

L=2 Run Settings & Metrics Summary

L=2 t=1.0 u=4.0 dv=0.0 boundary=periodic ordering=blocked initial_state_source=vqe t_final=20.0 num_times=201 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

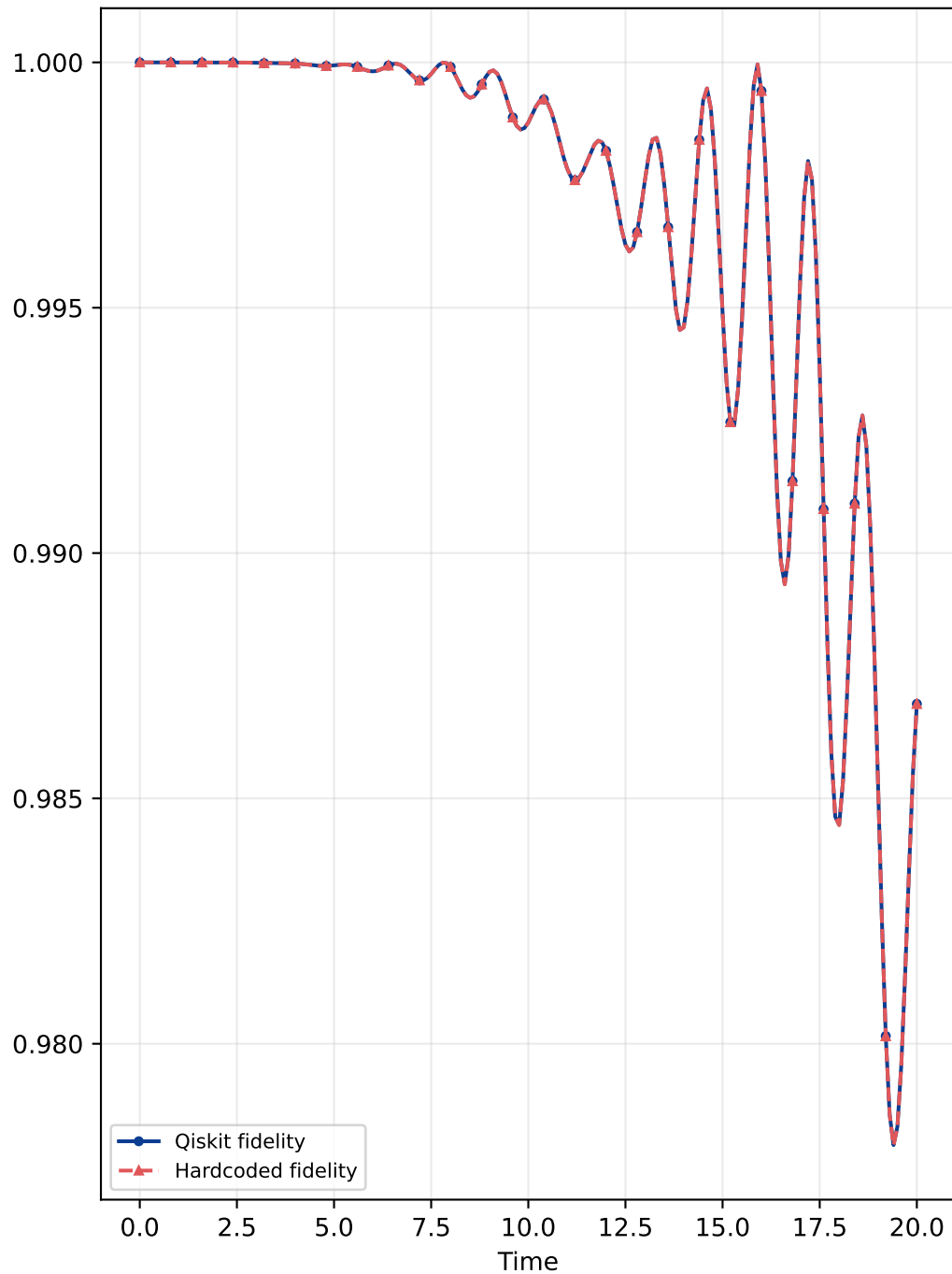
max $|\Delta|$:

gs_energy: 0.00e+00
doublon_trotter: 2.79e-06
energy_trotter: 2.35e-05
fidelity: 8.59e-06
n_dn_site0_trotter: 2.79e-05
n_up_site0_trotter: 2.78e-05

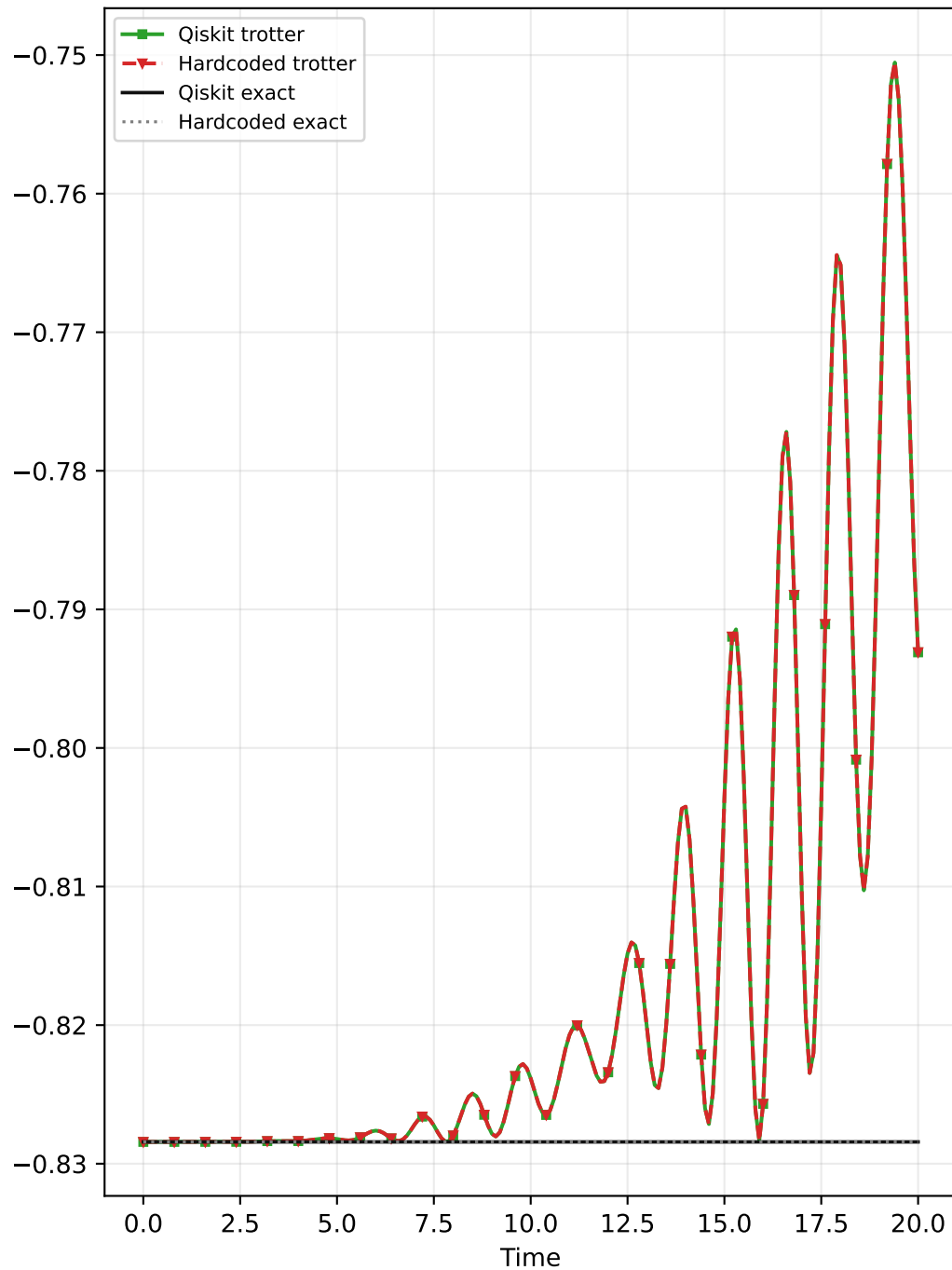
result: PASS

Pipeline Comparison L=2: Hardcoded vs Qiskit (Fidelity & Energy)

Fidelity

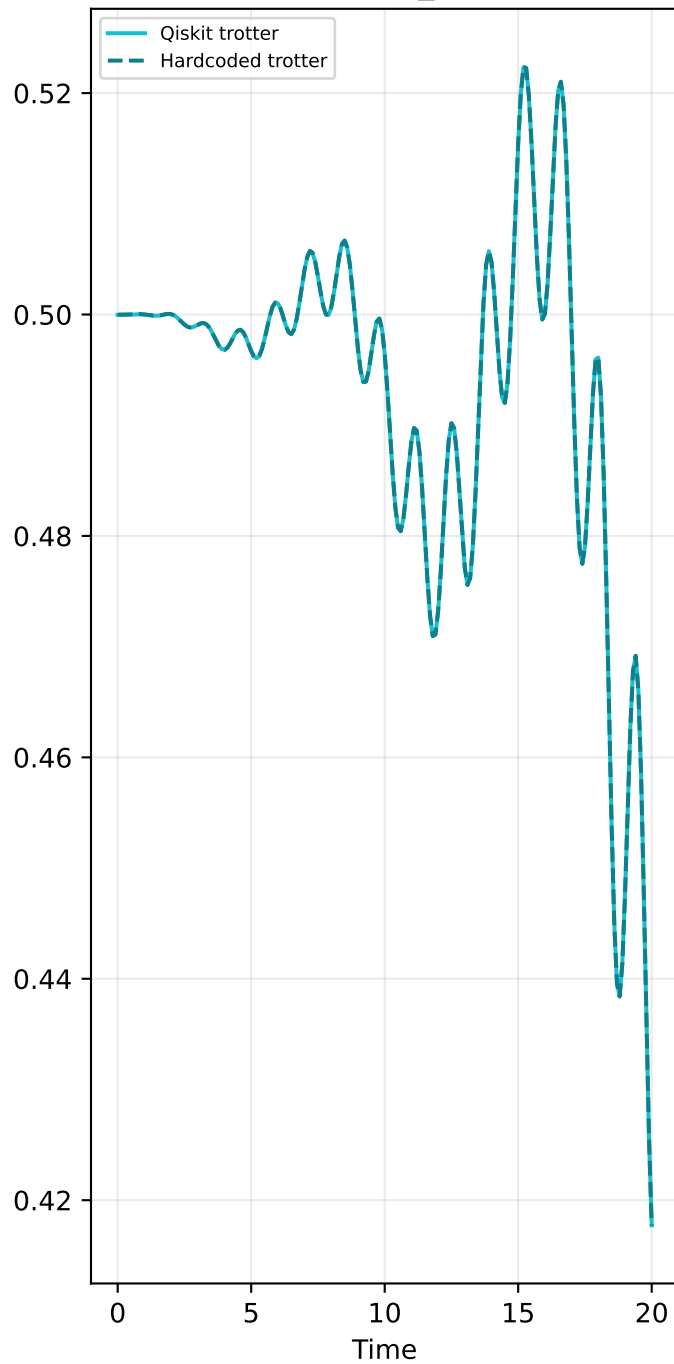


Energy

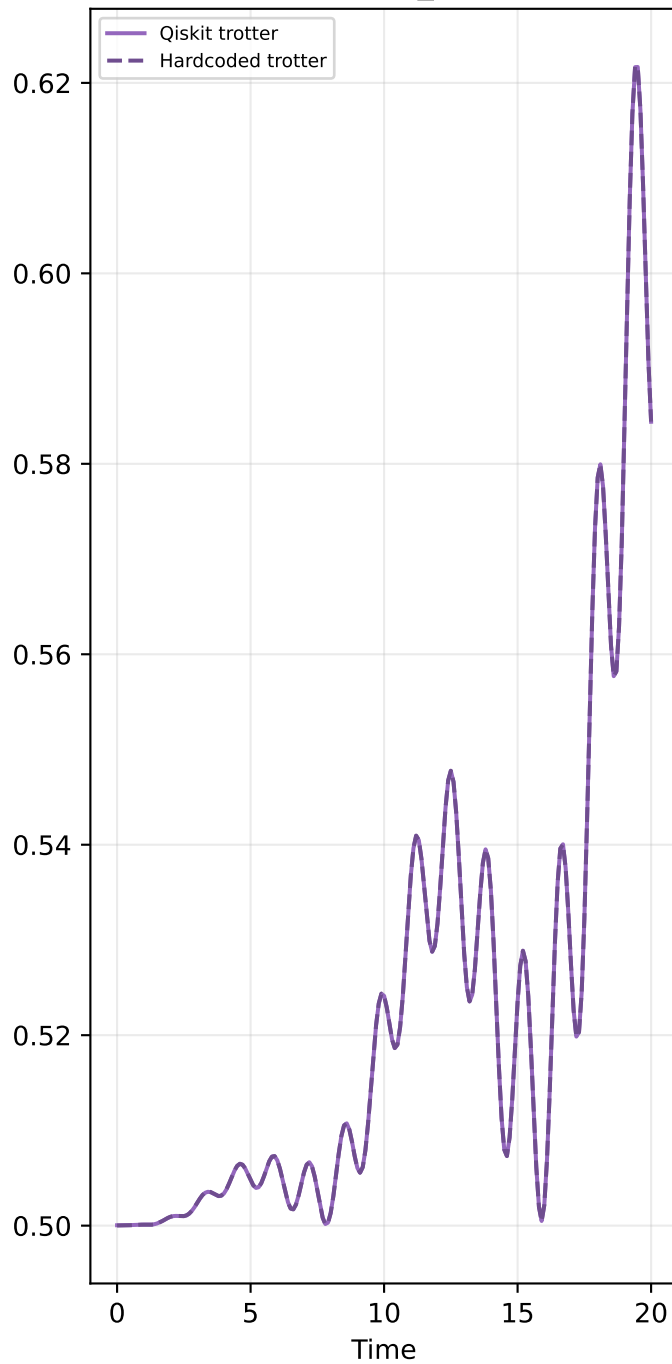


Pipeline Comparison L=2: Occupations & Doublon (auto-zoomed)

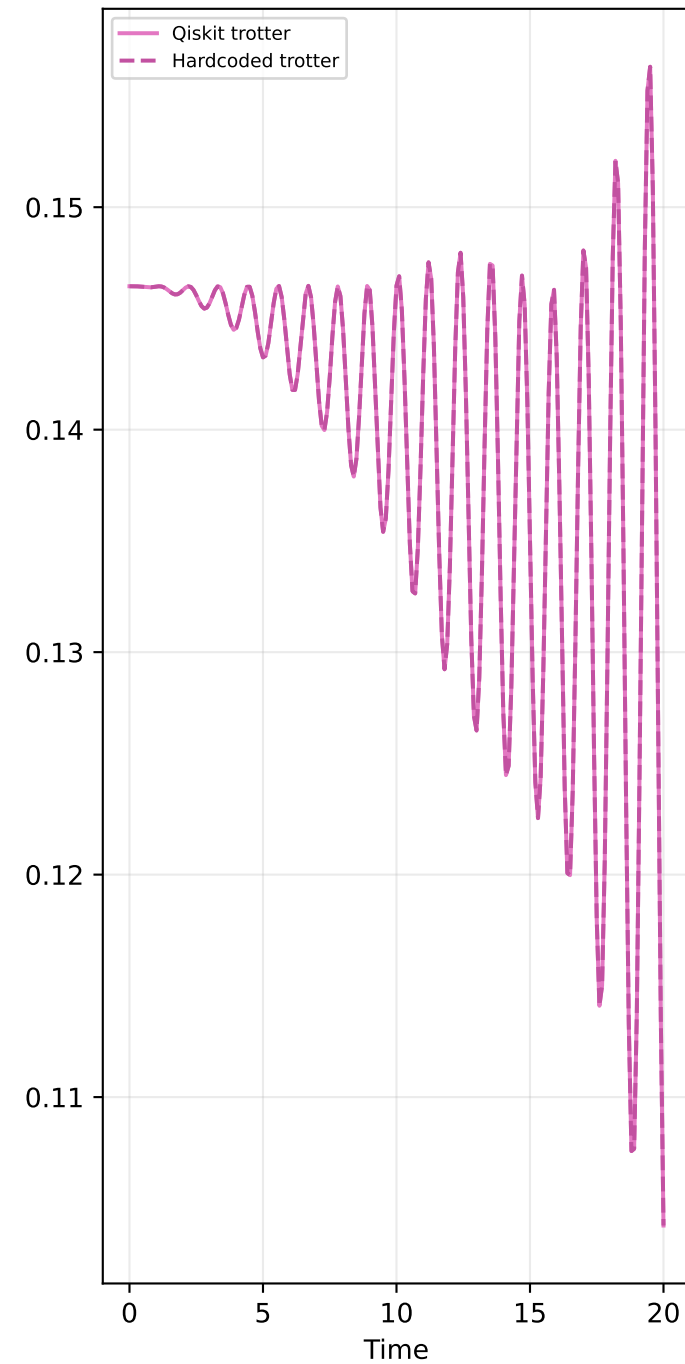
Site-0 n_{up}



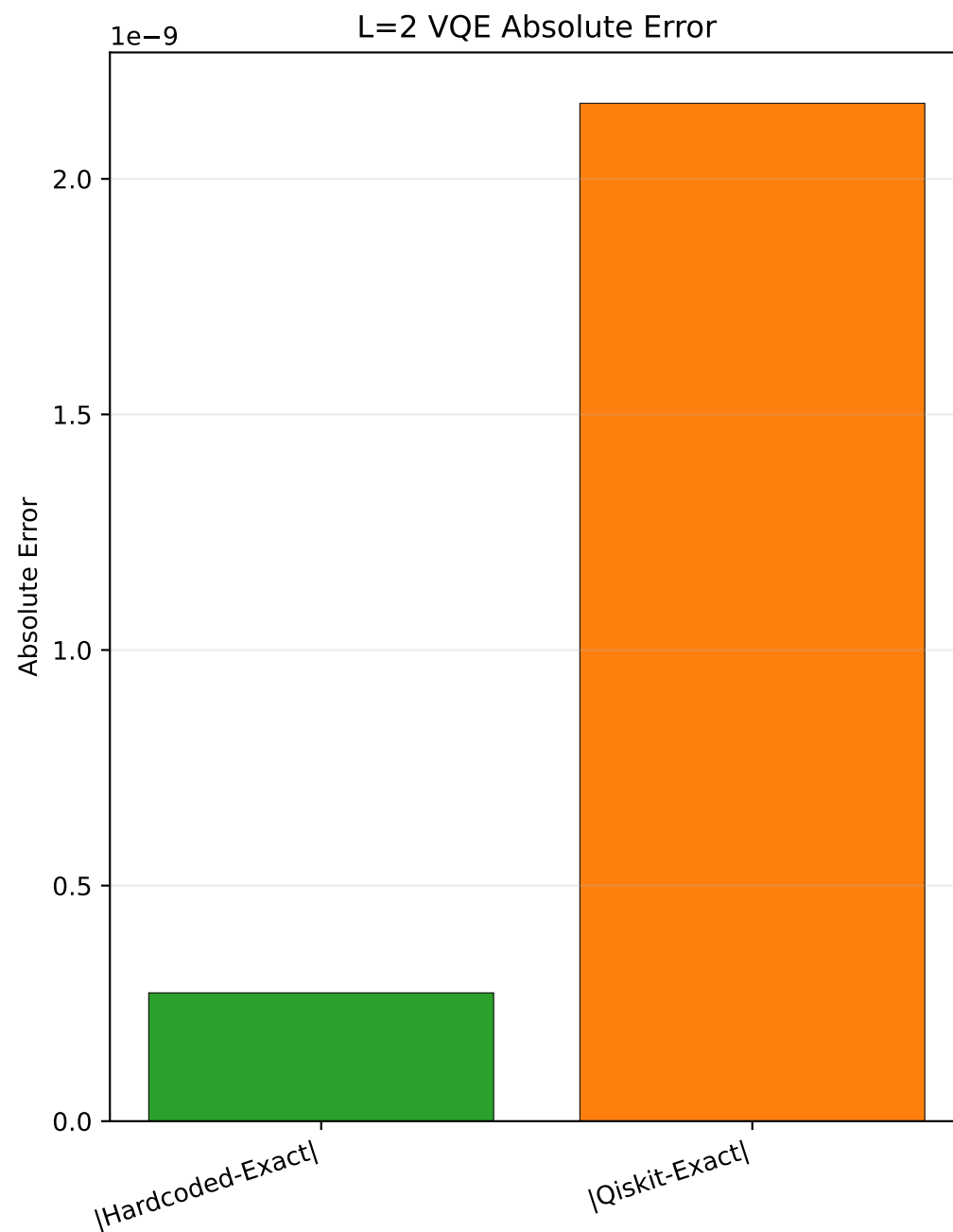
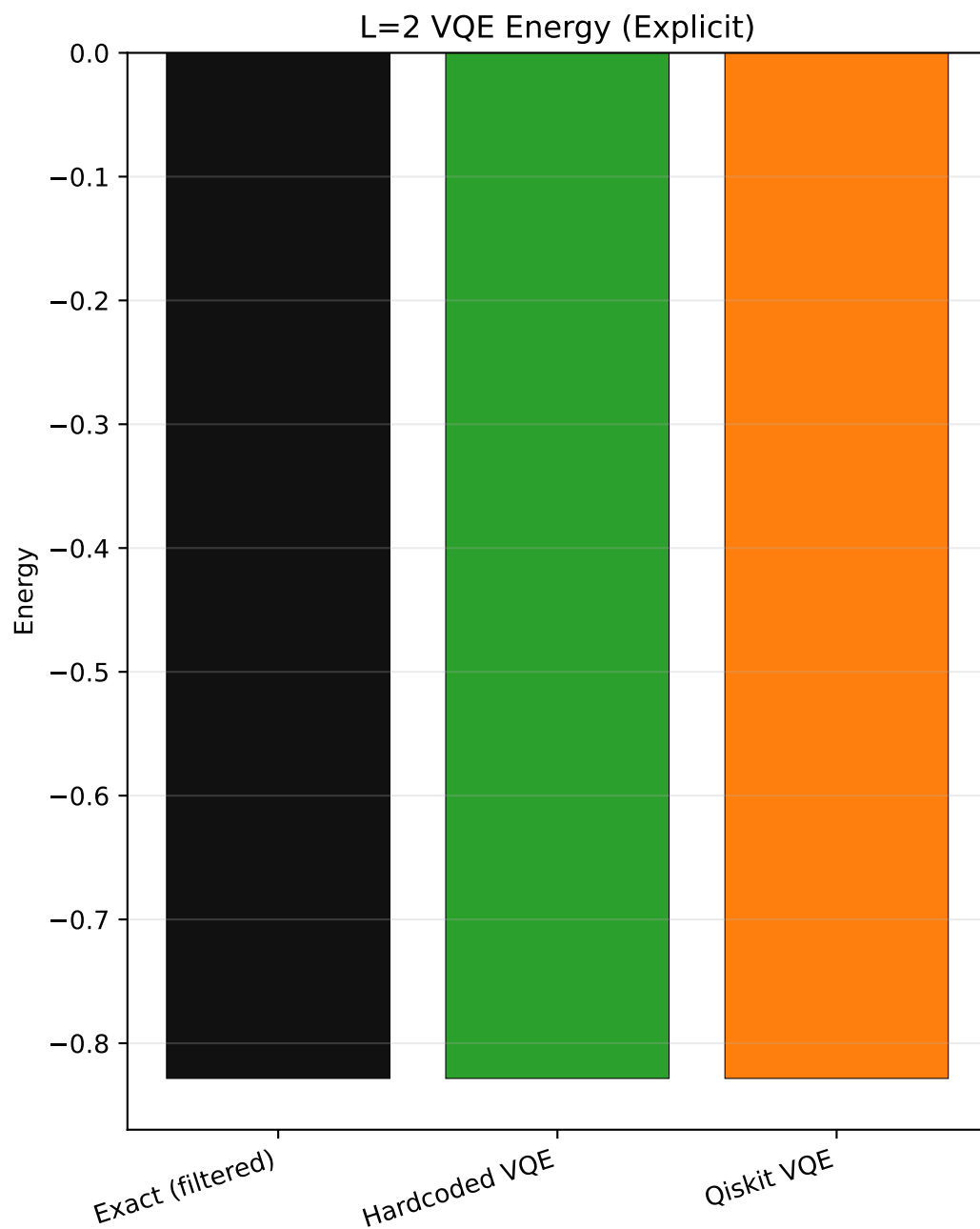
Site-0 n_{dn}



Doublon

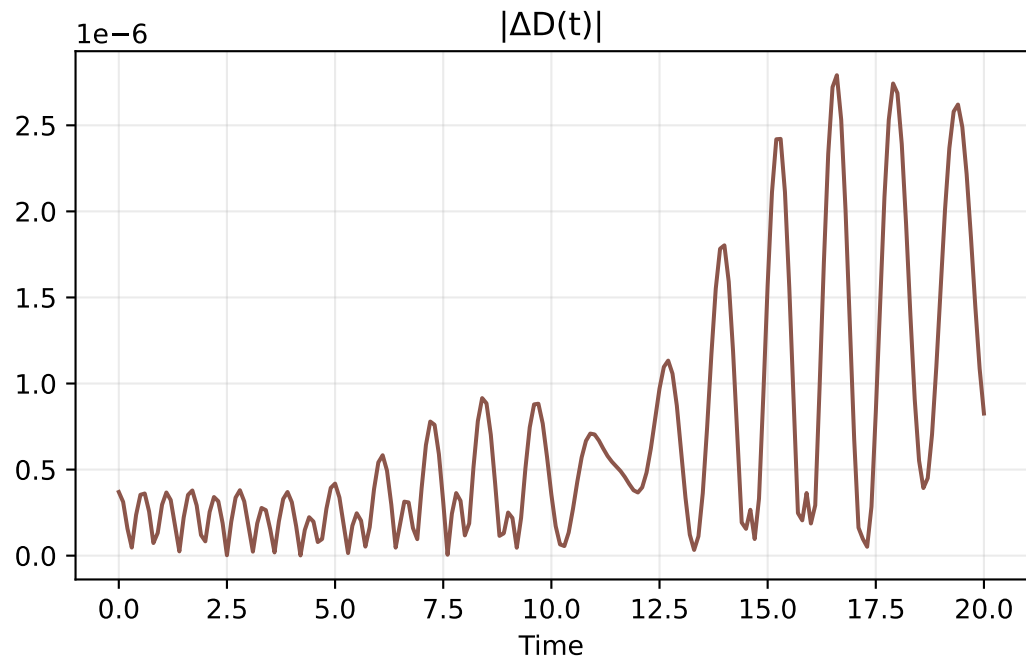
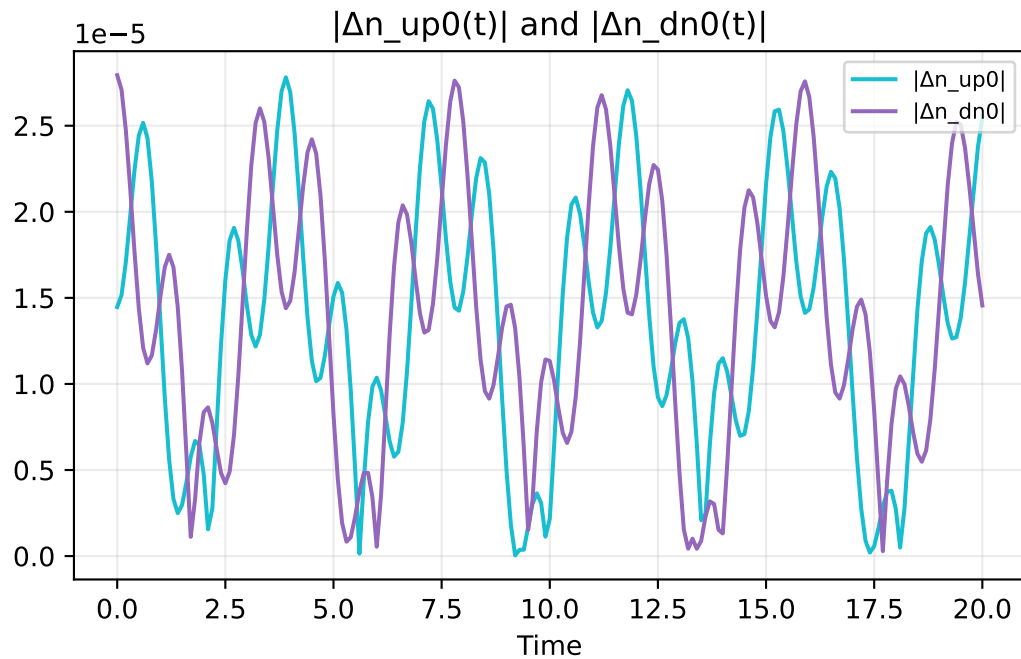
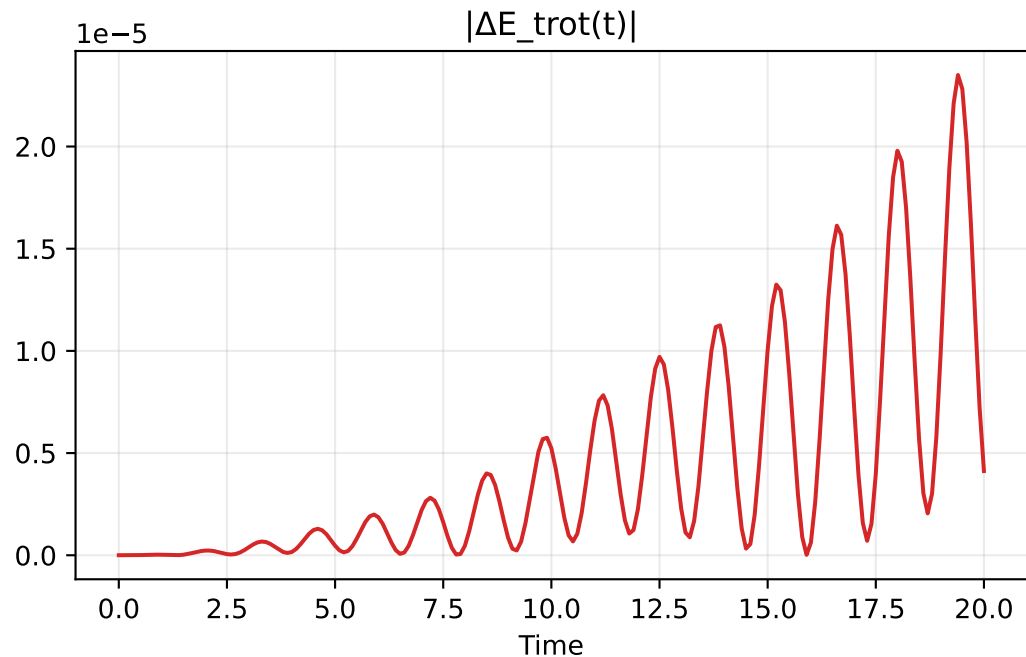
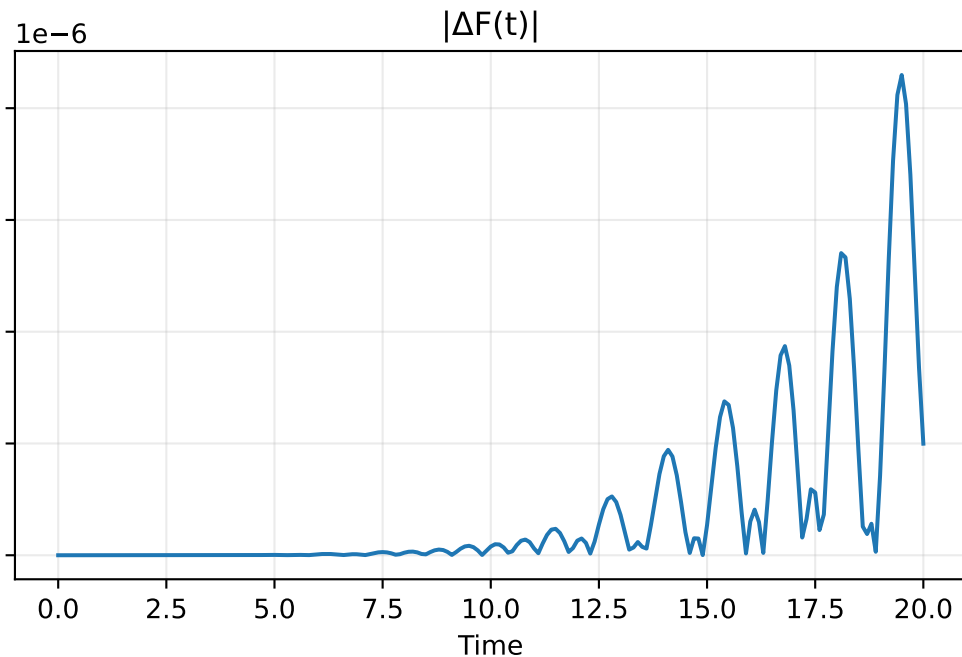


When initial_state_source=vqe, Trotter $E(t=0) = \langle \psi_{\text{vqe}} | H | \psi_{\text{vqe}} \rangle = \text{VQE energy}$.
VQE energy \neq exact ground state energy unless VQE fully converged.



Delta Diagnostics L=2

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



L=2 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 = 8.59377818263063e-06 / 8.005364268005184e-07 / 1.9968946775028584e-06

energy_trotter max/mean/final = 2.3499154368722408e-05 / 4.296069546226253e-06 / 4.121644446297701e-06

n_up_site0_trotter max/mean/final = 2.781282510533334e-05 / 1.3631273238300274e-05 / 2.545305309981094e-05

n_dn_site0_trotter max/mean/final = 2.7934482115687942e-05 / 1.3868963351504503e-05 / 1.4557018242267183e-05

doublon_trotter max/mean/final = 2.7910871213676636e-06 / 6.794619643993374e-07 / 8.256188262223407e-07

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