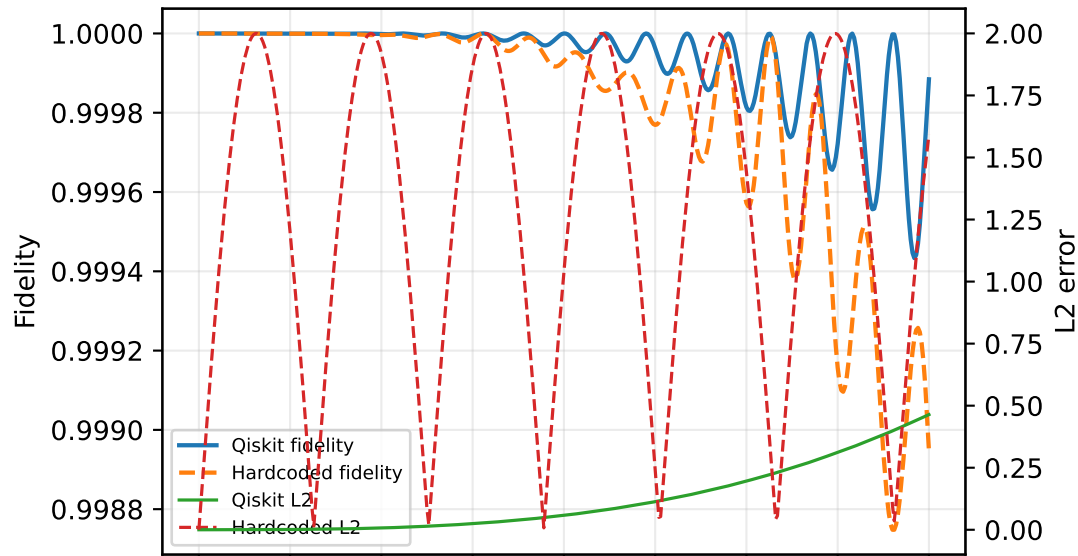
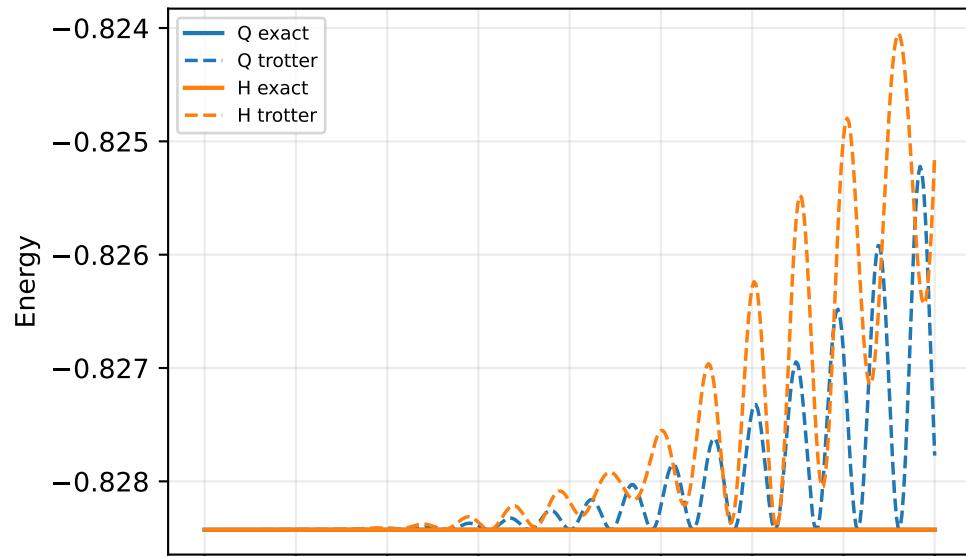


Phase 1 Comparison: Hardcoded vs Qiskit Dynamics (Locked Params)

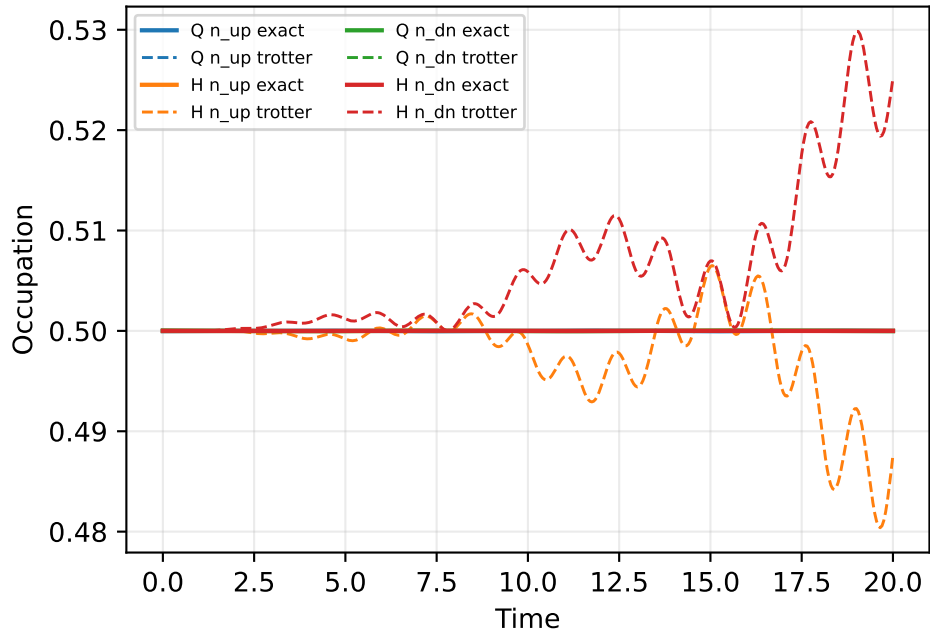
State Error Metrics



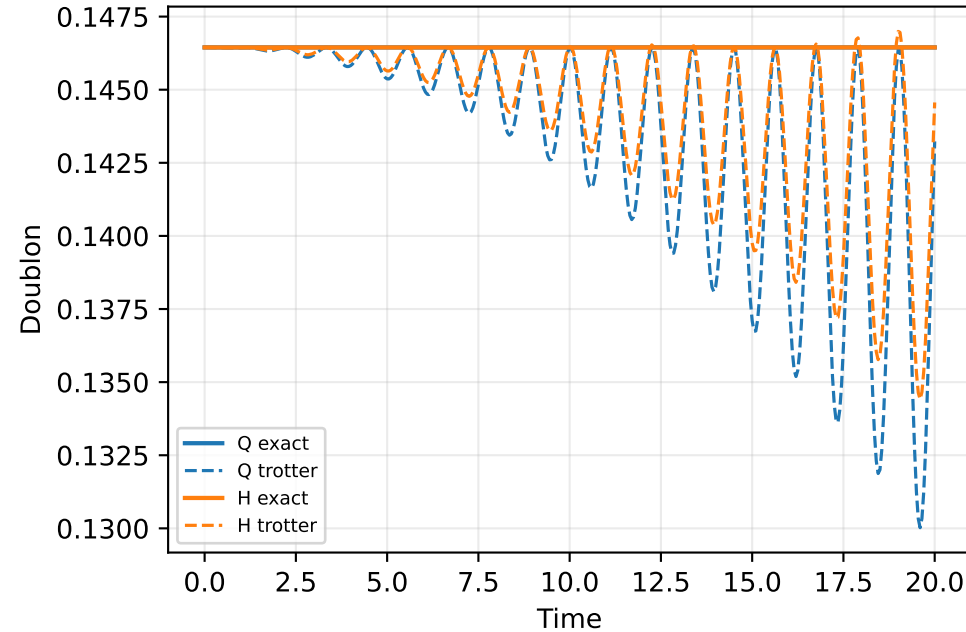
Energy Dynamics



Site-0 Occupations



Doublon Dynamics



Phase 1 Accuracy Comparison Summary

Parameter lock (from source files):

num_sites=2, hopping_t=1.0, onsite_u=4.0, dv=0.0, boundary=periodic, ordering=blocked
t_final=20.0, num_times=401, suzuki_order=2, trotter_steps=128
Qiskit ansatz=UCCSD(reps=2), restarts=3, maxiter=1800, seed=7, noiseless statevector
Hardcoded ansatz=HardcodedUCCSDAnsatz(reps=2), restarts=3, maxiter=1800, seed=7, noiseless numpy statevector

Ground-state energy: hardcoded=-0.828427124476, qiskit=-0.828427122588, abs_delta=1.888117e-09, rel_delta=2.279159e-09

Key max absolute deltas over time (hardcoded - qiskit):

fidelity: 1.249588e-03
state_l2_error: 1.999308e+00
energy_exact: 1.888131e-09
energy_trotter: 4.366136e-03
n_up_site0_trotter: 1.965088e-02
n_dn_site0_trotter: 2.987347e-02
doublon_trotter: 4.391465e-03

Runtime summary (wall, seconds):

qiskit runs: 78.76, 80.05 (mean 79.41)
hardcoded runs: 10.56, 10.53 (mean 10.54)
speedup hardcoded_vs_qiskit: 7.53x

Reproducibility check (run1 vs run2):

qiskit settings_equal=True, max_abs_summary_delta=0.000e+00, max_fidelity_delta=0.000e+00
hardcoded settings_equal=True, max_abs_summary_delta=0.000e+00, max_fidelity_delta=0.000e+00

Diagnosis:

material_difference=True

Differences are material for strict apples-to-apples dynamics: hardcoded and Qiskit runs use very similar but not id