Optimization of HEP Quantum Algorithms

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Acknowledgement

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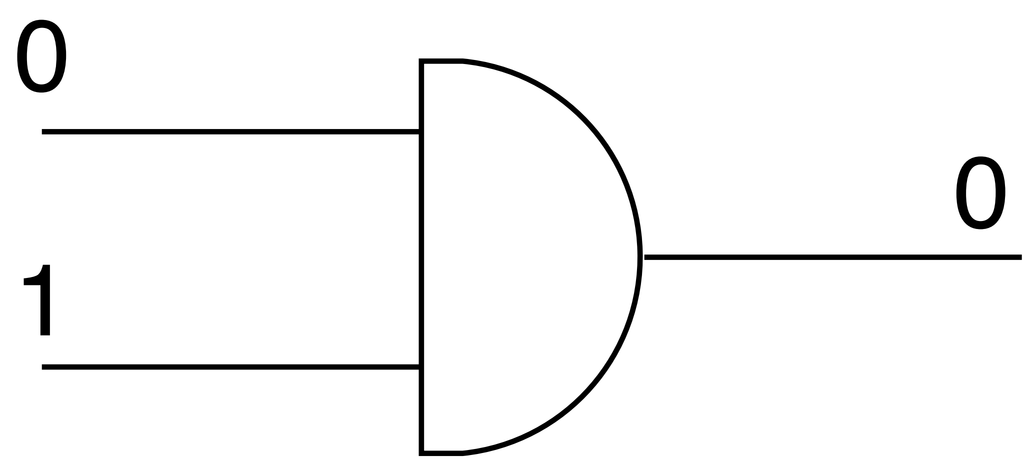
Main theme:
application of quantum computing
to HEP simulation

Quantum computing

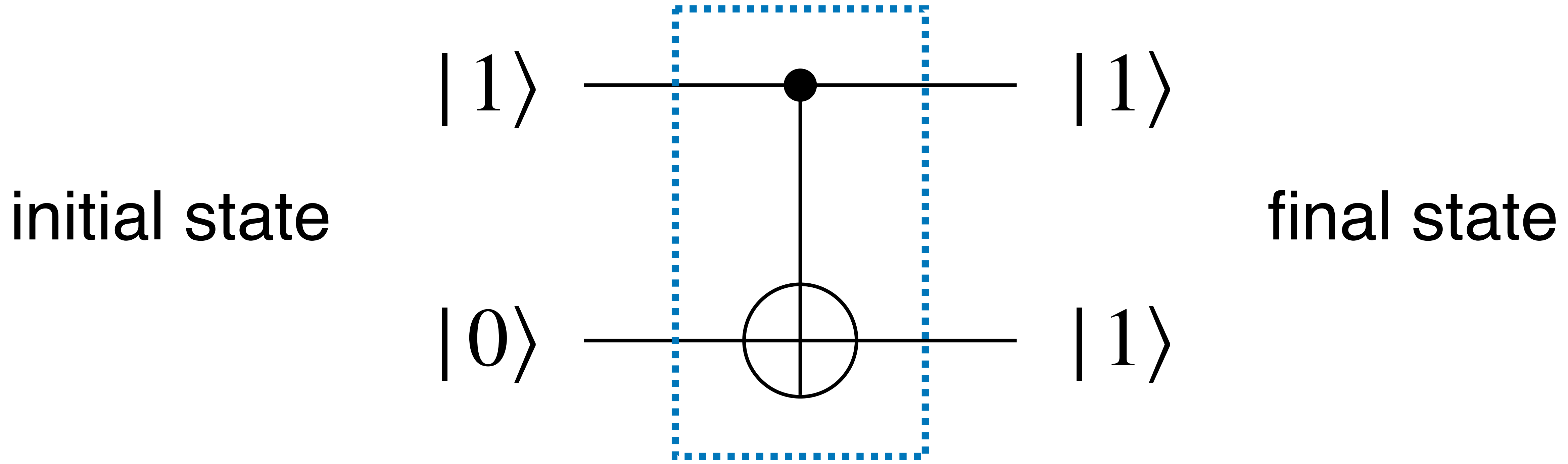
- classical computing
  - classical bit: $s \in \{0,1\}^n$
  - classical operation: $s \mapsto f(s)$

- quantum computing
  - quantum bit (**qubit**):
    $|\psi\rangle = \otimes_i (\alpha_i |0\rangle + \beta_i |1\rangle)$
    → superposition, entanglement
  - unitary operation (**quantum gate**):
    $|\psi\rangle \mapsto U|\psi\rangle$

classical (AND) gate

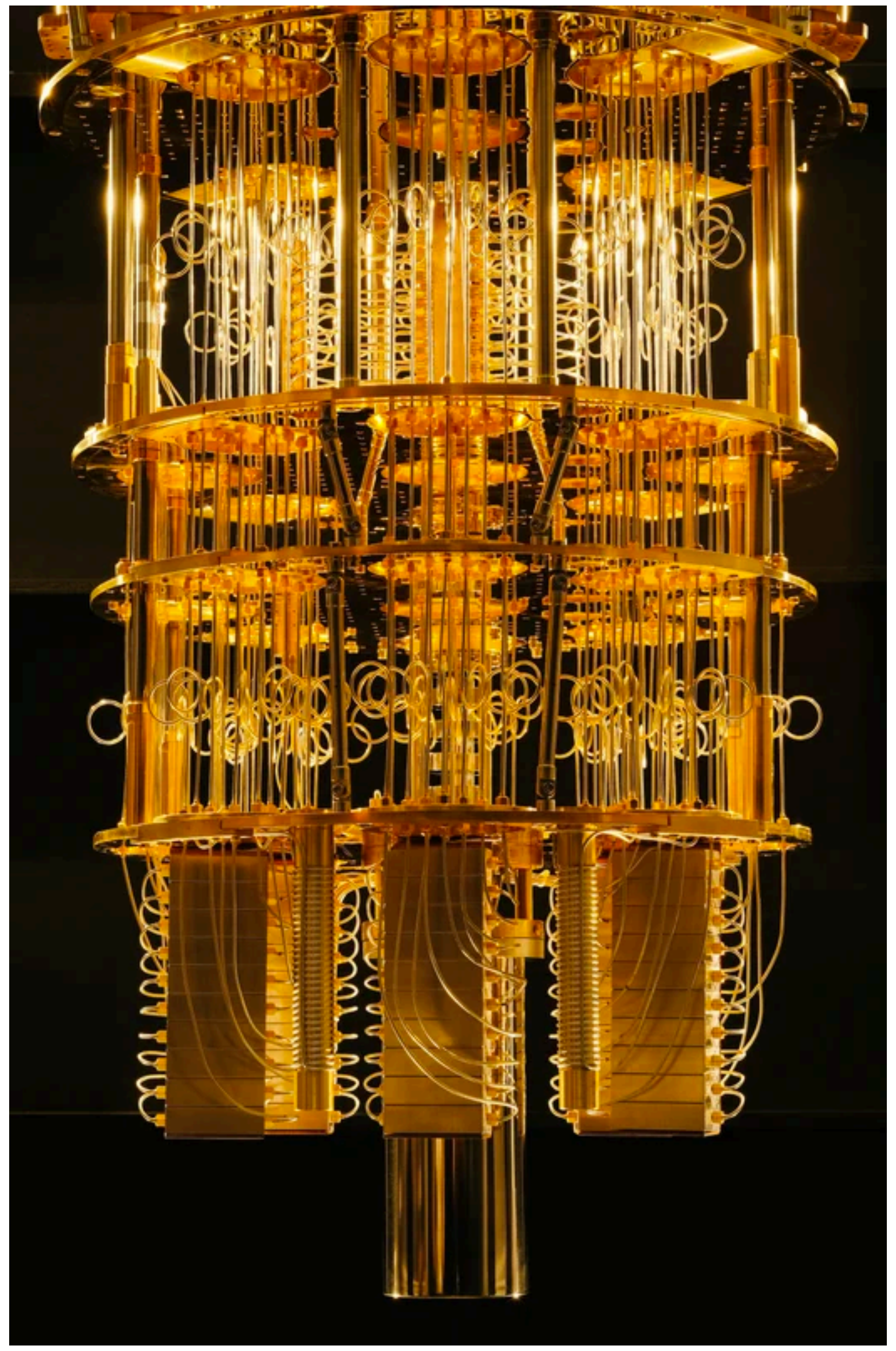


quantum (CNOT) gate



Quantum computer: current status

- hardware developments:
  - superconducting: IBM, google, etc
  - ion-trap: IONQ, Honeywell, etc.
  - photonic: Xanadu, etc.
- noisy intermediate-scale quantum: NISQ
  - the number of qubits $\sim \mathcal{O}(100)$
  - large quantum noise
  - cannot correct errors during calculation (no fault-tolerance) $\rightarrow$operating many gates is challenging
- useful applications in NISQ era?
- reducing (#gates, #qubits) is important!



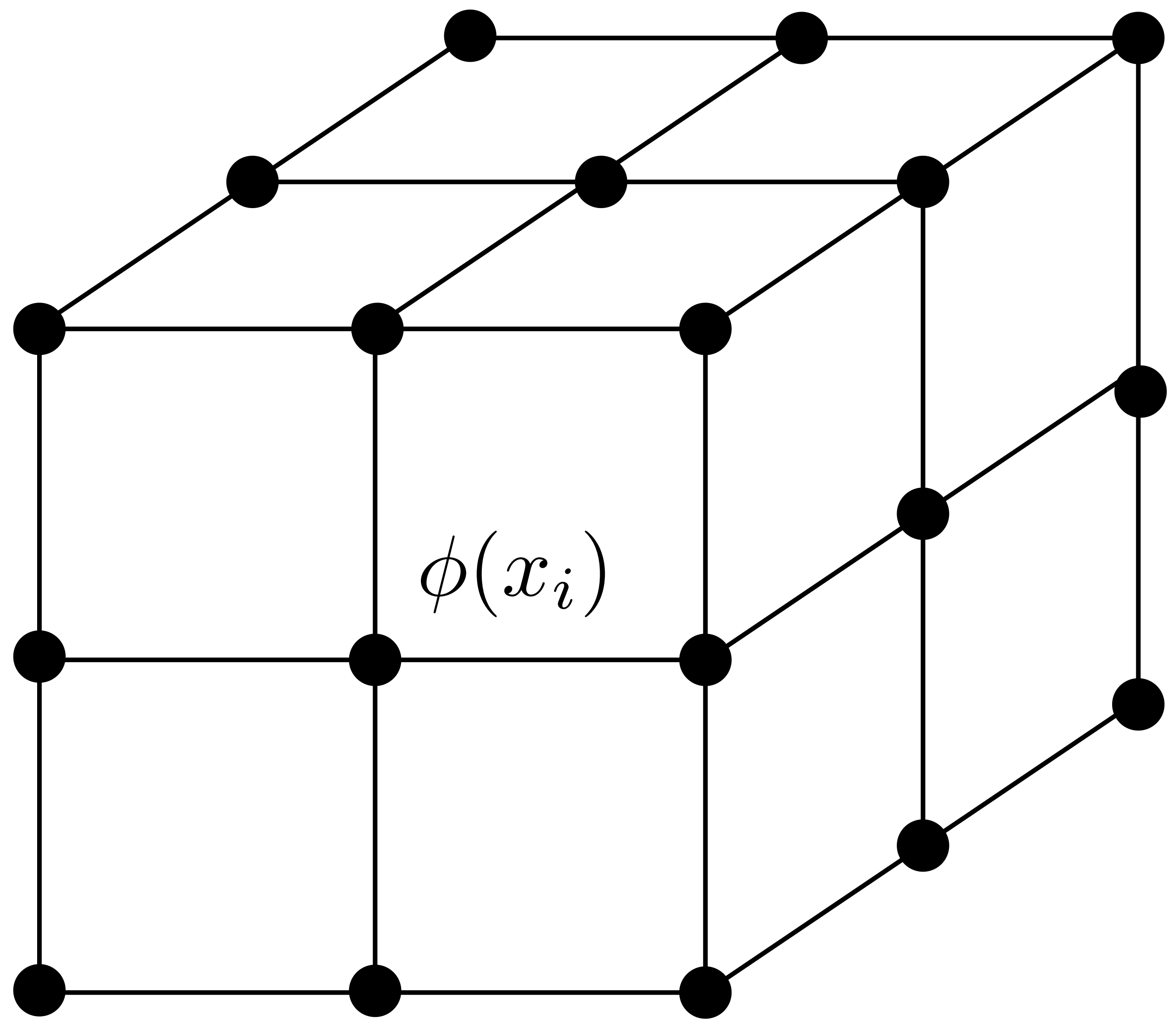
[IBM research, Flickr]

Numerical simulation of quantum field theory

- particle physics is described by quantum field theory (gauge theory)
- studying non-perturbative effects is (in general) very hard
- numerical simulation: lattice gauge theory
  - discretize **spacetime**

$$Z = \int [d\phi] e^{-S[\phi]} \rightarrow \sum_{\{\phi_i\}} \boxed{e^{-S(\phi_i)}}$$

regard as probability distribution



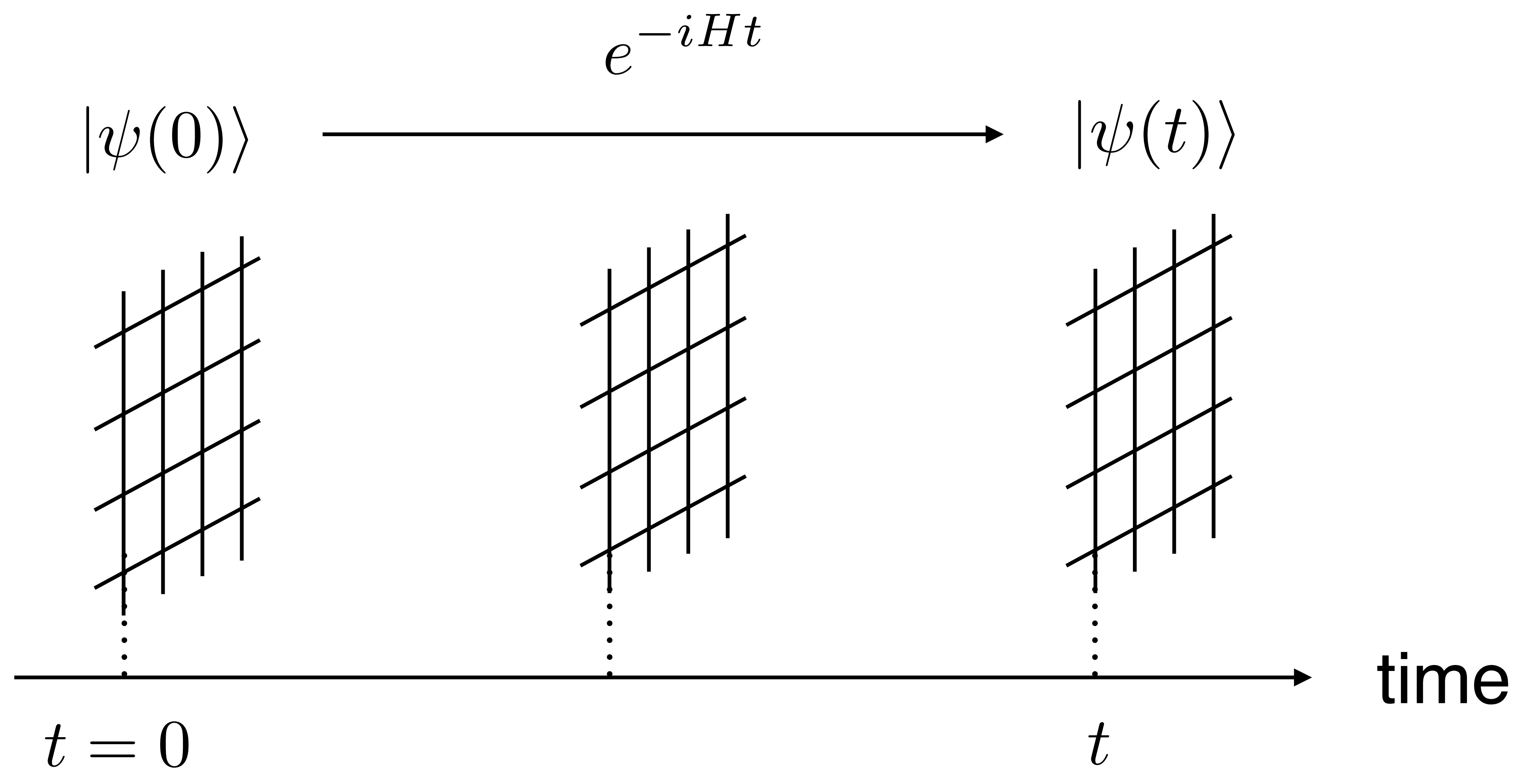
  - conventional method: using the Monte Carlo method
  - infamous sign problem
    - topological term
    - real-time dynamics, etc.

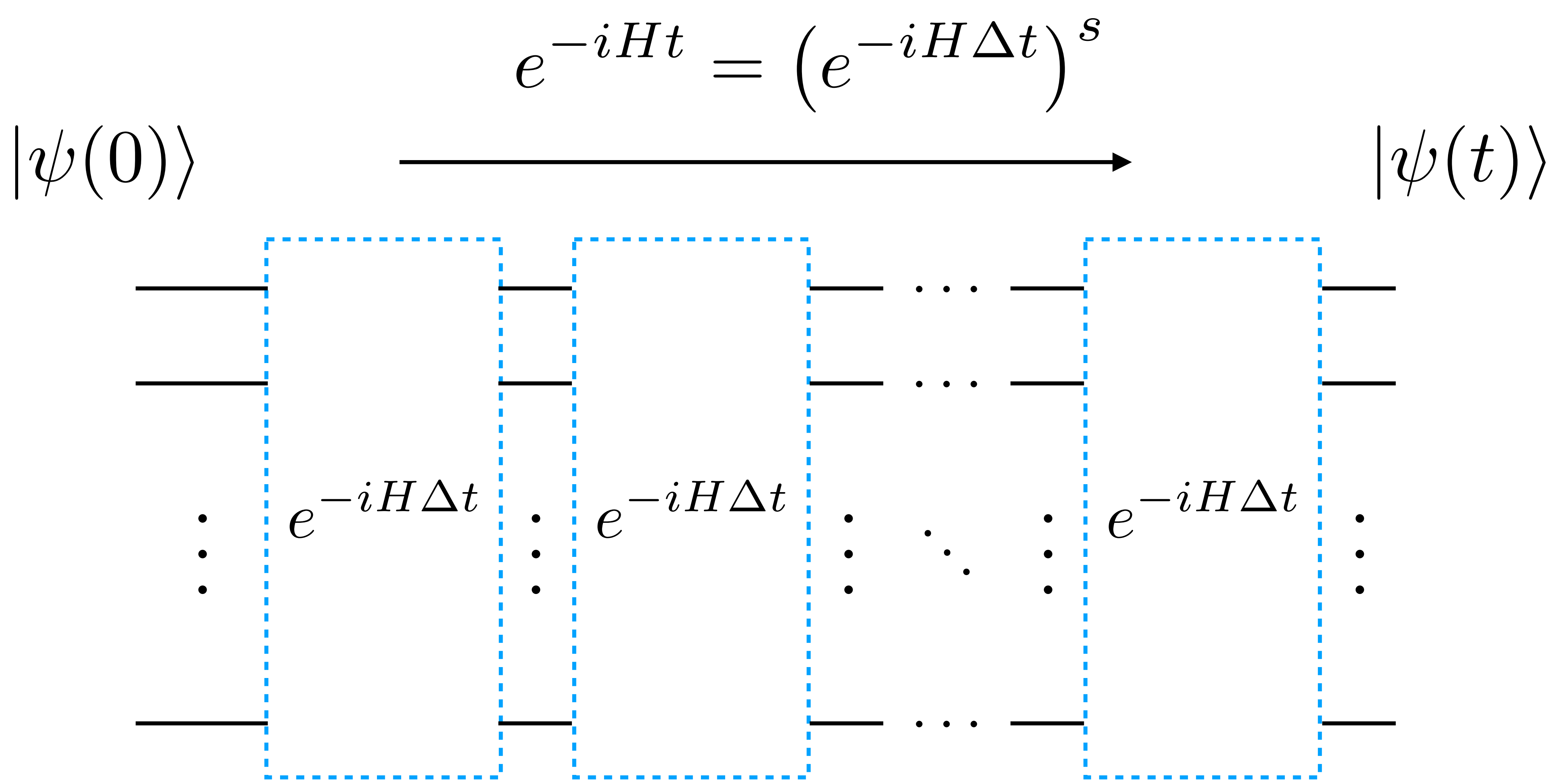
Hamiltonian simulation

- directly trace time evolution $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$
  - no sign problem!
  - need exponential resources…
- quantum simulation:
  simulation using a quantum computer
- applications to HEP: scattering problem

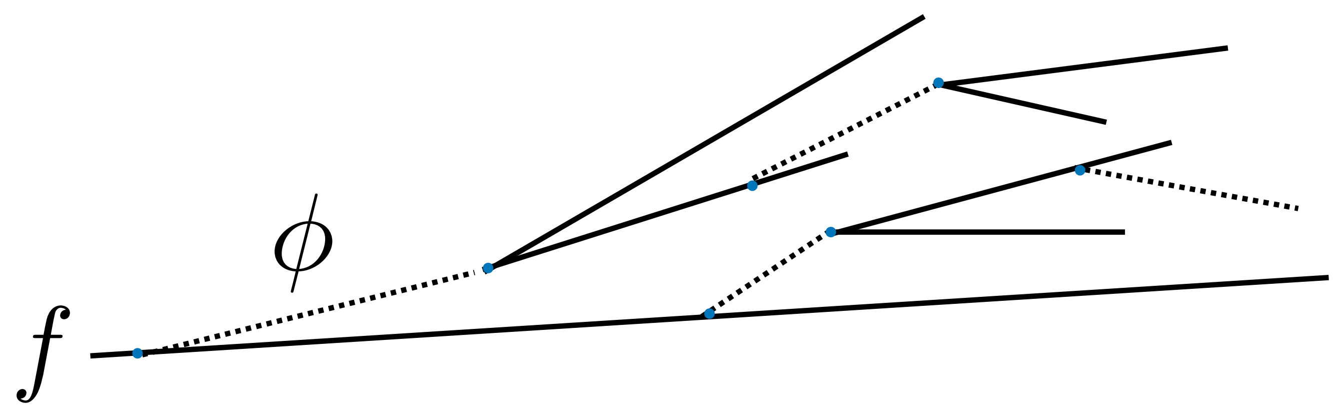
[Jordan, Lee, Preskill, Science 336, 1130-1133 (2012)]

  - pros: exponential advantage
  - cons:
    - still need many resources
    - near-term (NISQ) applications?





Collaboration I: Optimization of HEP-simulation circuit



- Parton shower simulation:

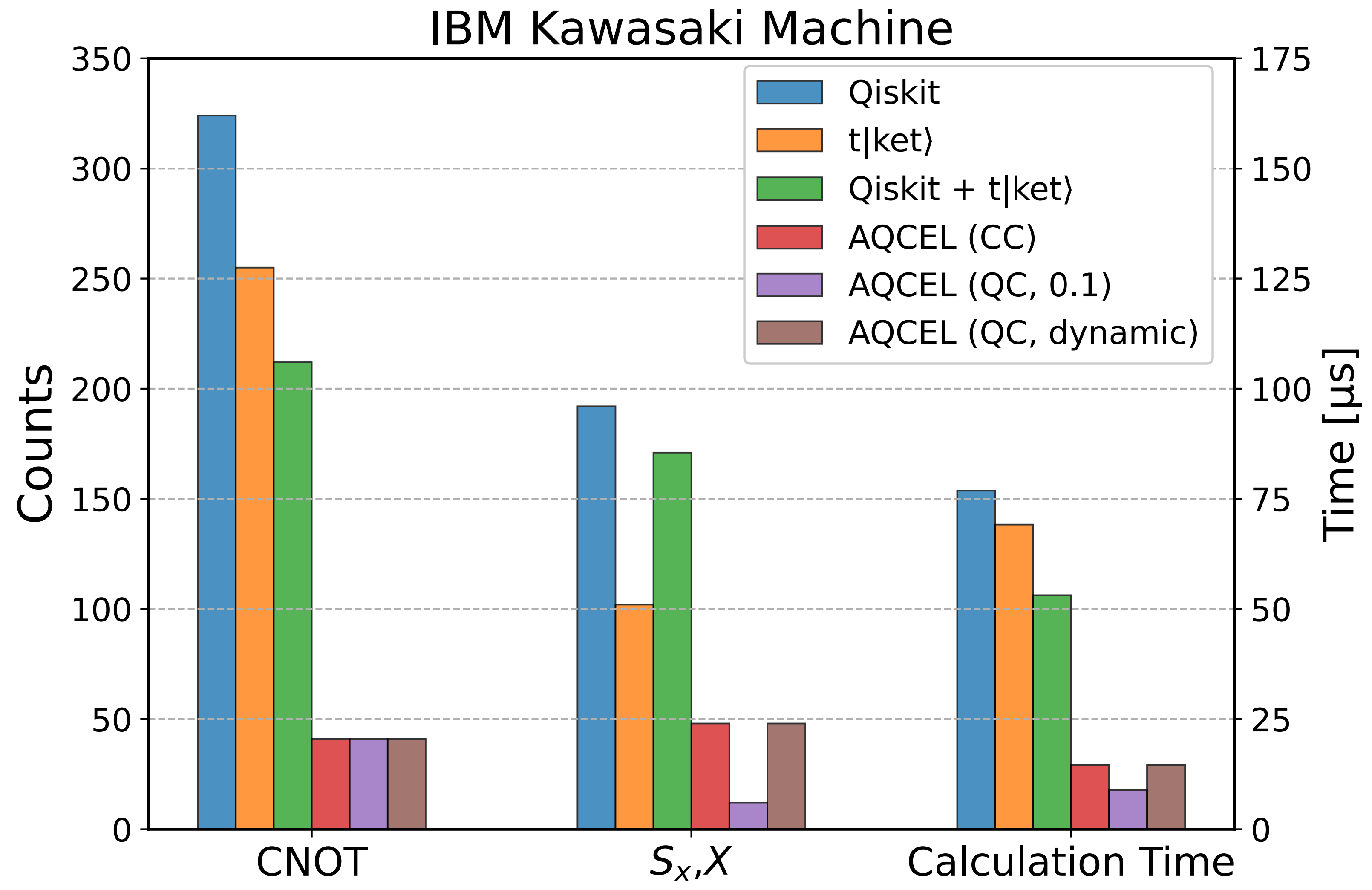
  [C. W. Bauer, W. A. de Jong, B. Nachman, D. Provasoli, PRL 126, 062001 (2021)]

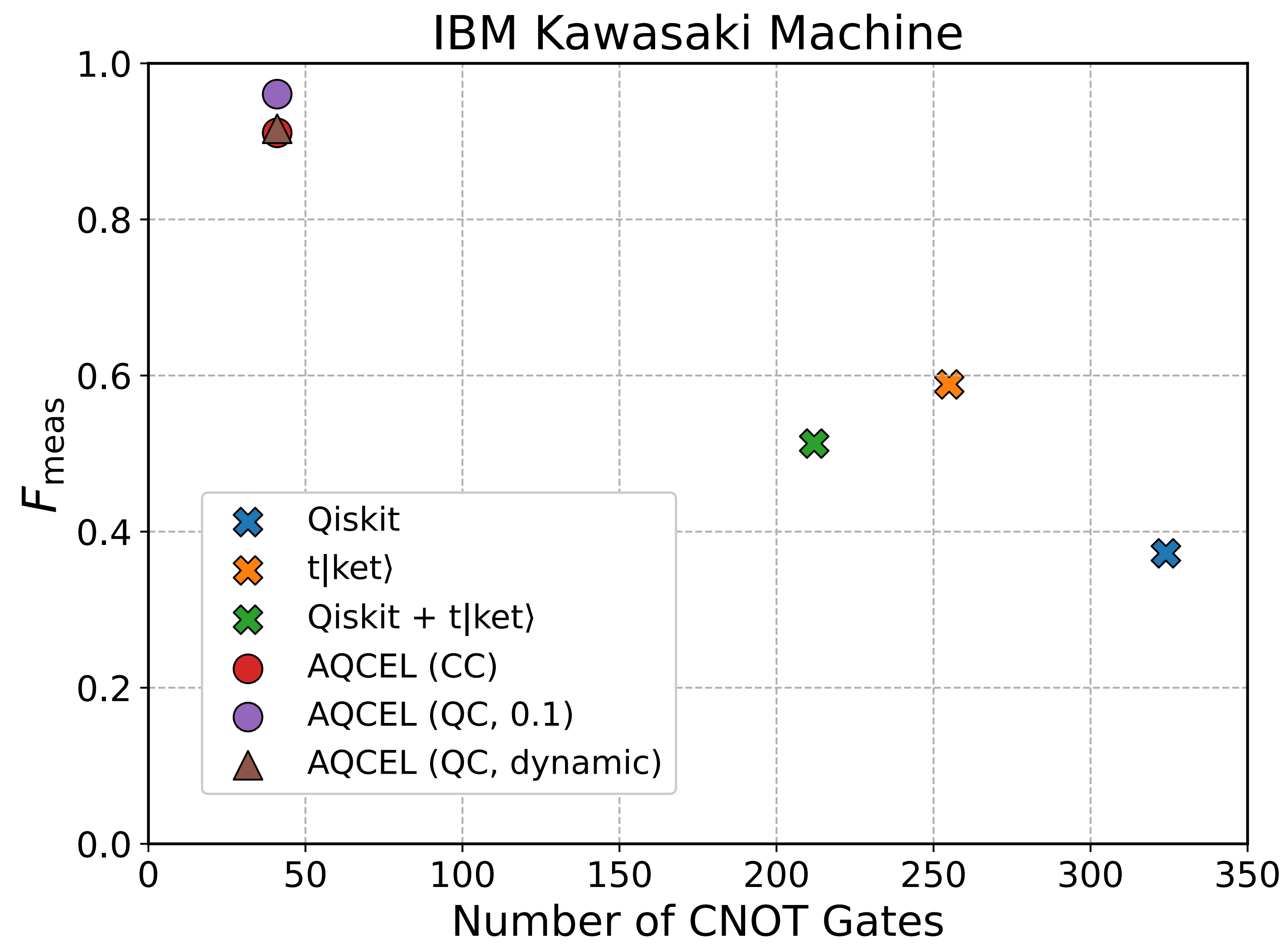
  - require many gates (depth)
  - need to be reduced for NISQ application

- AQCEL (**A**dvancin **Q**uantum **C**ircuits by IC**E**PP and **L**BNL) optimization protocol:

  [W. Jang, K. Terashi, M. Saito, C. W. Bauer, B. Nachman, Y. Iiyama, R. Okubo, and R. Sawada, Quantum 6, 798 (2022)]

  - identifying zero/low-amplitude basis states →remove redundant qubits or gates
  - identification of repeated sets of gates

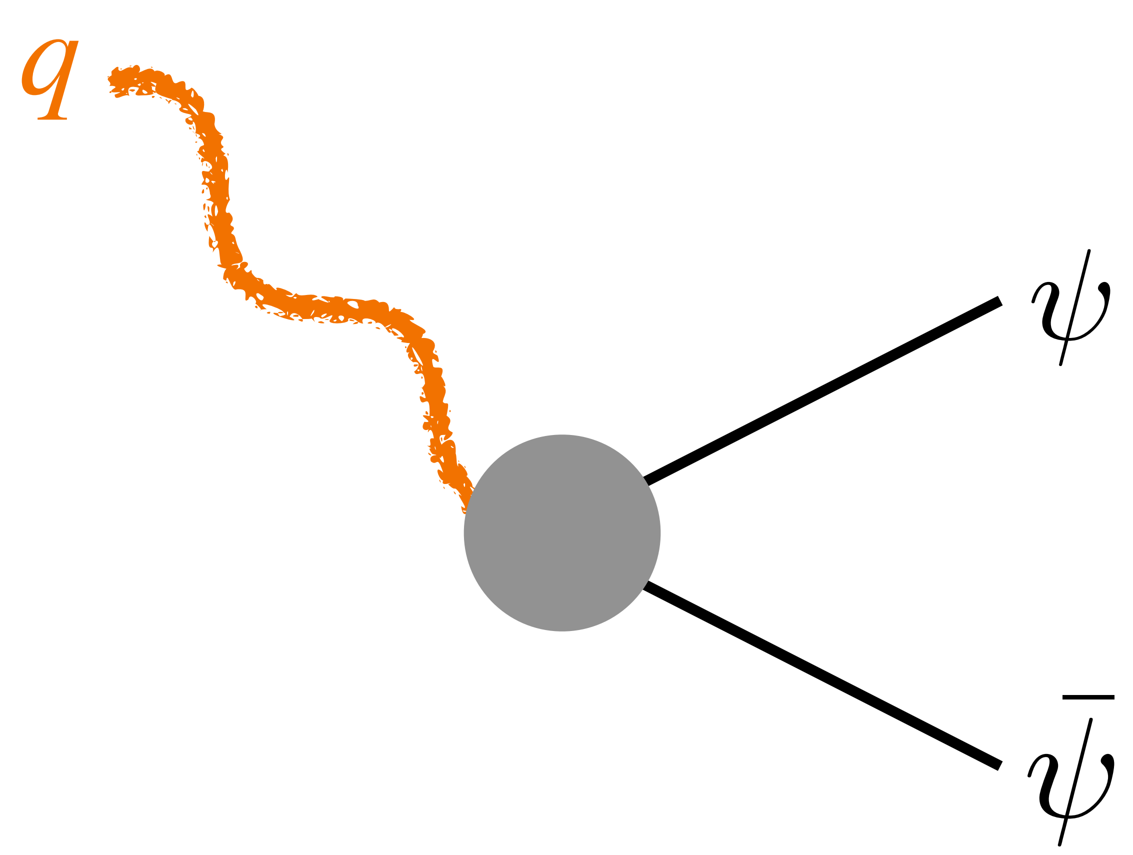




Collaboration II: quantum simulation of gauge theory

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{gq}{2}\epsilon^{\mu\nu}F_{\mu\nu} + \mathrm{i}\bar{\psi}\gamma^{\mu}\left(\partial_{\mu} + \mathrm{i}gA_{\mu}\right)\psi - m\bar{\psi}\psi$$

- simple toy model: 1+1d U(1) gauge theory = **Schwinger model** [Schwinger, Phys. Rev. 128, 2425]
- simple but still non-trivial
  - screening/confinement phenomena
  - we can include the topological term
    (cannot be treated in the MC method)
    →introduce the effects of the external field
- **Schwinger effect**: pair-creation due to strong external field
  [Schwinger, Phys. Rev. 82, 664, (1951)]
- our work: simulation using variational quantum algorithms
  →NISQ-friendly algorithms
  [LN, A. Bapat, C. W. Bauer, arXiv: 2302.10933 (2023)]



Model

Spin description of the Schwinger model

$$H = \int dx \left[\frac{1}{2} (\Pi - q)^2 - i\bar{\psi}\gamma^1(\partial_1 + igA_1 - m)\psi \right]$$

- continuum Hamiltonian→lattice Hamiltonian (Kogut-Susskind formulation)
- gauge symmetry→eliminate gauge fields
- lattice Hamiltonian→spin system (Jordan-Wigner transformation)

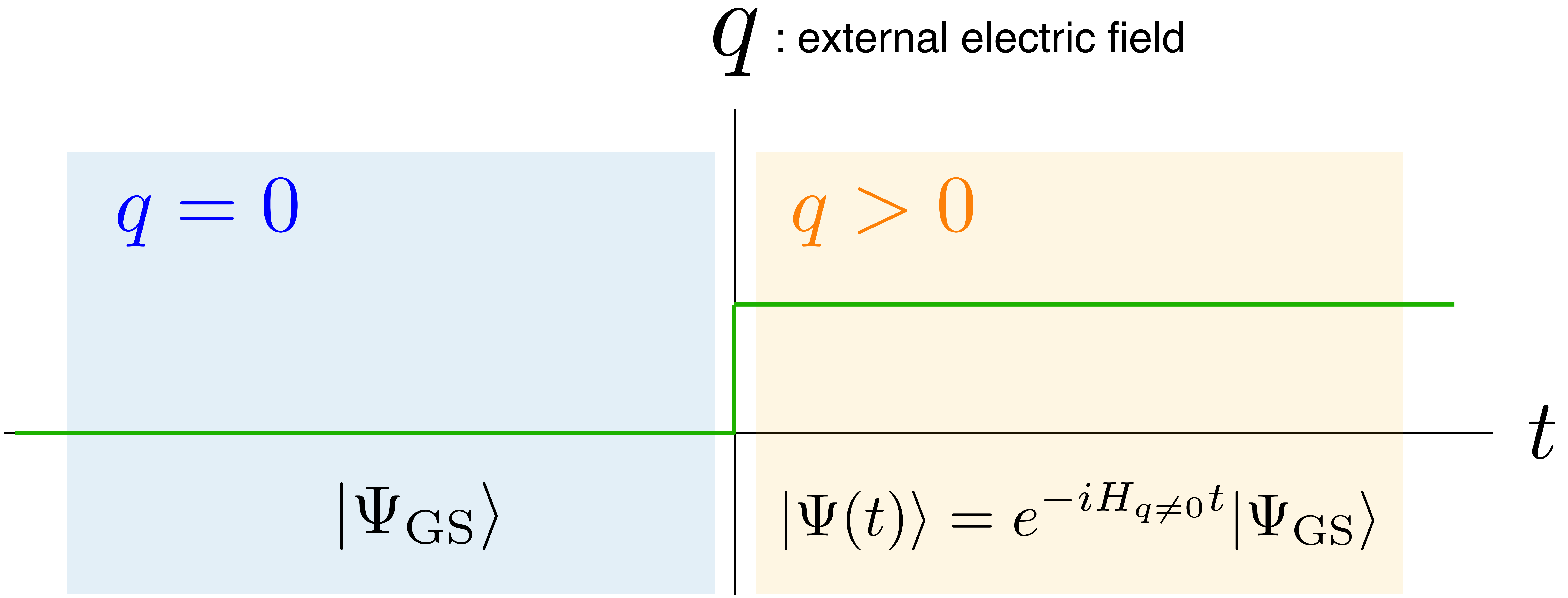
$$H_{\text{spin}} = J \sum_{n=0}^{N-2} \left(\sum_{k=0}^{n} \frac{Z_k + (-)^k}{2} + q \right)^2 + \frac{w}{2} \sum_{n=0}^{N-2} (X_n X_{n+1} + Y_n Y_{n+1}) + \frac{m}{2} \sum_{n=0}^{N-1} (-)^n Z_n$$

electric field — fermion kinetic term — fermion mass term

(X, Y, Z: Pauli matrices)

Quench dynamics in the Schwinger model

- Schwinger effect: particle pair creation due to strong external electric field [Schwinger, Phys. Rev. 82, 664, (1951)]



Ground state without external field

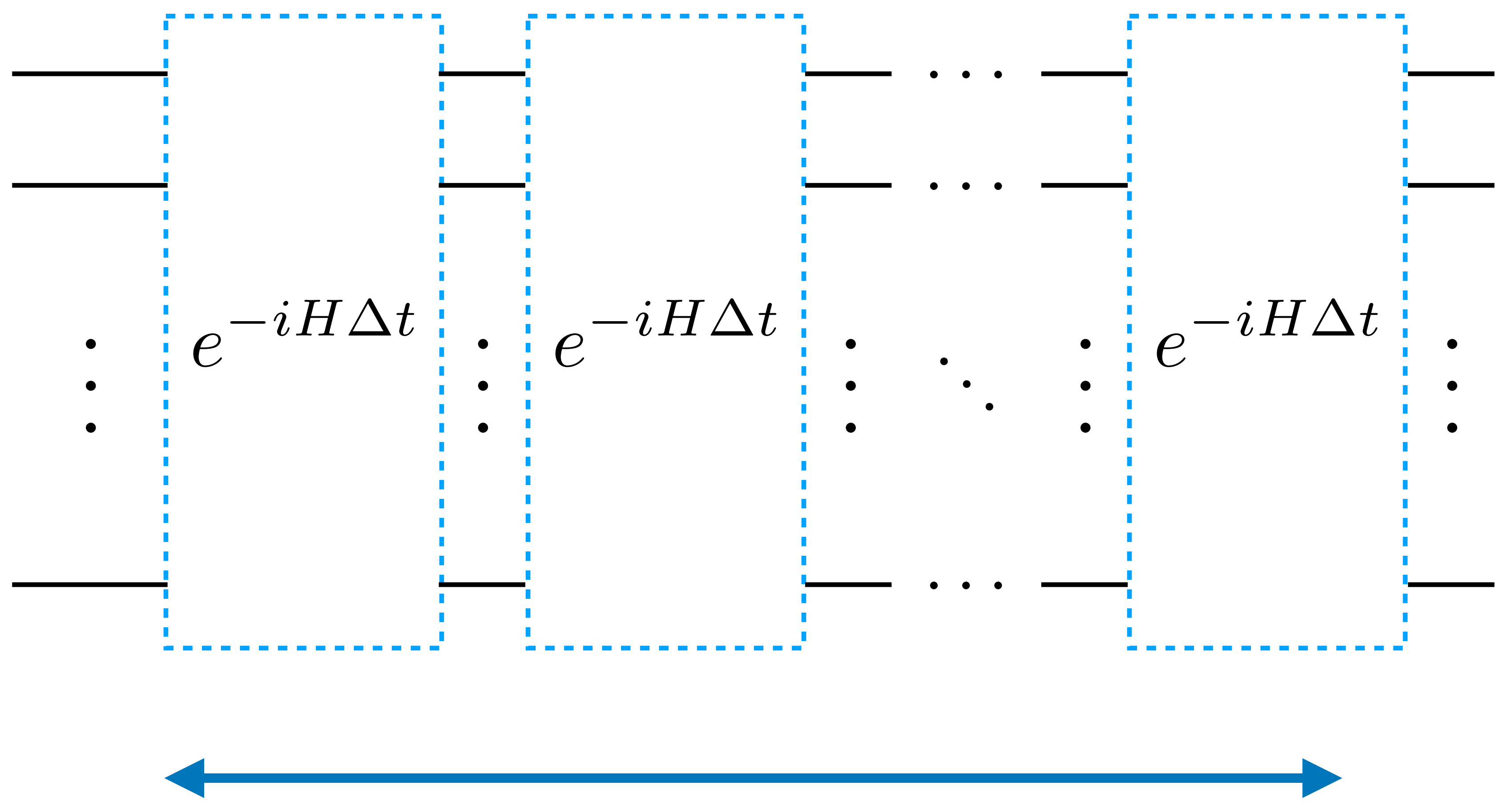
time evolution with external field
→pair-creation?

Method

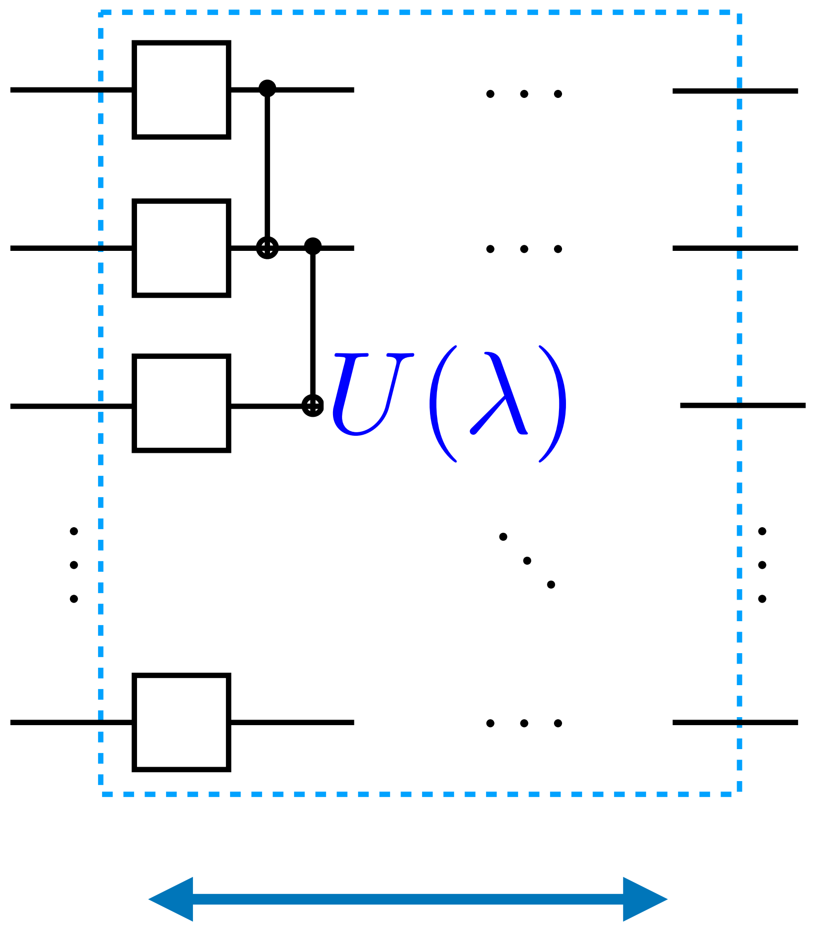
Suzuki-Trotter vs variational method

- Suzuki-Trotter method
  - #depth grows with #steps
  - decoherence problem on NISQ devices

- variational quantum algorithm (VQA)
  - approximate states by ansatz with fixed depth
  - state preparation: variational quantum eigensolver (VQE)
  - time-evolution: variational quantum simulation (VQS)



depth∝ (#step)



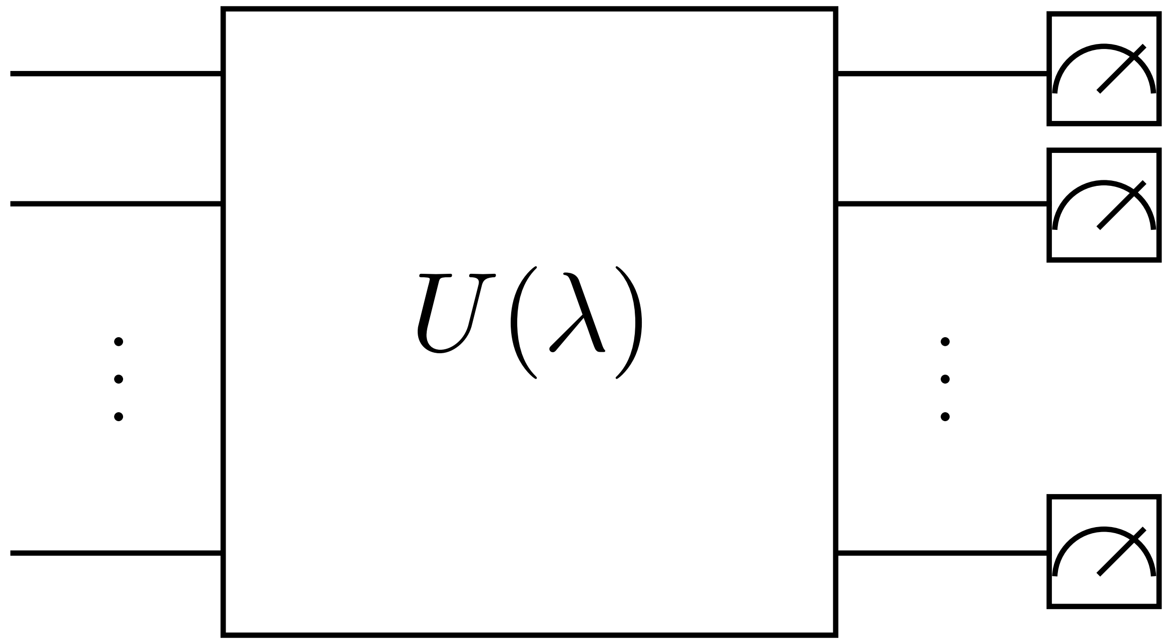
$$|\psi(\lambda)\rangle \approx \begin{cases} |\Psi_{\rm GS}\rangle & ({\rm VQE}) \\ e^{-iHt}|\psi(0)\rangle & ({\rm VQS}) \end{cases}$$

depth fixed

Variational quantum eigensolver

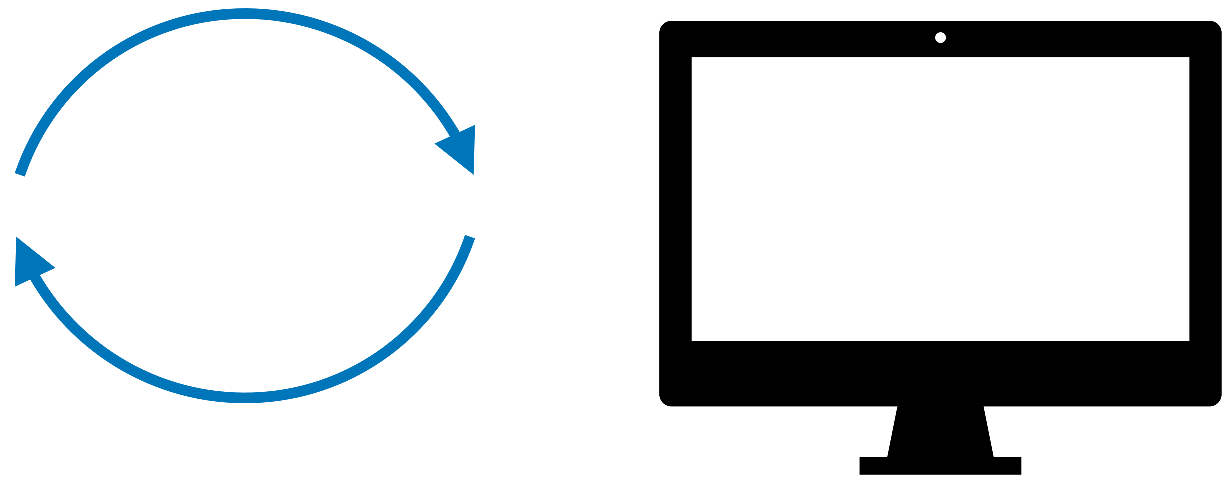
- goal: obtain the ground state
- approximate the ground state by ansatz $|\psi(\lambda)\rangle$
- optimize cost function $C(\lambda) = \langle\psi(\lambda)|H|\psi(\lambda)\rangle$ via classical computer
  $\rightarrow$ground state is given by $|\psi(\lambda_*)\rangle$

$$|\psi(\lambda)\rangle = U(\lambda)|0\rangle$$



$$C(\lambda) = \langle\psi(\lambda)|H|\psi(\lambda)\rangle$$

classical computer



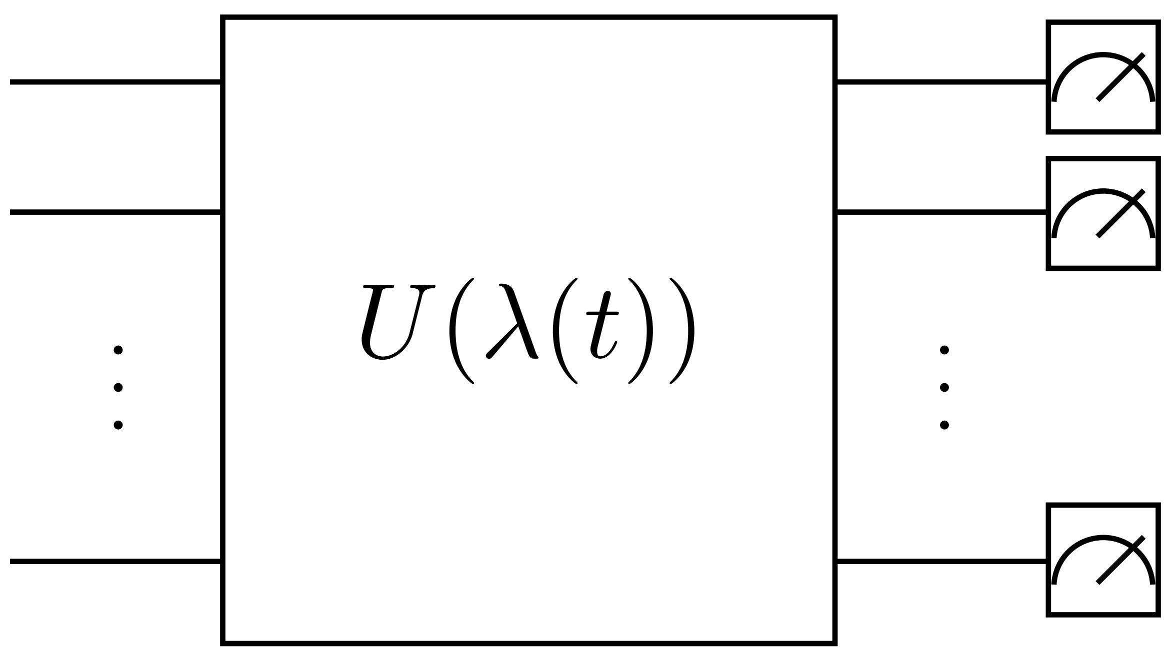
$$\lambda_* = \arg\min_{\lambda} C(\lambda)$$

Variational quantum simulation

[Li, Benjamin, Phys. Rev. X 7, 021050, (2017)]

- goal: obtain time-evolved state $|\Psi(t)\rangle = e^{-iHt}|\Psi(0)\rangle$
- approximate $|\Psi(t)\rangle$ by ansatz $|\psi(\lambda(t))\rangle$ with time-dependent parameters
- evolution of states → evolution of parameters $\lambda(t)$ via McLacran's variational principle
- we use the same ansatz for both VQE and VQS
  →quench dynamics: set $\lambda(0) = \lambda_*$ (obtained by VQE)

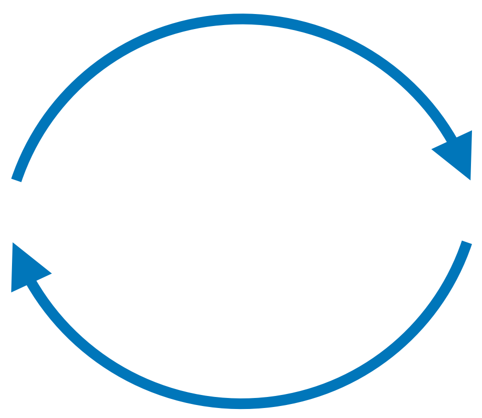
$$|\psi(\lambda(t))\rangle = U(\lambda(t))|0\rangle$$



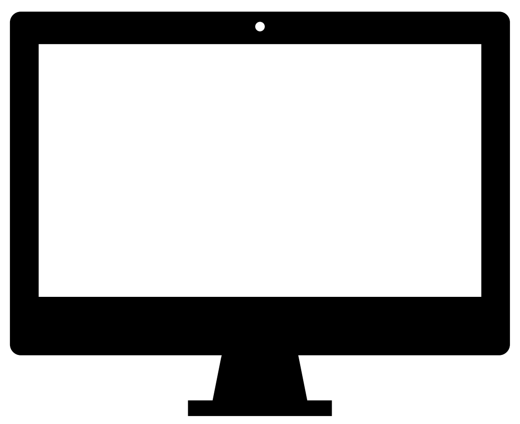
$$M_{ij} = \mathrm{Re}\frac{\partial\langle\psi(\lambda)|}{\partial\lambda_i}\frac{\partial|\psi(\lambda)\rangle}{\partial\lambda_j}$$

$$V_i = \mathrm{Im}\frac{\partial\langle\psi(\lambda)|}{\partial\lambda_i}H|\psi(\lambda)\rangle$$

(+correction terms)



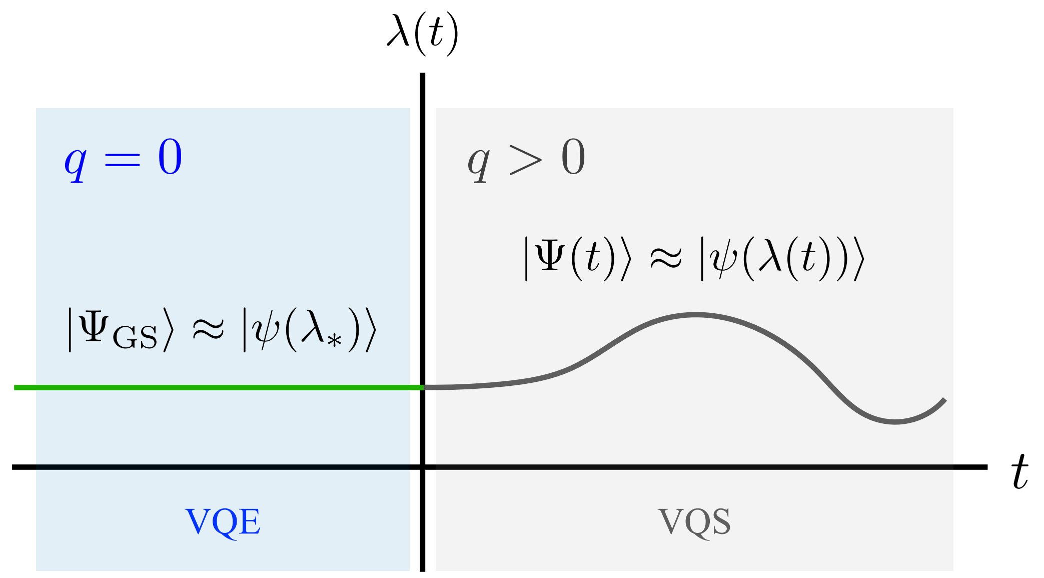
classical computer



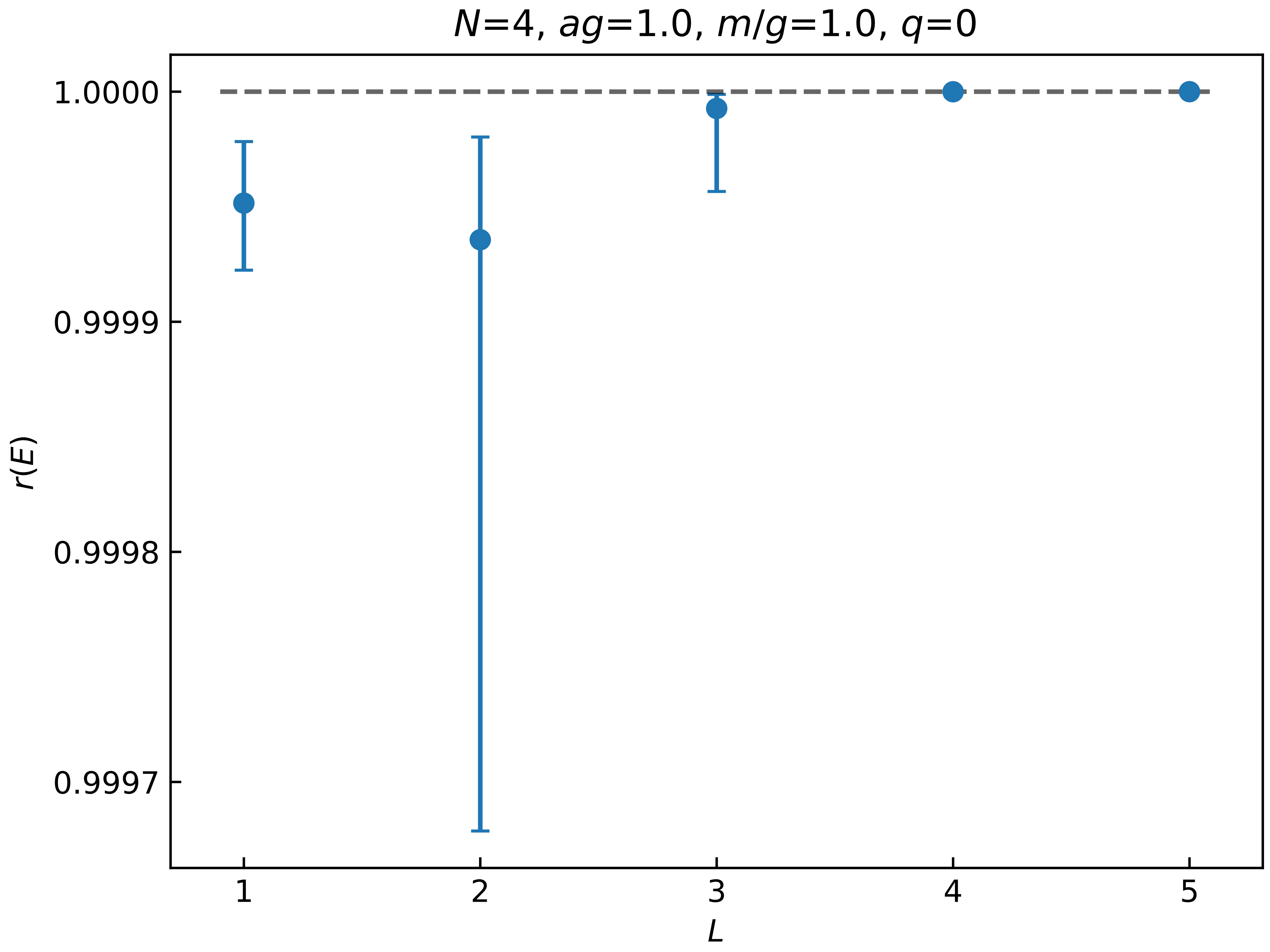
$$\sum_j M_{ij}\dot{\lambda}_j = V_i$$

Results

Ground state preparation via VQE

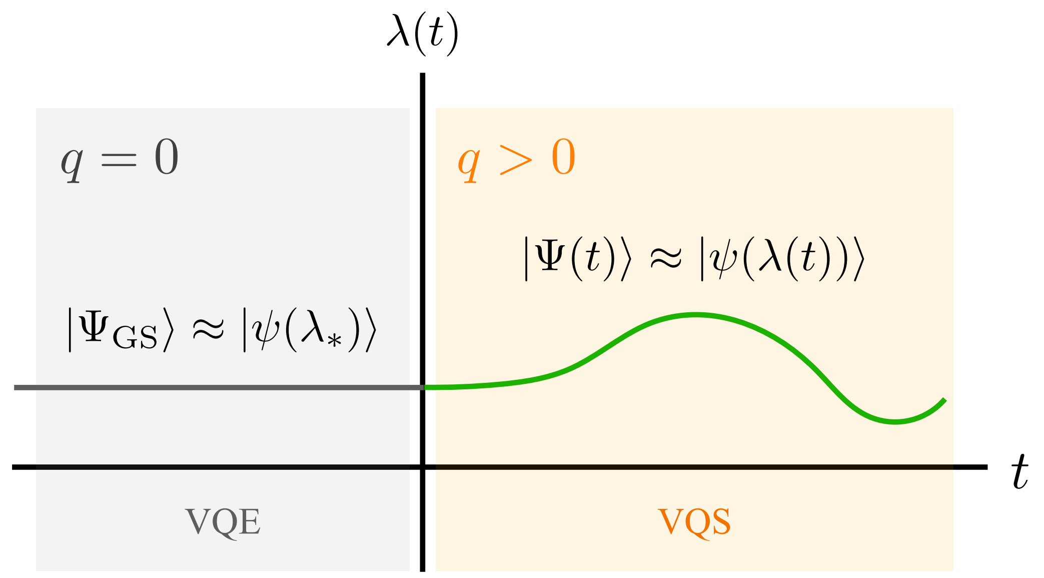


- use classical statevector simulator
- compare VQE with exact diagonalization (ED)
- a metric of accuracy: $r(E) = \dfrac{E_{\max} - E_{\mathrm{VQE}}}{E_{\max} - E_{\min}}$
  - $E_{\max}, E_{\min}$: max/min energy obtained by ED
  - $r(E) = 1$ for the best case
  - $r(E) = 0$ for the worst case
- L : depth of ansatz
- quality drastically improves for $L \geq 4$



- 20 samples with different initialization
- dots/bars represent medians and 25-75 percentiles

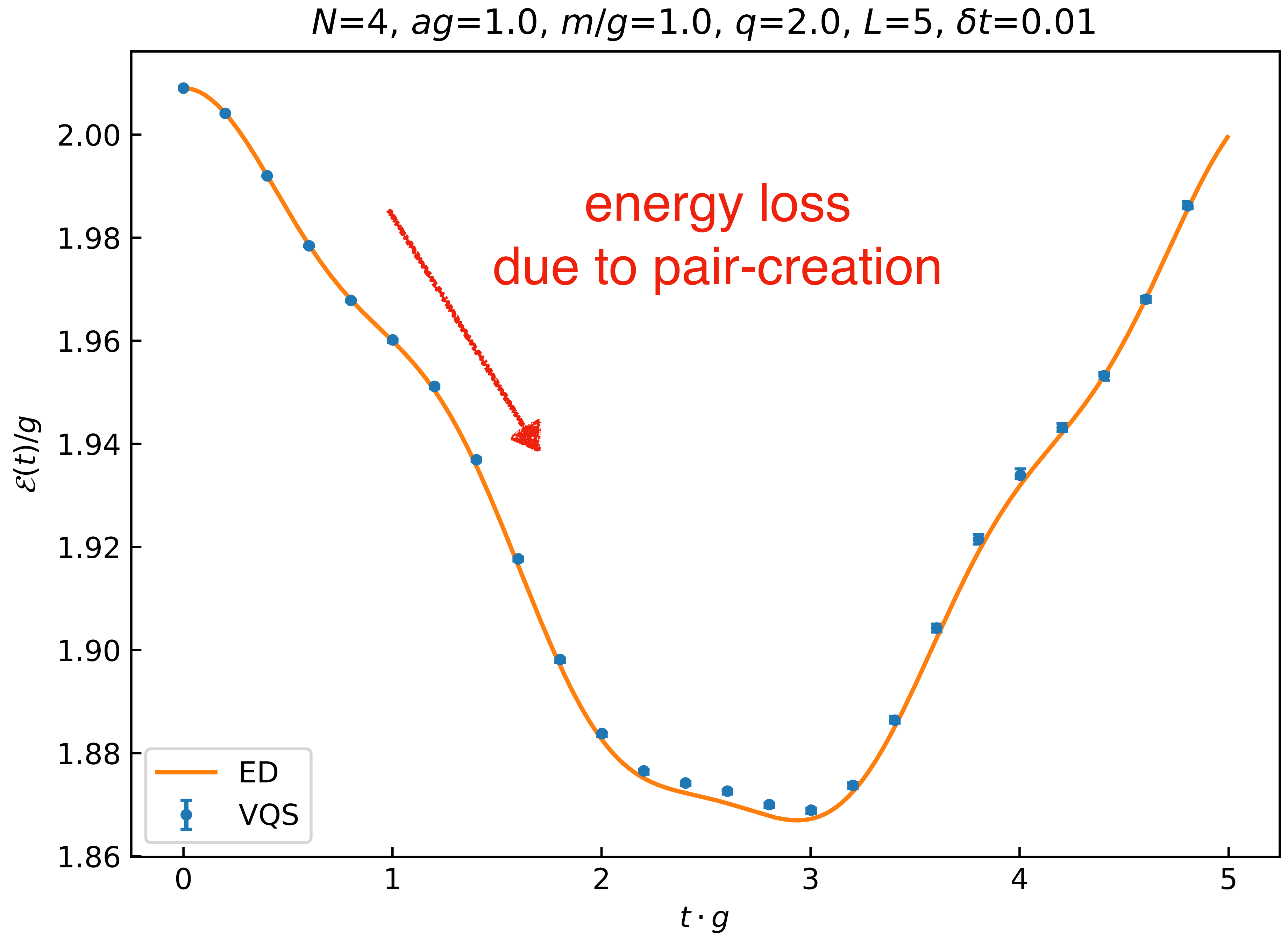
Real-time evolution via VQS



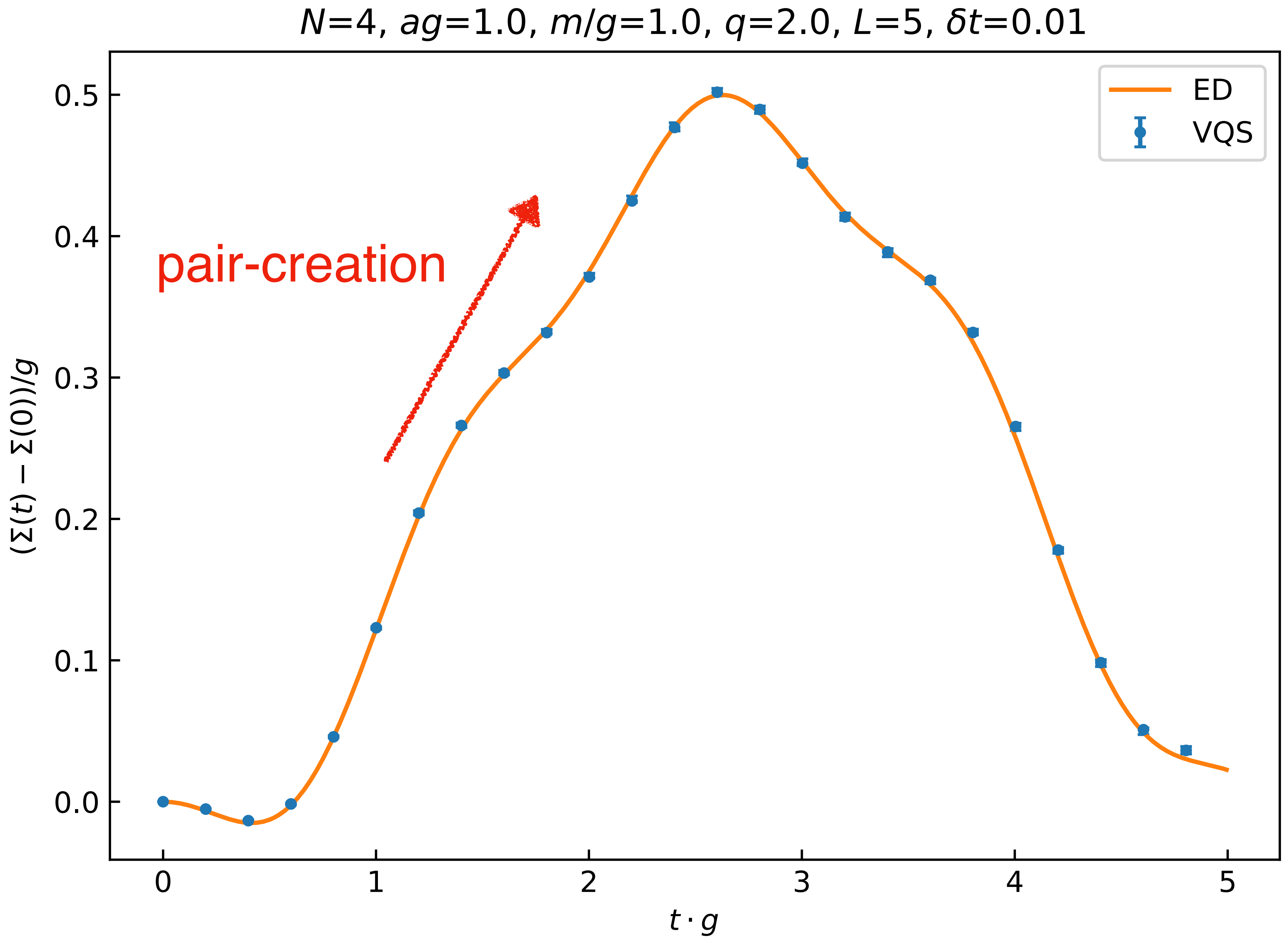
- two observables:
  - total electric field $\mathscr{E}$
  - chiral condensation $\langle \bar{\psi}\psi \rangle$ (~particle number density)
- observing energy loss and pair-creation!

- 20 samples with different initialization
- dots/bars represent medians and 25-75 percentiles

electric field

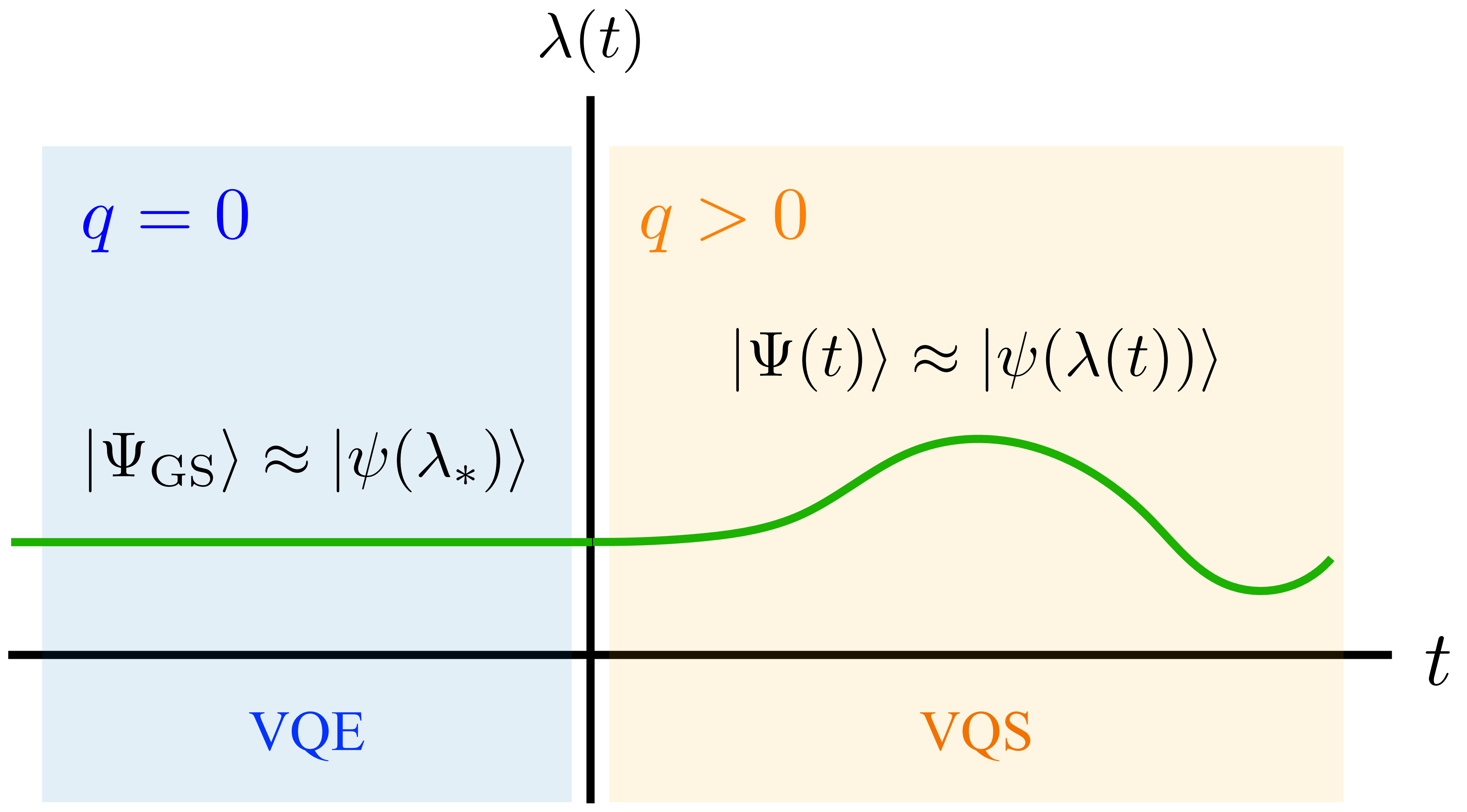


chiral condensation



Summary and outlooks

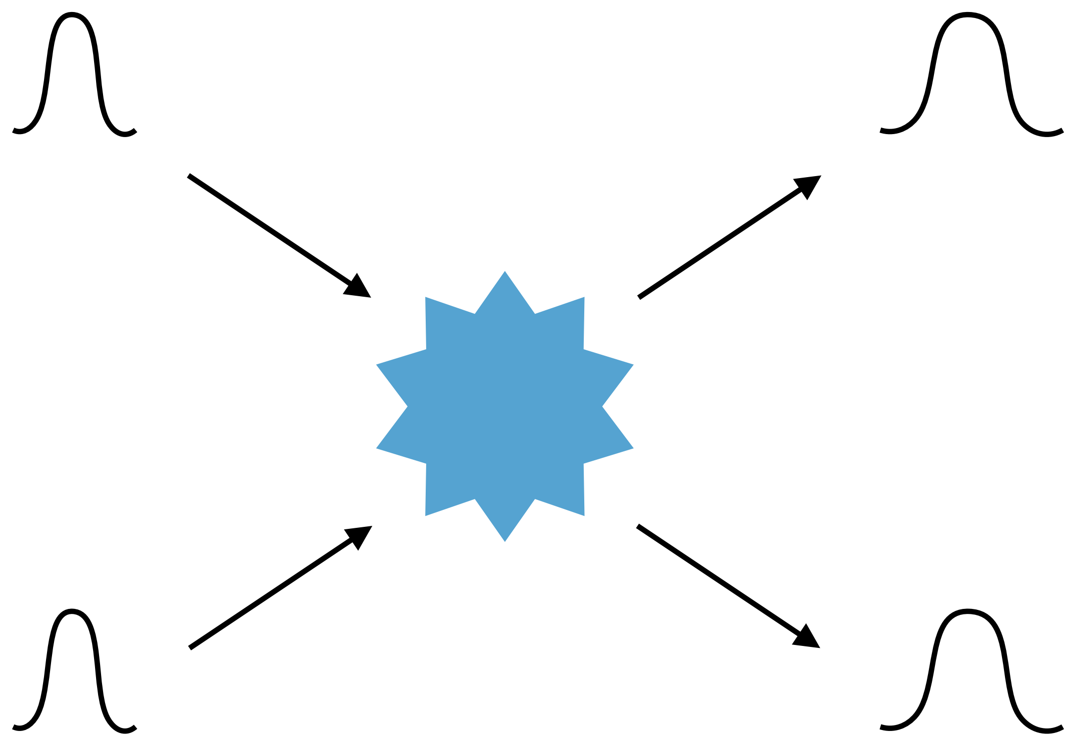
- circuit-optimization: reduction of CNOT counts!
- quench dynamics in the Schwinger model via VQAs
  - ground state w/o external field q via VQE
  - time evolution via Hamiltonian w/ external field q via VQS
  - we can reduce circuit depth
  - VQA results agree well with ED
- **future directions**:
  - scaling of resources/errors
  - extension to higher dimensional and/or non-Abelian theories
  - implementation of gauge theory simulation on real hardware with circuit optimization

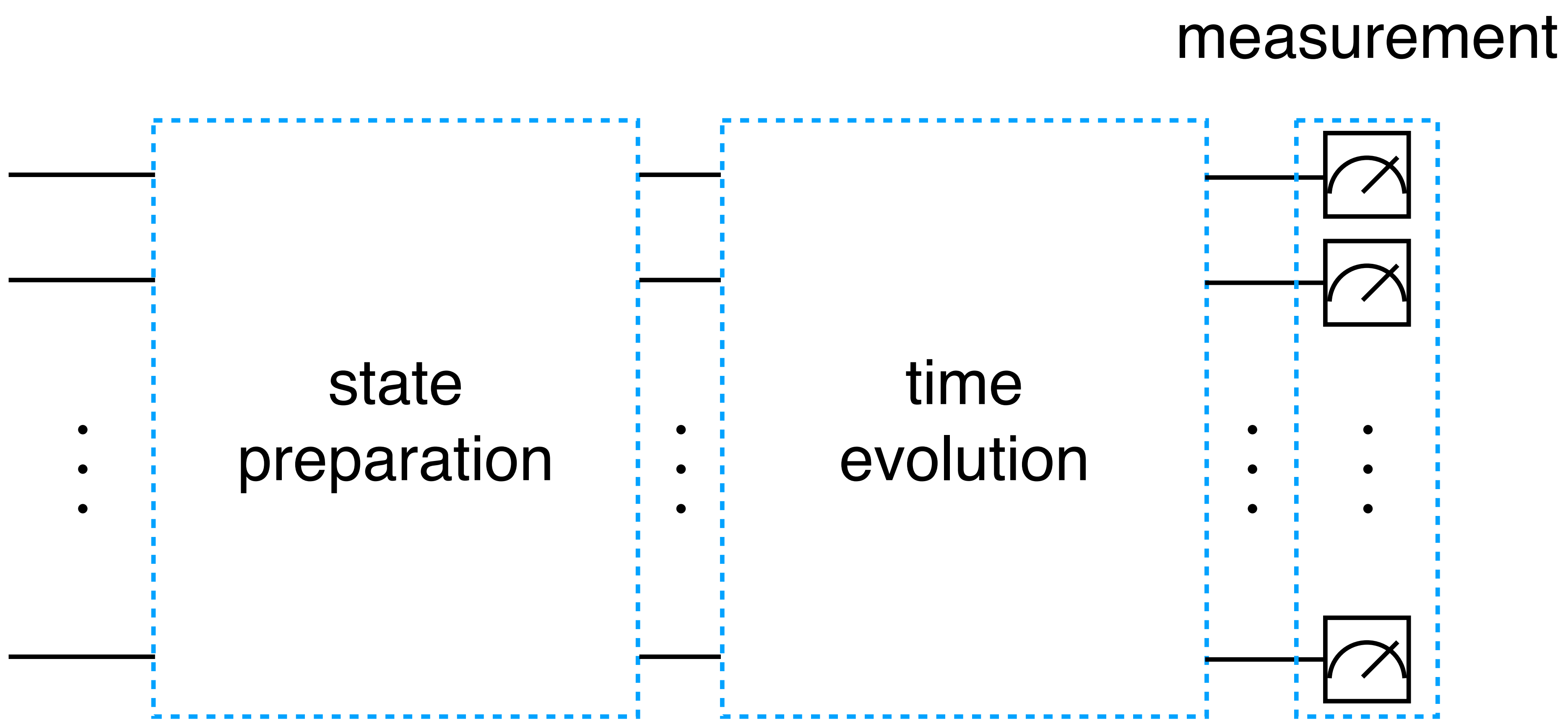


Backups

Quantum Simulation for HEP

- quantum computer = natural Hamiltonian simulator!
- application to HEP (ex. scattering) [e.g. Jordan-Lee-Preskill]
  - state preparation (vacuum/wave packet)
  - time evolution (scattering)
  - measurement
- exponential speedup!
  - but still need many resources…
  - assuming FTQC → NISQ simulation?



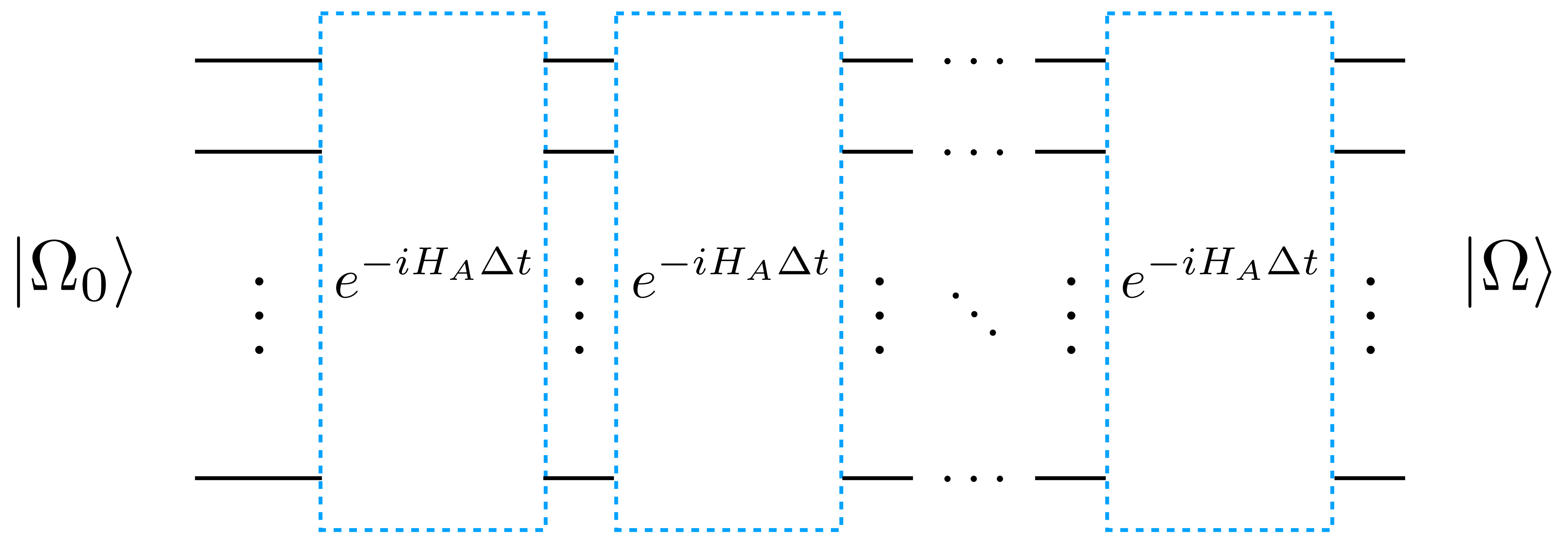


Suzuki-Trotter decomposition

- adiabatic state preparation

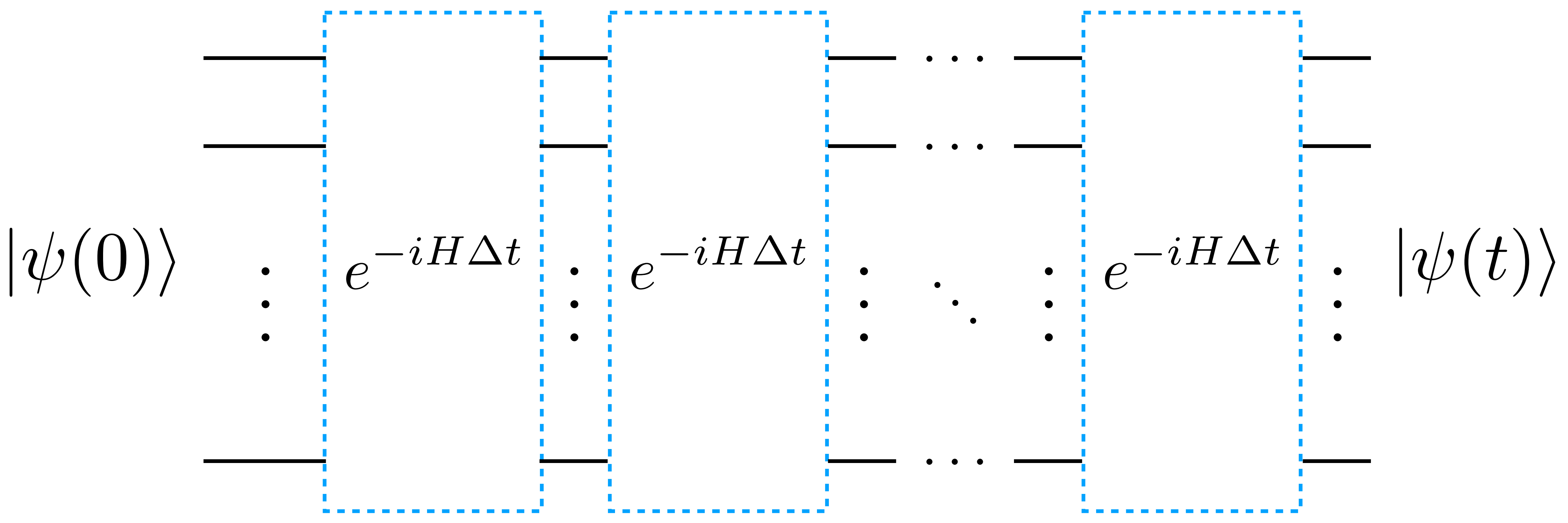
$$|\Omega\rangle = \lim_{T\to\infty} \mathrm{T}\exp\left(-\mathrm{i}\int_0^T \mathrm{d}t H_A(t)\right)|\Omega_0\rangle$$

$$\simeq \prod_s e^{-\mathrm{i}H_A(s\Delta t)\Delta t}|\Omega_0\rangle$$



- real-time evolution

$$|\psi(t)\rangle = e^{-\mathrm{i}Ht}|\psi(0)\rangle = \left(e^{-\mathrm{i}H\Delta t}\right)^s|\psi(0)\rangle$$



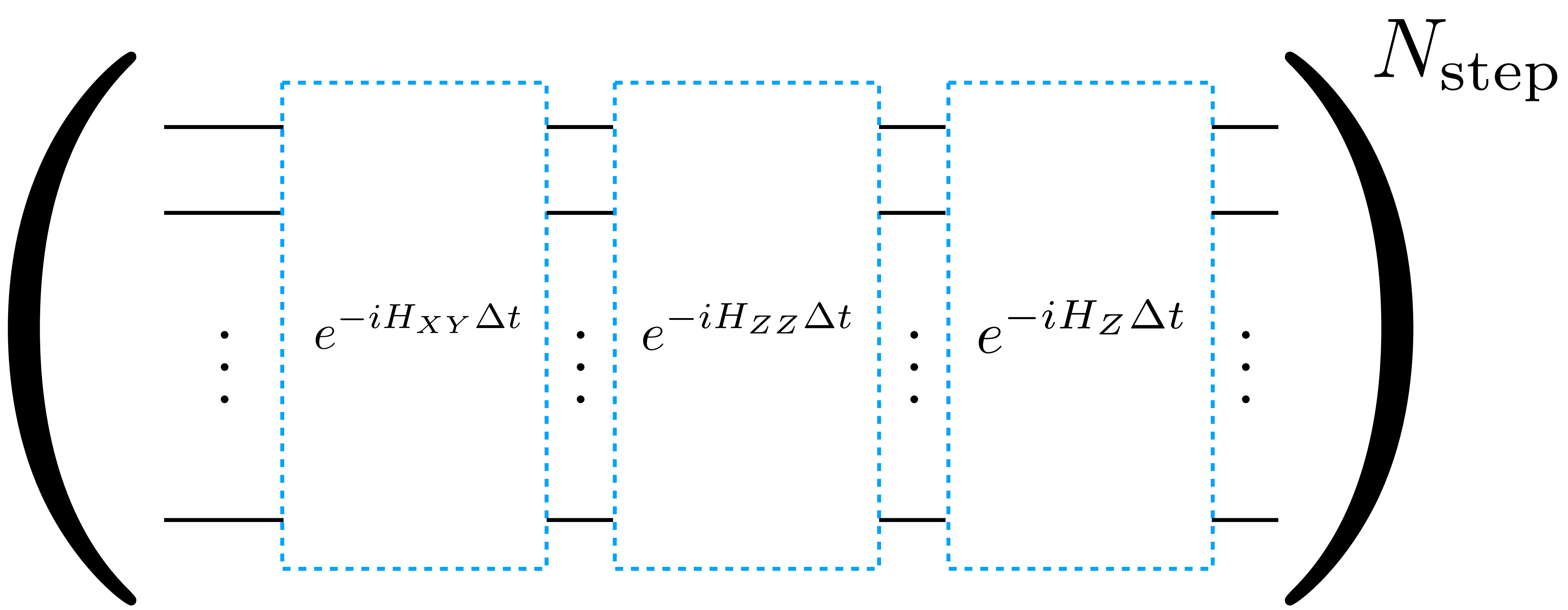
- drawback: #depth grows with #steps

Hamiltonian variational ansatz (HVA)

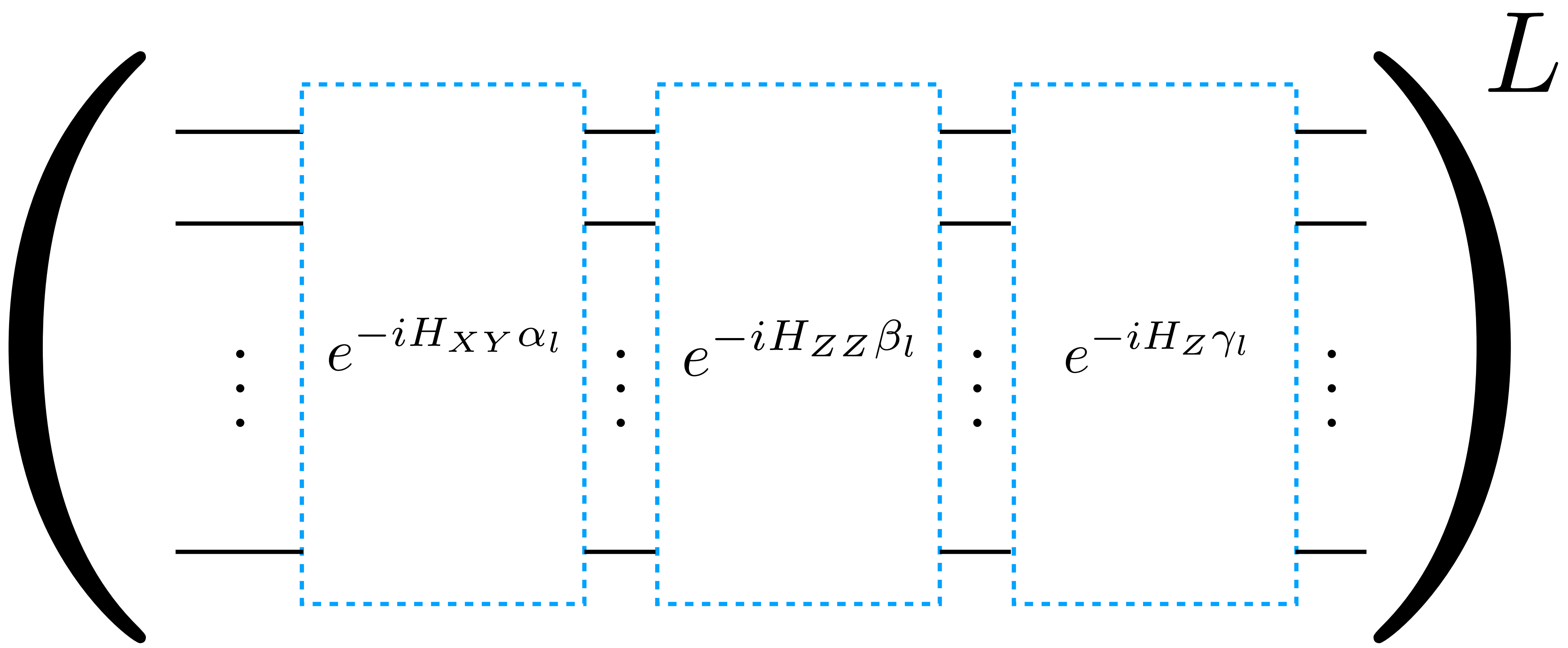
- motivation: mimic Suzuki-Trotter decomposition of adiabatic or real-time evolution
- parameters (α, β, γ) can depend on sites
- we use U(1) preserving decomposition

$$H = H_{XY} + H_{ZZ} + H_Z$$

Suzuki-Trotter evolution

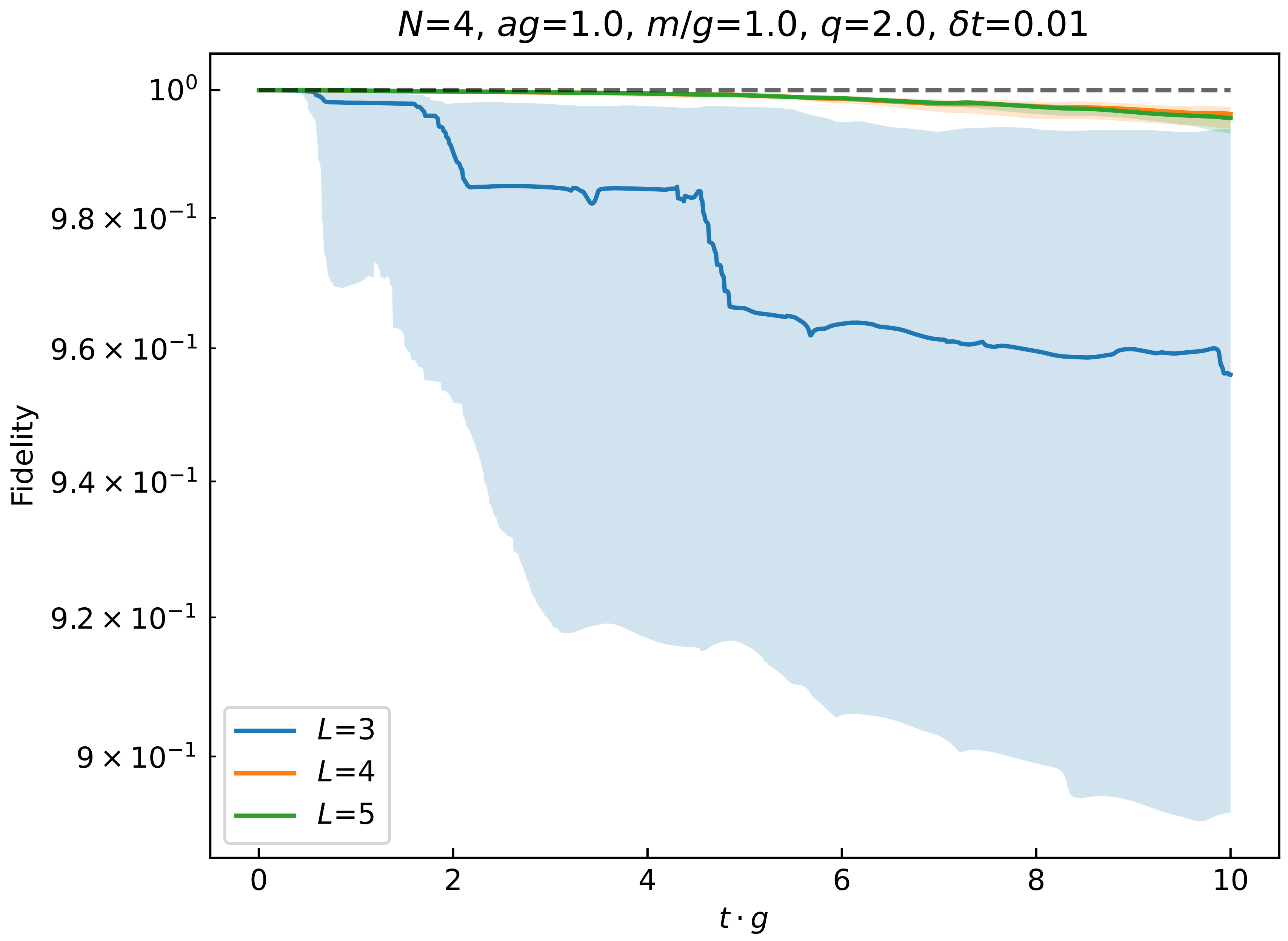


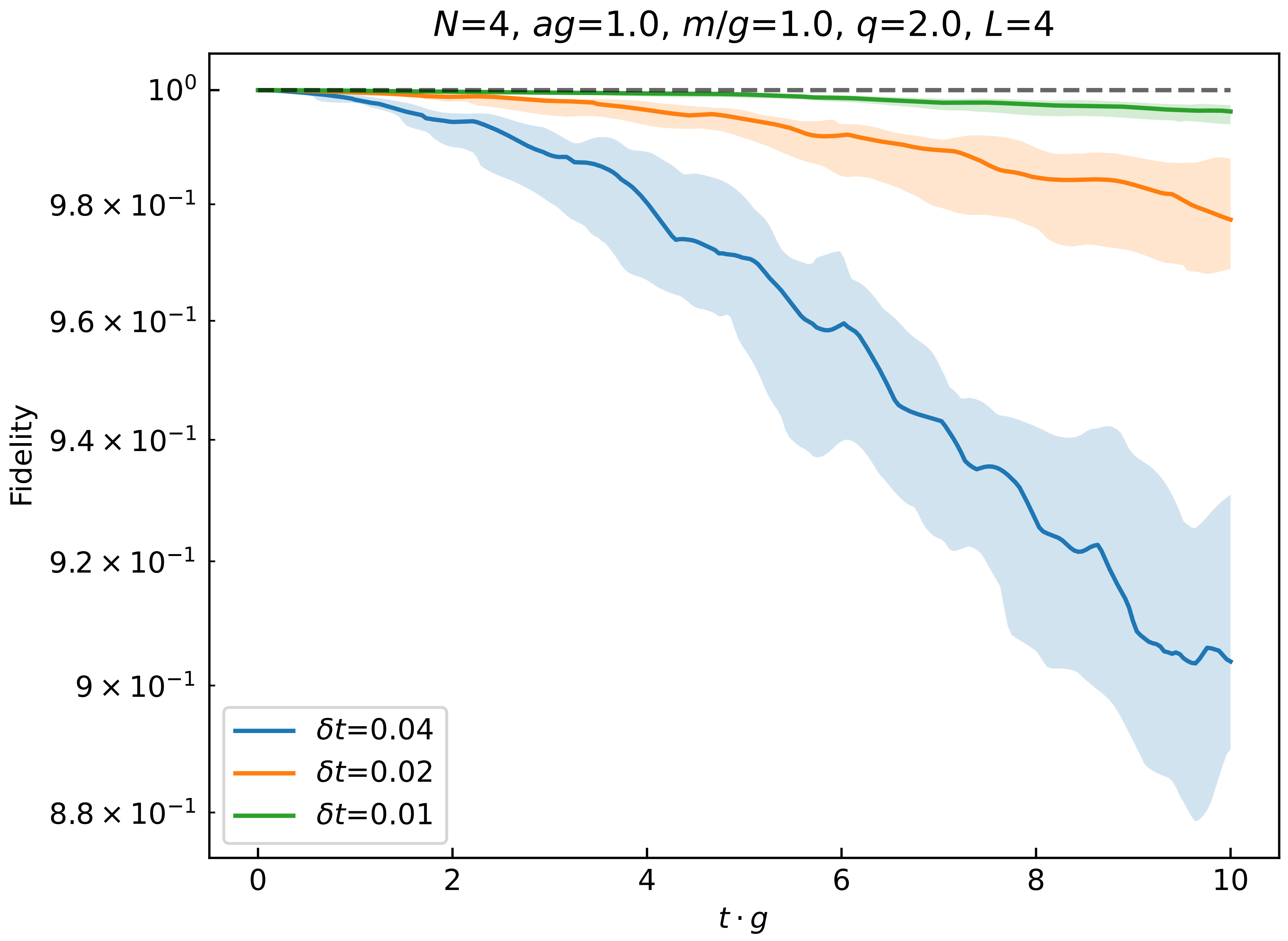
HVA



Fidelity and algorithmic errors

- fidelity improves as increasing L and/or decreasing $\delta t = T_{\rm max}/N_{\rm step}$
- effects from δt is significant





McLachlan's variational principle

$$\delta \left\| \left(\frac{d}{dt} + iH \right) |\psi(\lambda)\rangle \right\| = 0$$

$$\Rightarrow \sum_j M_{ij} \dot{\lambda}_j = V_i$$

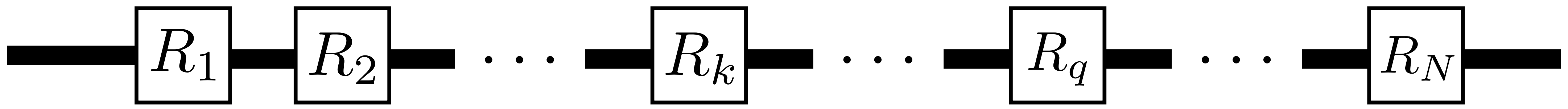
$$M_{ij} = \mathrm{Re} \frac{\partial \langle \psi(\lambda)|}{\partial \lambda_i} \frac{\partial |\psi(\lambda)\rangle}{\partial \lambda_j}$$

$$V_i = \mathrm{Im} \frac{\partial \langle \psi(\lambda)|}{\partial \lambda_i} H |\psi(\lambda)\rangle$$

Quantum circuit for VQS

[Li, Benjamin, Phys. Rev. X 7, 021050 (2017)]
[Yuan et al., Quantum 3, 191 (2019)]

$$U(\lambda) = R_N(\lambda_N) \cdots R_1(\lambda_N)$$



$$|\psi(\lambda)\rangle = U(\lambda)|\psi_0\rangle$$

- evaluation of matrix elements $M_{kq} = \mathrm{Re} \frac{\partial \langle \psi(\lambda)|}{\partial \lambda_k} \frac{\partial |\psi(\lambda)\rangle}{\partial \lambda_q}$
- derivative of each component w.r.t. parameters $\frac{\partial}{\partial \lambda_k} R_k(\lambda) = U_k R_k(\lambda)$
- quantum circuit:

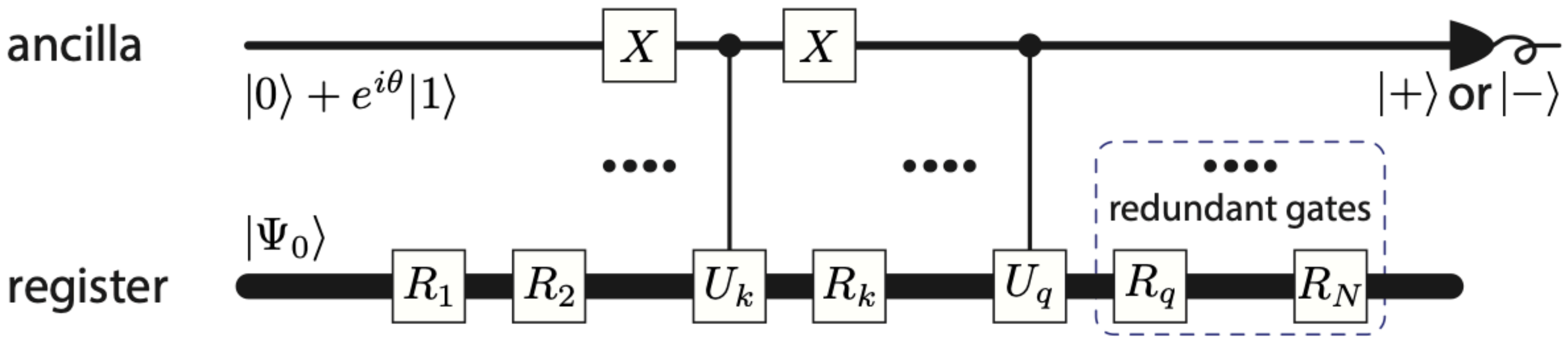


Figure from Yuan et al.