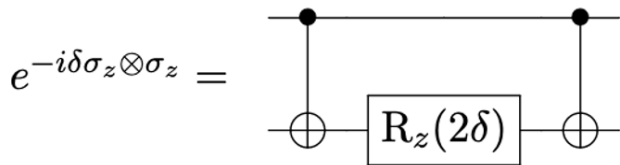

Solving Many-Body Problems on Quantum Computers

DQS: Solving the Schrödinger equation

- Step 1: Map the Hamiltonian onto an equivalent Pauli Hamiltonian
- Step 2: Decompose terms in Pauli Hamiltonian to native gate set.
- Step 3: Run time evolution circuit, measure observables and map back to original model



Great! Problem solved, right?

NISQ era

- Modern Quantum Computers are: **Noisy Intermediate-Scale Quantum (NISQ)** devices

Despite noise: Quantum Utility?

- > 100 Qubit kicked Ising time evolution
- But: reproduced by Tensor Networks

But we see progress

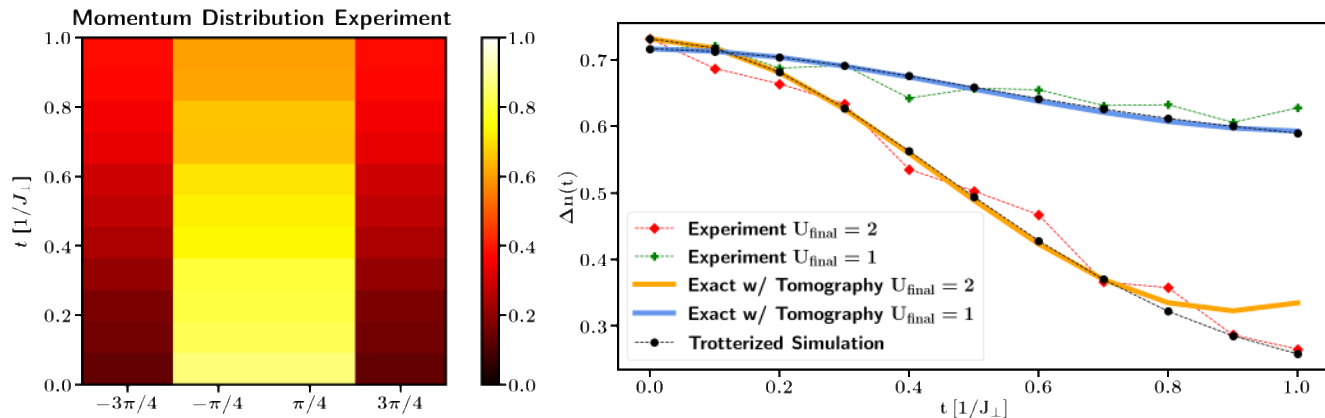
- Simulation of Spin plaquette and spin chain under a time-dependent magnetic field pulse

$$\mathcal{H} = \sum_{\langle i,j \rangle} J_{\perp} (S_i^x S_j^x + S_i^y S_j^y) + J_z S_i^z S_j^z + \sum_i \vec{H}_i(t) \vec{S}_i$$

Fauseweh, B., Zhu, JX. Digital quantum simulation of non-equilibrium quantum many-body systems. *Quantum Inf Process* **20**, 138 (2021).
<https://doi.org/10.1007/s11128-021-03079-z>

Simulation of strongly interacting fermions

- Observable: Momentum distribution and jump at Fermi Surface



Fauseweh, B., Zhu, JX.
Digital quantum
simulation of non-
equilibrium quantum
many-body systems.
Quantum Inf Process
20, 138 (2021).
<https://doi.org/10.1007/s11128-021-03079-z>

- The competition does not sleep, one month after posting our paper:

The right application!

Fauseweh, B. Quantum many-body simulations on digital quantum computers: State-of-the-art and future challenges. *Nat Commun* **15**, 2123 (2024). <https://doi.org/10.1038/s41467-024-46402-9>

- What problems can be tackled with digital quantum simulation to show quantum advantage?
 - Qualitative > Quantitative
 - Nonequilibrium > Equilibrium
 - 2D > 1D (large clusters > small clusters)

Application 1: Quantum computing Floquet bands

- Can we use quantum computers to describe time-periodically driven systems?

Use of Floquet theorem + parameterized quantum circuits

$$H(t) = H(t + T) \quad \Longrightarrow \quad |\Psi_\alpha(t)\rangle = |\Phi_\alpha(t)\rangle e^{-i\epsilon_\alpha t}, \quad |\Phi_\alpha(t + T)\rangle = |\Phi_\alpha(t)\rangle$$

Floquet quasi-energy

Floquet mode

- Use time evolution operator over full period

$$U_T |\Psi_\alpha(0)\rangle = |\Psi_\alpha(T)\rangle = e^{-i\epsilon_\alpha T} |\Psi_\alpha(0)\rangle$$

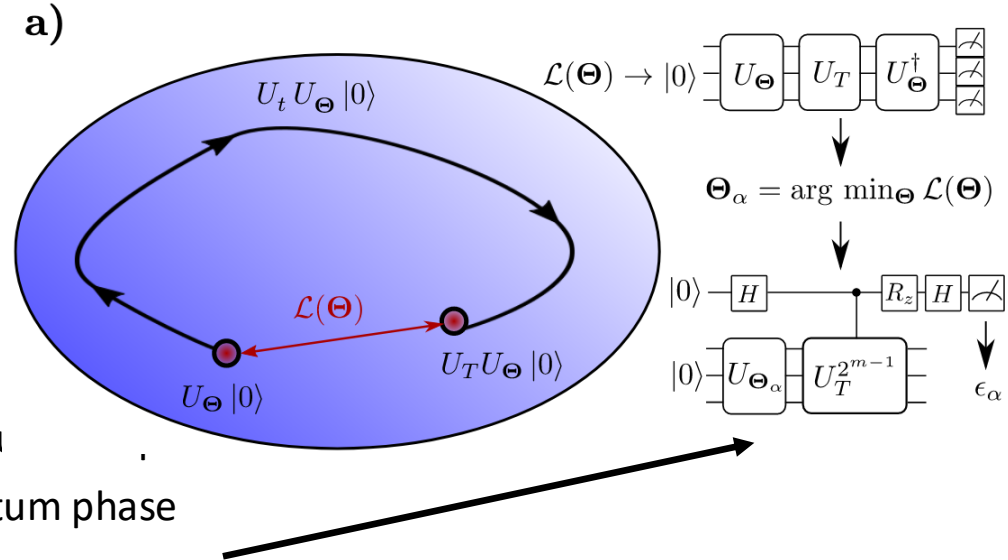
$$|\Psi_\alpha(0)\rangle \approx U_\Theta |0\rangle$$

B. Fauseweh, J.-X. Zhu, Quantum computing Floquet energy spectra Quantum 7, 1063 (2023)

<https://doi.org/10.22331/q-2023-07-20-1063>

New Algorithm : Time-domain approach

- Define target function as overlap between time evolved state and initial state
- $$\mathcal{L}(\Theta) = \left| \langle 0 | U_{\Theta}^{\dagger} U_T U_{\Theta} | 0 \rangle \right|^2$$
- Optimize target function in iterative hybrid scheme between classical and quantum
 - To obtain quasi-energy: use iterative quantum phase estimation

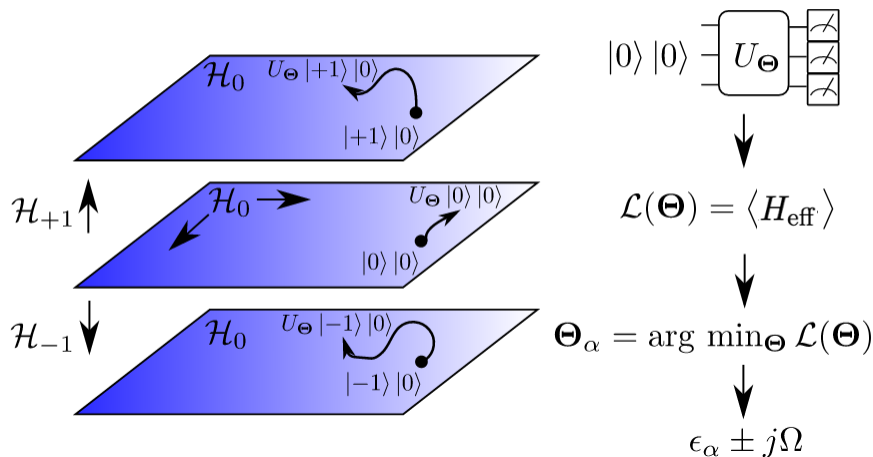


B. Fauseweh, J.-X. Zhu, Quantum computing Floquet energy spectra Quantum 7, 1063 (2023)

<https://doi.org/10.22331/q-2023-07-20-1063>

New Algorithm : Frequency-domain approach

b) $\mathcal{H}(t) \rightarrow \mathcal{H}_0 + \sum_j e^{ij\Omega t} \mathcal{H}_j \quad |\Psi\rangle \rightarrow |j\rangle |\Psi\rangle$



- Applying Fourier expansion leads to equivalent representation

$$H(t) = \sum_j e^{-ij\Omega t} H_j, \quad |\Phi_\alpha(t)\rangle = \sum_j e^{-ij\Omega t} |\Phi_\alpha^j\rangle$$

$$\Rightarrow \sum_j \underbrace{(H_{j-k} - j\Omega \delta_{j,k})}_{H_{\text{eff}}^{j,k}} |\Phi_\alpha^j\rangle = \epsilon_\alpha |\Phi_\alpha\rangle.$$

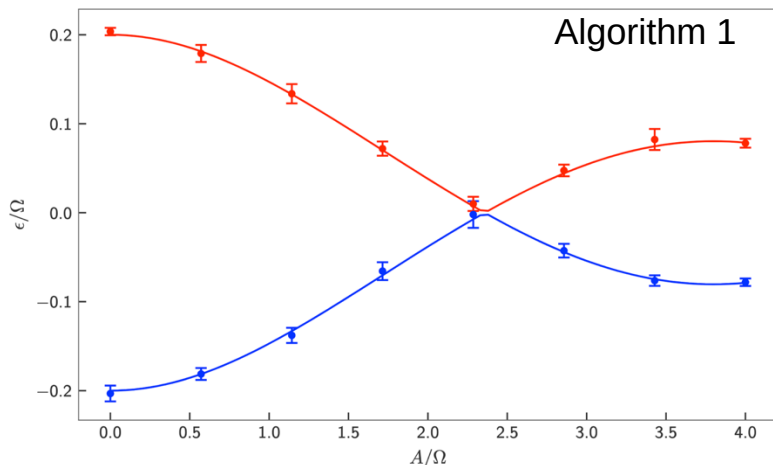
$$\Rightarrow \hat{H}\psi = E\psi$$

B. Fauseweh, J.-X. Zhu, Quantum computing Floquet energy spectra Quantum 7, 1063 (2023)

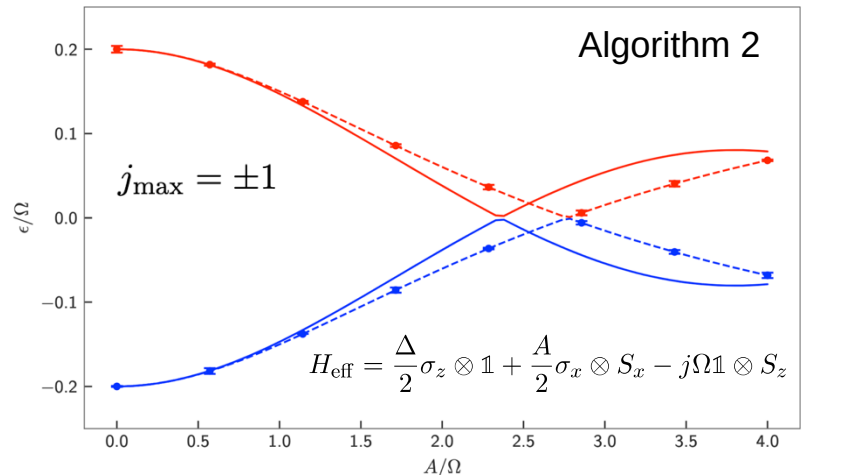
<https://doi.org/10.22331/q-2023-07-20-1063>

Test: linear driven spin-1/2

- Model: $H(t) = -\frac{\Delta}{2}\sigma_z + \frac{A}{2}\cos(\Omega t)\sigma_x$
- Task: compute Floquet quasi-energies as function of amplitude
- Test both algorithms on quantum computer simulator, taking finite sampling into account



$$U3(\theta, \phi, \nu) = \begin{pmatrix} \cos(\frac{\theta}{2}) & -e^{i\nu}\sin(\frac{\theta}{2}) \\ e^{i\phi}\sin(\frac{\theta}{2}) & e^{i(\phi+\nu)}\cos(\frac{\theta}{2}) \end{pmatrix}$$



$$U_{\Theta} = e^{i\Theta_1\sigma_y}e^{i\Theta_2S_4}e^{i\Theta_3S_5}e^{i\Theta_4S_x\sigma_x}e^{i\Theta_5\sigma_y}e^{i\Theta_6S_4}e^{i\Theta_7S_5}$$

Entangling gate

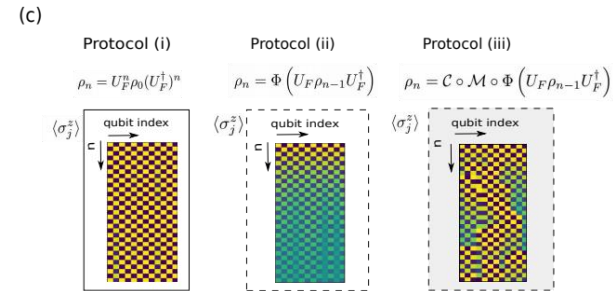
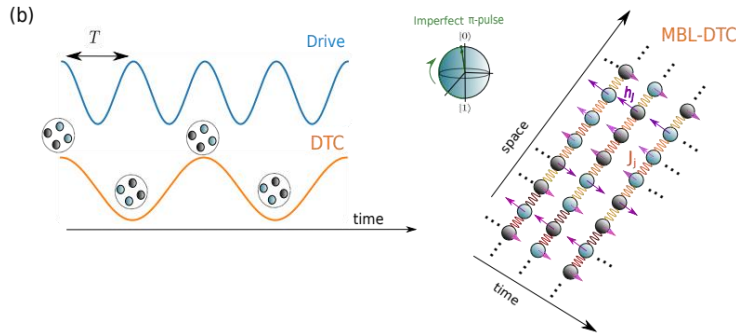
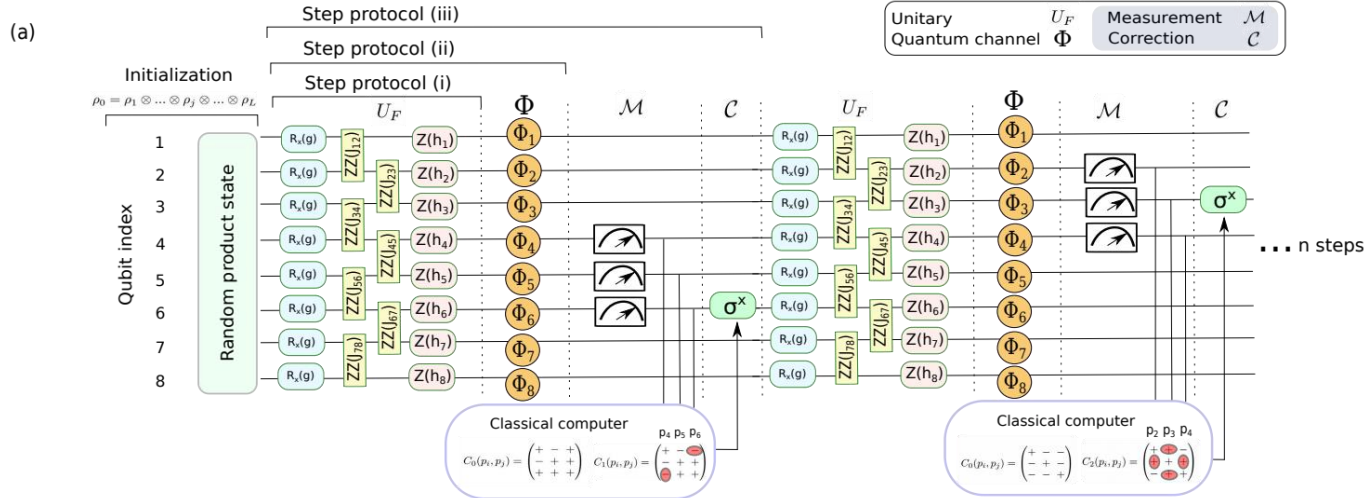
Application 2: Non-equilibrium phases of matter

- Continuously driving a many-body system typically leads to heating
- Possible work around: non-ergodic systems
- Example: discrete time crystals

Stabilizing discrete time crystals

- [illegible]

Quantum classical feedback protocol



Simulation results

- Results for protocol from classical simulation using matrix product density operators

Temporal Correlations

Spatial Correlations

G. Camacho, B. Fauseweh, **Prolonging a discrete time crystal by quantum-classical feedback**, Phys. Rev. Research 6, 033092 (2024)

<https://doi.org/10.1103/PhysRevResearch.6.033092>

Simulation results

$$\chi^{\text{SG}} = \frac{1}{L} \sum_{i,j} \langle \sigma_i^z \sigma_j^z \rangle^2$$

Dependence on number of corrected qubits

G. Camacho, B. Fauseweh, **Prolonging a discrete time crystal by quantum-classical feedback**, Phys. Rev. Research 6, 033092 (2024)

<https://doi.org/10.1103/PhysRevResearch.6.033092>

3T dynamical localization on a trapped ion qudit processor

- **Qutrit** 3T Floquet unitary

$$U_F = P_\epsilon^{\mathbb{Z}_3} e^{-i\frac{\theta_z}{2} \sum_{j=1}^{L-1} S_j^z S_{j+1}^z} e^{-i\frac{\theta_x}{2} \sum_{j=1}^{L-1} S_j^x S_{j+1}^x}$$

- Leads to non-ergodic time evolution for $|0\rangle^{\otimes n}$ product initial state

Application 3: Phase transitions on quantum computers

- Motivation: $\text{Ca}_3\text{Co}_2\text{O}_6$
- Frustrated triangular Ising chain w/ magnetization steps in external field
- Phase diagram of axial next-nearest neighbor Ising (ANNNI) model

$$\mathcal{H} = -J_1 \sum_i \sigma_i^z \sigma_{i+1}^z + J_2 \sum_i \sigma_i^z \sigma_{i+2}^z - B_x \sum_i \sigma_i^x$$

$$C^z(n) \equiv \langle s_j^z s_{j+n}^z \rangle - \langle s_j^z \rangle^2 \quad \text{with} \quad 0 < \phi_0 < \pi,$$

$$C^z(n) = A \frac{1}{\sqrt{n}} \cos[n(\pi - \phi_0)]$$

Phase determination via Fidelity susceptibility

- Use variational quantum eigensolver to find optimal parameters
- Detection of phase transition via fidelity susceptibility

$$F(\lambda, \delta) = | \langle \psi(\lambda - \delta) | \psi(\lambda + \delta) \rangle |$$
$$= 1 - \chi(\lambda)\delta^2 + \mathcal{O}(\delta^4)$$

K. Lively, T. Bode, J. Szangolies, J.-X. Zhu, B. Fauseweh, **Noise robust detection of quantum phase transitions**, Phys. Rev. Research 6, 043254 (2024),
<https://doi.org/10.1103/PhysRevResearch.6.043254>

Vision: Quantum Moore's Law

Thank you for your attention!