

Executed Command

Reference: pipelines/PIPELINE_RUN_GUIDE.md

Script: pipelines/compare_hardcoded_vs_qiskit_pipeline.py

```
/opt/anaconda3/bin/python3 pipelines/compare_hardcoded_vs_qiskit_pipeline.py --l-values 4 --with-per-l-pdfs  
--initial-state-source vqe --num-times 401 --trotter-steps 256 --hardcoded-vqe-reps 3 --hardcoded-vqe-  
restarts 8 --hardcoded-vqe-maxiter 3000 --hardcoded-vqe-seed 17 --qiskit-vqe-reps 2 --qiskit-vqe-restarts  
3 --qiskit-vqe-maxiter 800 --qiskit-vqe-seed 17 --skip-qpe
```

Hardcoded vs Qiskit Pipeline Comparison Summary

```
generated_utc: 2026-02-14T23:22:13.933442+00:00
all_pass: True
l_values: [4]
trajectory_comparison_basis: trotter trajectories start from
    each pipeline's selected initial_state_source (default: vqe)
exact_trajectory_labels: Exact_Hardcode, Exact_Qiskit
exact_trajectory_method: python_matrix_eigendecomposition

thresholds:
{'doublon_trotter_max_abs_delta': 0.001,
 'energy_trotter_max_abs_delta': 0.001,
 'fidelity_max_abs_delta': 0.0001,
 'ground_state_energy_abs_delta': 1e-08,
 'n_dn_site0_trotter_max_abs_delta': 0.005,
 'n_up_site0_trotter_max_abs_delta': 0.005}

hardcoded_qiskit_import_isolation:
{'offending_imports': [],
 'pass': True,
 'qiskit_imports': [{'line': 361, 'module': 'qiskit'},
                     {'line': 362, 'module': 'qiskit.circuit.library'},
                     {'line': 363, 'module': 'qiskit.primitives'},
                     {'line': 364, 'module': 'qiskit.quantum_info'},
                     {'line': 365, 'module': 'qiskit.synthesis'},
                     {'line': 366, 'module': 'qiskit_algorithms'},
                     {'line': 367, 'module': 'qiskit_algorithms.minimum_eigensolvers'}],
 'qpe_adapter_range': {'end_line': 463, 'start_line': 327}},

Delta metric definitions:
ΔF(t)      = |F_hc(t) - F_qk(t)|
ΔE_trot(t) = |E_trot_hc(t) - E_trot_qk(t)|
Δn_up0(t)  = |n_up0_hc(t) - n_up0_qk(t)|
```

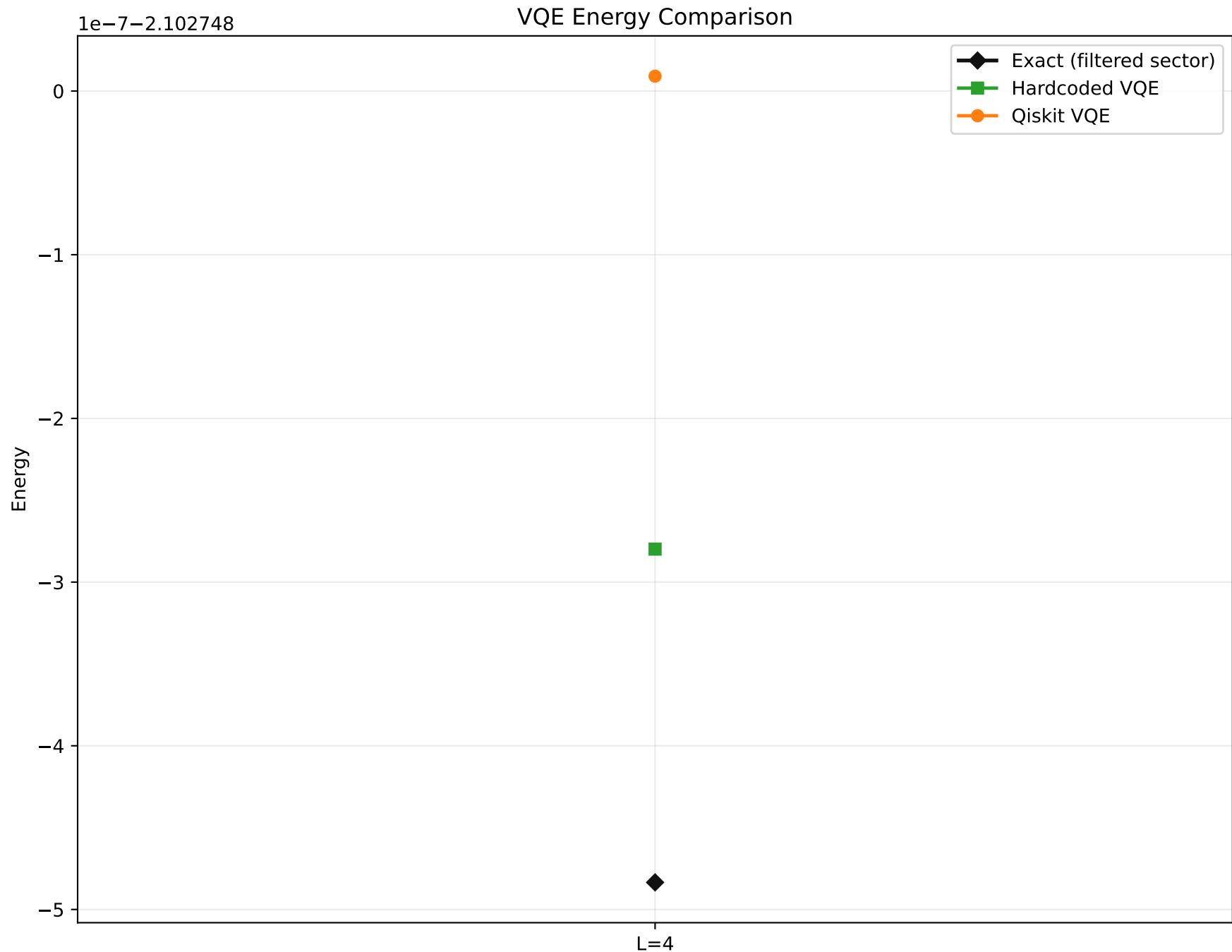
$\Delta n_{dn\theta}(t) = |n_{dn\theta}_{hc}(t) - n_{dn\theta}_{qk}(t)|$

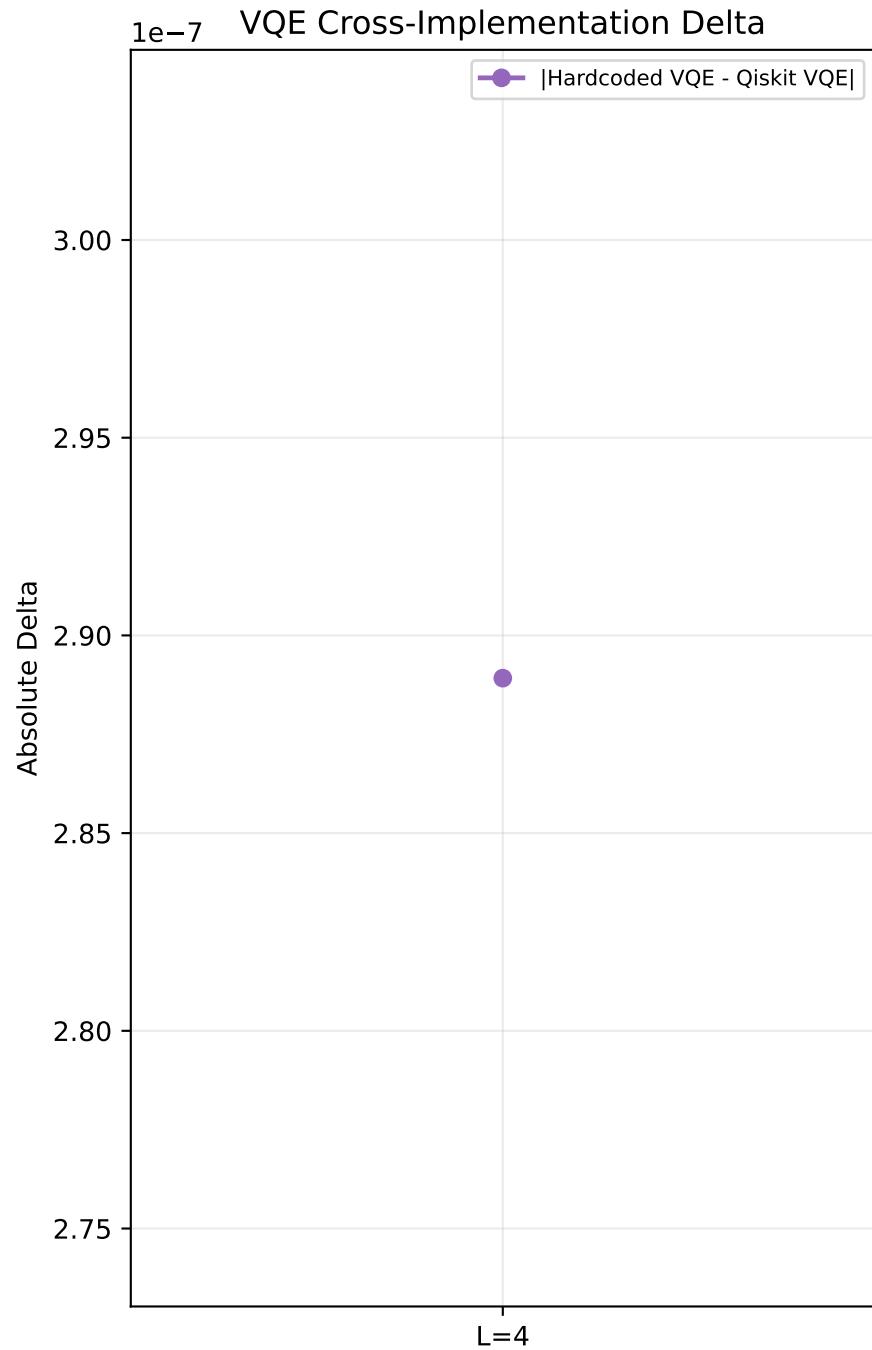
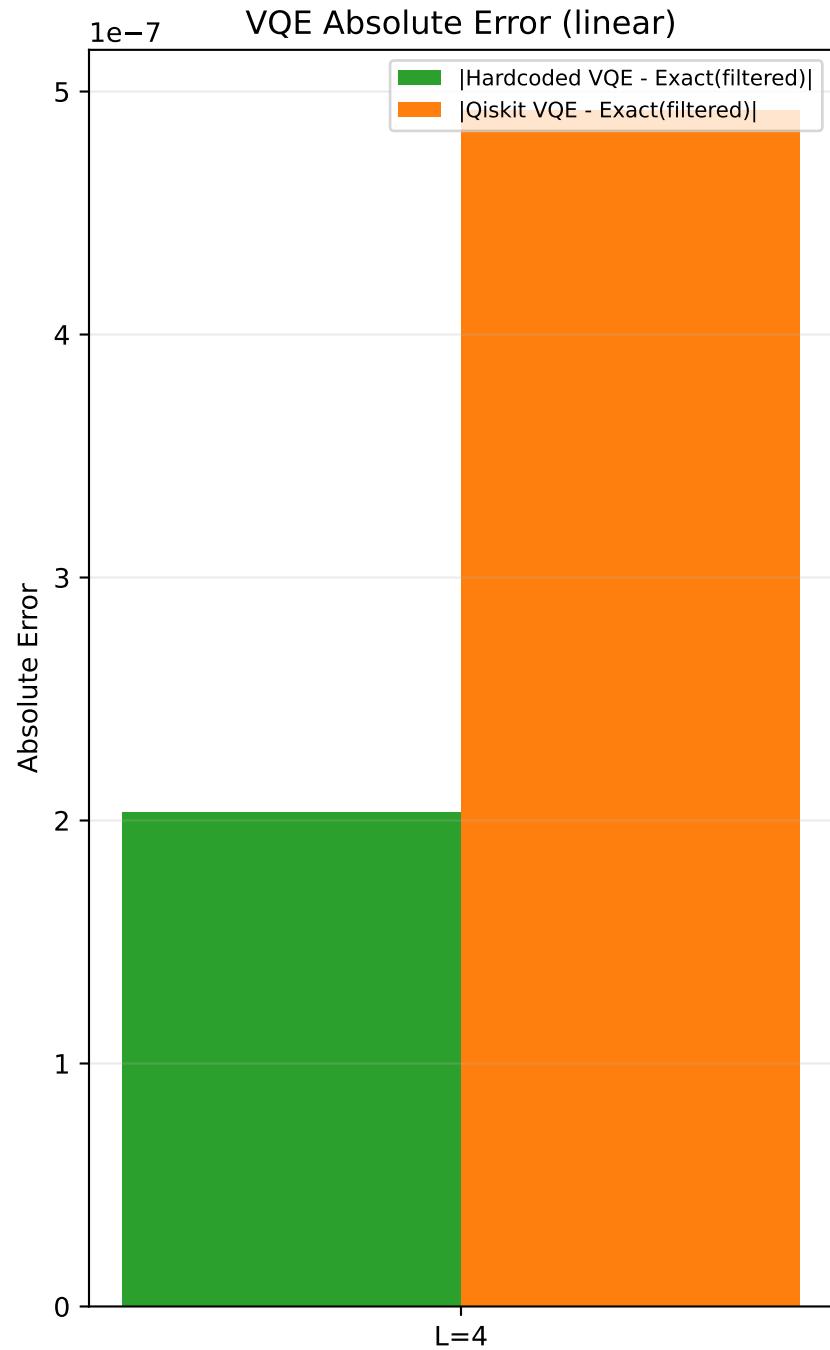
$\Delta D(t) = |D_{hc}(t) - D_{qk}(t)|$

$F_{pipeline}(t)$ is the pipeline's stored trajectory fidelity value (as computed internally vs that pipeline's exact evolution).

Per-L pass flags:

```
L=4 pass=True metrics_json=/Users/jakestrobel/Downloads/qdynamics-main/Fermi-Hamil-JW-VQE-TROTTER-  
PIPELINE/artifacts/hardcoded_vs_qiskit_pipeline_L4_metrics.json
```





QPE comparison skipped: no finite QPE energy estimates were found in per-L payloads.

Bundle L=4: Run Settings & Metrics Summary

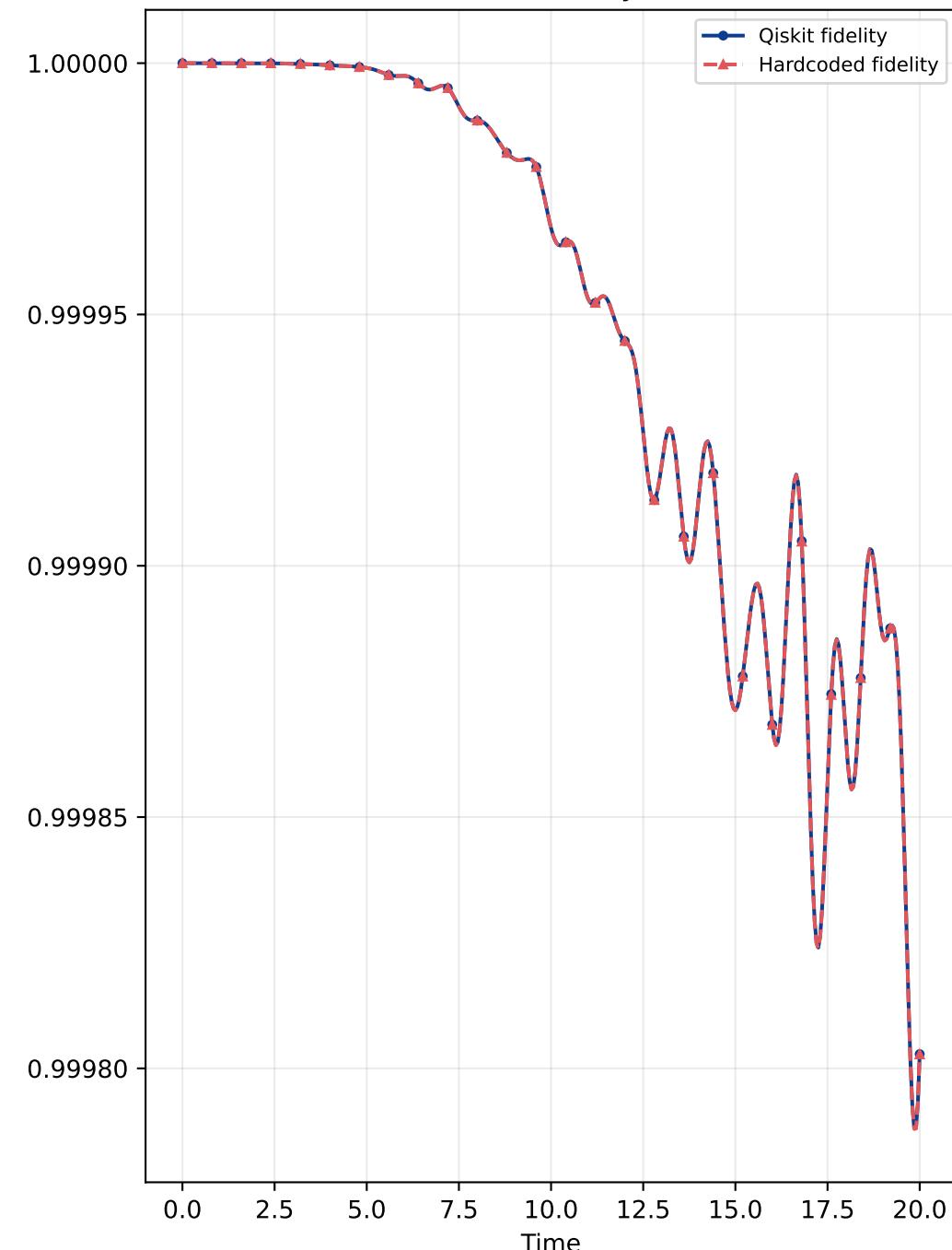
```
L=4  t=1.0  u=4.0  dv=0.0  boundary=periodic  ordering=blocked  initial_state_source=vqe  t_final=20.0  num_times=401  suz

thresholds:
doublon_trotter_max_abs_delta: 1.00e-03
energy_trotter_max_abs_delta: 1.00e-03
fidelity_max_abs_delta: 1.00e-04
ground_state_energy_abs_delta: 1.00e-08
n_dn_site0_trotter_max_abs_delta: 5.00e-03
n_up_site0_trotter_max_abs_delta: 5.00e-03

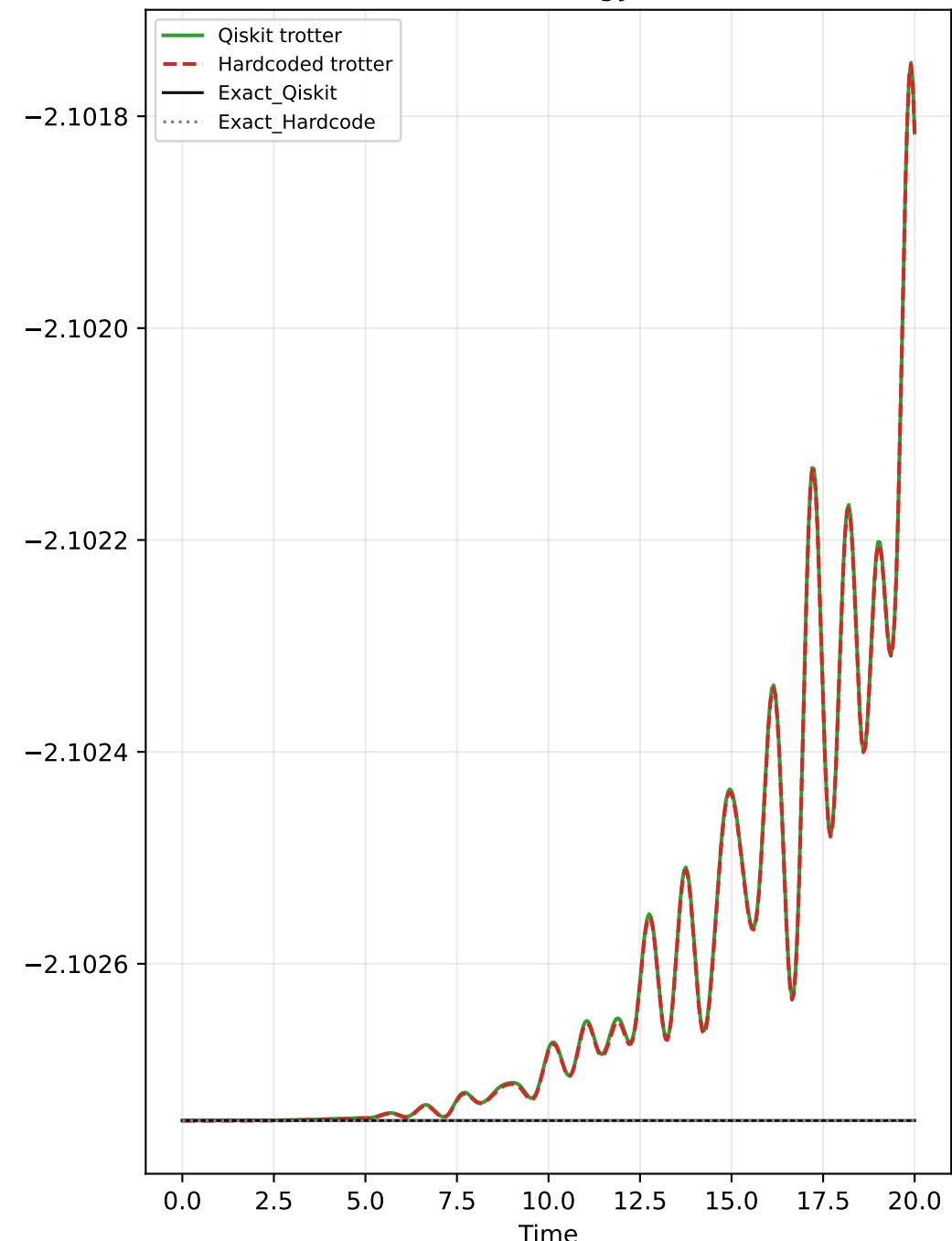
max |Δ|:
gs_energy: 0.00e+00
doublon_trotter: 1.98e-05
energy_trotter: 4.14e-06
fidelity: 2.21e-07
n_dn_site0_trotter: 3.24e-04
n_up_site0_trotter: 3.27e-04
result: PASS
```

Bundle Page: L=4 Fidelity & Energy

L=4 Fidelity

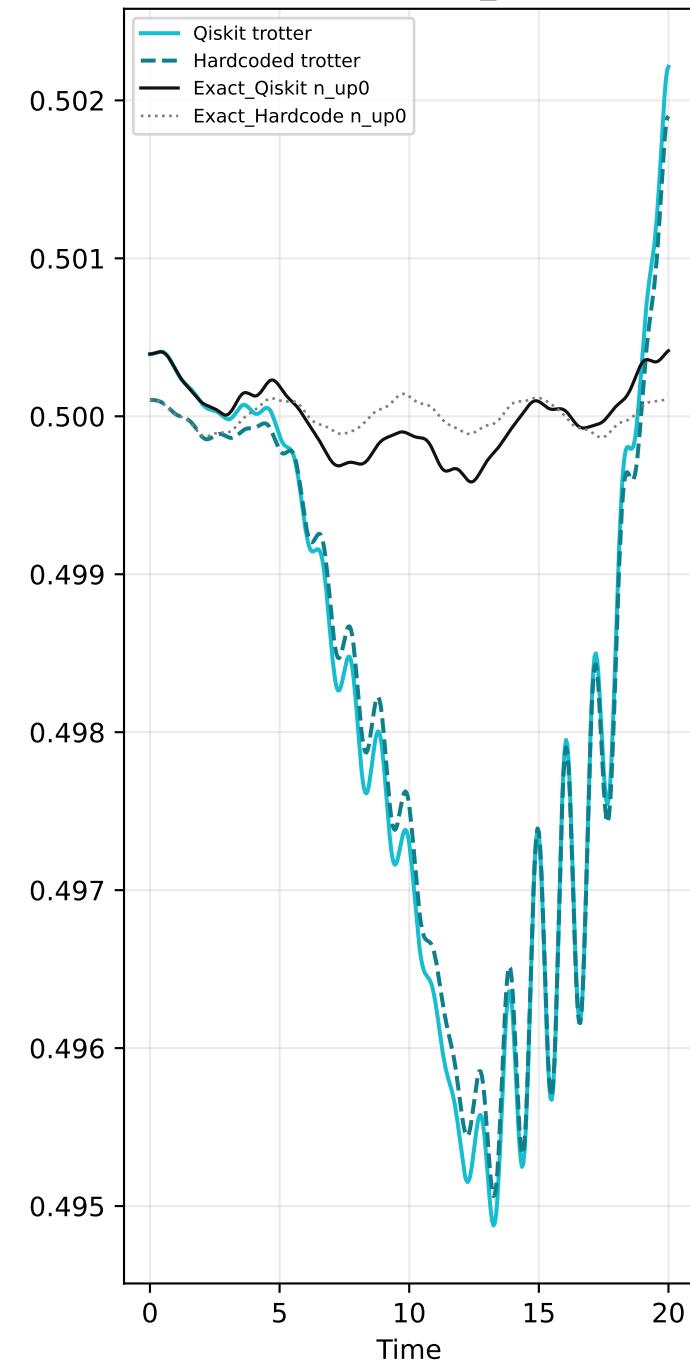


L=4 Energy

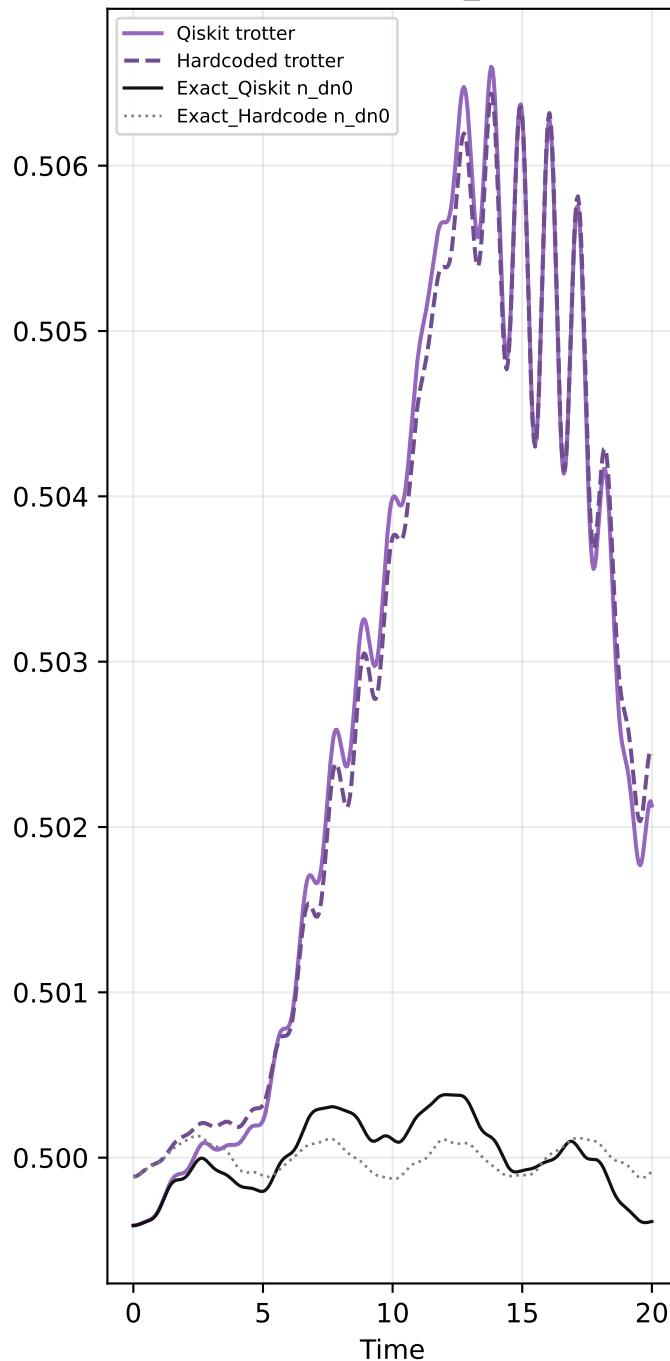


Bundle Page: L=4 Occupations & Doublon (auto-zoomed)

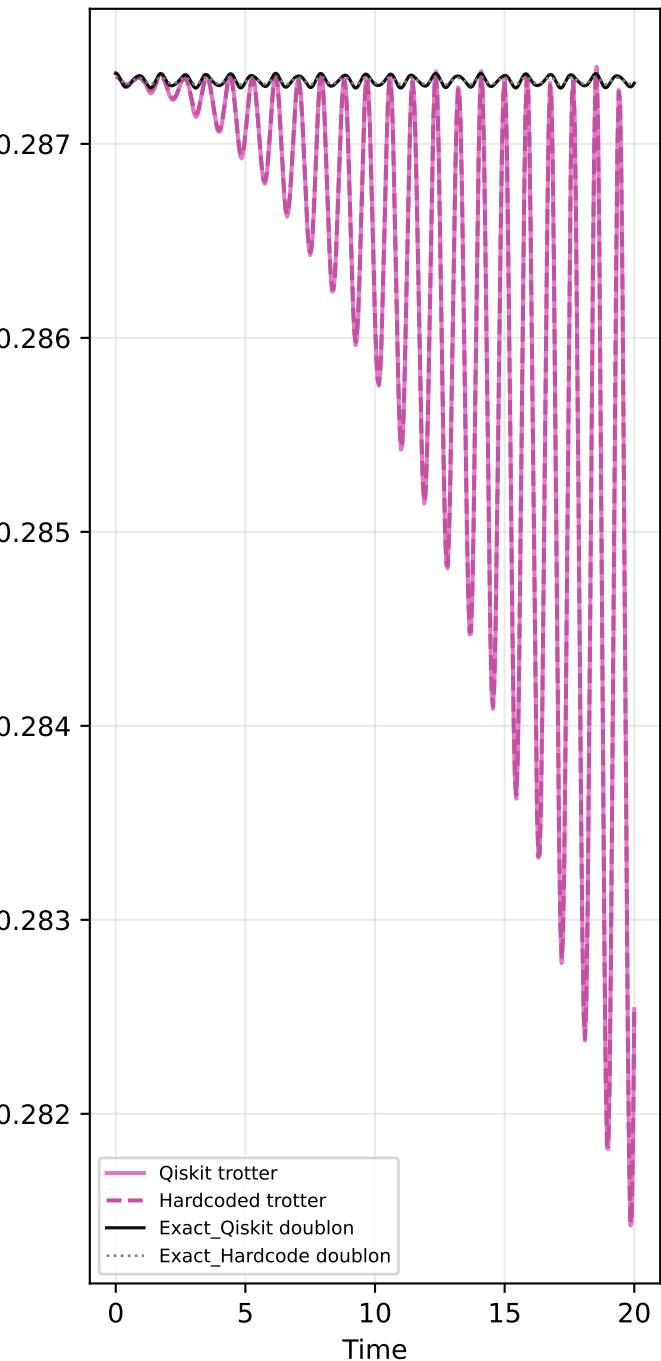
L=4 Site-0 n_up



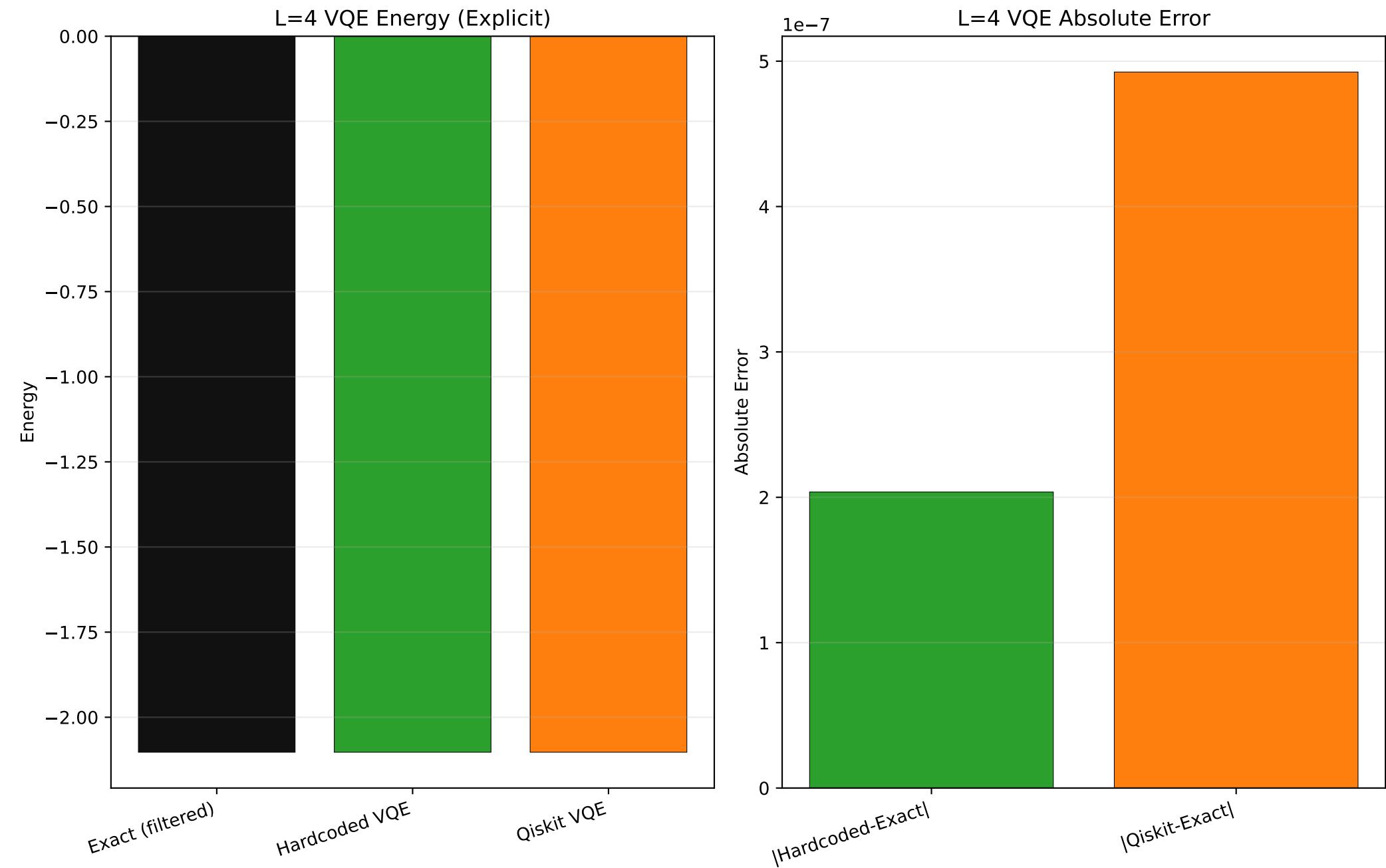
L=4 Site-0 n_dn



L=4 Doublon

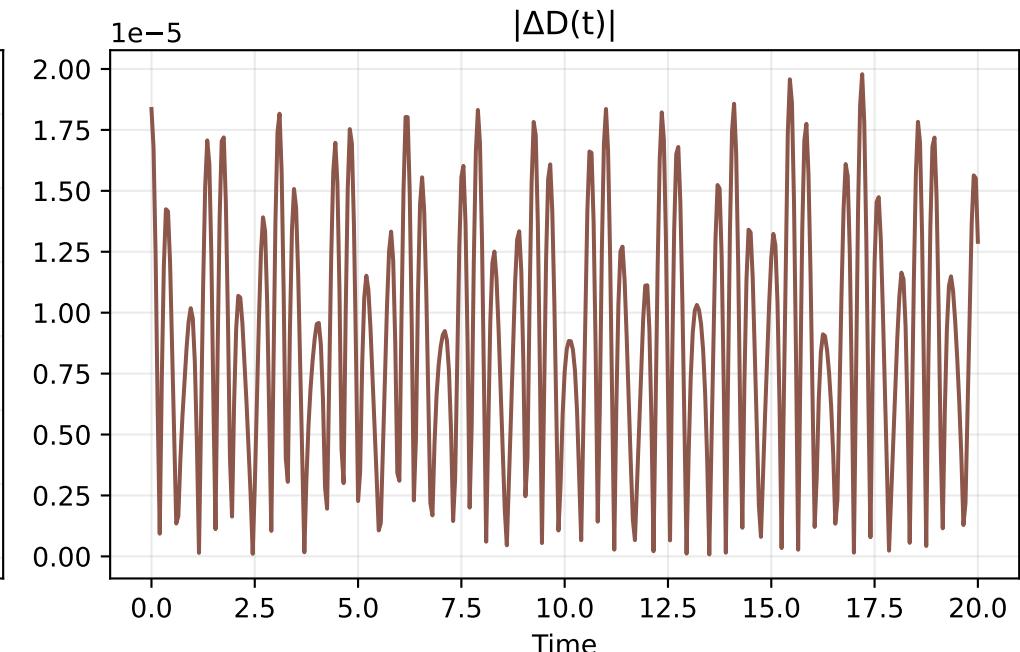
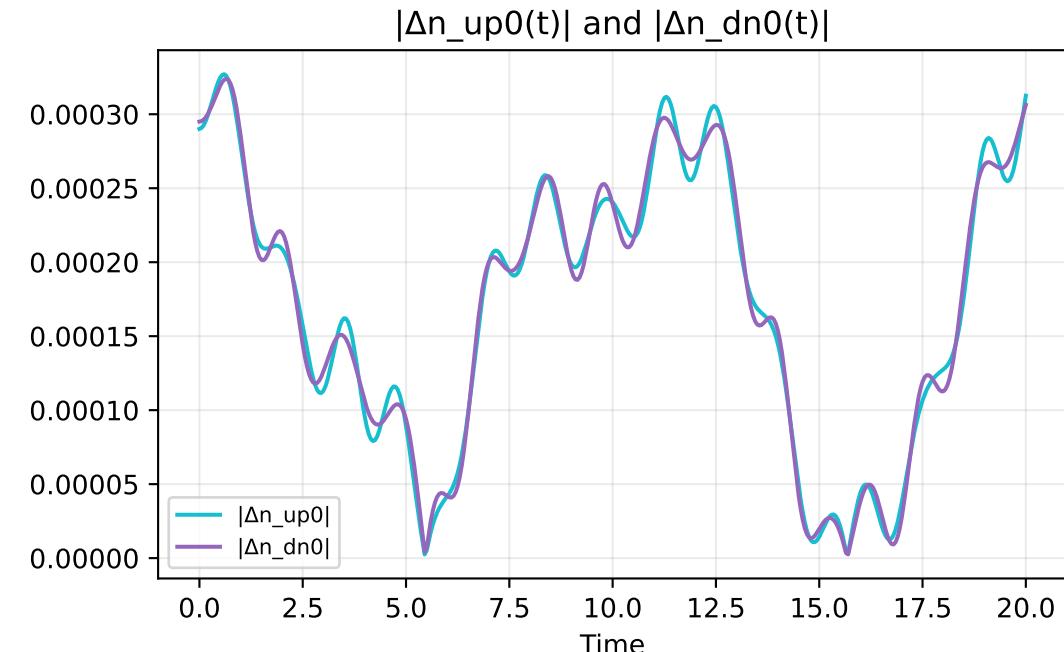
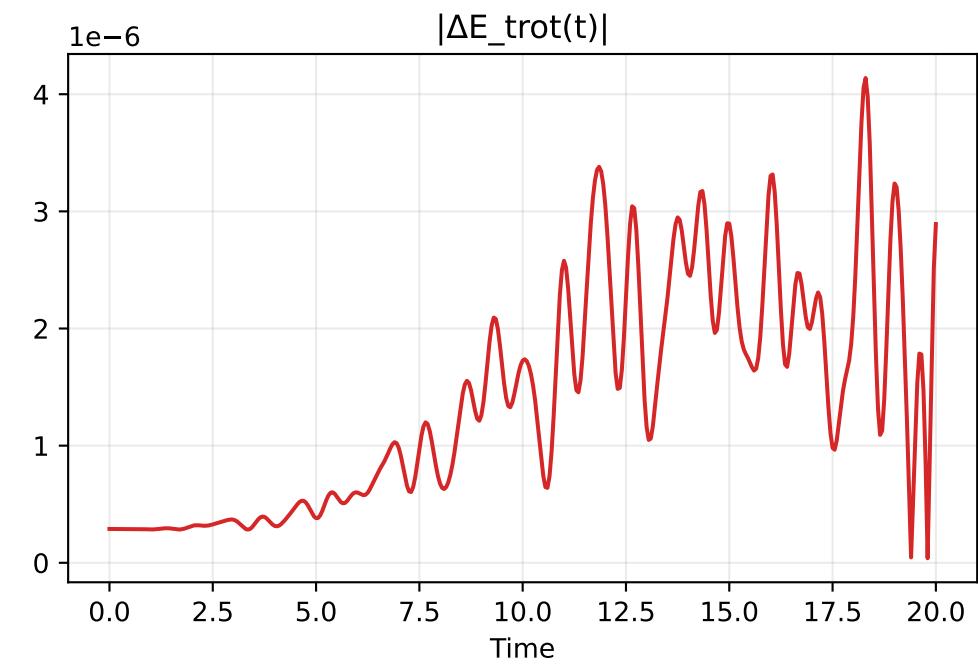
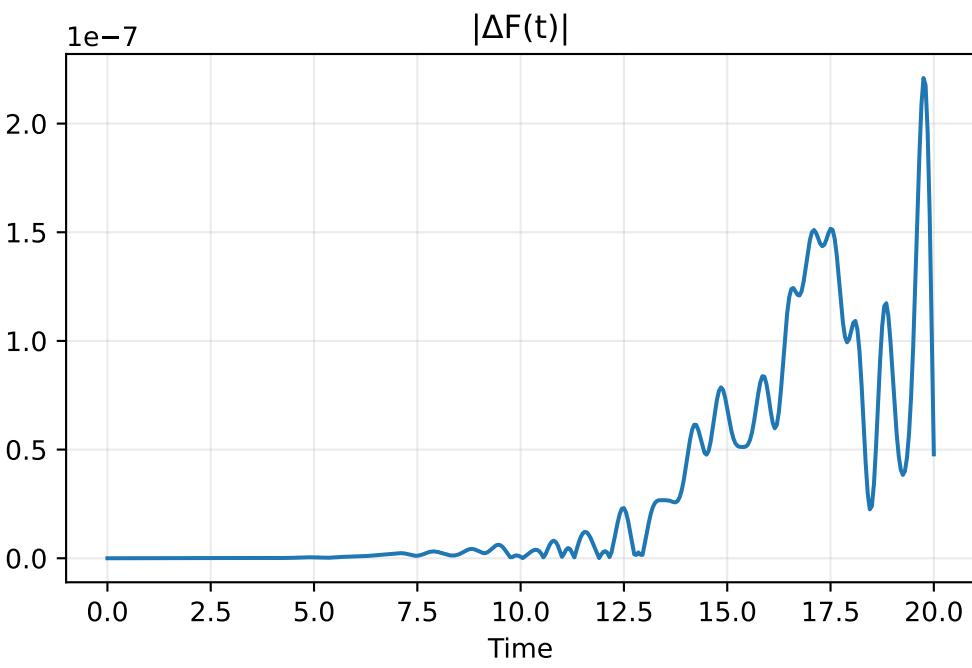


When `initial_state_source=vqe`, Trotter $E(t=0) = \langle \psi_{\text{vqe}} | H | \psi_{\text{vqe}} \rangle = \text{VQE energy}$.
VQE energy \neq exact ground state energy unless VQE fully converged.



Bundle Delta Diagnostics L=4

$\Delta X(t) = |X_{hc}(t) - X_{qk}(t)|$, where $X_{pipeline}(t)$ is that pipeline's stored trajectory value.



Bundle metrics page L=4

Trotterization comparison uses each path's configured initial state.

Trajectory labels: Exact_Hardcode and Exact_Qiskit.

Exact trajectory method: python_matrix_eigendecomposition.

For VQE-init runs, both exact(t) and trotter(t) start from the VQE ansatz state.

Delta metric definitions:

$\Delta F(t) = |F_{hc}(t) - F_{qk}(t)|$

$\Delta E_{trot}(t) = |E_{trot_hc}(t) - E_{trot_qk}(t)|$

$\Delta n_{up0}(t) = |n_{up0_hc}(t) - n_{up0_qk}(t)|$

$\Delta n_{dn0}(t) = |n_{dn0_hc}(t) - n_{dn0_qk}(t)|$

$\Delta D(t) = |D_{hc}(t) - D_{qk}(t)|$

$F_{pipeline}(t)$ is the pipeline's stored trajectory fidelity value (as computed internally vs that pipeline's exact evolution).

ground_state_energy_abs_delta = 0.0

fidelity max/mean/final = 2.209725978863375e-07 / 3.021212585926256e-08 / 4.7817899972990574e-08

energy_trotter max/mean/final = 4.138357329708242e-06 / 1.390849683424733e-06 / 2.8916515510957197e-06

n_up_site0_trotter max/mean/final = 0.00032705403848842796 / 0.0001690360931200569 / 0.0003125322846022627

n_dn_site0_trotter max/mean/final = 0.0003239662616169592 / 0.00016913479016976142 / 0.00030634941027374296

doublon_trotter max/mean/final = 1.9785792567172944e-05 / 9.157969656497664e-06 / 1.2908478513040667e-05

checks:

{'doublon_trotter_max_abs_delta': True,
'energy_trotter_max_abs_delta': True,
'fidelity_max_abs_delta': True,
'ground_state_energy_abs_delta': True,
'n_dn_site0_trotter_max_abs_delta': True,
'n_up_site0_trotter_max_abs_delta': True}

PASS = True