# Quantum Computing


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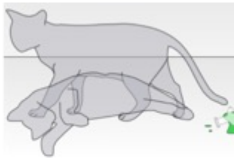
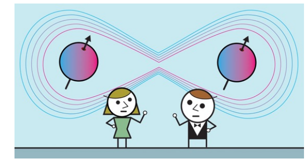
**Goal: Quantum dynamics simulation on quantum circuits**

# It’s Timely: 2022 Nobel Physics Prize



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



## The Nobel Prize in Physics 2022

Ill. Niklas Elmehed © Nobel Prize Outreach

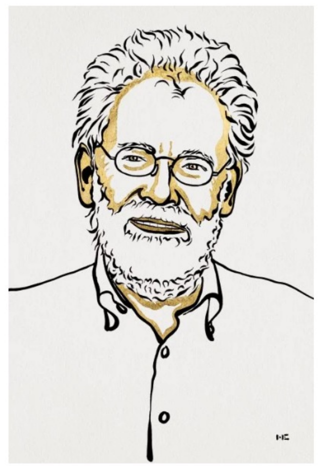
Alain Aspect

Prize share: 1/3

Ill. Niklas Elmehed © Nobel Prize Outreach

John F. Clauser

Prize share: 1/3



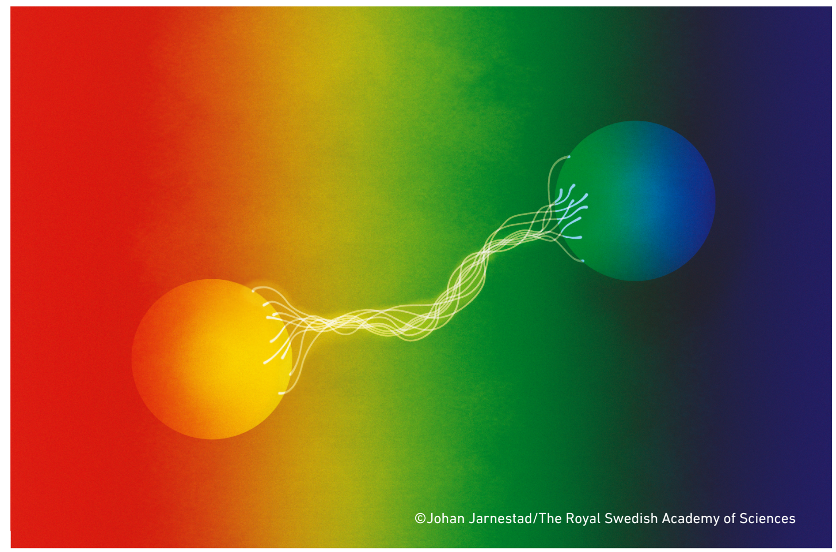
Ill. Niklas Elmehed © Nobel Prize Outreach

Anton Zeilinger

Prize share: 1/3

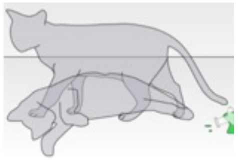
The Nobel Prize in Physics 2022 was awarded jointly to Alain Aspect, John F. Clauser and Anton Zeilinger "for experiments with entangled photons, establishing the violation of Bell inequalities and pioneering quantum information science"

***It’s entanglement!***

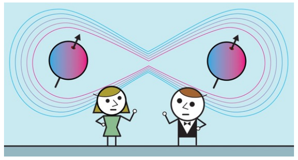



*cf*. Microsoft Majorana 1 chip (Feb. 19, ’25)
https://news.microsoft.com/azure-quantum/

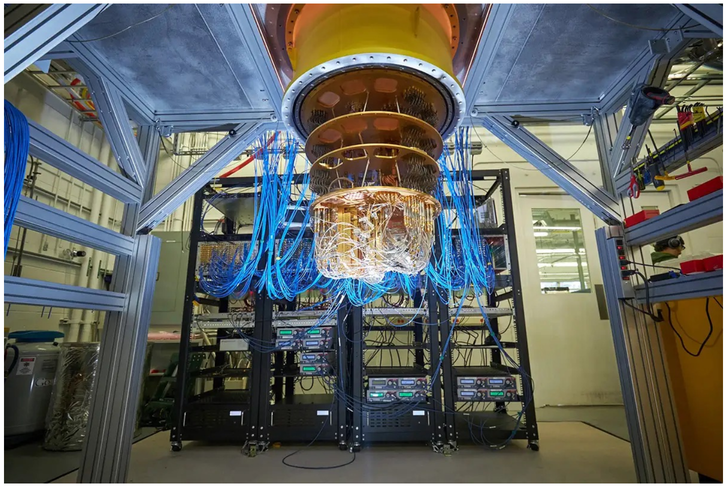
# Quantum Computing (QC) for Science

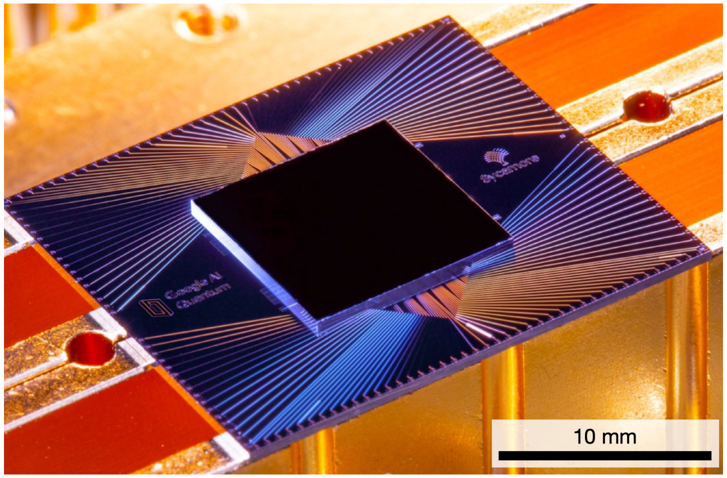


**Quantum computing utilizes quantum properties such as superposition & entanglement for computation**



- **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)






**54-qubit Google Sycamore**

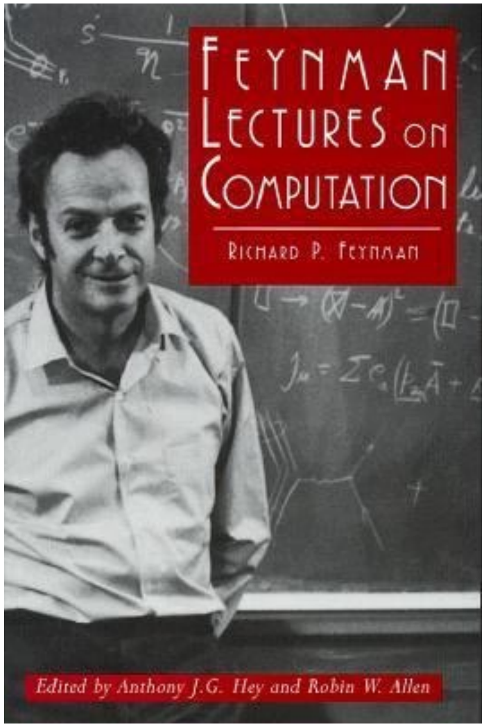
# Quantum Dynamics Simulations

- **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)]

  Watch Seth's movie: https://www.youtube.com/watch?v=EMzKshc6x2M

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

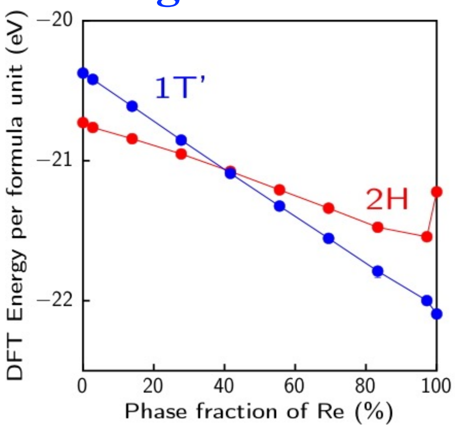


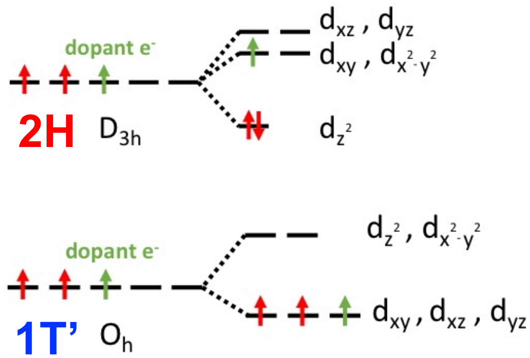

- **Simulated nontrivial quantum dynamics on publicly available IBM's Q16 Melbourne & Rigetti's Aspen NISQ computers, *i.e.*, ultrafast control of emergent magnetism by THz radiation in 2D material** [L. Bassman *et al.*, *Phys. Rev. B* **101**, 184305 ('20)]

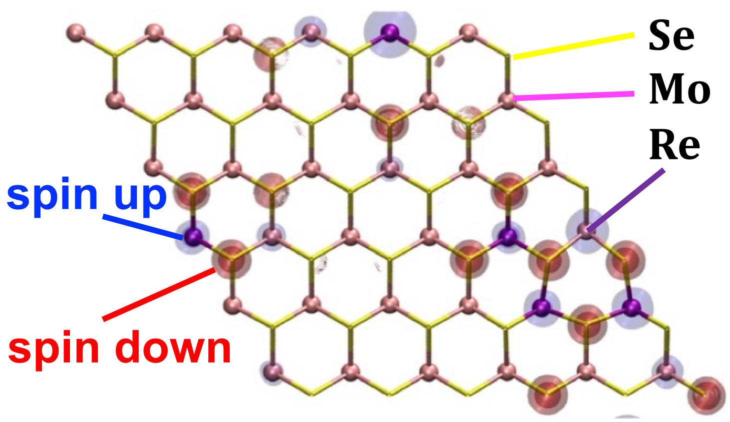
Do it yourself at https://quantum-computing.ibm.com

# Emergent Magnetism: Structural Transition *via* Doping

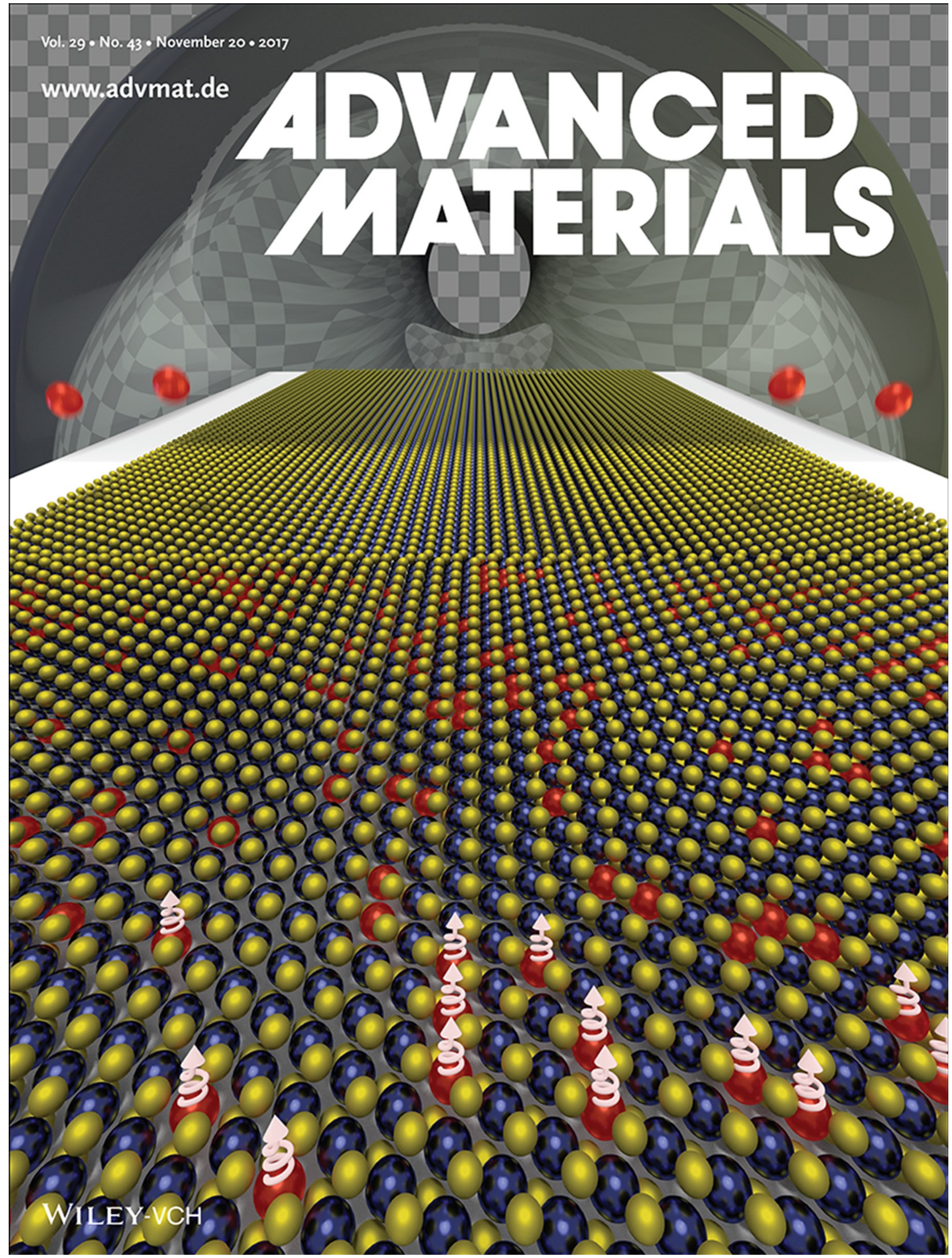
- **Experiment at Rice showed 2H-to-1T' phase transformation by alloying $MoSe_2$ with Re**
- **Simulations at USC elucidated its electronic origin**
- **Simulation & experiment showed novel magnetism centered at Re atoms**




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"**

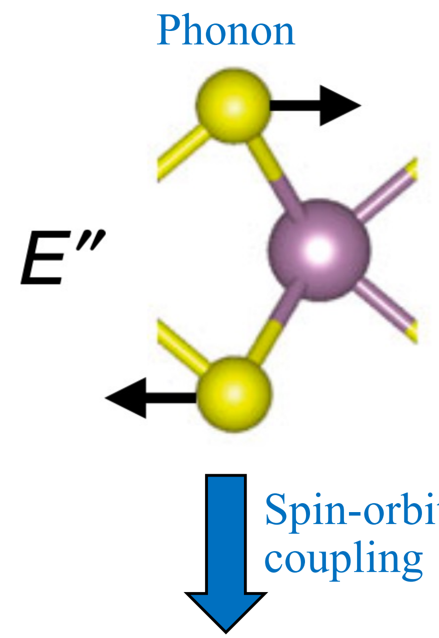
$$H(t) = -J_z \sum_{j=1}^{N-1} \sigma_z^j \sigma_z^{j+1} - \varepsilon_{ph} \sin(\omega_{ph} t) \sum_{j=1}^{N} \sigma_x^j$$

$$= H_z + H_x(t)$$

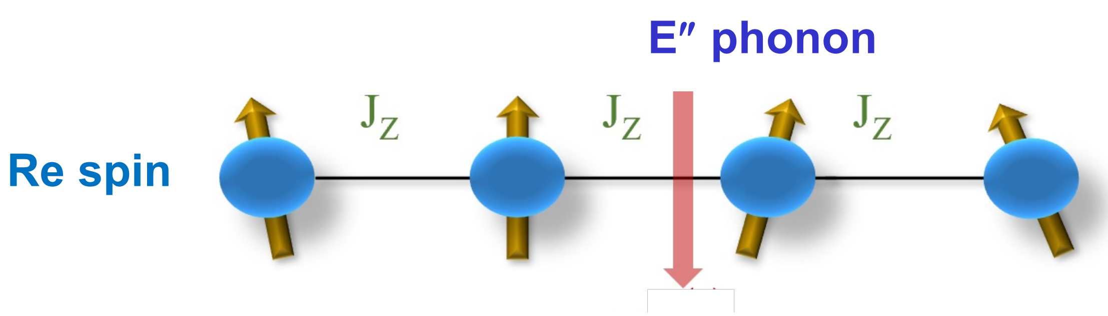
Phonon frequency

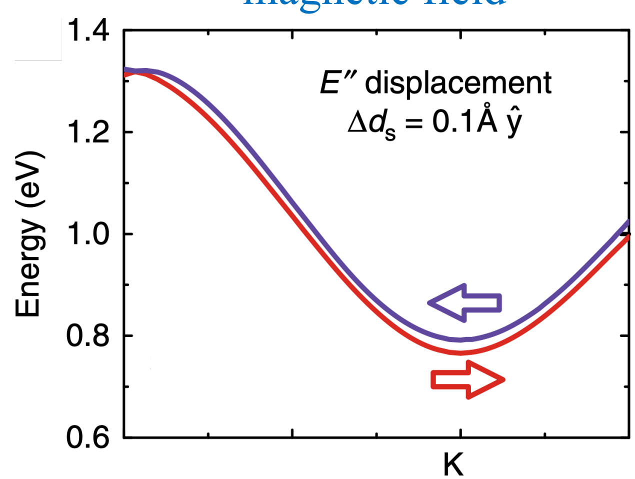
Phonon-induced energy split

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




Effective in-plane magnetic field



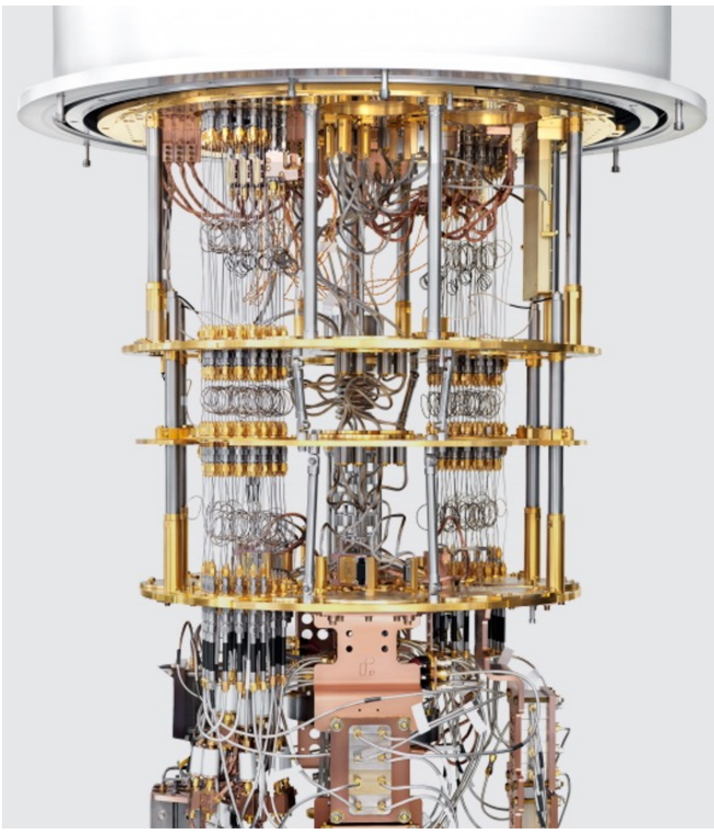




D. Shin *et al.*, *Nat. Commun.* **9**, 638 ('18)

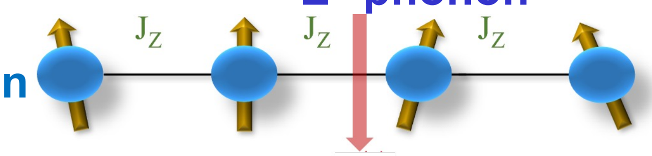
# Quantum Computing of Magnetism

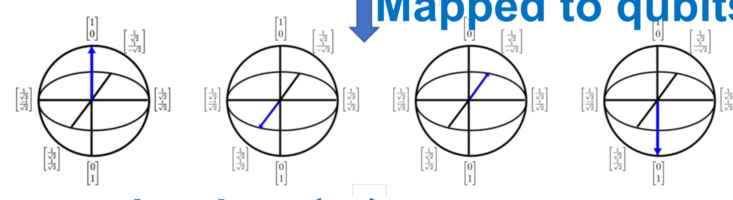
- **Simulated quantum many-body dynamics on IBM's Q16 Melbourne & Rigetti's Aspen quantum processors**

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

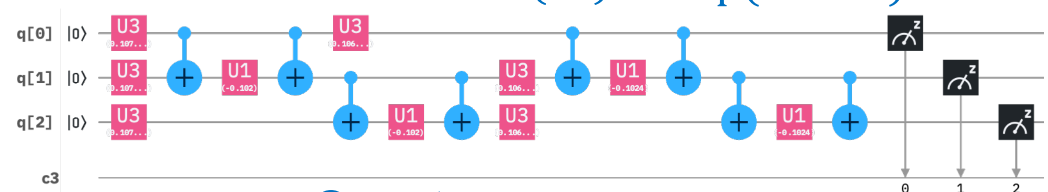


$$H(t) = -J_z \sum_{j=1}^{N-1} \boldsymbol{\sigma}_z^j \boldsymbol{\sigma}_z^{j+1} - \varepsilon_{ph} \sin(\omega_{ph} t) \sum_{j=1}^{N} \boldsymbol{\sigma}_x^j$$




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




**Quantum program**

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

**Will derive & implement the circuit in the hands-on session**

# Quantum Dynamics on NISQ Computers

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

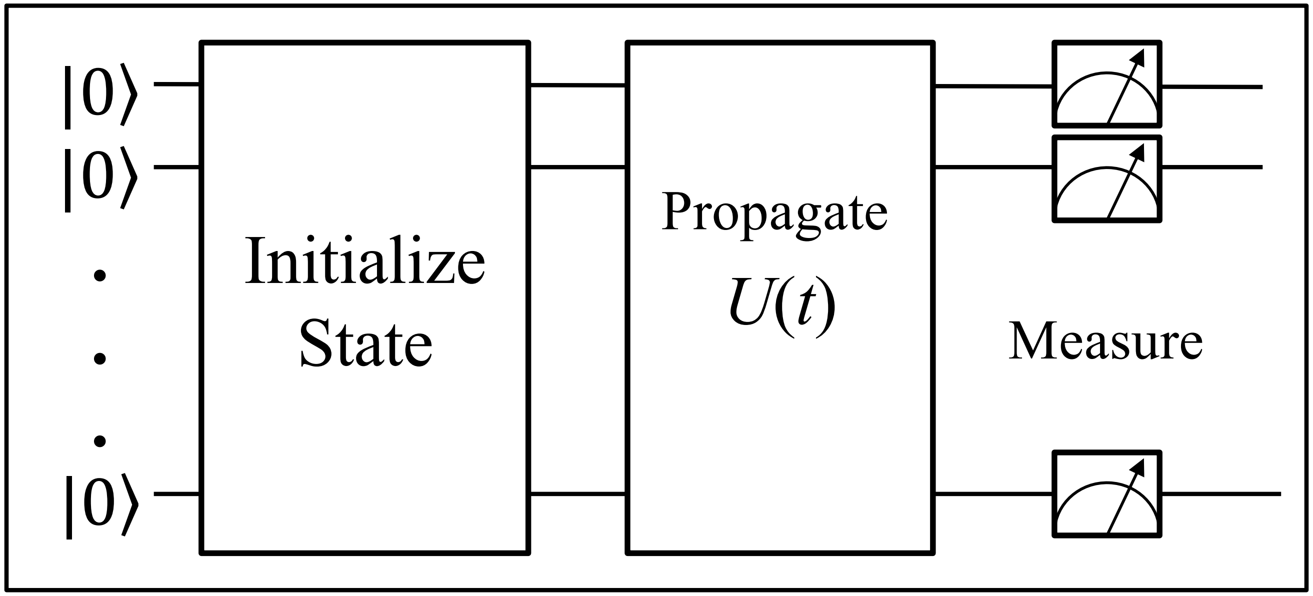
$$|\Psi(\Delta t)\rangle = U(\Delta t)|\Psi(t=0)\rangle$$
$$U(\Delta t) = \exp(-iH\Delta t)$$

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

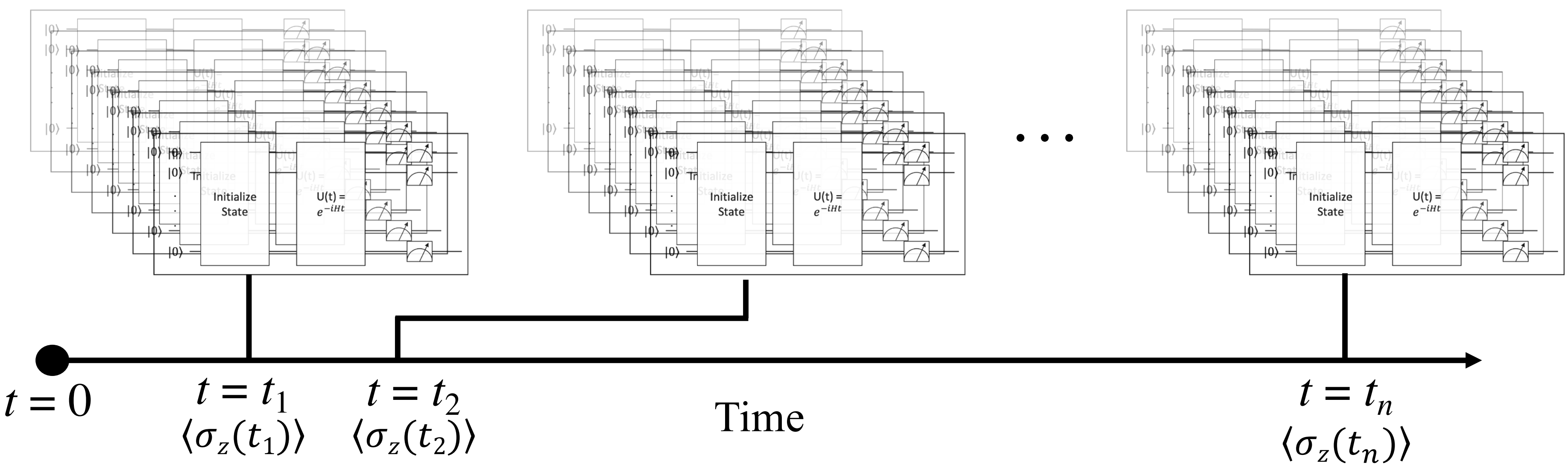
$$U(n\Delta t) \cong \prod_{k=0}^{n-1} \exp(-iH_z\Delta t)\exp(-iH_x((k+1/2)\Delta t)\Delta t)$$

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

# Quantum Computing Runs

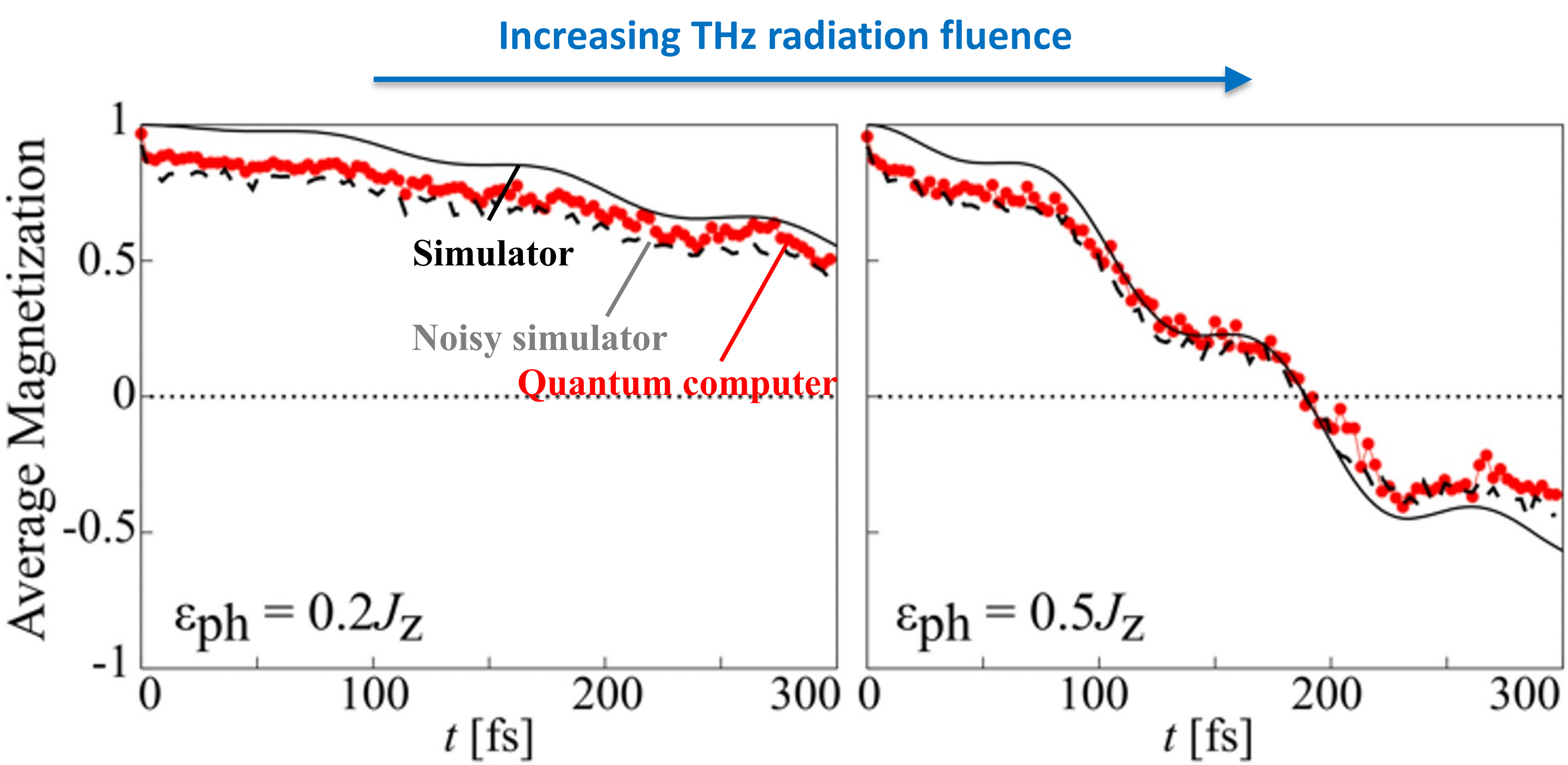



**For each time instance, many runs to obtain statistics**



# Quantum Computing Results

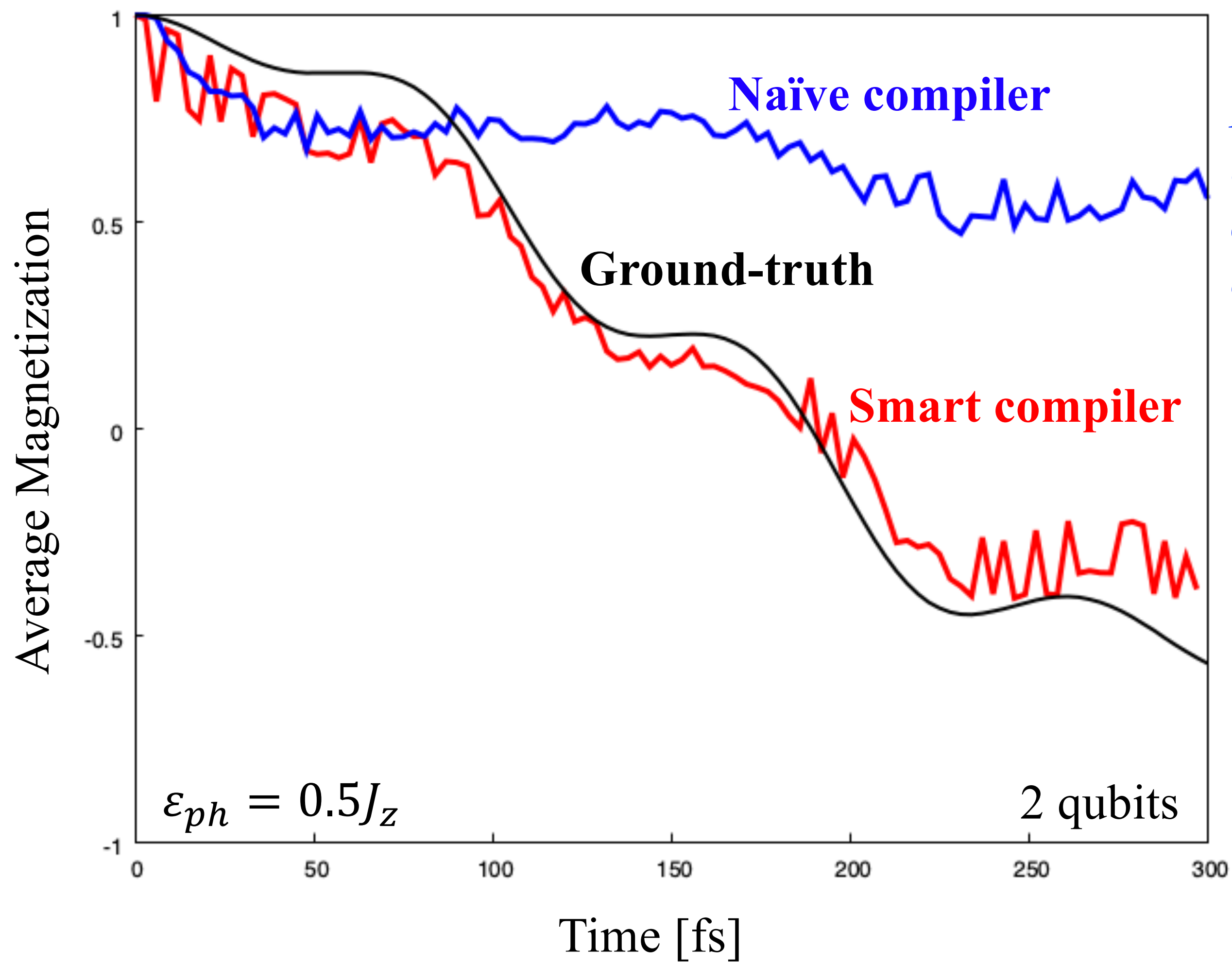
- **Quantum-dynamics simulations on NISQ computers show dynamic suppression of magnetization by THz radiation**




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

# Circuit Size *vs.* Simulation Fidelity

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



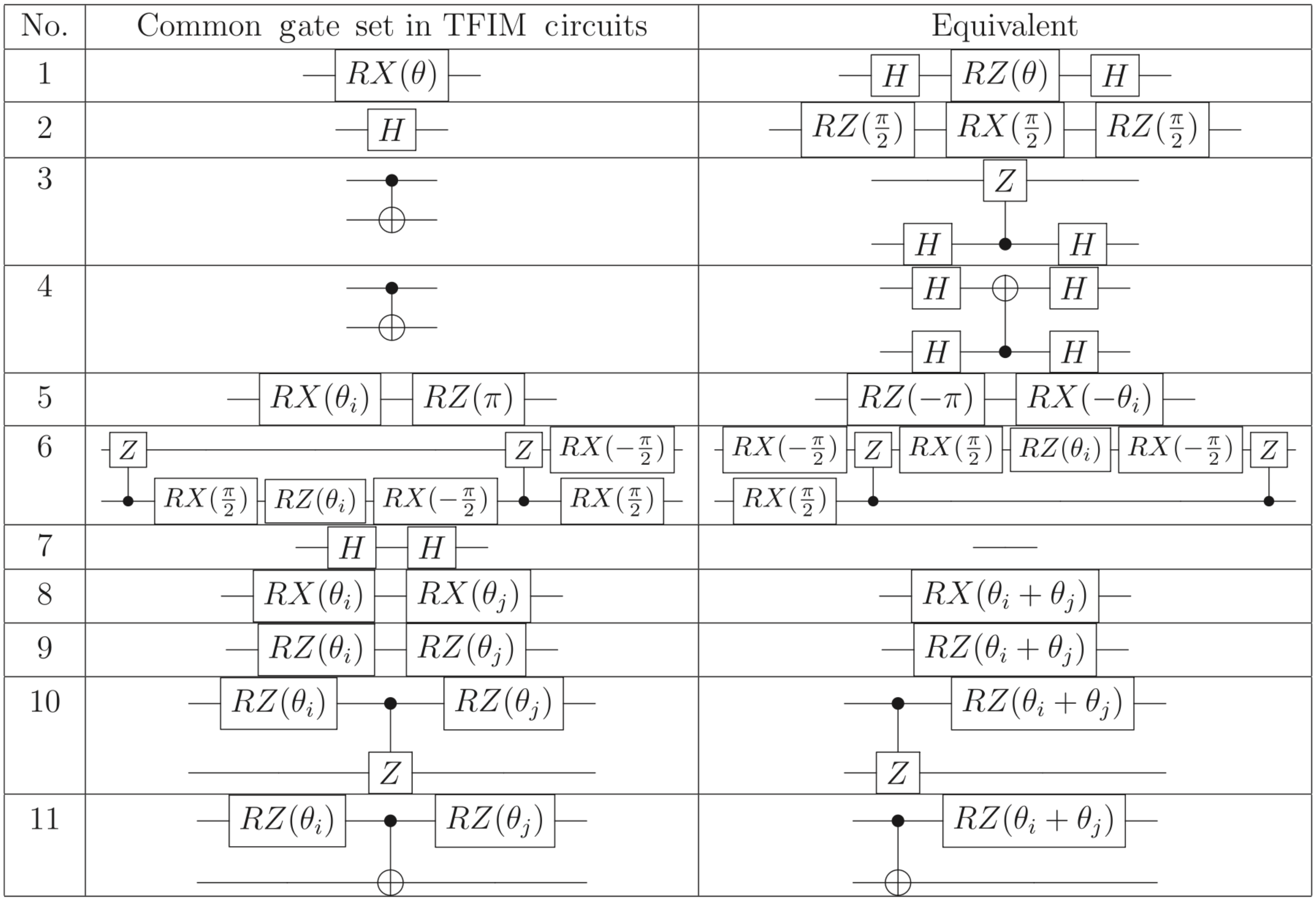

***Due to high cumulative quantum-gate errors!***

**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**

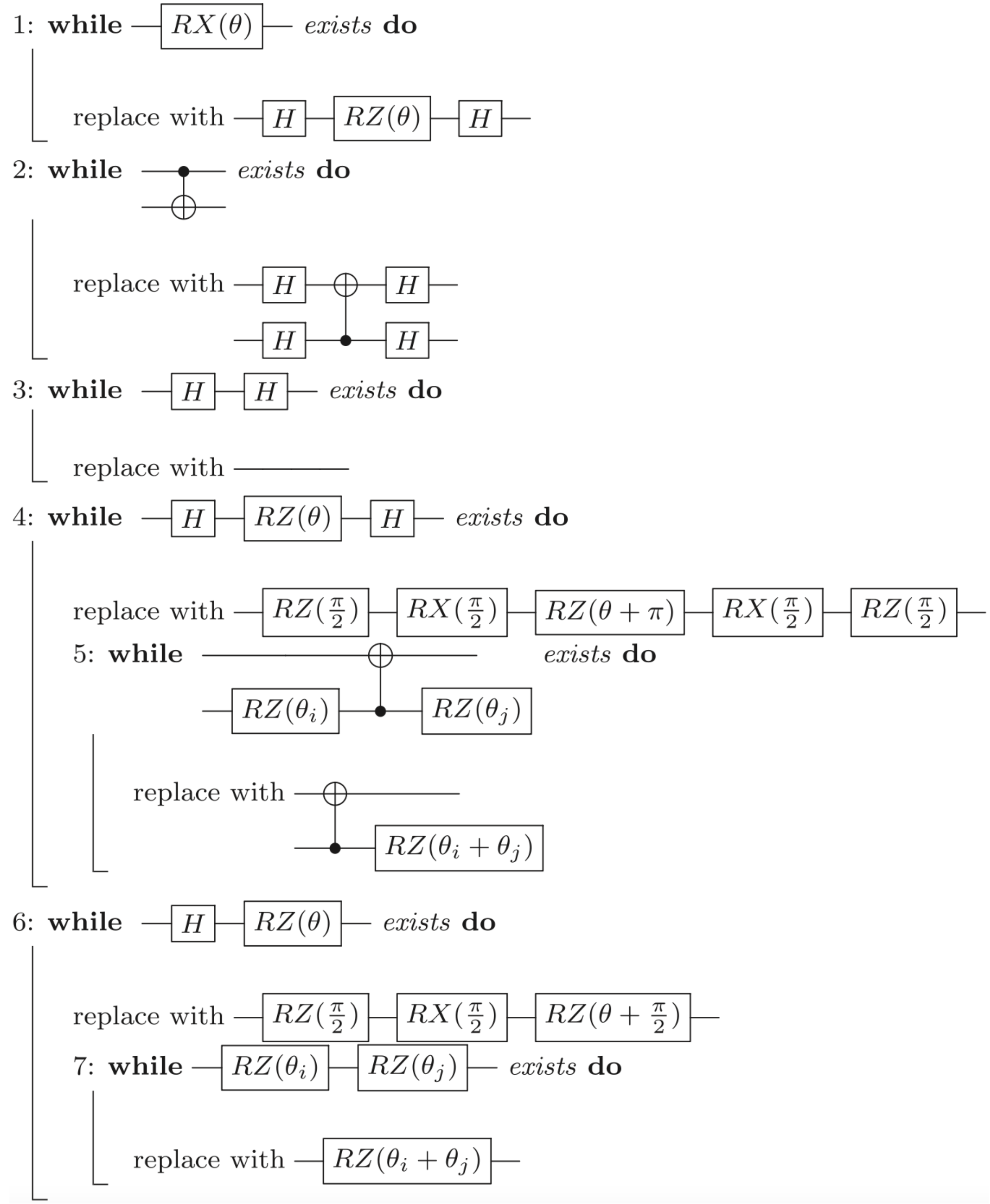



L. Bassman *et al.*, *Quantum Sci. Tech.* **6**, 014007 ('21)

# Algorithm for IBM Native Gates

- **Heuristic algorithm similar to unit propagation in artificial intelligence (AI)**

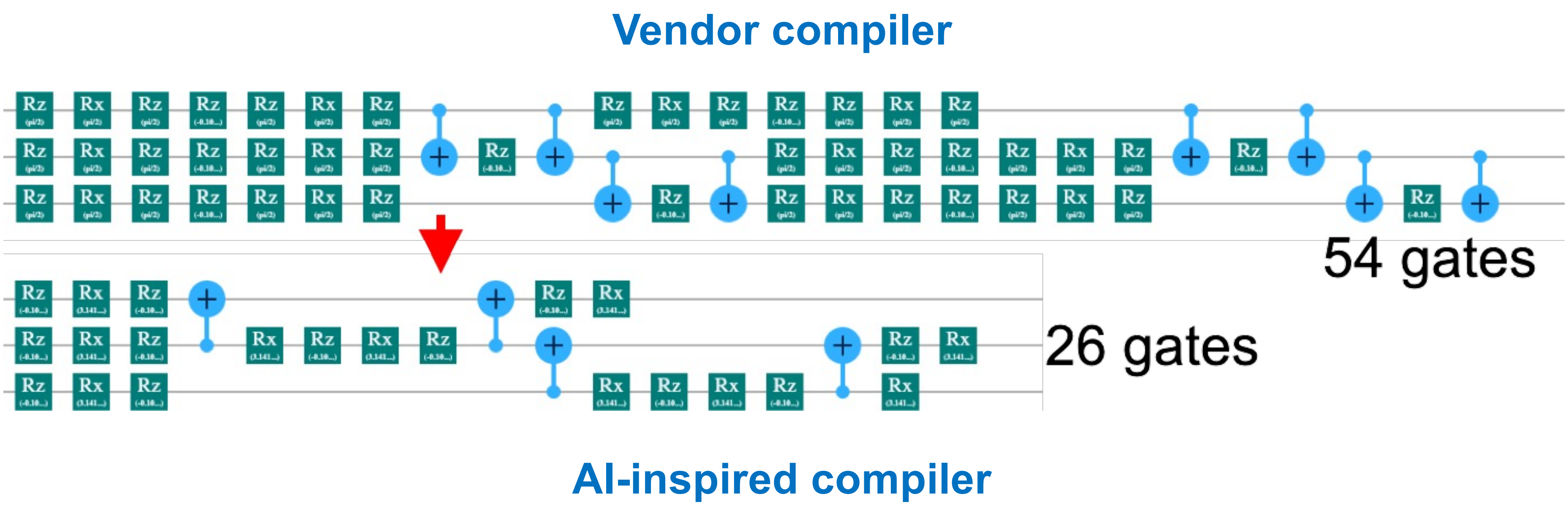
- **The heuristic order & types of identities applied are specific to the particular quantum dynamics we simulated**




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

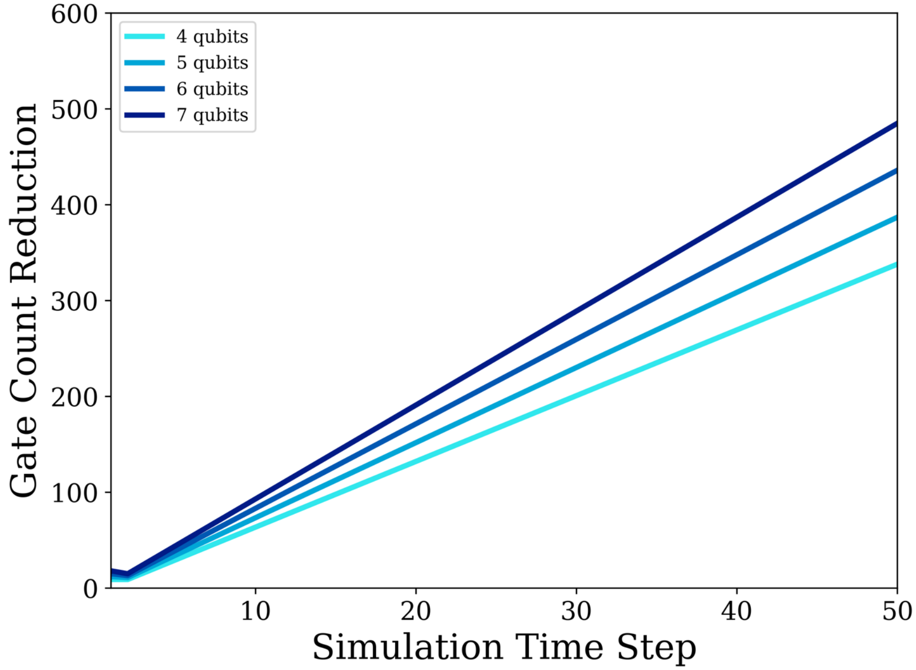



L. Bassman *et al.*, *Quantum Sci. Tech.* **6**, 014007 ('21)

# Performance of Domain-Specific Compiler

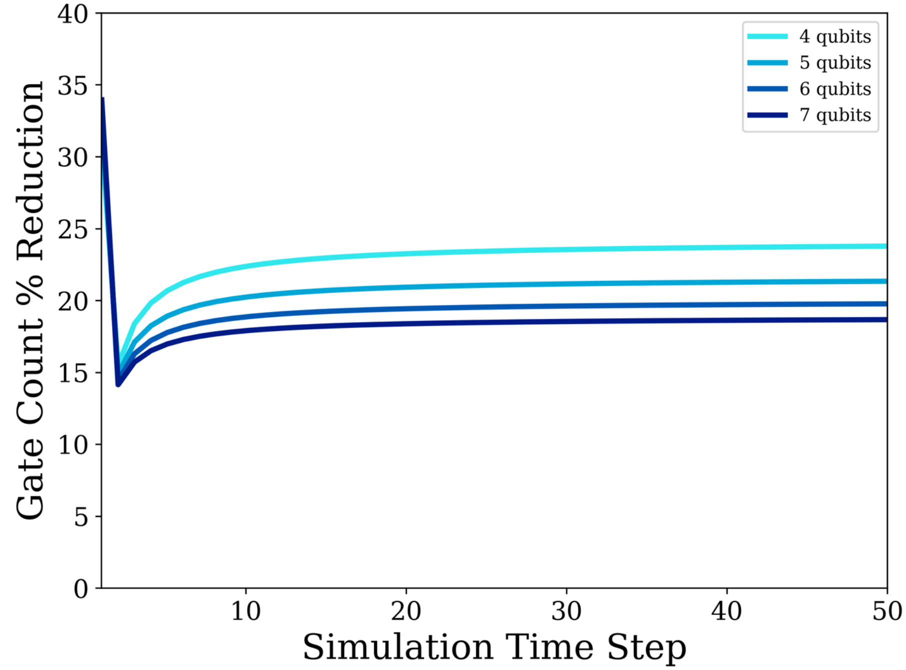
**Absolute gate count difference**

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




**Percent gate count difference**

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

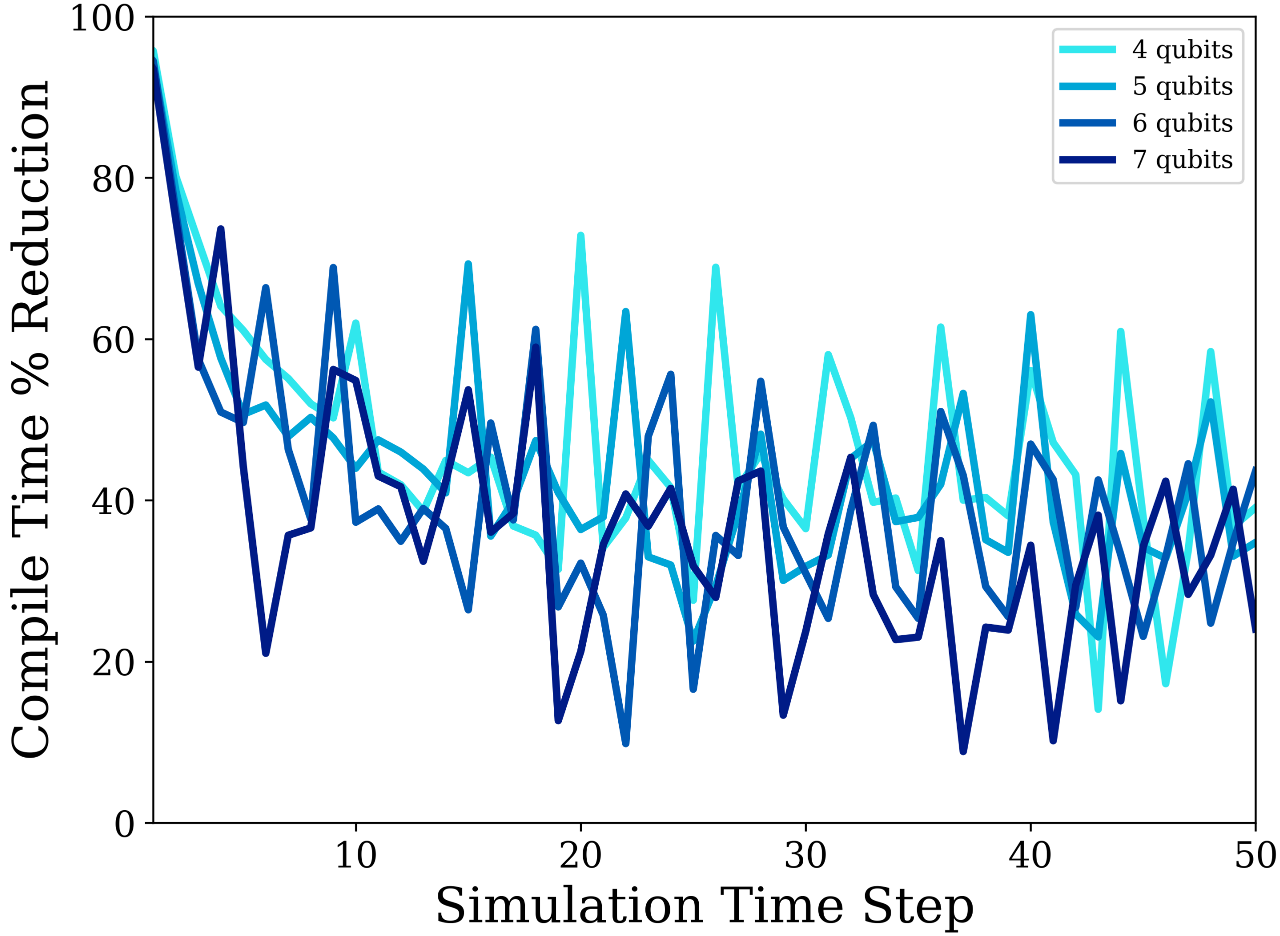



**Domain-specific compiler reduces gate count compared to IBM compiler**

# Speed of Domain-Specific Compiler

**Percent compile-time difference**

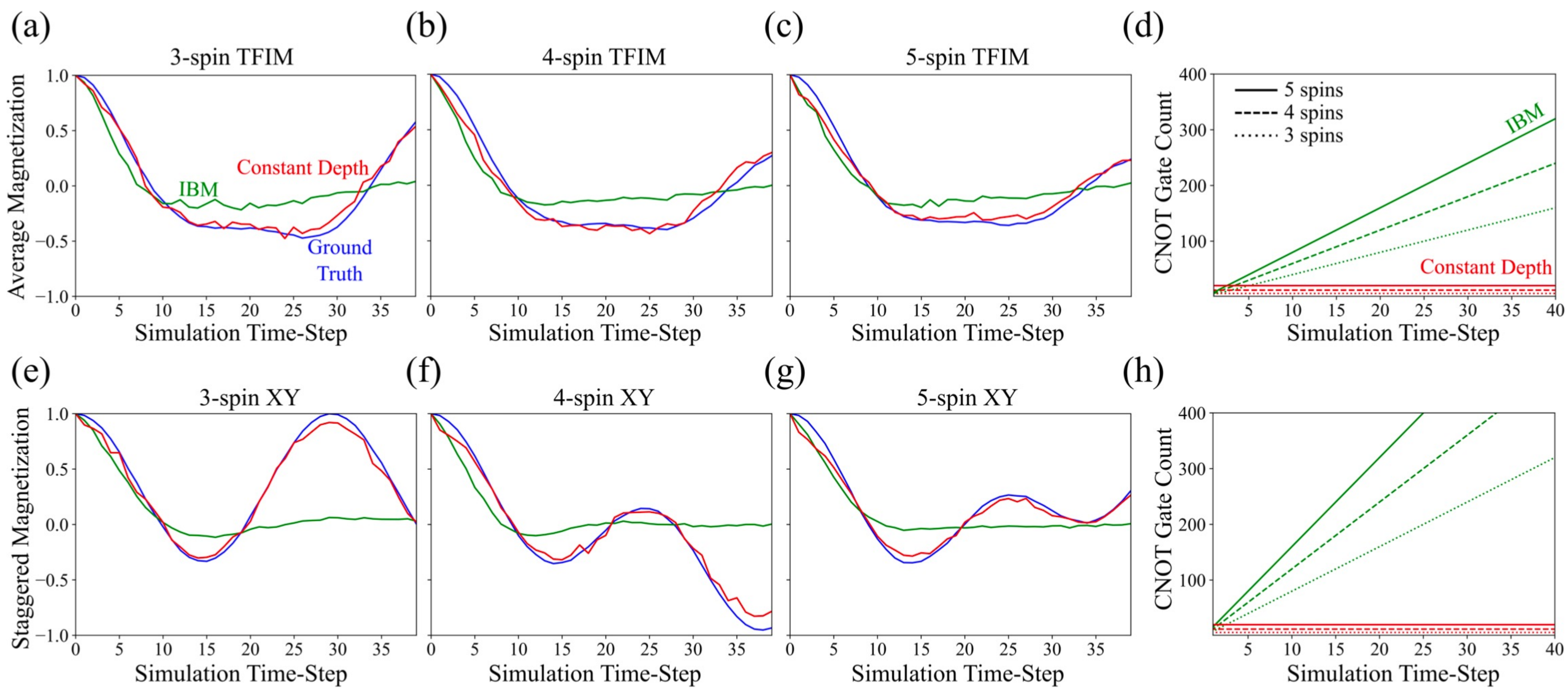
$$\frac{IBM\ Compiler - DS\ Compiler}{IBM\ Compiler} \times 100$$




**… 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"**

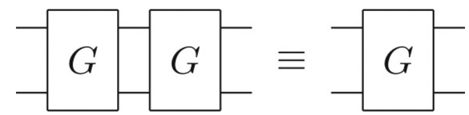
L. Bassman *et al.*, *Mater. Theo.* **6**, 13 ('22)

# Constant Circuit-Depth: How It is Done

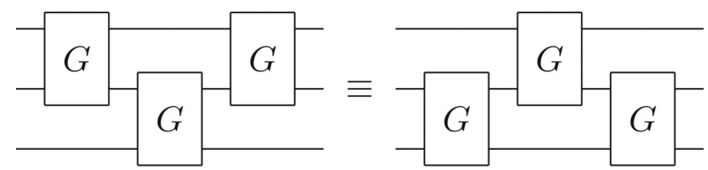
- **Matchgate (shifted 2×2 block diagonal)**

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

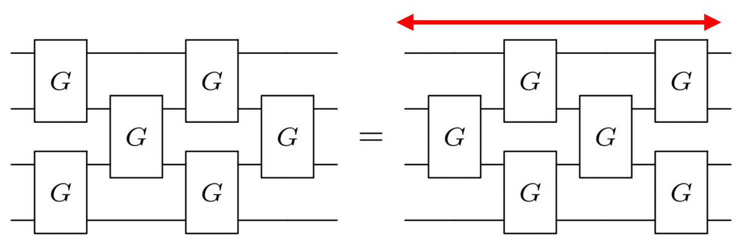
- **Contraction: product of matchgates is a matchgates**



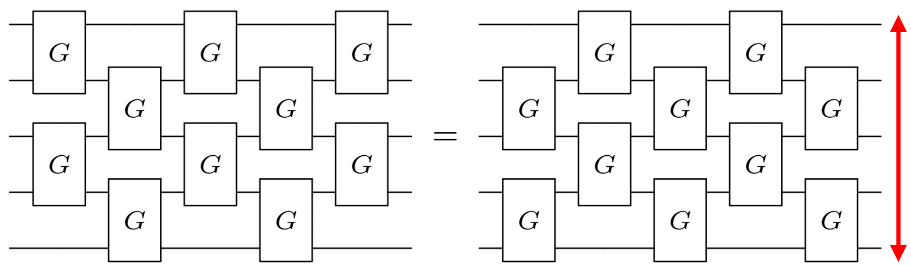

- **Conjecture: existence of flipped matchgates**
  *cf.* Yang-Baxter equation




- **Mirroring identities**



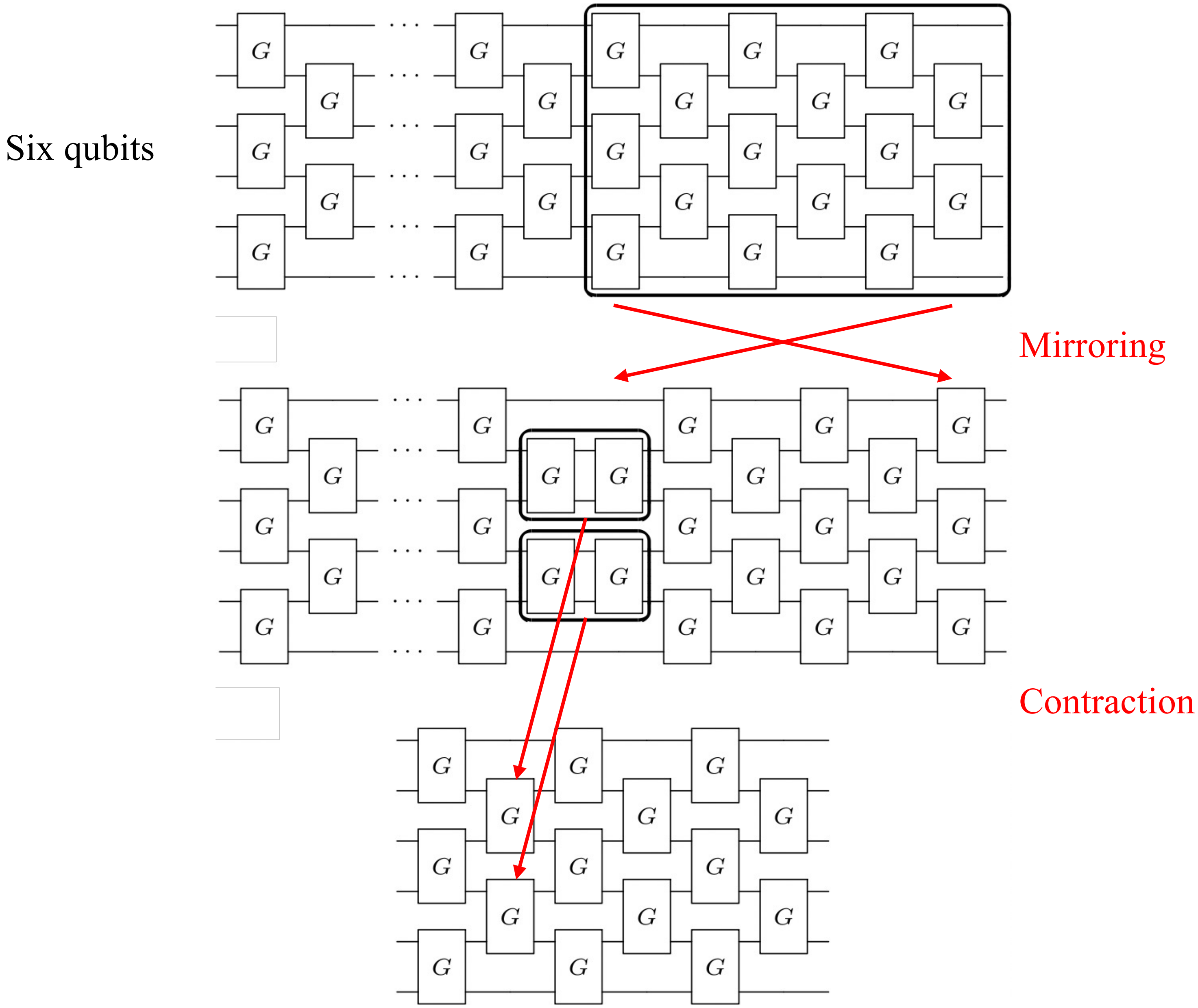
Even qubits



Odd qubits

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

# Downfolding to Constant-Depth




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

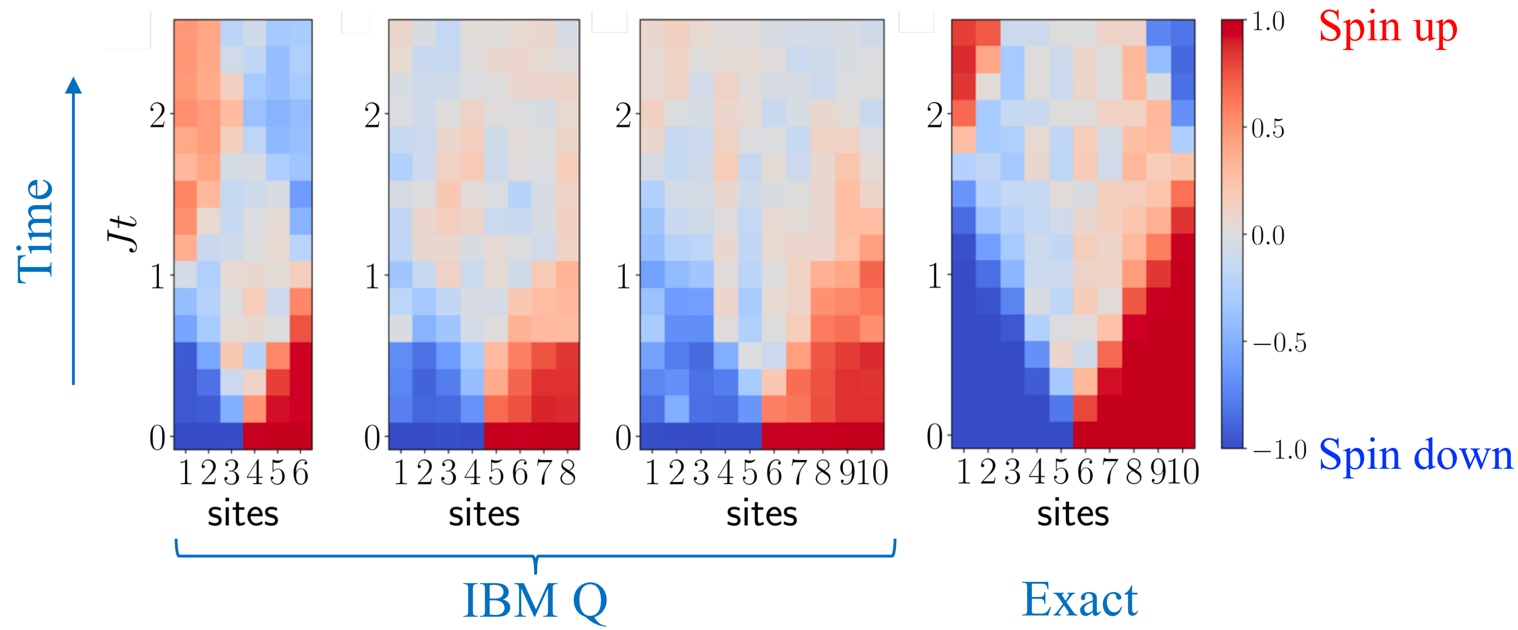
# Richer Physics: Heisenberg Model

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

**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

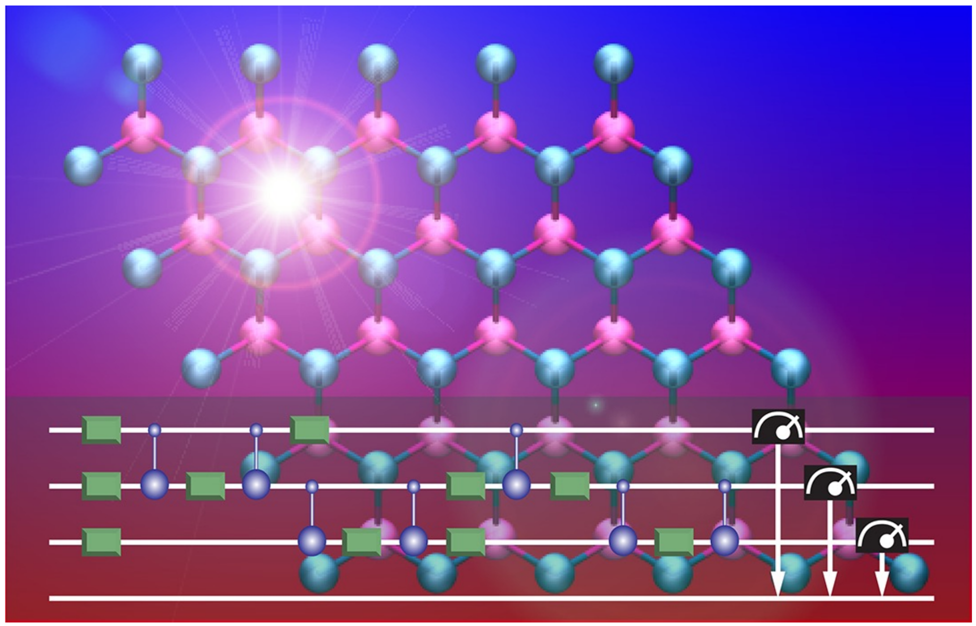
**Domain-wall dynamics (6-, 8- & 10-site spin chains)**




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

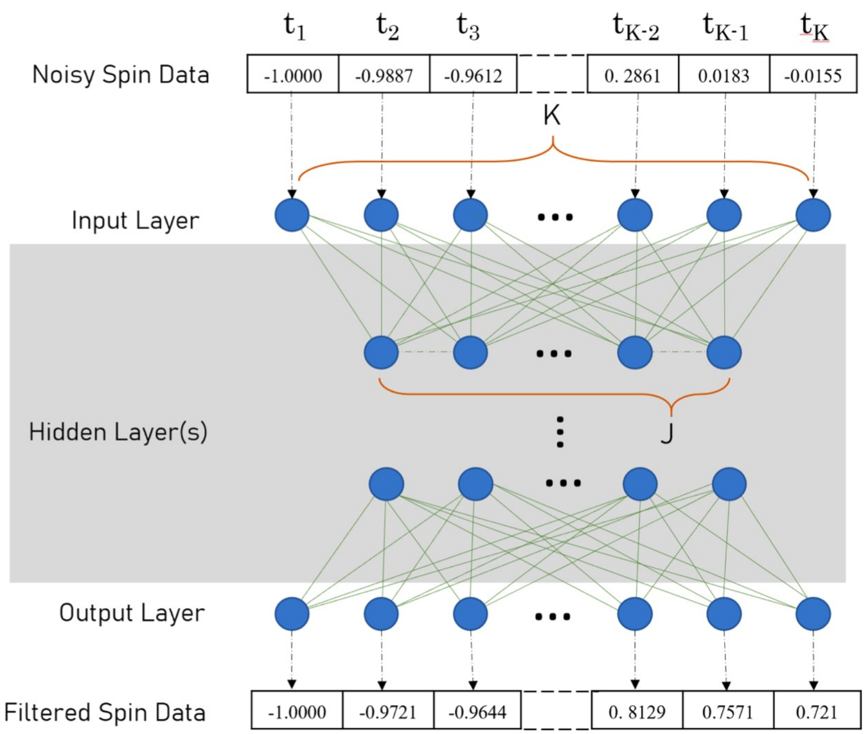
**M**ult**I**platform
**S**oftware for
**TI**me-dependent
**Q**uantum
**S**imulation

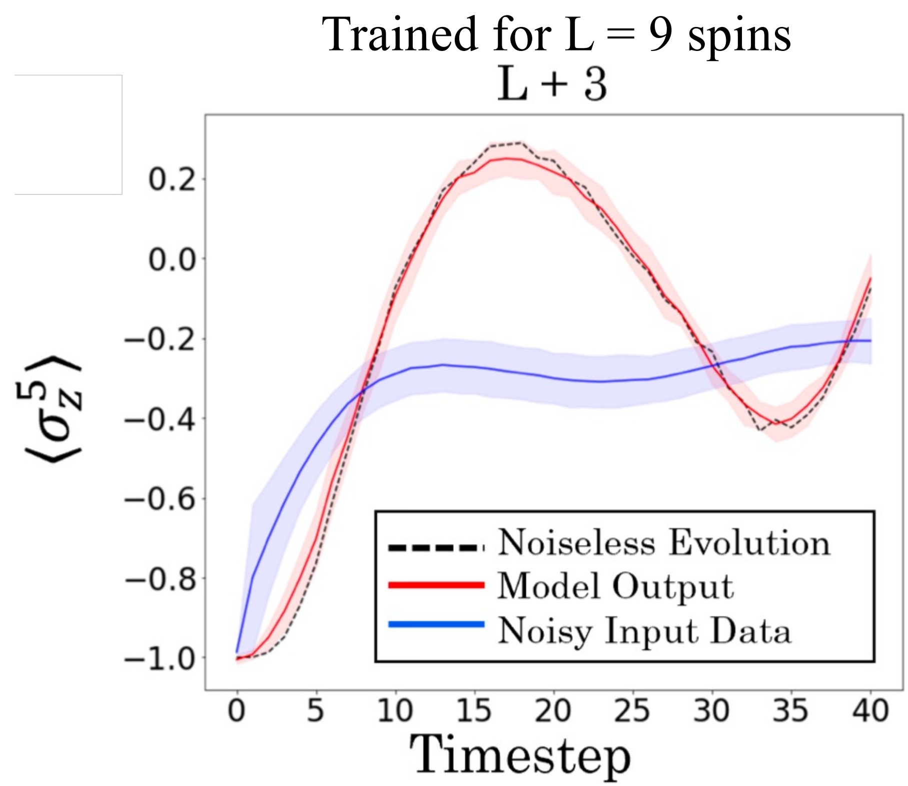
Paper: C. Powers *et al.*, *SoftwareX* **14**, 100696 ('21)

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**

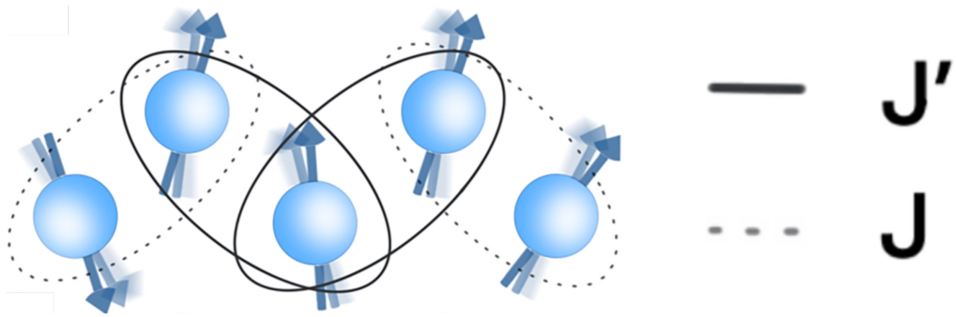



C. Powers *et al.*, *NeurIPS workshop* ('21)

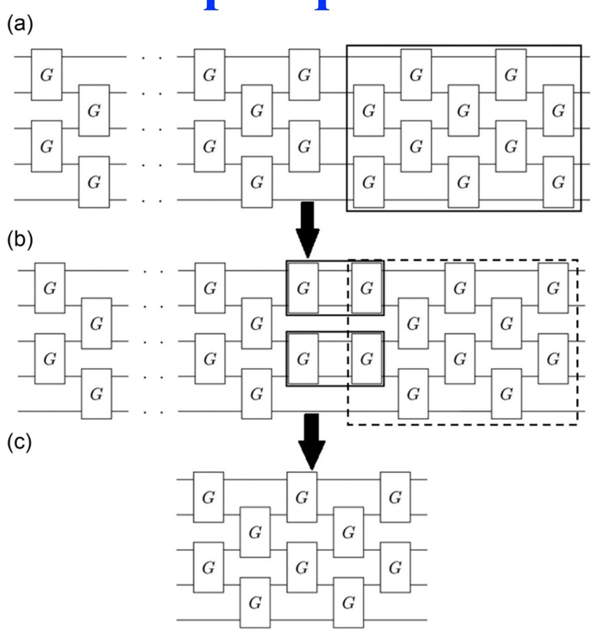
# Topological Quantum Dynamics

## Quantum spin chain

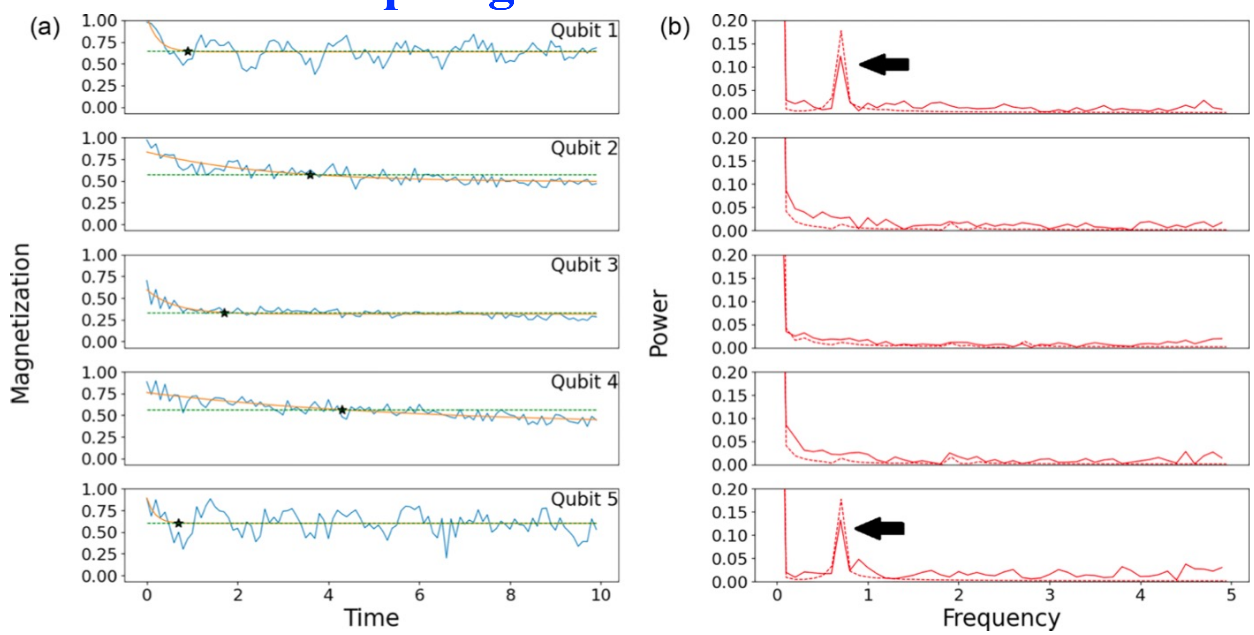




## Constant-depth quantum circuit




## Topological surface mode




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

## New: Periodically-driven Floquet topology simulated

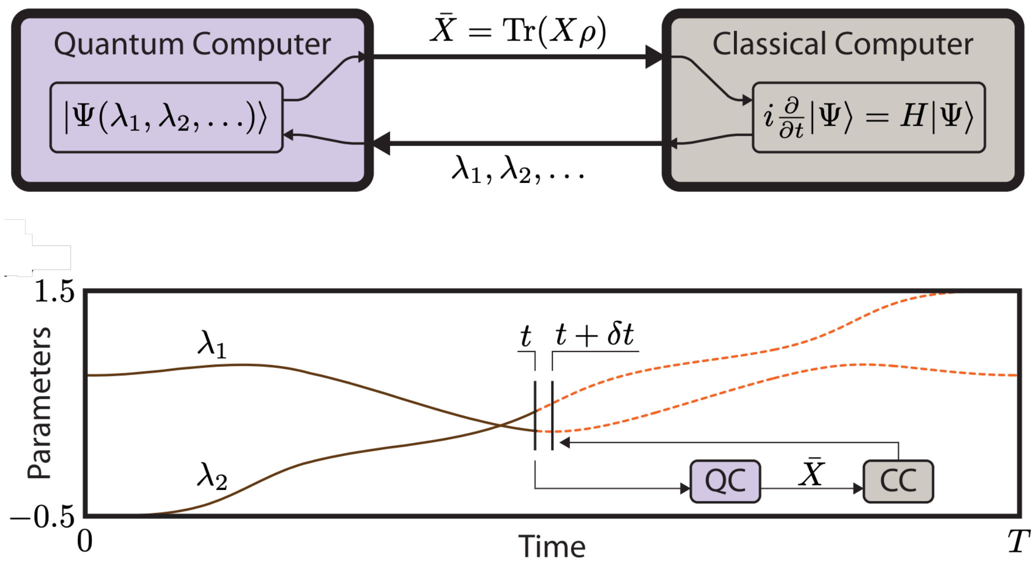
# Variational Quantum Simulator

**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**

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

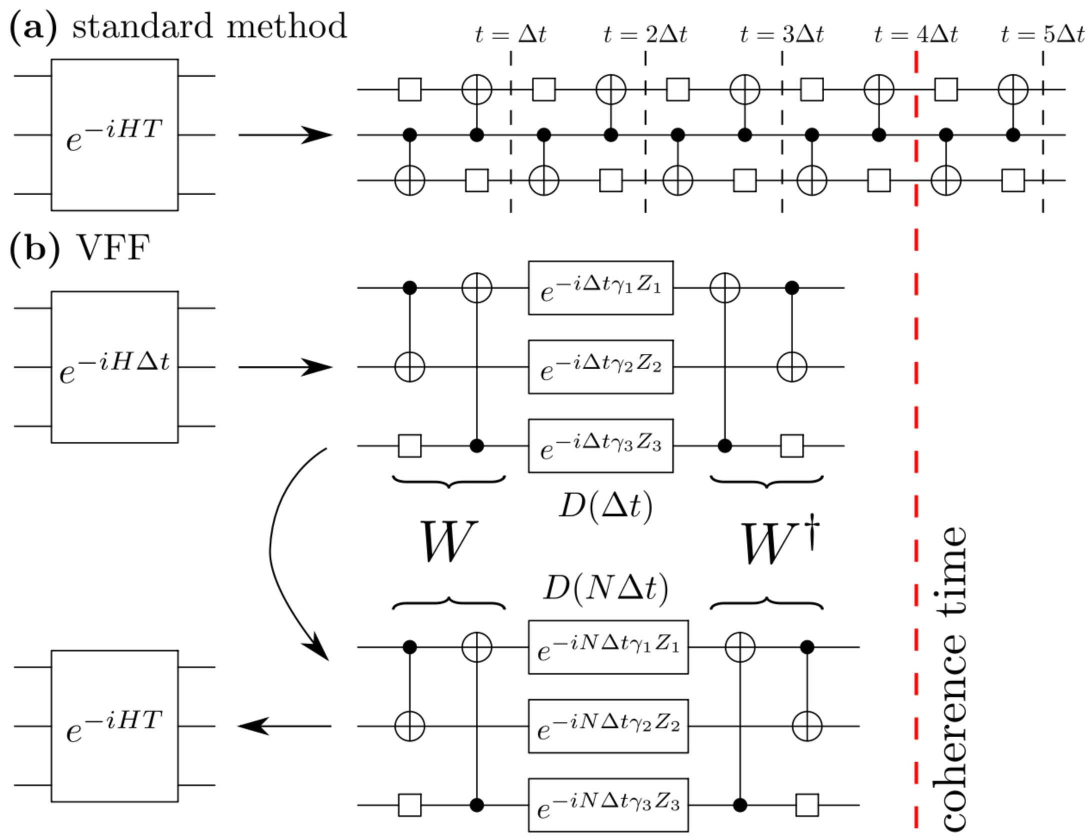
- **Short-time propagation of a many-body wave function on a quantum computer is mapped back to a parameterized variational wave function, $|\boldsymbol{\psi}(\boldsymbol{t})\rangle = |\boldsymbol{\psi}(\boldsymbol{\lambda_1}(\boldsymbol{t}), \ldots, \boldsymbol{\lambda_P}(\boldsymbol{t}))\rangle$, which 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

# 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 (this course), CSCI 596, CSCI 653: Elective for MSQIS