

Conserved charges in the quantum simulation of integrable spin chains

Takuya Okuda

Based on arXiv:2208.00576 (and some extra data)
with K. Maruyoshi, J. Pedersen, R. Suzuki, M. Yamazaki,
and Y. Yoshida

Jan. 18, 2023

Plan of the talk

- Motivations and background
- Integrable Trotterization of XXX spin chain
- Quantum gates and circuits
- Quantum devices
- Simulation results/theoretical analysis
- Summary and conclusions

Motivations and background

- Quantum technologies are developing very fast. Governments and companies are making huge investments. Universities and research institutes are hiring many researchers.
- Currently, we only have noisy intermediate-scale quantum (NISQ) devices. Their abilities are limited by noise (errors) and size.
- People hope for early ($\lesssim 10$ years) practical applications in chemistry (catalyst design) and finance (portfolio optimization).

- We expect that the quantum simulation of many-body systems (condensed matter systems and lattice quantum field theories) will be an important target application in the long term (\gtrsim 10 years).
- We wish to **do something interesting** even with the current quantum computers.
 - Q1: Can we quantify the effects of **quantum noise** using a many-body system?
 - Q2: Is there a way to put **discretization errors** under control?

- Because the realistic lattice gauge theories (such as lattice QCD) are hard to simulate on current devices, we consider a spin chain as a toy model.
- It is generally expected that integrable models provide useful benchmarks for quantum simulation because they allow greater analytical control, even when the system size is so large that classical simulation is impossible.
- Today I report the results of our quantum simulation of the Heisenberg spin $1/2$ XXX spin chain.

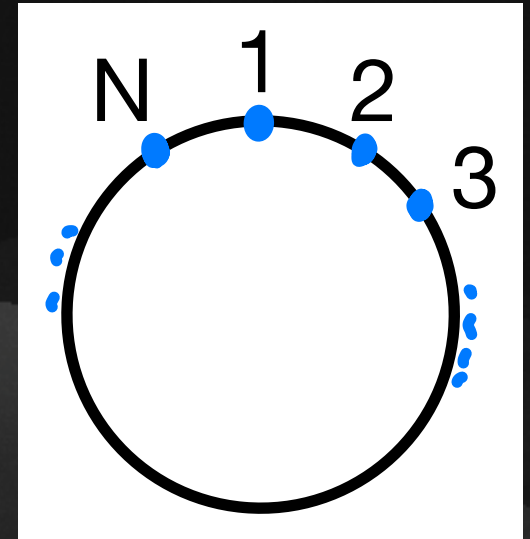
Integrable Trotterization

Integrable Trotterization

[Vanicat, Zadnik & Prosen '17]

- XXX Hamiltonian:

$$H \propto \sum_{j=1}^N \sigma_j \cdot \sigma_{j+1} = H_e + H_o .$$



- Ideally, we want to implement e^{-itH} . This is not possible and we resort to the Suzuki-Trotter **approximation**

$$\sigma \equiv (\sigma_x, \sigma_y, \sigma_z) \equiv (X, Y, Z)$$

$$(e^{-i(t/d)H_e} e^{-i(t/d)H_o})^d = e^{-it(H_e+H_o)}(1 + \mathcal{O}(d^{-1})) .$$

d : number of repetitions \sim depth

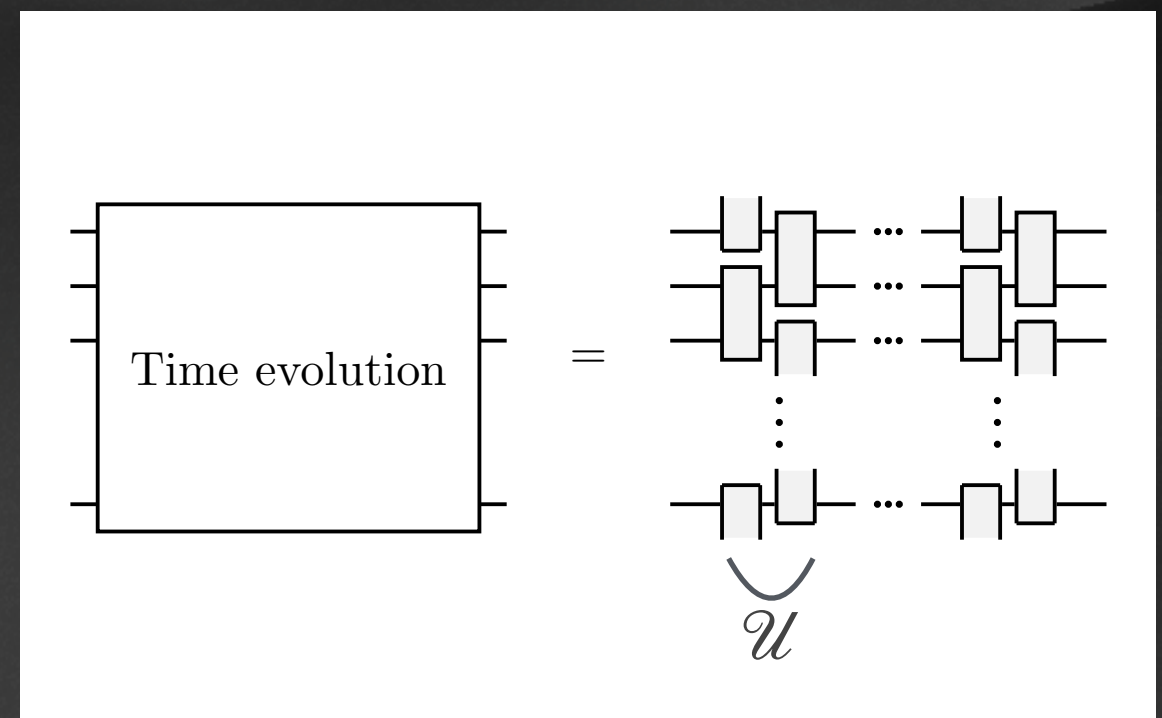
The Trotterized small-time evolution (even N , periodic b.c.) can be expressed in terms of the R(-check) matrix:

$$e^{-i\alpha H_e} e^{-i\alpha H_o} = \left(\prod_{j=1}^{N/2} R_{2j-1,2j}(\delta) \right) \left(\prod_{j=1}^{N/2} R_{2j,2j+1}(\delta) \right) =: \mathcal{U}(\delta),$$

$$R_{ij}(\delta) = (1 + i\delta P_{ij}) / (1 + i\delta)$$

$$= (\text{phase}) e^{i\alpha(X_i X_j + Y_i Y_j + Z_i Z_j)}.$$

$$(\delta = \tan \alpha)$$



Conserved charges

- $\mathcal{U}(\delta)$ commutes with the transfer matrix with specific inhomogeneity

$$T_\delta(\lambda) = \text{tr}_0 \left[\overleftarrow{\prod}_{1 \leq j \leq N} R_{0j}(\lambda - (-1)^j \delta) \right] \text{ for any } \lambda \in \mathbb{C}.$$

- Charges $Q_n^\pm(\delta) \sim \frac{d^n}{d\lambda^n} \log T_\delta(\lambda) \Big|_{\lambda=\pm\delta/2}$ are **exactly conserved** even with Trotterization, which give rise to time-discretization errors for other observables.
- $Q_n^{\text{dif}} \equiv [Q_n^+(\delta) - Q_n^-(\delta)]/\delta$ is also conserved.

- Densities $q_{j,j+1,\dots,j+2n}^{[n,\pm]}$ in higher charges

$$Q_n^+(\delta) = \sum_{j=1}^{N/2} q_{2j-2,2j-1,\dots,2j+2n-2}^{[n,+]}(\delta),$$

$$Q_n^-(\delta) = \sum_{j=1}^{N/2} q_{2j-1,2j,\dots,2j+2n-1}^{[n,-]}(\delta)$$

can be computed via the recursion relation $Q_{n+1}^\pm \sim [B, Q_n^\pm]$ on an infinite chain, where B is a discrete (Lorentz) boost transformation. [Vanicat et al.]

- We implemented the recursion in Mathematica programs.

known

$$q_{1,2,3}^{[1,\pm]}(\delta) = \sigma_1 \cdot \sigma_2 + \sigma_2 \cdot \sigma_3 \mp \delta \sigma_1 \cdot (\sigma_2 \times \sigma_3) + \delta^2 \sigma_2 \cdot \sigma_3,$$

$$q_{1,2,3,4,5}^{[2,\pm]}(\delta) = \mp 2\delta(\sigma_3 \cdot \sigma_4 + \sigma_4 \cdot \sigma_5 - \sigma_3 \cdot \sigma_5) - (1 - \delta^2)\sigma_3 \cdot (\sigma_4 \times \sigma_5) - \sigma_2 \cdot (\sigma_3 \times \sigma_4) - \delta^2 \sigma_2 \cdot (\sigma_3 \times \sigma_5) \\ - \delta^2 \sigma_1 \cdot (\sigma_3 \times \sigma_4) - \delta^4 \sigma_1 \cdot (\sigma_3 \times \sigma_5) \pm \delta \sigma_2 \cdot (\sigma_3 \times \sigma_4 \times \sigma_5) \pm \delta \sigma_1 \cdot (\sigma_2 \times \sigma_3 \times \sigma_4) \\ \pm \delta^3 \sigma_1 \cdot (\sigma_3 \times \sigma_4 \times \sigma_5) \pm \delta^3 \sigma_1 \cdot (\sigma_2 \times \sigma_3 \times \sigma_5) - \delta^2 \sigma_1 \cdot (\sigma_2 \times \sigma_3 \times \sigma_4 \times \sigma_5),$$

$$q_{1,2,3,4,5,6,7}^{[3,+]} = -4\sigma_6 \cdot \sigma_7 + 2\sigma_5 \cdot \sigma_7 - 4\sigma_5 \cdot \sigma_6 + 2\sigma_4 \cdot \sigma_6 + 2\sigma_4 \cdot (\sigma_5 \times \sigma_6 \times \sigma_7) + 2\sigma_3 \cdot (\sigma_4 \times \sigma_5 \times \sigma_6) \\ + \delta \left(10\sigma_5 \cdot (\sigma_6 \times \sigma_7) - 2\sigma_4 \cdot (\sigma_6 \times \sigma_7) - 4\sigma_4 \cdot (\sigma_5 \times \sigma_7) + 8\sigma_4 \cdot (\sigma_5 \times \sigma_6) - 4\sigma_3 \cdot (\sigma_5 \times \sigma_6) \right. \\ \left. - 2\sigma_3 \cdot (\sigma_4 \times \sigma_6) - 4\sigma_3 \cdot (\sigma_4 \times \sigma_5 \times \sigma_6 \times \sigma_7) - 2\sigma_2 \cdot (\sigma_3 \times \sigma_4 \times \sigma_5 \times \sigma_6) \right)$$

new

$$+ \delta^2 \left(2\sigma_6 \cdot \sigma_7 - 10\sigma_5 \cdot \sigma_7 + 2\sigma_5 \cdot \sigma_6 + 2\sigma_4 \cdot \sigma_7 + 2\sigma_4 \cdot \sigma_6 + 2\sigma_3 \cdot \sigma_6 \right. \\ \left. - 6\sigma_4 \cdot (\sigma_5 \times \sigma_6 \times \sigma_7) + 6\sigma_3 \cdot (\sigma_5 \times \sigma_6 \times \sigma_7) + 2\sigma_3 \cdot (\sigma_4 \times \sigma_6 \times \sigma_7) + 6\sigma_3 \cdot (\sigma_4 \times \sigma_5 \times \sigma_7) \right. \\ \left. - 6\sigma_3 \cdot (\sigma_4 \times \sigma_5 \times \sigma_6) + 2\sigma_2 \cdot (\sigma_3 \times \sigma_5 \times \sigma_6) \right. \\ \left. + 2\sigma_2 \cdot (\sigma_3 \times \sigma_4 \times \sigma_5 \times \sigma_6 \times \sigma_7) + 2\sigma_1 \cdot (\sigma_2 \times \sigma_3 \times \sigma_4 \times \sigma_5 \times \sigma_6) \right) \\ + \delta^3 \left(6\sigma_5 \cdot (\sigma_6 \times \sigma_7) - 2\sigma_4 \cdot (\sigma_6 \times \sigma_7) + 4\sigma_4 \cdot (\sigma_5 \times \sigma_7) - 2\sigma_3 \cdot (\sigma_6 \times \sigma_7) - 8\sigma_3 \cdot (\sigma_5 \times \sigma_7) \right. \\ \left. - 2\sigma_3 \cdot (\sigma_4 \times \sigma_6) + 4\sigma_3 \cdot (\sigma_5 \times \sigma_6) - 2\sigma_3 \cdot (\sigma_4 \times \sigma_7) + 4\sigma_3 \cdot (\sigma_4 \times \sigma_5 \times \sigma_6 \times \sigma_7) \right. \\ \left. - 2\sigma_2 \cdot (\sigma_3 \times \sigma_5 \times \sigma_6 \times \sigma_7) - 2\sigma_2 \cdot (\sigma_3 \times \sigma_4 \times \sigma_5 \times \sigma_7) - 2\sigma_1 \cdot (\sigma_3 \times \sigma_4 \times \sigma_5 \times \sigma_6) \right. \\ \left. - 2\sigma_1 \cdot (\sigma_2 \times \sigma_3 \times \sigma_5 \times \sigma_6) - 2\sigma_1 \cdot (\sigma_2 \times \sigma_3 \times \sigma_4 \times \sigma_5 \times \sigma_6 \times \sigma_7) \right) \\ + \delta^4 \left(-2\sigma_6 \cdot \sigma_7 - 8\sigma_5 \cdot \sigma_7 - 2\sigma_5 \cdot \sigma_6 + 2\sigma_4 \cdot \sigma_7 + 2\sigma_3 \cdot \sigma_6 + 2\sigma_3 \cdot \sigma_7 - 2\sigma_3 \cdot (\sigma_5 \times \sigma_6 \times \sigma_7) \right. \\ \left. + 2\sigma_3 \cdot (\sigma_4 \times \sigma_6 \times \sigma_7) - 2\sigma_3 \cdot (\sigma_4 \times \sigma_5 \times \sigma_7) + 2\sigma_2 \cdot (\sigma_3 \times \sigma_5 \times \sigma_7) + 2\sigma_1 \cdot (\sigma_3 \times \sigma_5 \times \sigma_6) \right. \\ \left. + 2\sigma_1 \cdot (\sigma_3 \times \sigma_4 \times \sigma_5 \times \sigma_6 \times \sigma_7) + 2\sigma_1 \cdot (\sigma_2 \times \sigma_3 \times \sigma_5 \times \sigma_6 \times \sigma_7) + 2\sigma_1 \cdot (\sigma_2 \times \sigma_3 \times \sigma_4 \times \sigma_5 \times \sigma_7) \right) \\ + \delta^5 \left(4\sigma_5 \cdot (\sigma_6 \times \sigma_7) - 2\sigma_3 \cdot (\sigma_6 \times \sigma_7) - 2\sigma_3 \cdot (\sigma_4 \times \sigma_7) - 2\sigma_1 \cdot (\sigma_3 \times \sigma_5 \times \sigma_6 \times \sigma_7) \right. \\ \left. - 2\sigma_1 \cdot (\sigma_3 \times \sigma_4 \times \sigma_5 \times \sigma_7) - 2\sigma_1 \cdot (\sigma_2 \times \sigma_3 \times \sigma_5 \times \sigma_7) \right) \\ + \delta^6 \left(-4\sigma_5 \cdot \sigma_7 + 2\sigma_3 \cdot \sigma_7 + 2\sigma_1 \cdot (\sigma_3 \times \sigma_5 \times \sigma_7) \right).$$

Densities and charges are traceless.

Here $\sigma_1 \cdot (\sigma_2 \times \sigma_3 \times \cdots \times \sigma_{\ell-1} \times \sigma_{\ell}) := \sigma_1 \cdot (\sigma_2 \times (\sigma_3 \times (\cdots \times (\sigma_{\ell-1} \times \sigma_{\ell}) \cdots)))$

Basics of quantum gates and circuits

Qubits

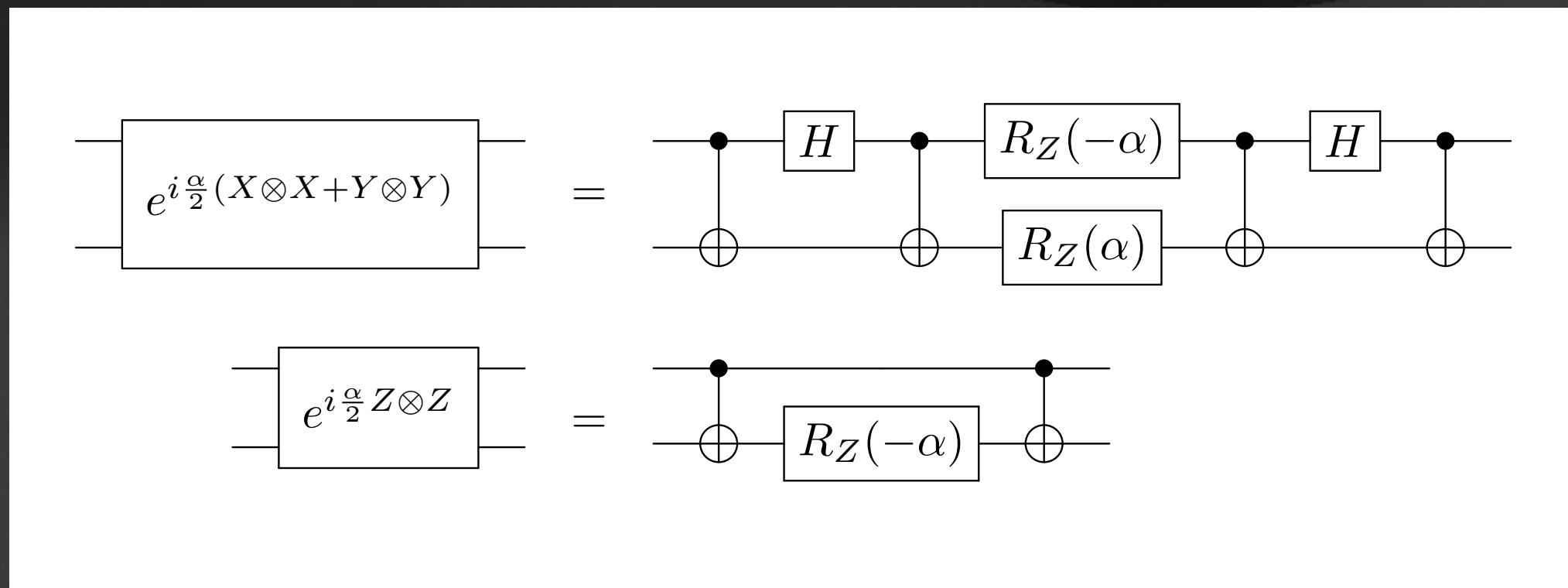
- A quantum computer comes with qubits.
- Each qubit is a 2-dimensional complex vector space spanned by the eigenstates $|0\rangle$ and $|1\rangle$ of Z with eigenvalues 1 and -1 .

Quantum gates

Gates are unitary transformations that act on a single qubit or multiplet qubits. We use

- Pauli gates X , Y , and Z ,
- Z-rotation $R_Z(\alpha) = e^{-i(\alpha/2)Z}$,
- Hadamard gate $H = 2^{-1/2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, $X \leftrightarrow Z$,
- Phase gate $S = \text{diag}(1, i)$, $X \leftrightarrow Y$,
- “controlled X ” = $CX = CNOT$: $CX_{12} |s_1, s_2\rangle = (X_2)^{s_1} |s_1, s_2\rangle$
($s_1, s_2 \in \{0, 1\}$).

The R matrix $R_{ij}(\delta) = (\text{phase})e^{i\alpha(X_iX_j+Y_iY_j+Z_iZ_j)}$ can be implemented by elementary gates.

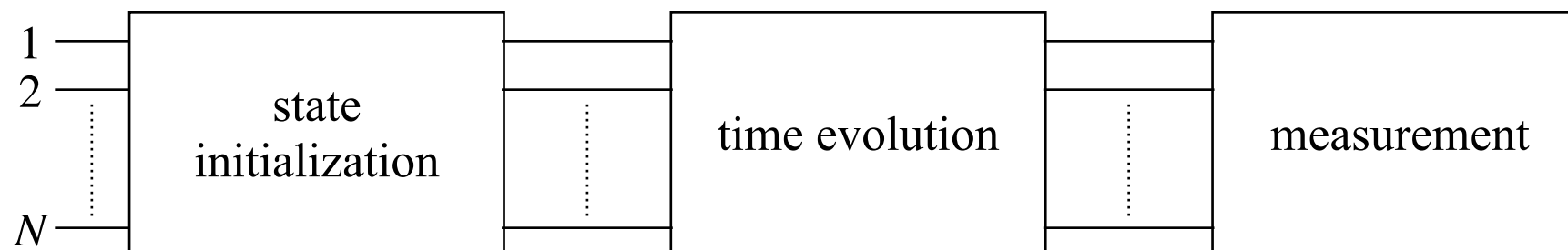


Quantum circuit

- Initialization: by default the quantum device prepares $|00\dots 0\rangle$. We further apply some of H , S , and Pauli gates (X , Y , and Z) to prepare a simultaneous eigenstate $|s_1\dots s_N\rangle_{P_1\dots P_N}$ of $P_i \in \{X, Y, Z\}$ with eigenvalues $(-1)^{s_i}$.
- Time evolution: d repetitions of

$$\mathcal{U}(\delta) = \left(\prod_{j=1}^{N/2} R_{2j-1,2j}(\delta) \right) \left(\prod_{j=1}^{N/2} R_{2j,2j+1}(\delta) \right).$$

- Measurement: we measure the eigenvalue of X , Y , or Z for each qubit.



Estimating observables

- One can compute (estimate) the expectation value of a charge

$$Q = \sum_{P \in \{I, X, Y, Z\}^{\otimes N}} c_{Q,P} P, \quad c_{Q,P} \in \mathbb{C},$$

from the measurement results in various measurement bases.

- See our paper for concrete formulas (no originality claimed) for the expectation value and the statistical uncertainty.

Quantum devices

IBM: Superconducting devices

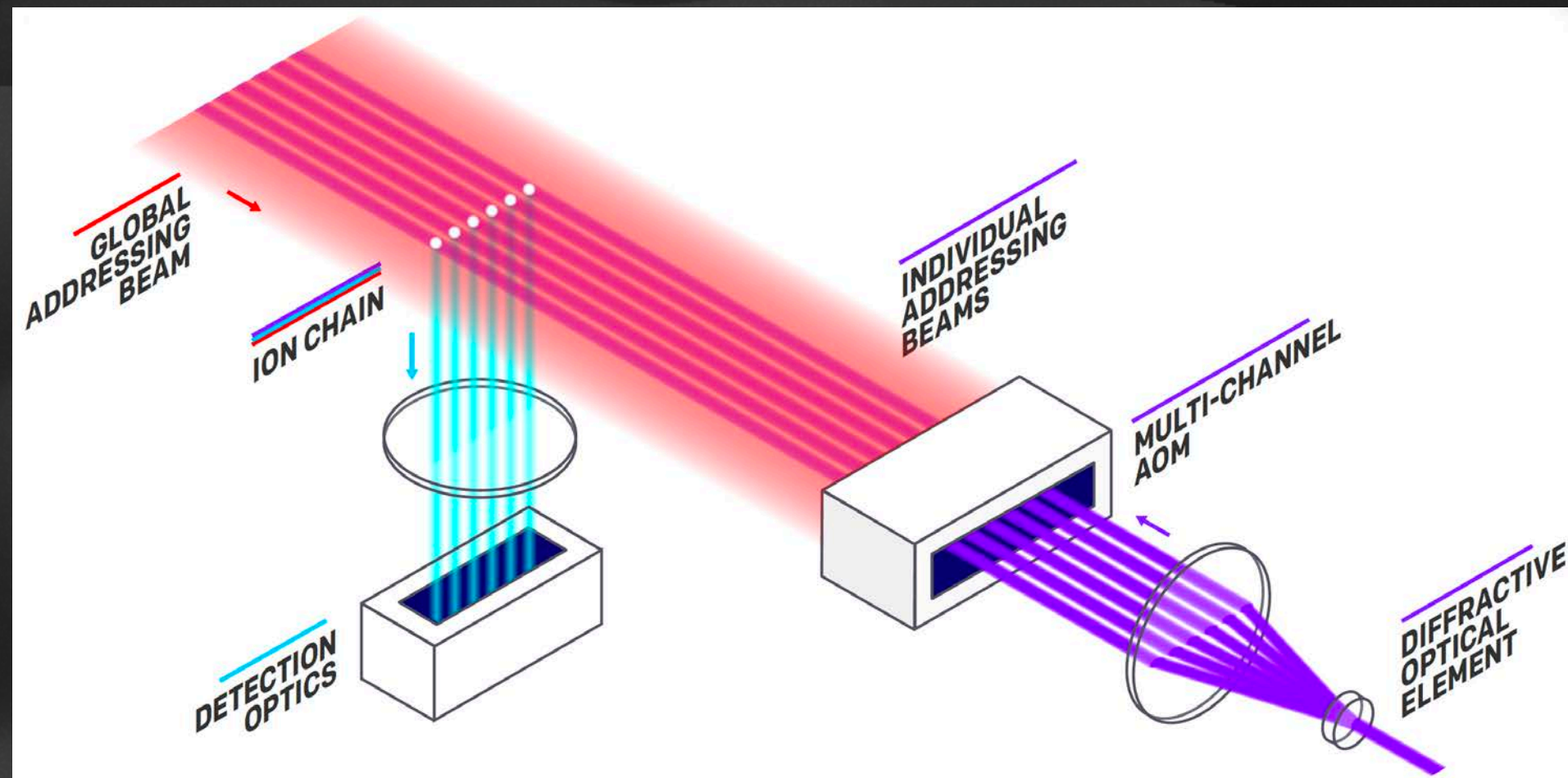
- IBM uses superconducting transmon qubits. These are made of materials such as niobium and aluminum placed on a silicon chip. Two energy-levels form an approximate qubit.
- We obtained access to the devices through the University of Tokyo. (Supported by UTokyo Quantum Initiative).
- We used the `ibm_kawasaki` and `ibm_washington` processors.



IonQ: trapped ion devices

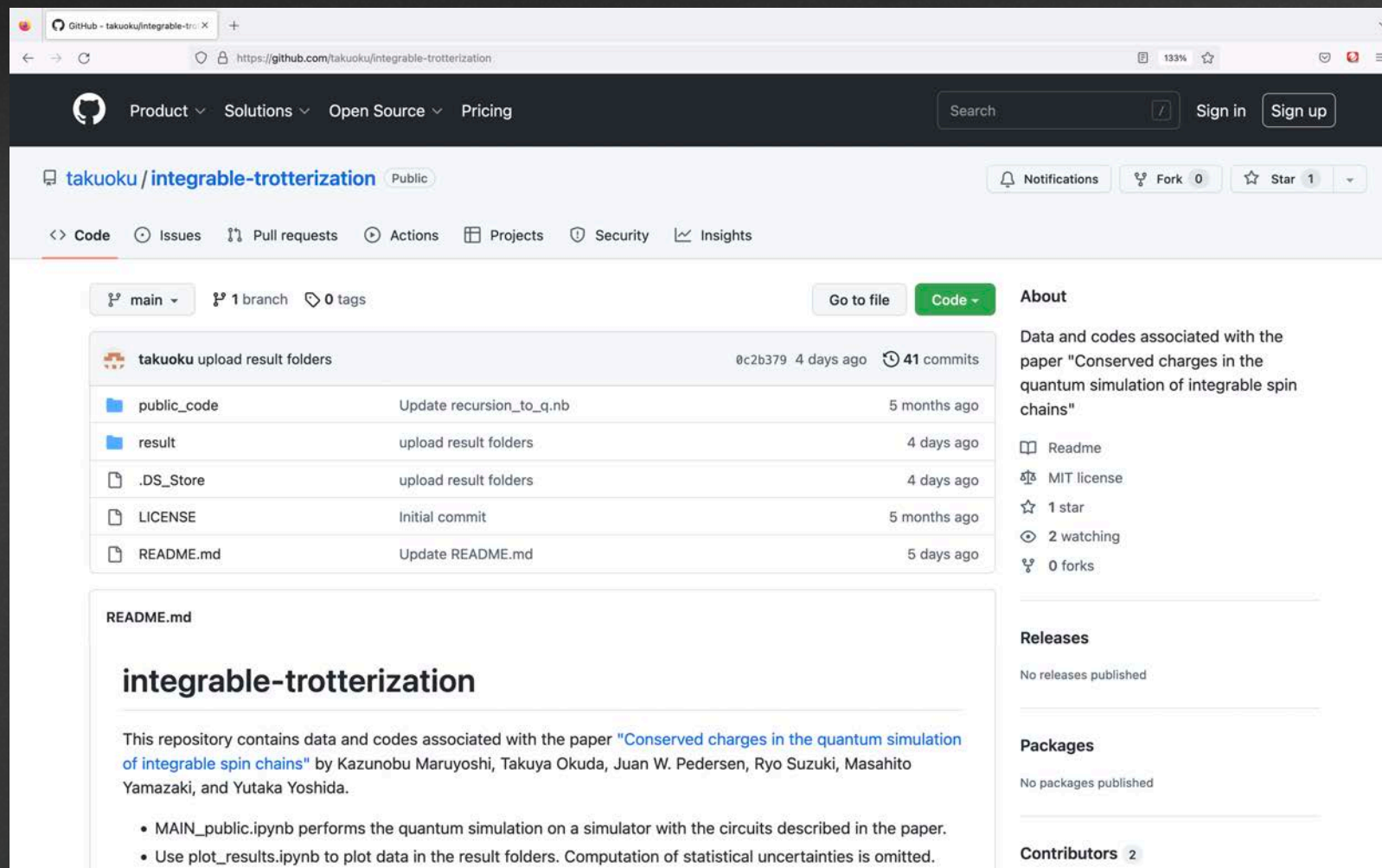
- We mainly used IonQ's device called Harmony. (Not in the current version of the e-print.)
- A linear chain of $^{171}\text{Yb}^+$ ions near an electrode trap.

- 11 qubits with all-to-all couplings.
- We got indirect access through Google Cloud and direct access through IonQ itself.



Cloud access via Qiskit

- We used the SDK called Qiskit to control the IBM and IonQ quantum computers.
- Our (mostly Python) programs are available via a GitHub repository.

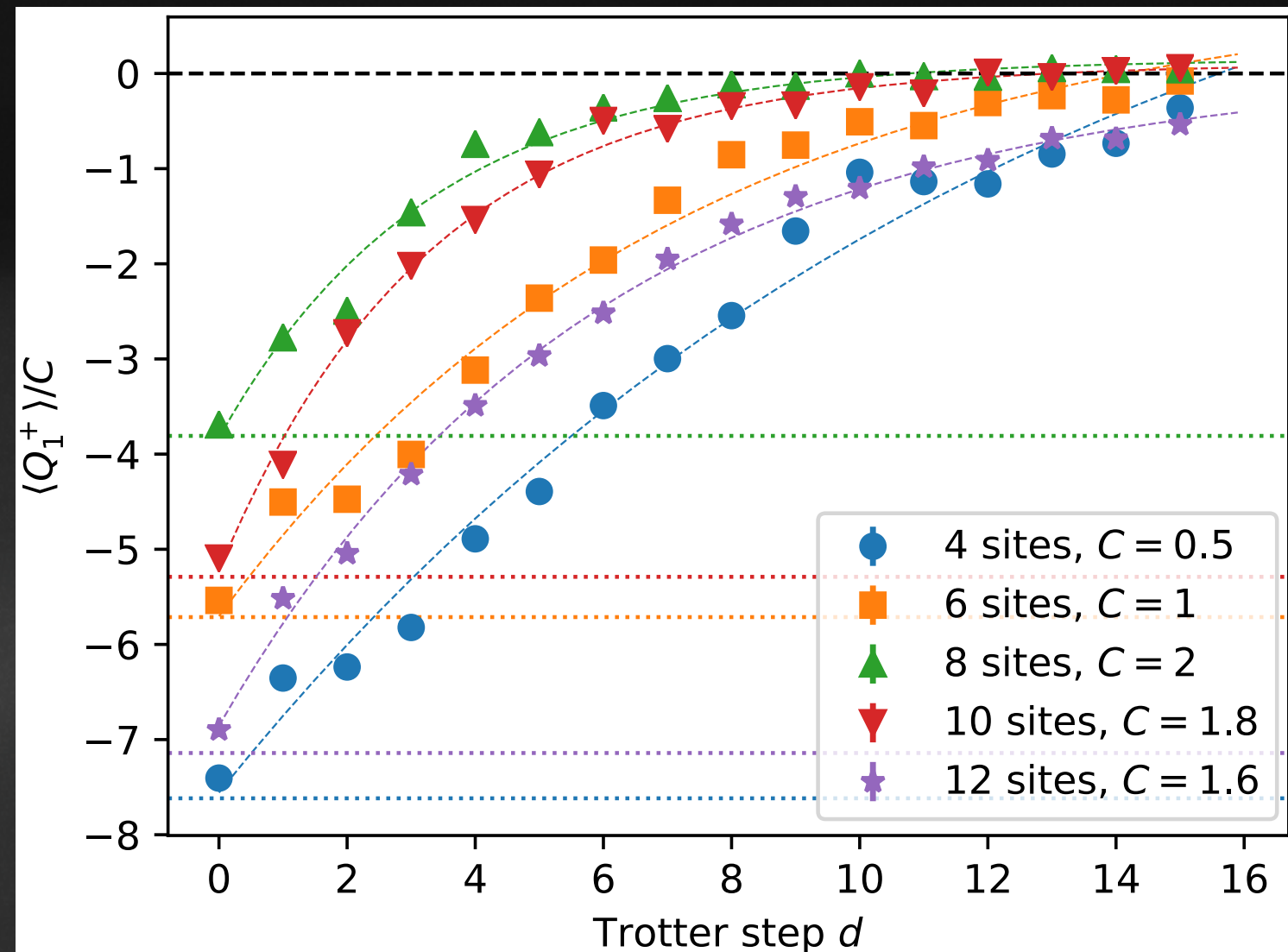


The screenshot shows a GitHub repository page for 'takuoku/integrable-trotterization'. The repository is public and has 1 star, 0 forks, and 2 watchers. The main branch is 'main' with 1 branch and 0 tags. The repository contains several files and folders, including 'public_code', 'result', '.DS_Store', 'LICENSE', and 'README.md'. The README.md file is displayed, containing the title 'integrable-trotterization' and a description of the repository's contents, which are associated with a paper titled 'Conserved charges in the quantum simulation of integrable spin chains' by Kazunobu Maruyoshi, Takuya Okuda, Juan W. Pedersen, Ryo Suzuki, Masahito Yamazaki, and Yutaka Yoshida. The README also lists two bullet points: 'MAIN_public.ipynb performs the quantum simulation on a simulator with the circuits described in the paper.' and 'Use plot_results.ipynb to plot data in the result folders. Computation of statistical uncertainties is omitted.'

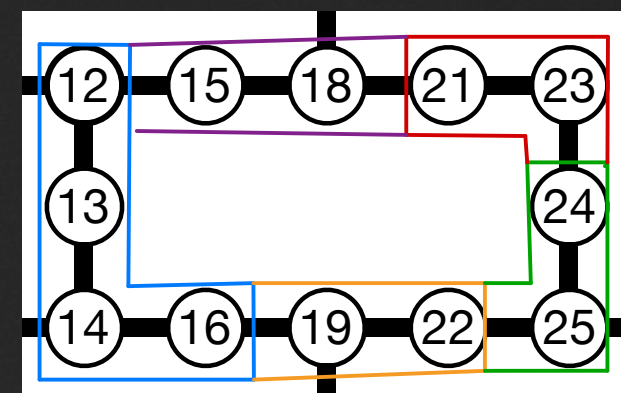
Results of real-device simulations

Simulation results for ibm_kawasaki

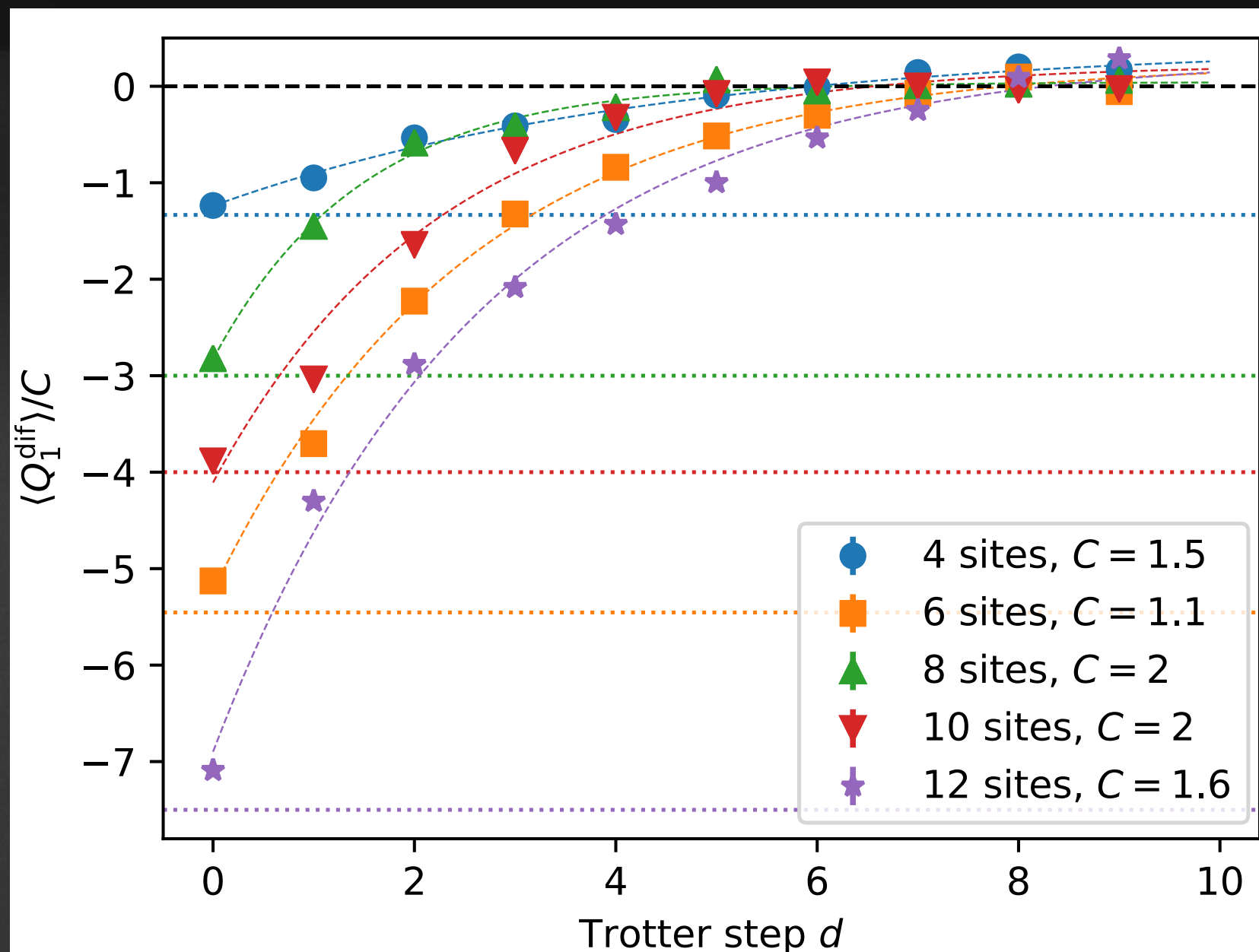
- $\langle Q_1^+ \rangle = \text{tr}(\rho Q_1^+)$ decays exponentially to zero asymptotically, due to noise. No error mitigation.
- Error bars are hidden by markers. Rescaled for better visibility. The theoretical values are shown by dotted lines. Fit by $c_1 e^{-\gamma d} + c_2$.
- The initial state is $|0101\dots 01\rangle$.
- Large fluctuations from one step to the next. (Due to change in device parameters?)



Only the 12-site simulation is for a circular topology.

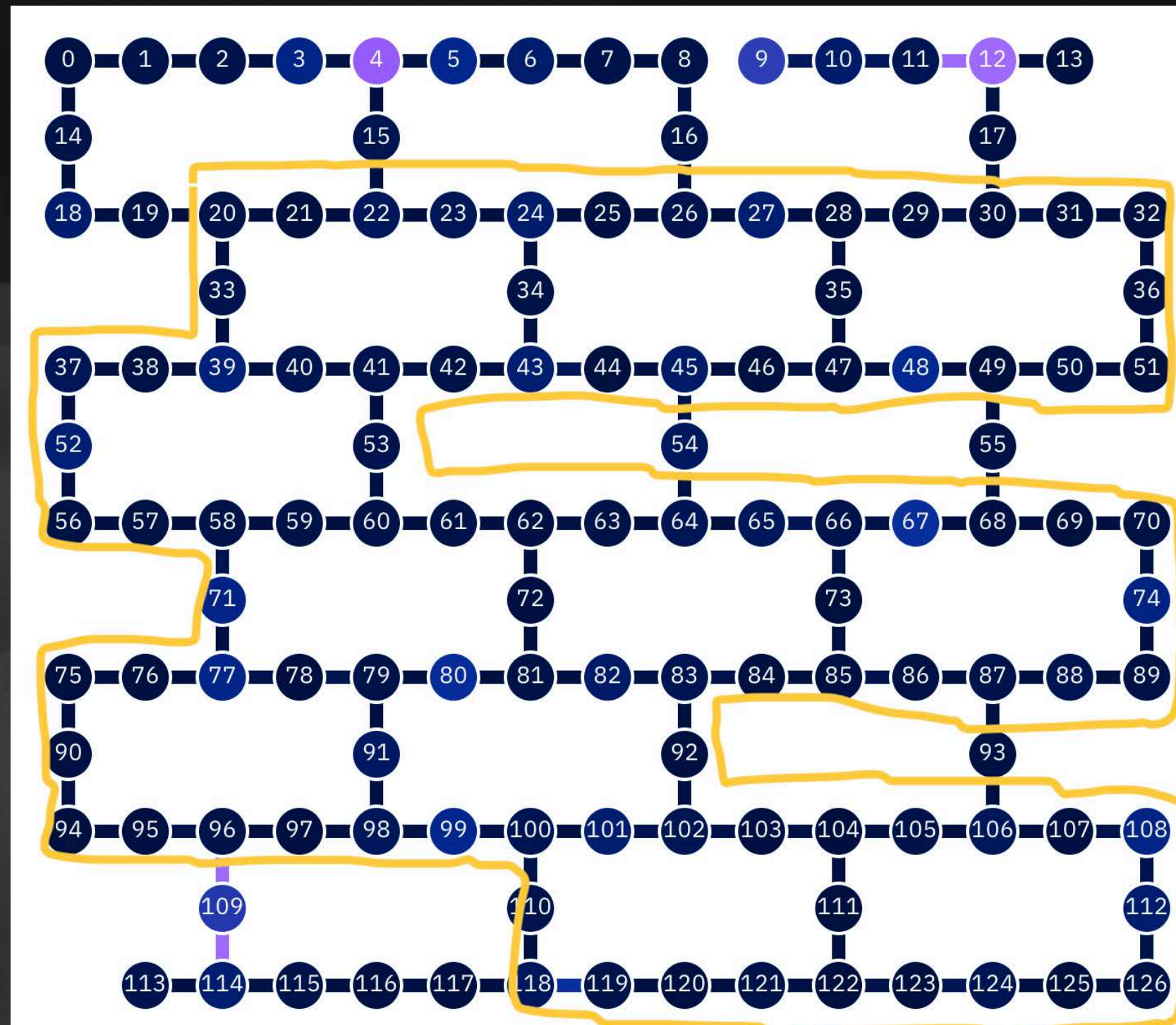


- Similar results for $Q_1^{\text{dif}} = [Q_1^+(\delta) - Q_1^-(\delta)]/2$.
- The initial states are chosen appropriately to give non-zero theoretical expectation values.



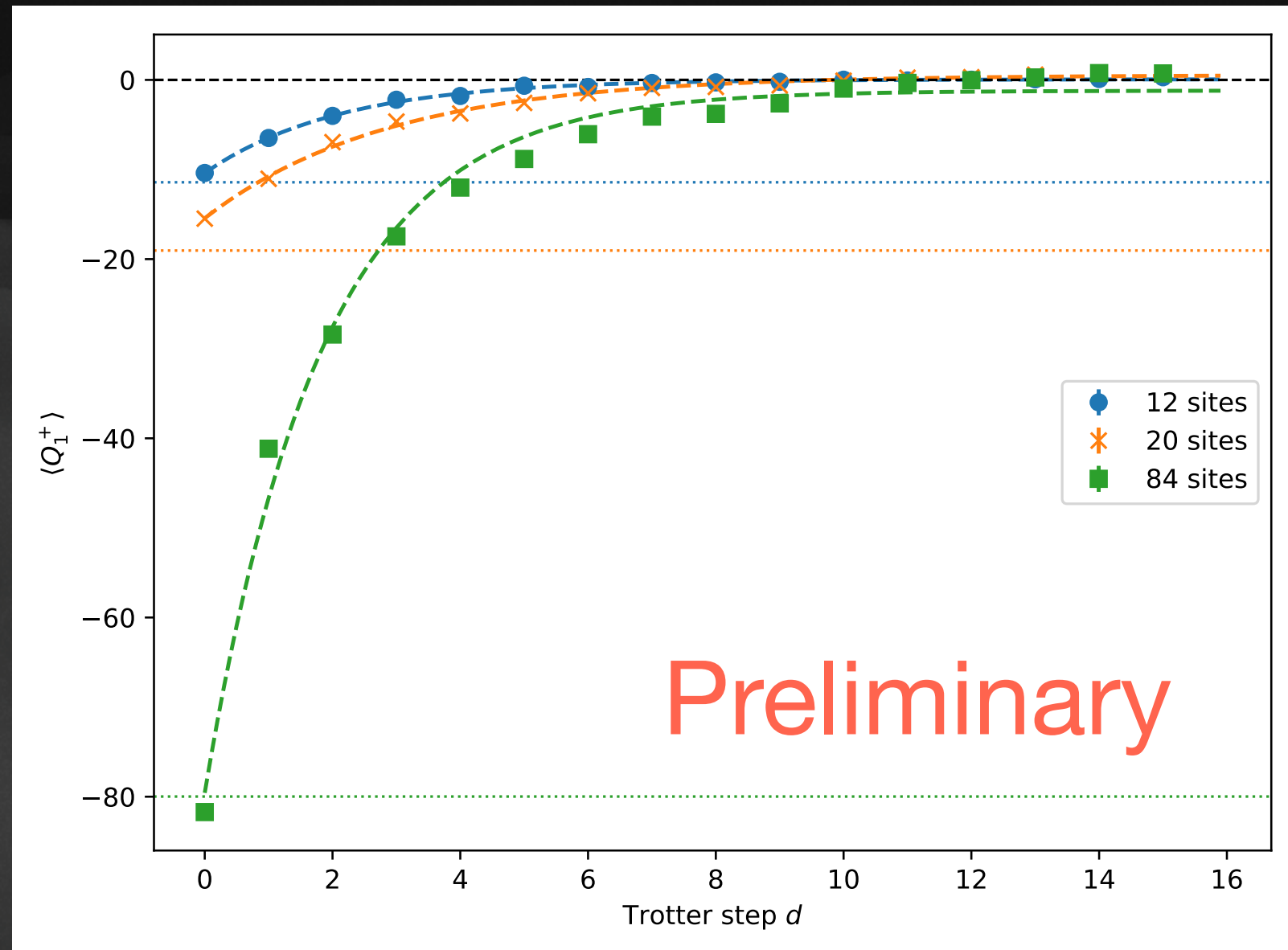
Simulations on a 127-qubit IBM device

- Quantum device `ibm_washington` with 127 qubits.
- We ran simulations with qubits on loops of size 12, 20, and 84. The 84-qubit loop is shown in the figure.
- To have slower decays, it is important to avoid faulty (purple) qubits and connections.



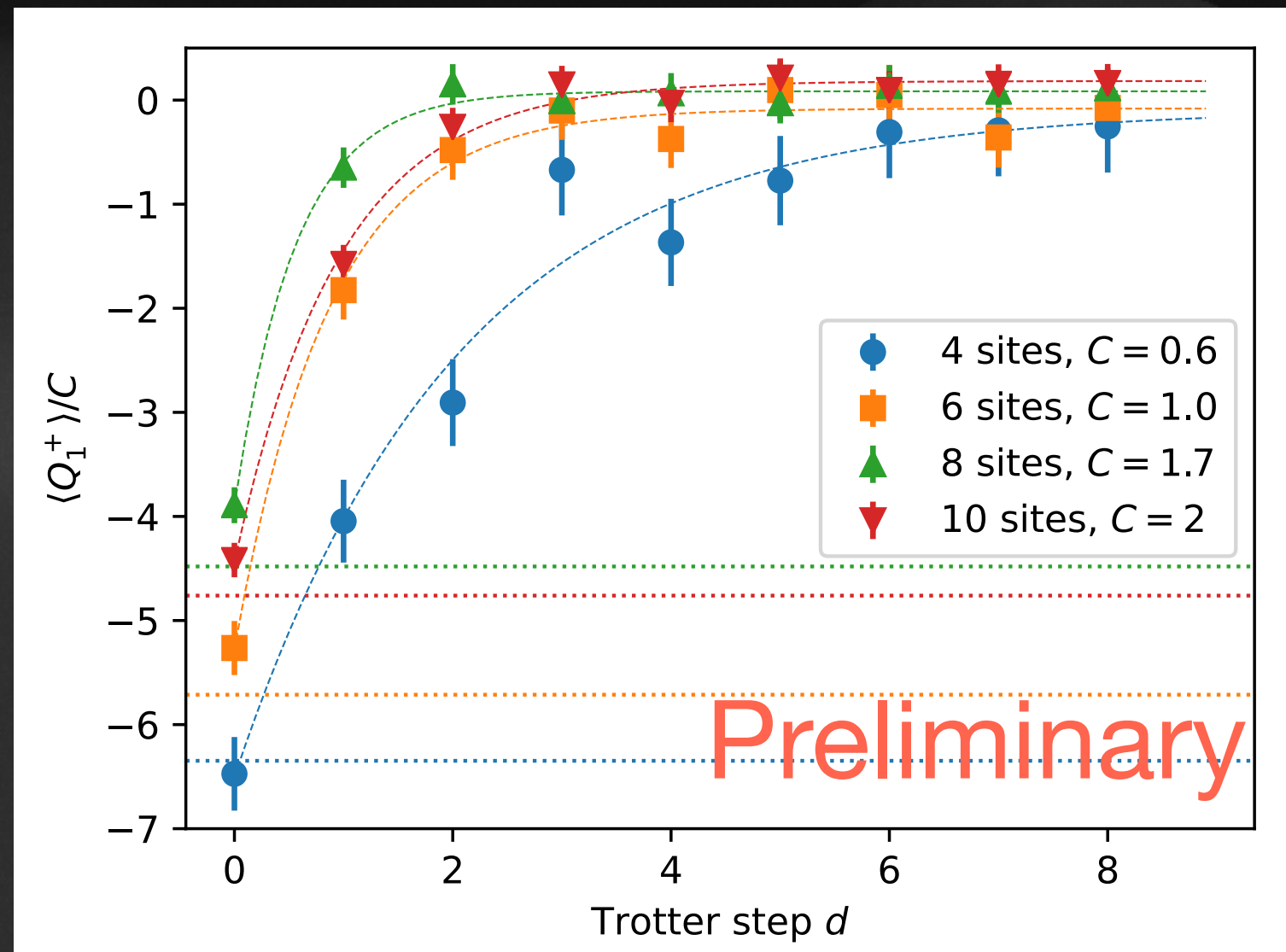
Simulation results on large chains

- Loops of size 12, 20, and 84.
- Similar exponential decays of $\langle Q_1^+ \rangle$.
- For the 84-site run, we had 10^6 shots (circuit executions) for each value of d .
- (There were significant time gaps between some data.)
- (Not in the current version of the e-print.)



Simulation results for IonQ Harmony

- Similar exponential decays.
- To have slower decays, it seems important to use the qubits (ions) in the middle of the linear chain.



Simulator results and theoretical analysis

Numerical noise models

- We ran digital quantum simulations on the Qiskit (classical) simulator with noise models.
- We considered two noise models:
 1. (1-qubit) depolarizing error channels inserted after 1- and 2-qubit gate operations.
 2. (1-qubit) amplitude-and-phase damping error channels inserted after 1- and 2-qubit gate operations.

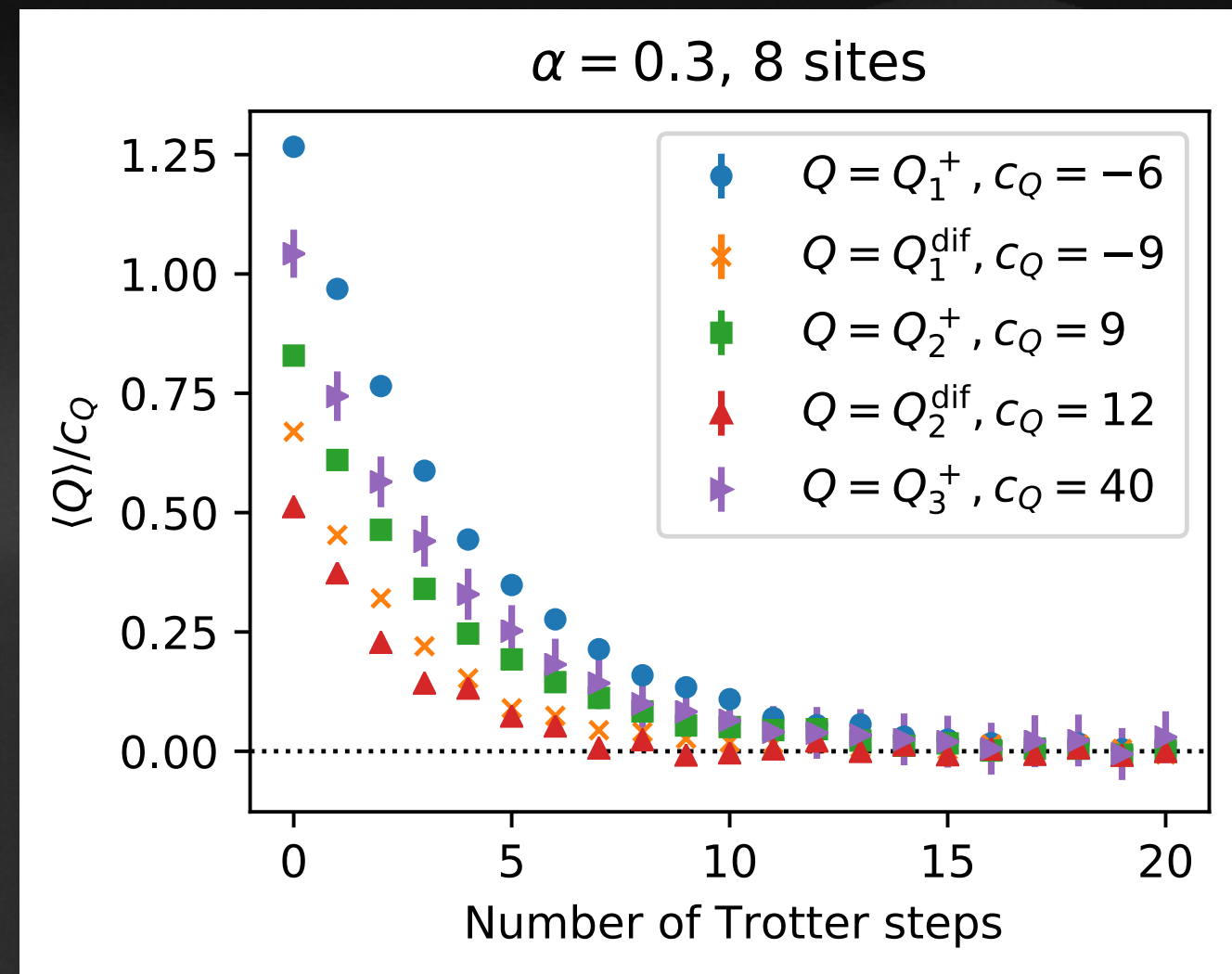
Classical emulation of quantum simulation with a depolarizing noise model

- $$\Phi_{\text{depo}}(\rho) = \sum_{j=1}^4 D_j \rho D_j^\dagger$$
 with

$$D_1 = \sqrt{1 - \frac{3p}{4}} I, \quad D_2 = \sqrt{\frac{p}{4}} X,$$

$$D_3 = \sqrt{\frac{p}{4}} Y, \quad D_4 = \sqrt{\frac{p}{4}} Z$$
 inserted after gate operations.

- $\langle Q_j^+ \rangle$ and $\langle Q_j^{\text{dif}} \rangle$ decay exponentially to zero. This suggests that the finite state is completely mixed.



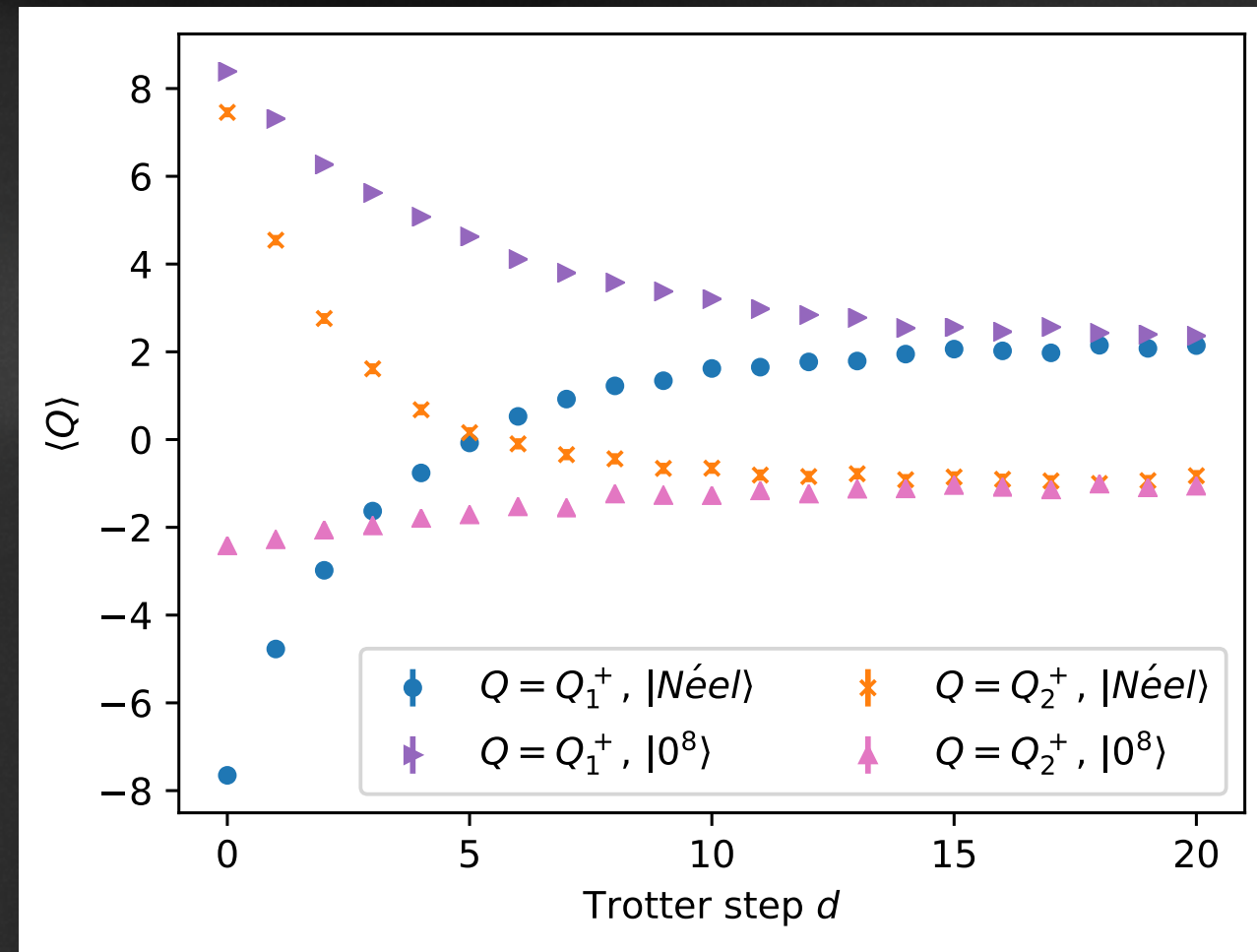
Classical emulation of quantum simulation with an amplitude-and-phase damping noise model

- $$\Phi_{\text{damp}}(\rho) = \sum_{j=1}^3 D_j \rho D_j^\dagger$$
 with

$$D_1 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1 - \lambda_a - \lambda_p} \end{pmatrix},$$

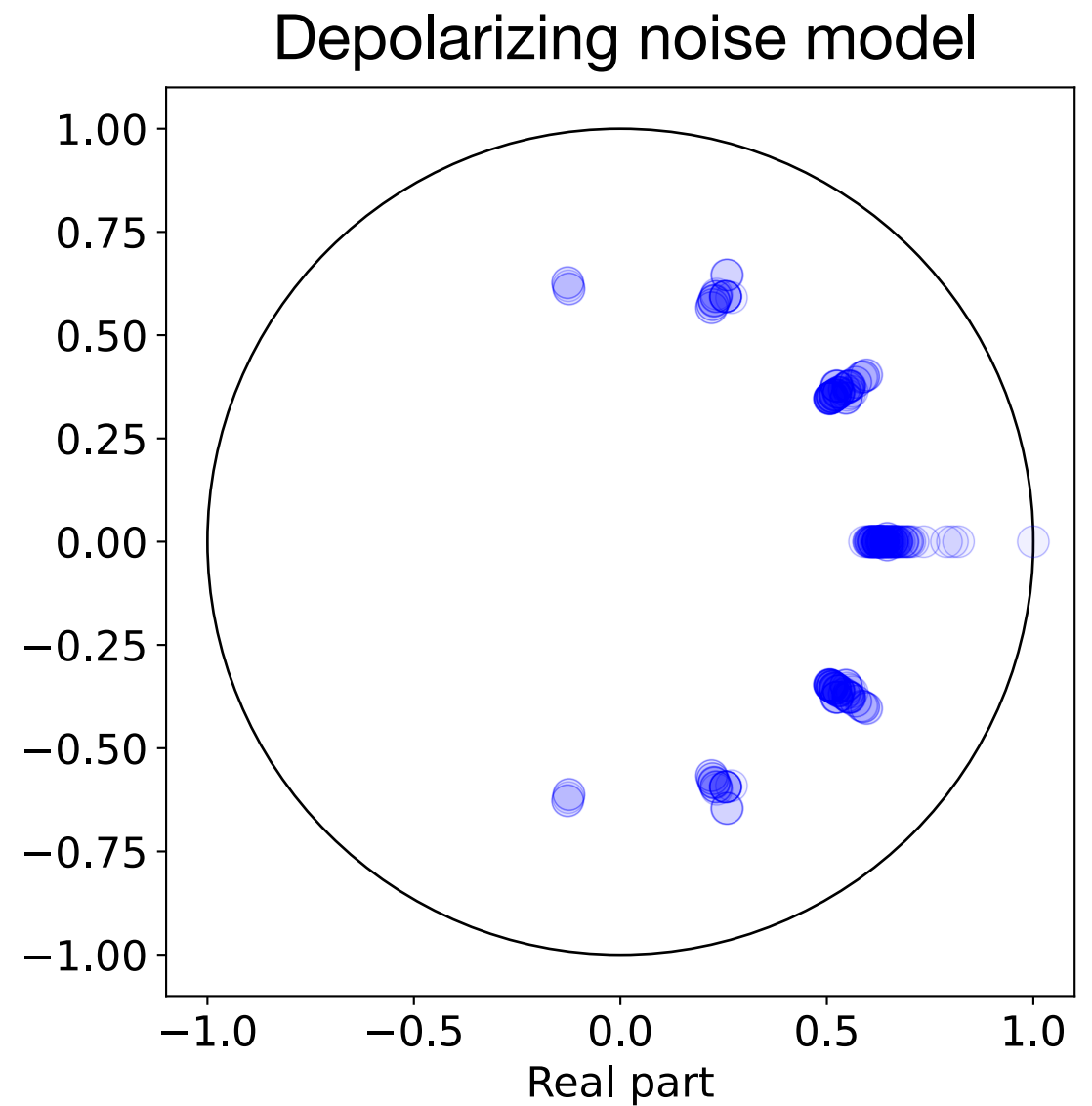
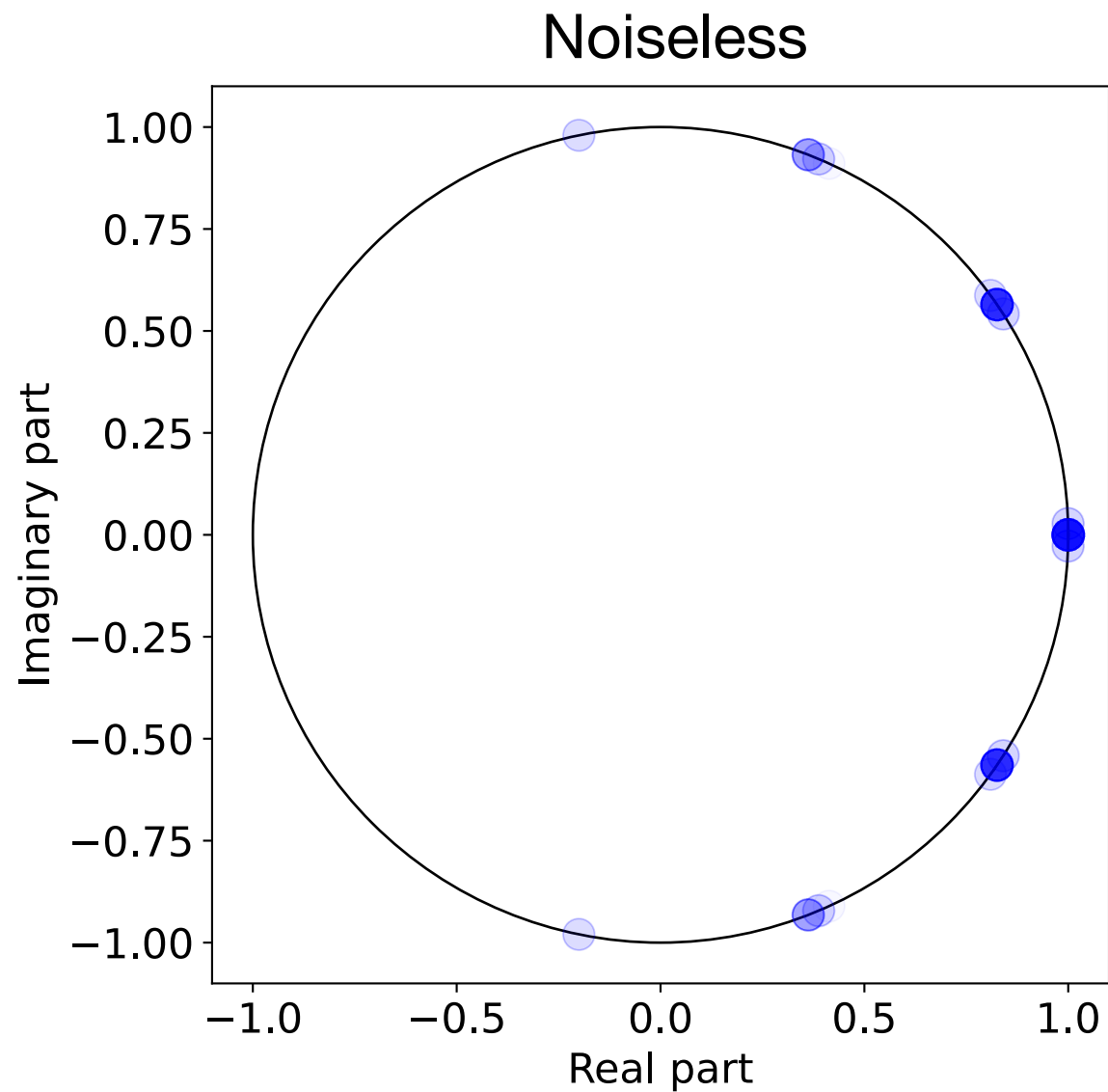
$$D_2 = \begin{pmatrix} 0 & \sqrt{\lambda_a} \\ 0 & 0 \end{pmatrix}, \quad D_3 = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{\lambda_p} \end{pmatrix}$$
 inserted after gate operations.

- $\langle Q_j^+ \rangle$ (and $\langle Q_j^{\text{dif}} \rangle$) asymptote to finite values. The finite state is unique and is NOT completely mixed. Checked by quantum tomography.



Analysis fo quantum channels

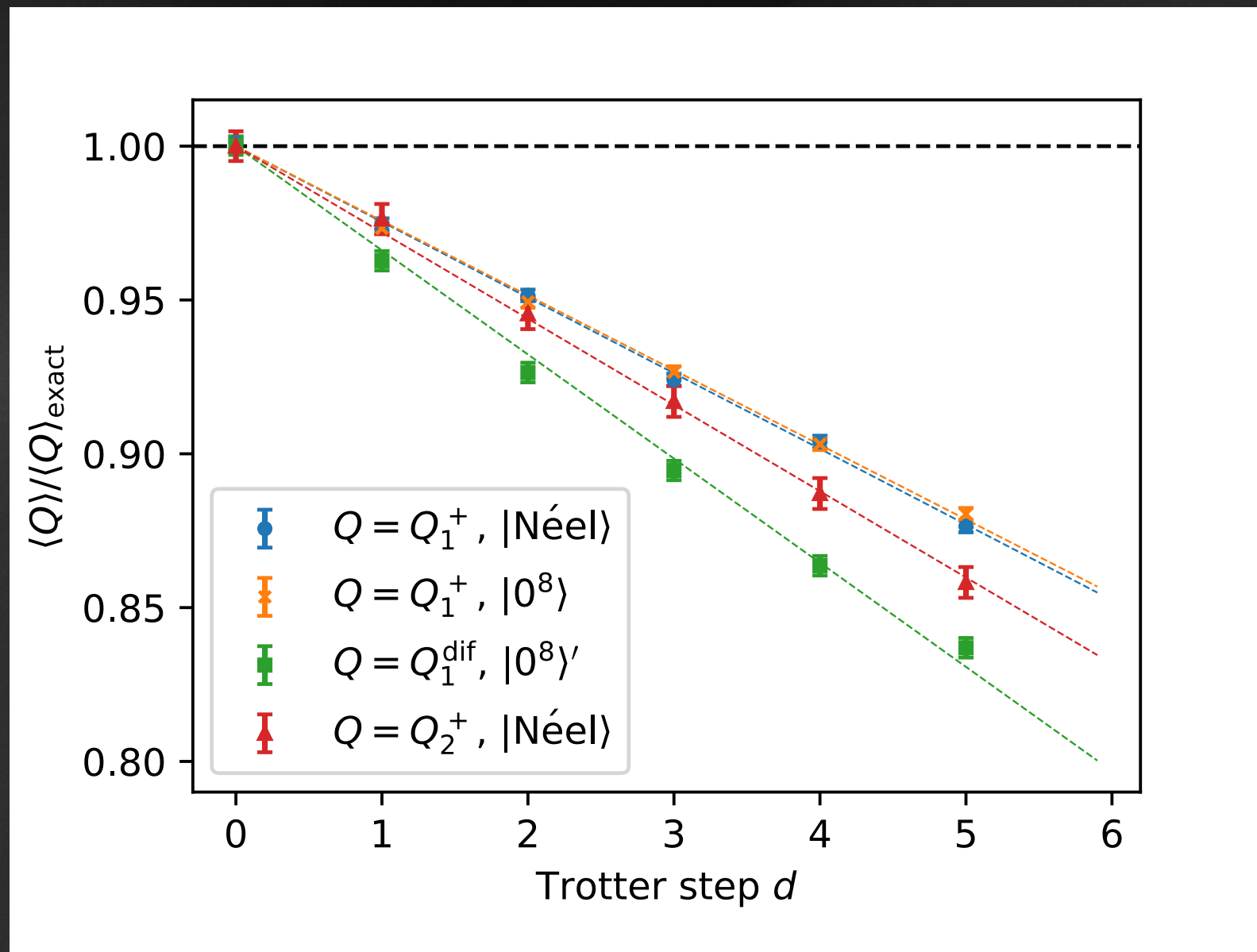
- The initial state $\rho_0 = |\psi_0\rangle\langle\psi_0|$ is mapped, at Trotter step d , to $\Phi^d(\rho)$, where Φ is a noisy time evolution for a single step.
- The expectation value of a conserved charge Q at step d is $\langle Q \rangle_d = \text{tr}[\Phi^d(\rho)Q]$.
- We studied the eigenvalue distribution of the linear map $\rho \rightarrow \Phi(\rho)$.



- The eigenvalues for the single time step Φ on 4 sites.
- In the noiseless case, the evolution is unitary and the eigenvalues are on a unit circle.
- In the depolarizing noise model, all the eigenvalues except one are strictly inside the unit circle. There remains a single eigenvalue 1, corresponding to the unique fixed point (completely mixed state) of Φ .

Possible use of conserved charges as benchmarks for future quantum computing

- For future quantum devices we expect smaller error rates. We propose to use the higher conserved charges of the integrable Trotterization as benchmarks.
- On a classical simulator, we numerically computed the time evolution on 8 sites.
- The slopes of early-time decays depend on the types and the degrees of the charges.



Summary and conclusions

- We implemented the integrable Trotterization of the Heisenberg spin $1/2$ XXX spin chain on real quantum computers and on classical simulators. We used superconducting devices of IBM and trapped ion devices of IonQ.
- As expected, conserved charges decay due to noise on the current quantum devices.
- The early-time decay rate seems to depend on the type and the degree of the charge. Higher charges are candidates of benchmarks for the future quantum simulation.