

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 3 --with-per-l-pdfs  
--initial-state-source vqe --num-times 401 --trotter-steps 256 --hardcoded-vqe-reps 2 --hardcoded-vqe-  
restarts 5 --hardcoded-vqe-maxiter 1800 --qiskit-vqe-reps 2 --qiskit-vqe-restarts 5 --qiskit-vqe-maxiter  
1800 --skip-qpe
```

L=3 Run Settings & Metrics Summary

L=3 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

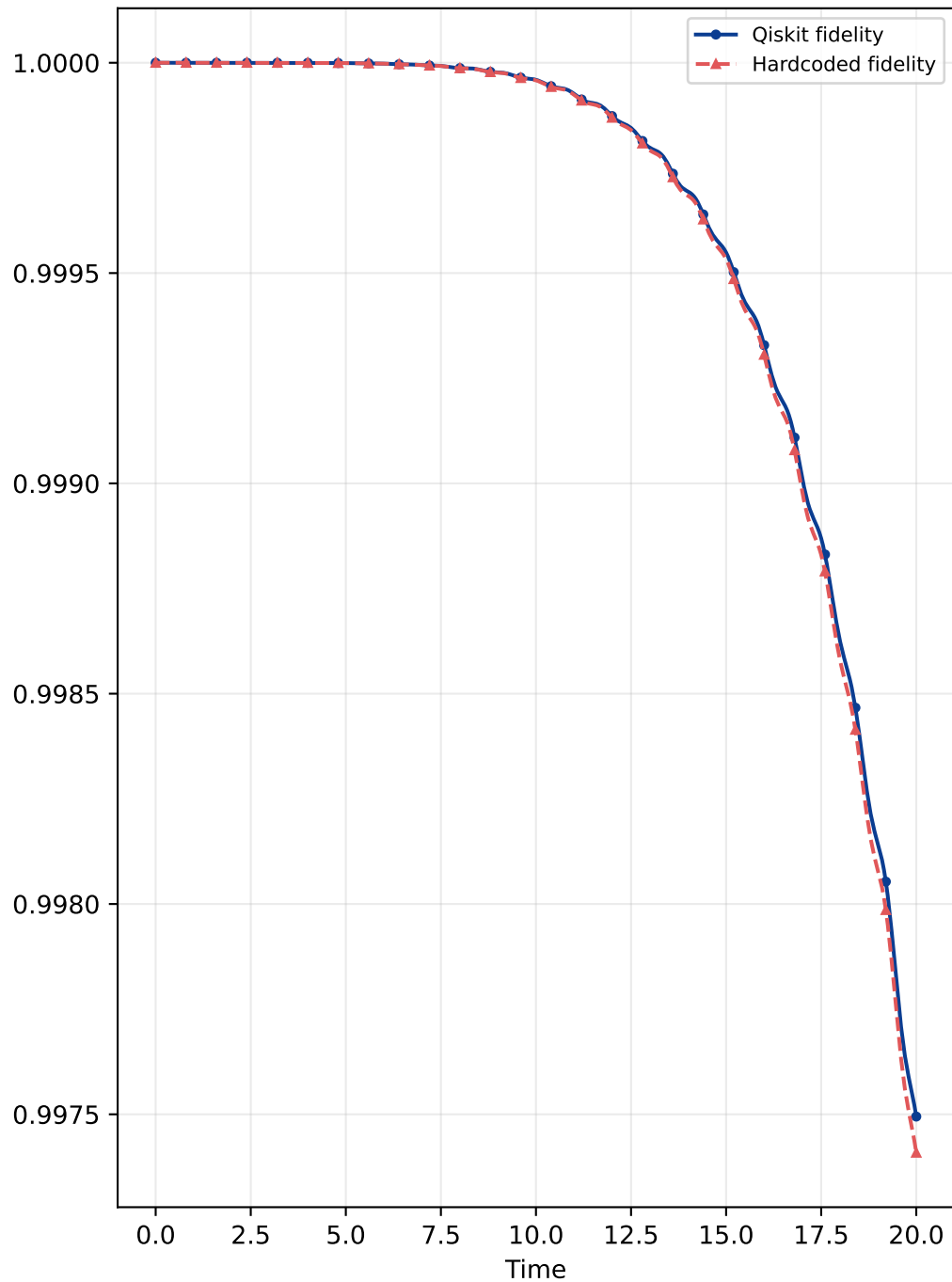
max $|\Delta|$:

gs_energy: 0.00e+00
doublon_trotter: 1.93e-05
energy_trotter: 2.57e-06
fidelity: 8.59e-05
n_dn_site0_trotter: 2.25e-03
n_up_site0_trotter: 2.97e-03

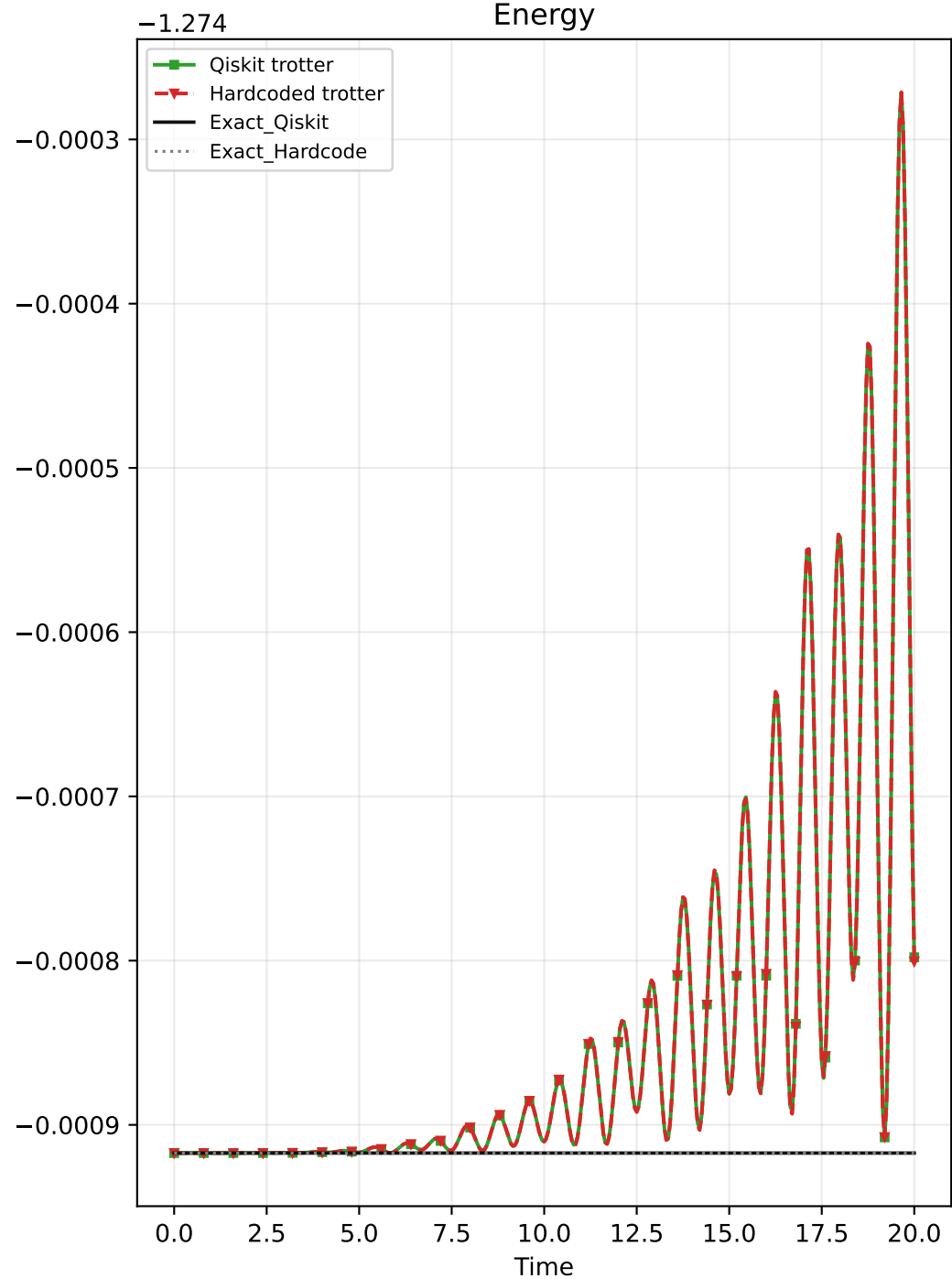
result: PASS

Pipeline Comparison L=3: Hardcoded vs Qiskit (Fidelity & Energy)

Fidelity

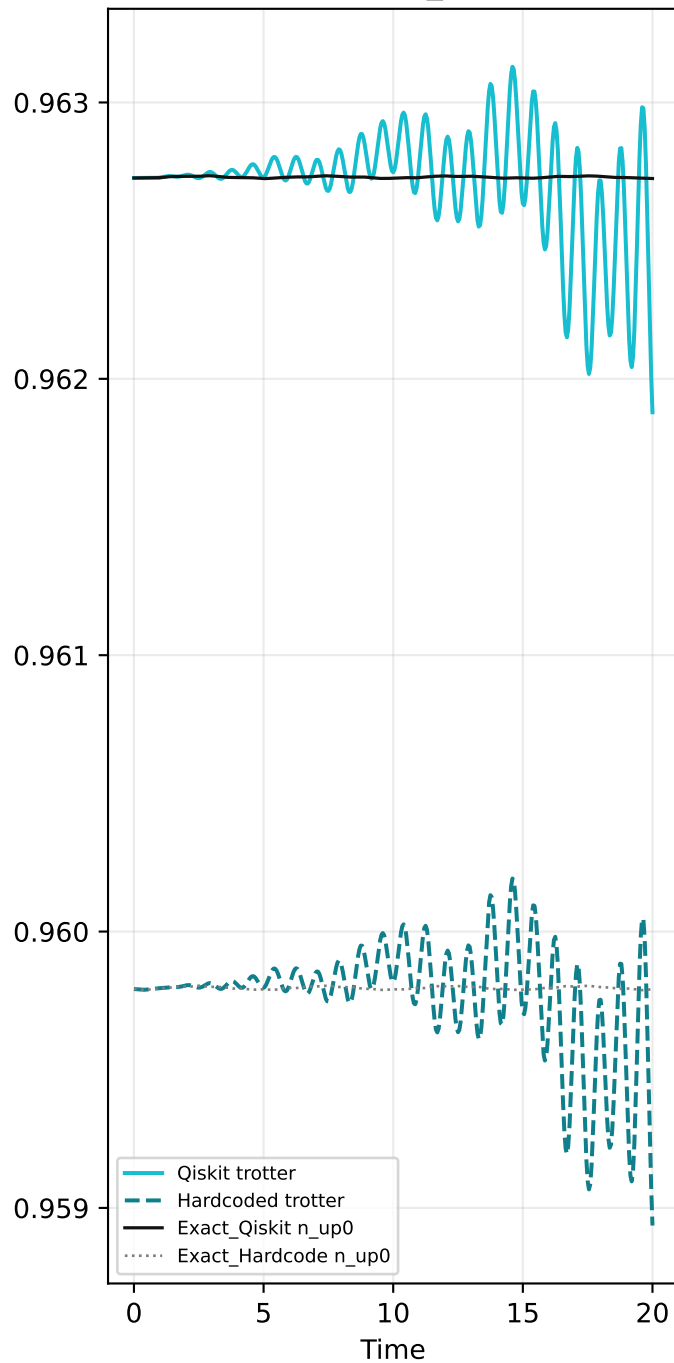


Energy

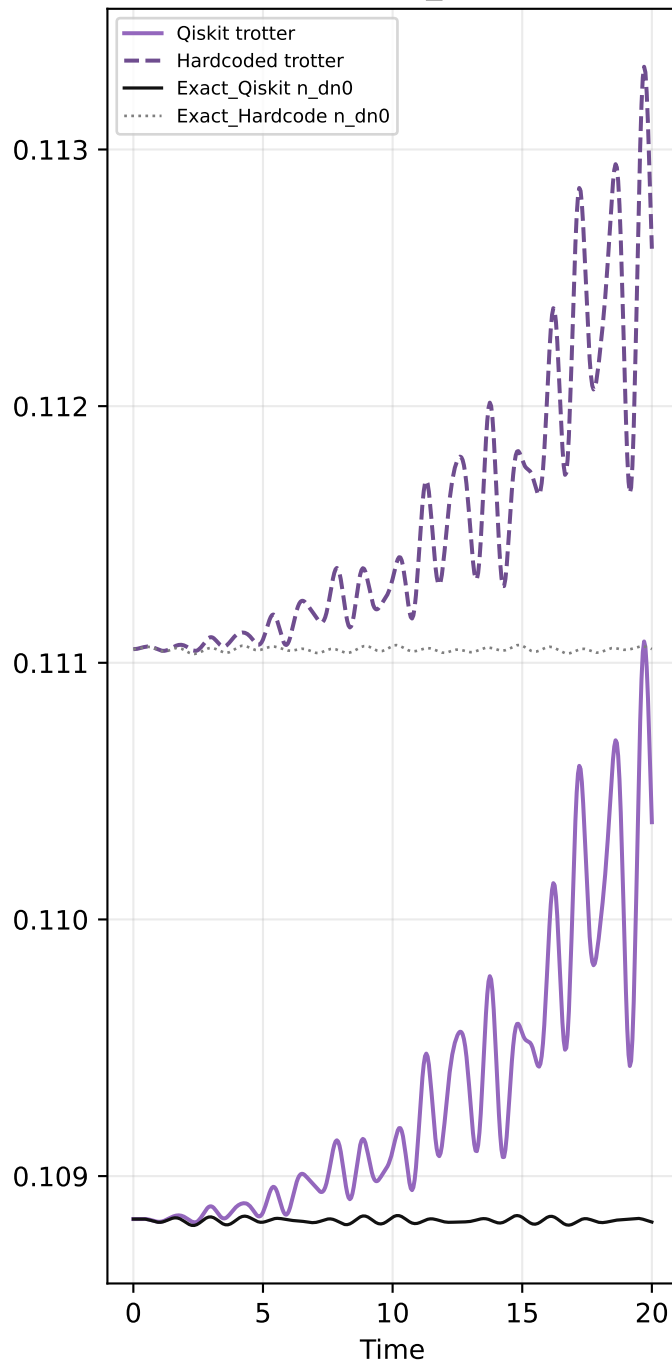


Pipeline Comparison L=3: Occupations & Doublon (auto-zoomed)

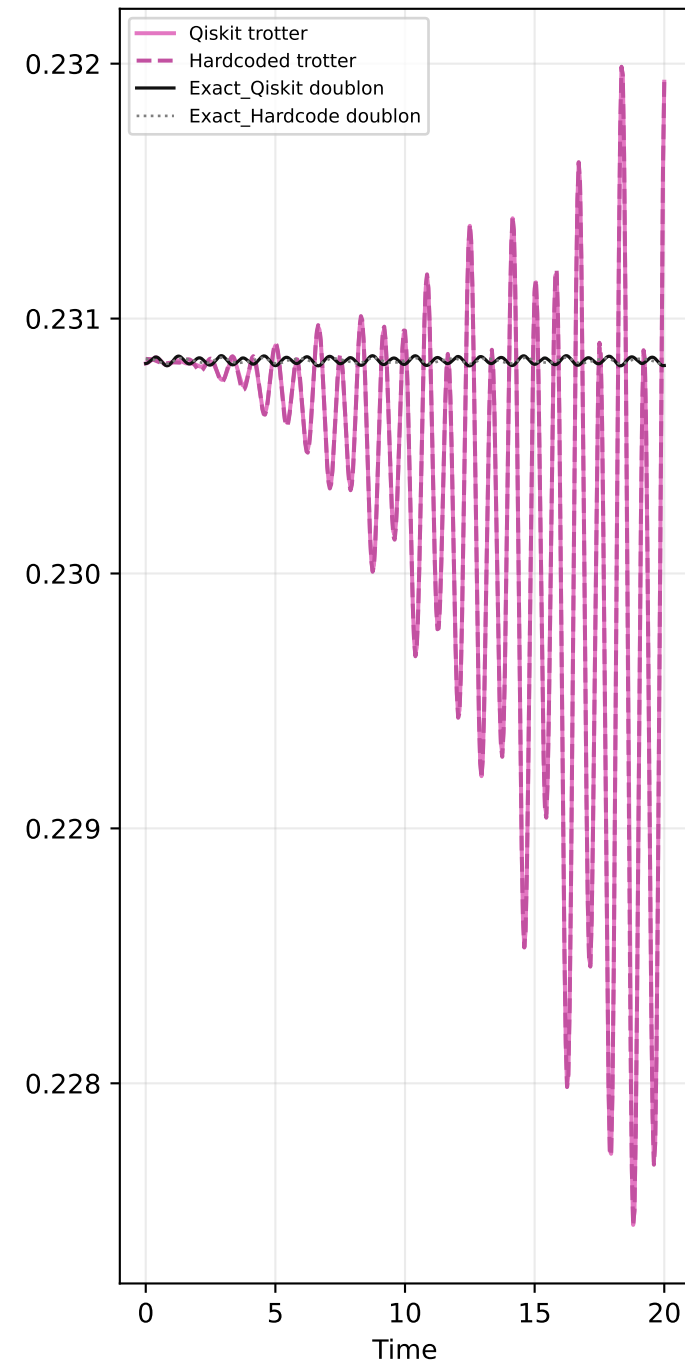
Site-0 n_{up}



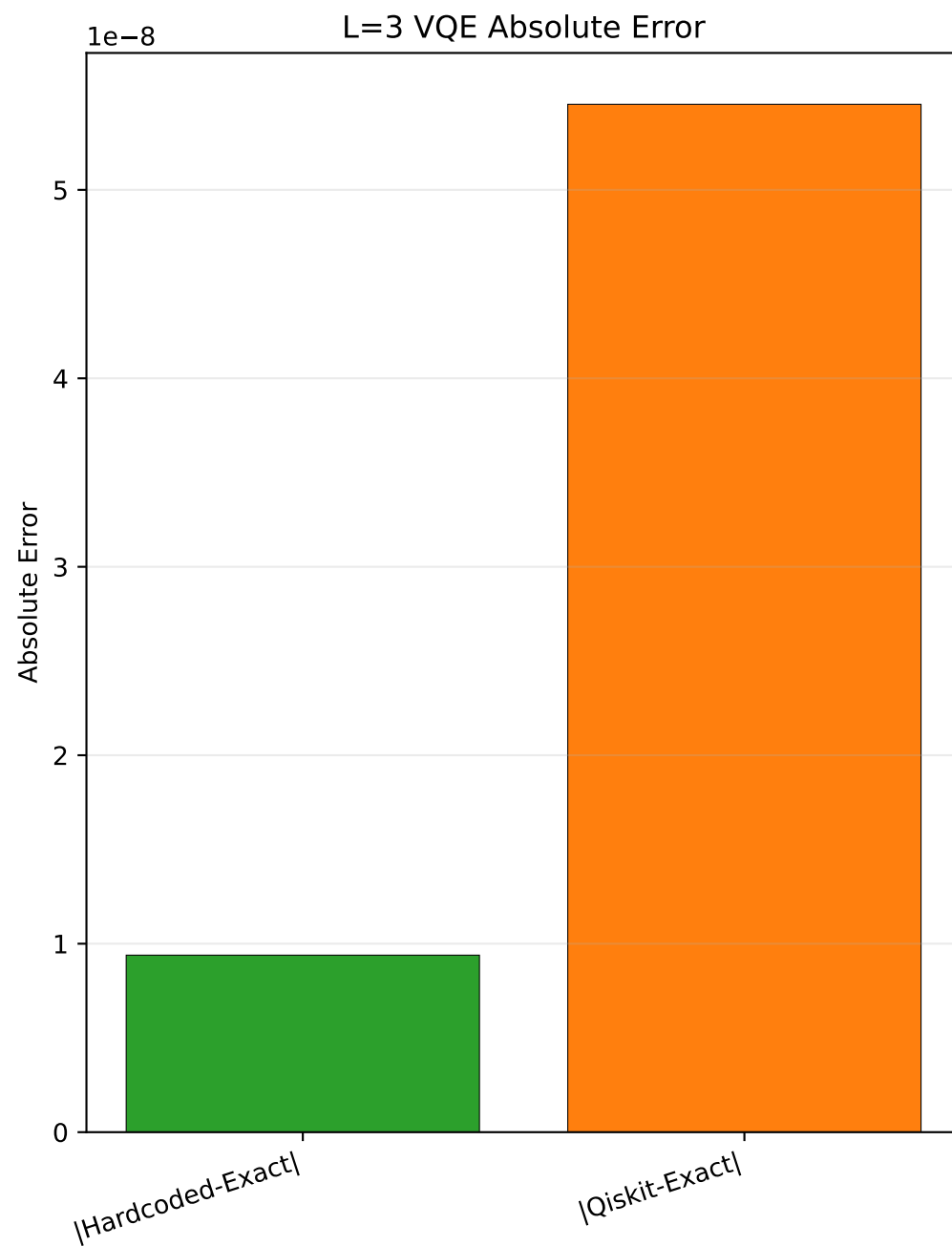
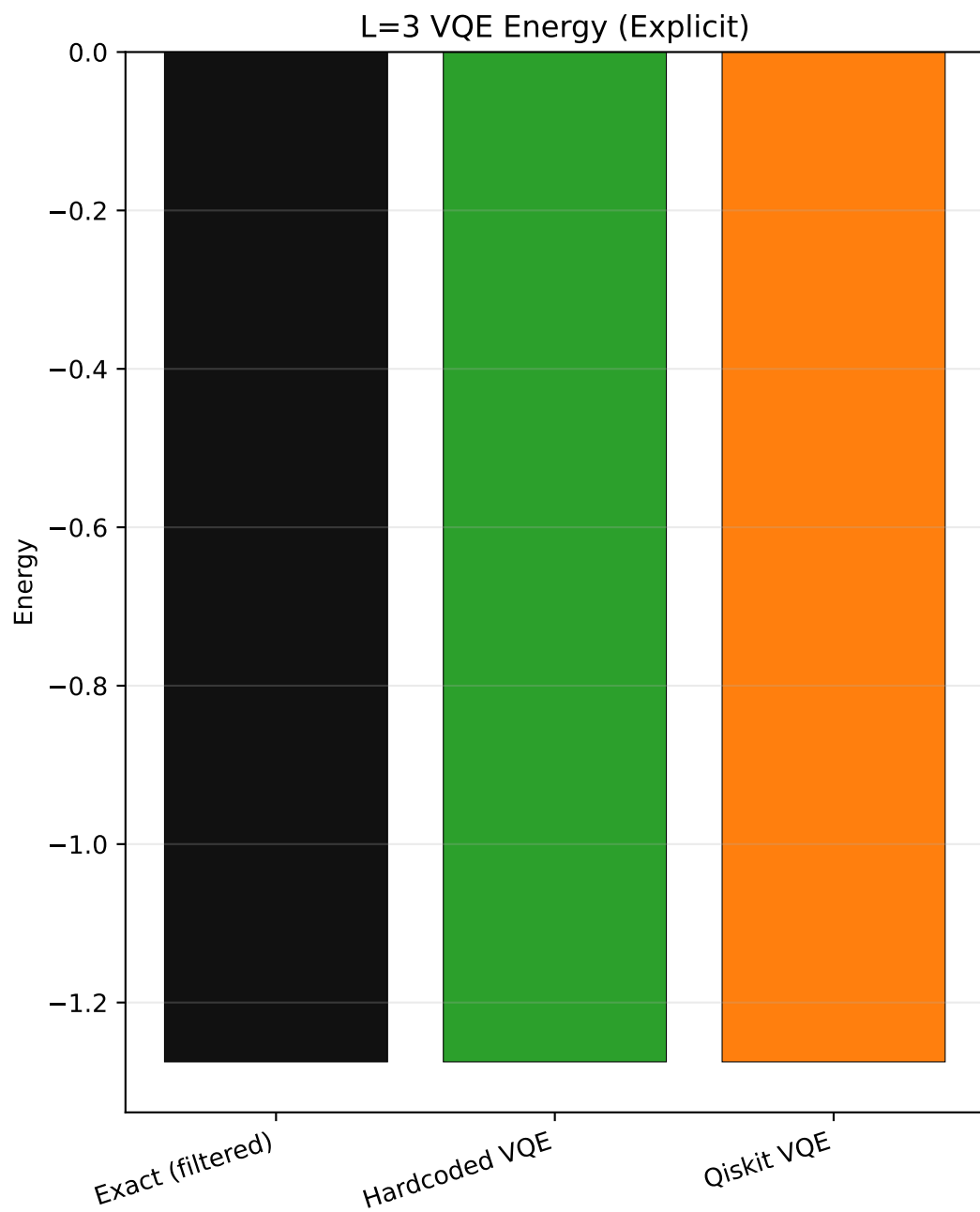
Site-0 n_{dn}



Doublon

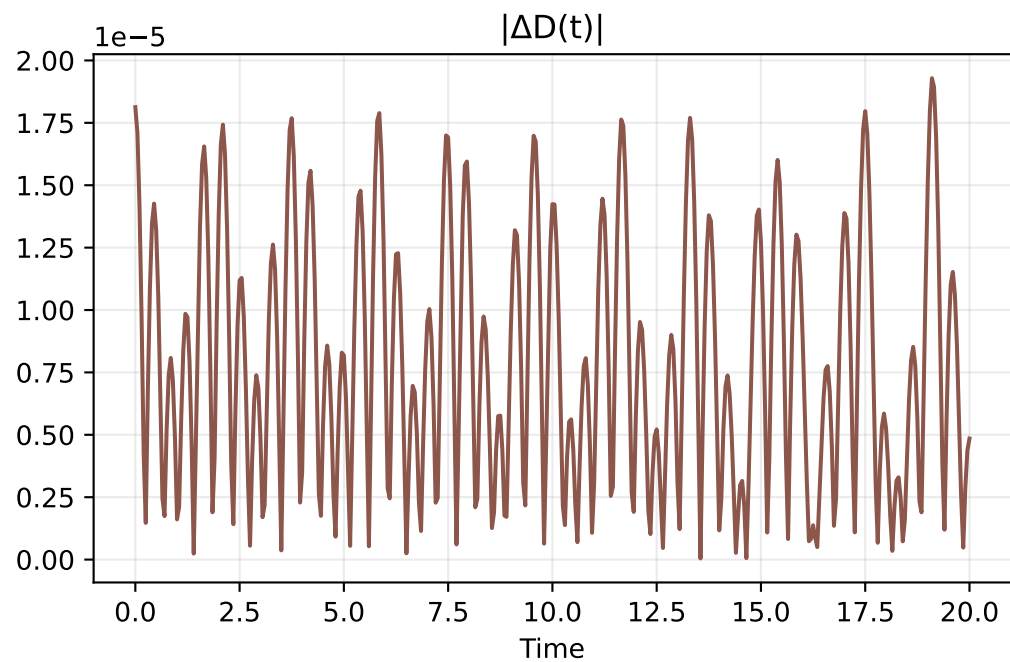
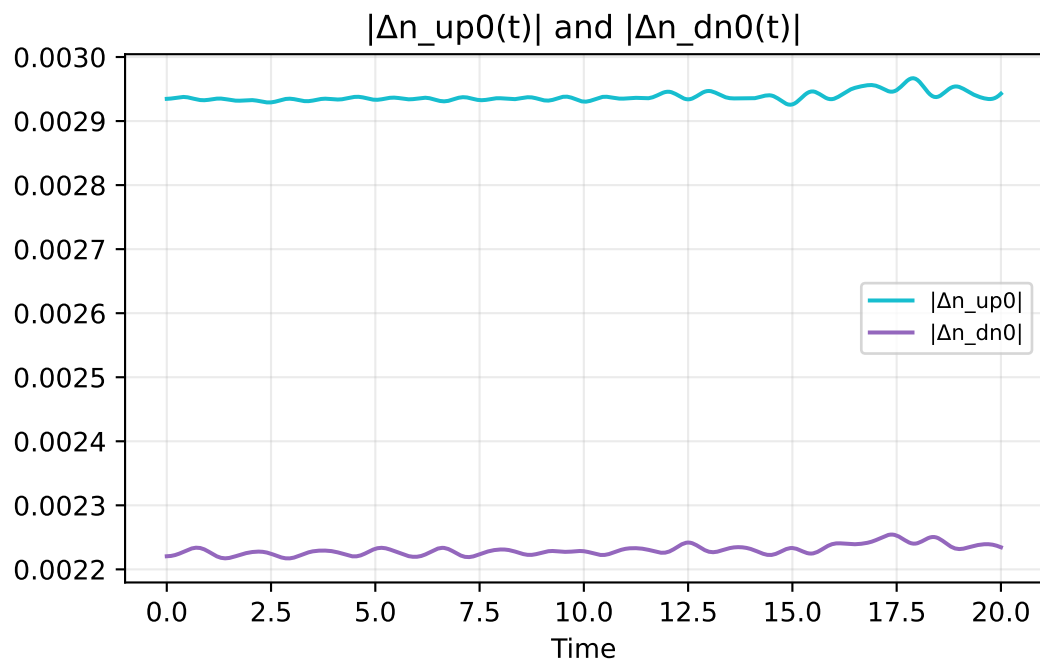
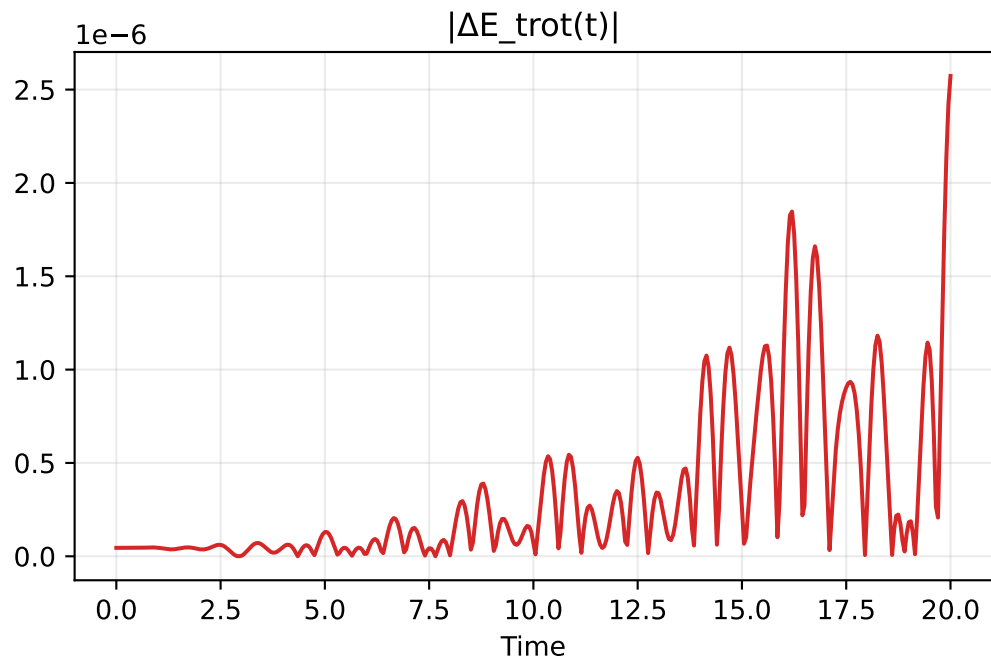
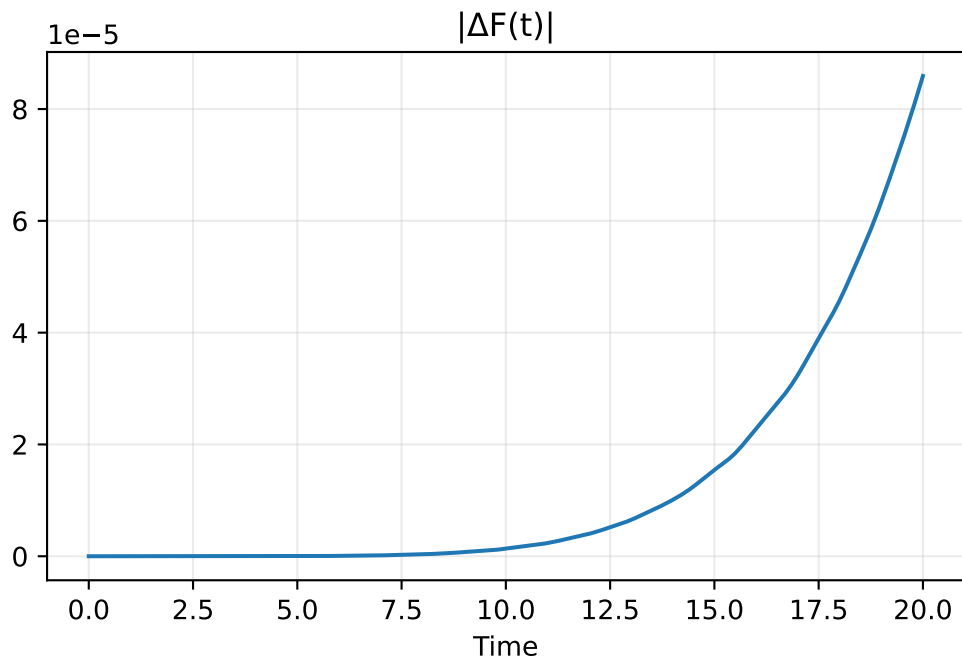


When initial_state_source=vqe, Trotter $E(t=0) = \langle \psi_{\text{vqe}} | H | \psi_{\text{vqe}} \rangle = \text{VQE energy}$.
VQE energy \neq exact ground state energy unless VQE fully converged.



Delta Diagnostics L=3

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



L=3 metrics summary

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 = 8.590937577102054e-05 / 1.2397428124140835e-05 / 8.590937577102054e-05

energy_trotter max/mean/final = 2.5727693202526325e-06 / 3.272323027216911e-07 / 2.5727693202526325e-06

n_up_site0_trotter max/mean/final = 0.0029669176457719493 / 0.002937995165993819 / 0.00294272903376791

n_dn_site0_trotter max/mean/final = 0.002254321495447492 / 0.002230267735052105 / 0.0022344932649621674

doublon_trotter max/mean/final = 1.928841137227577e-05 / 7.901033142319897e-06 / 4.8501852527027545e-06

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