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
```

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
```
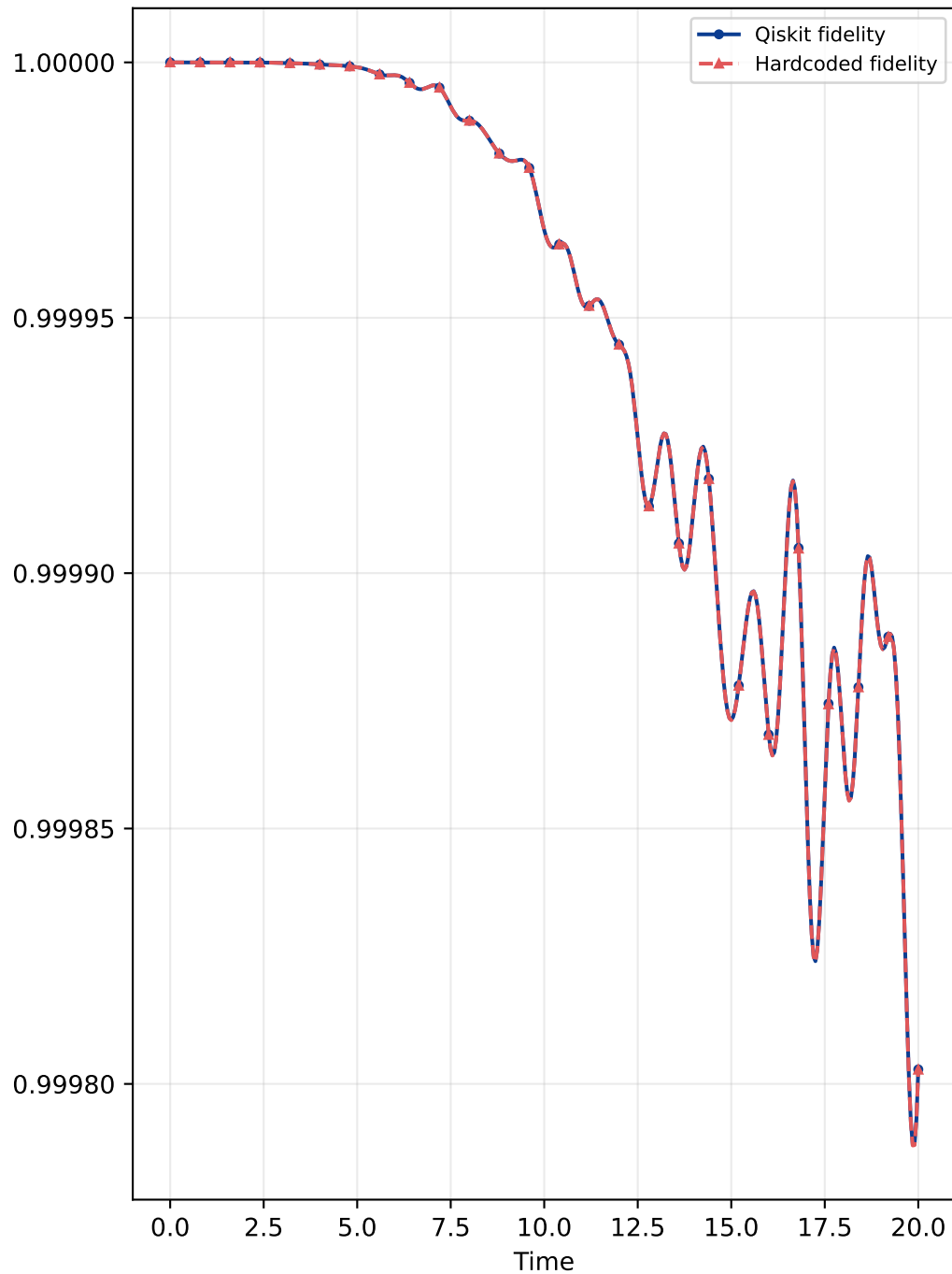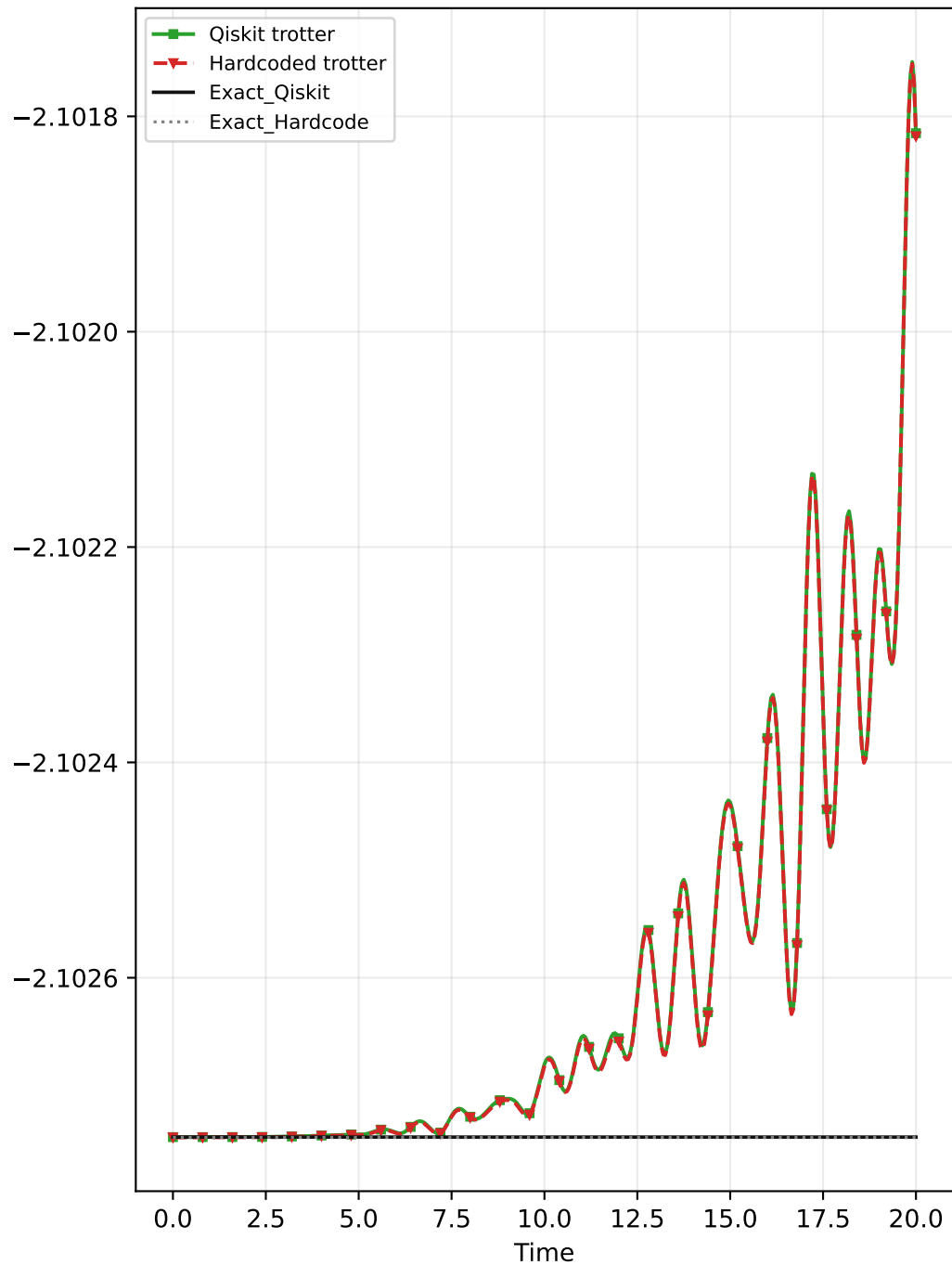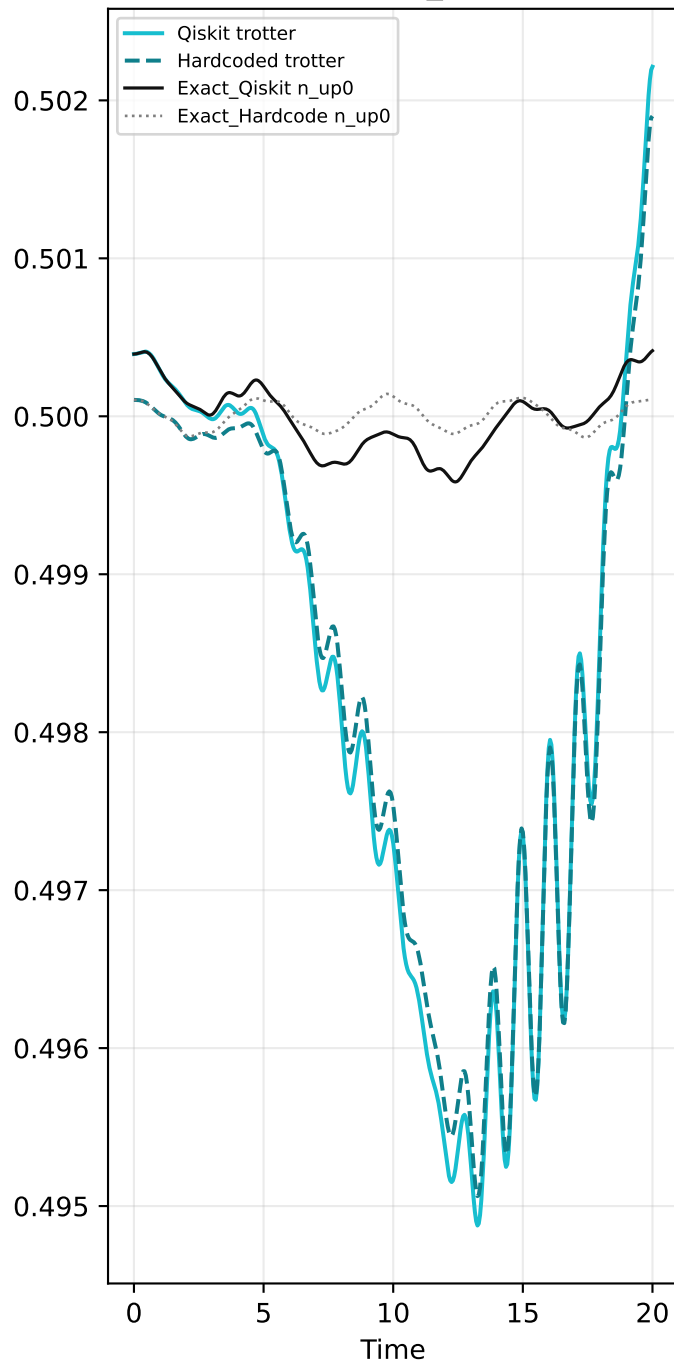
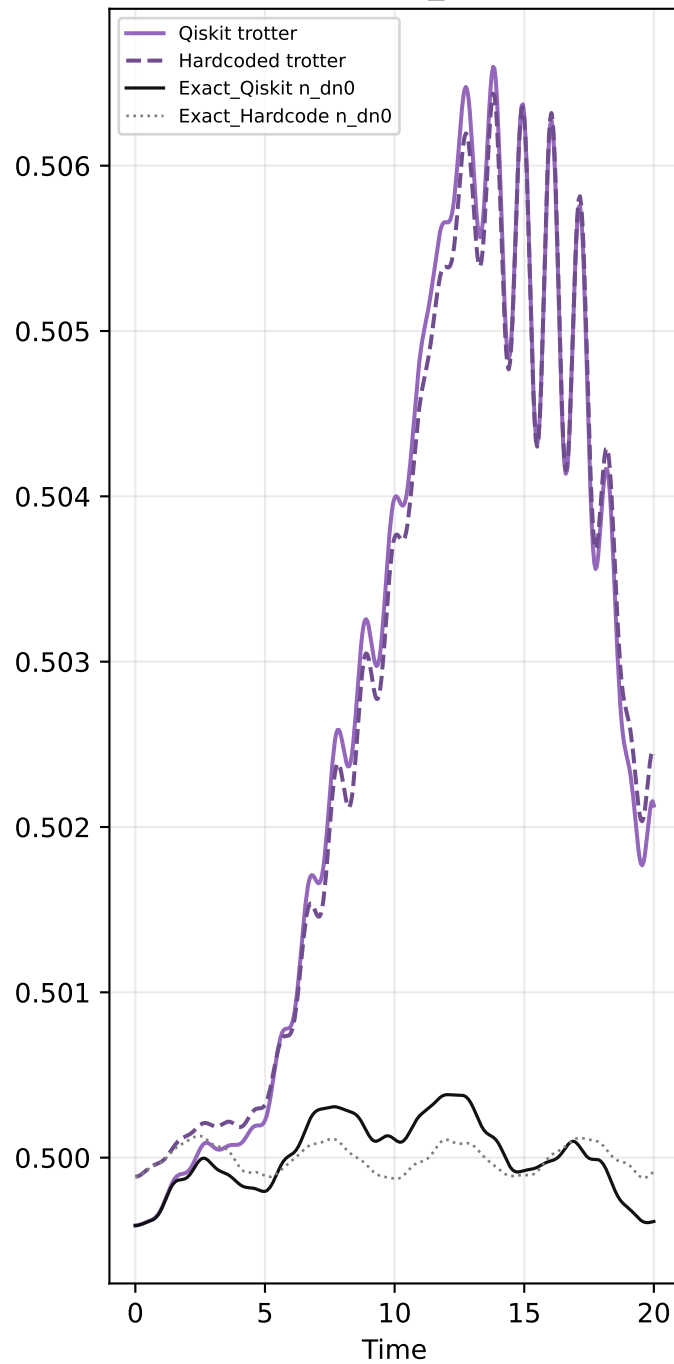Pipeline Comparison L=4: Hardcoded vs Qiskit (Fidelity & Energy)

Pipeline Comparison L=4: Occupations & Doublon (auto-zoomed)

Site-0 n_up
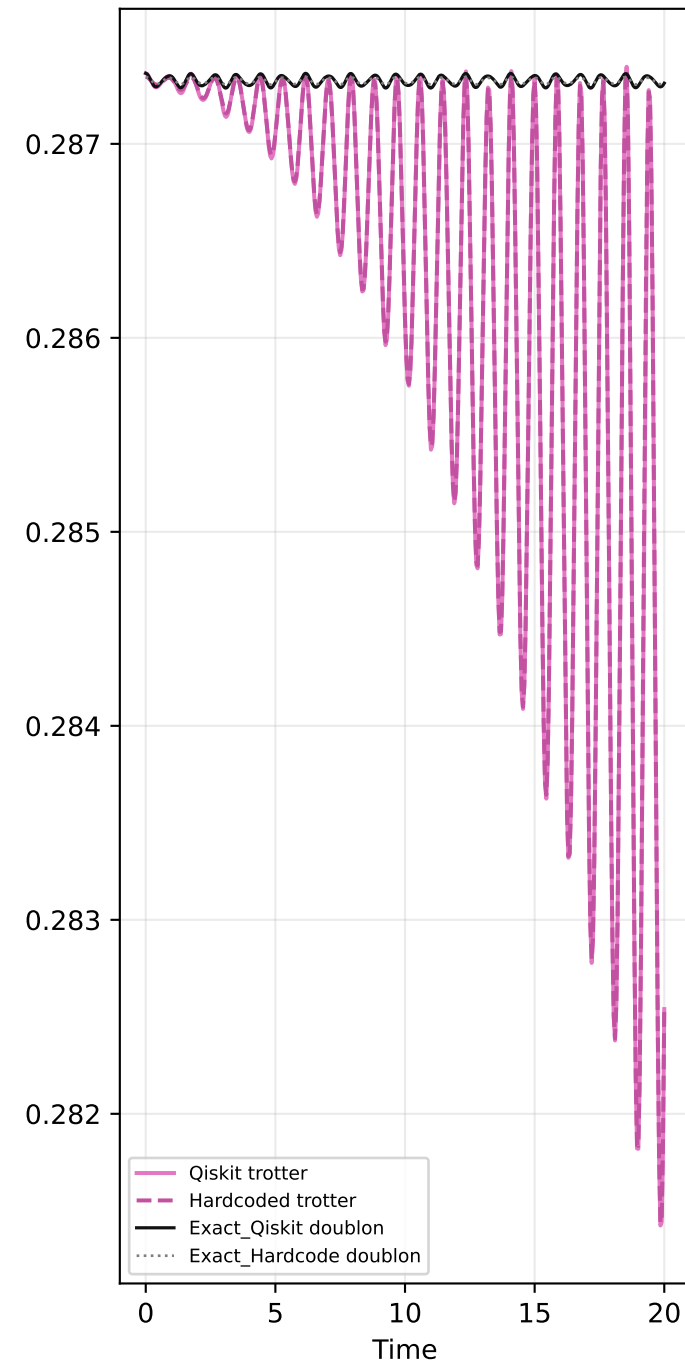
- Qiskit trotter
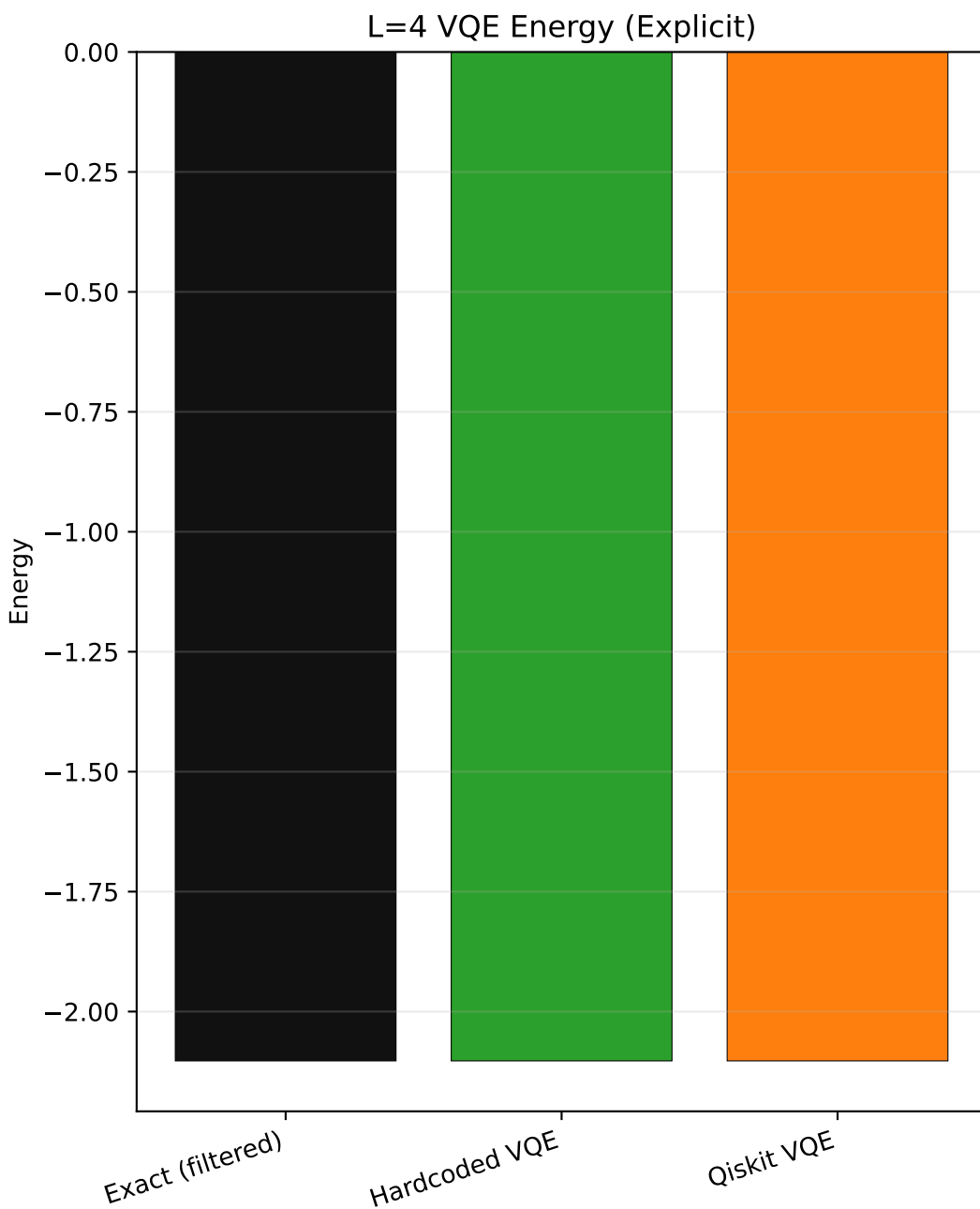- Hardcoded trotter
- Exact_Qiskit n_up0
- Exact_Hardcode n_up0

Site-0 n_dn

- Qiskit trotter
- Hardcoded trotter
- Exact_Qiskit n_dn0
- Exact_Hardcode n_dn0

Doublon

- Qiskit trotter
- Hardcoded trotter
- Exact_Qiskit doublon
- Exact_Hardcode doublon

When initial_state_source=vqe, Trotter E(t=0) = ⟨ψ_vqe|H|ψ_vqe⟩ = VQE energy.
VQE energy ≠ exact ground state energy unless VQE fully converged.
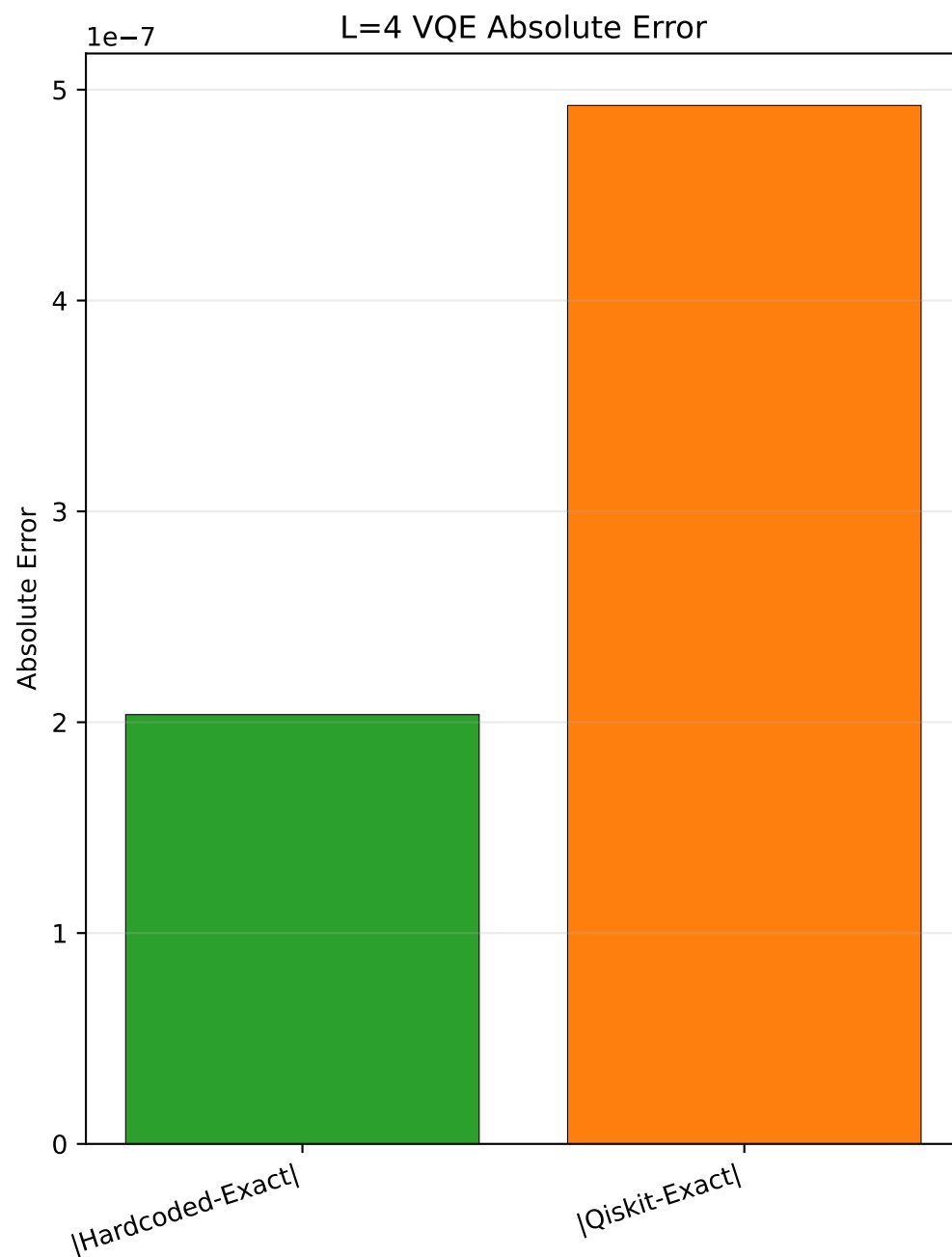
Delta Diagnostics L=4

$\Delta X(t) = |X\_hc(t) - X\_qk(t)|$, where $X\_pipeline(t)$ is that pipeline's stored trajectory value.
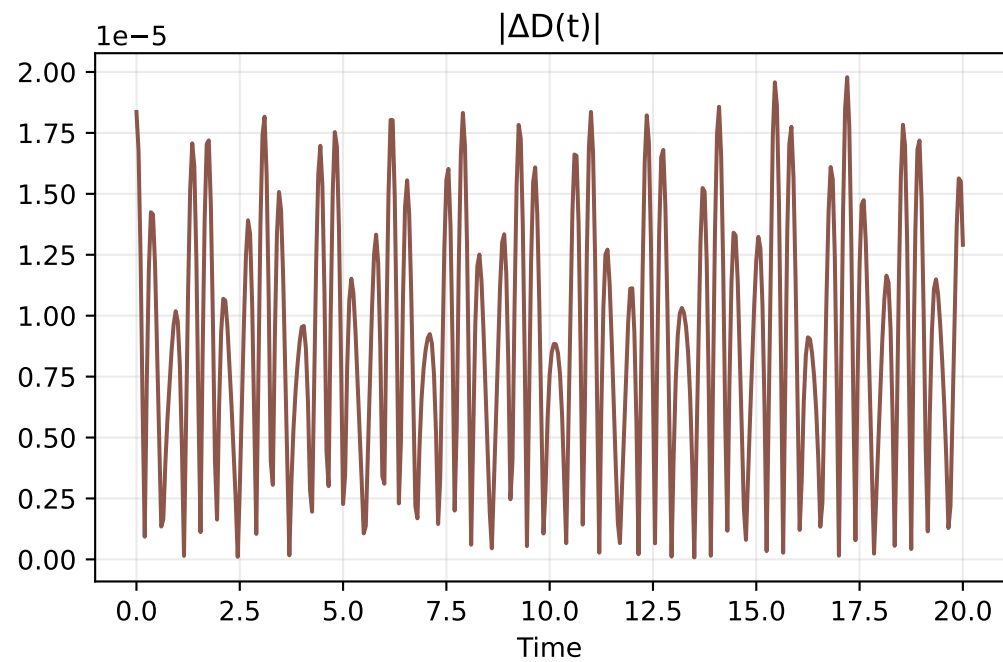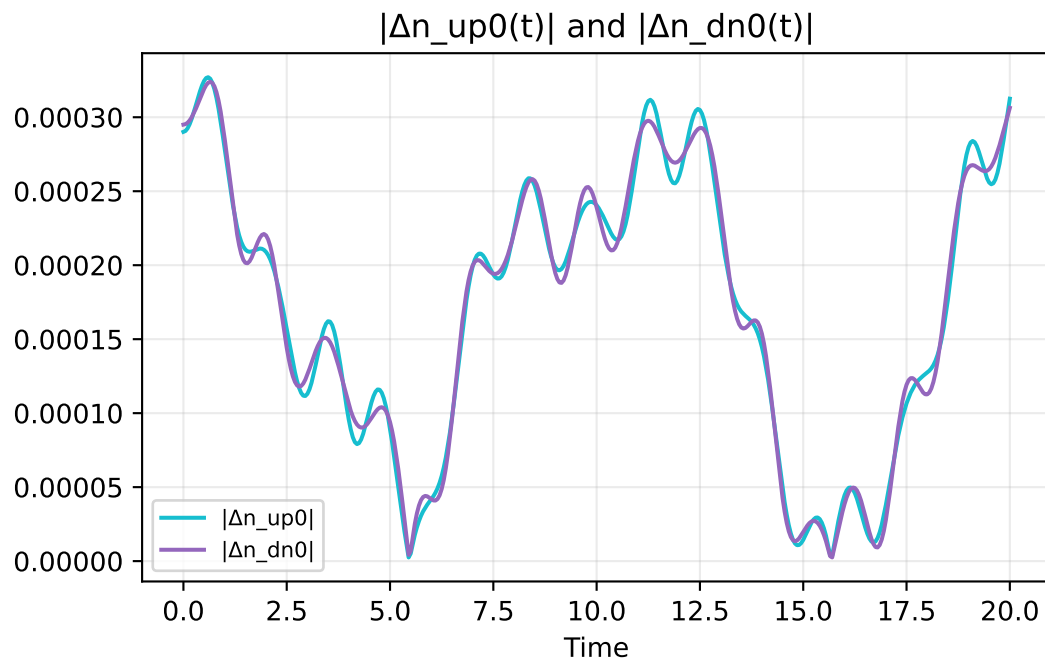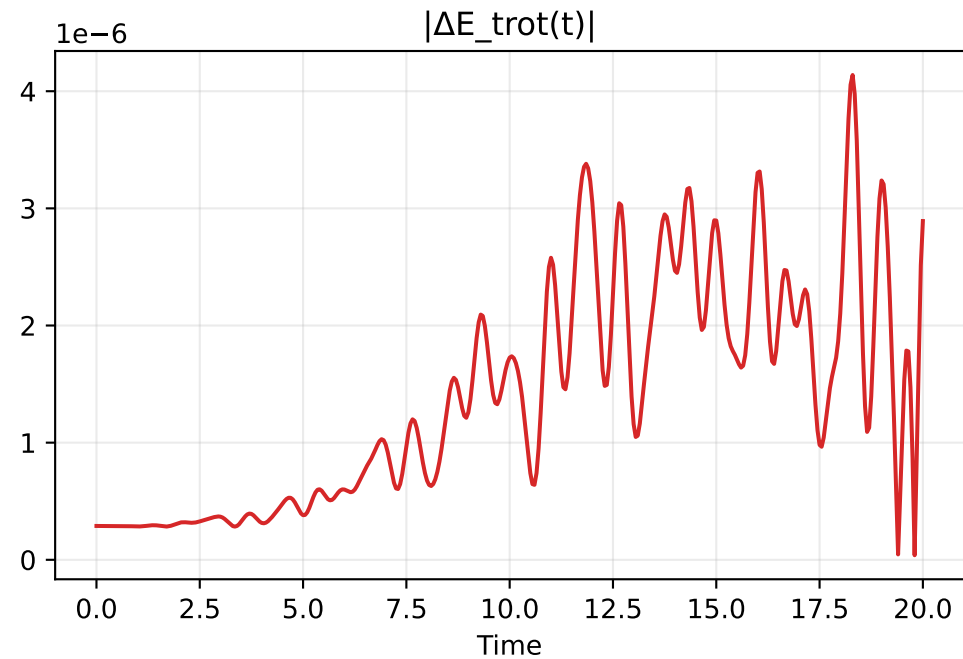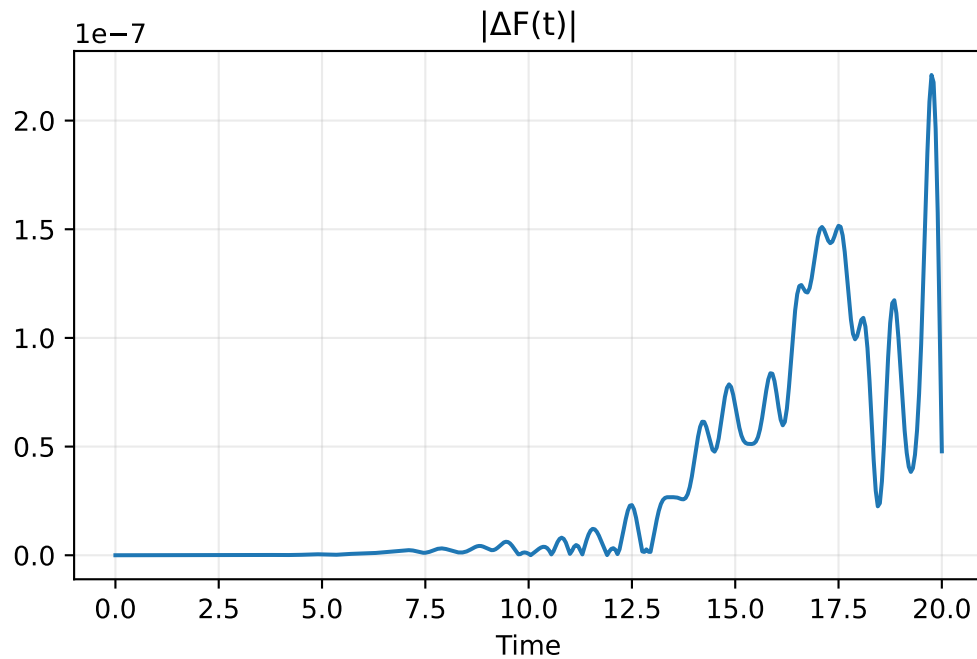
```
L=4 metrics summary

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)|
Δn_dn0(t)  = |n_dn0_hc(t) - n_dn0_qk(t)|
ΔD(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
```