Variational Quantum Dynamics Simulation

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IBM **Quantum**

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Quantum Time Evolution

Quantum Real Time Evolution

Study of real time dynamics for many-body physics systems, behavior under specific potential, etc. [1, 2, etc.]

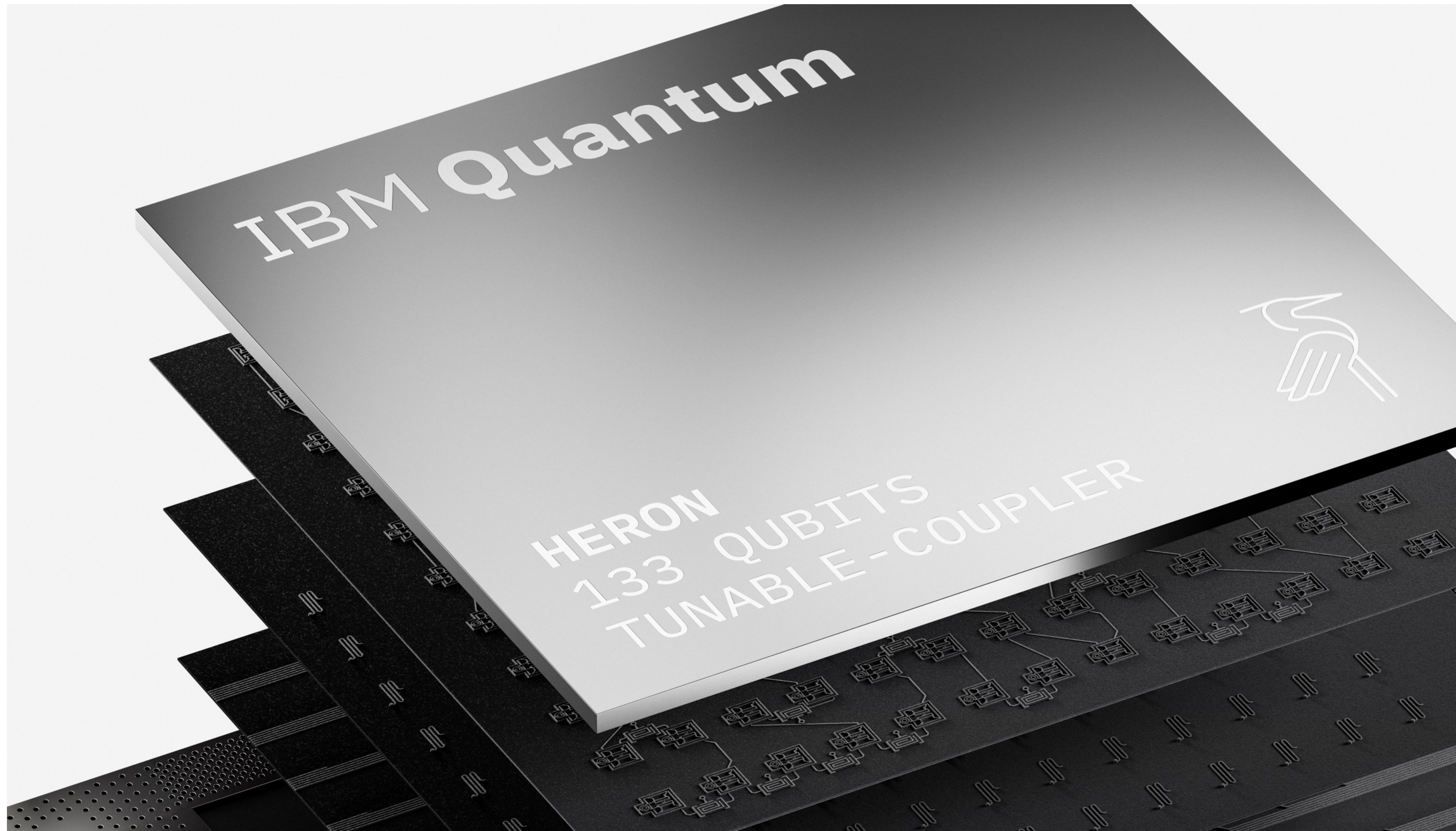
Solve PDEs via Schrödingerisation (such as heat equations)

Quantum Imaginary Time Evolution

Finding the ground state of Hamiltonian H [3]

Prepare a Gibbs state for a given Hamiltonian H [4]

Solve PDEs (such as Black Scholes model) [5, 6]



[1] Quantum algorithm for simulating real time evolution of lattice Hamiltonians, J. Haah et al.
[2] Simulating quantum many-body dynamics on a current digital quantum computer, A. Smith et al.
[3] Variational ansatz-based quantum simulation of imaginary time evolution, S. McArdle, et al.
[4] Variational Quantum Boltzmann Machines, C. Zoufal et al.
[5] Quantum option pricing using Wick rotated imaginary time evolution, S. K. Radha
[6] Variational quantum simulations of stochastic differential equations, K. Kubo et al.

Quantum Time Evolution

$$H = \sum_i \theta_i h_i$$

$$H \to \frac{H}{\hbar}$$

$$E_t = \langle\psi(t)|H|\psi(t)\rangle$$

Quantum Real Time Evolution

Schrödinger Equation

$$i\frac{\partial|\psi(t)\rangle}{\partial t} = H\,|\psi(t)\rangle$$

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$

Quantum Imaginary Time Evolution

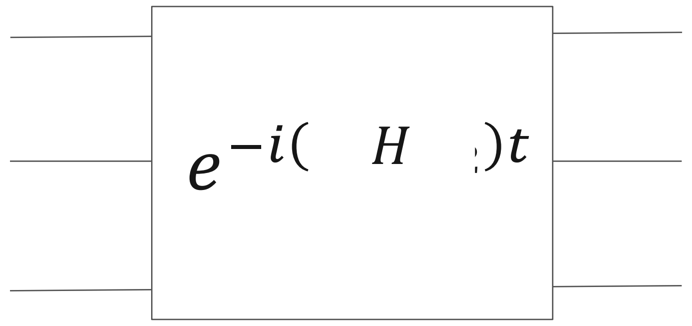
Wick-rotated
Schrödinger Equation

$$\frac{\partial|\psi(t)\rangle}{\partial t} = (E_t - H)\,|\psi(t)\rangle$$

$$|\psi(t)\rangle = \frac{e^{-Ht}}{\sqrt{Tr[e^{-2Ht}|\psi(0)\rangle\langle\psi\,(0)|]}}|\psi(0)\rangle$$

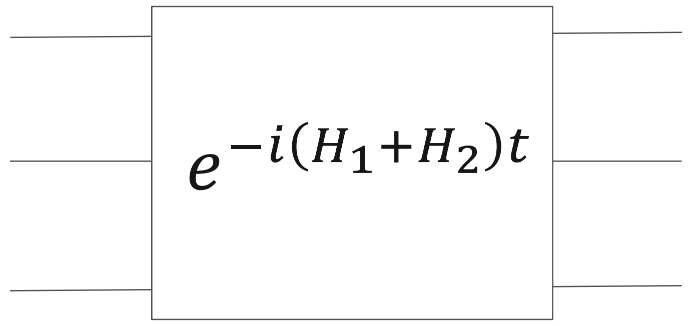
Product Formulas (PFs) for Real Time Dynamics

- Suppose H.



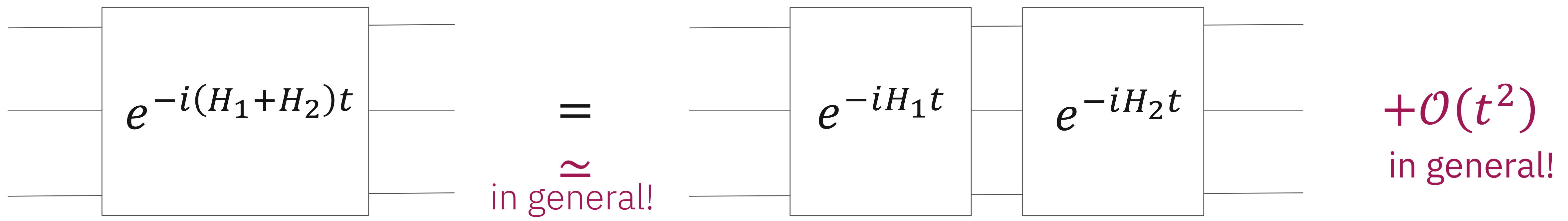
Product Formulas (PFs) for Real Time Dynamics

- Suppose $H = H_1 + H_2$.



Product Formulas (PFs) for Real Time Dynamics

- Suppose $H = H_1 + H_2$. If $[H_1, H_2] = 0$, we can add the circuits for $e^{-iH_1 t}$ and $e^{-iH_2 t}$ in sequence



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Product Formulas (PFs) for Real Time Dynamics

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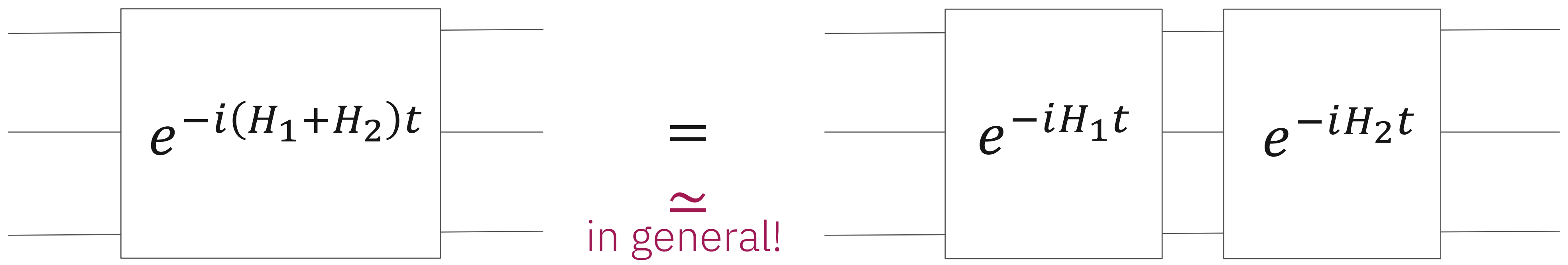
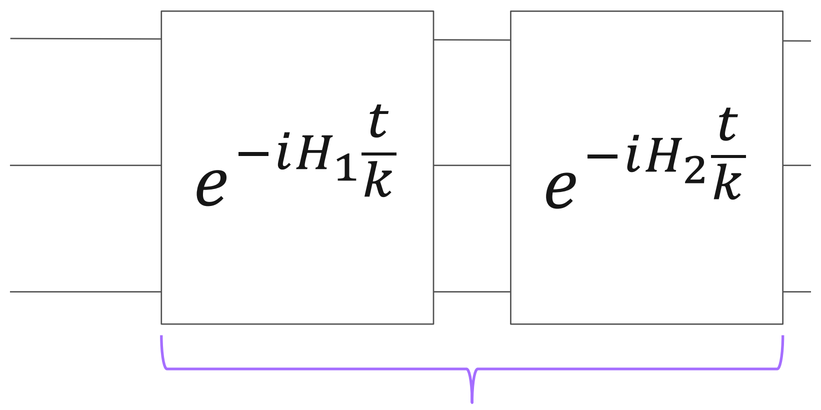


$+\mathcal{O}(t^2)$
in general!

- Otherwise, decreasing the time to t/k and repeating the sequence k times achieves a better approximation



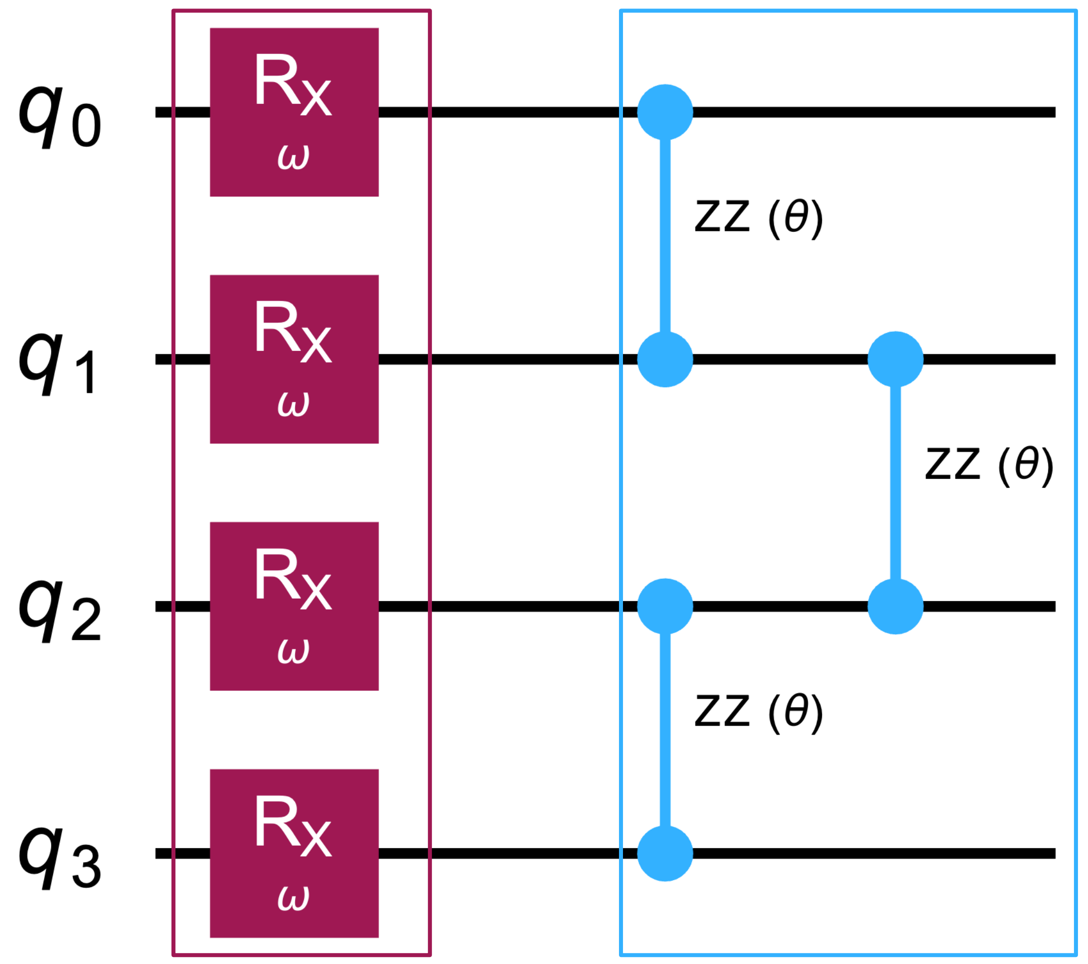
k ≔ number of Trotter steps

$+\mathcal{O}(t^2/k)$

$S_1^k\left(\frac{t}{k}\right)$ =: Lie-Trotter

H_1 H_2

$$H = -h \sum_i X_i - J \sum_{<i,j>} Z_i Z_j$$



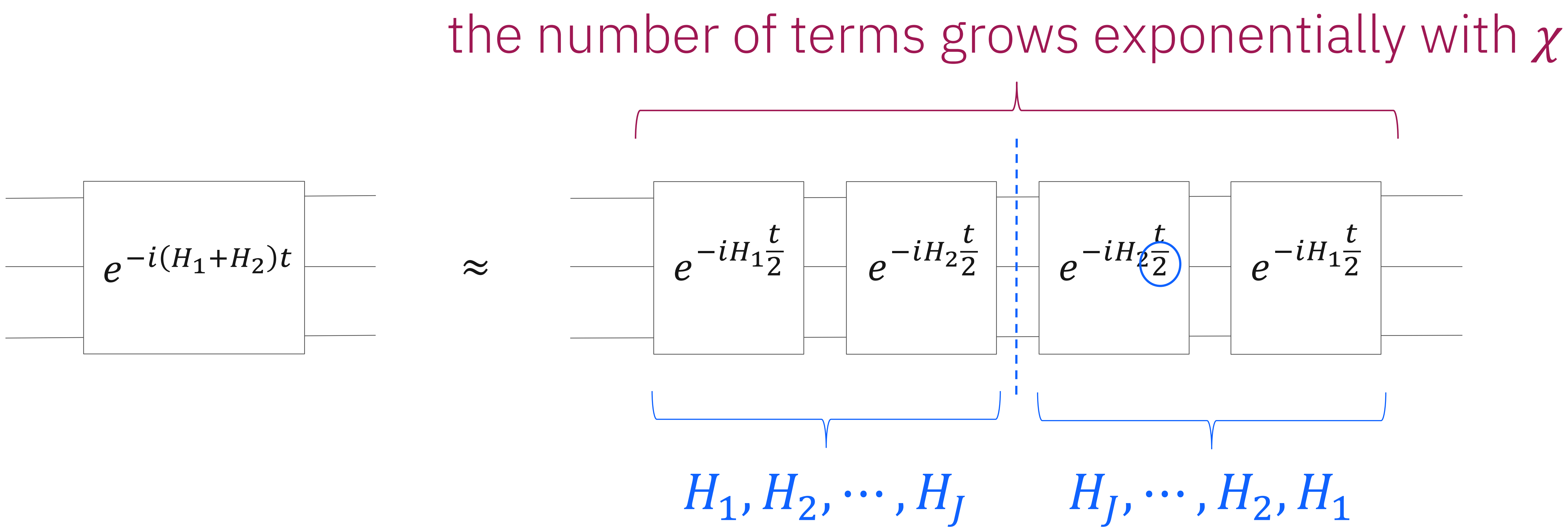
$$e^{-iH_1 t} \, e^{-iH_2 t}$$

Product Formulas (PFs) for Real Time Dynamics

- Higher order PFs: $S_{2\chi}^{k}\left(\frac{k}{t}\right) = e^{-iHt} + \mathcal{O}\left(t\left(\frac{t}{k}\right)^{2\chi}\right)$ — Trotter-Suzuki / Minimize cost

$$e^{(A+B)} = \lim_{\chi\to\infty}\left(e^{(A/\chi)}e^{(B/\chi)}\right)^{\chi}$$

- Example: 2nd order PF: $S_2^k = \left(e^{-iH_1\frac{t}{2k}}e^{-iH_2\frac{t}{k}}e^{-iH_1\frac{t}{2k}}\right)^k = e^{-iHt} + \mathcal{O}\left(\frac{t^3}{k^2}\right)$



How to improve accuracy?

1. Increase k
2. Increase χ

Product Formulas for Imaginary Time Dynamics

- By using the Hubbard-Stratonovich transformation for positive semidefinite H one can achieve a linear combination of unitary operators [1]

$$e^{-\beta H/2} = \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} dy\, e^{-\frac{y^2}{2}} e^{-iy\sqrt{\beta H}}$$

Requires the identification of $\sqrt{H}$ or at least $\widetilde{H}$ such that $\widetilde{H}^2 = H$

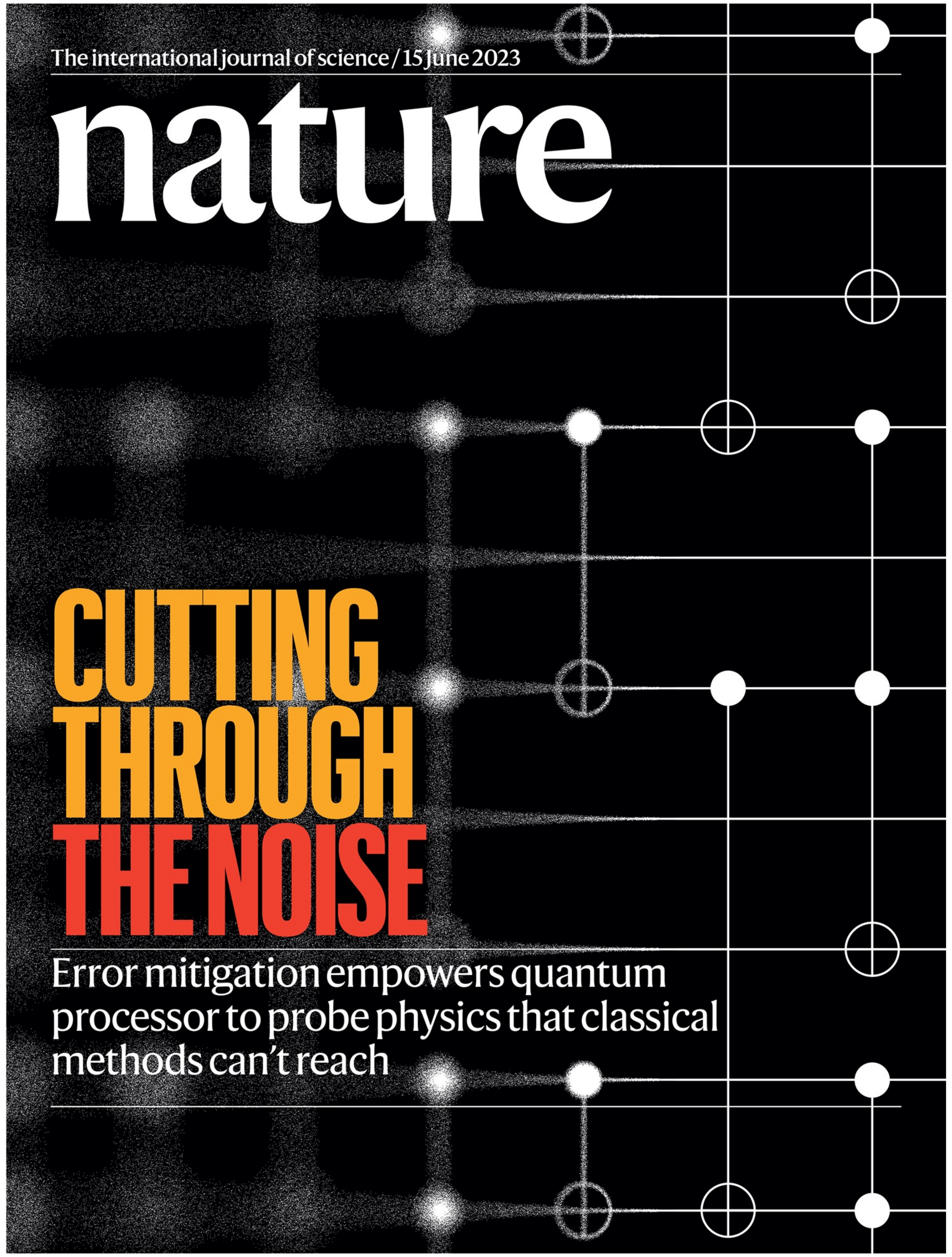
- For a geometric k-local $H = \sum_i \theta_i h_i$ one can apply a Trotter decomposition as

$$e^{-\beta H} = \left(e^{-\Delta\tau\theta_0 h_0} e^{-\Delta\tau\theta_1 h_1} \dots\right)^{\frac{\beta}{\Delta\tau}} + \mathcal{O}(\Delta\tau)$$

Approximate individual non-unitary transformations with unitary transformations $e^{-i\Delta\tau A}$ [2]
Expand A in the Pauli basis → fit coefficients via solving a linear system to approx. the imaginary dynamics.
Method cost generally scales **exponentially** in the **correlation** length

[1] Quantum algorithms with applications to simulating physical systems, A. Ch. N. Chowdhury
[2] Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution, M. Motta et al.

Exciting Times



- Simulation of an Ising model on 127 qubits
- Proof that error mitigation techniques work in practice
- Not yet a quantum advantage since sophisticated classical methods (tensor networks) exist for Ising models

We are getting close to showing a quantum advantage and doing useful things

Exciting Times

Chemistry Beyond Exact Solutions on a Quantum-Centric Supercomputer

Javier Robledo-Moreno, Mario Motta, Holger Haas, Ali Javadi-Abhari, Petar Jurcevic, William Kirby, Simon Martiel, Kunal Sharma, Sandeep Sharma, Tomonori Shirakawa, Iskandar Sitdikov, Rong-Yang Sun, Kevin J. Sung, Maika Takita, Minh C. Tran, Seiji Yunoki, Antonio Mezzacapo

arXiv:2405.05068

- Good approximate solutions to electronic structure calculations beyond exact diagonalization
- Upper bounds guarantee an unconditional quality metric for quantum advantage
  → certifiable by classical computers at polynomial cost
- Quantum circuits of up to 10570 (3590 2-qubit) quantum gates
  - N2 triple bond breaking (58 qubits)
  - Active-space electronic structure of [2Fe-2S] (45 qubits)
  - Active-space electronic structure of [4Fe-4S] clusters (77 qubits)

Combining powerful classical and quantum resources!

→ up to 6400 nodes of the supercomputer Fugaku + a Heron superconducting quantum processor

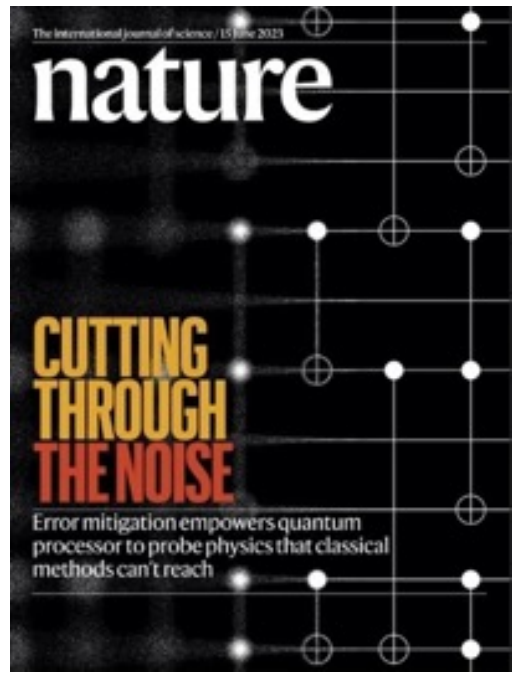
If you build it, they will use it…

Multiple utility-scale experiments within last 6 months (more to come)

Evidence for the utility of quantum computing before fault tolerance

127 qubits / 2880 CX gates

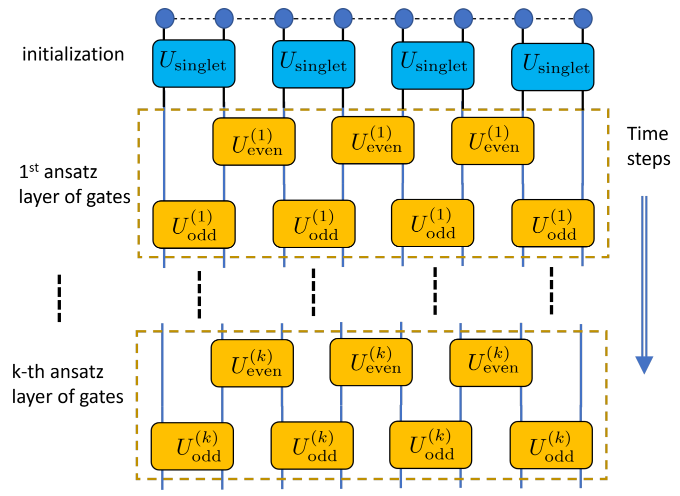
Nature, 618, 500 (2023)



Simulating large-size quantum spin chains on cloud-based superconducting quantum computers

102 qubits / 3186 CX gates

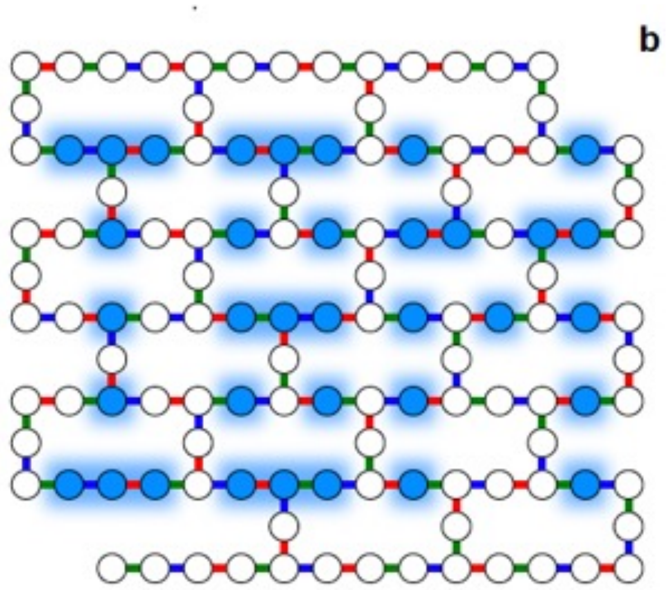
arXiv:2207.09994



Uncovering Local Integrability in Quantum Many-Body Dynamics

124 qubits / 2641 CX gates

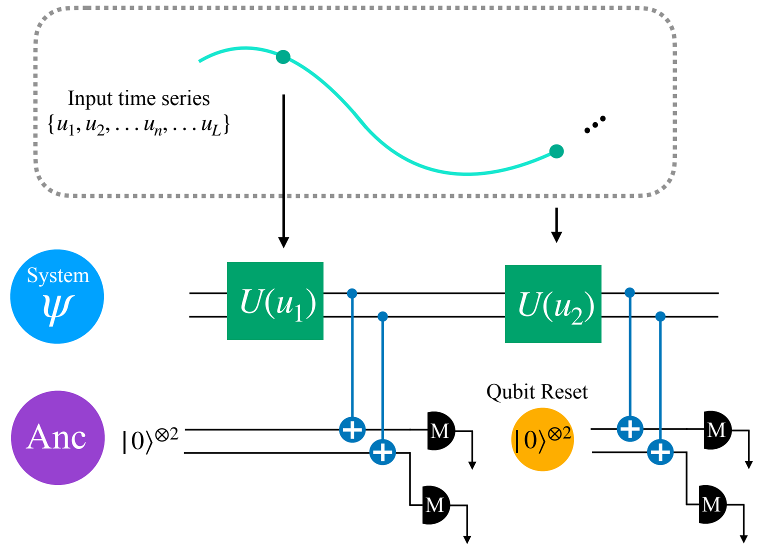
arXiv:2307.07552



Quantum reservoir computing with repeated measurements on superconducting devices

120 qubits / 49470 gates + meas.

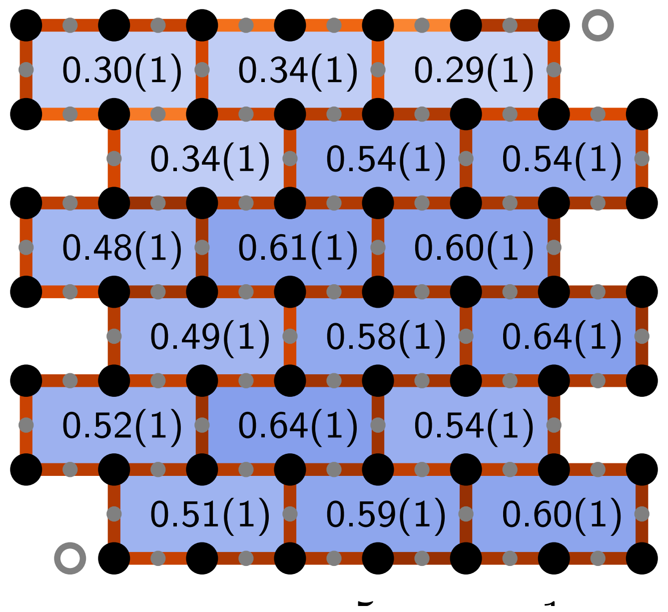
arXiv:2310.06706



Realizing the Nishimori transition across the error threshold for constant-depth quantum circuits

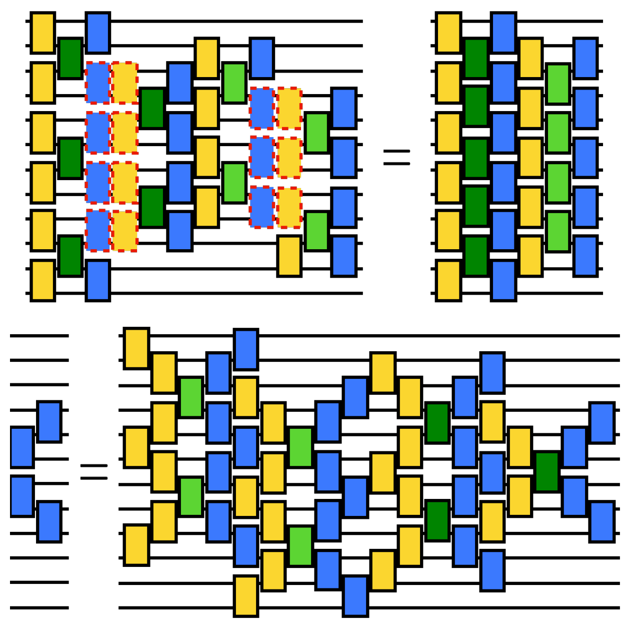
125 qubits / 429 gates + meas.

arXiv:2309.02863



Scalable Circuits for Preparing Ground States on Digital Quantum Computers: The Schwinger Model Vacuum on 100 Qubits

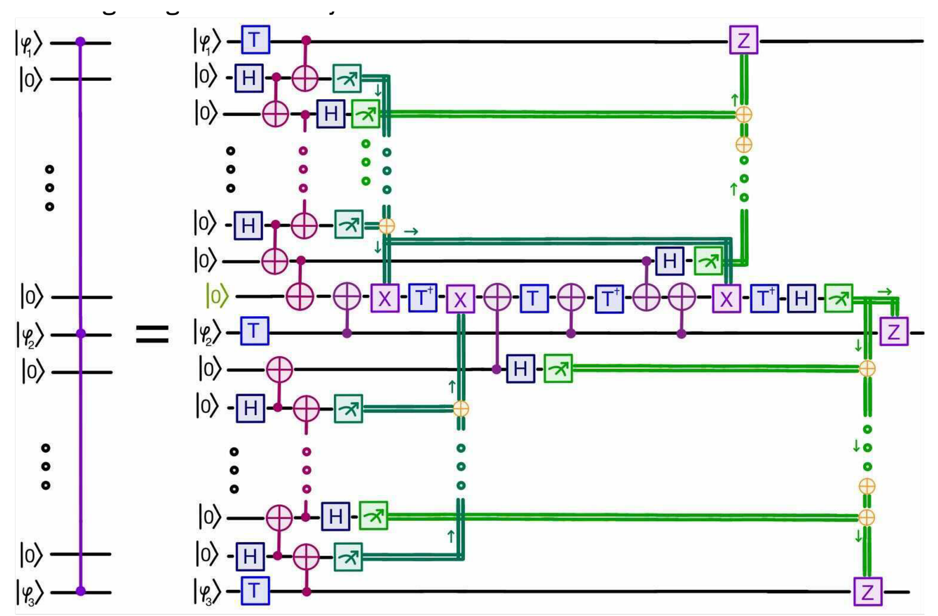
100 qubits / 788 CX gates
arXiv:2308.04481



Efficient Long-Range Entanglement using Dynamic Circuits

101 qubits / 504 gates + meas.

arXiv:2308.13065



Quantum Advantage

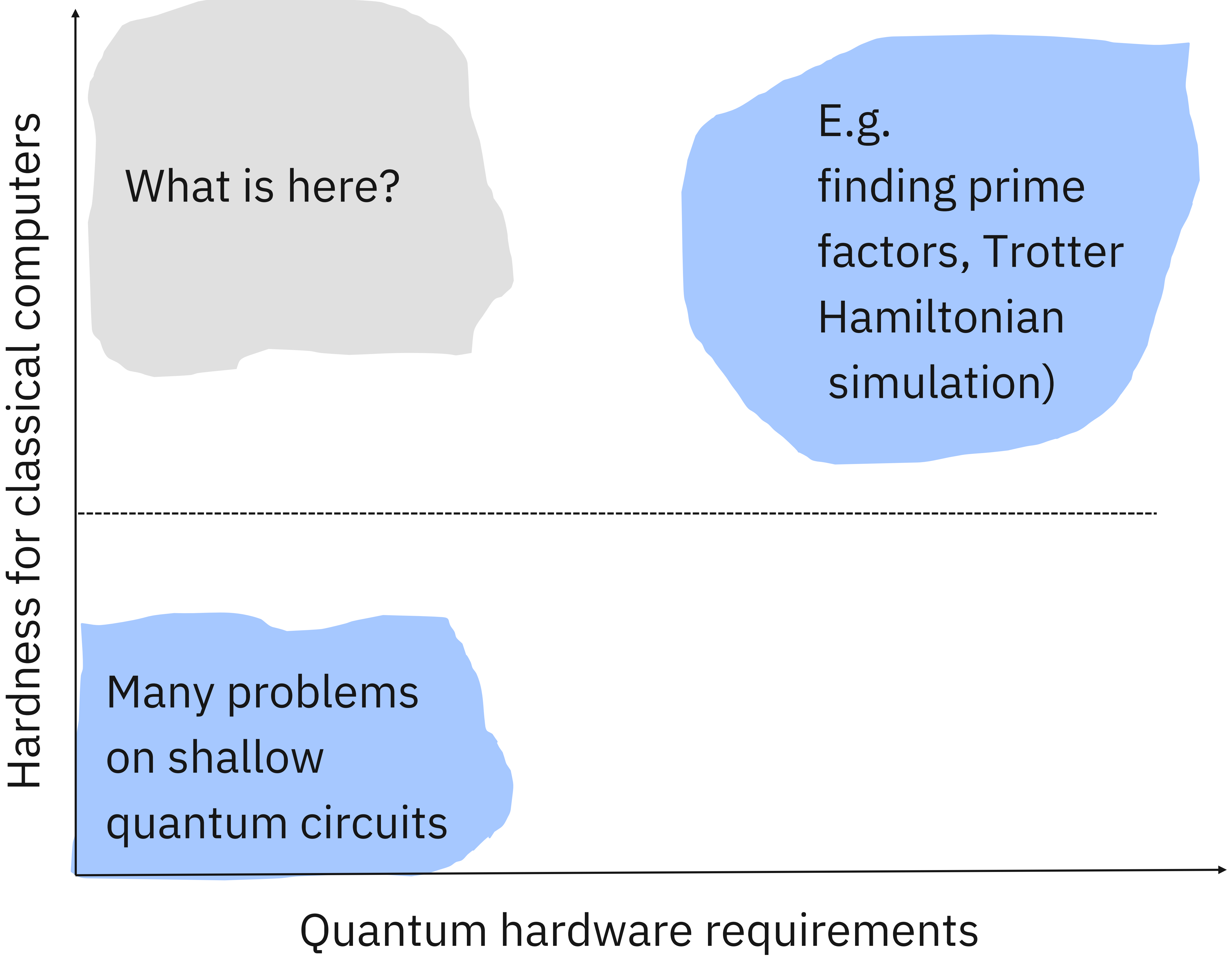
R. Feynman

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

Solve a *practically relevant* problem faster or better than any known classical algorithm on the best classical computer

(1) Fighting noise:
better error correction / fault-tolerance

(2) Finding new problems:
new quantum algorithms



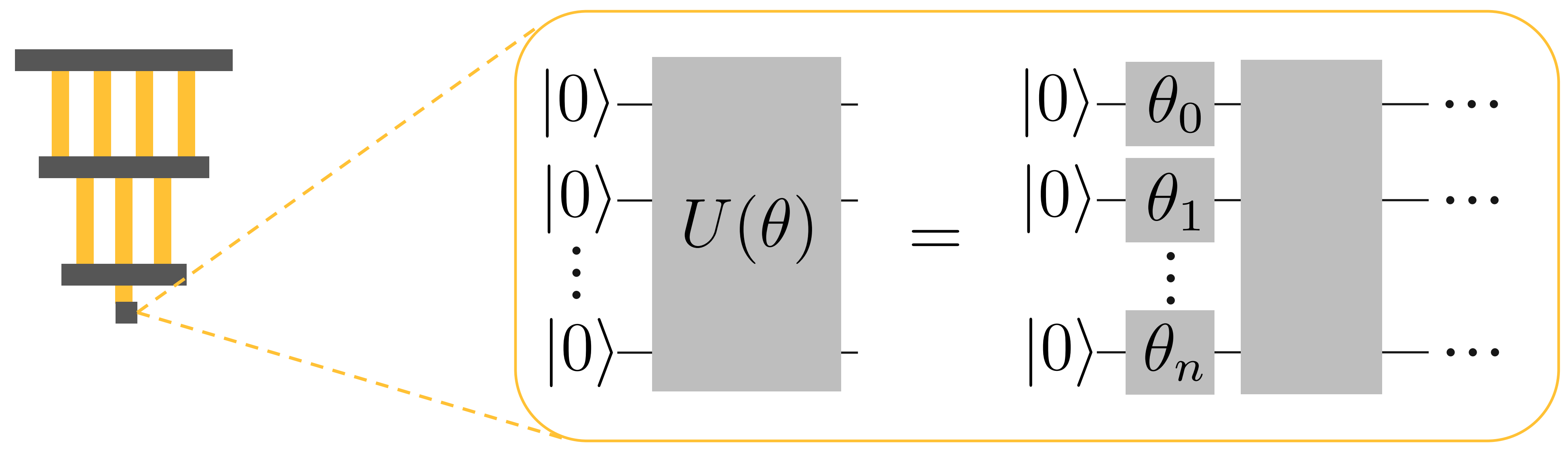
Variational Quantum Algorithms

Paradigm

Approximate the solution with a parameterized state

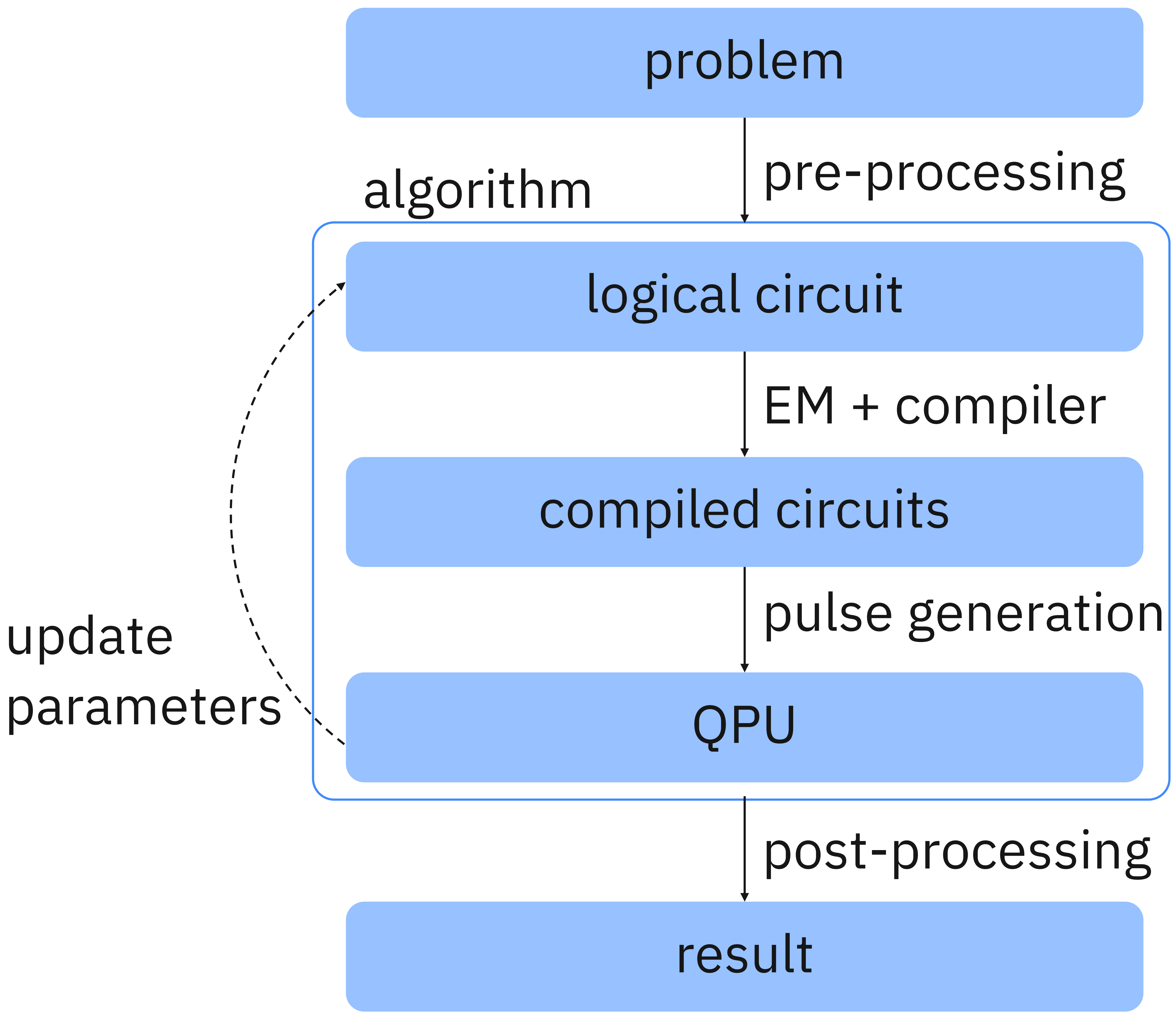
$$|\Psi\rangle \approx |\phi(\theta)\rangle, \ \theta \in \mathbb{R}^d$$

with $|\phi(\theta)\rangle = U(\theta)|0\rangle$ acting in the device's capabilities.



Ground-state preparation

$$E_0 \approx \min_\theta \langle\phi(\theta)|H|\phi(\theta)\rangle$$



Variational Quantum Time Evolution

$$H = \sum_i \theta_i h_i$$

Variational Ansatz

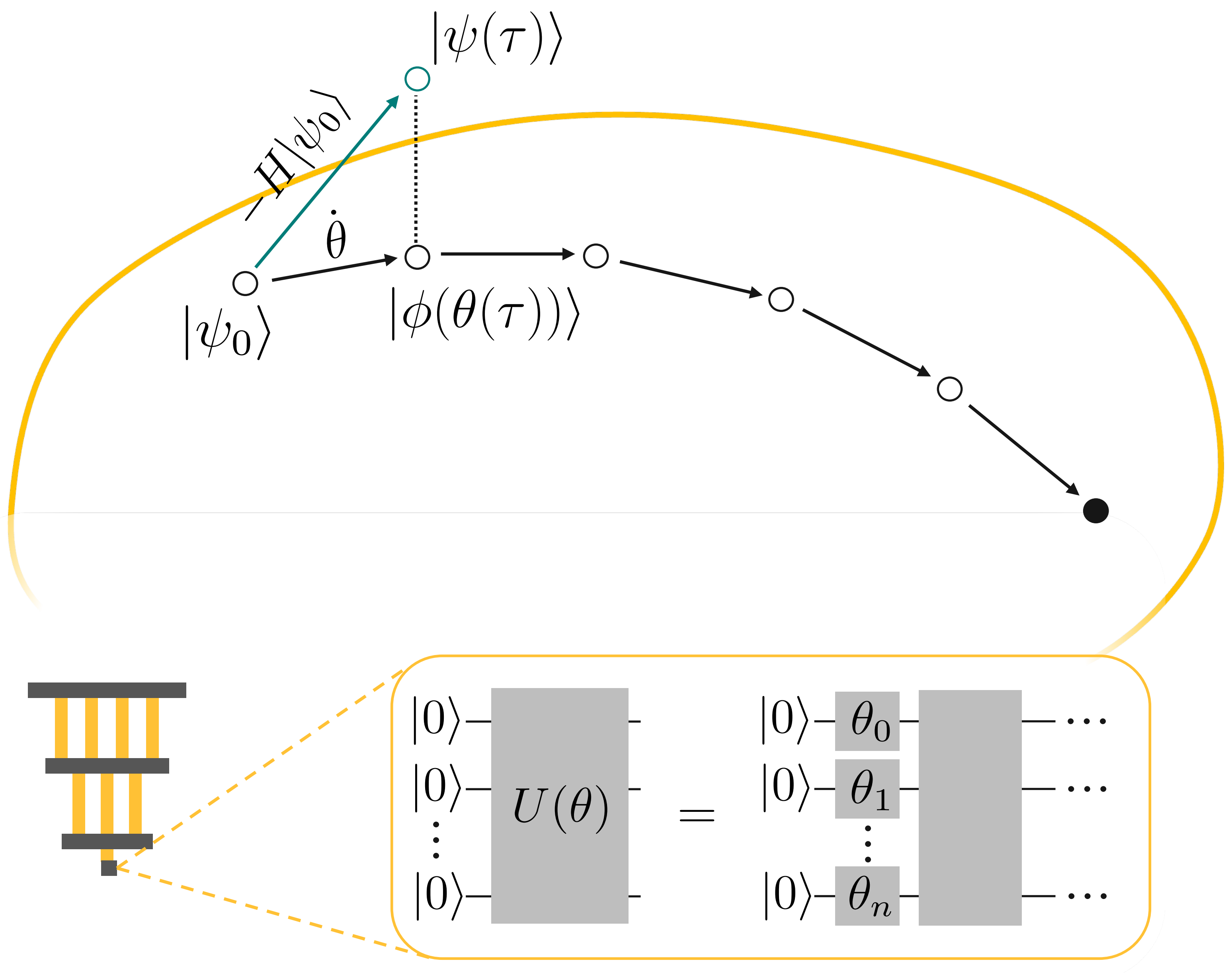
$$|\psi_\omega(t)\rangle = U\big(\omega(t)\big)|0\rangle$$

Approach:

- State evolution → Parameter evolution with McLachlan [1]
- Minimize the error between the variational trajectory and the actual gradient using a constant depth Ansatz

Properties:

- Ensures that $\omega \in \mathbb{R}$
- In the case of real time evolution not necessarily energy preserving
- Unlike PFs: circuit depth does not (necessarily) increase with the number time-steps and the locality of the system



[1] A variational solution of the time-dependent Schrödinger equation, A. McLachlan

McLachlan's Variational Principle

$$H = \sum_i \theta_i h_i$$

Variational Ansatz

$$|\psi_{\omega}(t)\rangle = U\big(\omega(t)\big)|0\rangle$$

Quantum Real Time Evolution
➔ VarQRTE

$$\delta \left\| \left(i\frac{\partial}{\partial t} - H \right) |\psi_{\omega}(t)\rangle \right\|_2 = 0$$

Quantum Imaginary Time Evolution
➔ VarQITE

$$\delta \left\| \left(\frac{\partial}{\partial t} + H - E_t \right) |\psi_{\omega}(t)\rangle \right\|_2 = 0$$

Derivation for VarQRTE

Let’s move to the blackboard

McLachlan's Variational Principle

$$H = \sum_i \theta_i h_i$$

Variational Ansatz

$$|\psi_\omega(t)\rangle = U(\omega(t))|0\rangle$$

Quantum Real Time Evolution

$$\delta \left\| \left(i\frac{\partial}{\partial t} - H \right) |\psi_\omega(t)\rangle \right\|_2 = 0$$

$$\mathrm{Re}\left(\frac{\partial\langle\psi_\omega(t)|}{\partial\omega_i} \frac{\partial|\psi_\omega(t)\rangle}{\partial\omega_j} - \frac{\partial\langle\psi_\omega(t)|}{\partial\omega_i} |\psi_\omega(t)\rangle\langle\psi_\omega(t)| \frac{\partial|\psi_\omega(t)\rangle}{\partial\omega_j} \right) \dot{\omega}_j = \mathrm{Im}\left(\frac{\partial\langle\psi_\omega(t)|}{\partial\omega_i} H|\psi(t)\rangle - \frac{\partial\langle\psi_\omega(t)|}{\partial\omega_i} |\psi_\omega(t)\rangle\langle\psi_\omega(t)|H|\psi_\omega(t)\rangle \right)$$

Quantum Imaginary Time Evolution

$$\delta \left\| \left(\frac{\partial}{\partial t} + H - E_t \right) |\psi_\omega(t)\rangle \right\|_2 = 0$$

$$\mathrm{Re}\left(\frac{\partial\langle\psi_\omega(t)|}{\partial\omega_i} \frac{\partial|\psi_\omega(t)\rangle}{\partial\omega_j} - \frac{\partial\langle\psi_\omega(t)|}{\partial\omega_i} |\psi_\omega(t)\rangle\langle\psi(t)| \frac{\partial|\psi_\omega(t)\rangle}{\partial\omega_j} \right) \dot{\omega}_j = -\mathrm{Re}\left(\frac{\partial\langle\psi_\omega(t)|}{\partial\omega_i} H|\psi_\omega(t)\rangle \right)$$

McLachlan's Variational Principle

Quantum Real Time Evolution

$$\delta \left\| \left(i\frac{\partial}{\partial t} - H \right) |\psi_{\boldsymbol{\omega}}(t)\rangle \right\|_2 = 0$$

Quantum Geometric Tensor (QGT)
prop. to the Quantum Fisher Information (QFI) →

$$F^Q_{ij}\dot{\omega}_j = \mathrm{Im}\left(C_i - \frac{\partial \langle \psi_{\boldsymbol{\omega}}(t)|}{\partial \omega_i} |\psi_{\boldsymbol{\omega}}(t)\rangle E_t \right)$$

Quantum Imaginary Time Evolution

$$\left\| \left(\frac{\partial}{\partial t} + H - E_t \right) |\psi_{\boldsymbol{\omega}}(t)\rangle \right\|_2 = 0$$

$$F^Q_{ij}\dot{\omega}_j = -\mathrm{Re}(C_i) \quad \propto \frac{\partial \langle E_{\boldsymbol{\omega}}(t)\rangle}{\partial \omega_i}$$

➔ Application to ground state search!

$$H = \sum_i \theta_i h_i$$

Variational Ansatz

$$|\psi_{\boldsymbol{\omega}}(t)\rangle = U(\omega(t))|0\rangle$$

Real

$$i\frac{\partial |\psi(t)\rangle}{\partial t} = H\,|\psi(t)\rangle$$

Imaginary

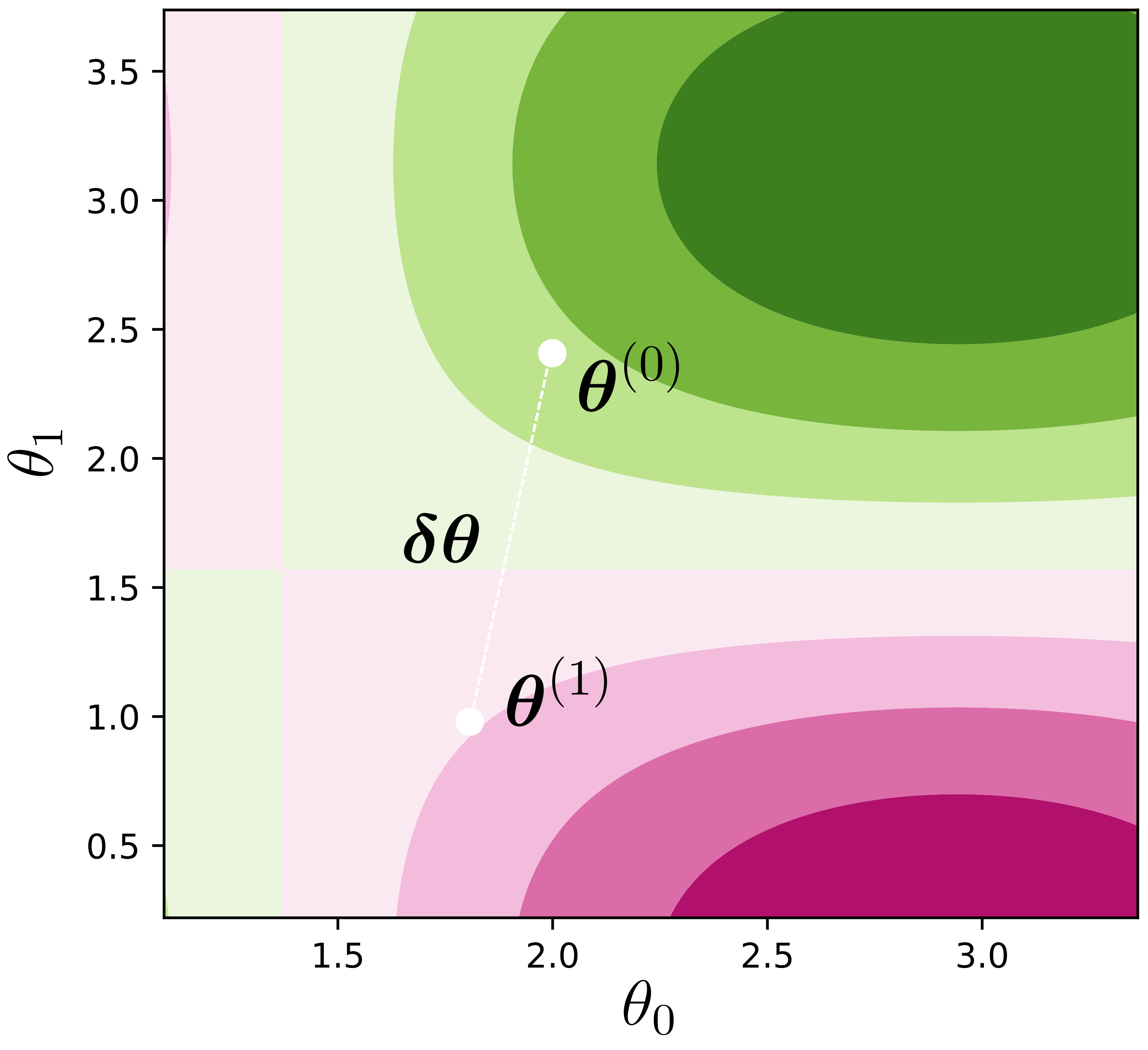
$$\frac{\partial |\psi(t)\rangle}{\partial t} = (E_t - H)\,|\psi(t)\rangle$$

Quantum Geometric Tensor – Interpretation

Slightly different notation...

F: fidelity
g: QGT

$$\ell(\boldsymbol{\theta}) = \langle\phi(\boldsymbol{\theta})|H|\phi(\boldsymbol{\theta})\rangle$$



What's the *distance* of the parameters?

Model-independent measure:

$$\left\|\boldsymbol{\theta}^{(0)} - \boldsymbol{\theta}^{(1)}\right\|_2$$

Model-aware measure:

$$F(\boldsymbol{\theta}^{(0)}, \boldsymbol{\theta}^{(1)}) = \left|\langle\phi(\boldsymbol{\theta}^{(0)})|\phi(\boldsymbol{\theta}^{(1)})\rangle\right|^2$$

For $\boldsymbol{\delta\theta}$ → 0, we can Taylor expand the fidelity

$$F(\boldsymbol{\theta}, \boldsymbol{\theta}+\boldsymbol{\delta\theta}) = \underbrace{F(\boldsymbol{\theta}, \boldsymbol{\theta})}_{1} + \boldsymbol{\delta\theta}^\top \underbrace{\nabla_{\boldsymbol{\theta}} F(\boldsymbol{\theta}, \boldsymbol{\theta}')}_{0}\Big|_{\boldsymbol{\theta}'=\boldsymbol{\theta}} + \frac{\boldsymbol{\delta\theta}^\top \overbrace{\nabla\nabla_{\boldsymbol{\theta}}^\top F(\boldsymbol{\theta}, \boldsymbol{\theta}')}^{-2g(\boldsymbol{\theta})}\boldsymbol{\delta\theta}}{2}\Bigg|_{\boldsymbol{\theta}'=\boldsymbol{\theta}} + \mathcal{O}(\|\boldsymbol{\delta\theta}\|_2^3)$$

$$= 1 - \boldsymbol{\delta\theta}^\top g(\boldsymbol{\theta})\boldsymbol{\delta\theta} + \mathcal{O}(\|\boldsymbol{\delta\theta}\|_2^3)$$

➡ the QGT captures the *local model sensitivity to parameter changes*

Fisher Information in Noisy Intermediate-Scale Quantum Applications, J. J. Meyer, 2021

Numerical Solution to ODE

Variational Quantum Time Evolution (VarQTE)
➔ Ordinary Differential Equation (ODE)

Initial value problem (IVP)

$$\dot{\boldsymbol{\omega}}(t) = f\left(t, \boldsymbol{\omega}(t)\right)$$

VarQRTE

$$f_{\text{std}}\left(\boldsymbol{\omega}\right) = \left(\mathcal{F}^{Q}\right)^{-1} \text{Im}\left(\boldsymbol{C} - \frac{\partial \langle \psi_t^{\omega} |}{\partial \boldsymbol{\omega}} | \psi_t^{\omega} \rangle E_t^{\omega}\right)$$

VarQITE

$$f_{\text{std}}\left(\boldsymbol{\omega}\right) = -\left(\mathcal{F}^{Q}\right)^{-1} \text{Re}\left(C_i\right)$$

State evolution → Parameter evolution

Residual Errors

Quantum Real Time Evolution

$$\||e_t\rangle\|_2 = \left\|\left(i\frac{\partial}{\partial t} - H\right)|\psi_{\boldsymbol{\omega}}(t)\rangle\right\|_2$$

$$H = \sum_i \theta_i h_i$$

Quantum Imaginary Time Evolution

Variational Ansatz

$$|\psi_{\boldsymbol{\omega}}(t)\rangle = U\big(\omega(t)\big)|0\rangle$$

$$\||e_t\rangle\|_2 = \left\|\left(\frac{\partial}{\partial t} + H - E_t\right)|\psi_{\boldsymbol{\omega}}(t)\rangle\right\|_2$$

Derivation for the VarQRTE Error Bound

Let's move to the blackboard

Residual Errors

$$H = \sum_i \theta_i h_i$$

Variational Ansatz

$$|\psi_{\boldsymbol{\omega}}(t)\rangle = U\big(\omega(t)\big)|0\rangle$$

Quantum Real Time Evolution

$$\||e_t\rangle\|_2 = \left\|\left(i\frac{\partial}{\partial t} - H\right)|\psi_{\boldsymbol{\omega}}(t)\rangle\right\|_2$$

$$\||e_t\rangle\|_2{}^2 = \sum_i \sum_j \dot{\omega}_i\, \dot{\omega}_j F_{ij}^Q - 2\sum_i \dot{\omega}_i\, Im\left(C_i - \frac{\partial\langle\psi_{\boldsymbol{\omega}}(t)|}{\partial\omega_i}|\psi_{\boldsymbol{\omega}}(t)\rangle E_t\right) + \mathrm{Var}(H)_t$$

Quantum Imaginary Time Evolution

$$\||e_t\rangle\|_2 = \left\|\left(\frac{\partial}{\partial t} + H - E_t\right)|\psi_{\boldsymbol{\omega}}(t)\rangle\right\|_2$$

$$\||e_t\rangle\|_2{}^2 = \sum_i \sum_j \dot{\omega}_i\, \dot{\omega}_j F_{ij}^Q + 2\sum_i \dot{\omega}_i\, Re(C_i) + \mathrm{Var}(H)_t$$

$$\mathrm{Var}(H)_t = \langle\psi_{\boldsymbol{\omega}}(t)|H^2|\psi_{\boldsymbol{\omega}}(t)\rangle - \langle\psi_{\boldsymbol{\omega}}(t)|H|\psi_{\boldsymbol{\omega}}(t)\rangle^2$$

Numerical Solution to ODE

VarQTE given as an Ordinary Differential Equation (ODE)

Initial value problem (IVP)

$$\dot{\boldsymbol{\omega}}(t) = f(t, \boldsymbol{\omega}(t))$$

VarQRTE

$$f_{\text{std}}(\boldsymbol{\omega}) = \left(\mathcal{F}^{Q}\right)^{-1} \operatorname{Im}\left(\boldsymbol{C} - \frac{\partial \langle \psi_t^{\omega} |}{\partial \boldsymbol{\omega}} |\psi_t^{\omega}\rangle E_t^{\omega}\right)$$

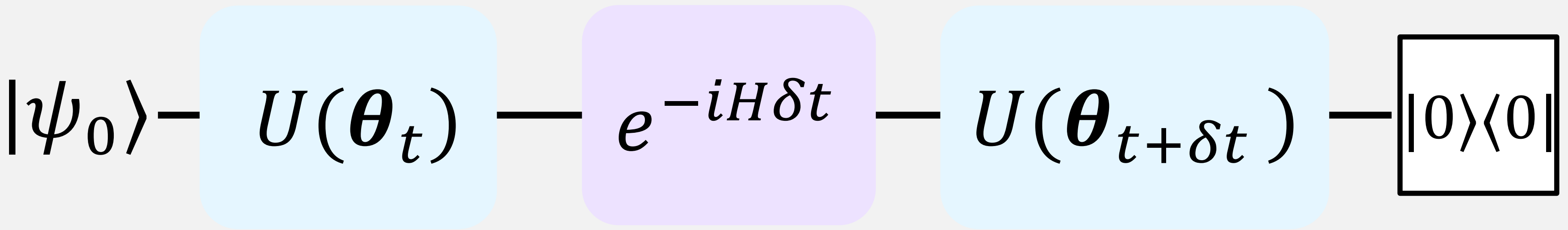
VarQITE

$$f_{\text{std}}(\boldsymbol{\omega}) = -\left(\mathcal{F}^{Q}\right)^{-1} \operatorname{Re}(C_i)$$

$$f_{\min}(\boldsymbol{\omega}) = \underset{\dot{\boldsymbol{\omega}} \in \mathbb{R}^{k+1}}{\operatorname{argmin}} \| \, |e_t\rangle \, \|_2^2$$

Alternative Variational Quantum Time Evolution Methods

Projected Variational Quantum Dynamics [1] *(pVQD)*



$$\min_{\boldsymbol{\theta}_{t+\delta t}} 1 - \left|\langle\psi(\boldsymbol{\theta}_{t+\delta t})\right| e^{-iH\delta t} \left|\psi(\boldsymbol{\theta}_t)\rangle\right|$$

$$|\psi(\boldsymbol{\theta}_t)\rangle = U(\boldsymbol{\theta}_t)|\psi_0\rangle$$
$$|\psi(\boldsymbol{\theta}_{t+\delta t})\rangle = U(\boldsymbol{\theta}_{t+\delta t})|\psi_0\rangle$$

For $\boldsymbol{\delta t} \rightarrow \mathbf{0}$ pVQD is equivalent to VarQRTE

Variational & Trotterized Imaginary Time Evolution [2]

Geometric k-local $H = \sum_i \theta_i h_i$

$$e^{-\beta H} = \left(e^{-\Delta\tau\theta_0 h_0} e^{-\Delta\tau\theta_1 h_1} \ldots\right)^{\frac{\beta}{\Delta\tau}} + \mathcal{O}(\Delta\tau)$$

After a single Trotter step

$$|\psi'\rangle = e^{-\Delta\tau\theta_m h_m}|\psi\rangle$$

Unitary approximation

$$|\widetilde{\psi'}\rangle = \frac{|\psi'\rangle}{\||\psi'\rangle\|} \approx e^{-i\Delta\tau A_m}|\psi\rangle, \qquad A_m = \sum_i a_m^i \sigma_i$$

$$\min \||\psi'\rangle - (1 - i\Delta\tau i\Delta\tau A_m)|\psi\rangle\|_2$$

$$S a_m = b$$

$$S_{k,l} = \langle\psi|\sigma_k\sigma_l|\psi\rangle \quad b_k = \frac{-i}{\sqrt{c}}\langle\psi|\sigma_k h_m|\psi\rangle$$

$$c = 1 - 2\Delta\tau\langle\psi|h_m|\psi\rangle + \mathcal{O}(\Delta\tau^2)$$

Complexity

Number of measurements for a single time:

$\mathcal{O}\left(e^{C^d}\right)$ with C correlation length, d: domain size

[1] An efficient quantum algorithm for the time evolution of parameterized circuits, Stefano Barison, et al. 2021
[2] Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution, M. Motta, et al. 2020

Now back to VarQTE…

How can we verify the preparation accuracy?

Bures Metric

Target state

$$|\psi^*(t)\rangle$$
$$\rho^*(t) = |\psi^*(t)\rangle\langle\psi^*(t)|$$

Prepared variational state

$$|\psi(t)\rangle$$
$$\rho(t) = |\psi(t)\rangle\langle\psi(t)|$$

Fidelity ⟶ $F\big(\rho^*(t), \rho(t)\big) = |\langle\psi(t)|\psi^*(t)\rangle|^2$

$$B\big(\rho^*(t), \rho(t)\big) = \sqrt{2 - 2\sqrt{F\big(\rho^*(t), \rho(t)\big)}} \leq \epsilon_t$$

Further

$$B\big(\rho^*(t), \rho(t)\big) = \min_\phi \left\| |\psi^*(t)\rangle - e^{i\phi}|\psi(t)\rangle \right\|_2$$

If $\epsilon_t^2 \in [0, 2]$ ➔ $F\big(\rho^*(t), \rho(t)\big) \geq \left(1 - \frac{\epsilon_t^2}{2}\right)^2$

➔ Global phase independent

Errors

Target state

$$|\psi^*(t)\rangle$$
$$\rho^*(t) = |\psi^*(t)\rangle\langle\psi^*(t)|$$

Exact variational state

$$|\psi'(t)\rangle$$
$$\rho'(t) = \left|\psi'^{(t)}\right\rangle\langle\psi'(t)|$$

Prepared variational state

$$|\psi_{\boldsymbol{\omega}}(t)\rangle$$
$$\rho_{\boldsymbol{\omega}}(t) = |\psi_{\boldsymbol{\omega}}(t)\rangle\langle\psi_{\boldsymbol{\omega}}(t)|$$

What we want

$$B\big(\rho^*(t), \rho_{\boldsymbol{\omega}}(t)\big) \leq \epsilon_t$$

$$B\big(\rho^*(t), \rho_{\boldsymbol{\omega}}(t)\big) \leq \underbrace{B\big(\rho^*(t), \rho'(t)\big)}_{\text{Error due to variational approximation}} + \underbrace{B\big(\rho'(t), \rho_{\boldsymbol{\omega}}(t)\big)}_{\text{Error due to numerical ODE solution}}$$

Errors

Target state

$$|\psi^*(t)\rangle$$
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Exact variational state

$$|\psi'(t)\rangle$$
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Error due to variational approximation

Mitigate locally using suitable ODE solvers

VarQTE

Error Bounds

Target state

$$|\psi^*(t)\rangle$$
$$\rho^*(t) = |\psi^*(t)\rangle\langle\psi^*(t)|$$

Prepared variational state

$$|\psi_{\boldsymbol{\omega}}(t)\rangle$$
$$\rho_{\boldsymbol{\omega}}(t) = |\psi_{\boldsymbol{\omega}}(t)\rangle\langle\psi_{\boldsymbol{\omega}}(t)|$$

$$B\big(\rho^*(t), \rho_{\boldsymbol{\omega}}(t)\big) \leq \epsilon_t$$

$$\epsilon_t = \int_{\tau=0}^{t} \| |e_\tau\rangle \|_2 \, d\tau$$

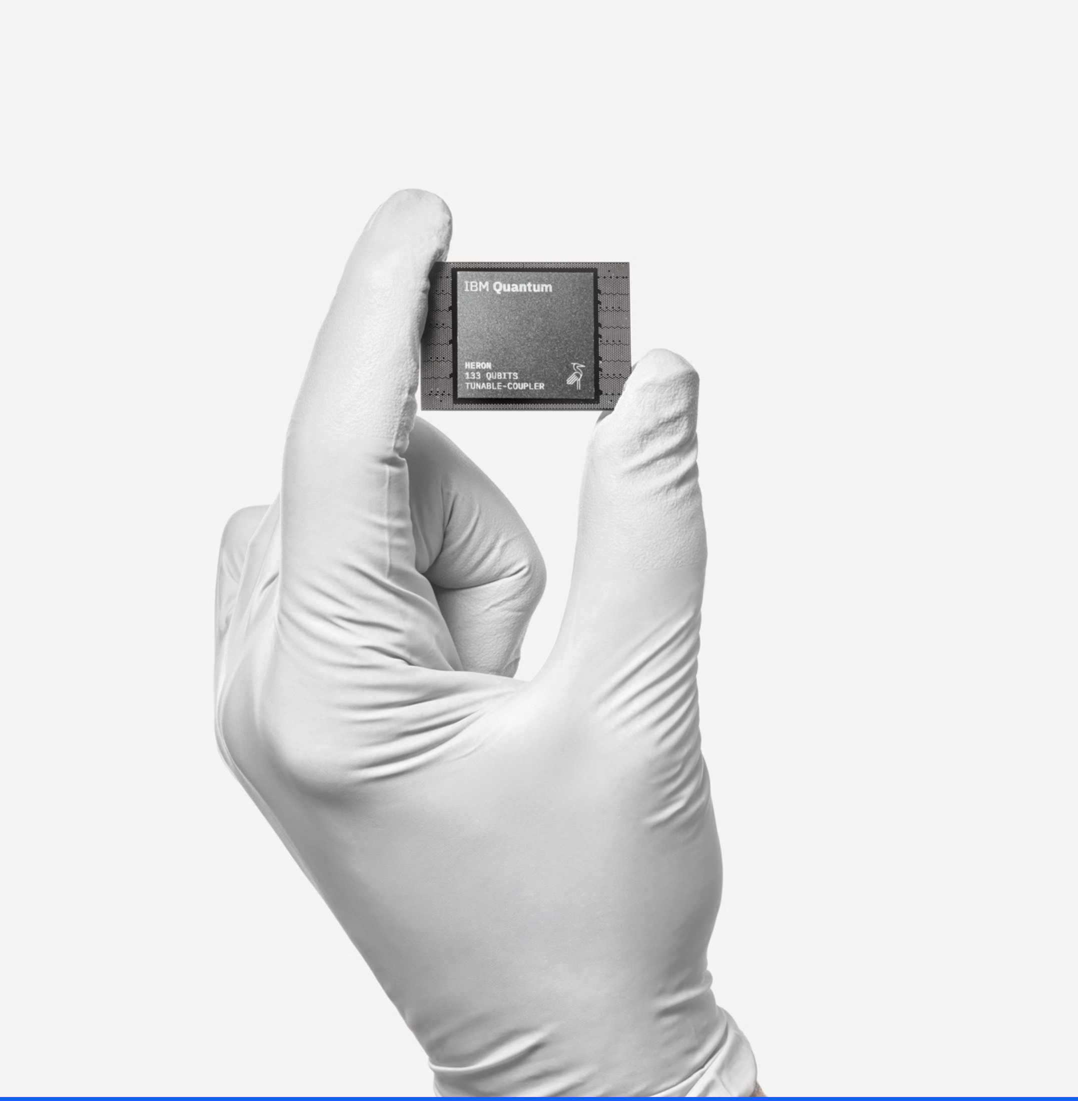
Error Bounds Derivation

Let’s move to the blackboard

What about the ODE implementation?

Solving the IVP

Making the right choices when solving the different components of the system is imperative for a successful VarQTE simulation.



Methods

$$x = g^{-1} b$$

Exact inversion ideally g is always invertible if all parameters are linearly independent → not true for sampled appr

$$min_x \|b - gx\|$$

Least squares → more stable

$$min_x \|b - gx\| + \boldsymbol{\lambda} \|\boldsymbol{f}\|$$

Regularized least squares, e.g., eigenvalue cut-off or ridge → even more stable but possibly unphysical

Solving the Ordinary Differential Equation

Main ODE solvers:

- Euler
- Runge-Kutta

Solving the Ordinary Differential Equation

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- Euler
- Runge-Kutta

Explicit methods: Calculation of update by using the system state at the current time.
Pro: Simple to evaluate
Con: For stiff problems the time steps become impractically small

➔Evolve $\vec{\omega}\,(\tau)$ e.g. with explicit Euler

$$\vec{\omega}\,(\tau) \simeq \vec{\omega}\,(\tau - \delta\tau) + \dot{\vec{\omega}}(\tau - \delta\tau)\delta\tau$$

Solving the Ordinary Differential Equation

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➔Evolve $\vec{\omega}\,(\tau)$ e.g. with explicit Euler

$$\vec{\omega}\,(\tau) \simeq \vec{\omega}\,(\tau - \delta\tau) + \dot{\vec{\omega}}(\tau - \delta\tau)\delta\tau$$

Implicit methods: Calculation of update by using the system state at the current time and for a time that lies in the future of the current time.

Pro: Can improve numerical stability Con: Expensive evaluation

➔Evolve $\vec{\omega}\,(\tau)$ e.g. with implicit Euler

$$\vec{\omega}\,(\tau) \simeq \vec{\omega}\,(\tau - \delta\tau) + \dot{\vec{\omega}}(\tau)\delta\tau$$

VarQRTE

Error Bound

Open chain transverse field Ising model on 3 qubits

$$H = 0.5\left(\sum_{ij} Z_i Z_j - 0.5\sum_i X\right)$$

$$EfficientSU2(3, \text{reps} = 1)$$

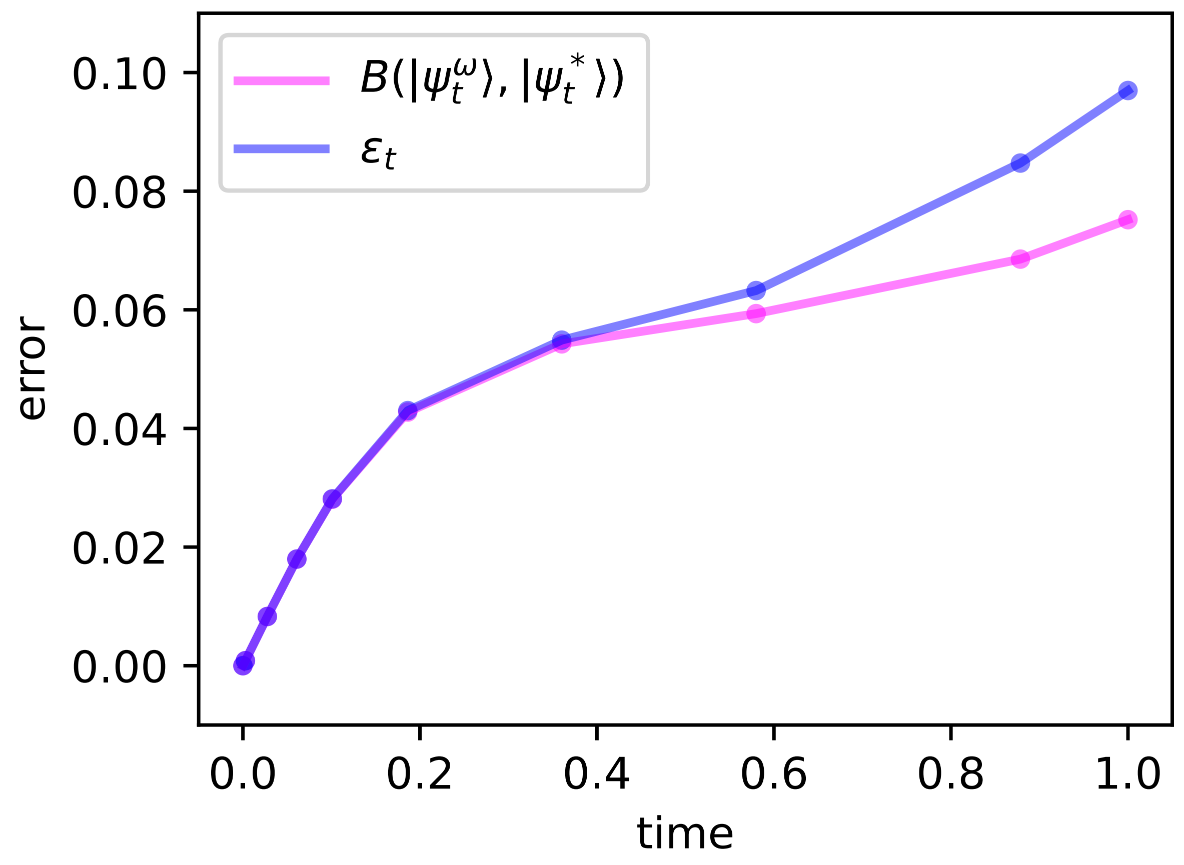
$$t = 1$$

$$|\psi(0)\rangle = e^{-i\gamma}|000\rangle$$

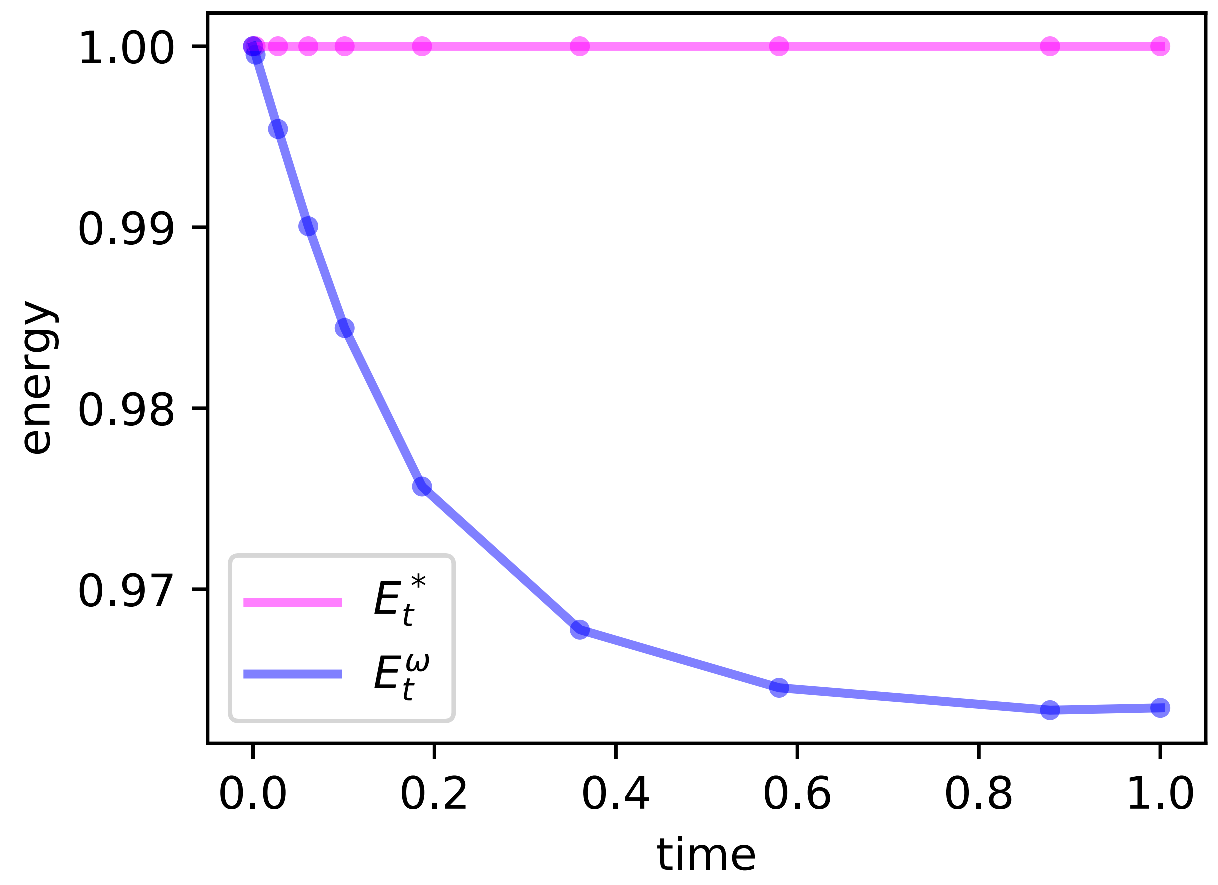
Runge Kutta

f_{std}

State Error



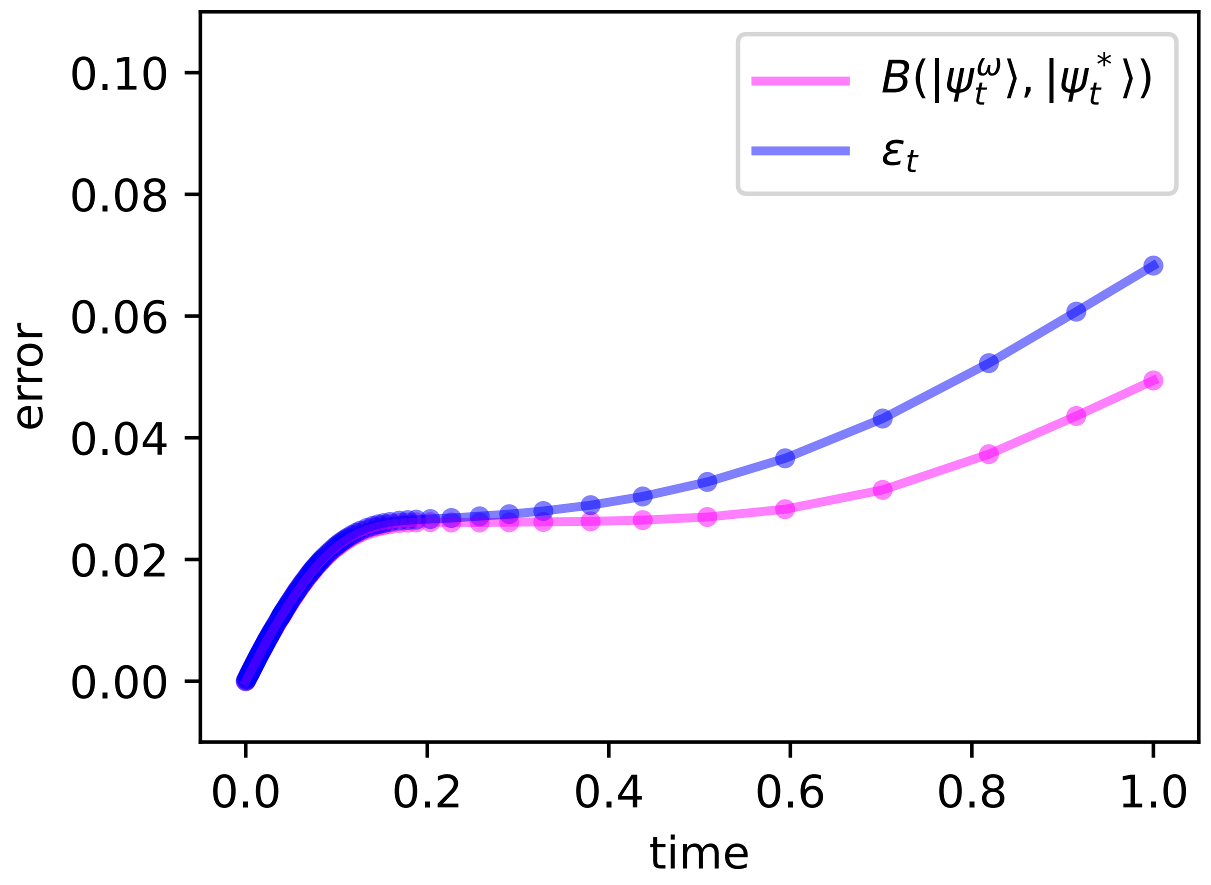
Energy



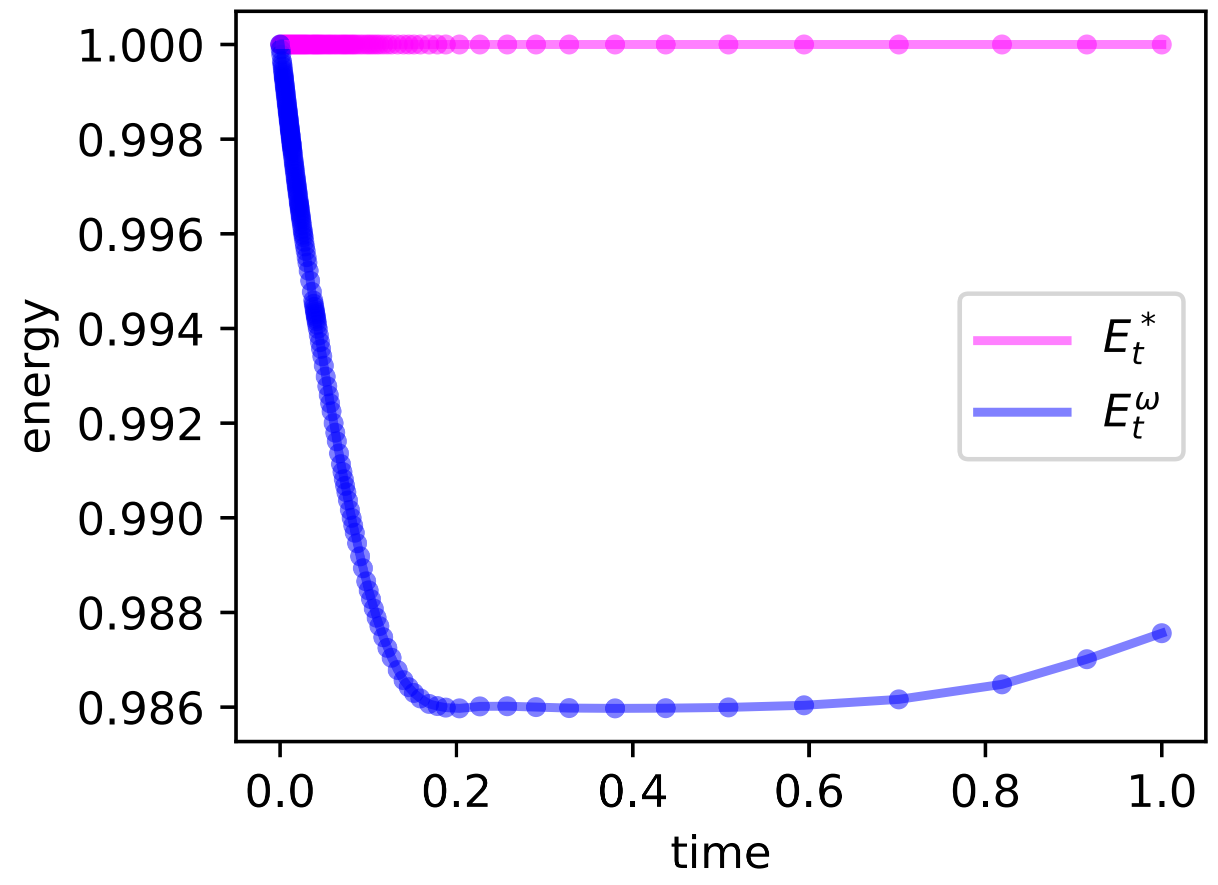
Runge Kutta

f_{res}

State Error



Energy



VarQITE Error Bound

Hydrogen [1]

$$H = 0.2252\ II + 0.5716\ ZZ + 0.3435\ IZ - 0.4347\ ZI + 0.091\ YY + 0.091\ XX$$

$$EfficientSU2(2, reps = 1)$$

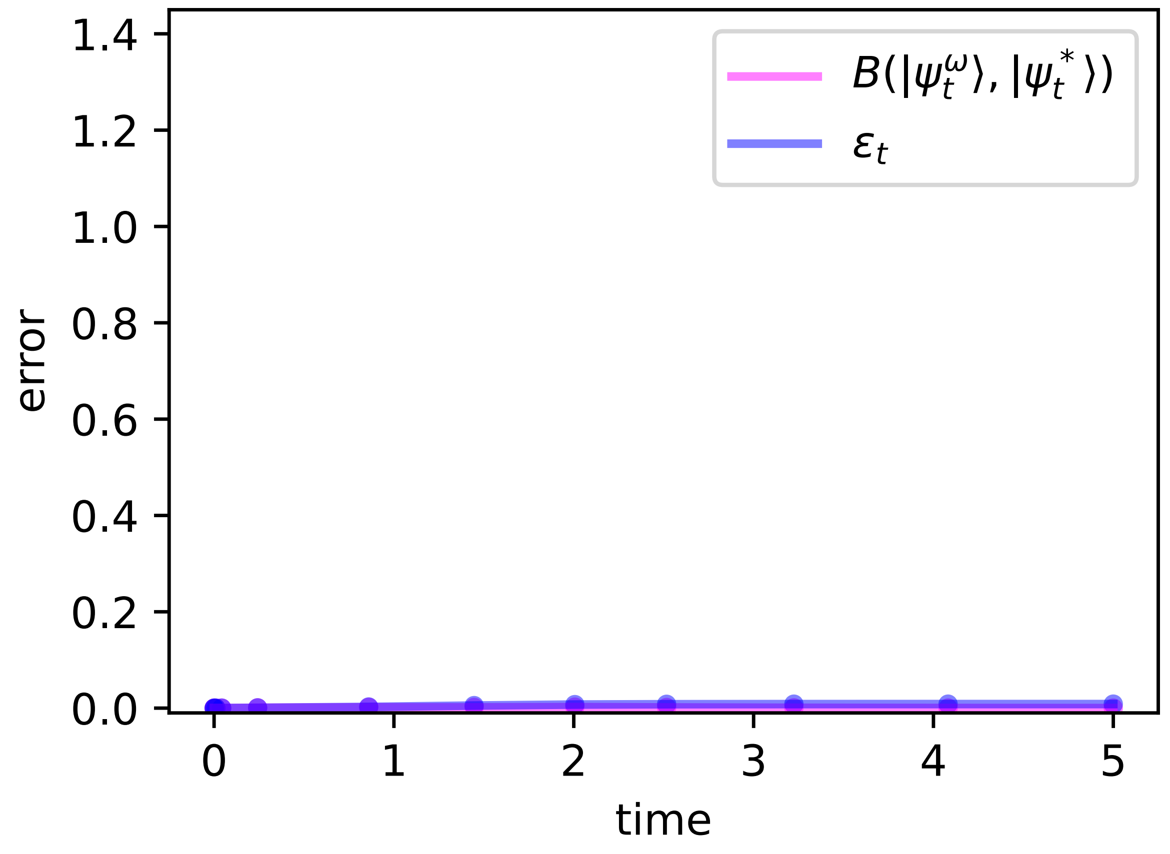
$$t = 1$$

$$|\psi(0)\rangle = |+\rangle \otimes |+\rangle$$

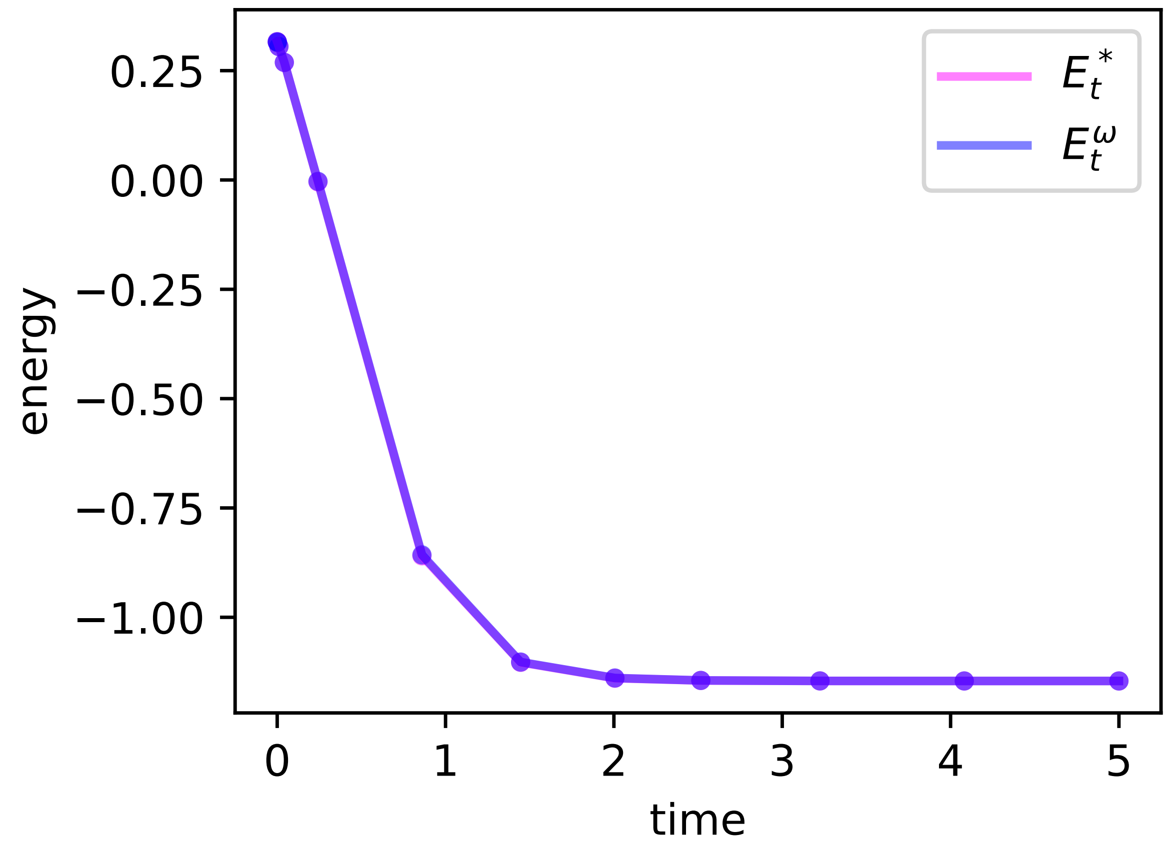
Runge Kutta

f_{std}

State Error



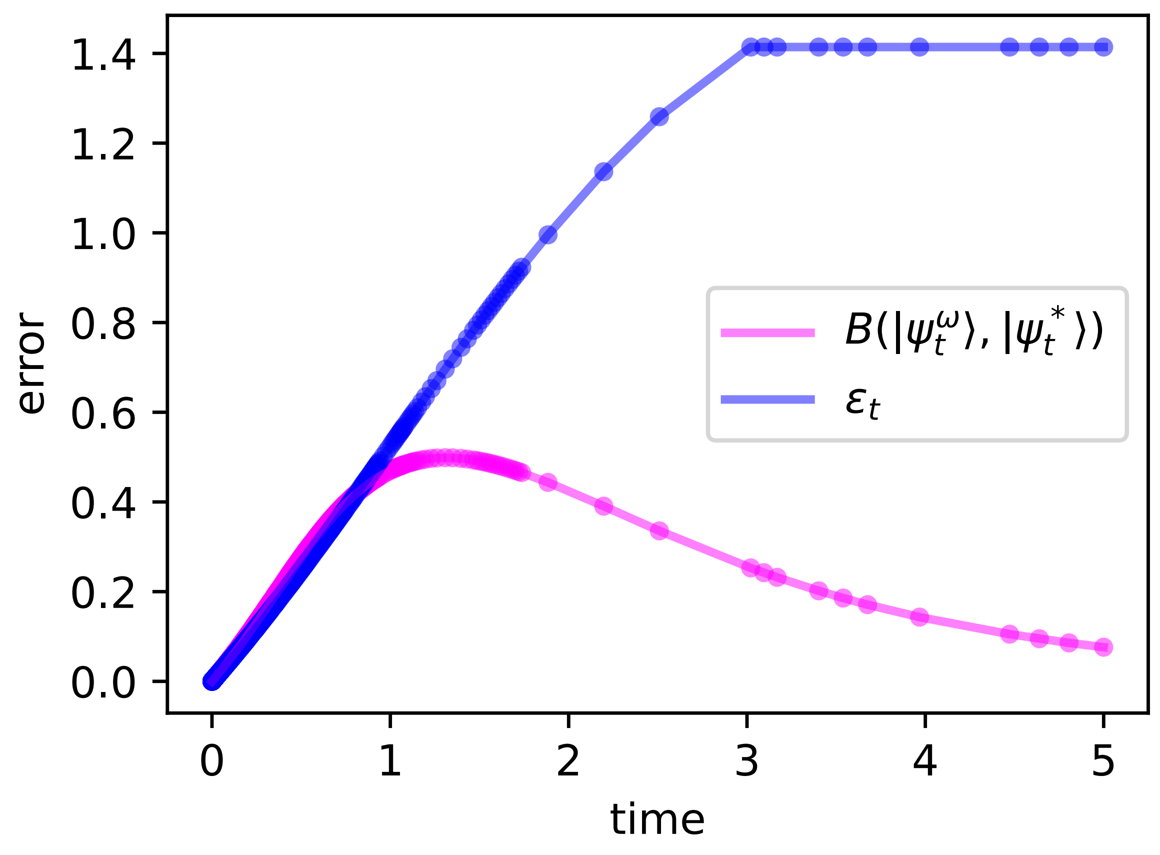
Energy



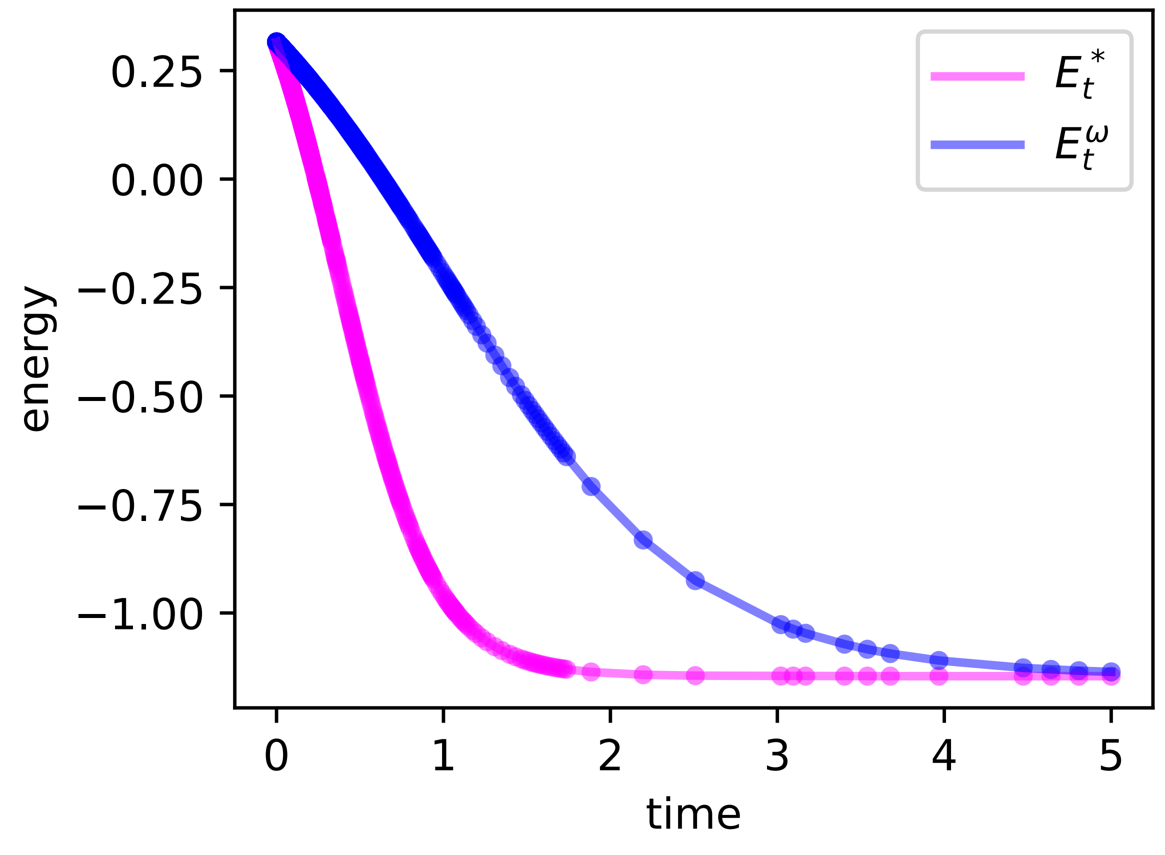
Runge Kutta

f_{err}

State Error



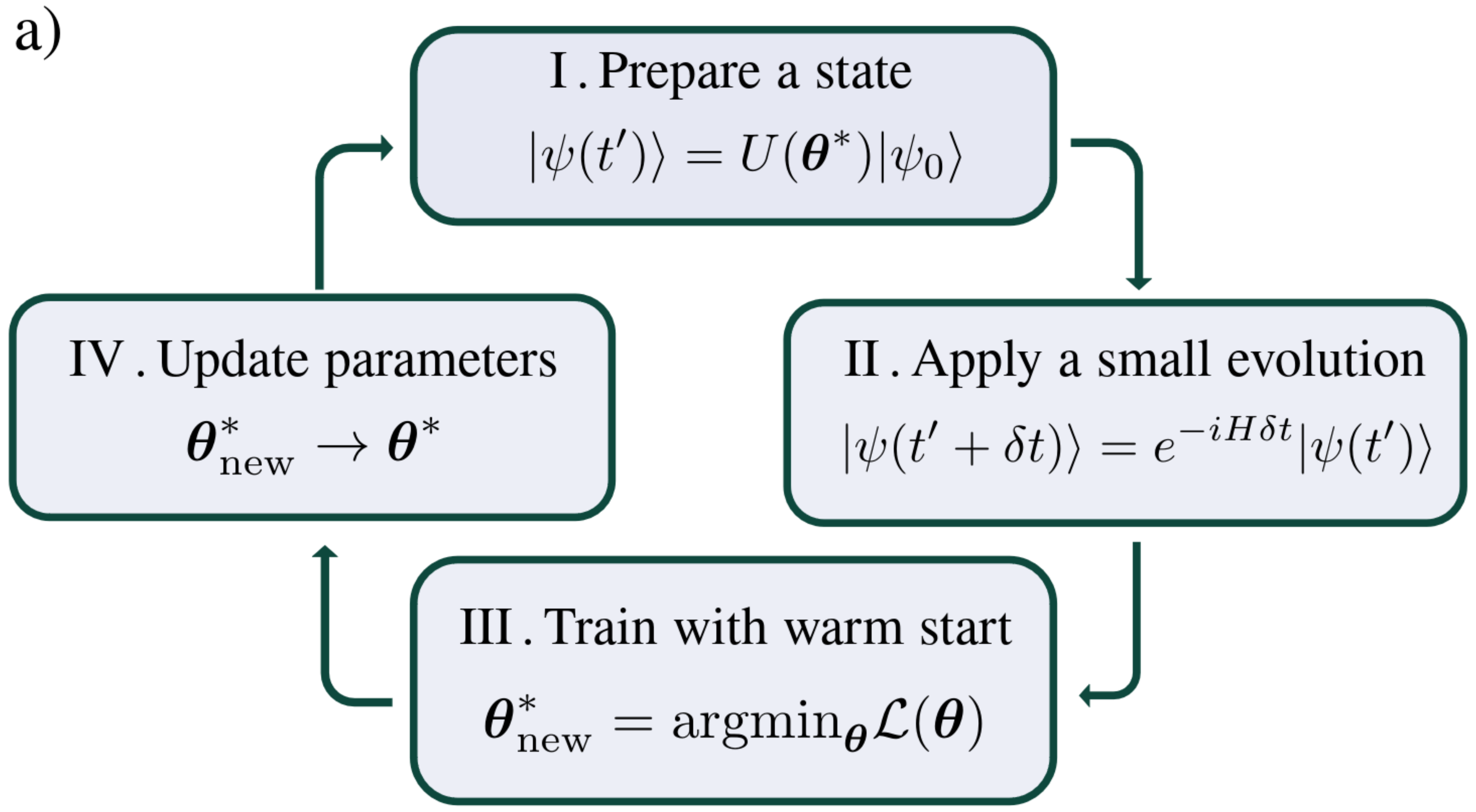
Energy

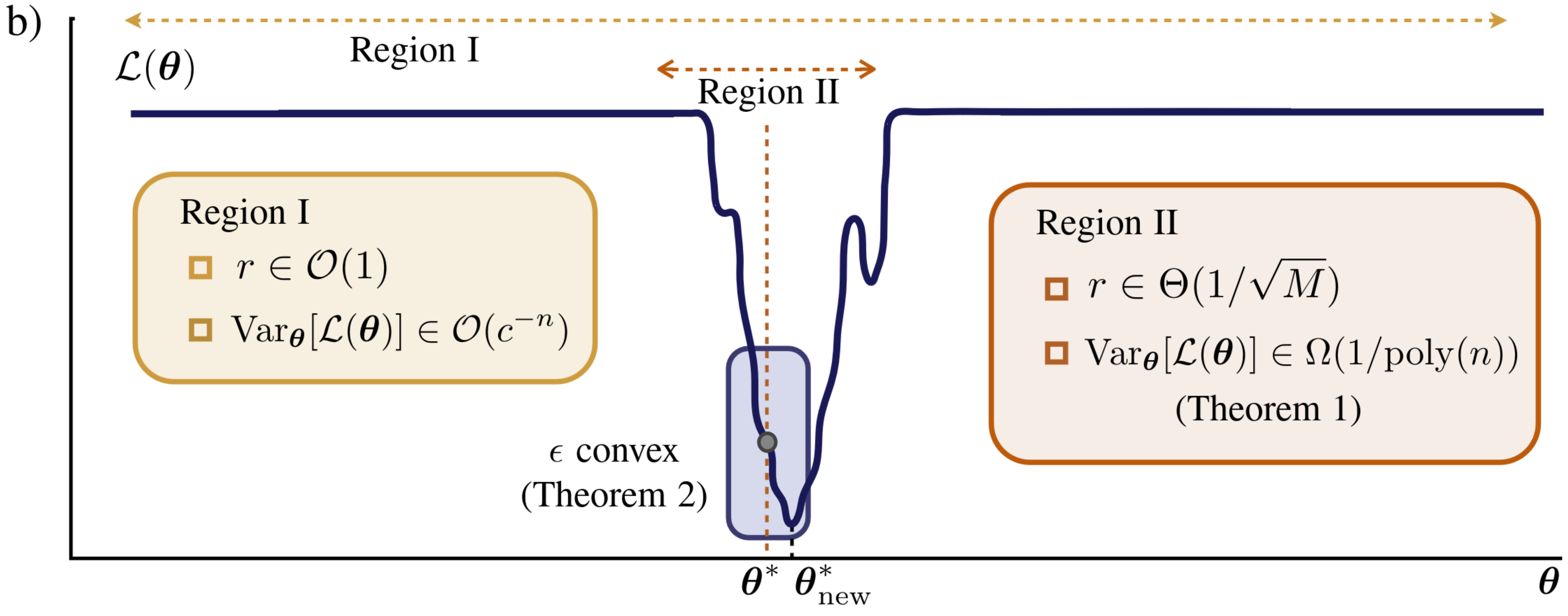


[1] Variational ansatz-based quantum simulation of imaginary time evolution - S. McArdle, et al

What about the trainability?

Trainability of Variational Time Evolution





$$\mathcal{L}(\theta) = 1 - \left|\langle\psi_0\middle|U^\dagger(\boldsymbol{\theta})e^{-iH\delta t}U(\boldsymbol{\theta}^*)\middle|\psi_0\rangle\right|$$

→ In the limit pVQD and VarQTE are equivalent

Conditions sufficed

1. Non-vanishing variance in poly large surrounding region
2. (ϵ-)Convexity guarantees for poly large time steps

Variational quantum simulation: a case study for understanding warm starts, R. Puig-i-Valls, M. Drudis, et al. 2024

Complexity

VarQTE Complexity

$$H = \sum_{i=0}^{m-1} \theta_i h_i$$

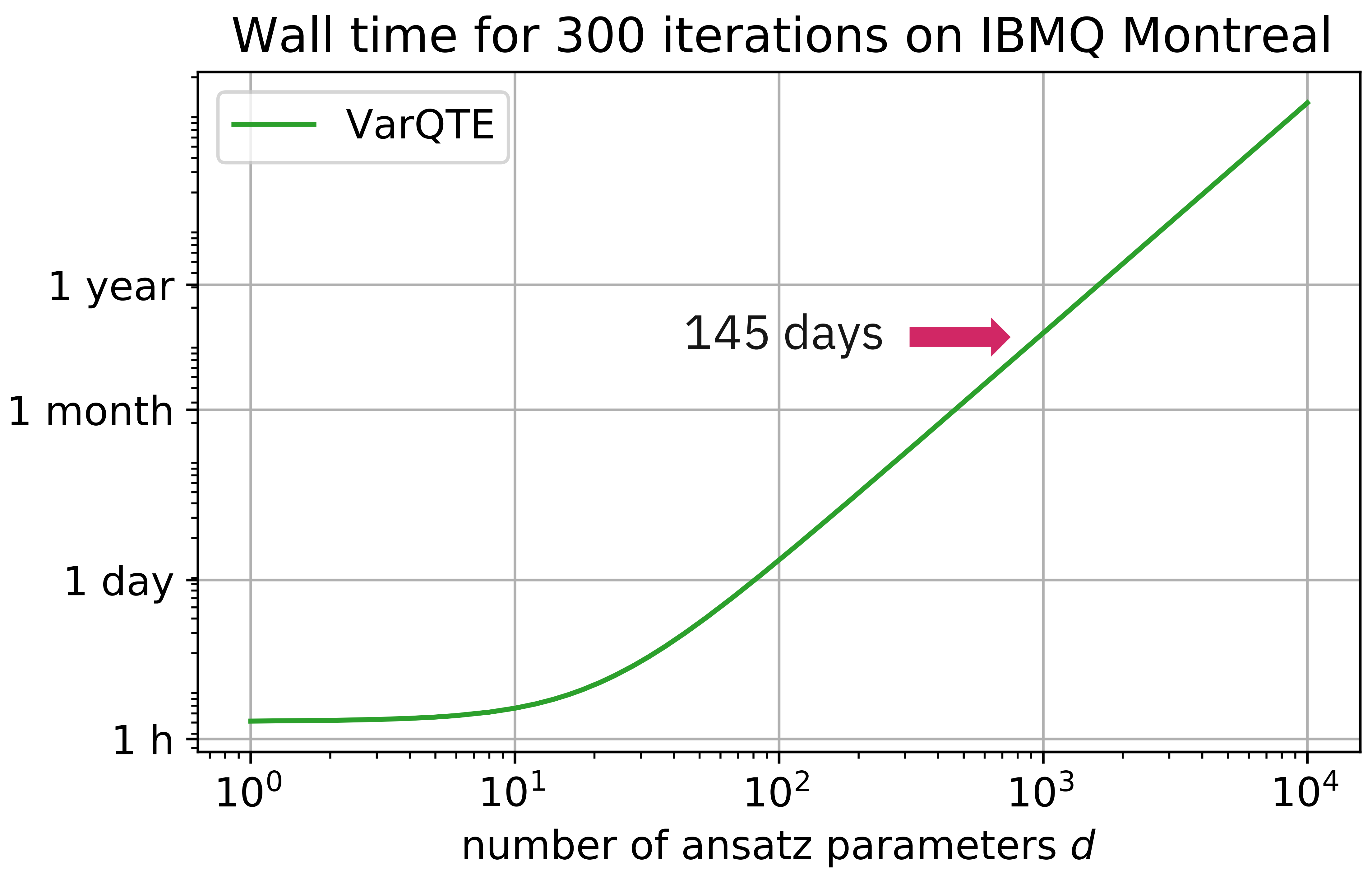
$$\boldsymbol{\omega} \in \mathbb{R}^d$$

Number time steps

Number of expectation values $\mathbf{O}\left(\mathbf{T}\left(\mathbf{md} + \mathbf{d}^2\right)\right)$

$\mathrm{Im}\left(C_i - \frac{\partial\langle\psi_{\boldsymbol{\omega}}(t)|}{\partial\omega_i}|\psi_{\boldsymbol{\omega}}(t)\rangle E_t\right)$ and $\mathrm{Re}(C_i) \in \mathbb{R}^d$

$$F_{ij}^Q = \left(\frac{\partial\langle\psi_{\boldsymbol{\omega}}(t)|}{\partial\omega_i}\frac{\partial|\psi_{\boldsymbol{\omega}}(t)\rangle}{\partial\omega_j} - \frac{\partial\langle\psi_{\boldsymbol{\omega}}(t)|}{\partial\omega_i}|\psi_{\boldsymbol{\omega}}(t)\rangle\langle\psi_{\boldsymbol{\omega}}(t)|\frac{\partial|\psi_{\boldsymbol{\omega}}(t)\rangle}{\partial\omega_j}\right) \in \mathbb{R}^{dxd}$$



IBM Quantum – Christa Zoufal ouf@Zurich.ibm.com

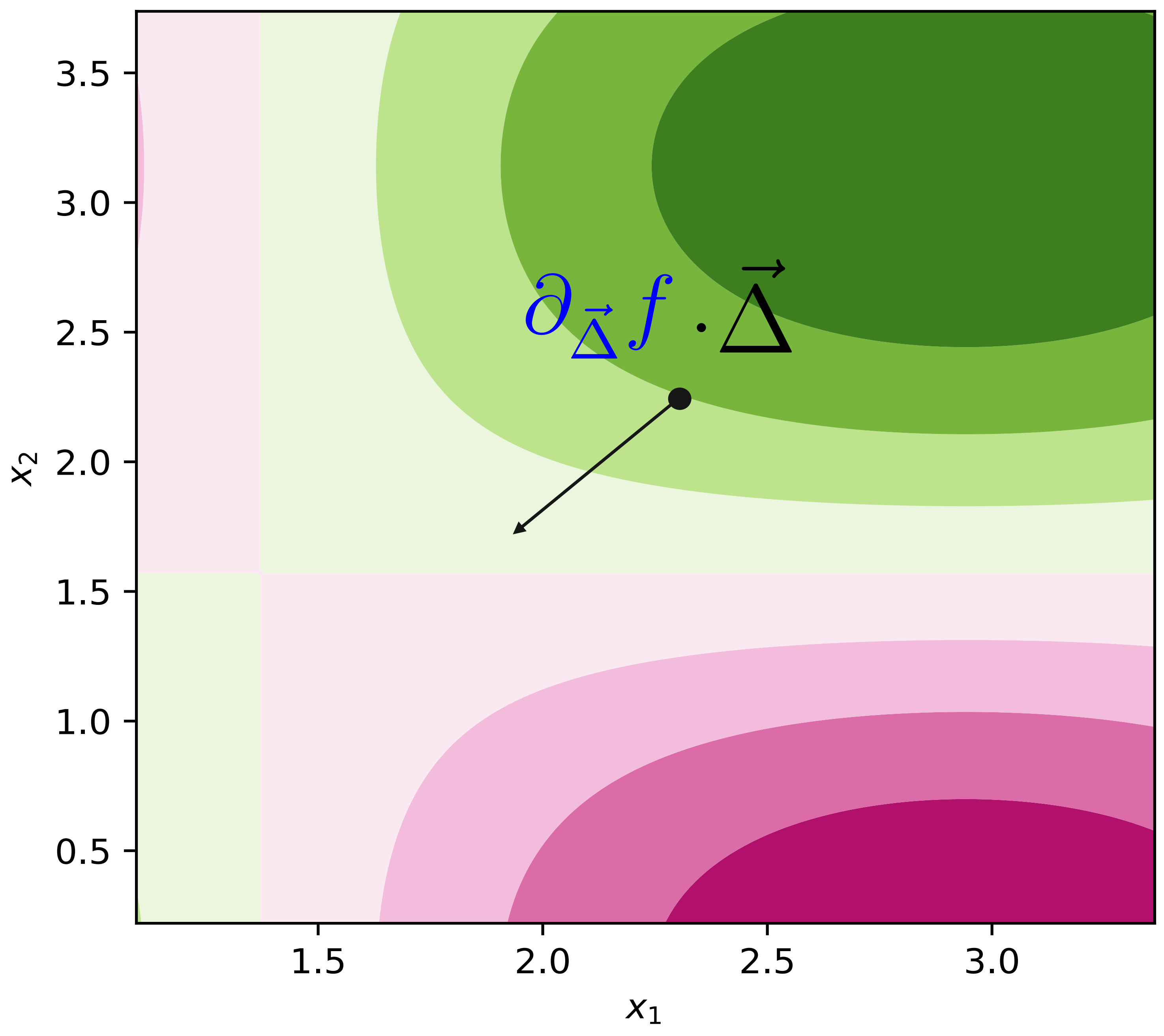
How can we reduce this complexity?

Simultaneous Perturbation Stochastic Approximation (SPSA)

Quantum
the open journal for quantum science

Simultaneous Perturbation Stochastic Approximation of the Quantum Fisher Information

Julien Gacon[1,2], Christa Zoufal[1,3], Giuseppe Carleo[2], and Stefan Woerner[1]



$$\frac{f(\theta + \epsilon\vec{\Delta}) - f(\theta - \epsilon\vec{\Delta})}{2\epsilon}\vec{\Delta} \approx \nabla f(\theta)$$

with $\vec{\Delta} \sim \text{Bernoulli}\{\pm 1\}$

➡ SPSA is (in the limit) an unbiased estimator of the gradient [1]

Note: Does not apply to real time evolution

[1] Spall. IEEE Transactions on Automatic Control 37(3) (1992)

Can we evaluate the QGT via SPSA?

Step 1

Write QGT as Hessian

$$F_{ij}^{Q} = -\frac{1}{2}\partial\omega_i\partial\omega_j \left|\langle\psi(\omega'(t))|\psi(\omega(t))\rangle\right|^2\Big|_{\omega'=\omega}$$

Step 2

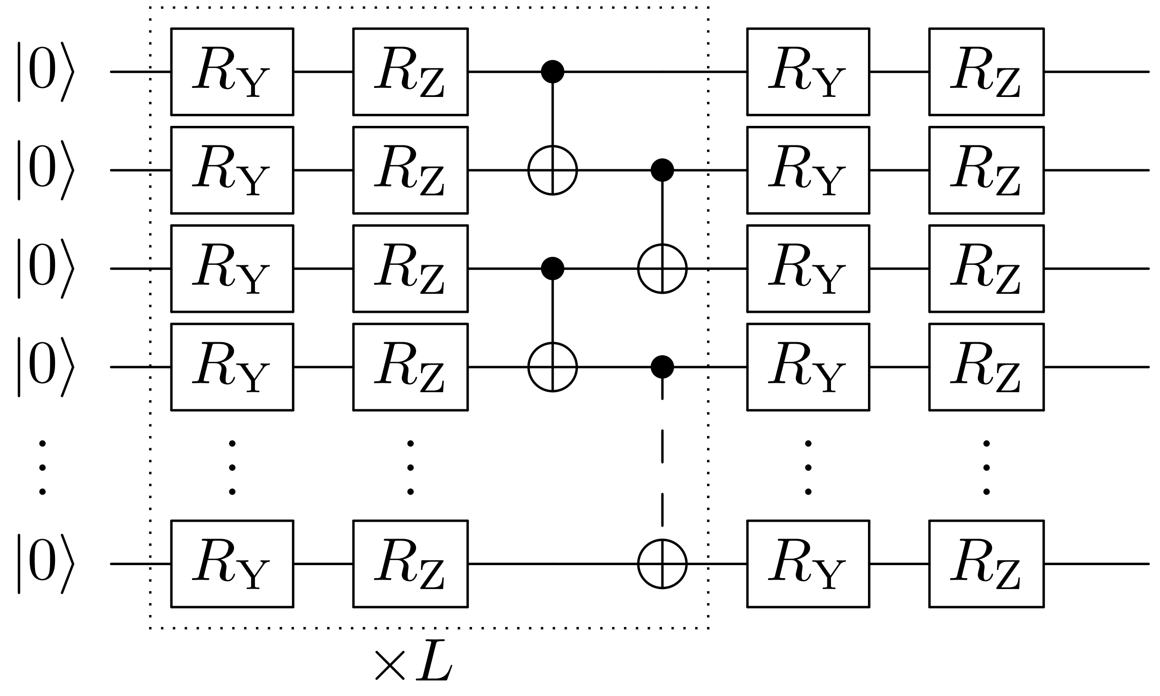
Generalize SPSA for Hessians

Resource reduction

- Ising model with a transversal field $(J = 0.5,\ h = 1)$

$$H = J \sum_{i=1}^{n-1} Z_i Z_{i+1} + h \sum_{i=1}^{n} X_i$$

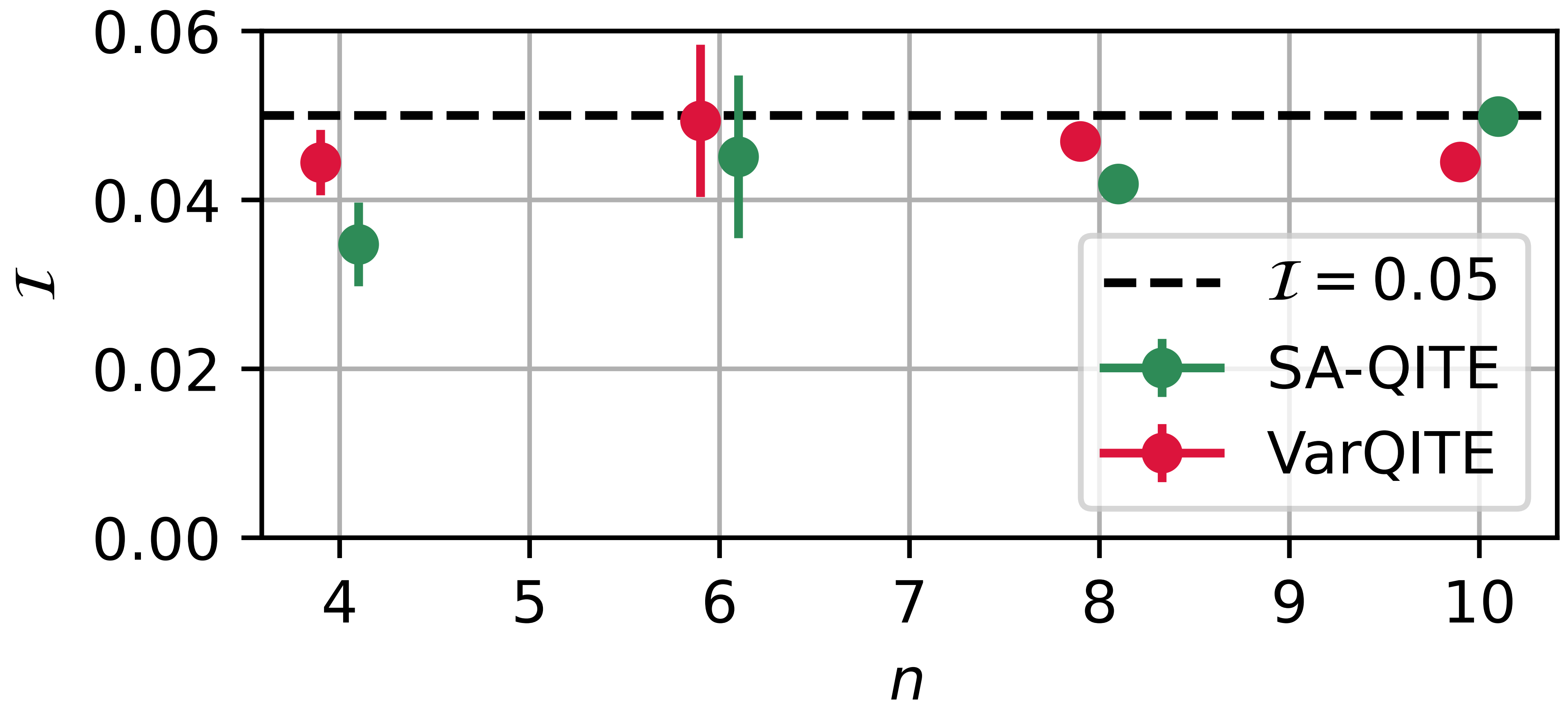
- Hardware-efficient ansatz with $L = \log(n)$

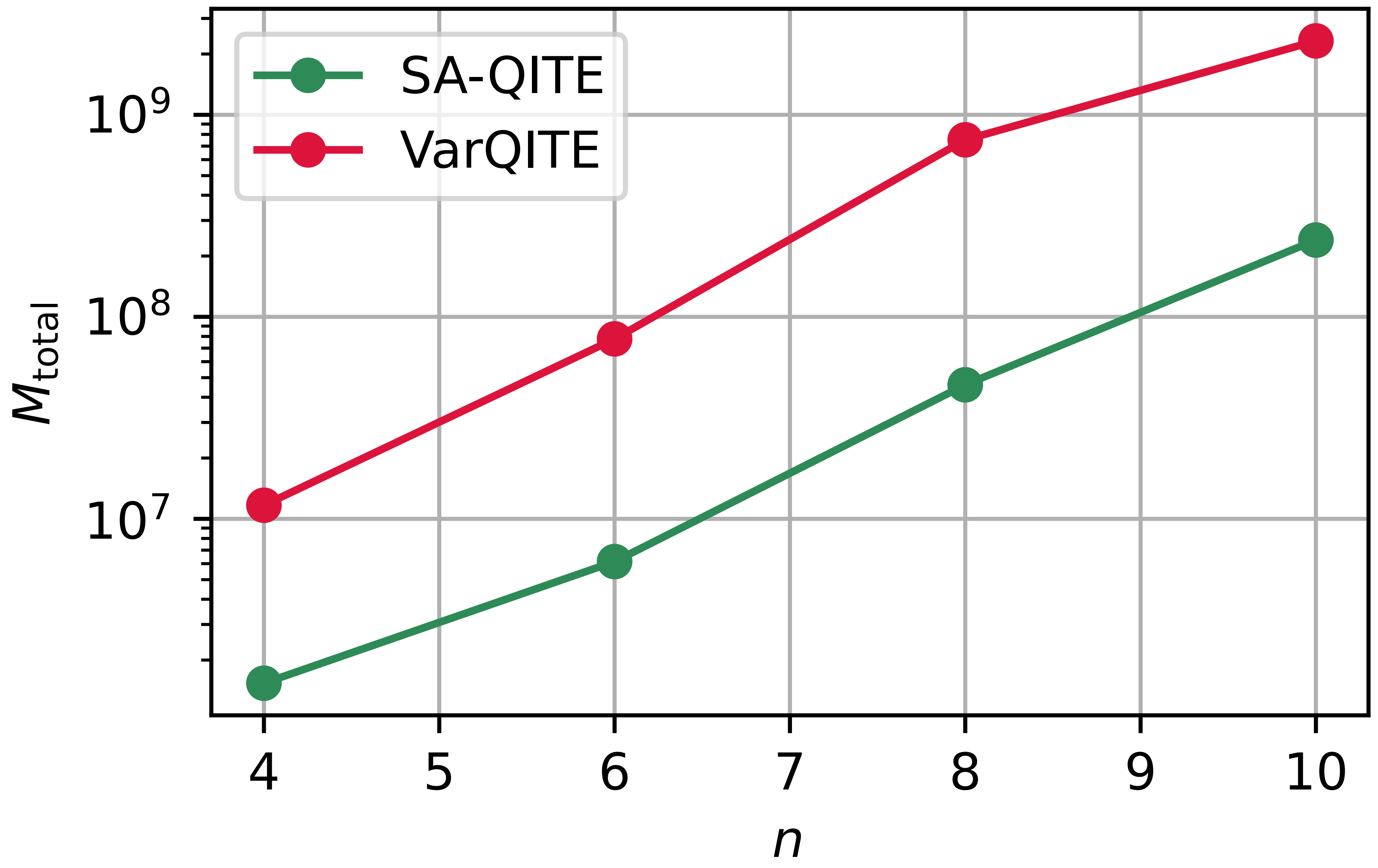


- Measure total number of shots M to achieve $\mathcal{I} \leq 0.05$

$$\mathcal{I} = \frac{1}{T} \int_0^T \left(1 - |\langle \phi(\theta(\tau)) | \psi(\tau) \rangle|^2\right) \mathrm{d}\tau$$

exact solution





10x less samples required

Resource reduction

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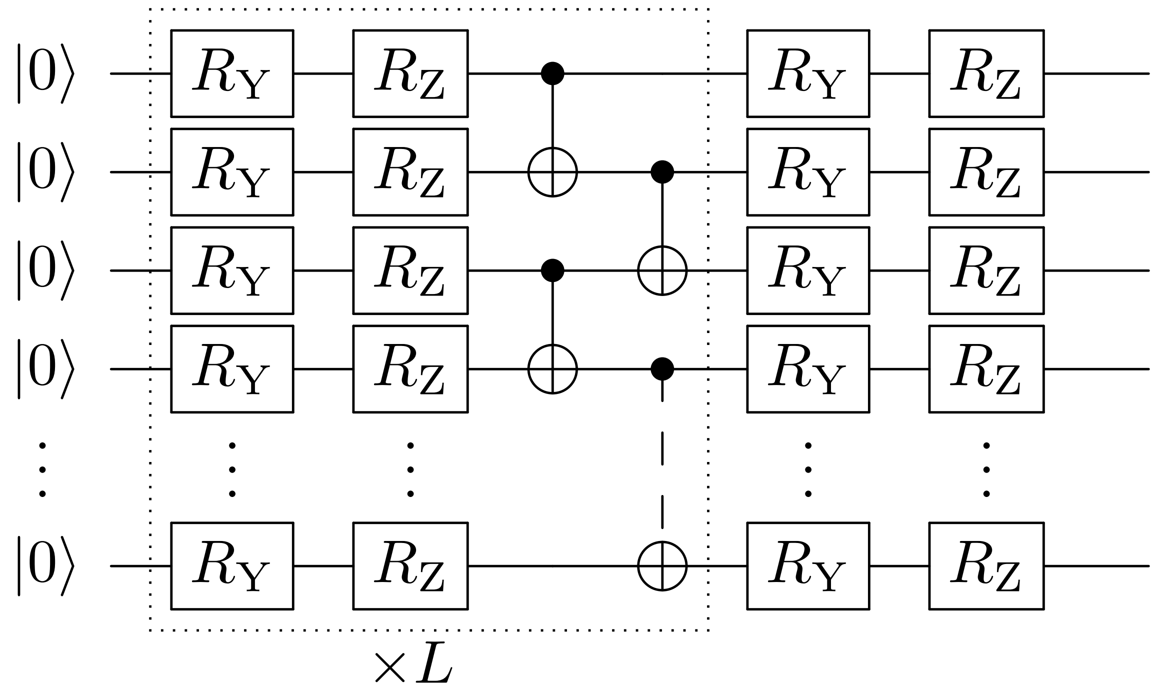

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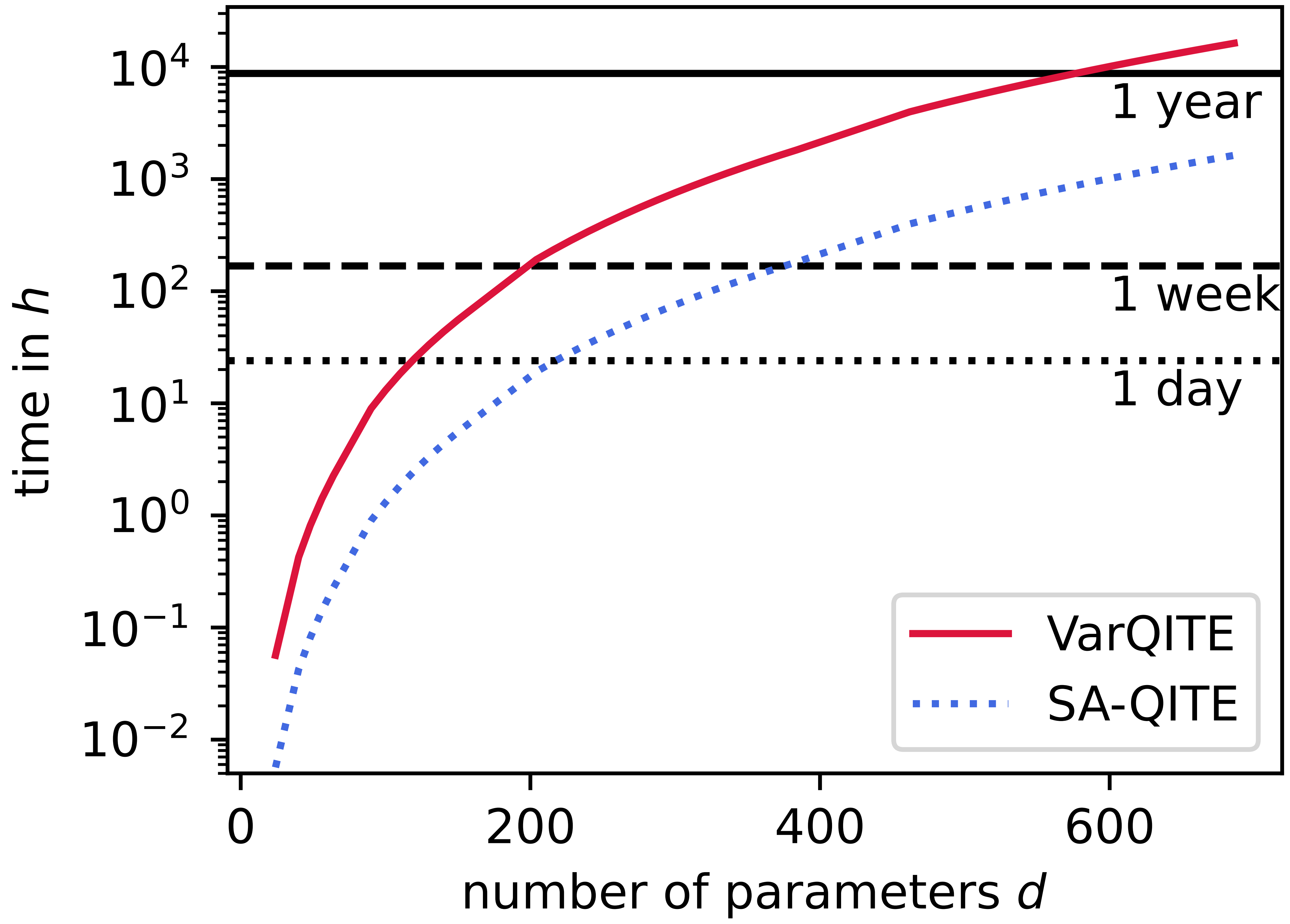


…or we employ classical shadows.

$$\mathrm{Im}\left(C_i - \frac{\partial\langle\psi_\omega(t)|}{\partial\omega_i}|\psi_\omega(t)\rangle E_t\right) \text{ and } \mathrm{Re}(C_i) \in \mathbb{R}^d$$

$$C_i = \frac{\partial\langle\psi_\omega(t)|}{\partial\omega_i} H|\psi_\omega(t)\rangle$$

$$2\mathrm{Re}(C_i) = \frac{\partial E_t}{\partial\omega_i}$$

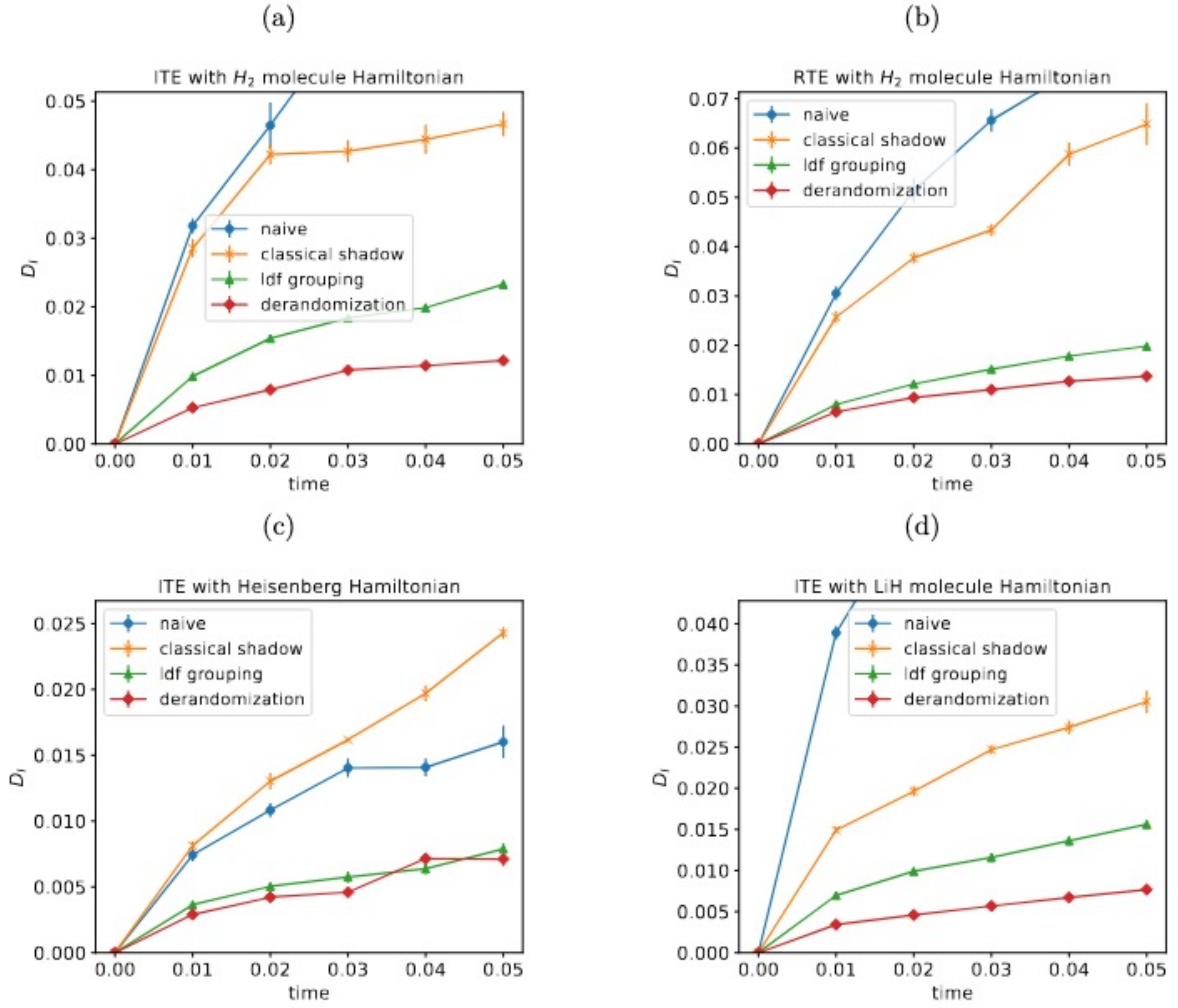
$$E_t = \langle\psi_\omega(t)|H|\psi_\omega(t)\rangle$$

$$H = \sum_i \alpha_i \bigotimes_j \sigma_{ij},\ \sigma_{ij} \in \{I, X, Y, Z\}$$

Shadows

Prediction of M observables with $O(\log M)$ measurements up to additive error

→ Can also help to reduce the impact of shot noise [1]



Credits [1]
The evolutions of the infidelity $D_I(|\psi^{\text{target}}\rangle, |\psi_\omega\rangle)$ for each time step. (a) QITE for H_2, (b) QRTE for H_2, (c) QITE with Heisenberg model Hamiltonian, and (d) ITE with LiH. For a bricklayer HEA with d=4, n=8

Largest degree first (LDF) grouping [2]: smart combination of Pauli terms to reduce number of required measurements
Derandomization [3]: variant of classical shadows which aims at minimizing the confidence bound

[1] Measurement optimization of variational quantum simulation by classical shadow and derandomization, K. Nakaji, S. Endo, Y. Matsuzaki, and H. Hakoshima
[2] Measurement optimization in the variational quantum eigensolver using a minimum clique cover, V. Verteletskyi, T.-C. Yen, and A. F Izmaylov.
[3] Efficient estimation of Pauli observables by derandomization, H.-Y. Huang, R. Kueng, and J. Preskill

Summary

- VarQTE could help to model time dynamics for **non-local** Hamiltonians or **longer times** respectively
- The power of the method strongly relies on
  - Ansatz, ODE solver, IVP model **choice**
  - Shot and hardware **noise**

  } Algorithm and hardware development should go hand in hand
- This will not be a universal solution but it would be great if we could find a relevant system with a good ansatz → possibly better suited for **imaginary dynamics**

Resources

IBM Quantum Platform: https://quantum.ibm.com/
Access to quantum hardware and related information, e.g., about system noise, tutorials, learning platform, etc.

Qiskit Documentation: https://docs.quantum.ibm.com/
How to build a circuit, transpile a circuit, debug, execute with simulators, or hardware, etc.

Qiskit Github: https://github.com/qiskit
Code, building blocks, algorithms, etc.
Special note to: https://github.com/qiskit-community

Thank you for your attention!

A big thank you also goes to my colleagues for all their work!
→ foundation for this lecture

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IBM