

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 2 --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
```

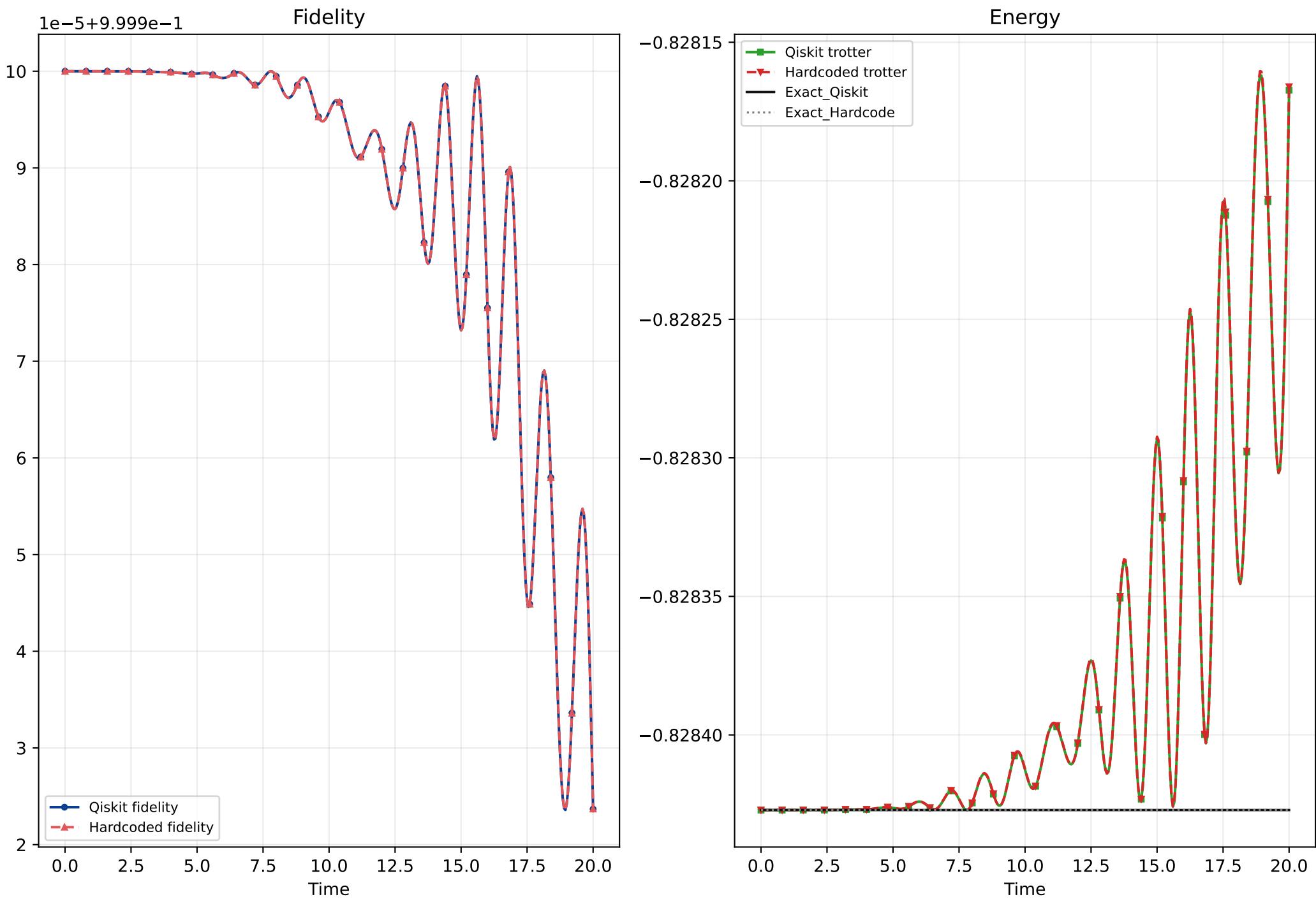
L=2 Run Settings & Metrics Summary

```
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=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

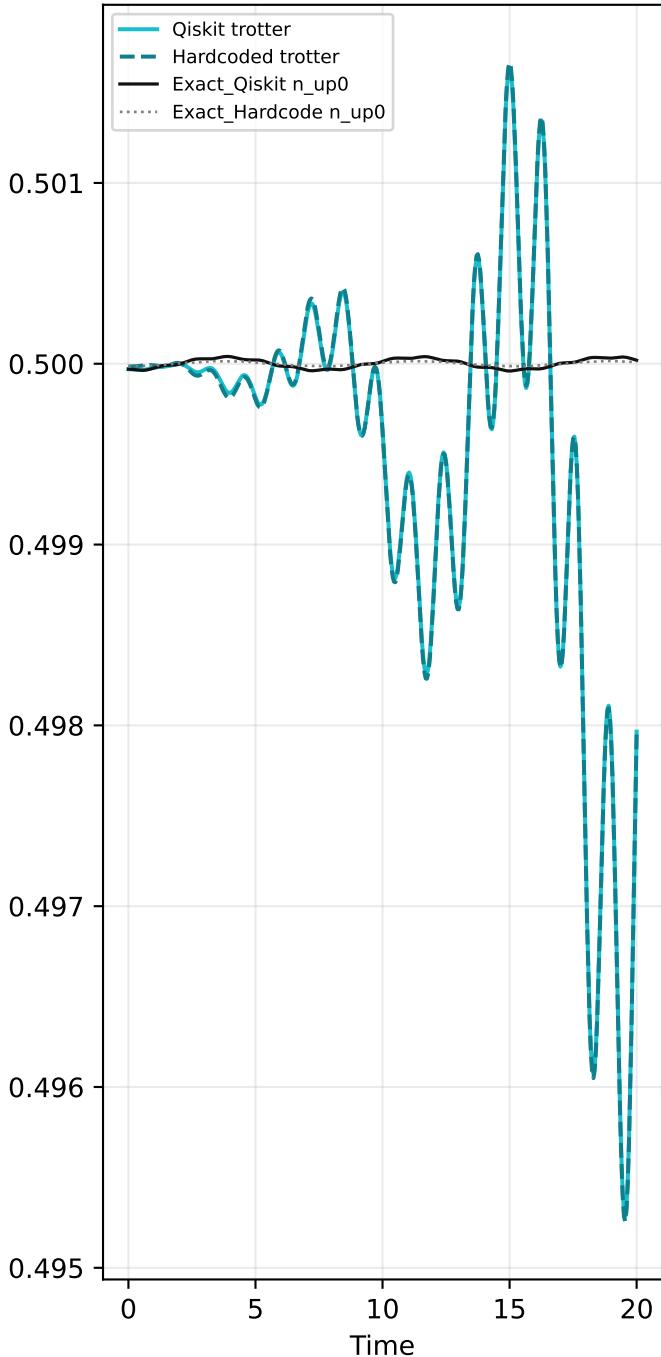
max |Δ|:
gs_energy: 0.00e+00
doublon_trotter: 4.84e-07
energy_trotter: 1.40e-06
fidelity: 2.26e-08
n_dn_site0_trotter: 2.79e-05
n_up_site0_trotter: 2.78e-05
result: PASS
```

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

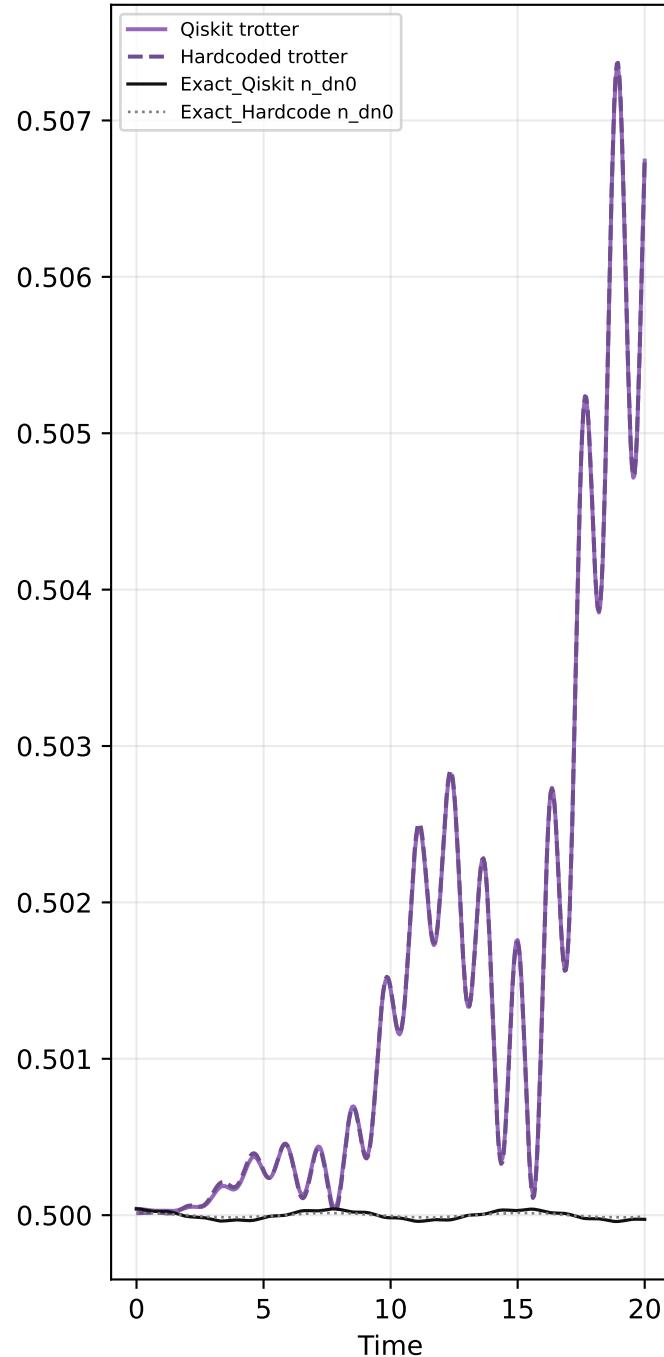


Pipeline Comparison L=2: Occupations & Doublon (auto-zoomed)

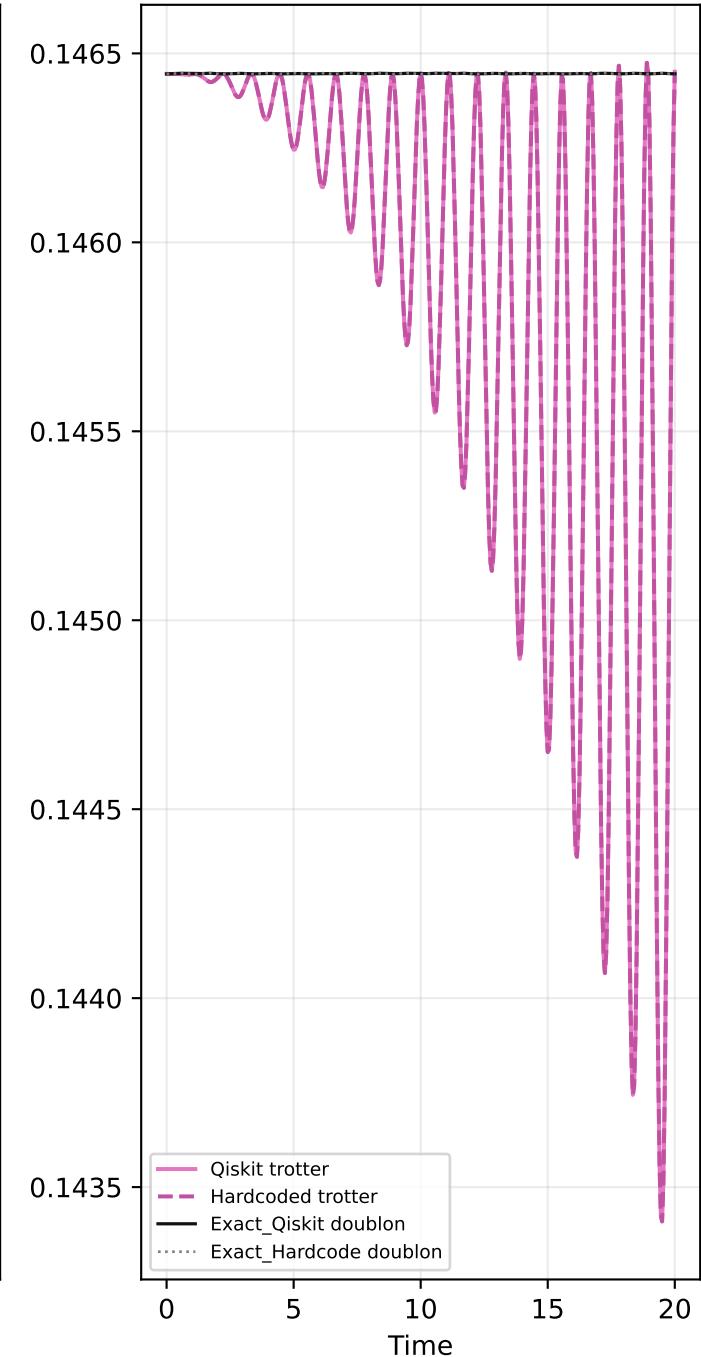
Site-0 n_up



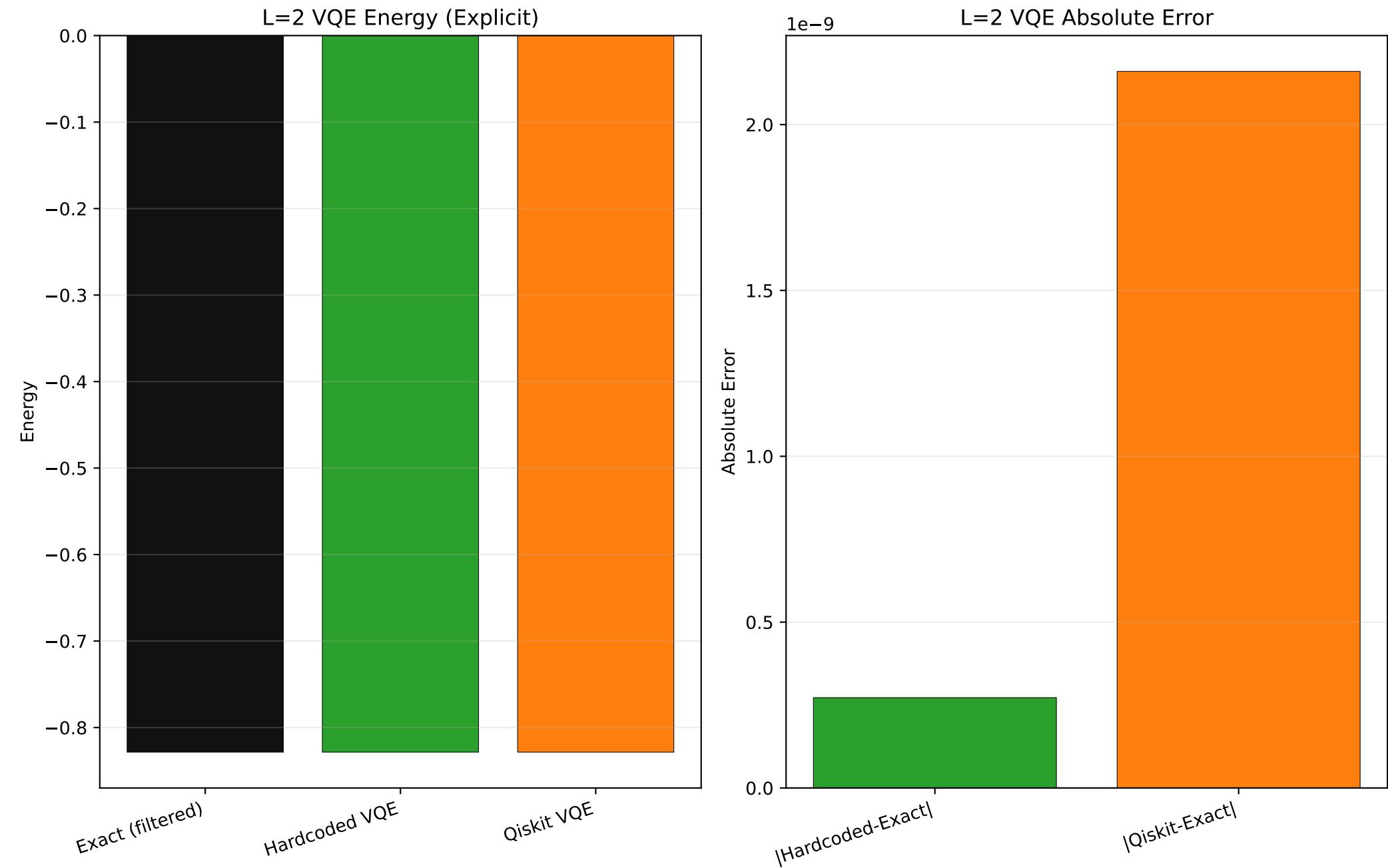
Site-0 n_dn



Doublon

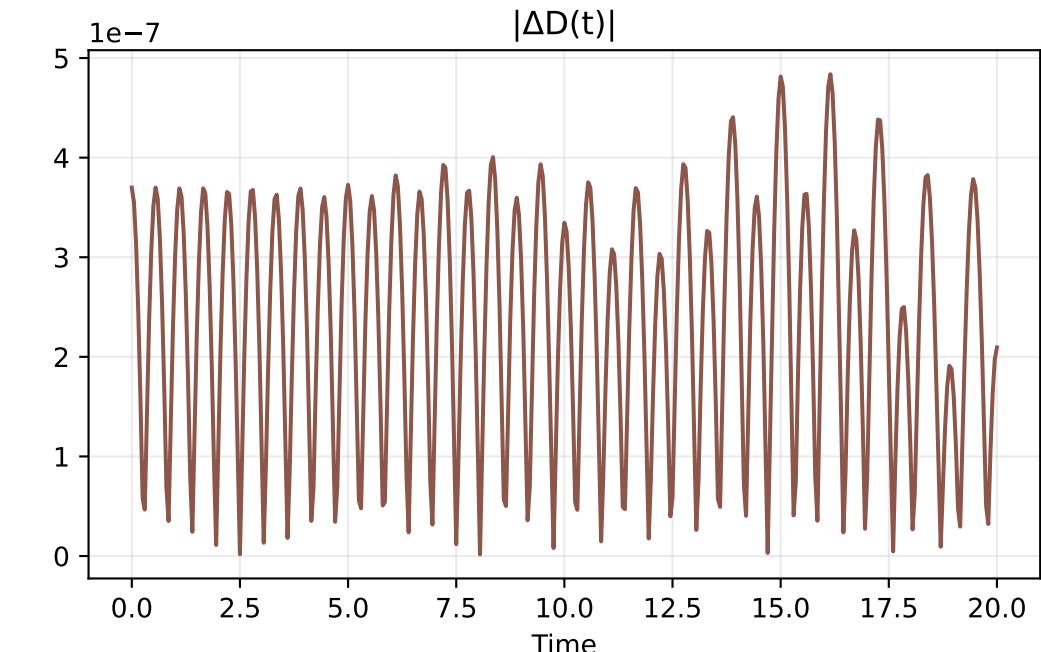
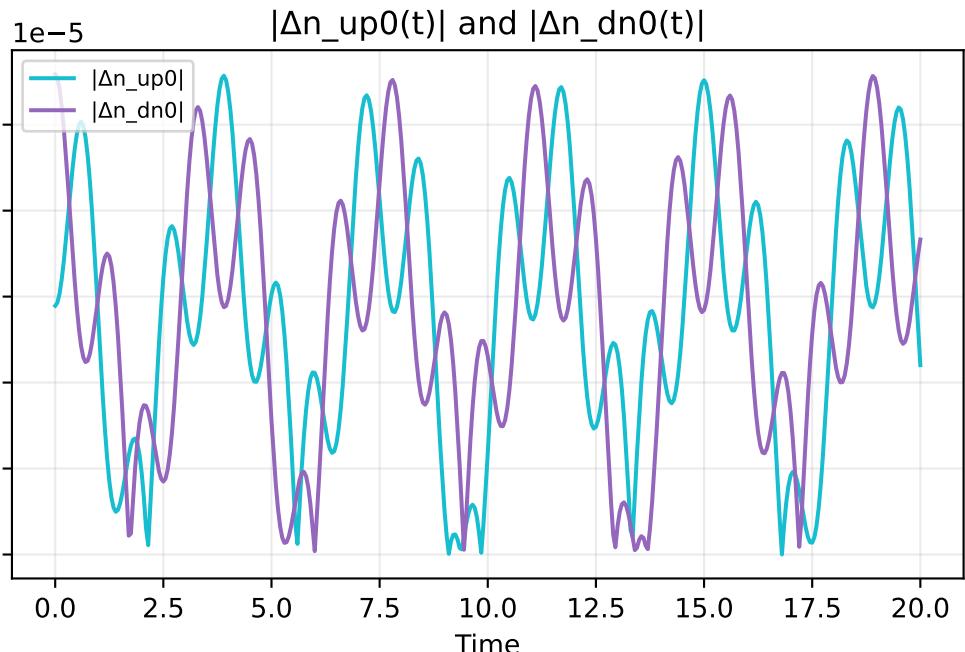
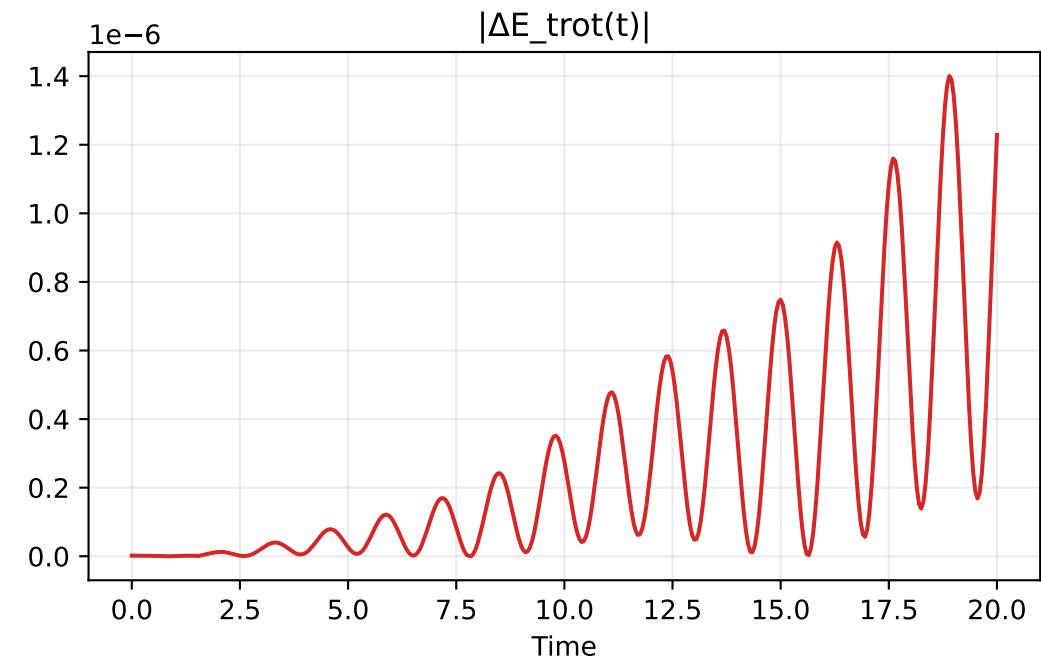
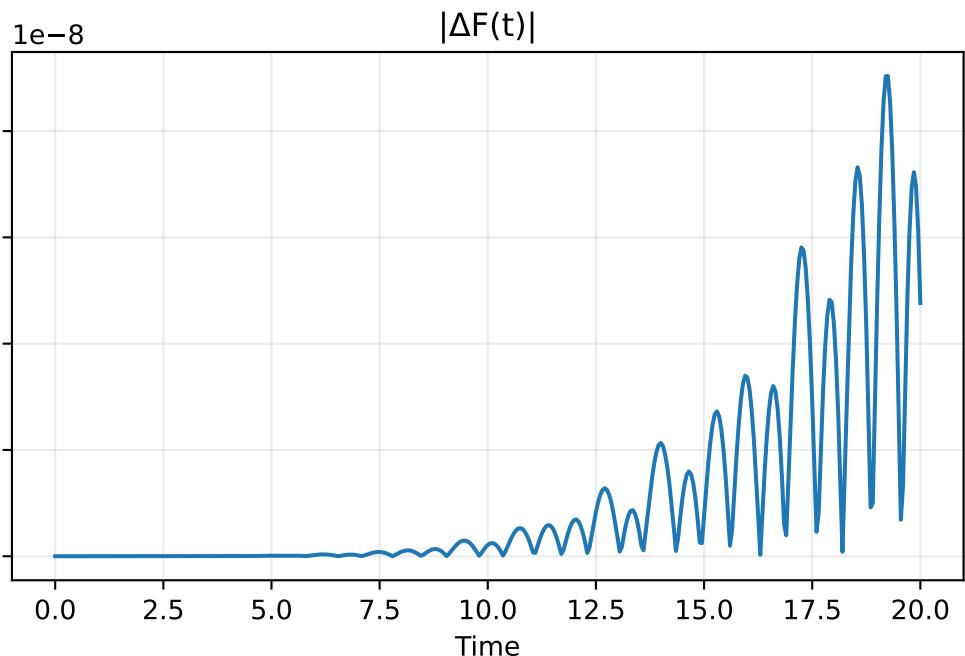


When initial_state_source=vqe, Trotter $E(t=0) = \langle \psi_{\text{vqe}} | H | \psi_{\text{vqe}} \rangle$ = VQE energy.
VQE energy \neq exact ground state energy unless VQE fully converged.



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:
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```
 $\Delta F(t) = |F_{hc}(t) - F_{qk}(t)|$ 
 $\Delta E_{trot}(t) = |E_{trot\_hc}(t) - E_{trot\_qk}(t)|$ 
 $\Delta n_{up0}(t) = |n_{up0\_hc}(t) - n_{up0\_qk}(t)|$ 
 $\Delta n_{dn0}(t) = |n_{dn0\_hc}(t) - n_{dn0\_qk}(t)|$ 
 $\Delta D(t) = |D_{hc}(t) - D_{qk}(t)|$ 
```

```
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 = 2.2590508352848815e-08 / 2.6804744024278294e-09 / 1.190507825654663e-08
energy_trotter max/mean/final = 1.400460892919675e-06 / 2.561722049860173e-07 / 1.228592043989174e-06
n_up_site0_trotter max/mean/final = 2.7846824668553705e-05 / 1.4103046424698389e-05 / 1.1012572472712812e-05
n_dn_site0_trotter max/mean/final = 2.7934482115687942e-05 / 1.406226762311699e-05 / 1.8319372432129555e-05
doublon_trotter max/mean/final = 4.837666837398391e-07 / 2.3529349619561587e-07 / 2.0937875369608783e-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
```