

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

Fidelity

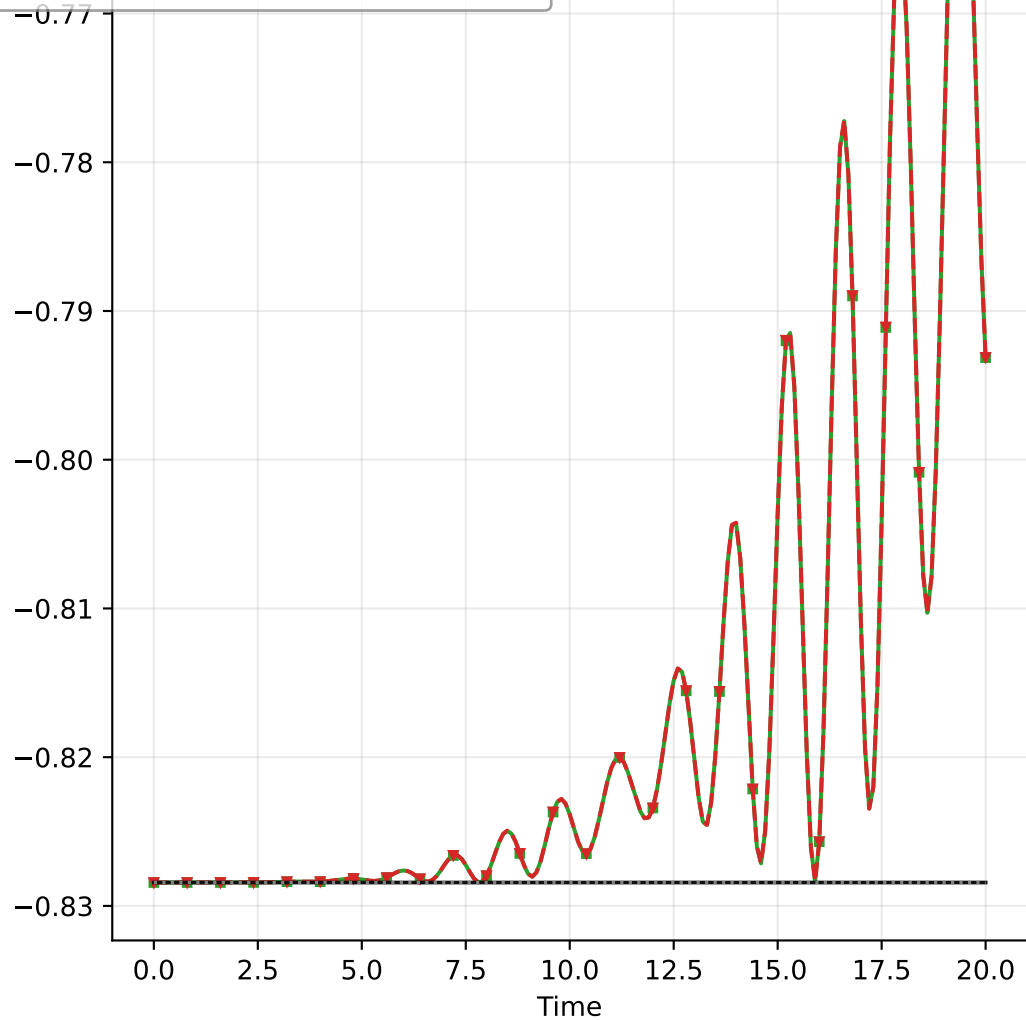
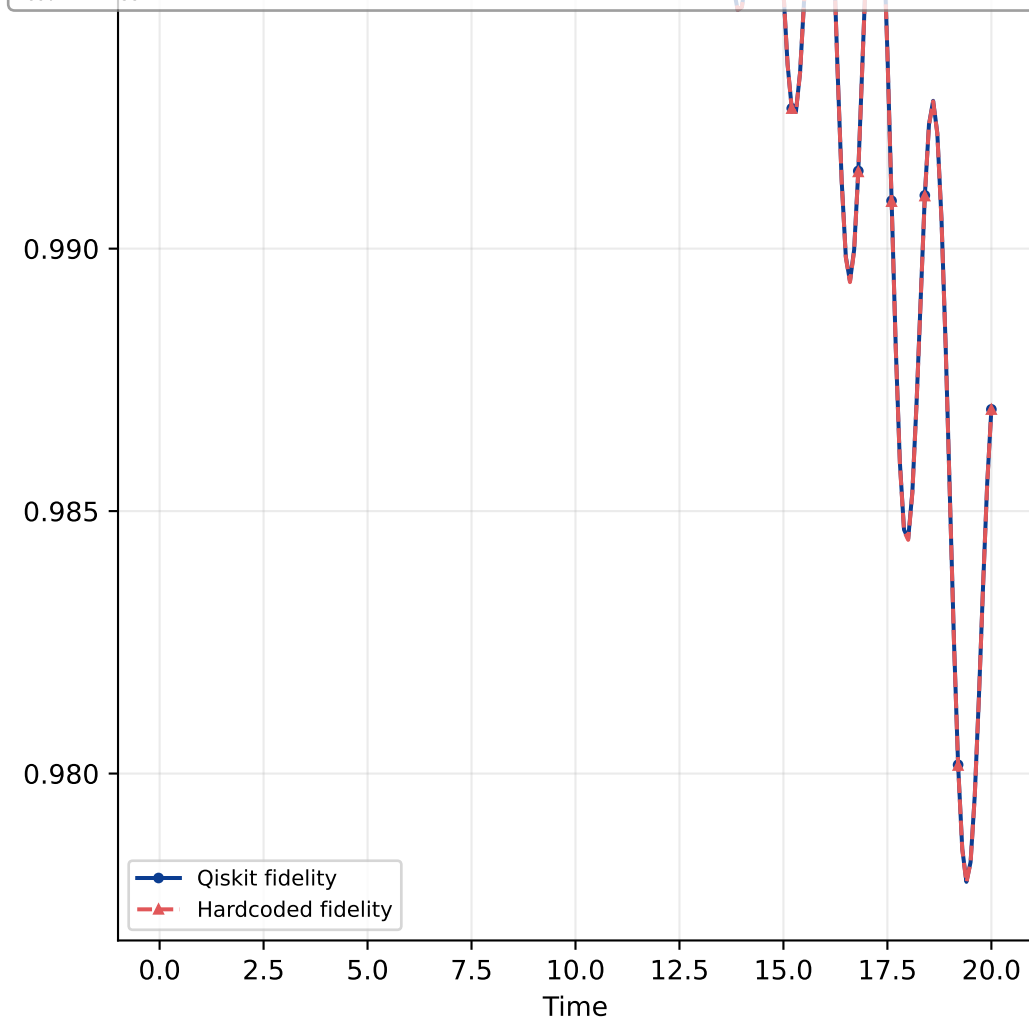
Energy

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 suzuki_order=2 trotter steps=64

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: 4.65e-05
energy_trotter: 5.14e-05
fidelity: 2.41e-05
n_dn_site0_trotter: 2.13e-04
n_up_site0_trotter: 2.13e-04
result: PASS

Qiskit trotter
Hardcoded trotter
Qiskit exact
Hardcoded exact

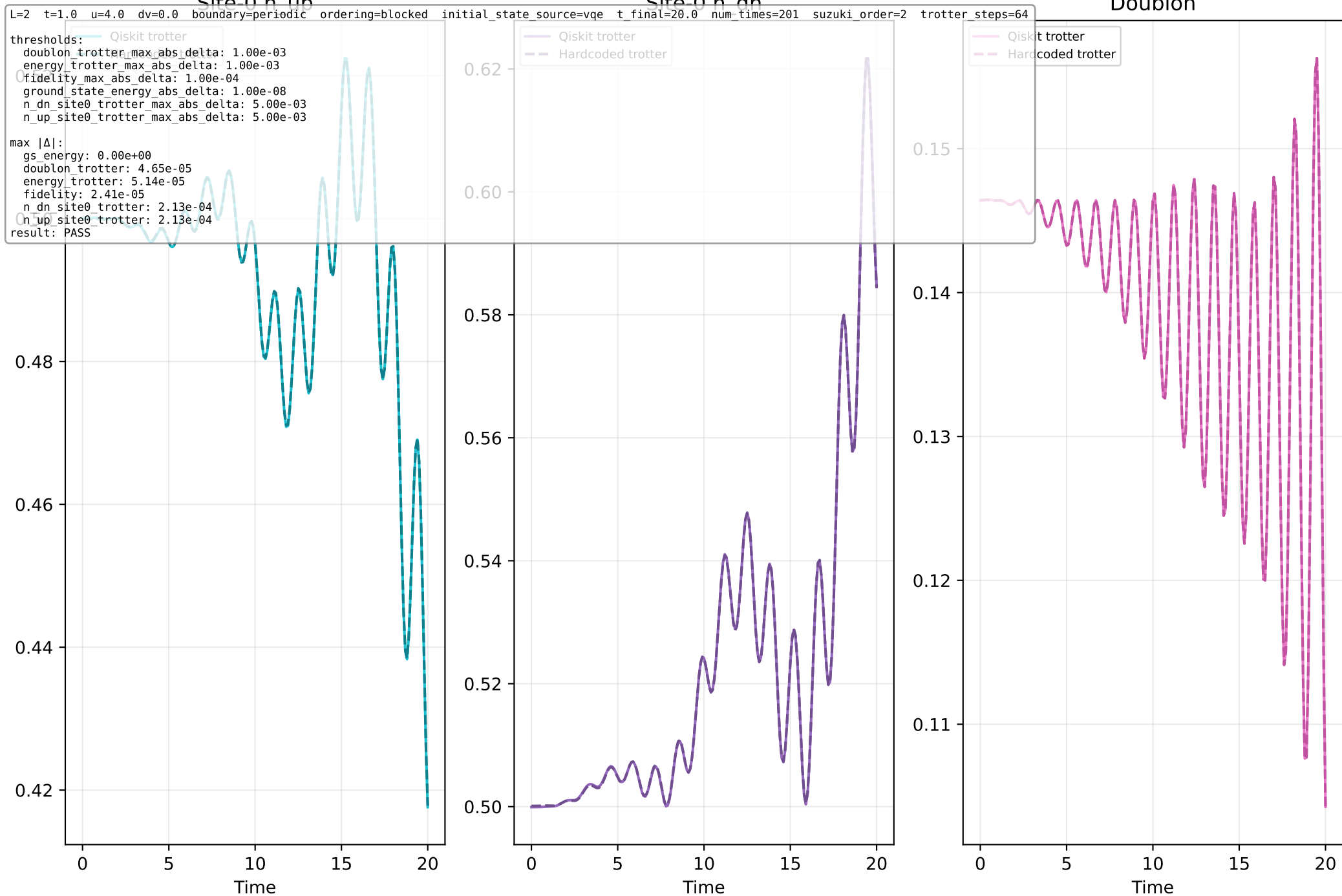


Pipeline Comparison L=2: Occupations & Doublon (auto-zoomed)

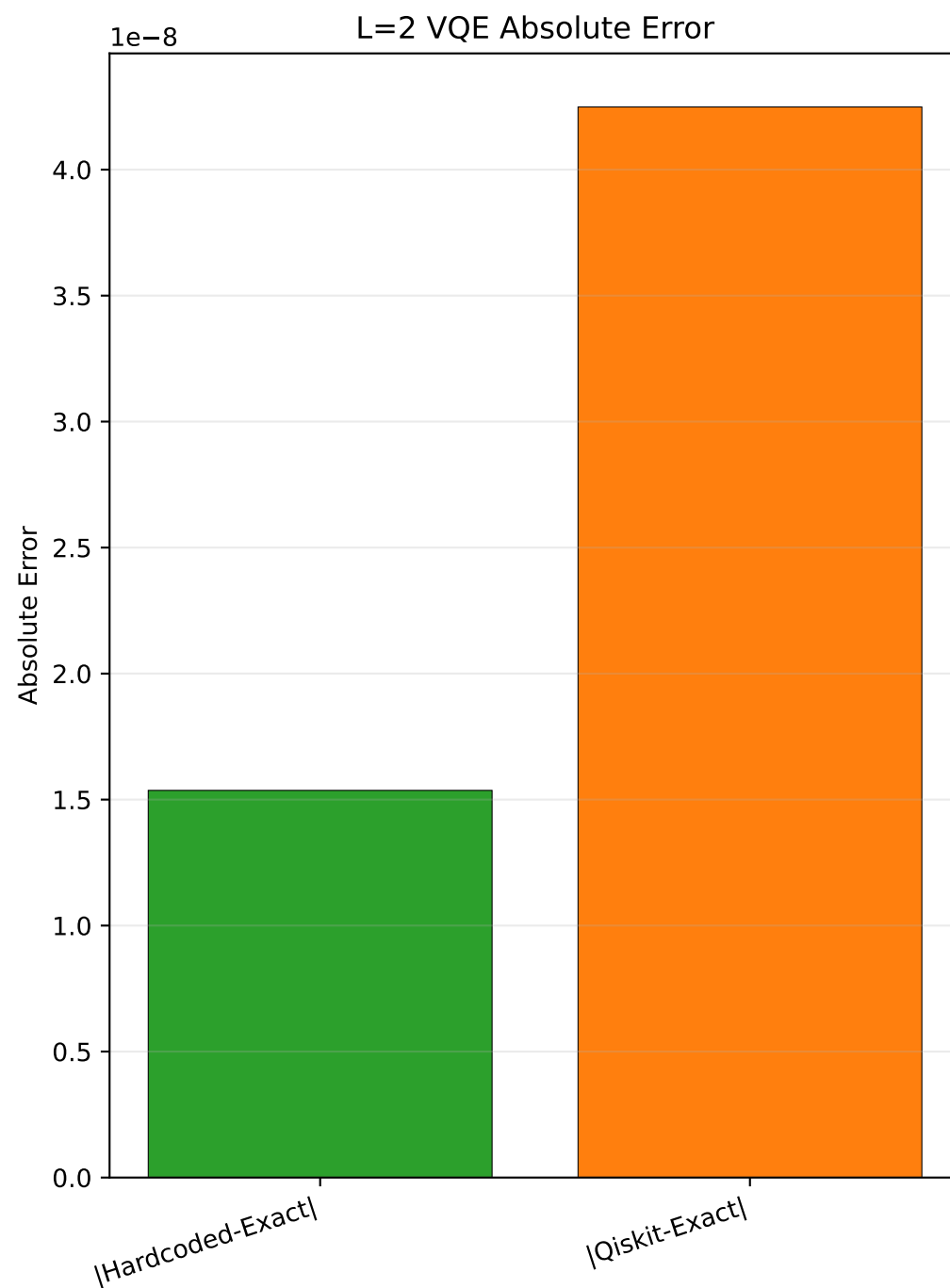
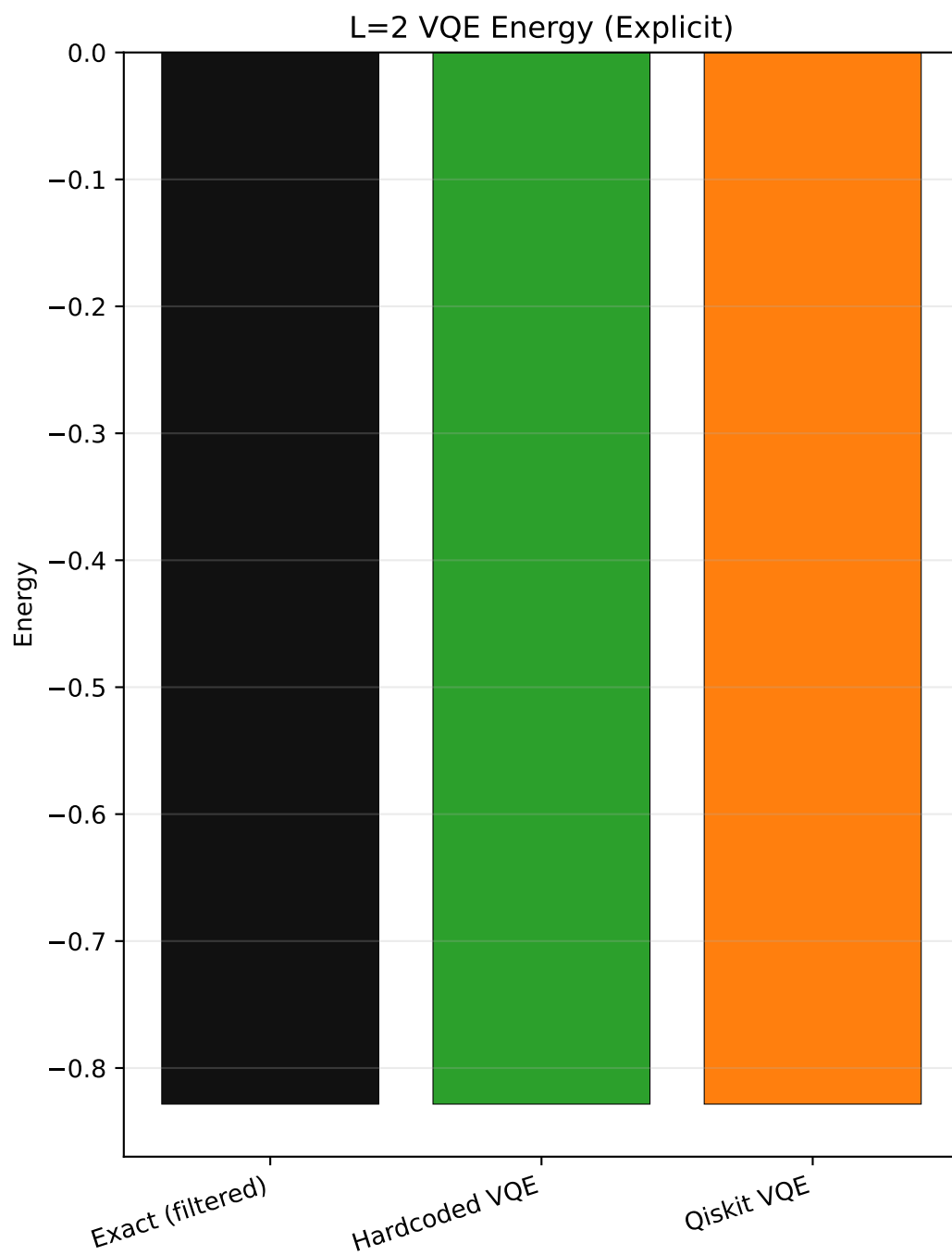
Site 0 n_{up}

Site 0 n_{dn}

Doublon



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



Delta Diagnostics L=2

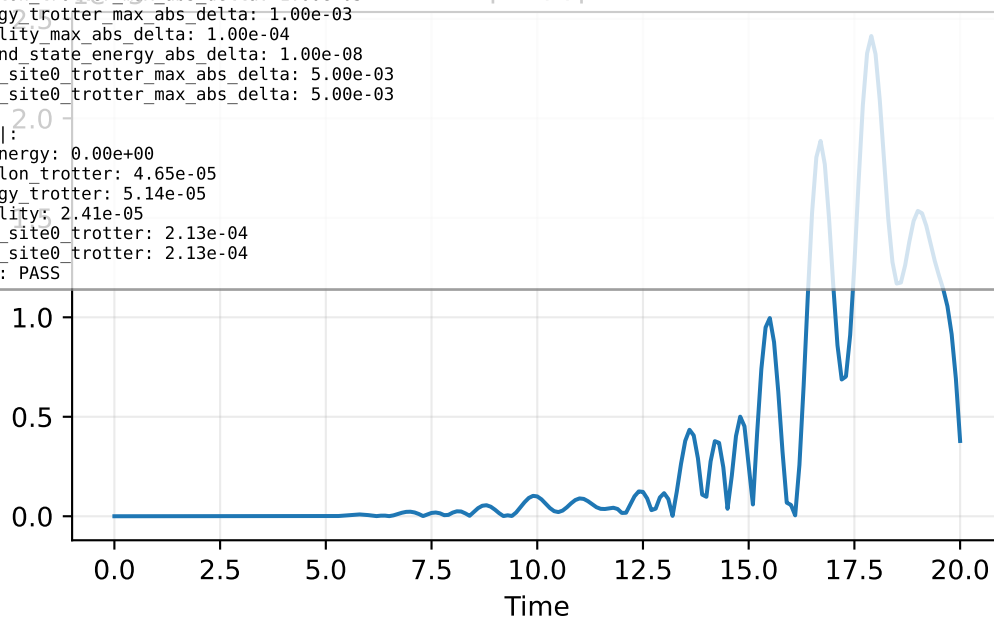
$\Delta X(t) = |X_{hc}(t) - X_{qk}(t)|$, where $X_{pipeline}(t)$ is that pipeline's stored trajectory value.

L=2 t=1.0 u=4.0 dv=0.0 boundary=periodic ordering=blocked initial_state_source=vqe t_final=20.0 num_times=201 suzuki_order=2 trotter_steps=64

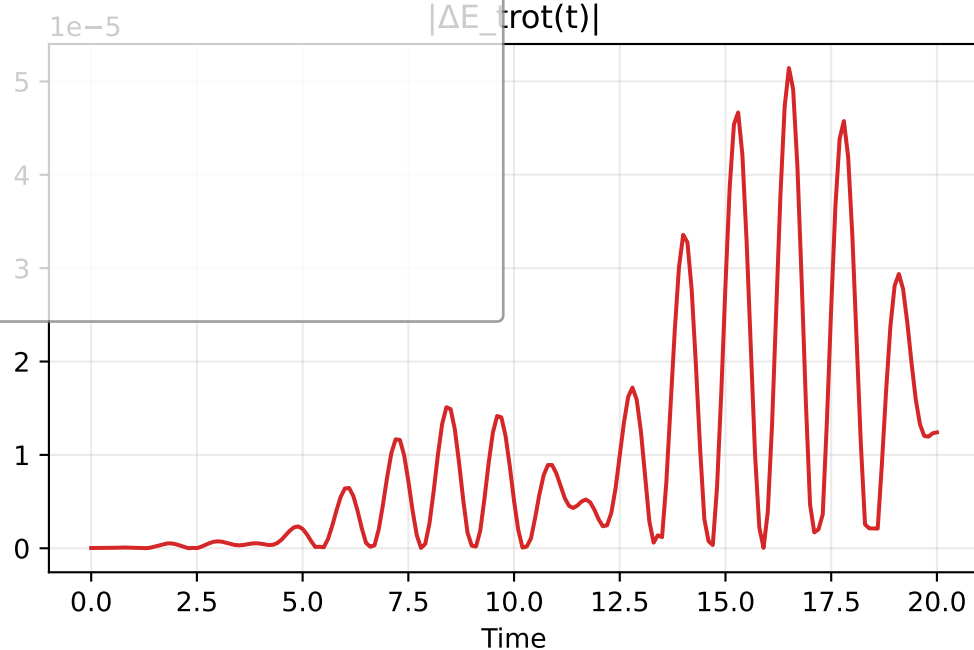
thresholds:
doublon_trotter_max_abs_delta: 1.00e-03
energy_trotter_max_abs_delta: 1.00e-03
fidelity_max_abs_delta: 1.00e-04
ground_state_energy_abs_delta: 1.00e-08
n_dn_site0_trotter_max_abs_delta: 5.00e-03
n_up_site0_trotter_max_abs_delta: 5.00e-03

max $|\Delta|$:
gs.energy: 0.00e+00
doublon_trotter: 4.65e-05
energy_trotter: 5.14e-05
fidelity: 2.41e-05
n_dn_site0_trotter: 2.13e-04
n_up_site0_trotter: 2.13e-04
result: PASS

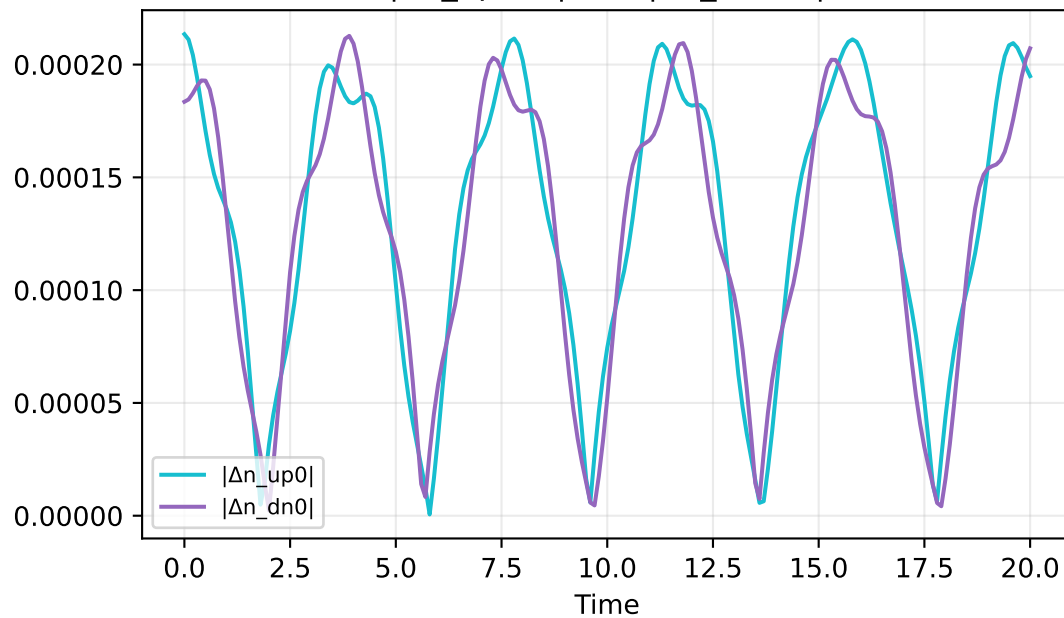
$|\Delta F(t)|$



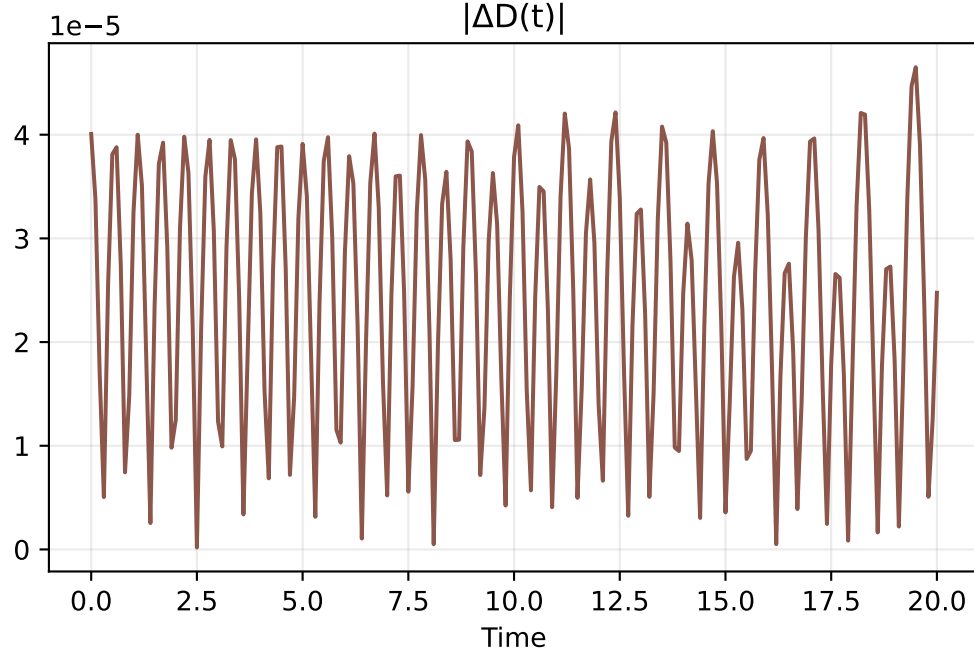
$|\Delta E_{trot}(t)|$



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



$|\Delta D(t)|$



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 = 2.4137975728866223e-05 / 3.2780993371204888e-06 / 3.783465616358228e-06

energy_trotter max/mean/final = 5.1436108605140696e-05 / 9.344796006301634e-06 / 1.2411196367745347e-05

n_up_site0_trotter max/mean/final = 0.00021346380603026738 / 0.000129601417068683 / 0.00019487823333519394

n_dn_site0_trotter max/mean/final = 0.0002127320858726911 / 0.00012600310926826942 / 0.00020719542794467305

doublon_trotter max/mean/final = 4.6510415792039295e-05 / 2.4404822266394123e-05 / 2.4752750301254567e-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