

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

Fidelity

Energy

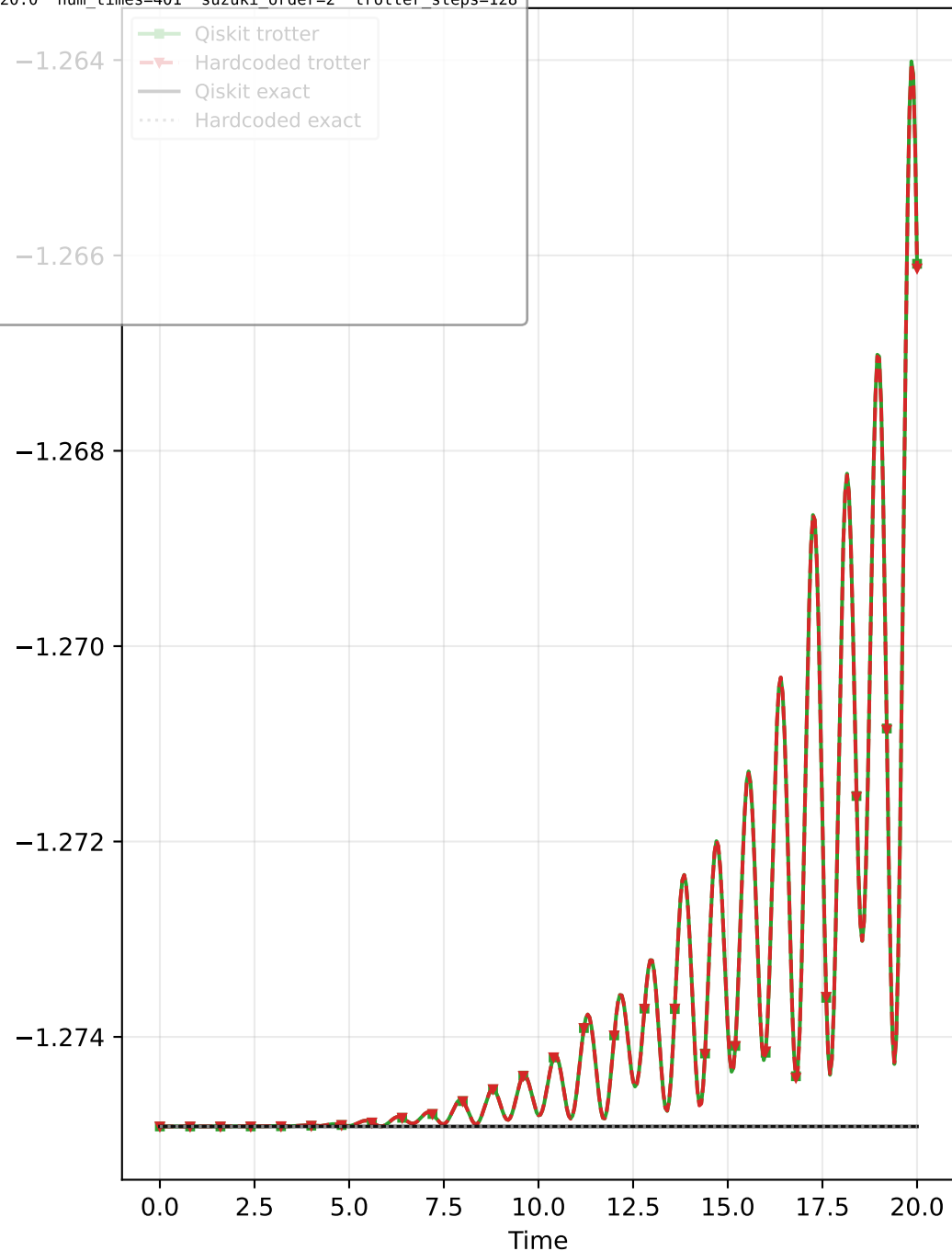
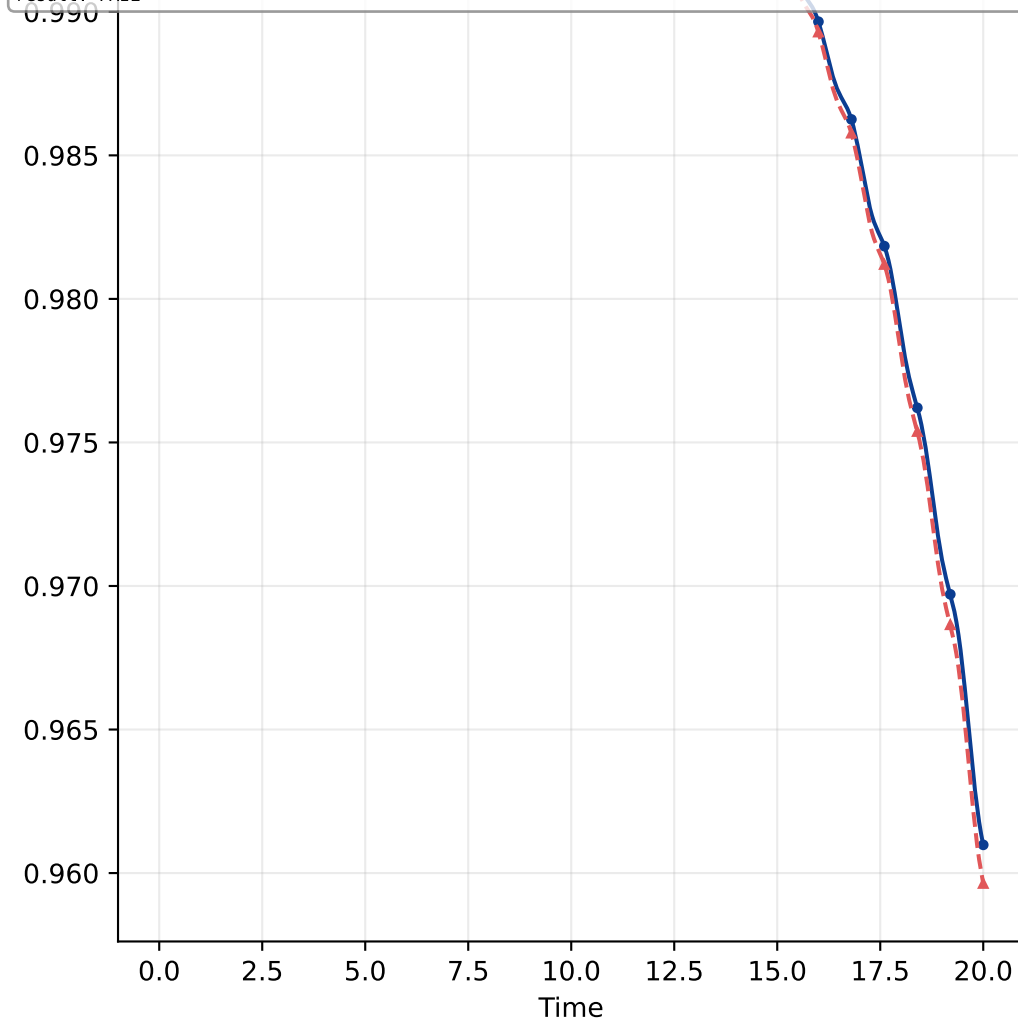
L=3 t=1.0 u=4.0 dv=0.0 boundary=periodic ordering=blocked initial_state source=vqe t_final=20.0 num_times=401 suzuki_order=2 trotter_steps=128

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

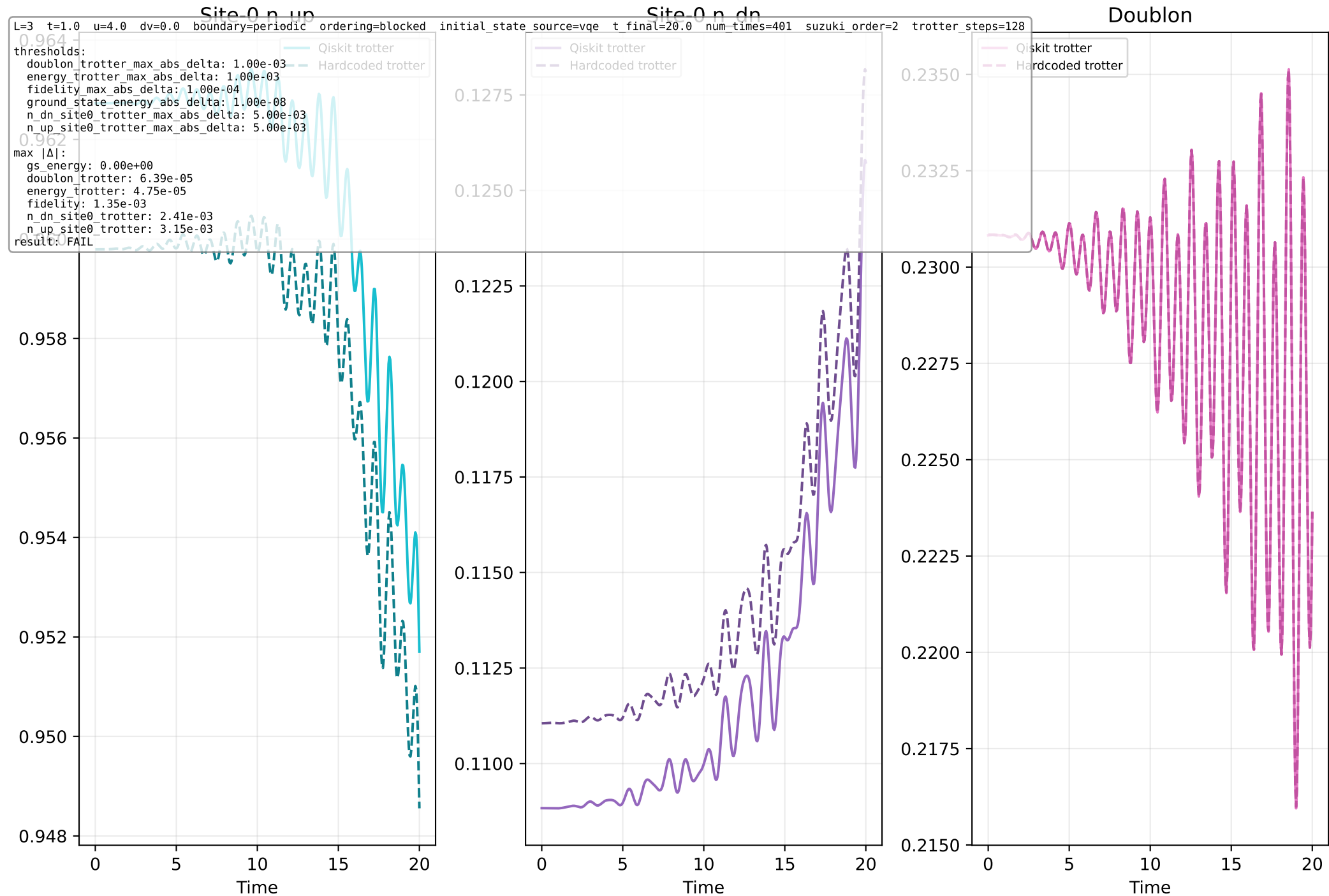
max |Δ|:
 gs_energy: 0.00e+00
 doublon_trotter: 6.39e-05
 energy_trotter: 4.75e-05
 fidelity: 1.35e-03
 n_dn_site0_trotter: 2.41e-03
 n_up_site0_trotter: 3.15e-03
 result: FAIL

Qiskit fidelity
 Hardcoded fidelity

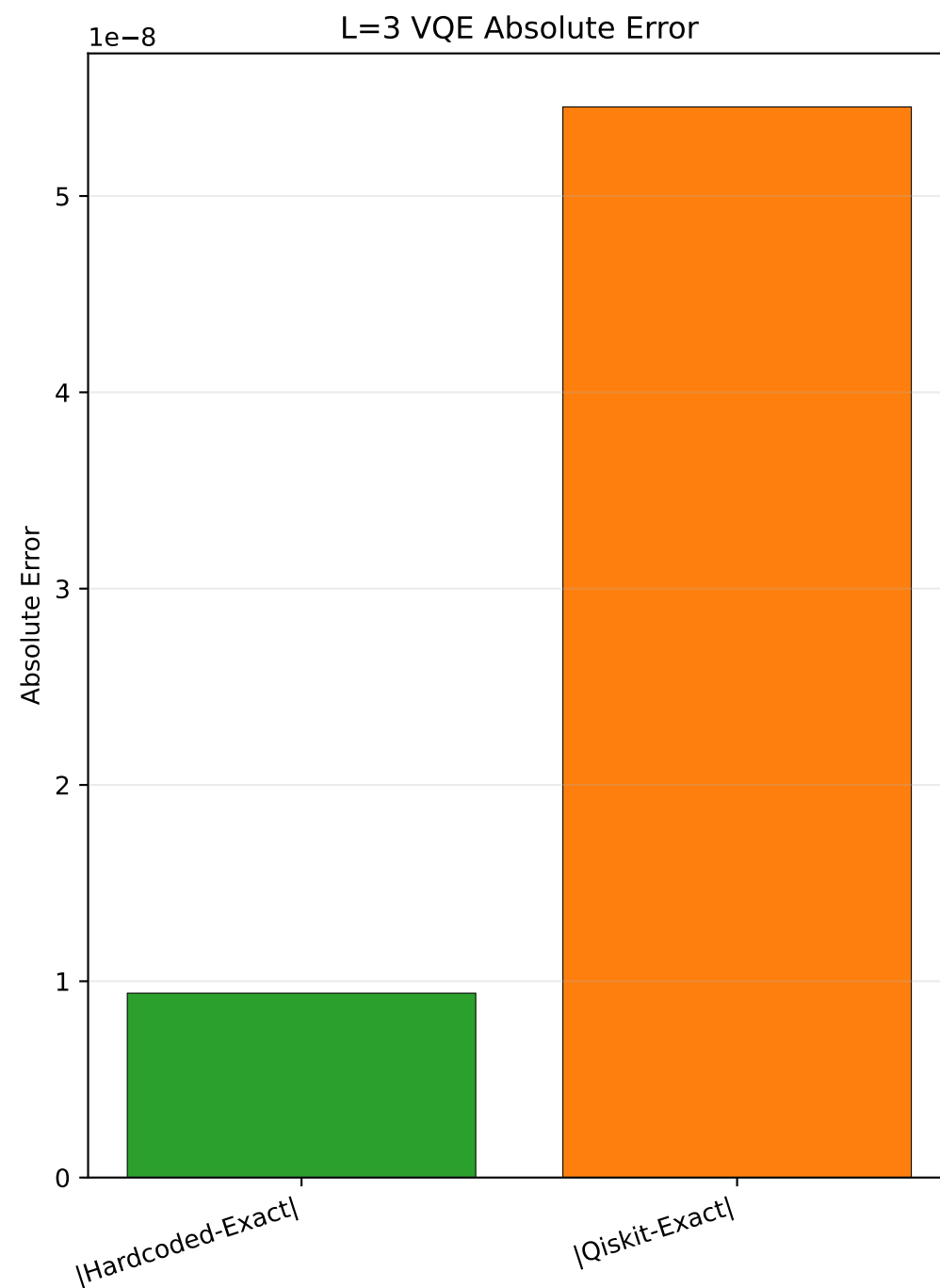
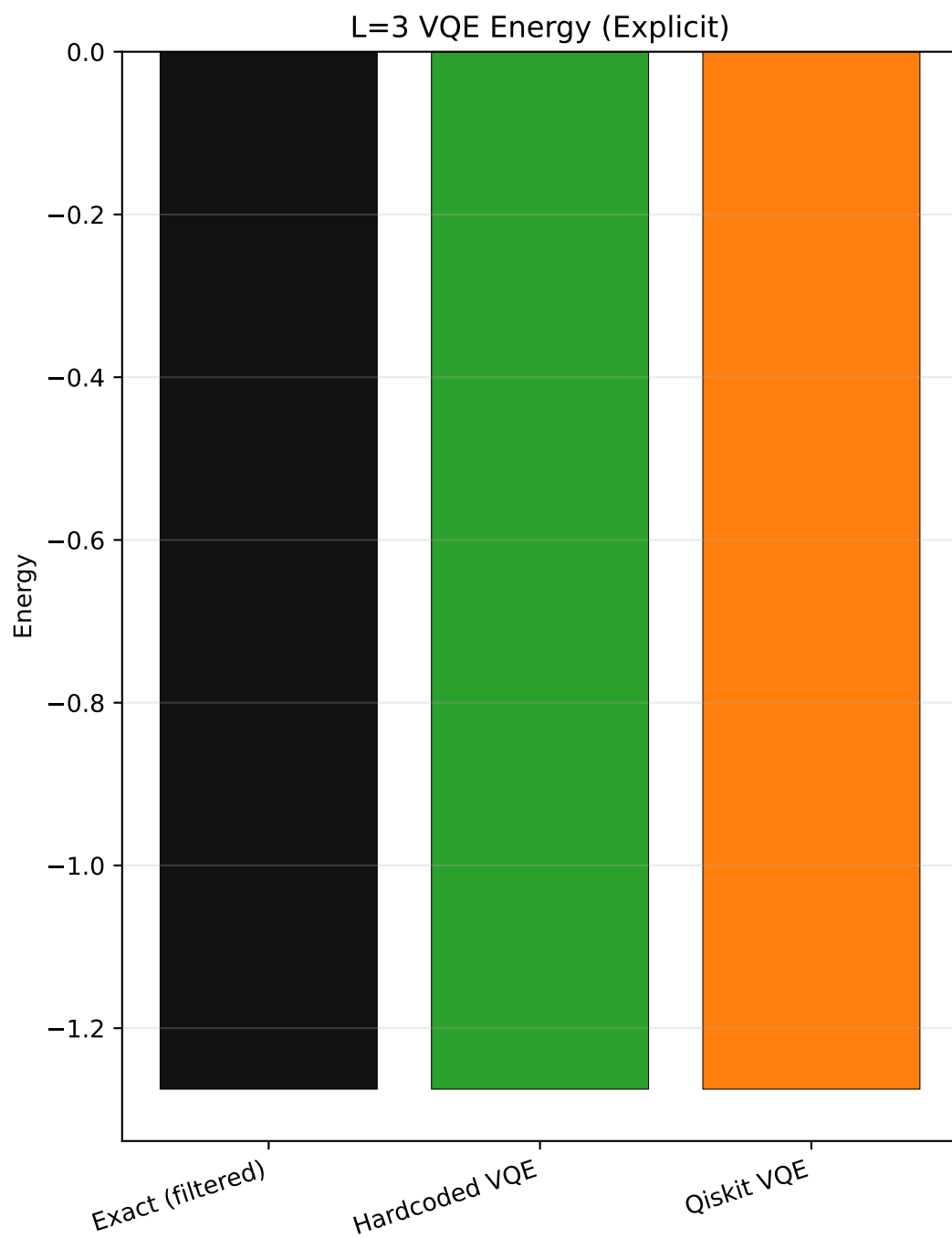
Qiskit trotter
 Hardcoded trotter
 Qiskit exact
 Hardcoded exact



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



VQE is a separate quantity from the Trotter $t=0$ value; do not infer VQE energy from trajectory plots.



Delta Diagnostics L=3

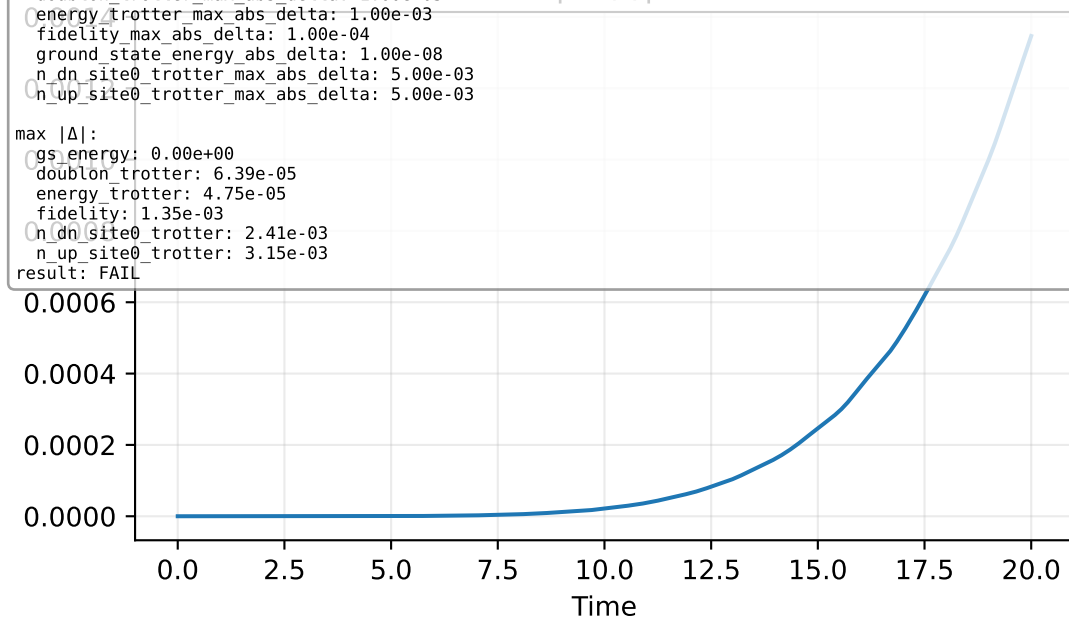
$\Delta X(t) = |X_{hc}(t) - X_{qk}(t)|$, where $X_{pipeline}(t)$ is that pipeline's stored trajectory value.

L=3 t=1.0 u=4.0 dv=0.0 boundary=periodic ordering=blocked initial_state_source=vqe t_final=20.0 num_times=401 suzuki_order=2 trotter_steps=128

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

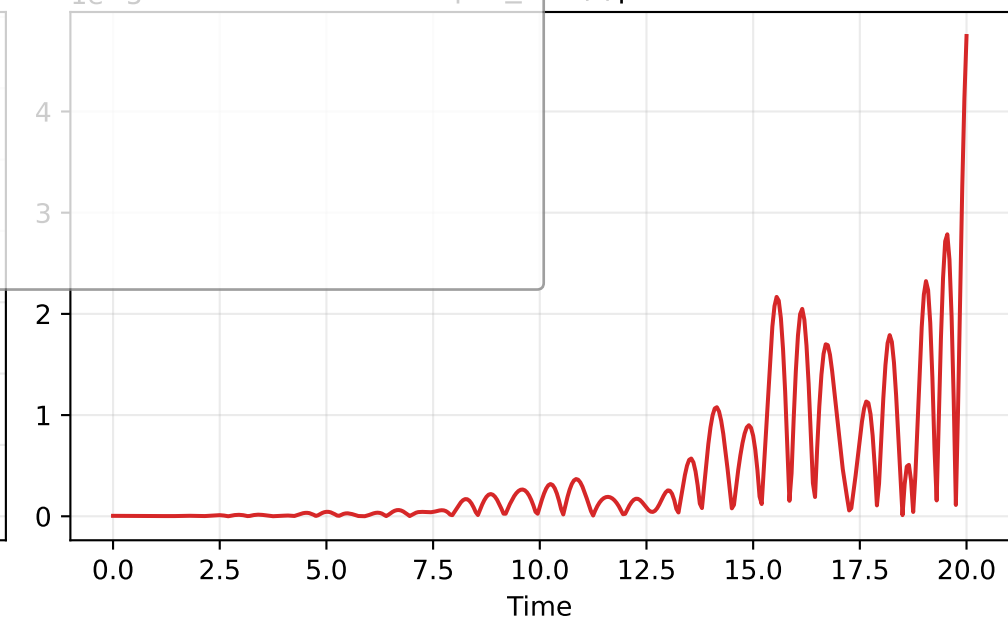
max $|\Delta|$:
gs_energy: 0.00e+00
doublon_trotter: 6.39e-05
energy_trotter: 4.75e-05
fidelity: 1.35e-03
n_dn_site0_trotter: 2.41e-03
n_up_site0_trotter: 3.15e-03
result: FAIL

$|\Delta F(t)|$

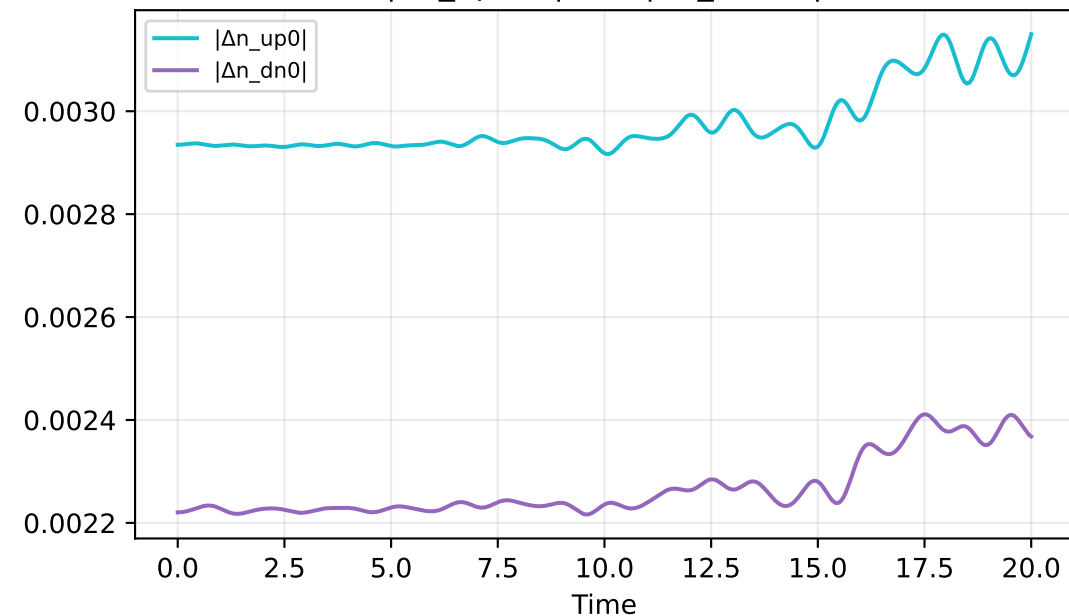


$1e-5$

$|\Delta E_{trot}(t)|$

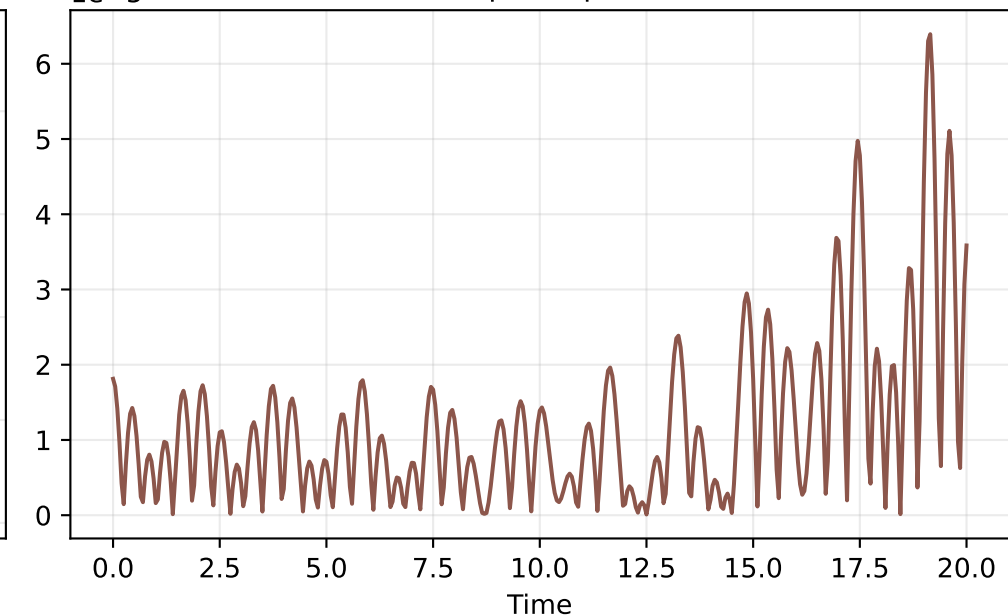


$|\Delta n_{up0}(t)|$ and $|\Delta n_{dn0}(t)|$



$1e-5$

$|\Delta D(t)|$



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 = 0.0013464071626839713 / 0.00019665025721909328 / 0.0013464071626839713

energy_trotter max/mean/final = 4.7458908048580994e-05 / 3.99668035453194e-06 / 4.7458908048580994e-05

n_up_site0_trotter max/mean/final = 0.0031496651890847716 / 0.002975898354829075 / 0.0031496651890847716

n_dn_site0_trotter max/mean/final = 0.0024109550934178353 / 0.00226718670337712 / 0.002368035185029038

doublon_trotter max/mean/final = 6.39293585977807e-05 / 1.1616930205037722e-05 / 3.5848731140875056e-05

checks:

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

PASS = False