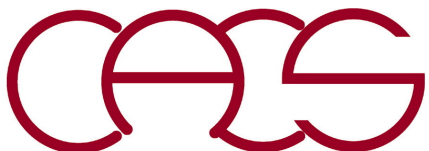# Quantum Computational Science

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Department of Physics & Astronomy
Department of Quantitative & Computational Biology
University of Southern California

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Goal: Quantum dynamics simulation on quantum circuits

2022 Nobel Physics Prize

It's entanglement!

The Nobel Prize in Physics 2022

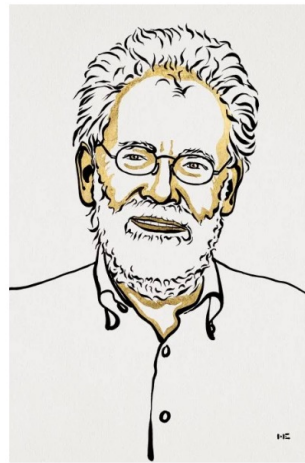Ill. Niklas Elmehed © Nobel Prize Outreach
Alain Aspect
Prize share: 1/3

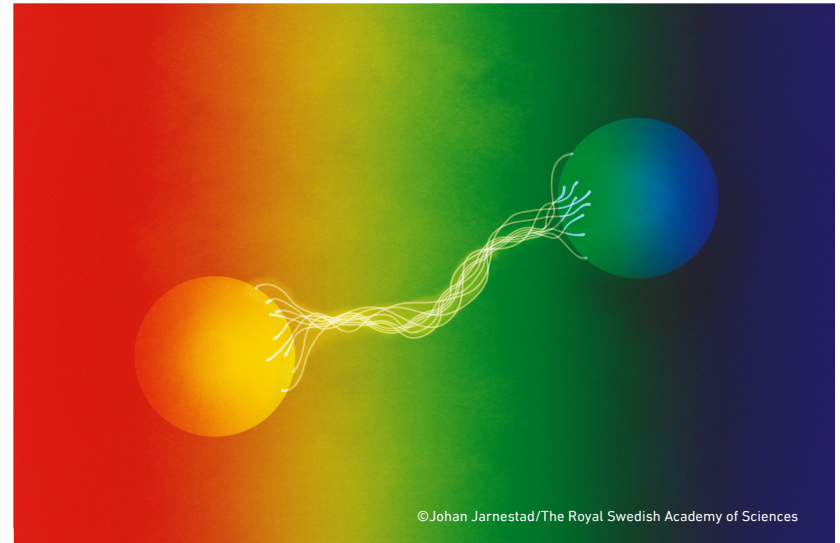Ill. Niklas Elmehed © Nobel Prize Outreach
John F. Clauser
Prize share: 1/3

Ill. Niklas Elmehed © Nobel Prize Outreach
Anton Zeilinger
Prize share: 1/3

©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"

Quantum Computing (QC) for Science

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

- **U.S. Congress (Dec. 21, '18) signed National Quantum Initiative Act to ensure leadership in quantum computing & its applications**

- **Quantum supremacy demonstrated by Google**
  F. Arute, *Nature* **574**, 505 ('19)

- **Quantum computing for science:**
  Universal simulator of quantum many-body systems

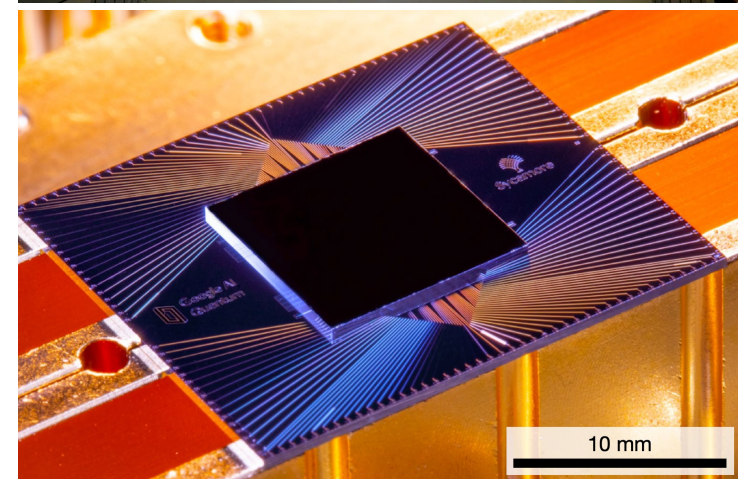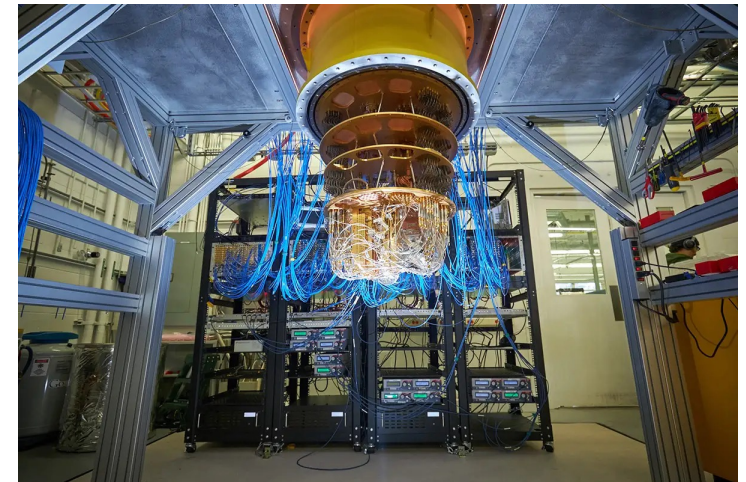 R. P. Feynman, *Int. J. Theo. Phys.* **21**, 467 ('82);
  S. Lloyd, *Science* **273**, 1073 ('96)

- **Success in simulating *static* properties of quantum systems (*i.e.*, ground-state energy of small molecules)**
  A. 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)

10 mm

**54-qubit Google Sycamore**

Quantum Dynamics Simulations

- **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)]

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

- **Simulated nontrivial quantum dynamics on publicly available IBM's Q16 Melbourne & Rigetti's Aspen NISQ computers, *i.e.*, ultrafast control of emergent magnetism by THz radiation in 2D material** [L. Bassman *et al., Phys. Rev. B* **101**, 184305 ('20)

Do it yourself at https://quantum-computing.ibm.com
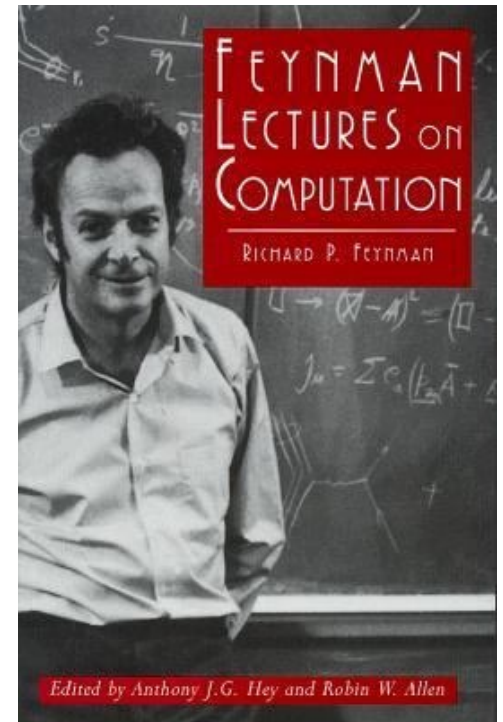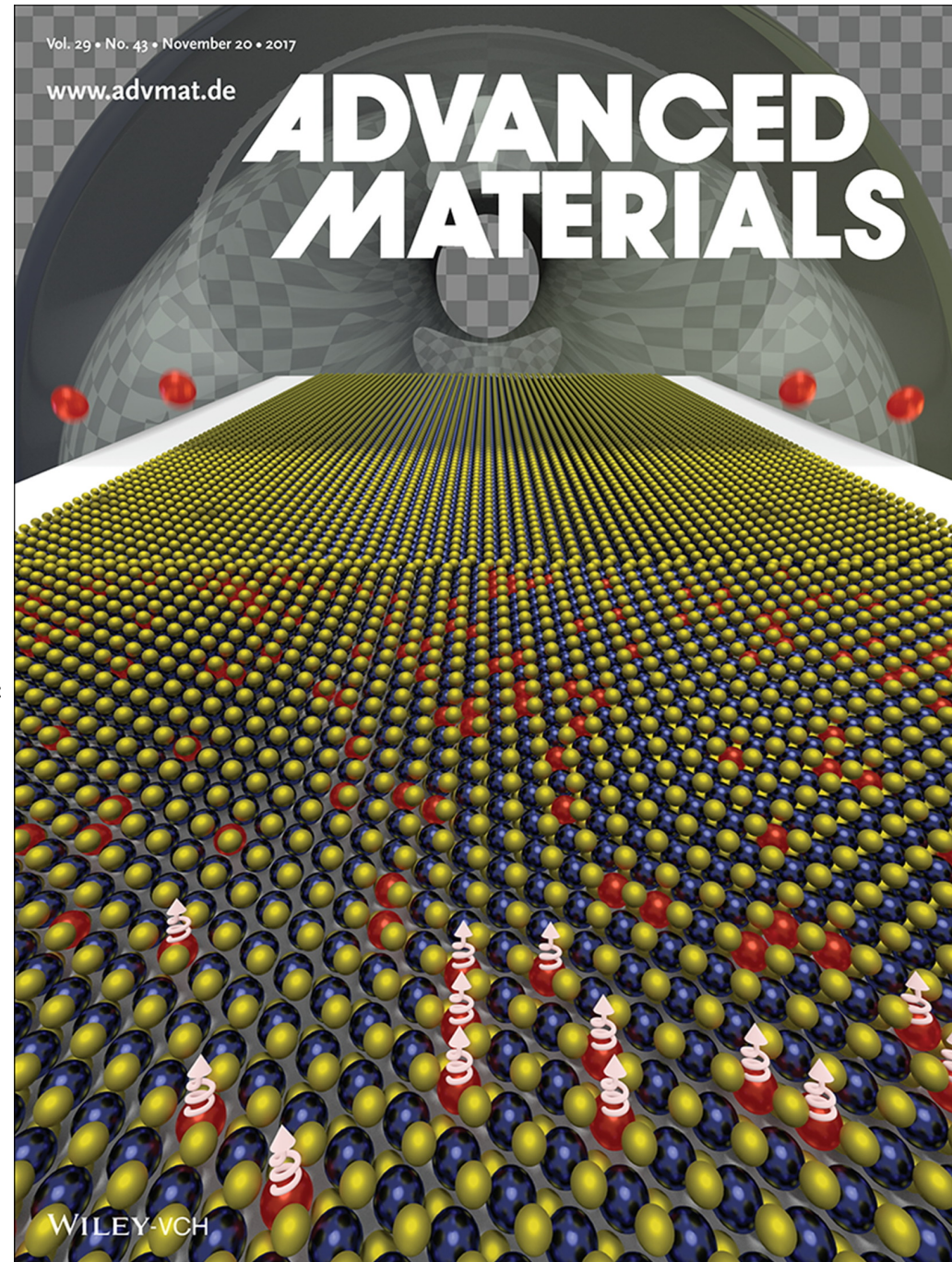
Emergent Magnetism: Structural Transition *via* Doping

- 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
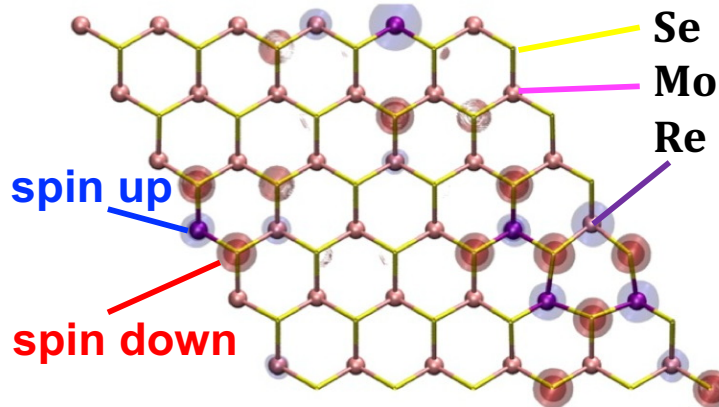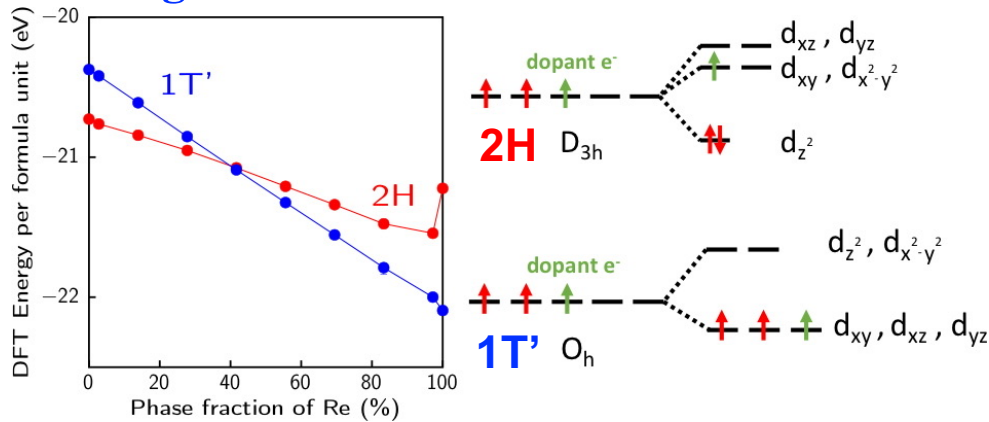
V. Kochat *et al.*, *Adv. Mater.* **29**, 1703754 ('17)
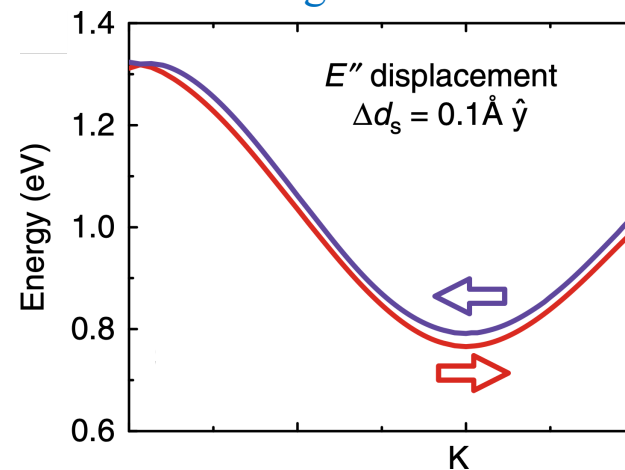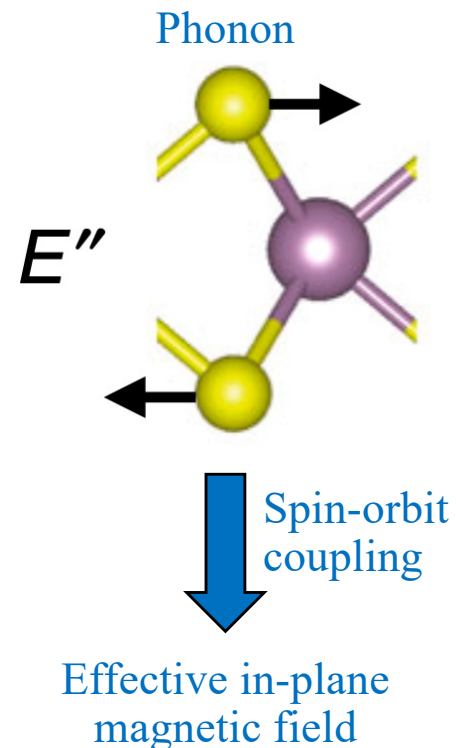
Transverse Field Ising Model

- **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

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

Phonon

E''

Spin-orbit coupling

Effective in-plane magnetic field

E″ phonon

Re spin

J$_Z$ J$_Z$ J$_Z$

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

E″ displacement
$\Delta d_s = 0.1$Å $\hat{y}$

Energy (eV)

1.4
1.2
1.0
0.8
0.6

K
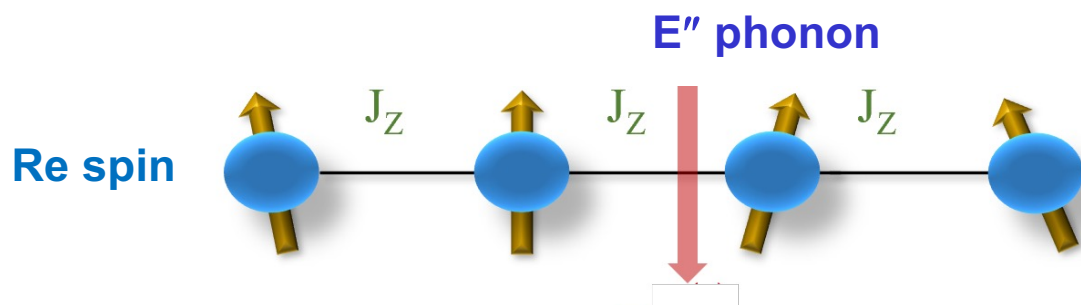
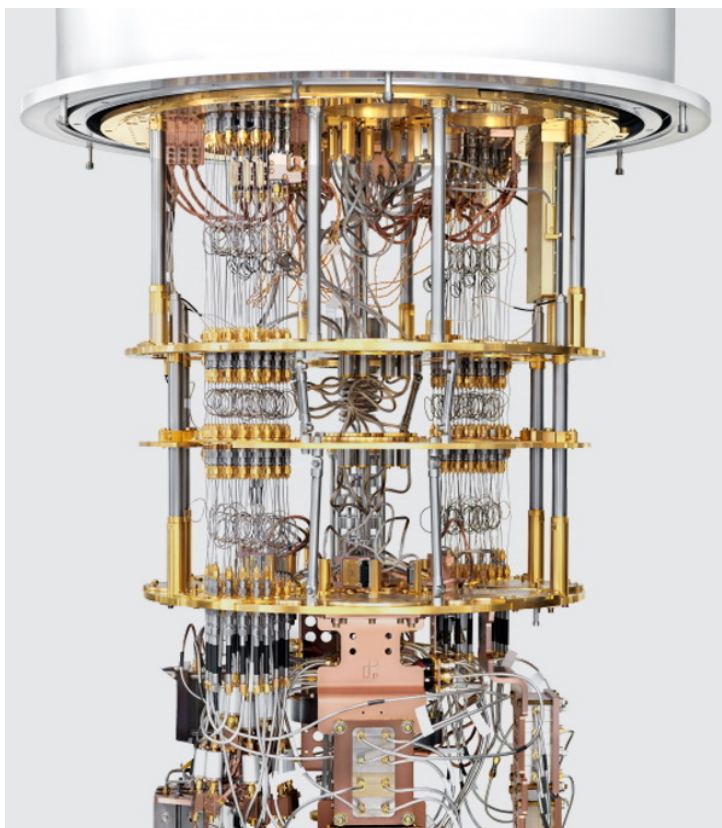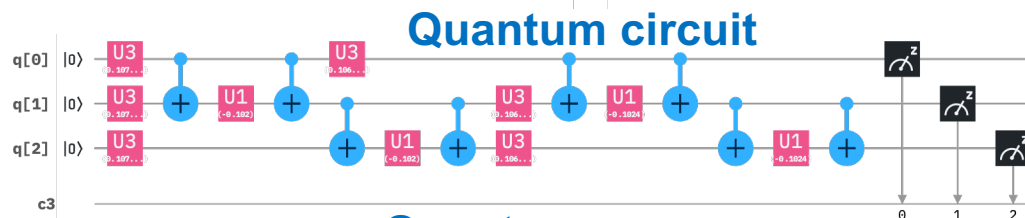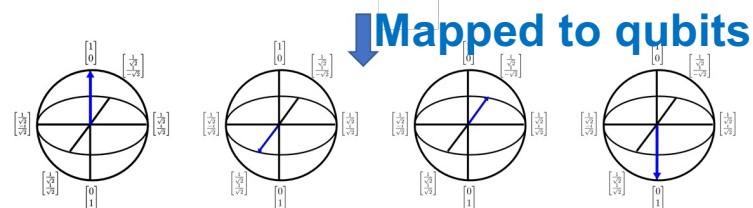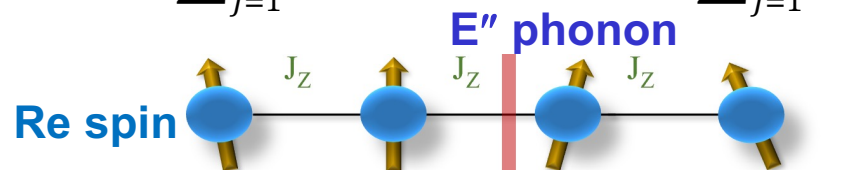# Quantum Computing of Magnetism

- **Simulated quantum many-body dynamics 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

Re spin — J_Z — J_Z — J_Z

Mapped to qubits

Quantum circuit

```
q[0] |0⟩  U3          U3                              Z
q[1] |0⟩  U3  +  U1 +        U3  +  U1  +              Z
q[2] |0⟩  U3       + U1 + U3        +  U1  +           Z
c3                                          0  1  2
```

Quantum program

```
32    ····#define·the·two·non-commuting·terms·that·comprise·the·Hamiltonian¬
33    ····Hz·=·PauliTerm("Z",·0,·epsilon_0)¬
34    ····Hy·=·PauliTerm("Y",·0,·epsilon_ph*np.sin(w_ph*t))¬
35    ····#exponentiate·the·terms·of·the·Hamiltonian·for·use·in·Trotter·approx¬
36    ····exp_Hz·=·exponential_map(Hz)(delta_t/(2.0*hbar))¬
37    ····exp_Hy·=·exponential_map(Hy)(delta_t/hbar)¬
```

Quantum Dynamics on NISQ Computers

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

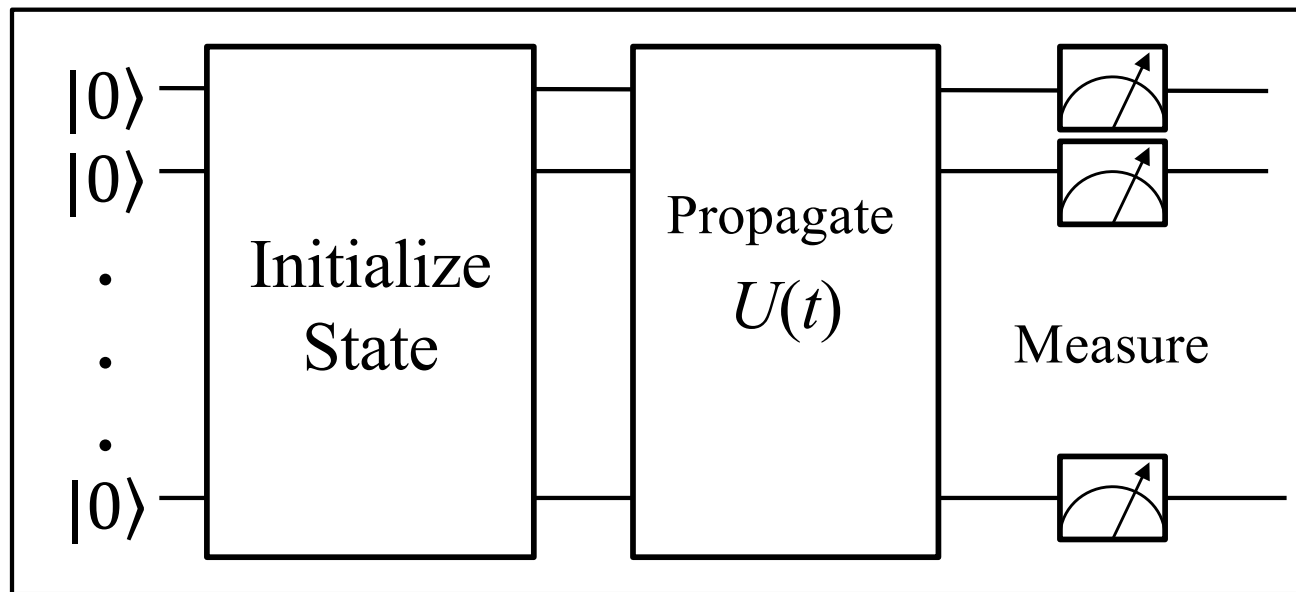$$|\Psi(\Delta t)\rangle = U(\Delta t)|\Psi(t = 0)\rangle$$

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

- **Time discretization with time-step Δt and Trotter expansion**

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

- **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

For each time instance, many runs to obtain statistics

$t = 0$ $t = t_1$ $t = t_2$ Time $t = t_n$

$\langle \sigma_z(t_1) \rangle$ $\langle \sigma_z(t_2) \rangle$ $\langle \sigma_z(t_n) \rangle$
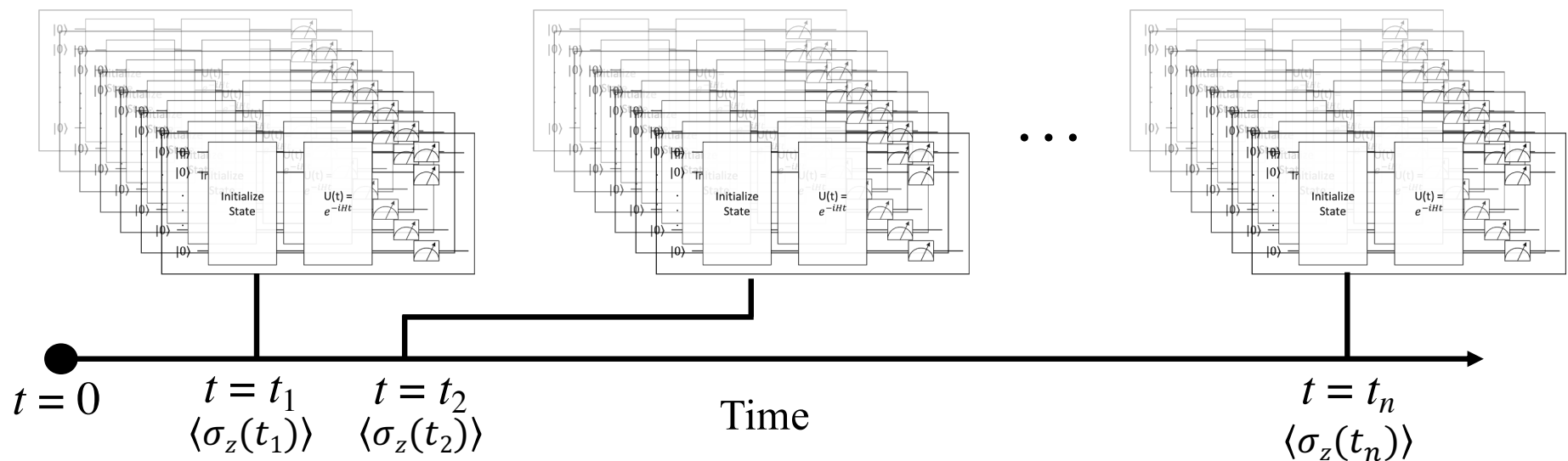
Quantum Computing Results

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

Increasing THz radiation fluence

L. Bassman *et al., Phys. Rev. B* **101**, 184305 ('20)
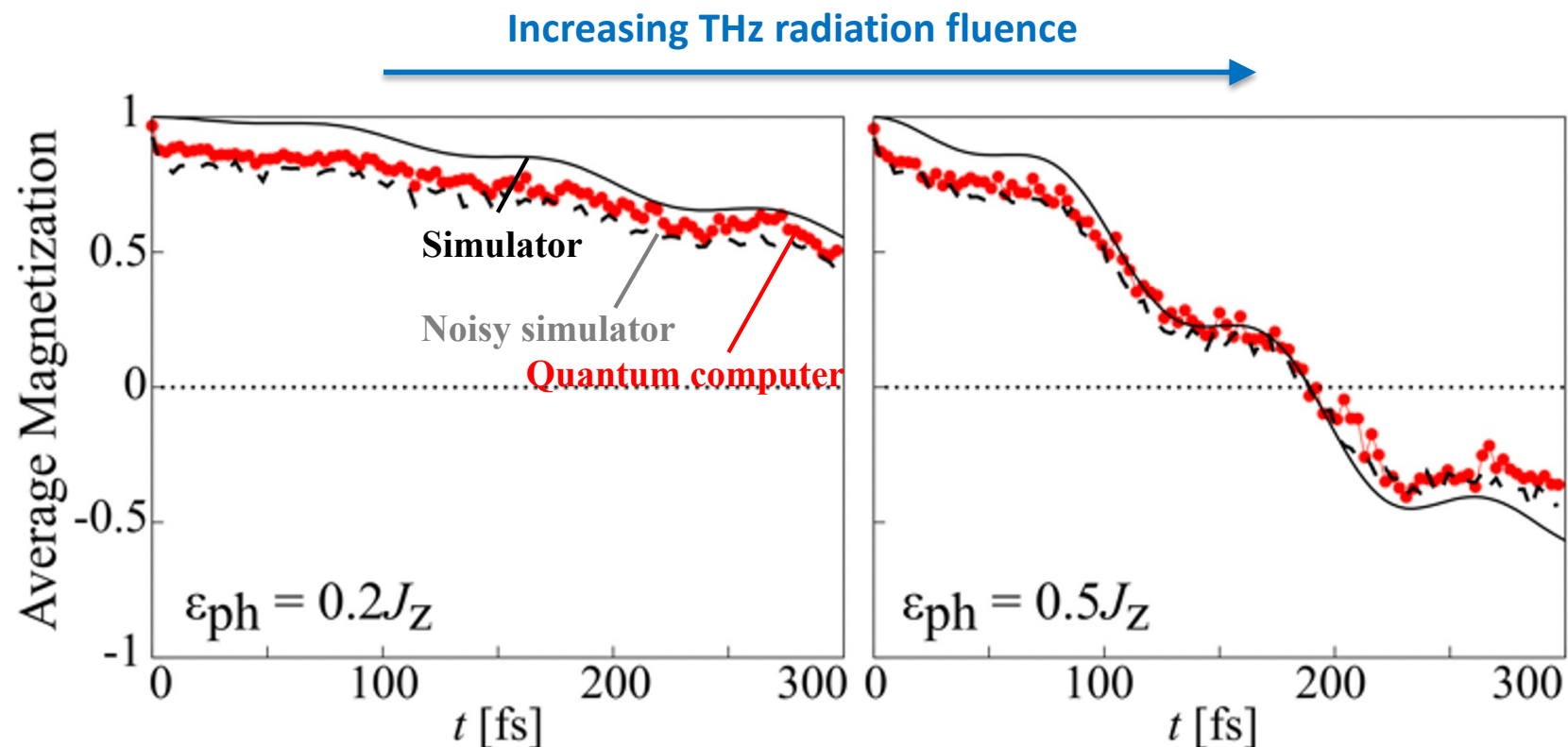
Circuit Size *vs.* Simulation Fidelity

- **Reduced circuit size improves the fidelity of simulation**
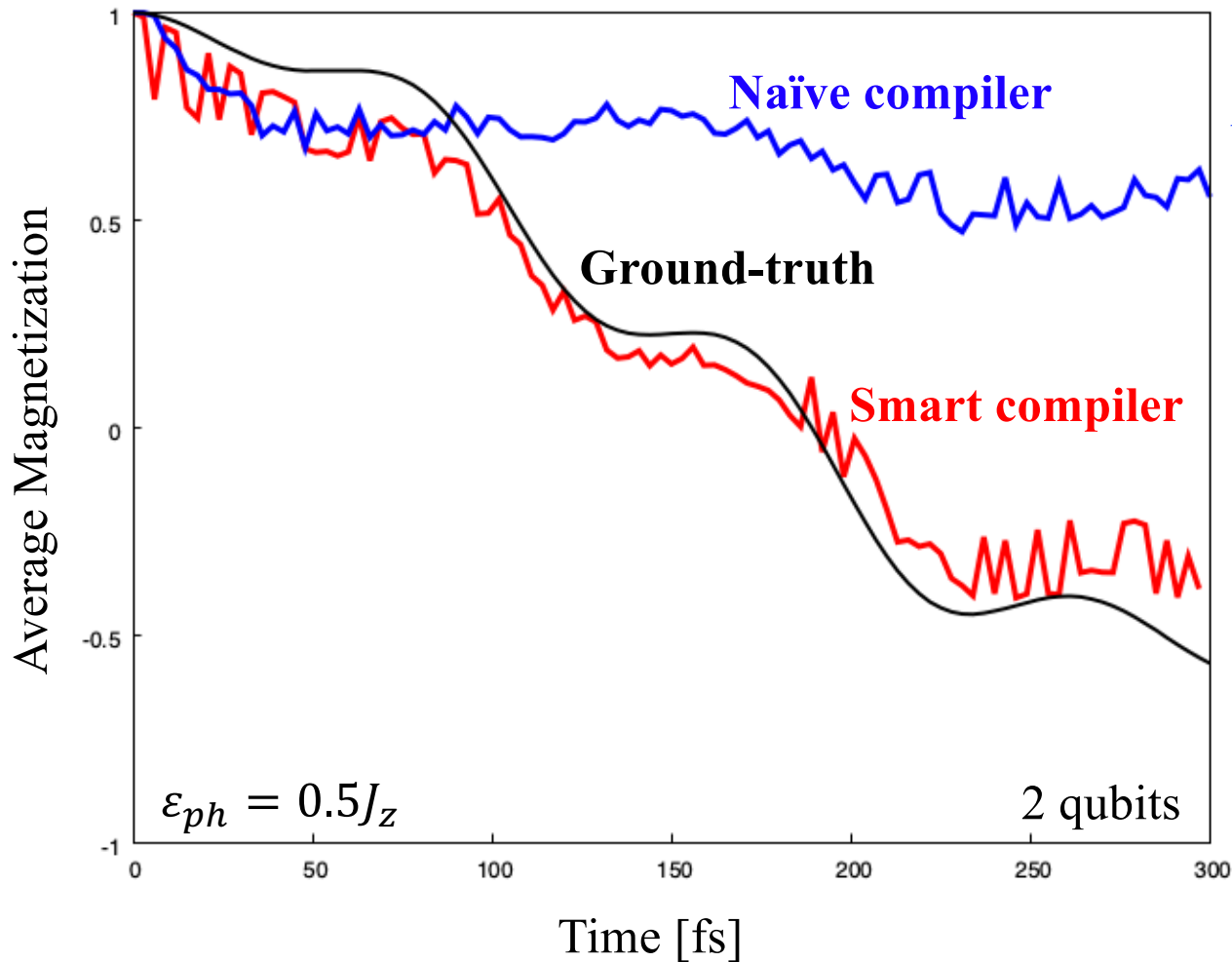
Naïve compiler: circuit size ∝ time
Smart compile: Constant circuit size w.r.t. time

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**

No.	Common gate set in TFIM circuits	Equivalent
1	$RX(\theta)$	H — $RZ(\theta)$ — H
2	H	$RZ(\frac{\pi}{2})$ — $RX(\frac{\pi}{2})$ — $RZ(\frac{\pi}{2})$
3	$\bullet$ / $\oplus$ (CNOT)	Z controlled-Z
4	$\bullet$ / $\oplus$ (CNOT)	H — $\bullet$ — H / H — $\oplus$ — H / H — $\bullet$ — H
5	$RX(\theta_i)$ — $RZ(\pi)$	$RZ(-\pi)$ — $RX(-\theta_i)$
6	Z ... Z — $RX(-\frac{\pi}{2})$ / $\bullet$ — $RX(\frac{\pi}{2})$ — $RZ(\theta_i)$ — $RX(-\frac{\pi}{2})$ — $\bullet$ — $RX(\frac{\pi}{2})$	$RX(-\frac{\pi}{2})$ — Z — $RX(\frac{\pi}{2})$ — $RZ(\theta_i)$ — $RX(-\frac{\pi}{2})$ — Z / $RX(\frac{\pi}{2})$ — $\bullet$
7	H — H	——
8	$RX(\theta_i)$ — $RX(\theta_j)$	$RX(\theta_i + \theta_j)$
9	$RZ(\theta_i)$ — $RZ(\theta_j)$	$RZ(\theta_i + \theta_j)$
10	$RZ(\theta_i)$ — $\bullet$ — $RZ(\theta_j)$ / Z	$\bullet$ — $RZ(\theta_i + \theta_j)$ / Z
11	$RZ(\theta_i)$ — $\bullet$ — $RZ(\theta_j)$ / $\oplus$	$\bullet$ — $RZ(\theta_i + \theta_j)$ / $\oplus$

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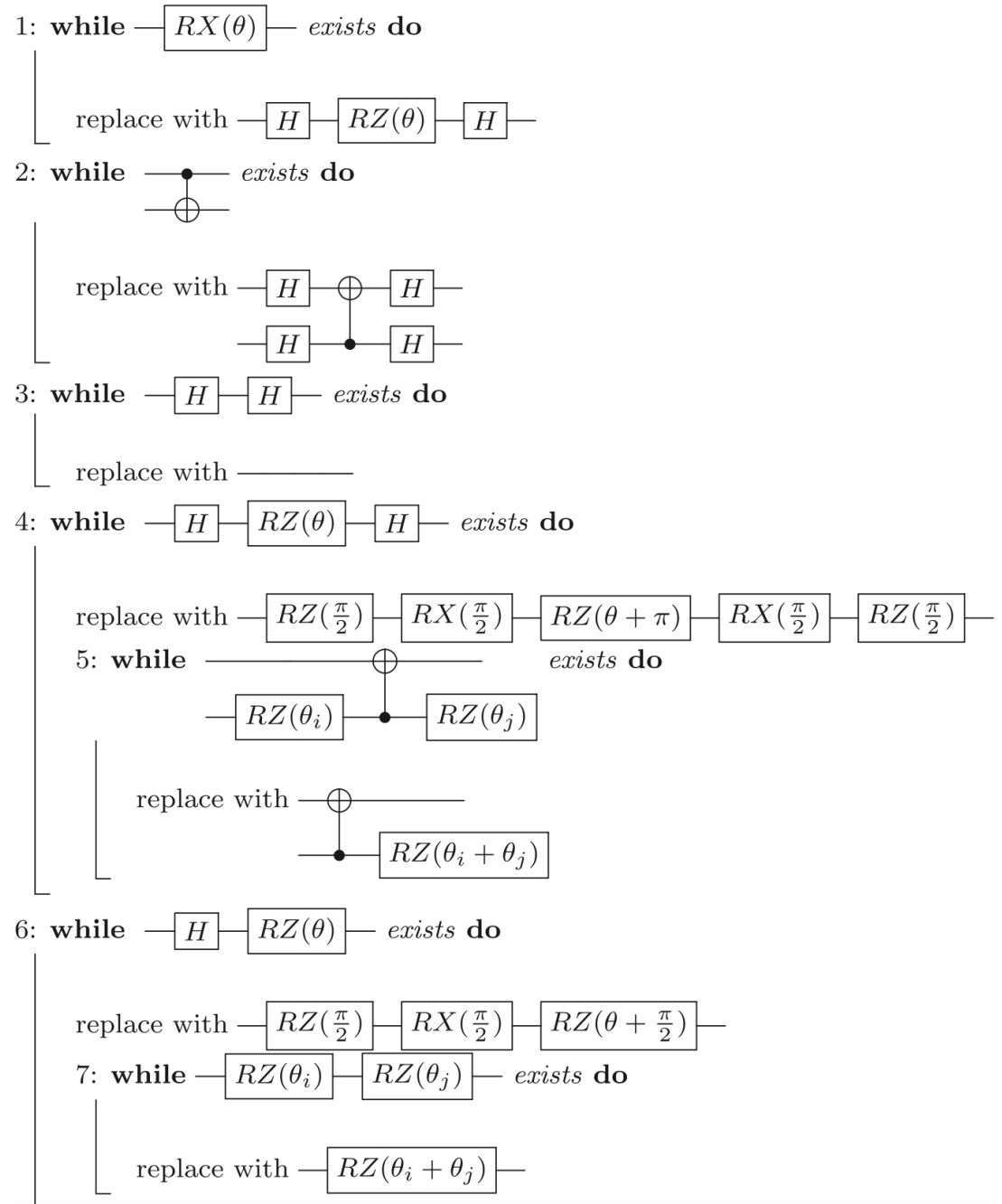
L. Bassman *et al.*,
*Quantum Sci. Tech.* **6**, 014007 ('21)

Domain-Specific Quantum Compiler

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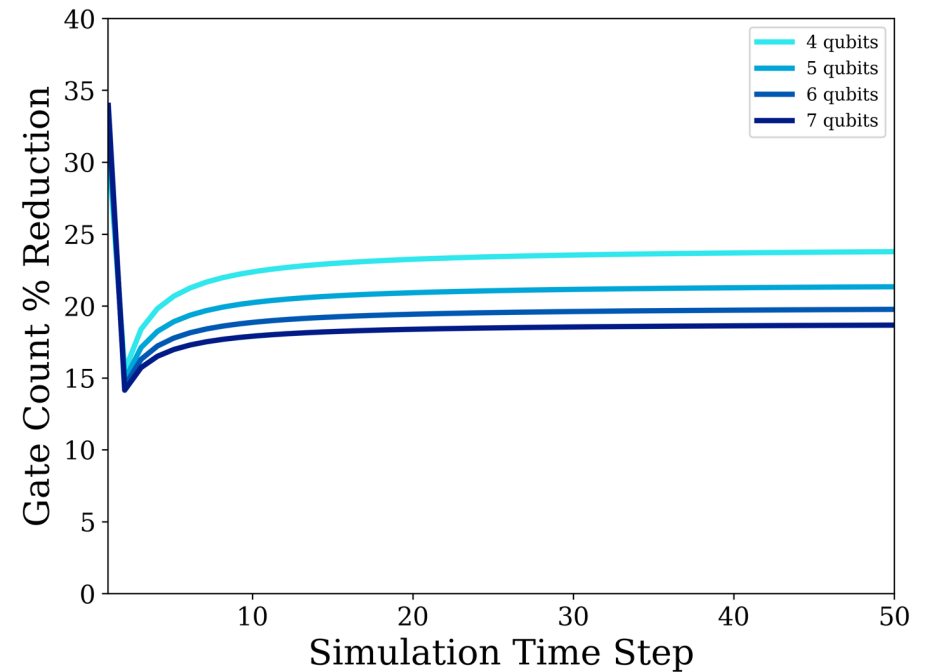
Vendor compiler

54 gates

26 gates

AI-inspired compiler

L. Bassman *et al.*, *Quantum Sci. Tech.* **6**, 014007 ('21)
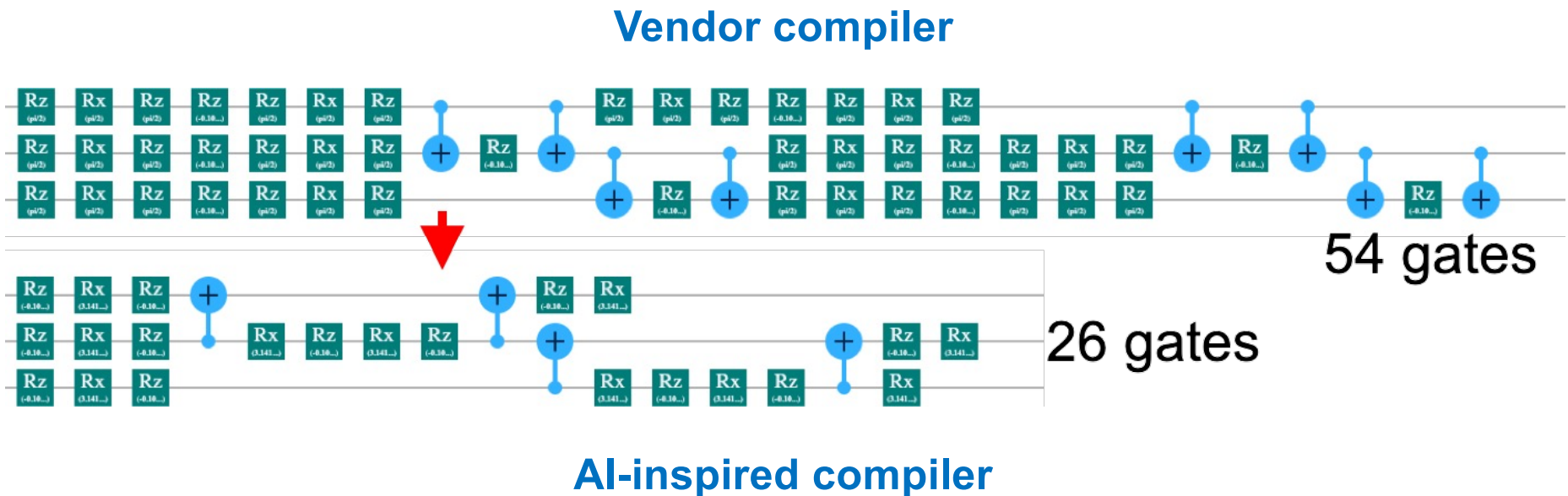
Performance of Domain-Specific Compiler

Absolute gate count difference
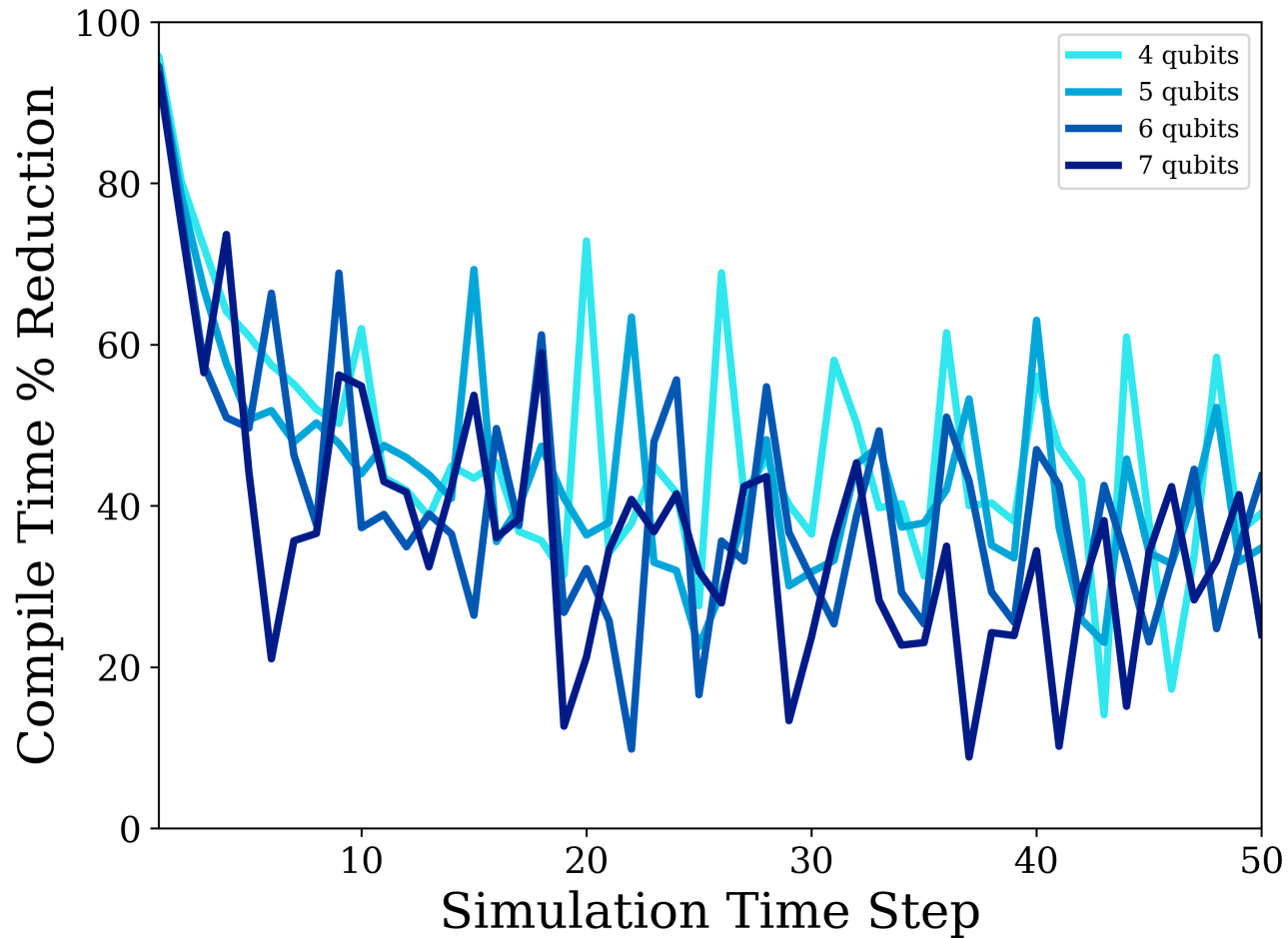*(IBM Compiler − DS Compiler)*
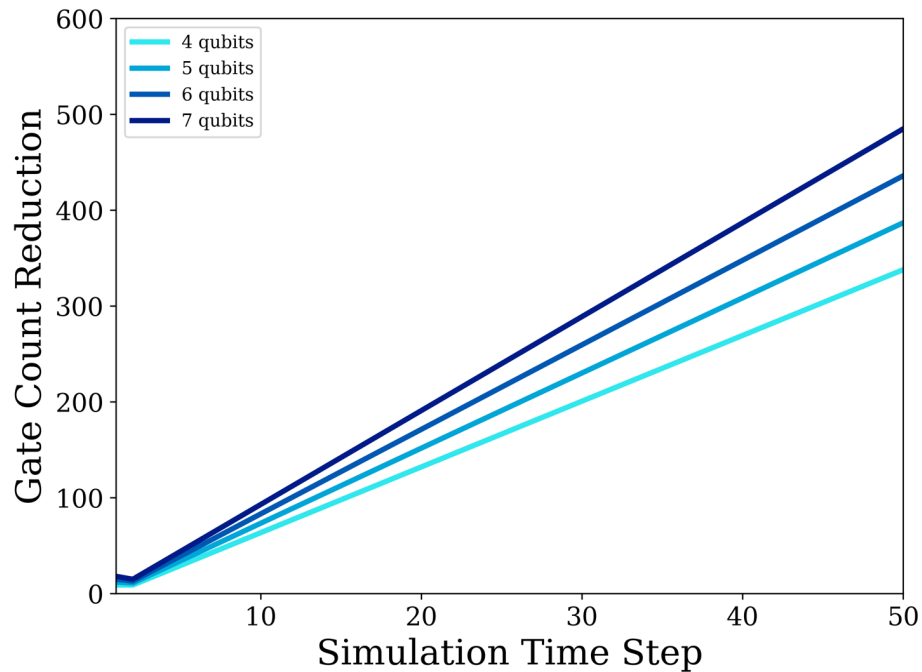
Percent gate count difference

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

Domain-specific compiler reduces gate count compared to IBM compiler
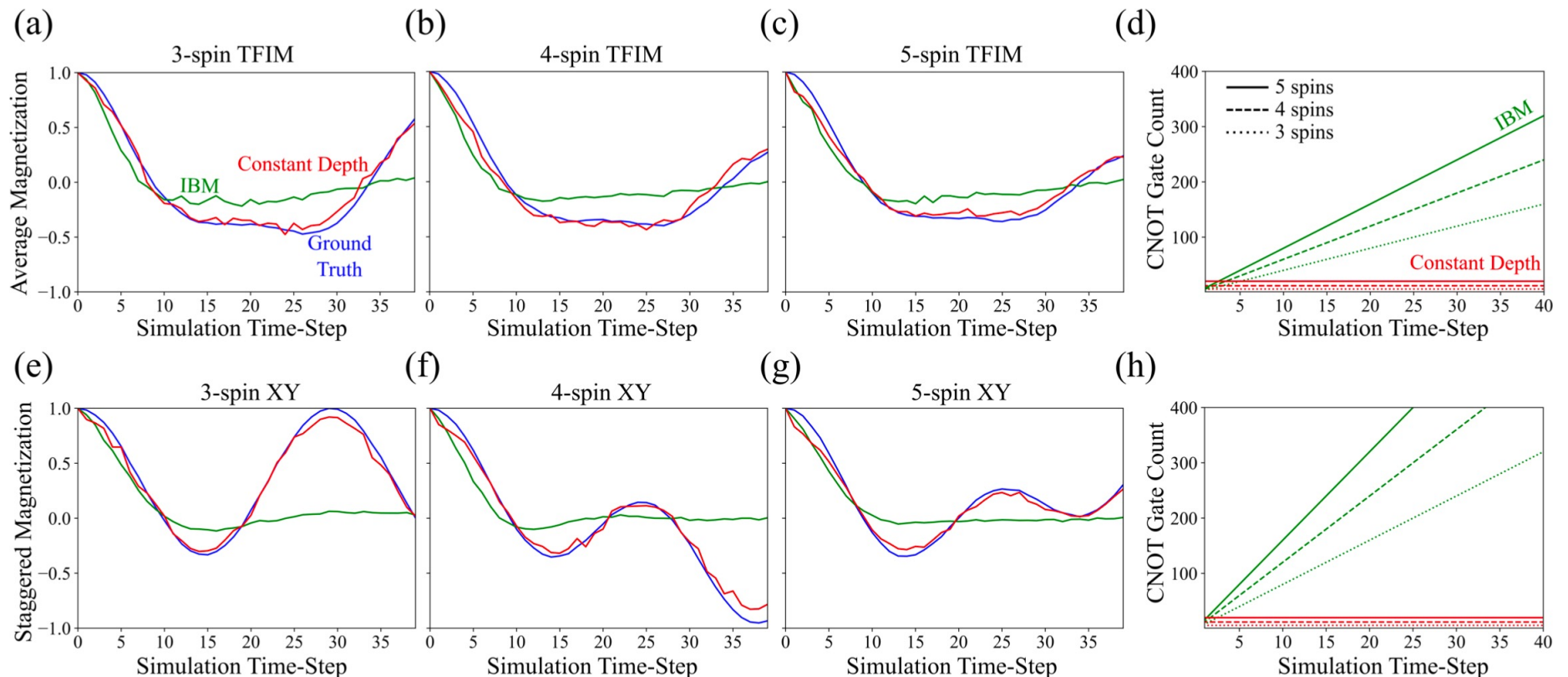
Speed of Domain-Specific Compiler

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**
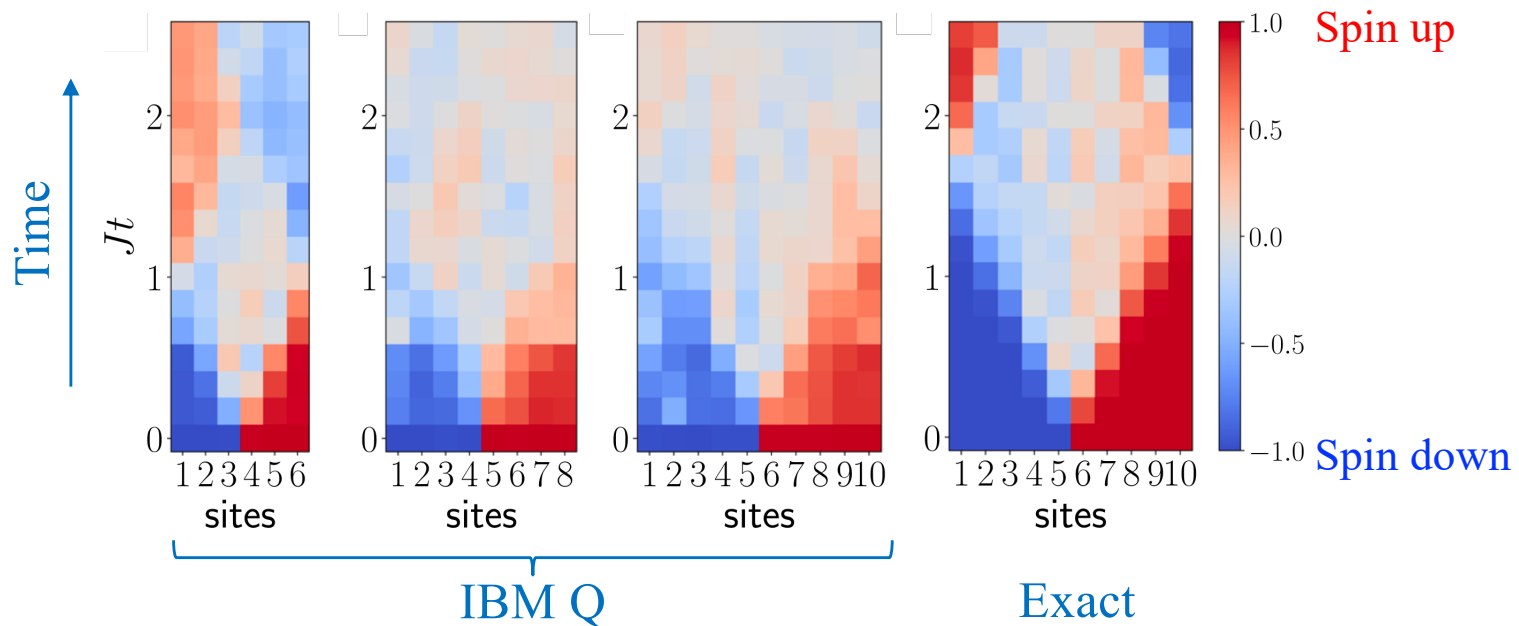

L. Bassman *et al., arXiv*: 2103.07429v4 ('21)

Richer Physics: Heisenberg Model

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

Exchange coupling   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)

IBM Q   Exact

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**
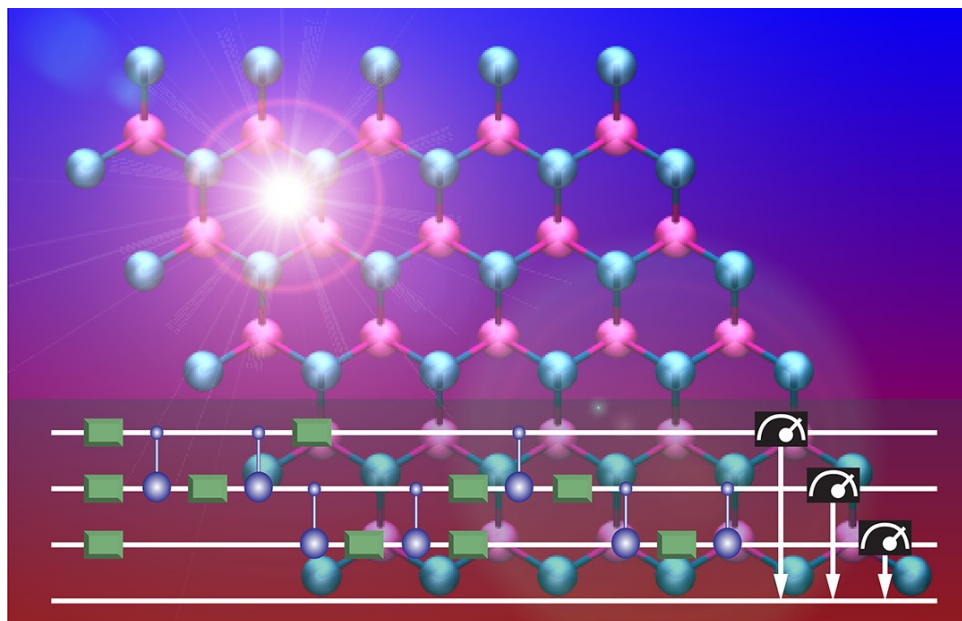

MISTIQS

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)
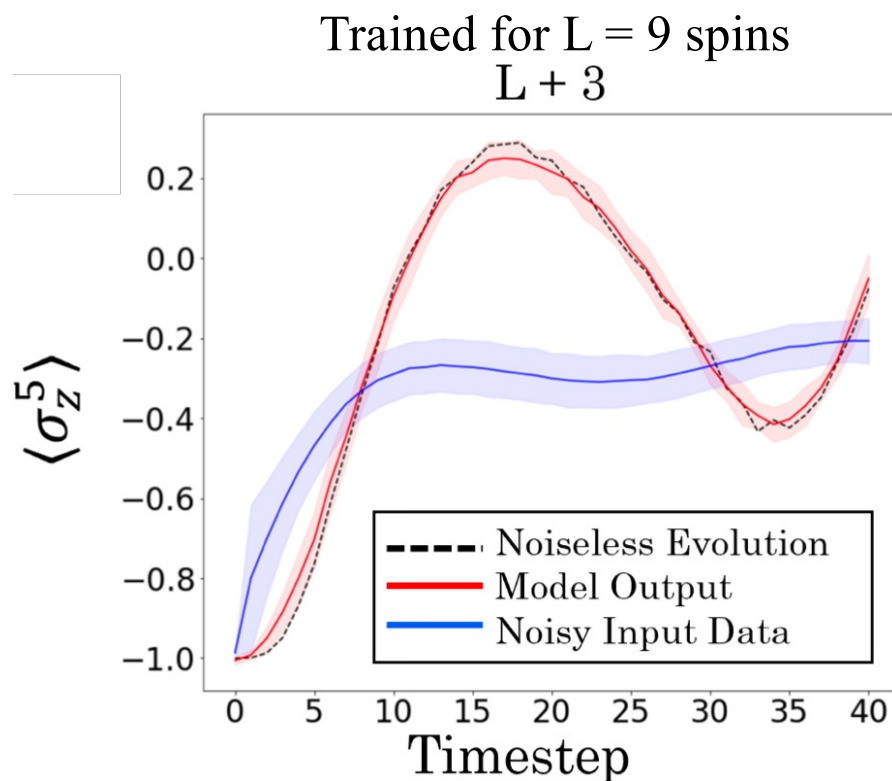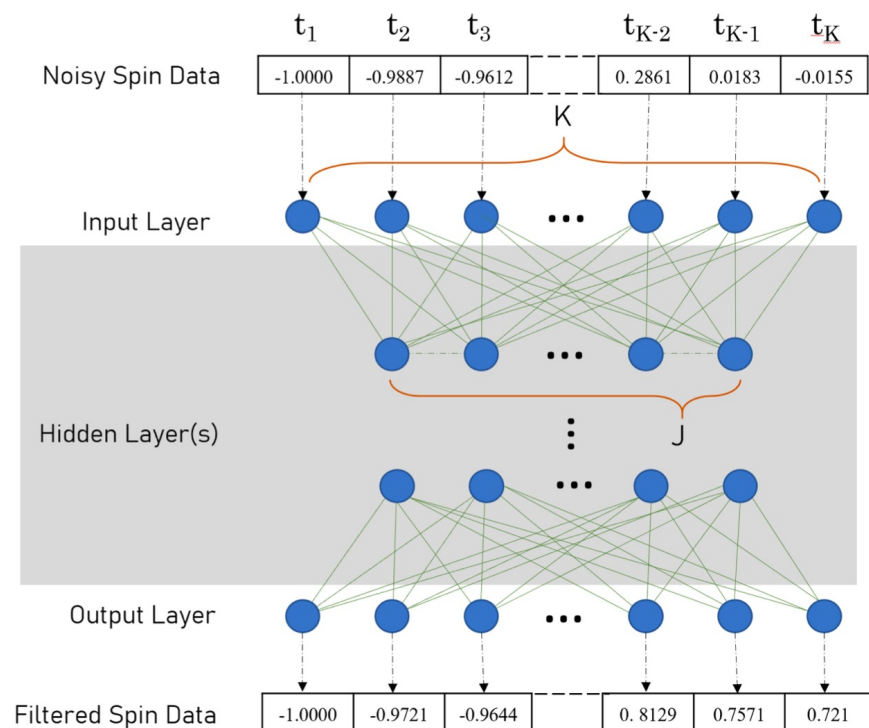
Variational Quantum Simulator

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, $|\psi(t)\rangle = |\psi(\lambda_1(t), \ldots, \lambda_P(t))\rangle$, which is tractable on a classical computer**

Y. Li & S. Benjamin, *Phys. Rev. X* **7**, 021050 ('17)
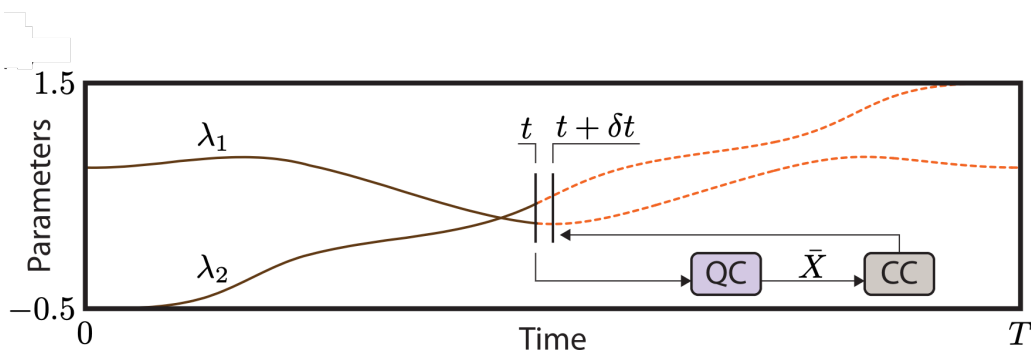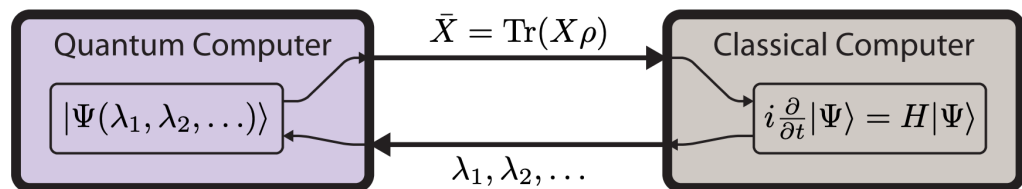
Where to Go from Here

- **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 (this course): Elective for MSQIS**