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Sandia National Laboratories

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Lyapunov Control-Inspired Quantum Algorithms for Ground State Preparation

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Motivation

Goal: study the ground state properties of quantum many-body systems

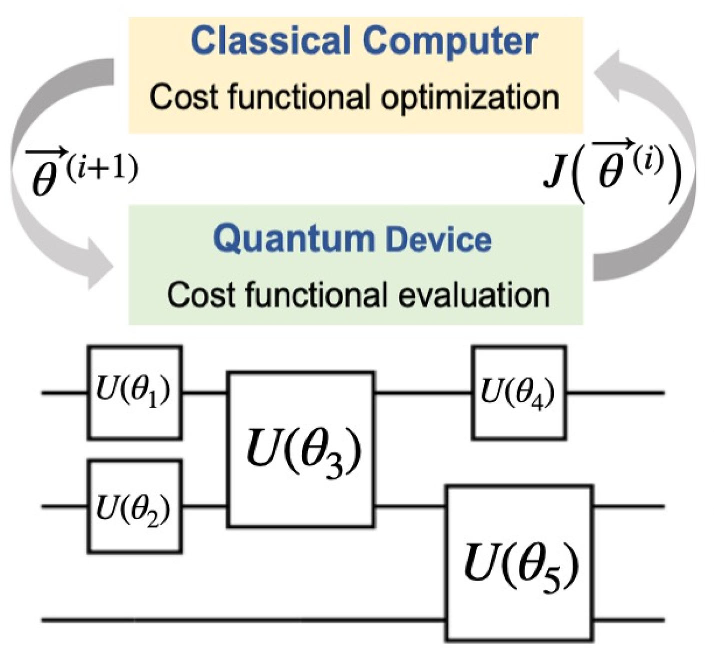


Figure 2: Illustration of VQE

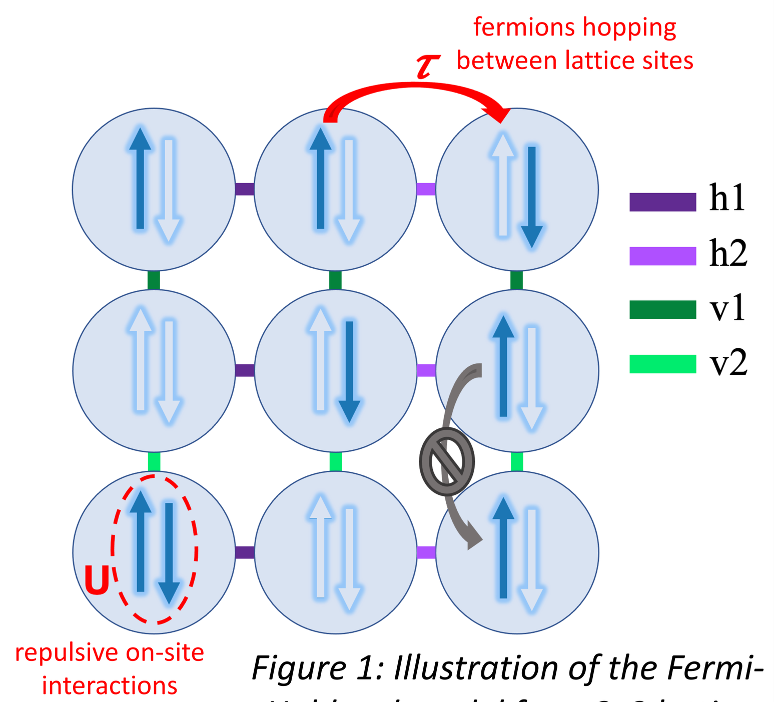


Figure 1: Illustration of the Fermi-Hubbard model for a 3x3 lattice

Variational Quantum Eigensolver (VQE) for ground state preparation on quantum computers:

- parameterize quantum circuit and seek to minimize $J(\boldsymbol{\theta}) = \langle\psi(\boldsymbol{\theta})|\, Hp \,|\psi(\boldsymbol{\theta})\rangle$
- classically optimize over $\boldsymbol{\theta}$ to solve

Problem: VQE optimization might become prohibitively expensive in high dimensions

Solution: prepare ground states without optimization, using feedback-based method

Theory

Quantum Lyapunov Control

Consider a time evolution defined by:

$$i\frac{d}{dt}|\psi(t)\rangle = (H_p + H_d\beta(t))|\psi(t)\rangle$$

"problem" Hamiltonian (H_p); "driver" Hamiltonian (H_d); control function ($\beta(t)$)

We define an objective function:

$$J(|\psi(t)\rangle) = \langle\psi(t)|H_p|\psi(t)\rangle$$

where

$$\frac{dJ}{dt} = \langle\psi(t)|i[H_d, H_p]|\psi(t)\rangle\beta(t)$$

so if

$$\beta(t) = -\langle\psi(t)|i[H_d, H_p]|\psi(t)\rangle$$

then

$$\frac{dJ}{dt} \le 0, \forall t$$

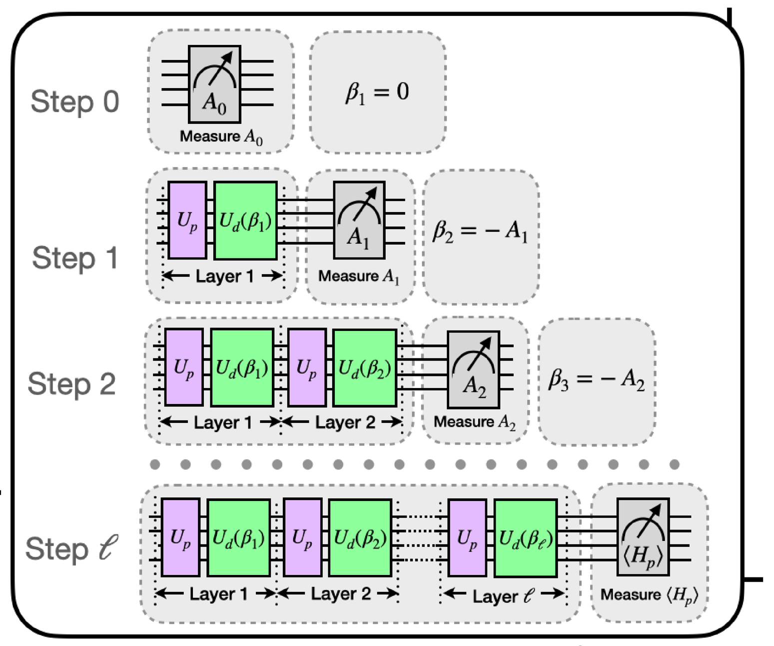


Figure 3: FALQON circuit for Fermi-Hubbard ground state preparation

Fermi-Hubbard Model

- describes strongly correlated solid-state systems
- has phenomenology that might be related to the mechanism for high-temperature superconductivity
- notoriously difficult to solve, complete phase diagram remains open topic of research

$$H_{FH} = T + V$$

$$T = -\sum_{\langle m,n\rangle} t_{m,n}(\hat{a}^\dagger_{m\uparrow}\hat{a}_{n\uparrow} + \hat{a}^\dagger_{n\uparrow}\hat{a}_{m\uparrow} + \hat{a}^\dagger_{m\downarrow}\hat{a}_{n\downarrow} + \hat{a}^\dagger_{n\downarrow}\hat{a}_{m\downarrow})$$

"hopping" terms of the Hamiltonian, $t_{m,n} = \tau \;\; \forall m,n$ (see Figure 1)

on-site interaction terms

$$V = U\sum_{k=1}^{N} \hat{n}_{k\uparrow}\hat{n}_{k\downarrow}$$

Feedback-based Algorithm for Quantum OptimizatioN (FALQON)

Magann, Rudinger, Grace, Sarovar, arXiv:2103.08619 & arXiv:2108.05945 (2021)

We digitize the evolution of the wave function into discrete timesteps:

$$|\psi(t+\Delta t)\rangle = e^{-i(H_p+\beta(t)H_d)\Delta t}|\psi(t)\rangle$$

Then, we can Trotterize the full evolution:

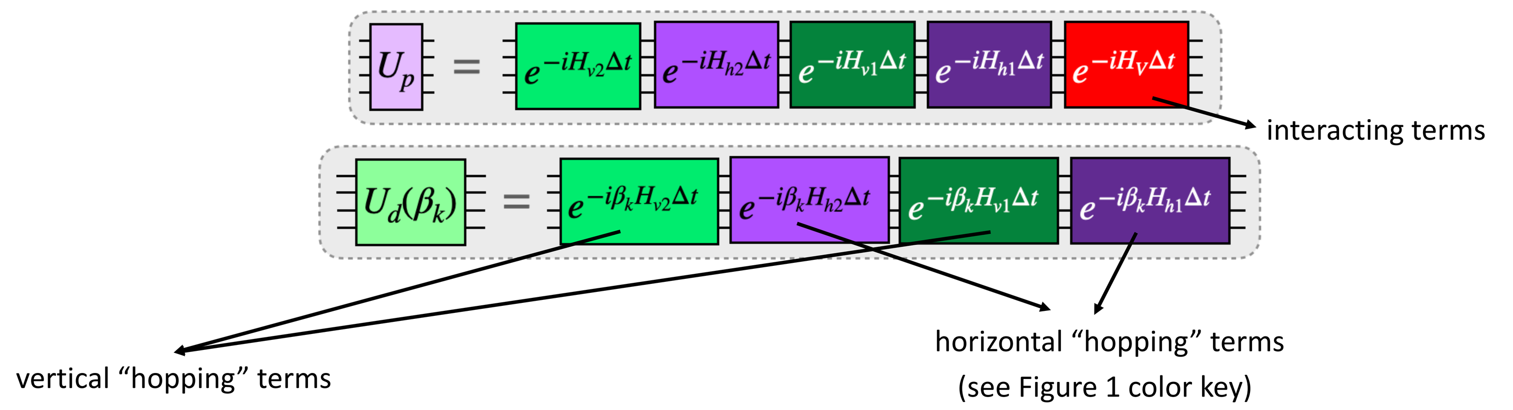
$$|\psi_\ell\rangle = e^{-i\beta_\ell H_d\Delta t}e^{-iH_p\Delta t}\cdots e^{-i\beta_1 H_d\Delta t}e^{-iH_p\Delta t}|\psi_0\rangle = U_d(\beta_\ell)U_p \ldots U_d(\beta_1)U_p|\psi_0\rangle$$

And set each β_k according to the Lyapunov-control inspired feedback law:

$$\beta_k = -\langle\psi_{k-1}|i[H_d, H_p]|\psi_{k-1}\rangle$$

For the Fermi-Hubbard model, we can separate H_{FH} into 5 terms.

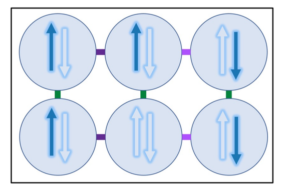
We can decompose the unitaries according to the Hamiltonian Variational Ansatz:



Wecker, Hastings, Troyer, *Phys Rev A* **92**, 042303 (2015)
Cade, Mineh, Montanaro, Stanisic, *Phys Rev B* **102**, 235122 (2020)

We use the Jordan-Wigner encoding to represent fermionic operators as Pauli operators

Numerical Results



FALQON for the Fermi-Hubbard Model

Performance of Lyapunov control-inspired approach for finding ground states of Fermi-Hubbard model, shown here for 2x3 instance

Figure 4: 2D Fermi-Hubbard Simulation

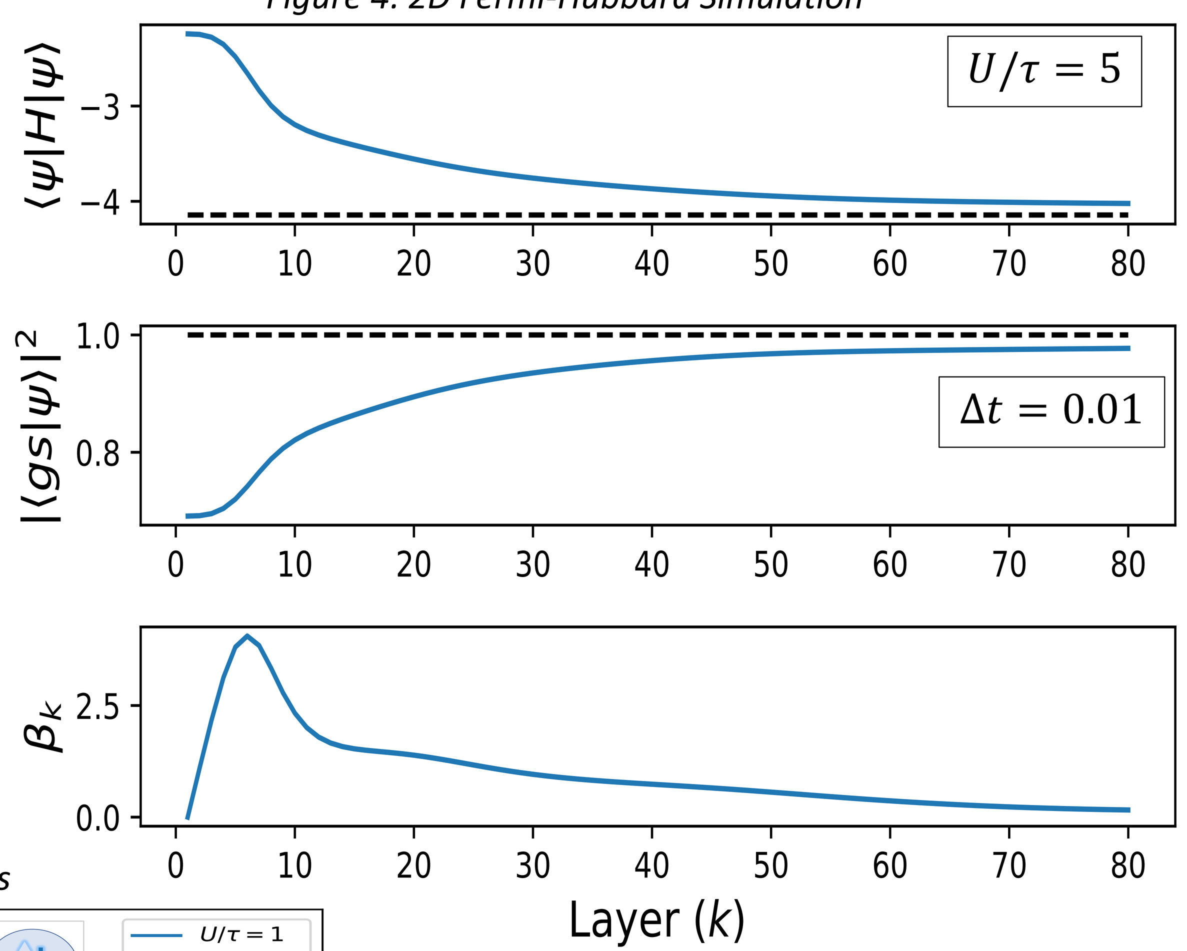
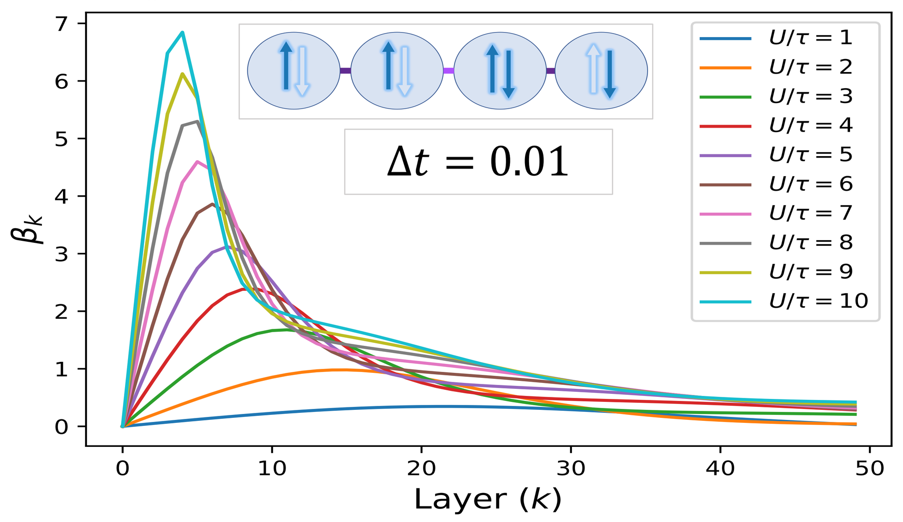


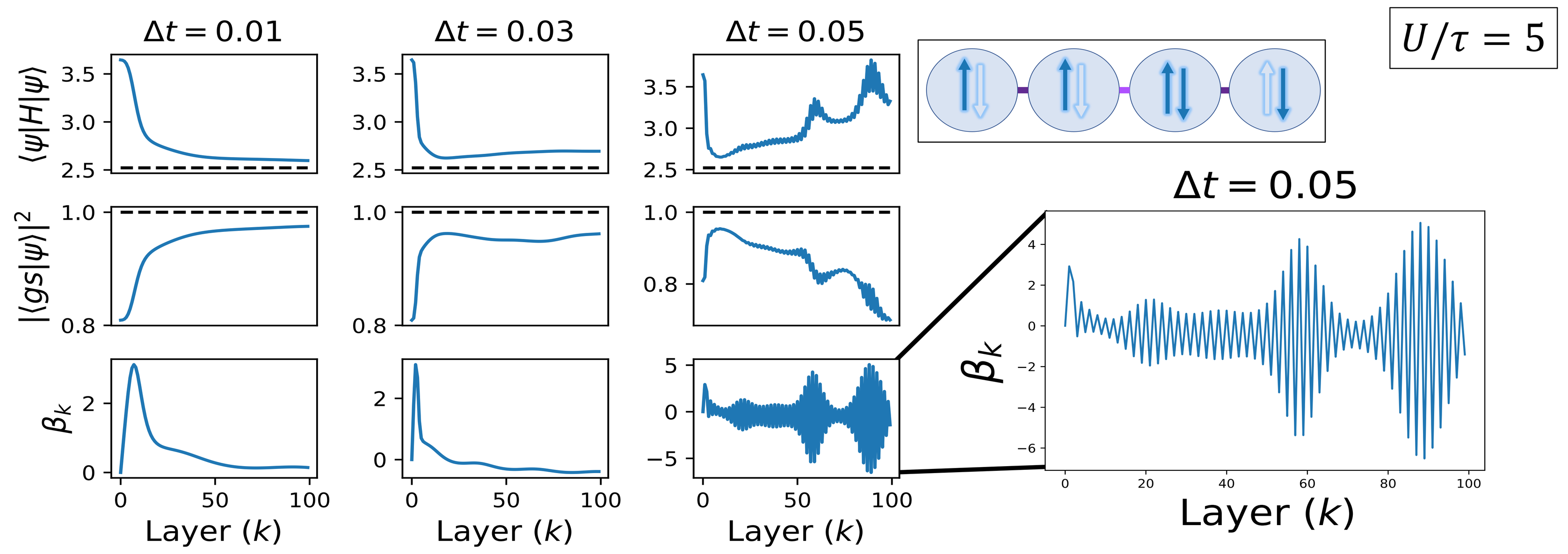
Figure 5: different parameters



Impact of varying U/τ on β

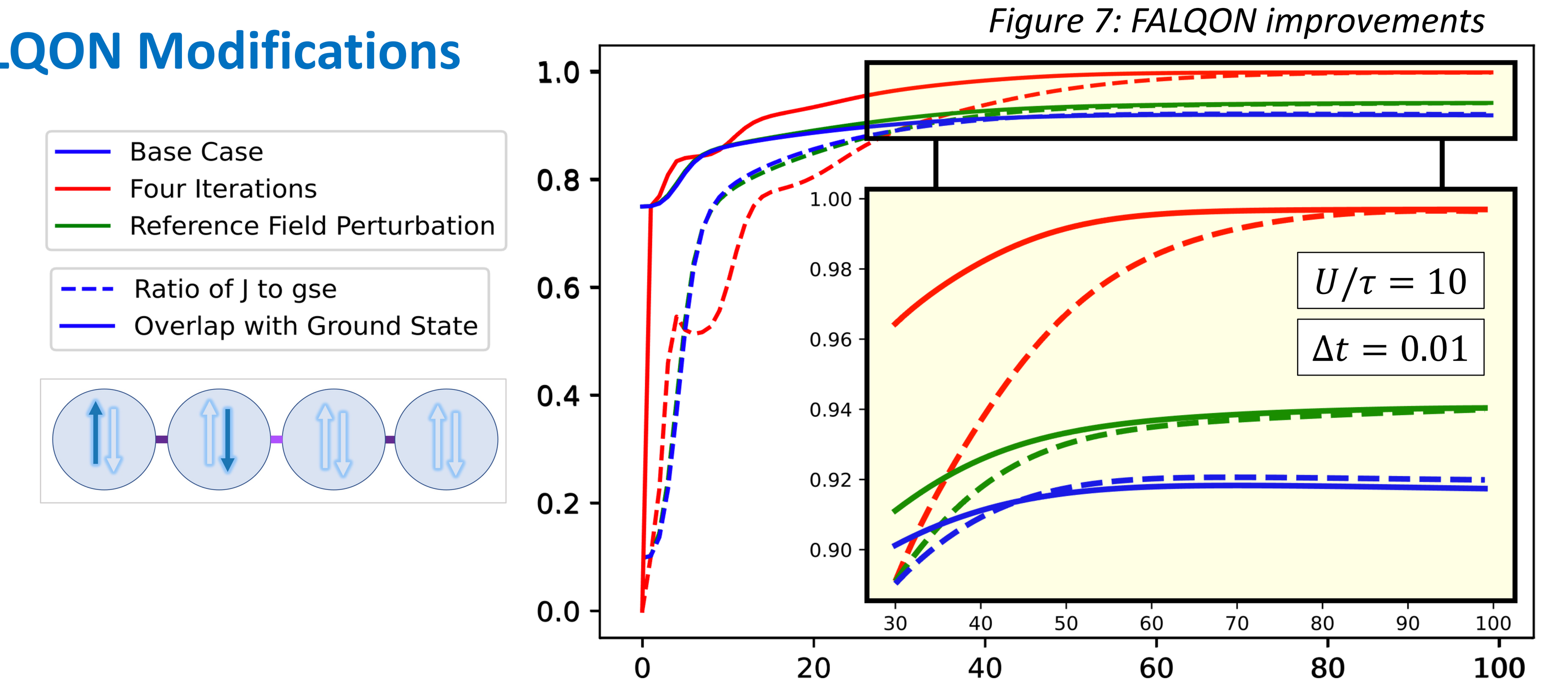
Dependence on Timestep

Figure 6: timestep analysis



FALQON Modifications

Figure 7: FALQON improvements



We can improve the performance and convergence in FALQON in two ways:

- Run all layers for several iterations, adding previous β values at each iteration
- Add a reference field perturbation to β values

Robustness to Sampling Noise

Number of measurements of $i[H_d, H_p]$ used to estimate each β_k

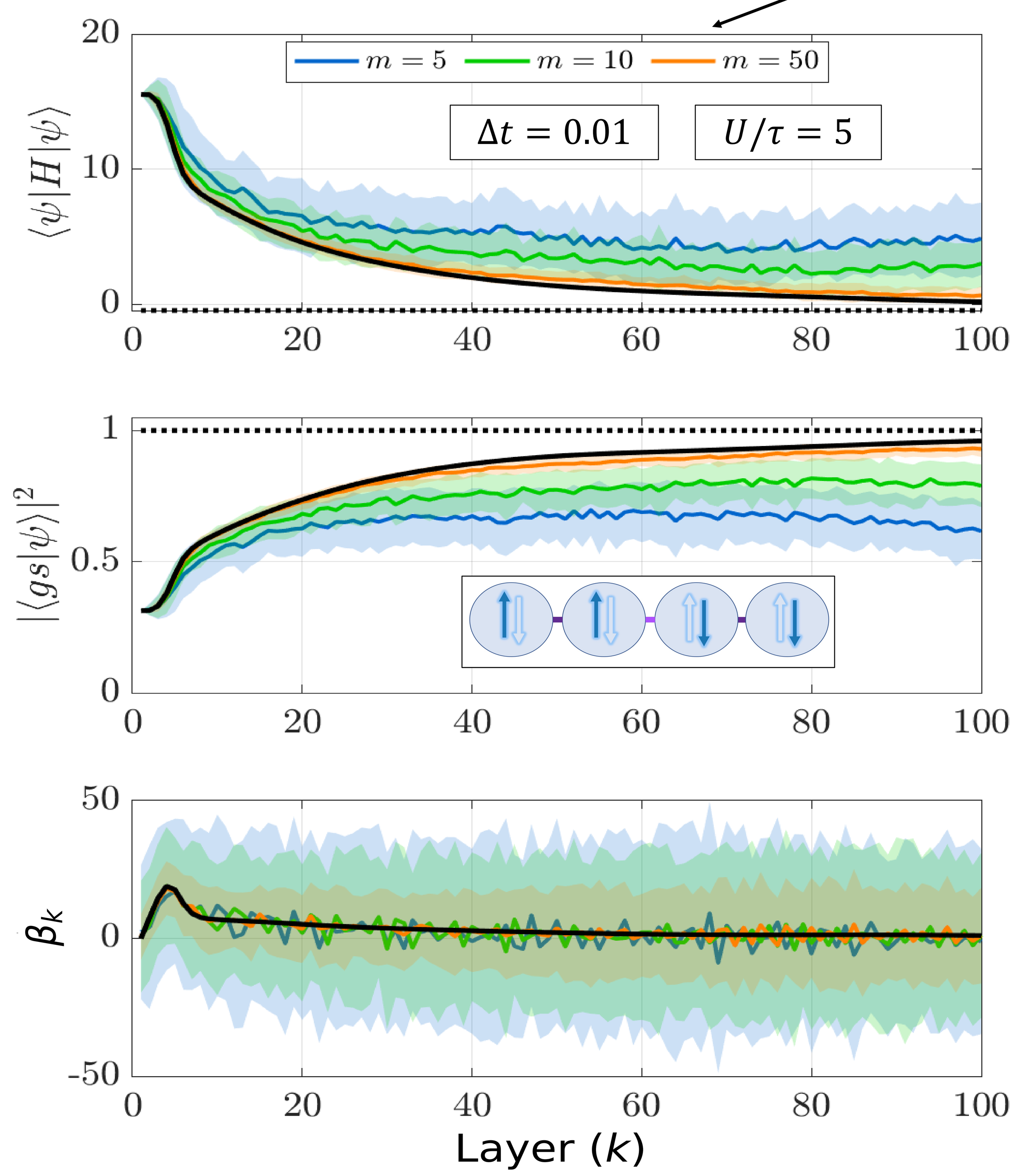


Figure 8: FALQON single parameter noise analysis