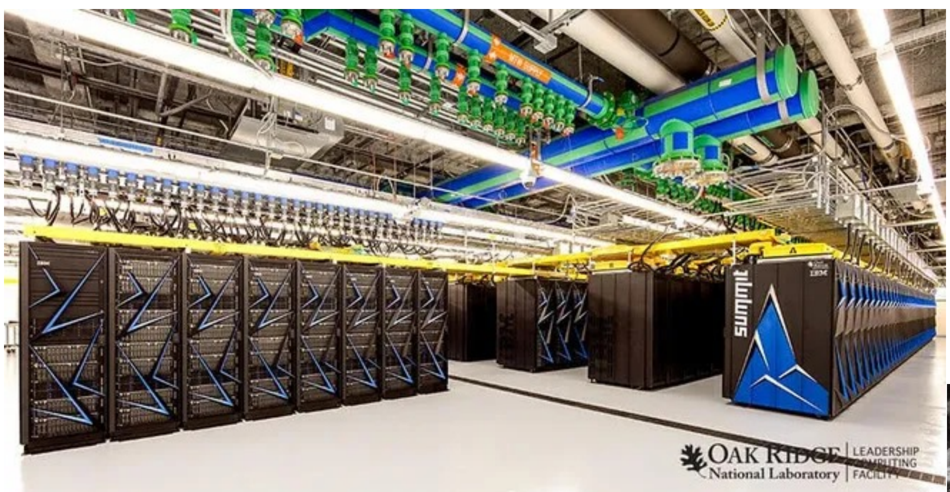


cf. Microsoft Majorana 1 chip (Feb. 19, '25)
https://news.microsoft.com/azure-quantum/

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**

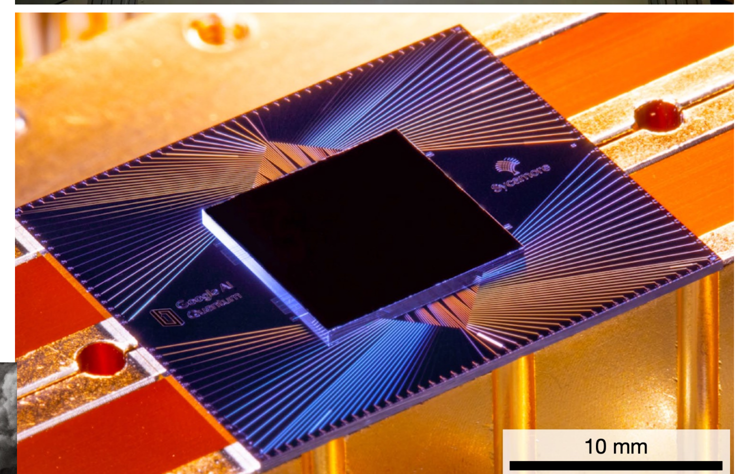




9,216-CPU & 27,648-GPU Summit

<

Fast & frugal



53-qubit Google Sycamore

Quantum Computing Gets Hotter

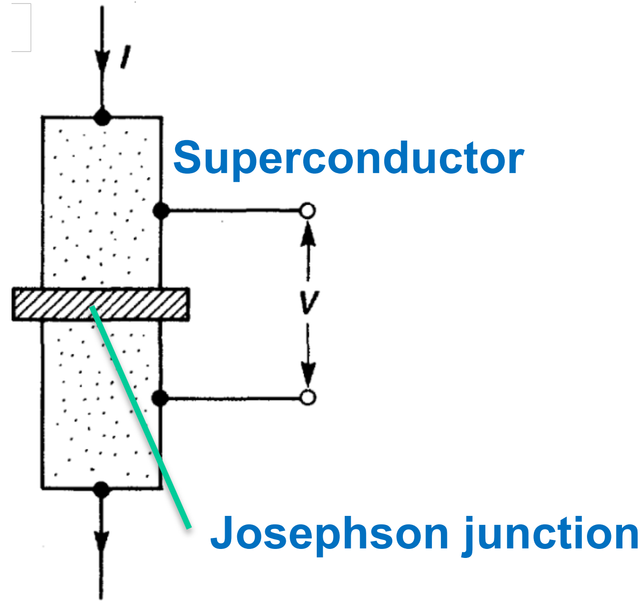
Nobel Prize in Physics 2025

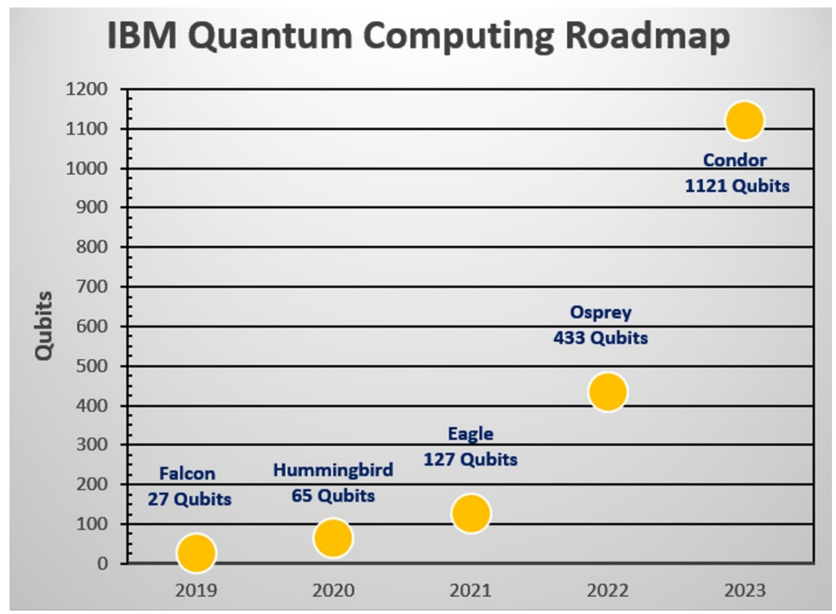
Ill. Niklas Elmehed © Nobel Prize Outreach
John Clarke
Prize share: 1/3

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

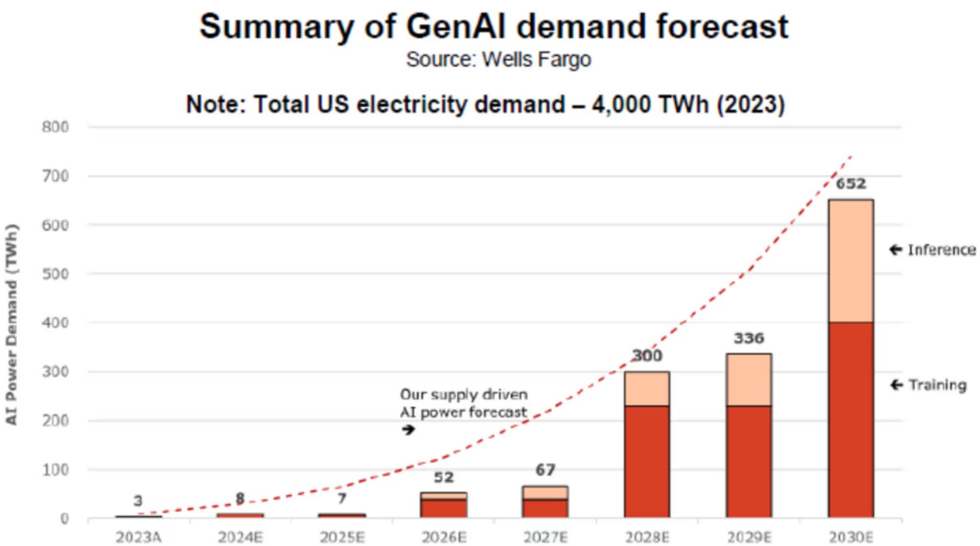
The Nobel Prize in Physics 2025 was awarded jointly to John Clarke, Michel H. Devoret and John M. Martinis "for the discovery of macroscopic quantum mechanical tunnelling and energy quantisation in an electric circuit"



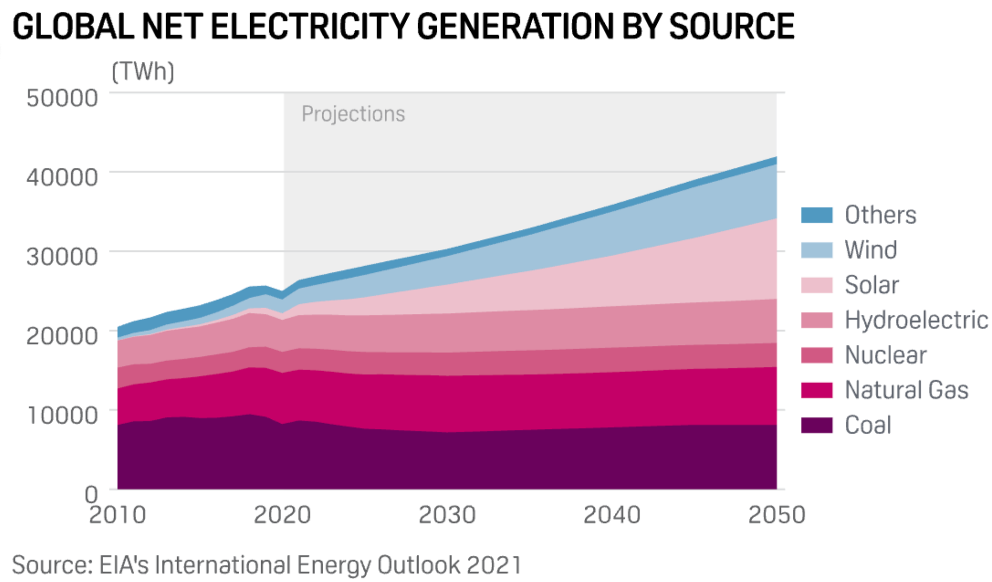


Foundation of superconducting quantum circuits

Why Care?



- **Exponential growth of energy demand for AI-computing**



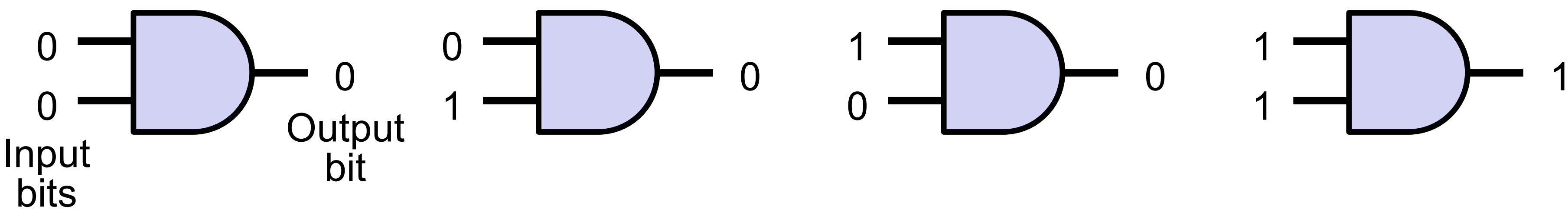
- **Linear growth of global energy supply (don't forget the growing CO_2 emission)**

- **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**

One of these input/output combinations happens at a time

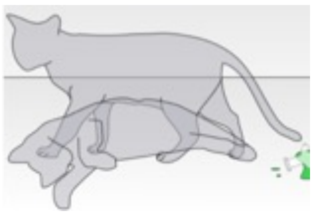


von Neumann computer architecture (1944)

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**

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



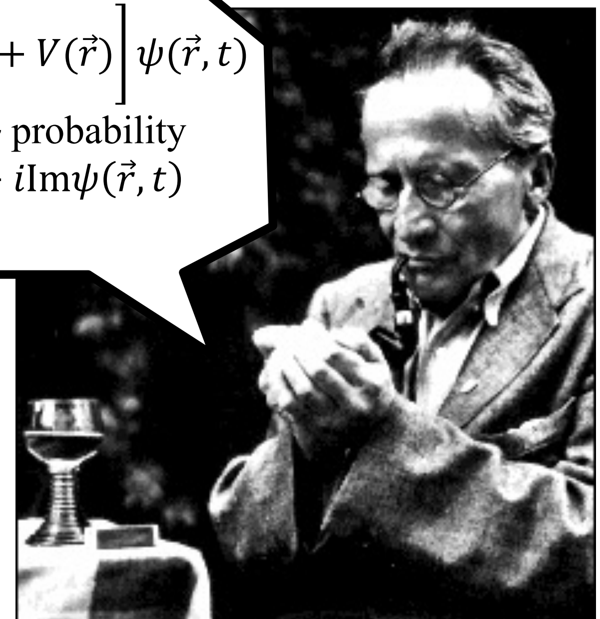
$$|cat\rangle = a|\text{alive}\rangle + b|\text{dead}\rangle$$

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r},t)$$

$$P(\vec{r},t) = |\psi(\vec{r},t)|^2 \sim \text{probability}$$

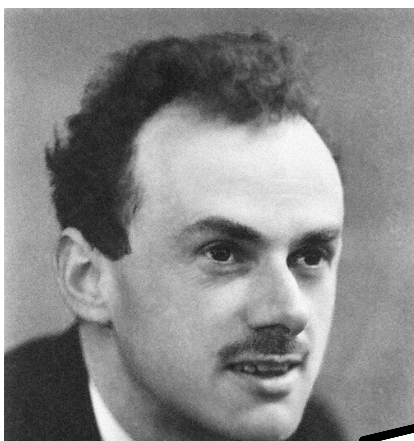
$$\psi(\vec{r},t) = \text{Re}\psi(\vec{r},t) + i\text{Im}\psi(\vec{r},t)$$

$$i = \sqrt{-1}$$



Erwin Schrödinger
1933 Nobel physics prize

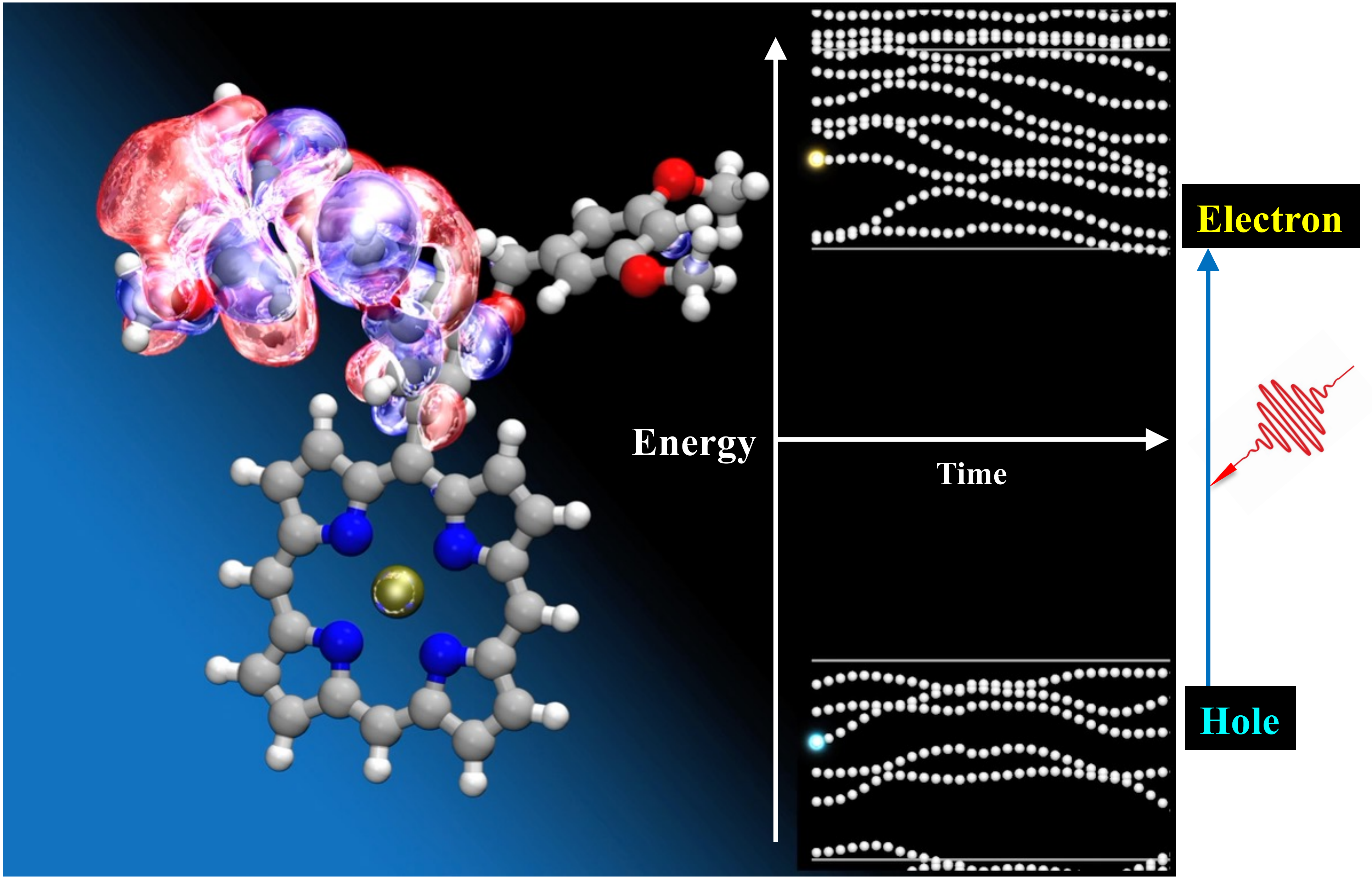
- **Quantum mechanics is exponentially hard — just describing *n*-qubit quantum state requires 2^n coefficients (*e.g.*, $2^{100} \sim 10^{30}$)**



Paul Dirac
1933 Nobel
physics prize

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 7×10^5 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.

Richard Feynman
1965 Nobel physics prize

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

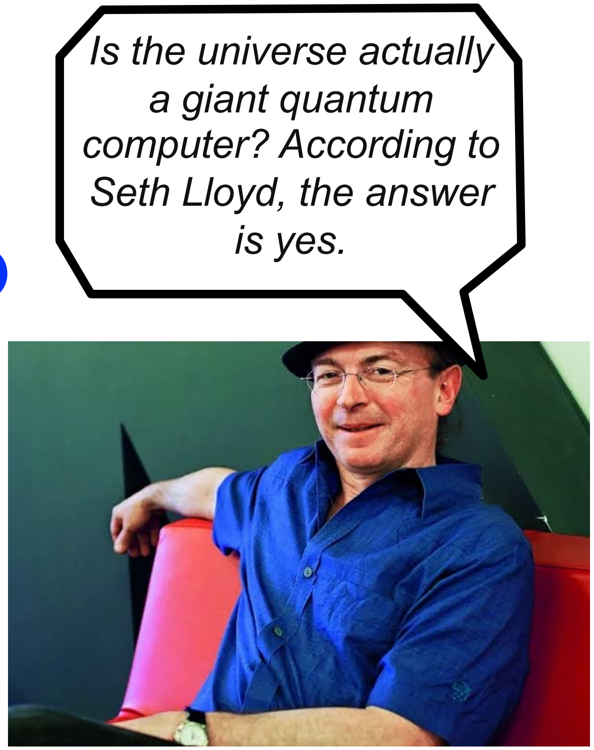
Int. J. Theor. Phys. **21**, 467 ('82)

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



- **Success in simulating *static* properties of quantum systems (*i.e.*, ground-state energy of small molecules)**
  Aspuru-Guzik *et al*., *Science* **309**, 1704 ('05)

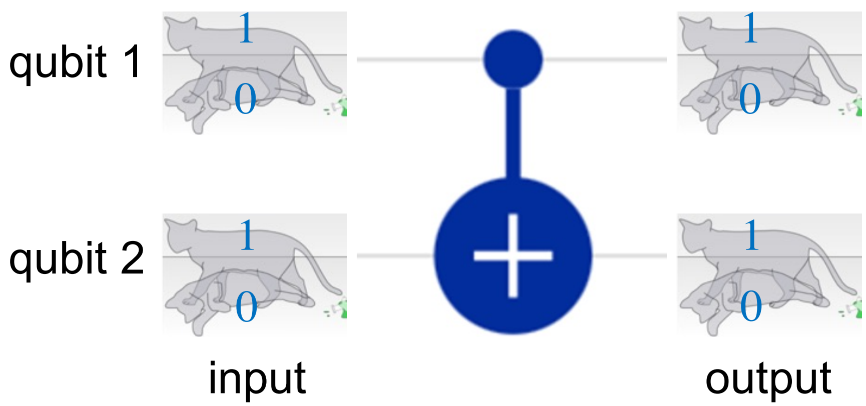
- **Challenge: Simulate quantum many-body *dynamics* on current-to-near-future noisy intermediate-scale quantum (NISQ) computers**
  J. Preskill, *Quantum* **2**, 79 ('18)

- **Second edition of *Feynman Lectures on Computation* (2023) added a section on "Simulating quantum dynamics" by John Preskill** *arXiv*:2106.10522 ('21)

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

How Quantum Computing Works

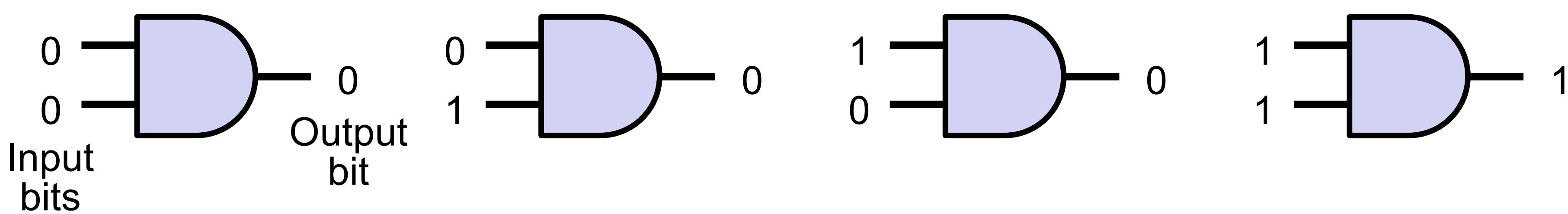
- **Quantum parallelism:** ***Quantum*** **gate acting on** ***n*****-qubit computes** ***all*** **2^n** ***case works all at once*****, thus achieving exponential speedup**
- **Example: Quantum CNOT (conditional not) gate**



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

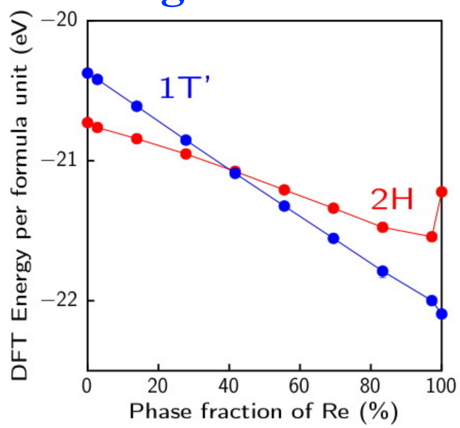
$$U_{\text{CNOT}} = \begin{array}{c} \text{input } 00 \quad 01 \quad 10 \quad 11 \\ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \end{array} \begin{array}{c} \\ 00 \\ 01 \\ 10 \\ 11 \\ \text{output} \end{array}$$

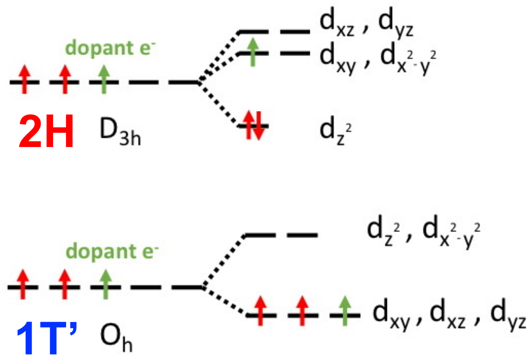
cf. Classical gate computes *only one case at a time*

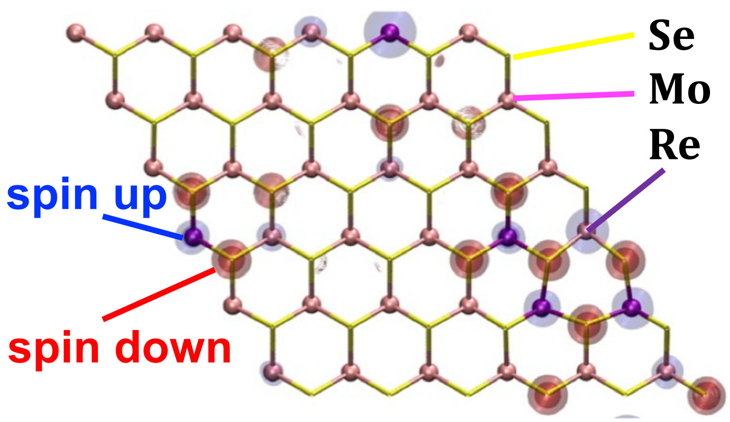


Emergent Magnetism: Structural Transition *via* Doping

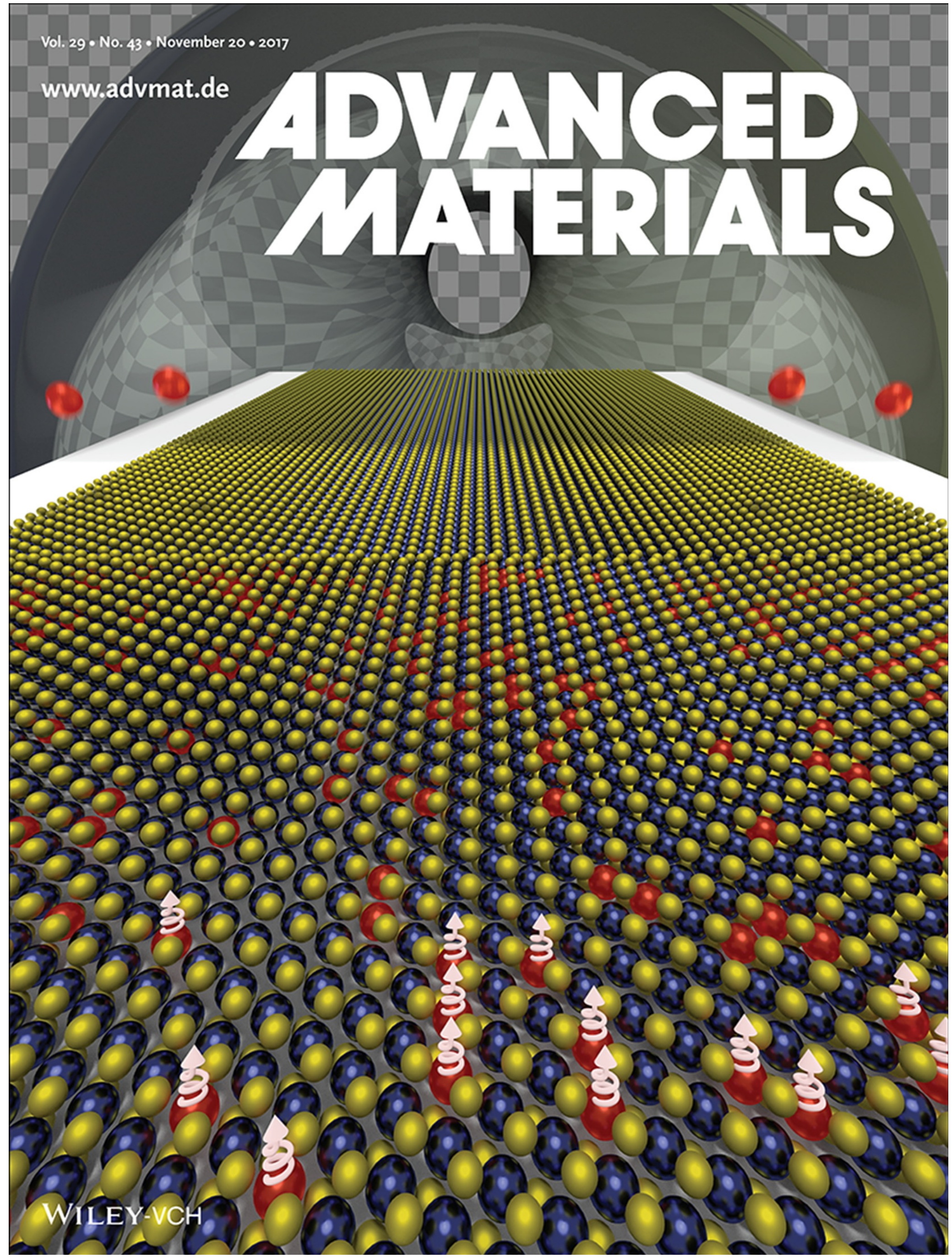
- Experiment at Rice showed 2H-to-1T' phase transformation by alloying $MoSe_2$ with Re
- Simulations at USC elucidated its electronic origin
- Simulation & experiment showed novel magnetism centered at Re atoms







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 $MoSe_2$ monolayer to realize desired material properties on demand, thereby pushing the envelope of "quantum materials science"**

$$H(t) = -J_z \sum_{j=1}^{N-1} \sigma_z^j \sigma_z^{j+1} - \varepsilon_{ph} \sin(\omega_{ph} t) \sum_{j=1}^{N} \sigma_x^j$$

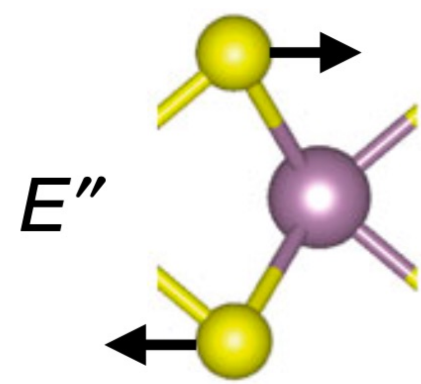
$$= H_z + H_x(t)$$

Phonon frequency

Phonon-induced energy split

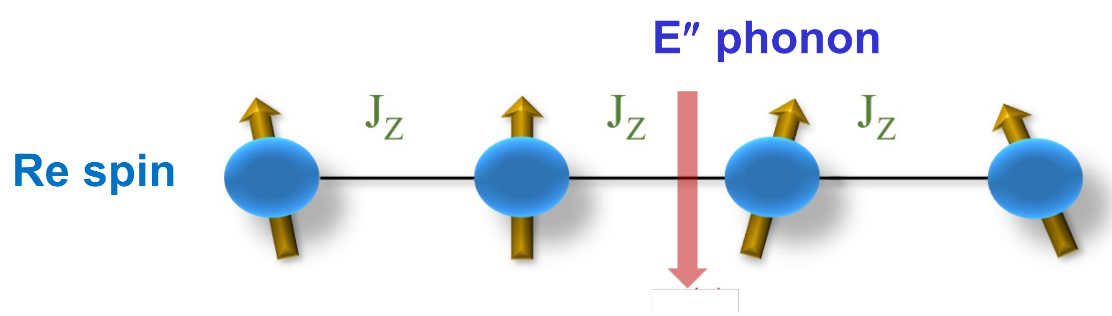
$$\sigma_z^j = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix};\ \sigma_x^j = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$ // Act on *j*-th qubit

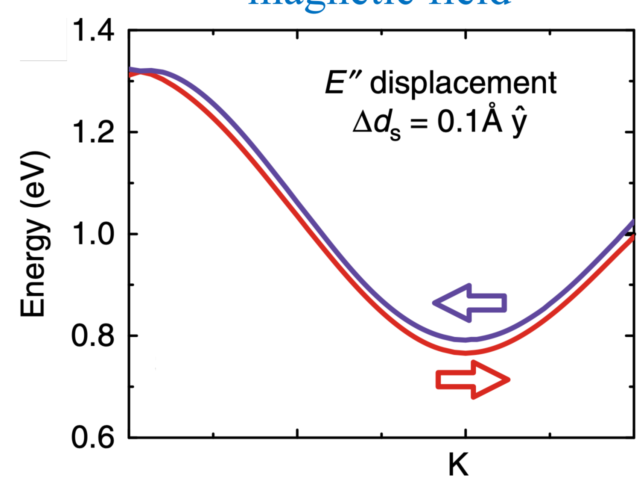
Phonon



Spin-orbit coupling

Effective in-plane magnetic field



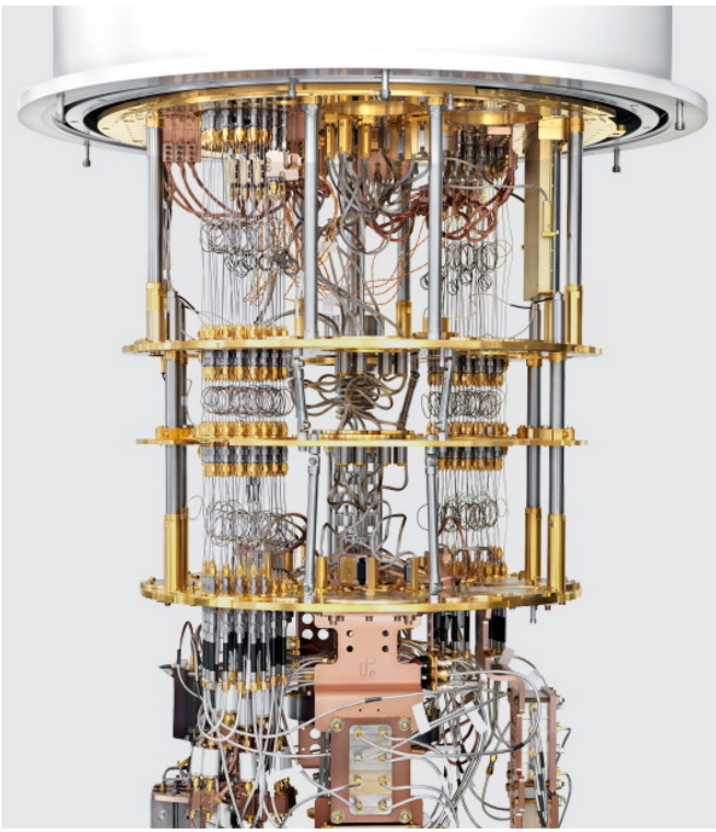


D. Shin *et al.*, *Nat. Commun.* **9**, 638 ('18)

Quantum Computing of Magnetism

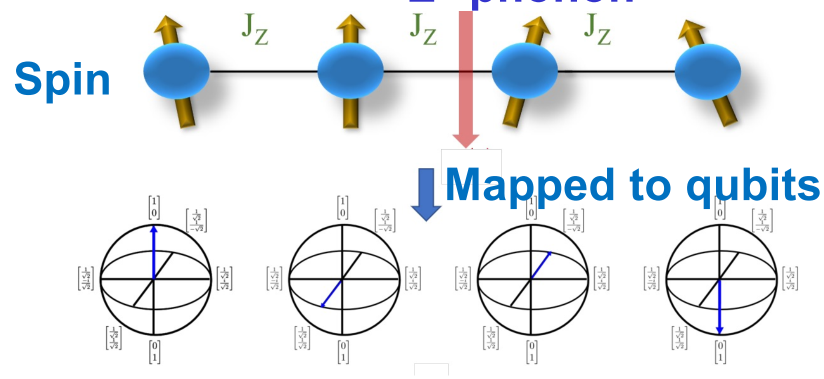
- **Simulated quantum many-body dynamics of magnetic spins on IBM's Q16 Melbourne & Rigetti's Aspen quantum processors**

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

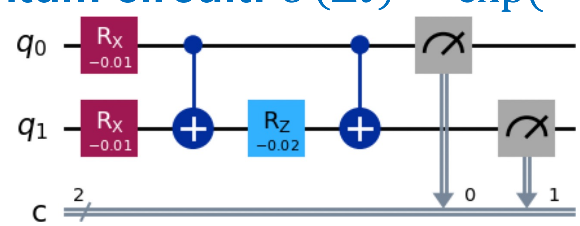


$$H(t) = -J_z \sum_{j=1}^{N-1} \boldsymbol{\sigma}_z^j \boldsymbol{\sigma}_z^{j+1} - \varepsilon_{ph} \sin(\omega_{ph} t) \sum_{j=1}^{N} \boldsymbol{\sigma}_x^j$$

E″ phonon



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*J, 1)
circ.cx(0, 1)
```

Quantum Dynamics on NISQ Computers

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

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

$$U(\Delta t) = \exp(-iH\Delta t)$$

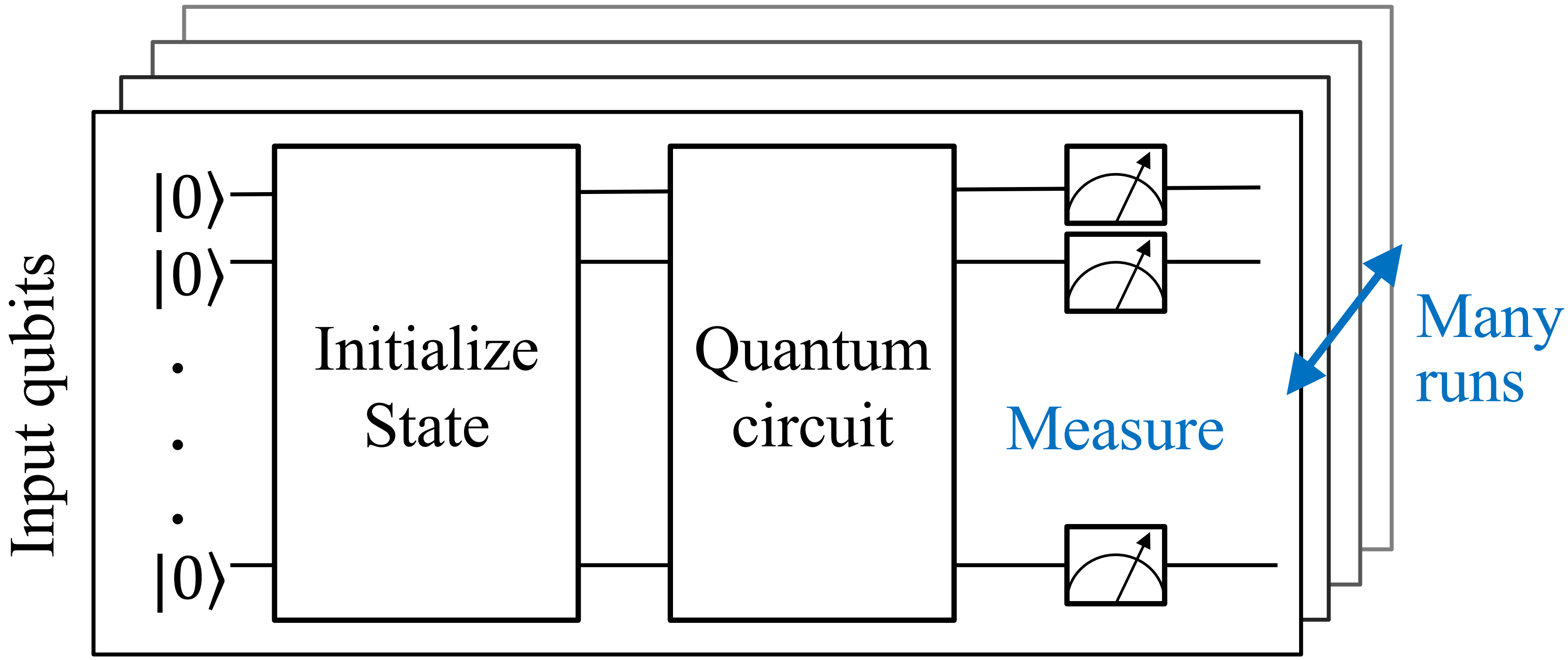
- **Time discretization with time-step $\Delta \boldsymbol{t}$ and Trotter expansion**

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

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

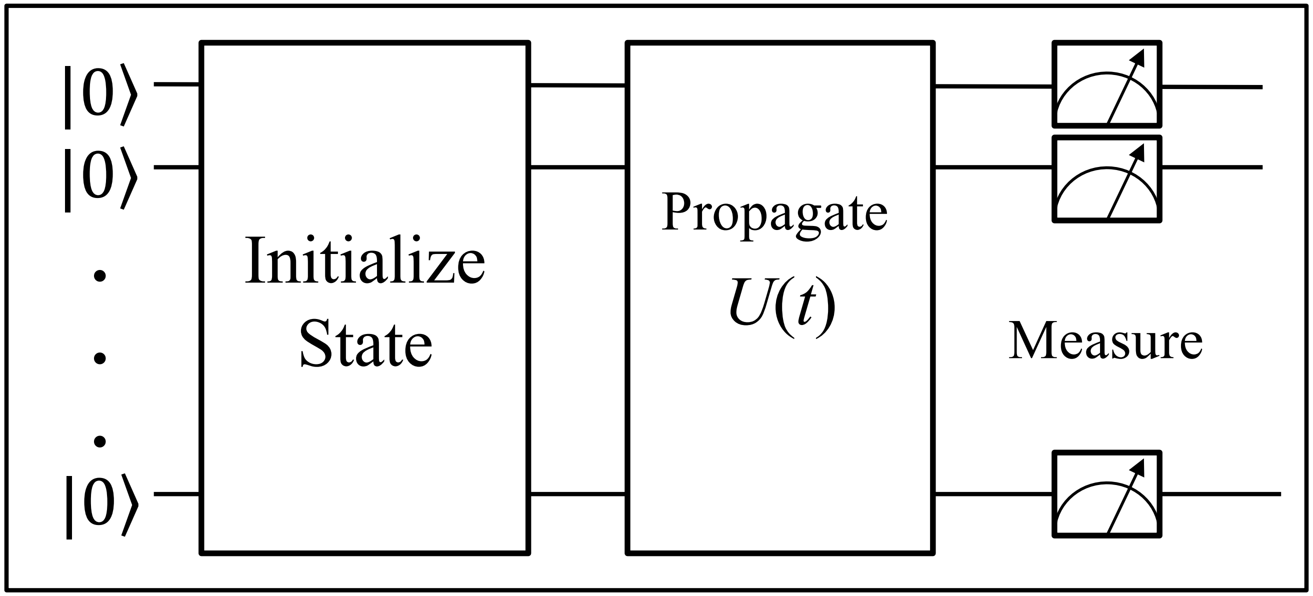
Quantum Computing Runs & Measurements

- 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

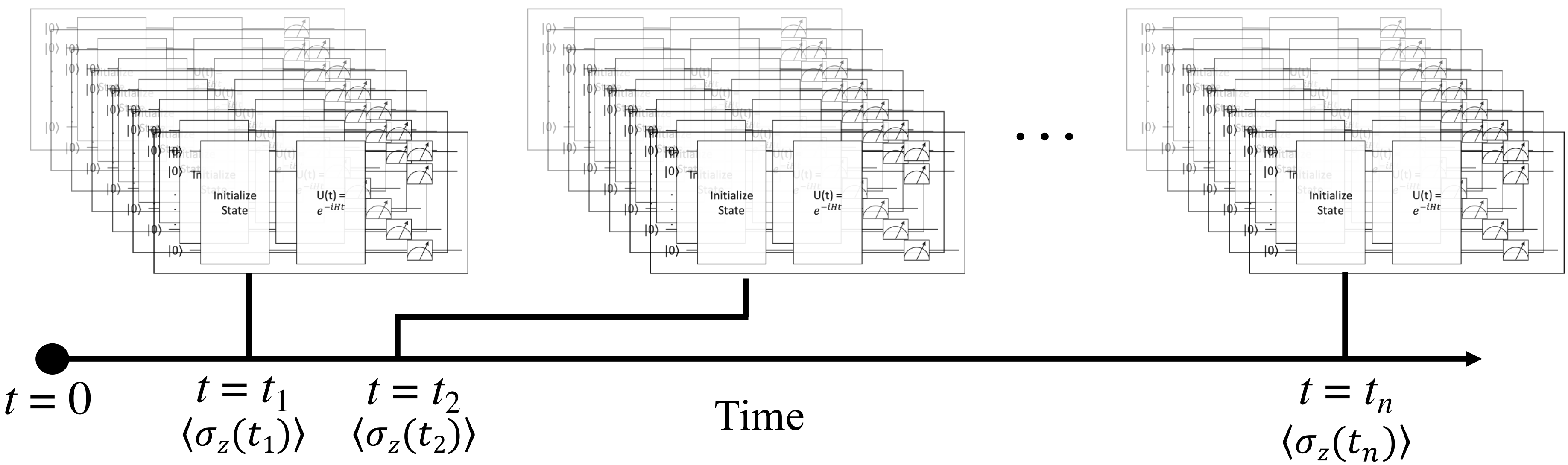


- For each program, thousands of runs need be performed on a quantum computer to obtain statistics

More Runs for Quantum Dynamics



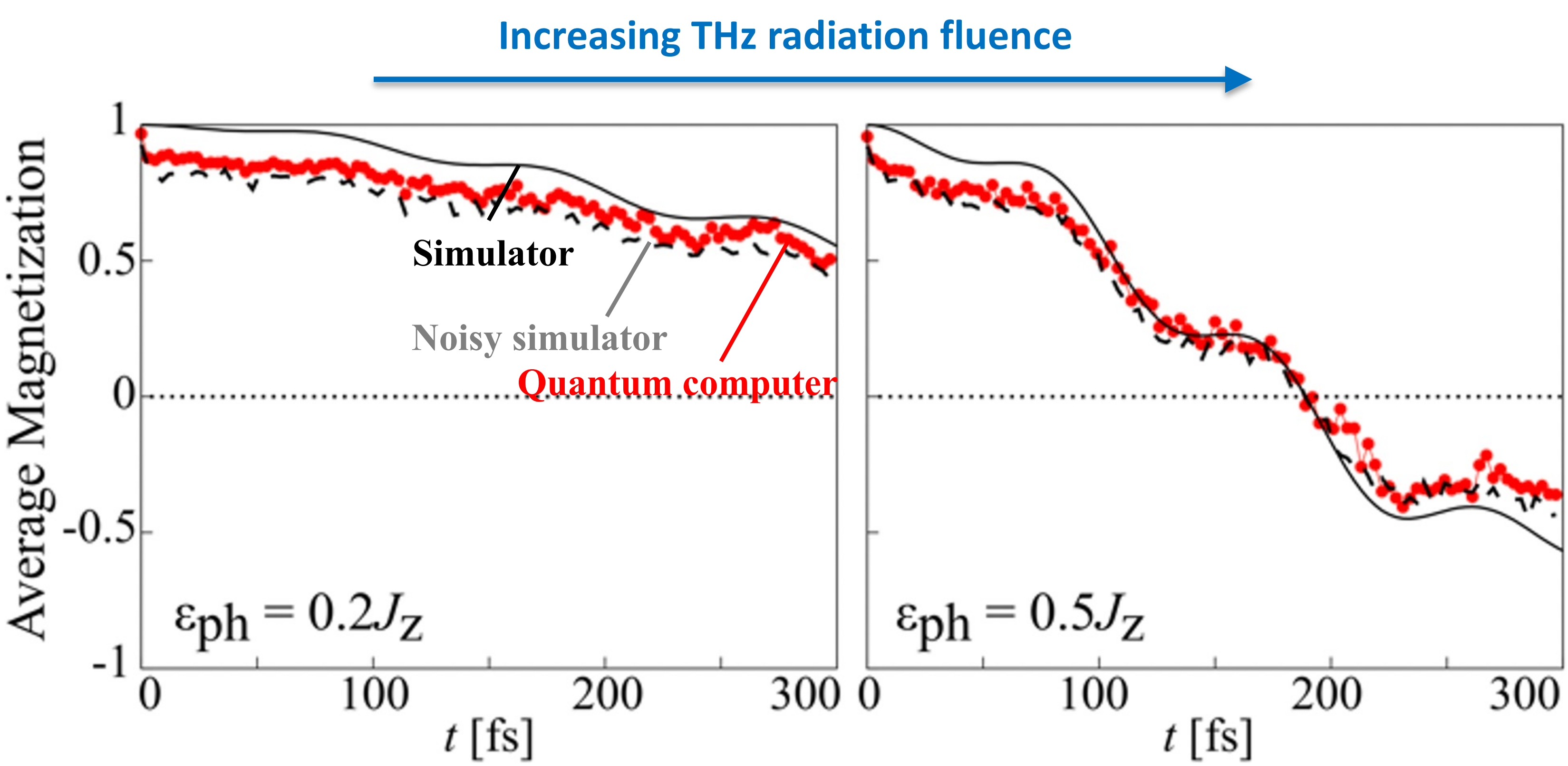
For *each of many time instances*, many runs to obtain statistics



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

Quantum Computing Results

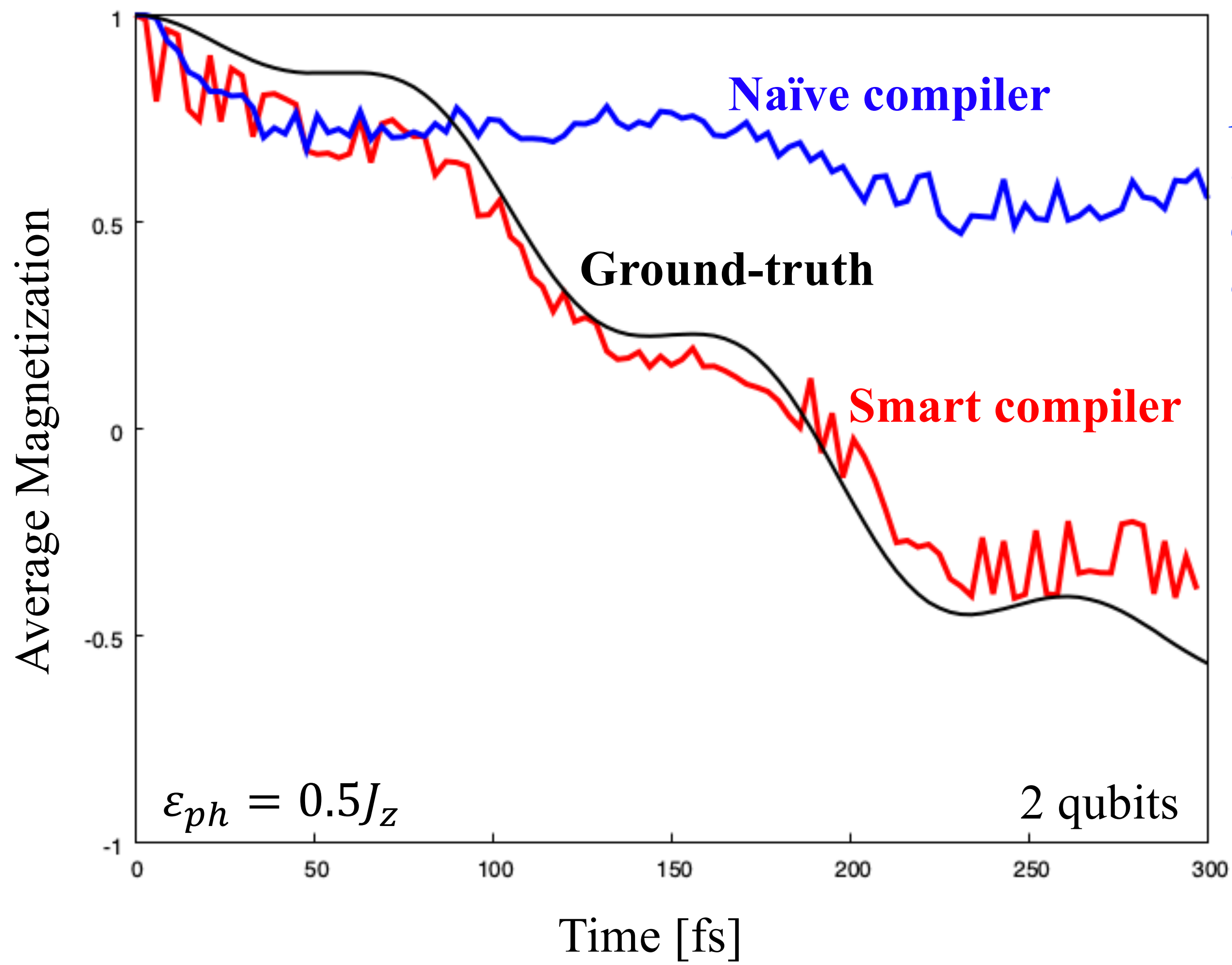
- **Quantum-dynamics simulations on NISQ computers show dynamic suppression of magnetization by THz radiation**



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

Circuit Size *vs.* Simulation Fidelity

- **Reduced circuit size improves the fidelity of simulation**



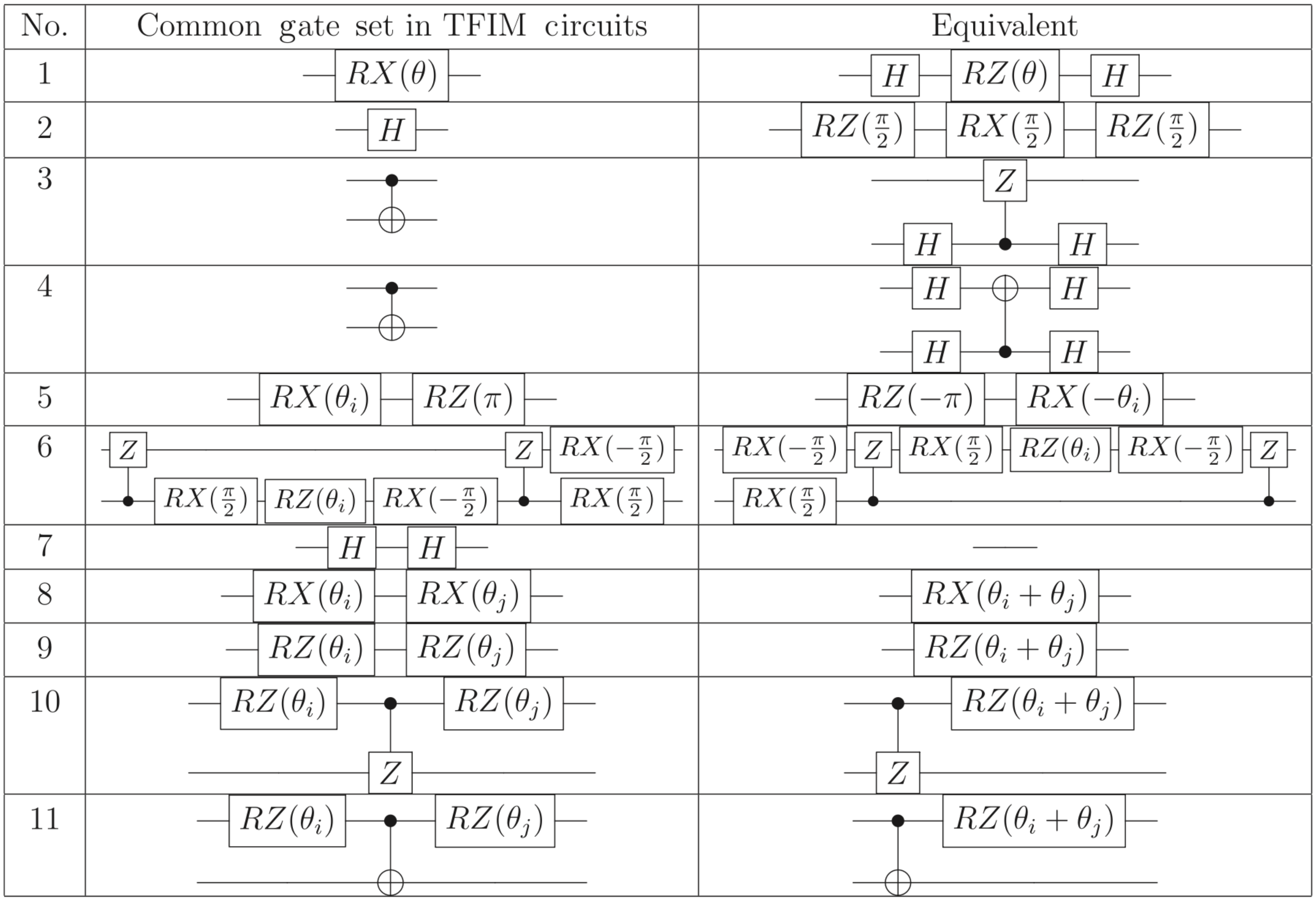
Due to high cumulative quantum-gate errors!

Naïve compiler: circuit size ∝ time

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

Quantum Compiler: Math

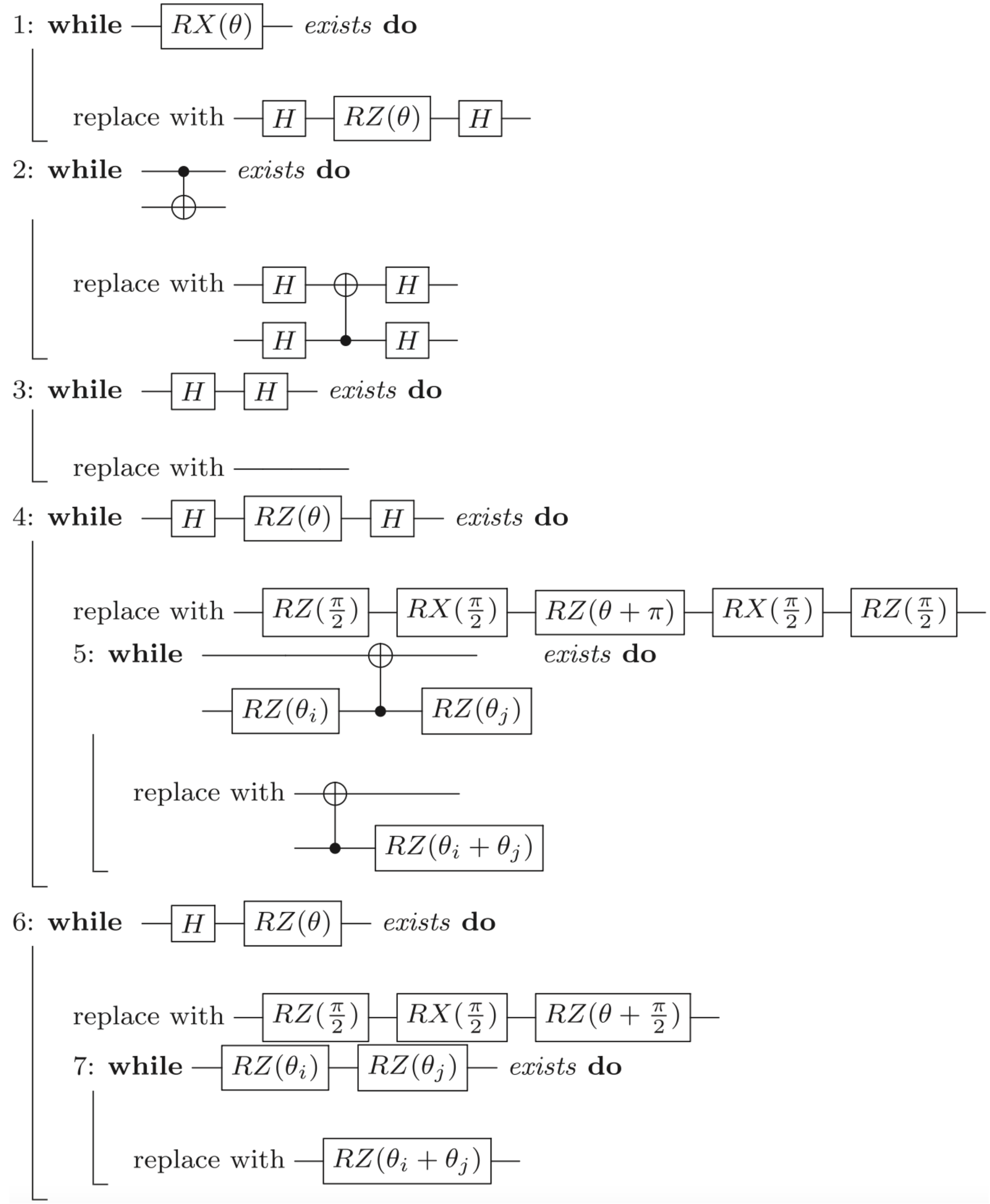
- **Problem: High gate errors make long-time simulations impractical**
- **Solution: Domain-specific compiler = use algebraic identities to derive an equivalent circuit with reduced circuit size**



L. Bassman *et al.*, *Quantum Sci. Tech.* **6**, 014007 ('21)

Algorithm for IBM Native Gates

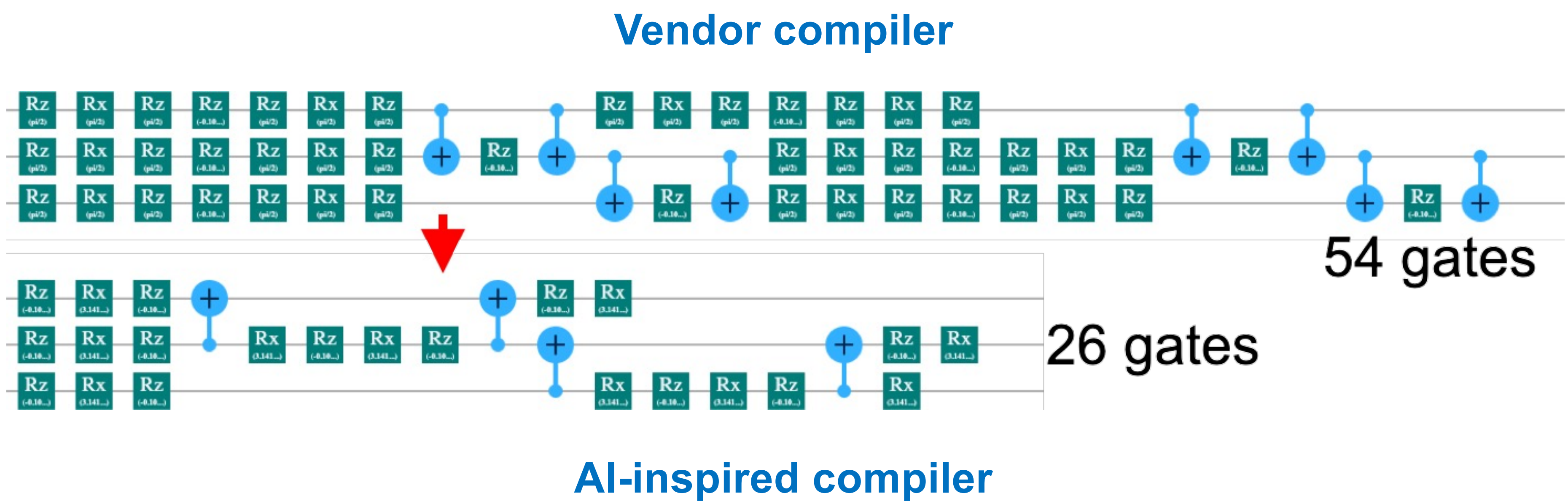
- **Heuristic algorithm similar to unit propagation in artificial intelligence (AI)**
- **The heuristic order & types of identities applied are specific to the particular quantum dynamics we simulated**



L. Bassman *et al.*,
Quantum Sci. Tech. **6**, 014007 ('21)

Domain-Specific Quantum Compiler

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

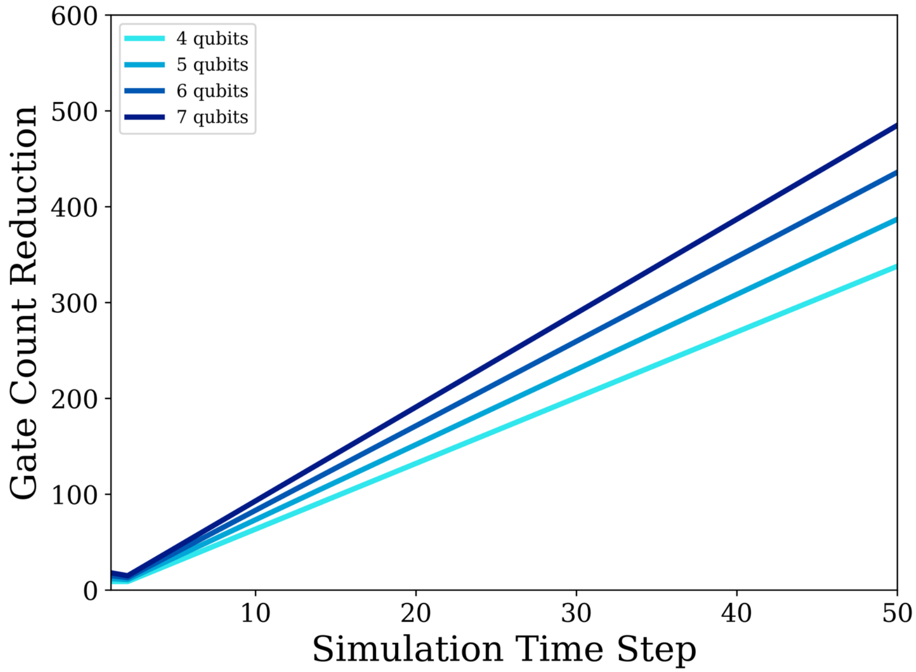


L. Bassman *et al.*, *Quantum Sci. Tech.* **6**, 014007 ('21)

Performance of Domain-Specific Compiler

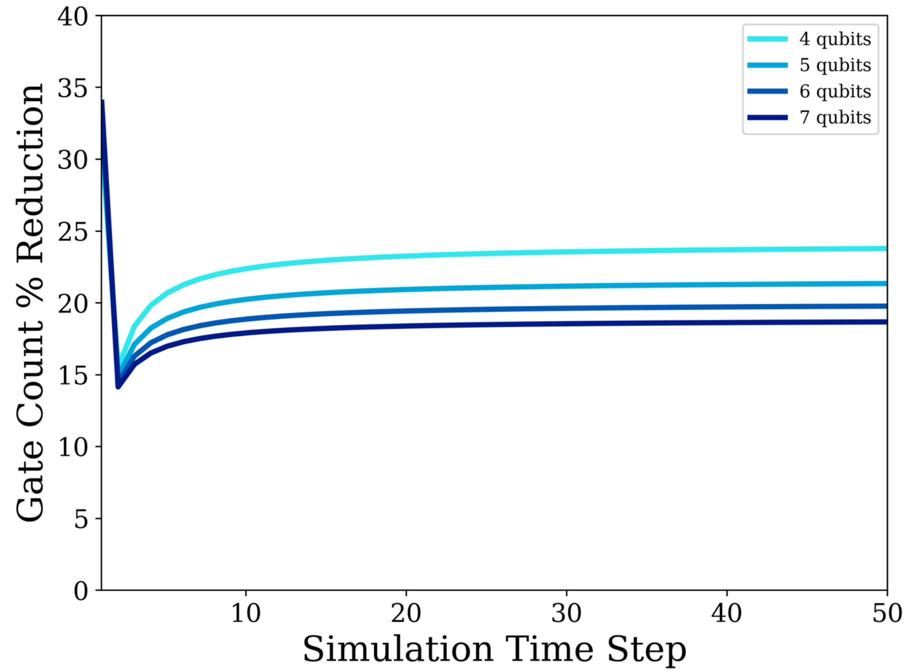
Absolute gate count difference

$$(IBM\ Compiler - DS\ Compiler)$$



Percent gate count difference

$$\frac{IBM\ Compiler - DS\ Compiler}{IBM\ Compiler} \times 100$$

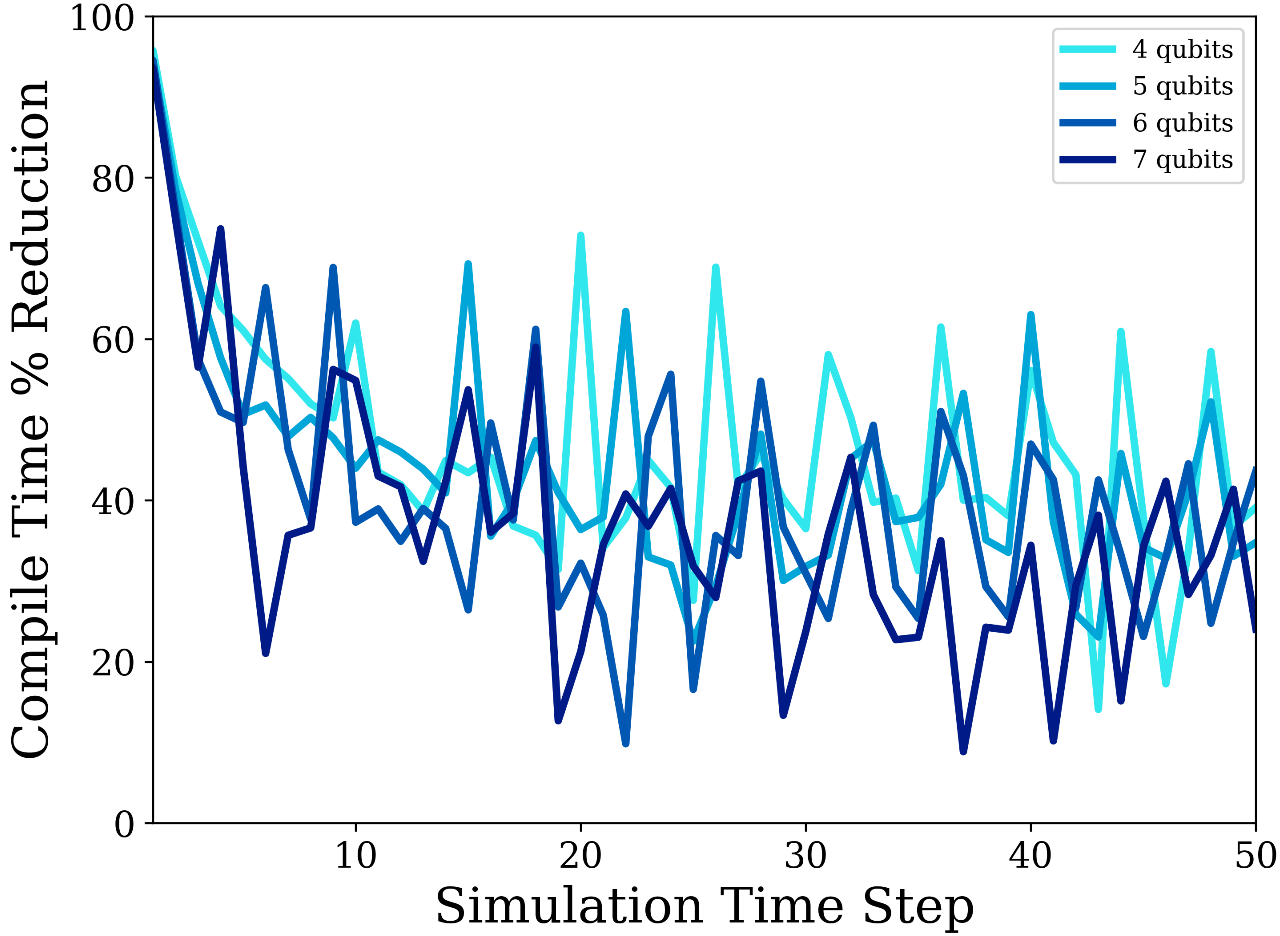


Domain-specific compiler reduces gate count compared to IBM compiler

Speed of Domain-Specific Compiler

Percent compile-time difference

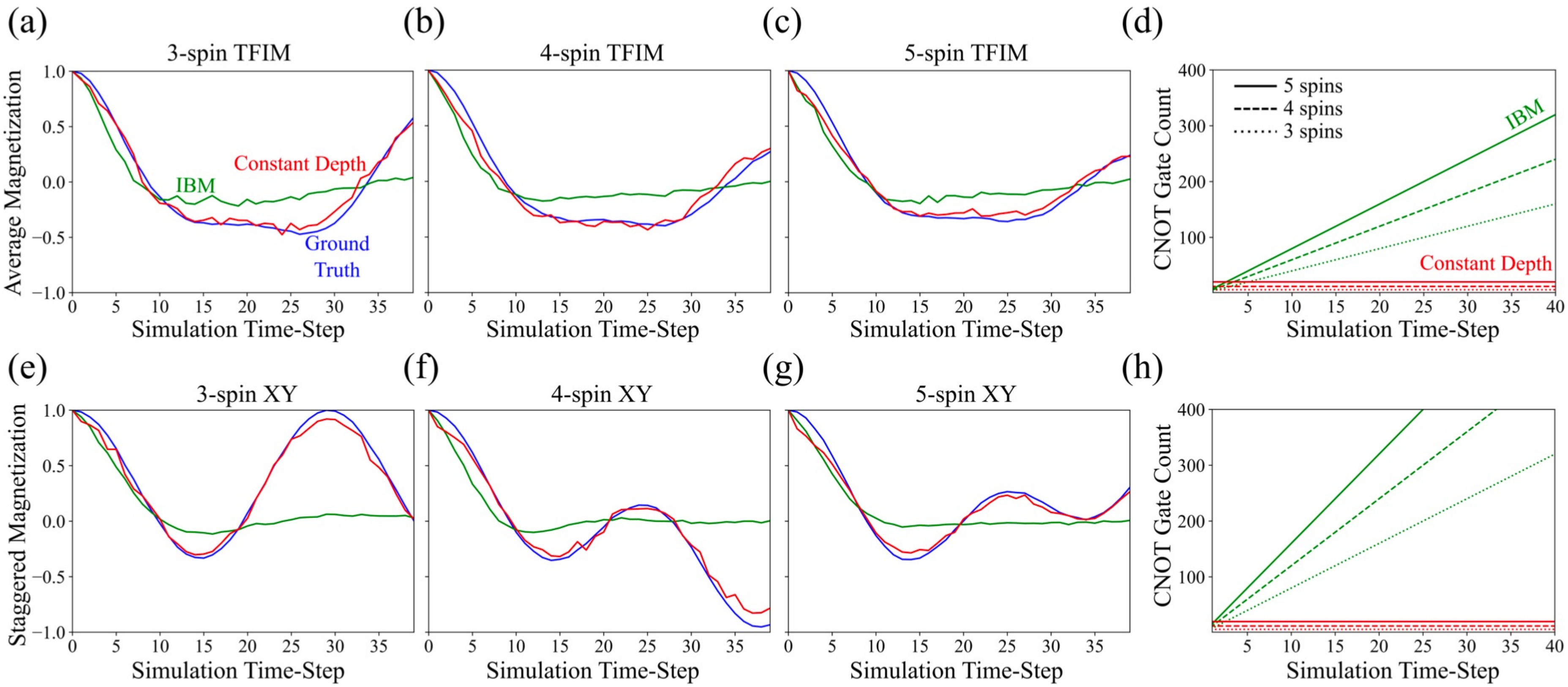
$$\frac{IBM\ Compiler - DS\ Compiler}{IBM\ Compiler} \times 100$$



… 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"

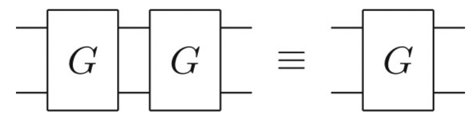
L. Bassman *et al.*, *Mater. Theo.* **6**, 13 ('22)

Constant Circuit-Depth: How It is Done

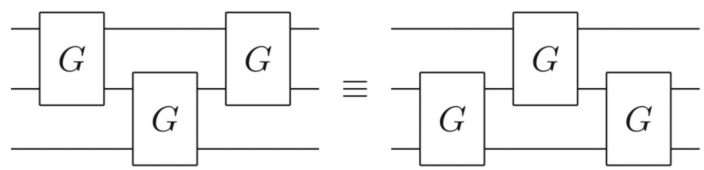
- **Matchgate (shifted 2×2 block diagonal)**

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

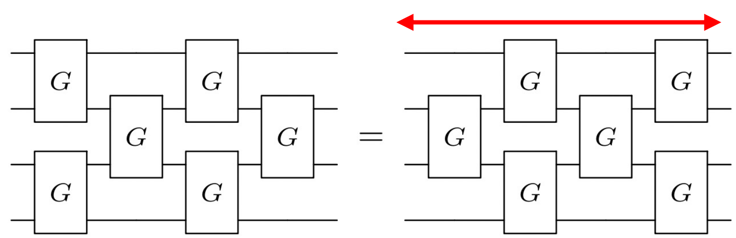
- **Contraction: product of matchgates is a matchgates**



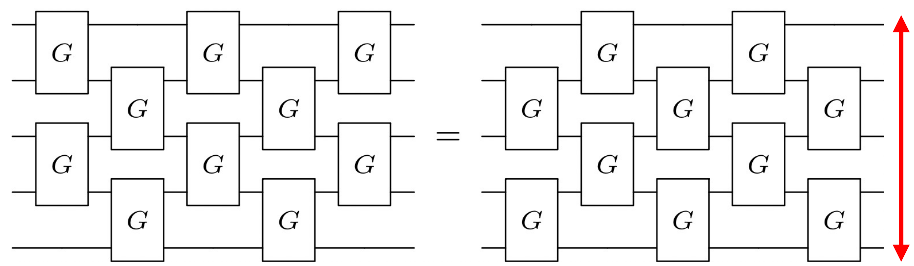
- **Conjecture: existence of flipped matchgates**
  cf. Yang-Baxter equation



- **Mirroring identities**



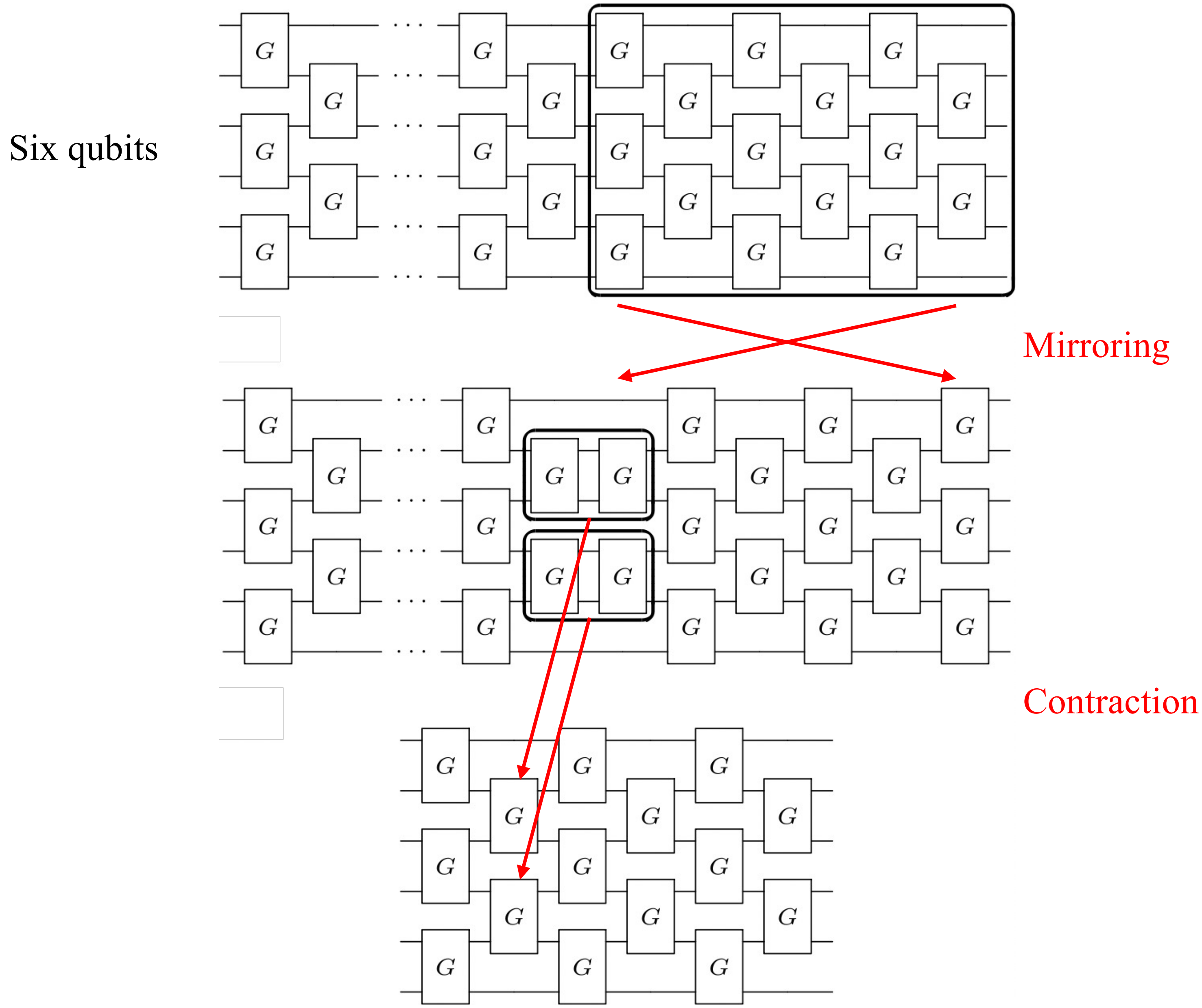
Even qubits



Odd qubits

L. Bassman *et al.*, *Mater. Theo.* **6**, 13 ('21)

Downfolding to Constant-Depth



L. Bassman *et al.*, *Mater. Theo.* **6**, 13 ('21)

Richer Physics: Heisenberg Model

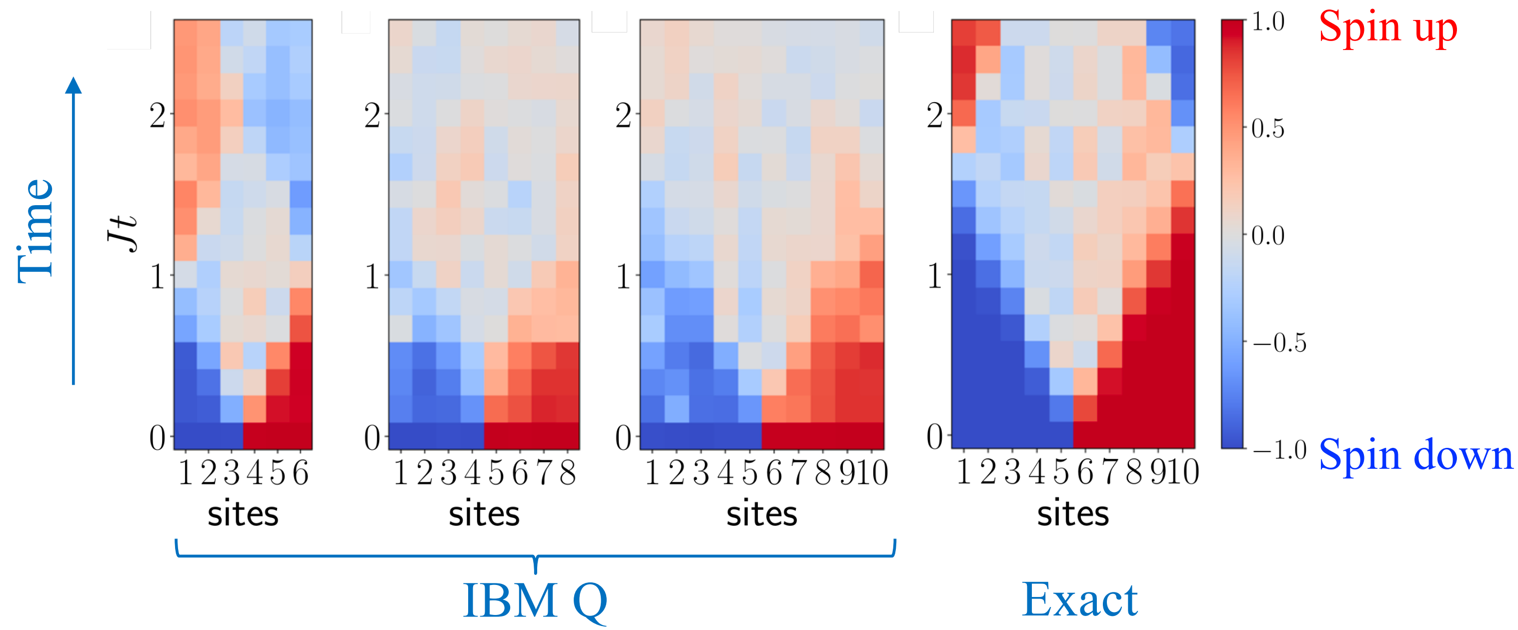
$$H = -\sum_{j=1}^{N-1}\underbrace{\left(J_x\sigma_x^j\sigma_x^{j+1} + J_y\sigma_y^j\sigma_y^{j+1} + J_z\sigma_z^j\sigma_z^{j+1}\right)}_{\text{Exchange coupling}} - h\sum_{j=1}^{N}\sigma_z^j$$

Magnetic field

Pauli spin-1/2 matrices

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

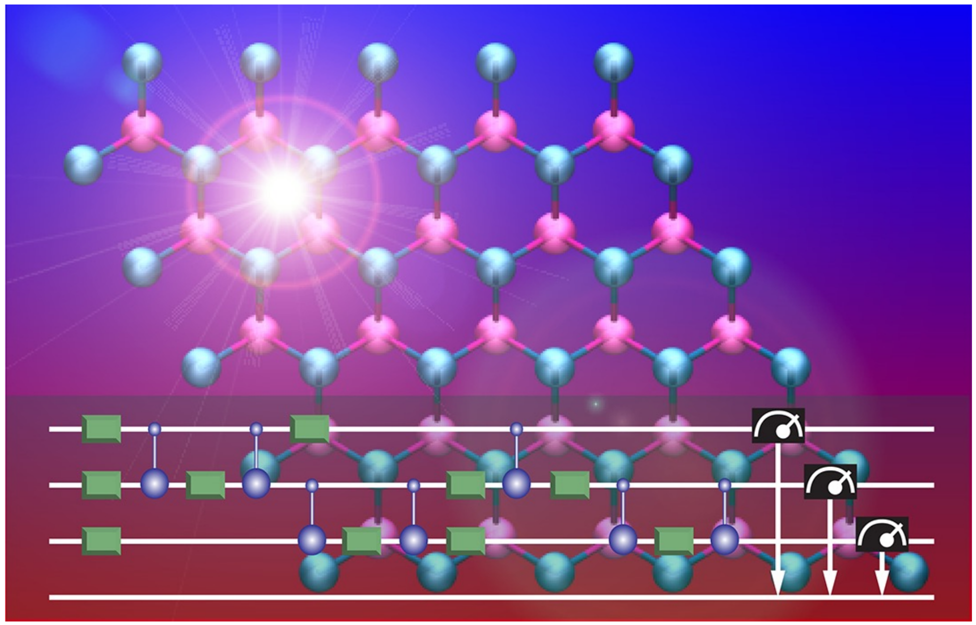
Domain-wall dynamics (6-, 8- & 10-site spin chains)



A. Smith *et al.*, *npJ Quantum Info.* **5**, 106 ('19)

Open-Source Quantum Software

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



MISTIQS

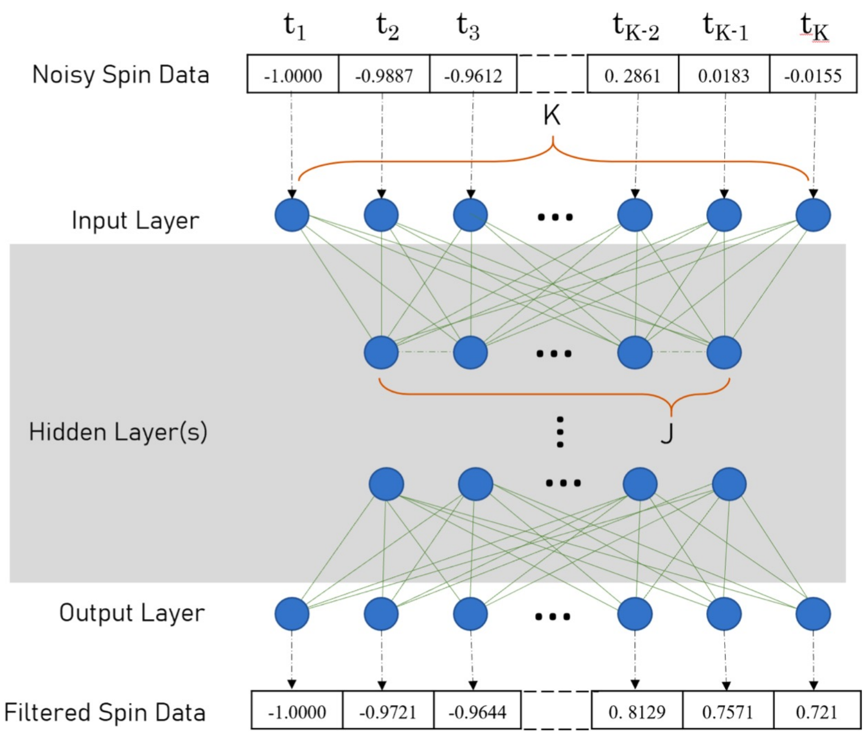
Mult**I**platform
Software for
TIme-dependent
Quantum
Simulation

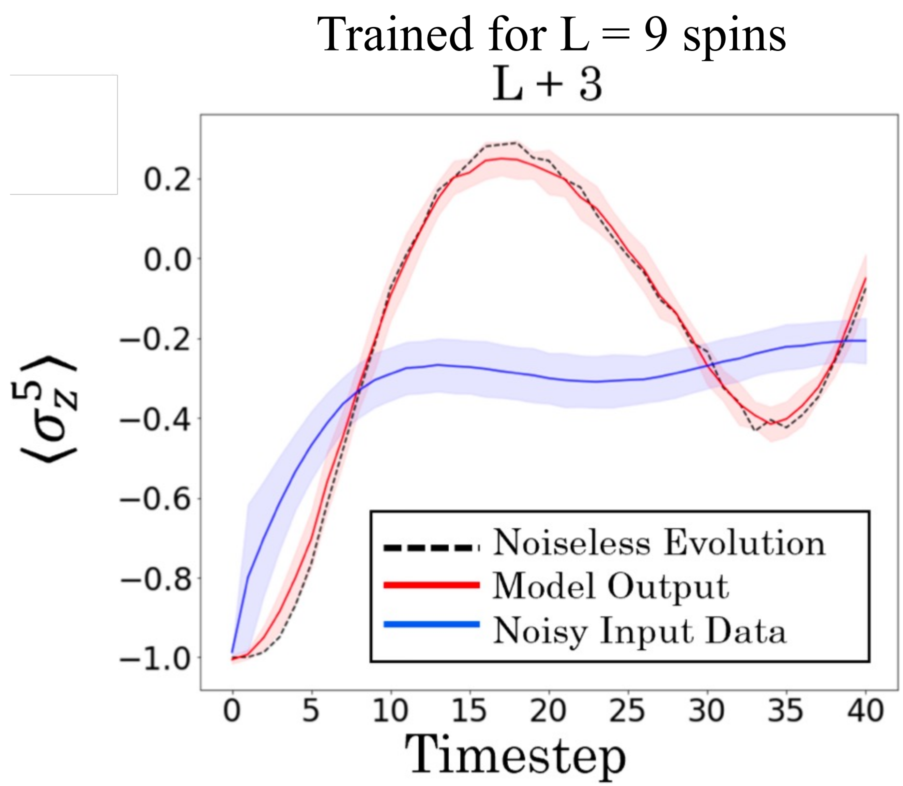
Paper: C. Powers *et al.*, *SoftwareX* **14**, 100696 ('21)

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**

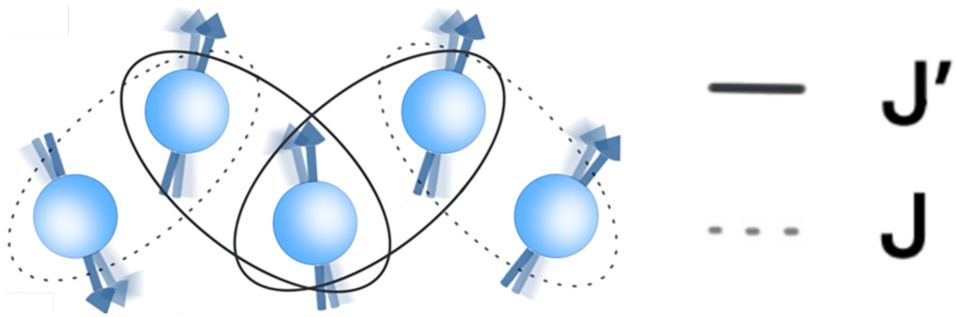




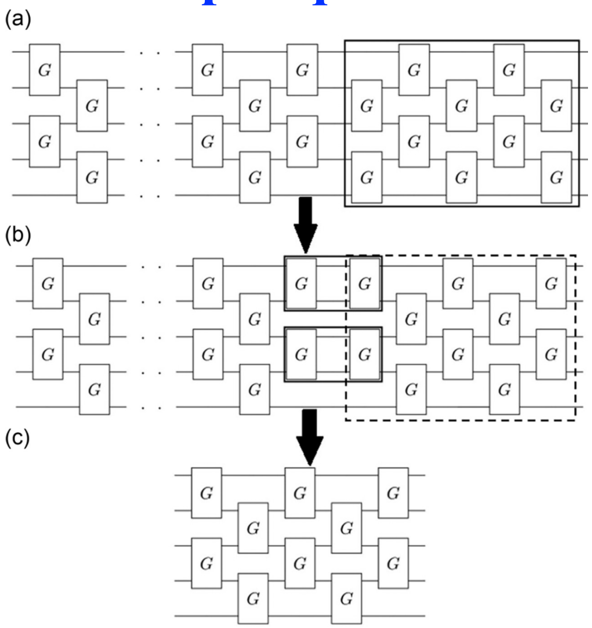
C. Powers *et al.*, *NeurIPS workshop* ('21)

Topological Quantum Dynamics

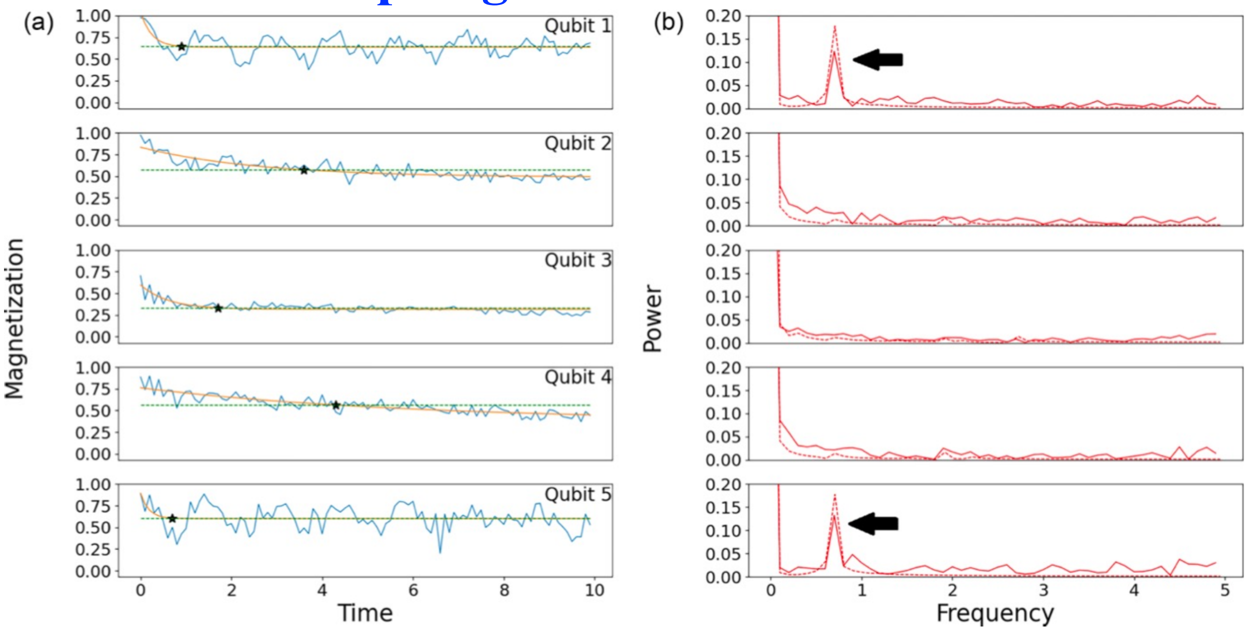
Quantum spin chain



Constant-depth quantum circuit



Topological surface mode



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

New: Periodically-driven Floquet topology simulated

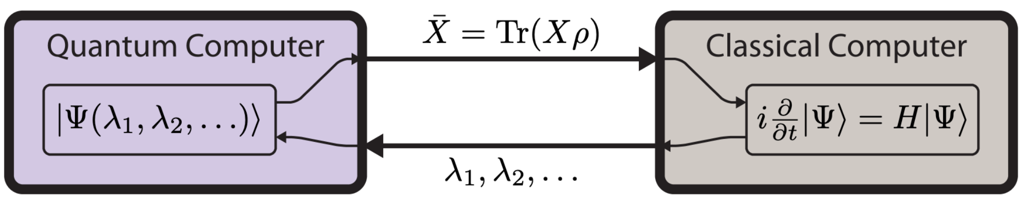
Variational Quantum Simulator

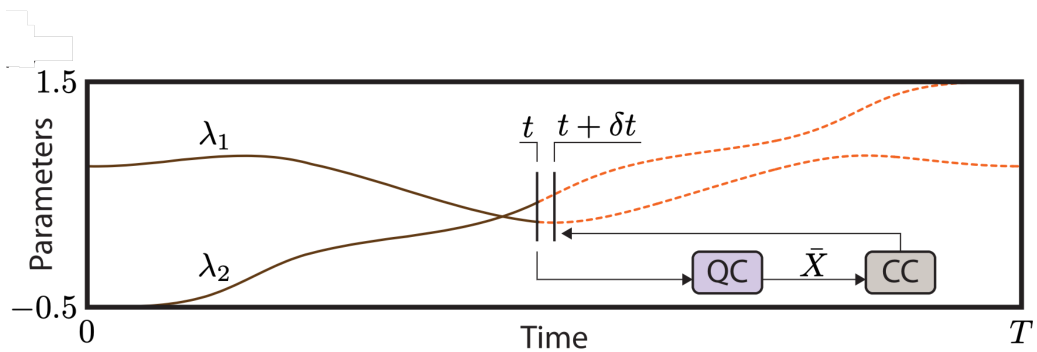
Hybrid quantum/classical approach: Boost the power of a classical supercomputer using a quantum co-processor

- **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, $|\boldsymbol{\psi}(\boldsymbol{t})\rangle = |\boldsymbol{\psi}(\boldsymbol{\lambda_1}(\boldsymbol{t}), \dots, \boldsymbol{\lambda_P}(\boldsymbol{t}))\rangle$, which is tractable on a classical computer**

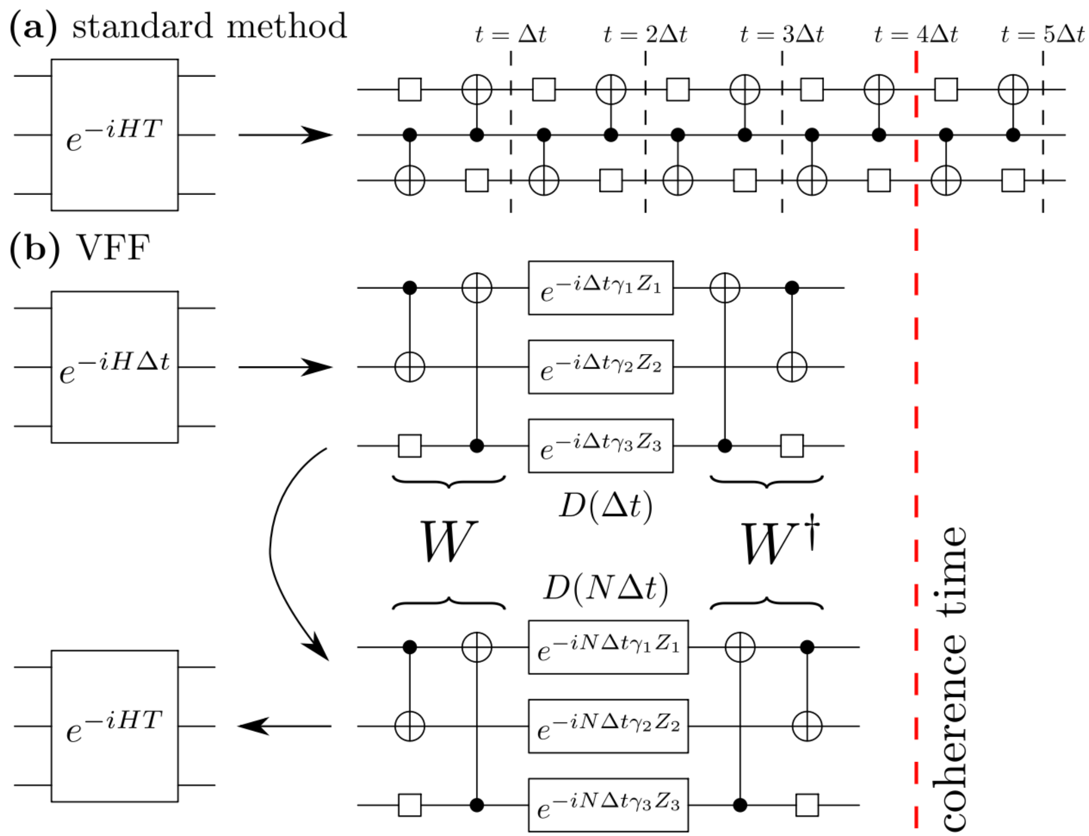




Y. Li & S. Benjamin, *Phys. Rev. X* **7**, 021050 ('17)

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**

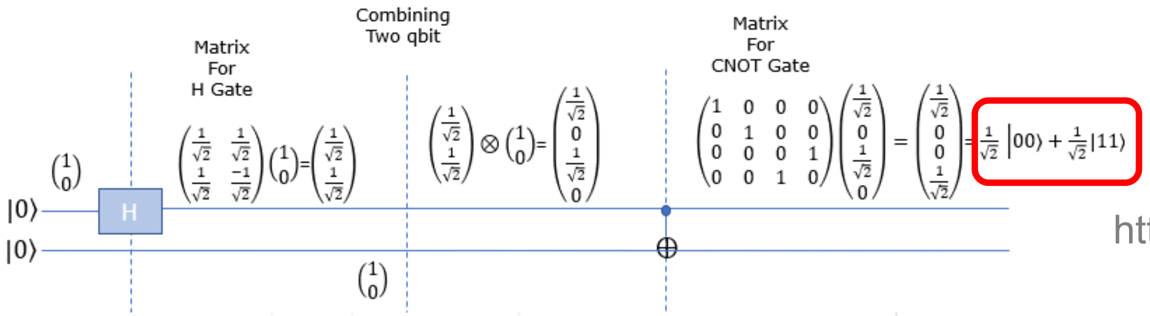


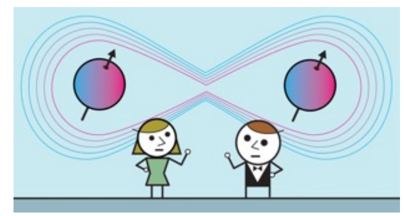
C. Cirstoiu *et al.*, *npjQI* **6**, 82 ('20)

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

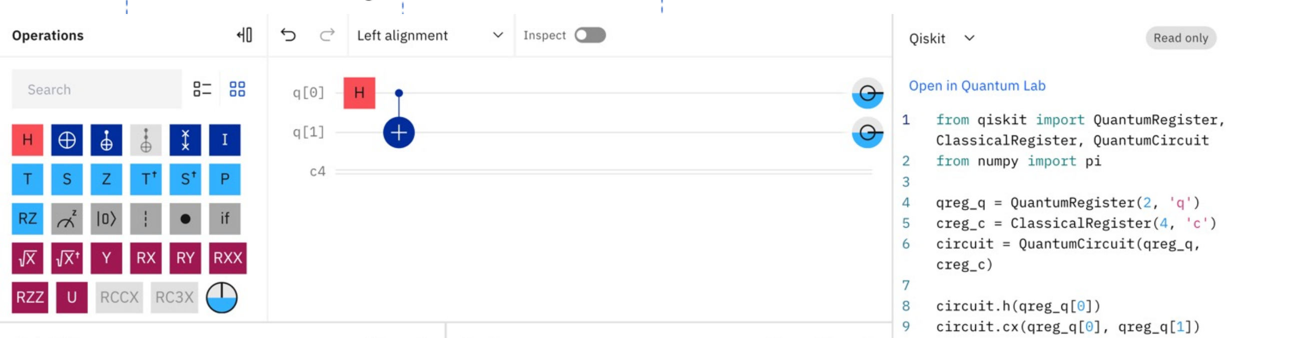
Do-It-Yourself Quantum Computing

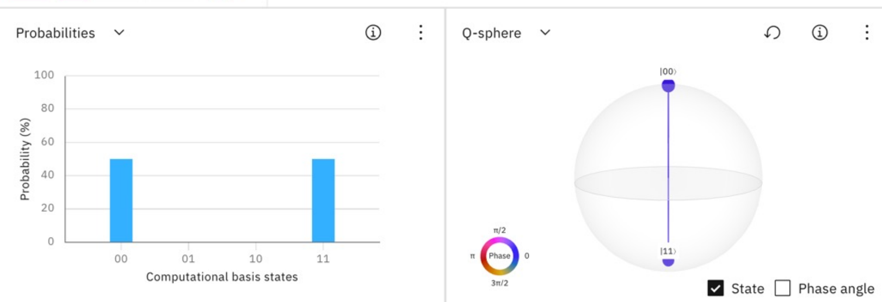
- **Sign up & sign in to IBM Quantum cloud**
  https://quantum.cloud.ibm.com
- **Open Composer (GUI-based quantum programming platform)**
- **Build a quantum circuit to prepare an *entangled Bell's state*, which has played an essential role in quantum information science (2022 Nobel physics prize), using Hadamard & CNOT gates**

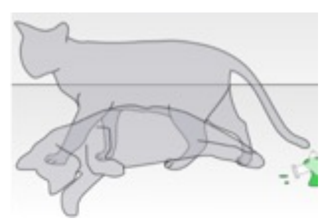




https://en.wikipedia.org/wiki/Bell_state







Hadamard gate transforms a pure qubit (|0⟩ or |1⟩) into a superposition of |0⟩ & |1⟩:

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

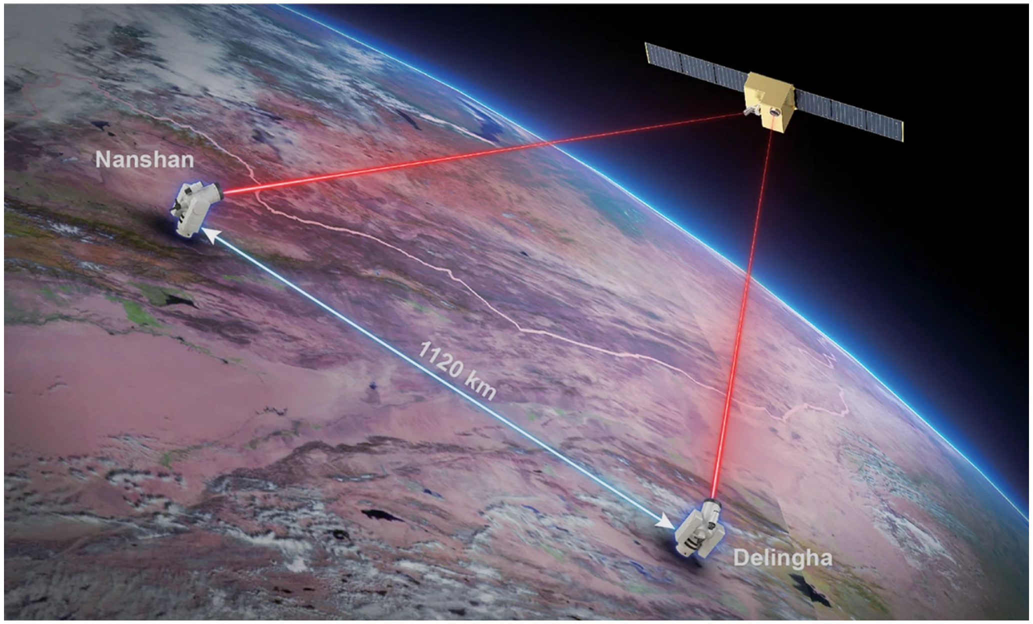
$$H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

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