

Executed Command

Script: pipelines/compare_adapt_pipelines.py

```
/opt/anaconda3/bin/python3 pipelines/compare_adapt_pipelines.py --l-values 3 --run-pipelines --hc-adapt-max-  
depth 50 --hc-adapt-eps-grad 1e-6 --hc-adapt-eps-energy 1e-10 --hc-adapt-maxiter 1000 --qk-adapt-max-  
iterations 50 --qk-adapt-gradient-threshold 1e-6 --qk-adapt-cobyla-maxiter 1000
```

Hardcoded ADAPT-VQE vs Qiskit ADAPT-VQE Comparison Summary

generated_utc: 2026-02-25T03:59:34.286724+00:00

all_pass: False

l_values: [3]

trajectory_comparison_basis: trotter trajectories start from
each pipeline's ADAPT-VQE ground state (default: adapt_vqe)

exact_trajectory_labels: Exact_Hardcode, Exact_Qiskit

exact_trajectory_method: python_matrix_eigendecomposition

thresholds:

```
{'doublon_trotter_max_abs_delta': 0.001,  
 'energy_trotter_max_abs_delta': 0.001,  
 'fidelity_max_abs_delta': 0.0001,  
 'ground_state_energy_abs_delta': 1e-08,  
 'n_dn_site0_trotter_max_abs_delta': 0.005,  
 'n_up_site0_trotter_max_abs_delta': 0.005}
```

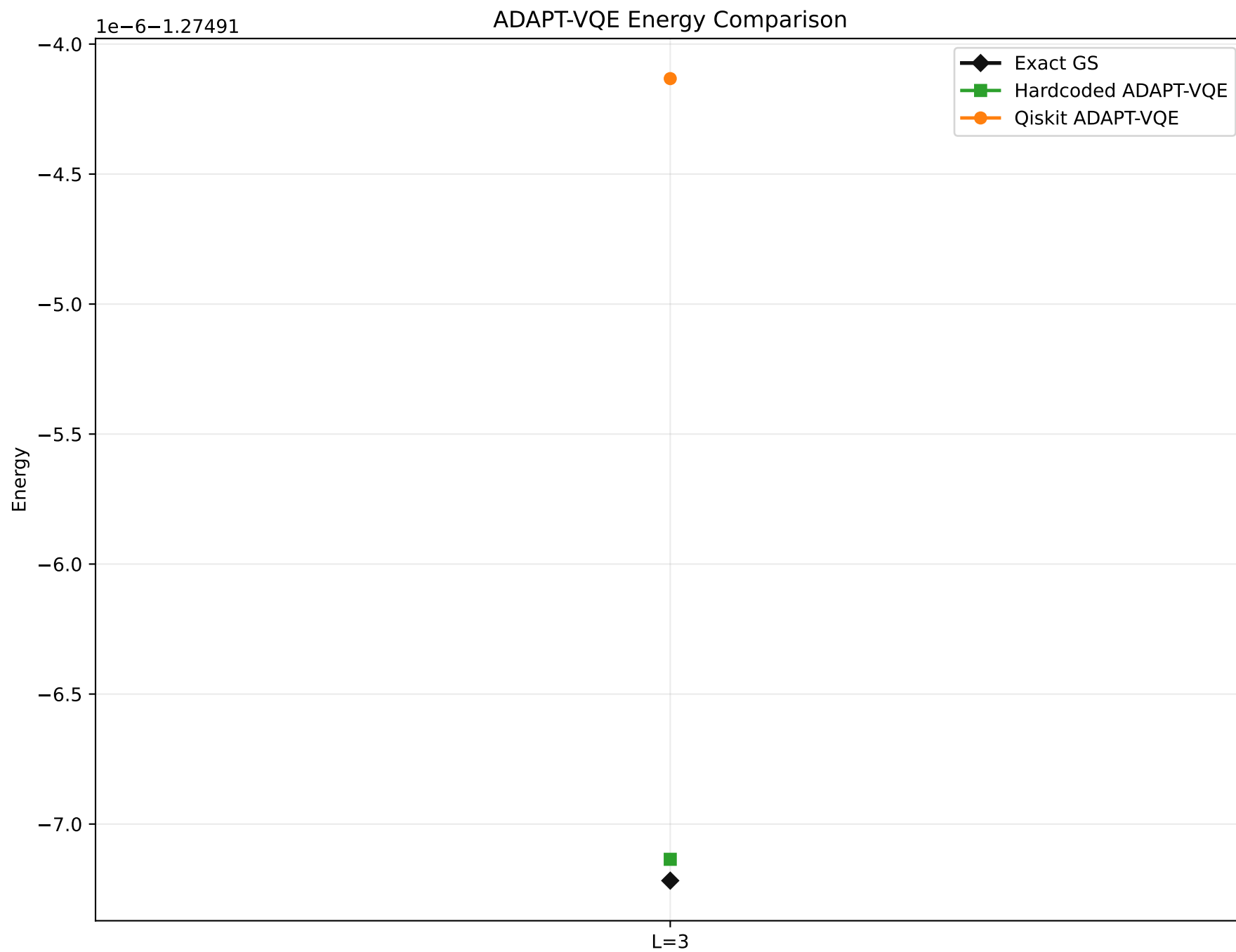
Delta metric definitions:

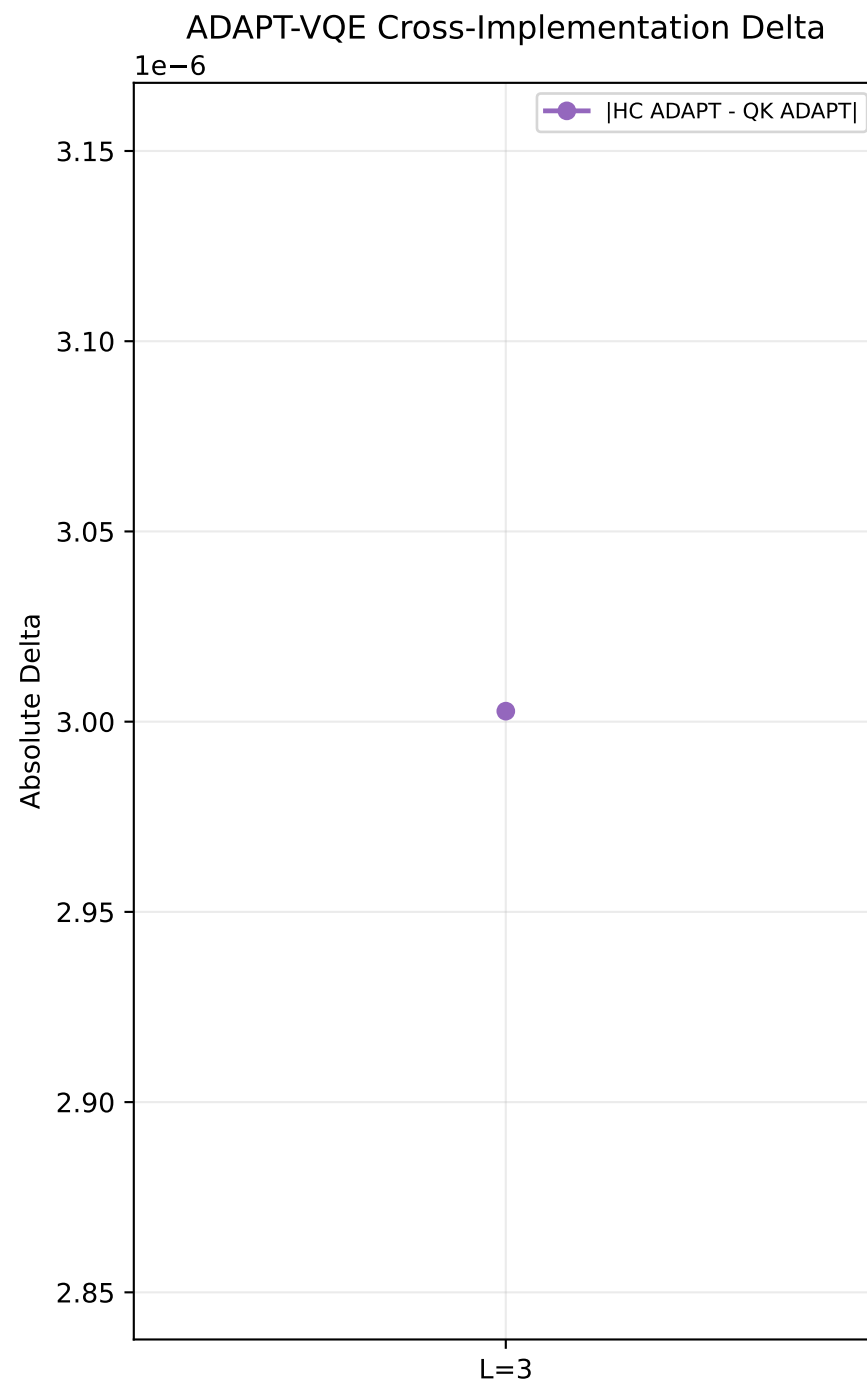
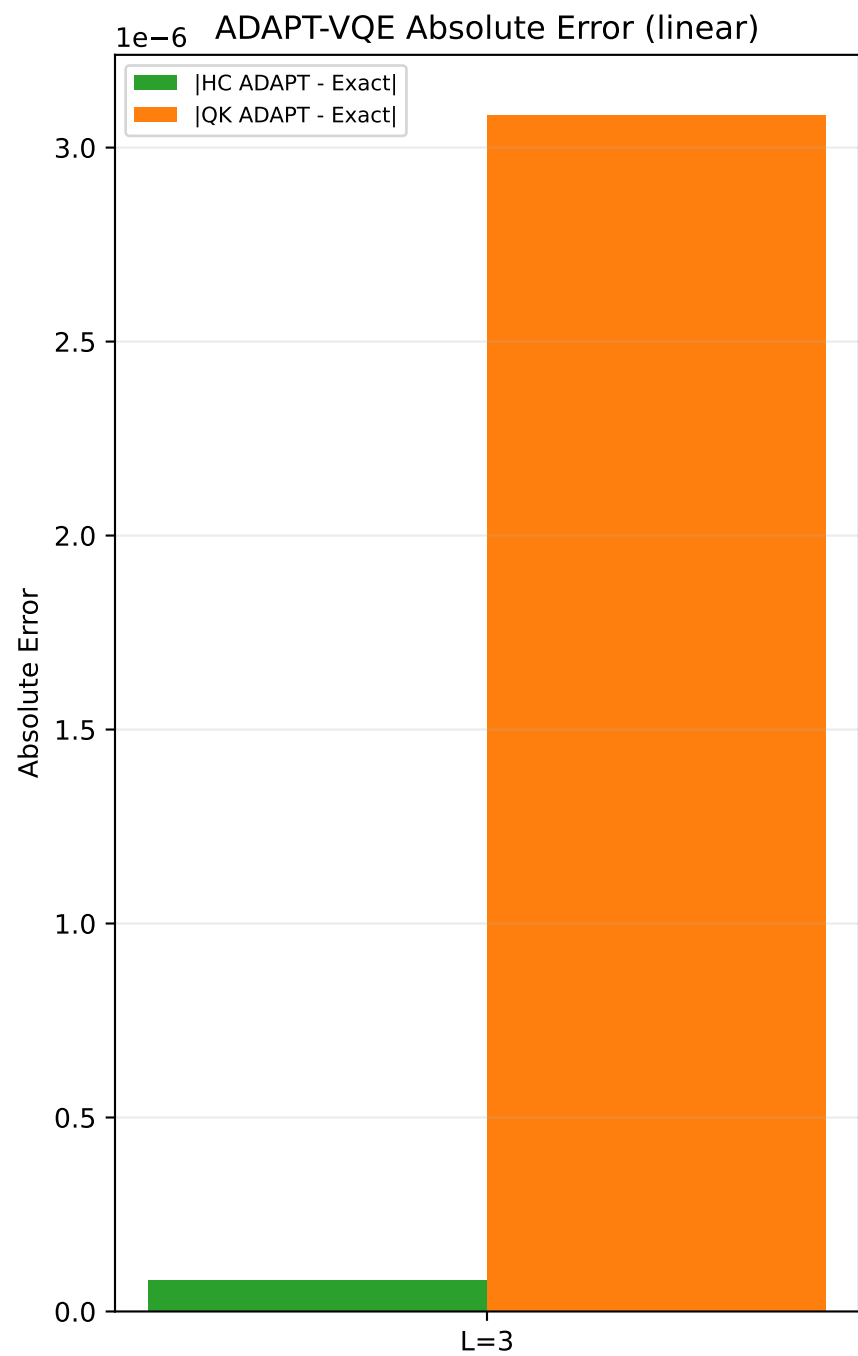
$$\Delta F(t) = |F_{hc}(t) - F_{qk}(t)|$$
$$\Delta E_{trot}(t) = |E_{trot_{hc}}(t) - E_{trot_{qk}}(t)|$$
$$\Delta n_{up0}(t) = |n_{up0_{hc}}(t) - n_{up0_{qk}}(t)|$$
$$\Delta n_{dn0}(t) = |n_{dn0_{hc}}(t) - n_{dn0_{qk}}(t)|$$
$$\Delta D(t) = |D_{hc}(t) - D_{qk}(t)|$$

$F_{pipeline}(t)$ is the pipeline's stored trajectory fidelity value (as computed internally vs that pipeline's exact evolution).

Per-L pass flags:

L=3 pass=False metrics_json=/Users/jakestrobels/Downloads/Holstein_test/Adapt-VQE-Pipeline/artifacts/hardcoded_vs_qiskit_adapt_L3_metrics.json



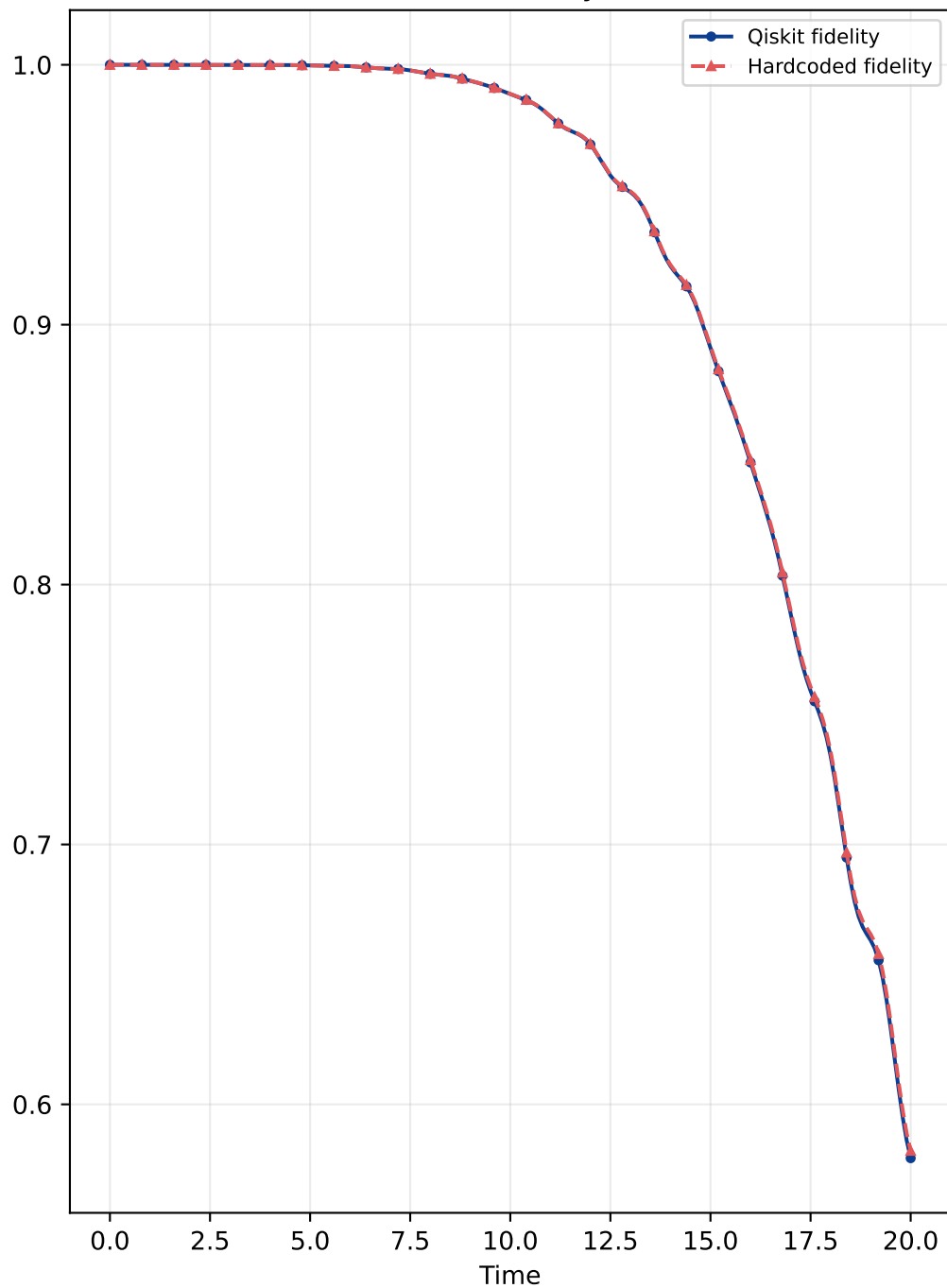


Bundle L=3: ADAPT-VQE Settings & Metrics

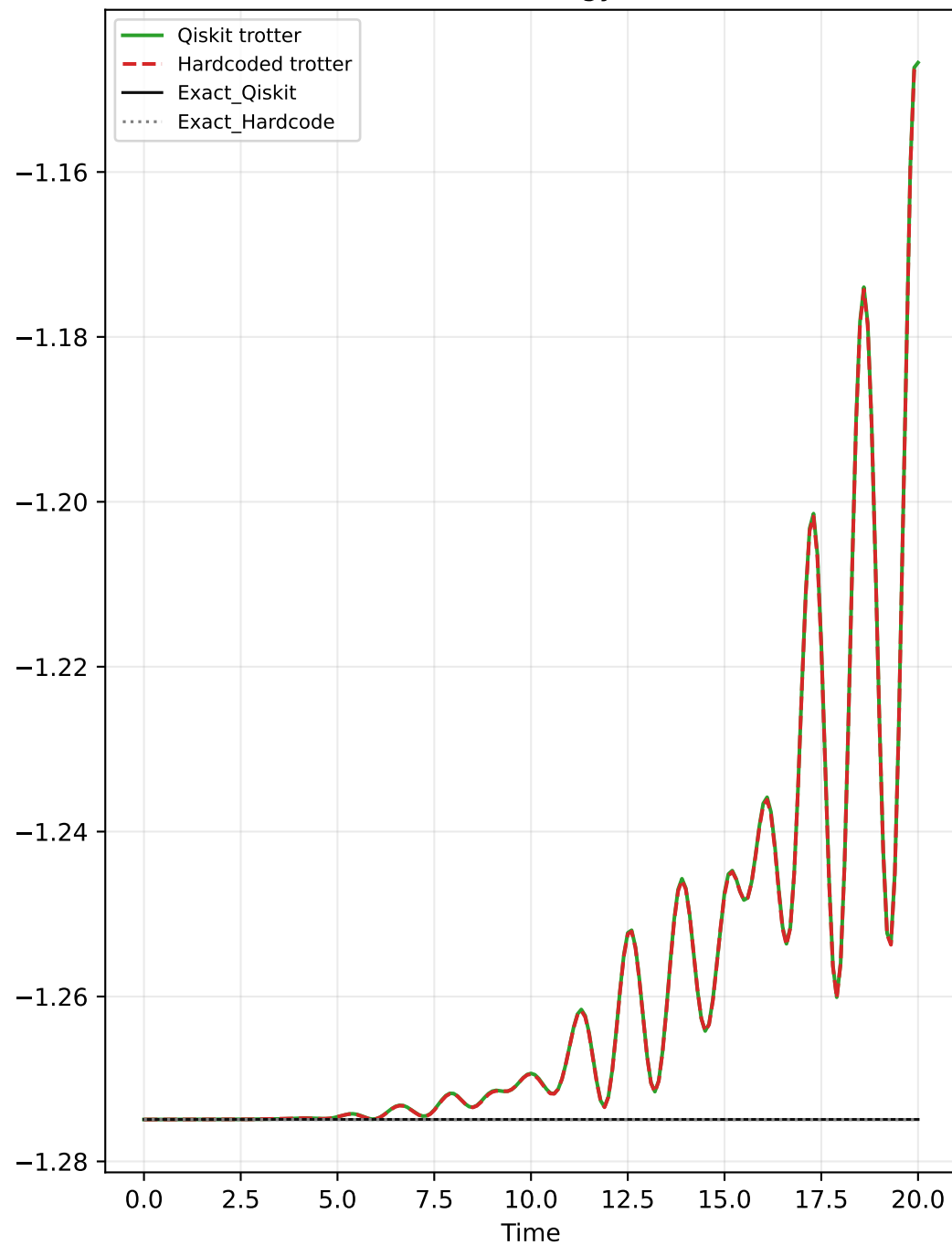
```
L=3  t=1.0  u=4.0  dv=0.0  boundary=periodic  ordering=blocked  initial_state_source=adapt_vqe  t_final=20.0  num_times=20  
thresholds:  
  doublon_trotter_max_abs_delta: 1.00e-03  
  energy_trotter_max_abs_delta: 1.00e-03  
  fidelity_max_abs_delta: 1.00e-04  
  ground_state_energy_abs_delta: 1.00e-08  
  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: 2.94e-04  
  energy_trotter: 4.04e-04  
  fidelity: 2.85e-03  
  n_dn_site0_trotter: 1.26e-03  
  n_up_site0_trotter: 1.56e-03  
result: FAIL
```

Bundle: L=3 ADAPT-VQE Fidelity & Energy

L=3 Fidelity

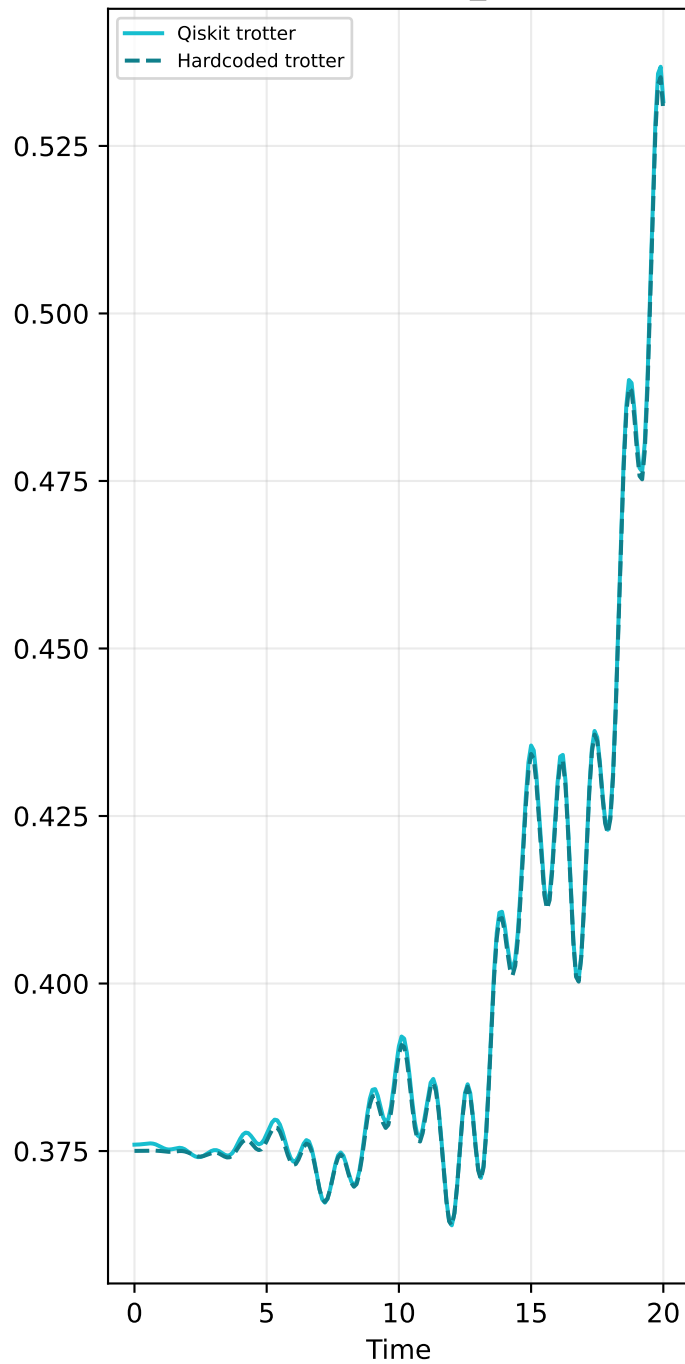


L=3 Energy

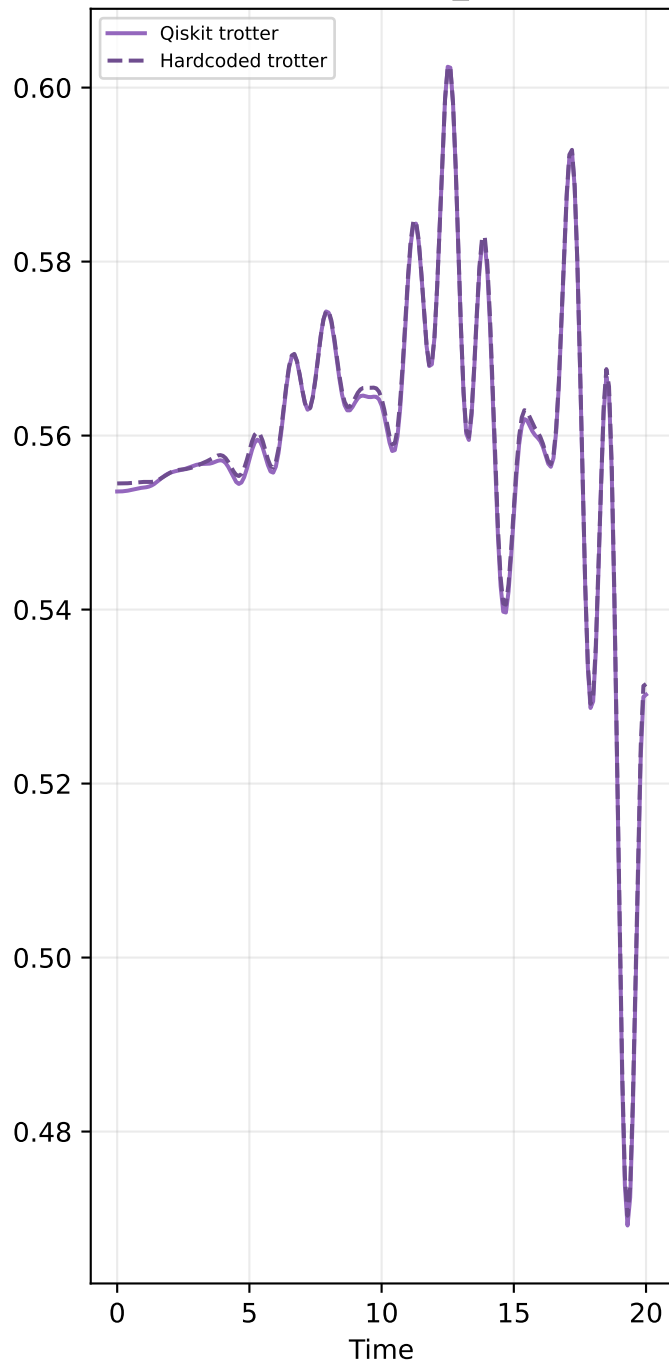


Bundle: L=3 Occupations & Doublon

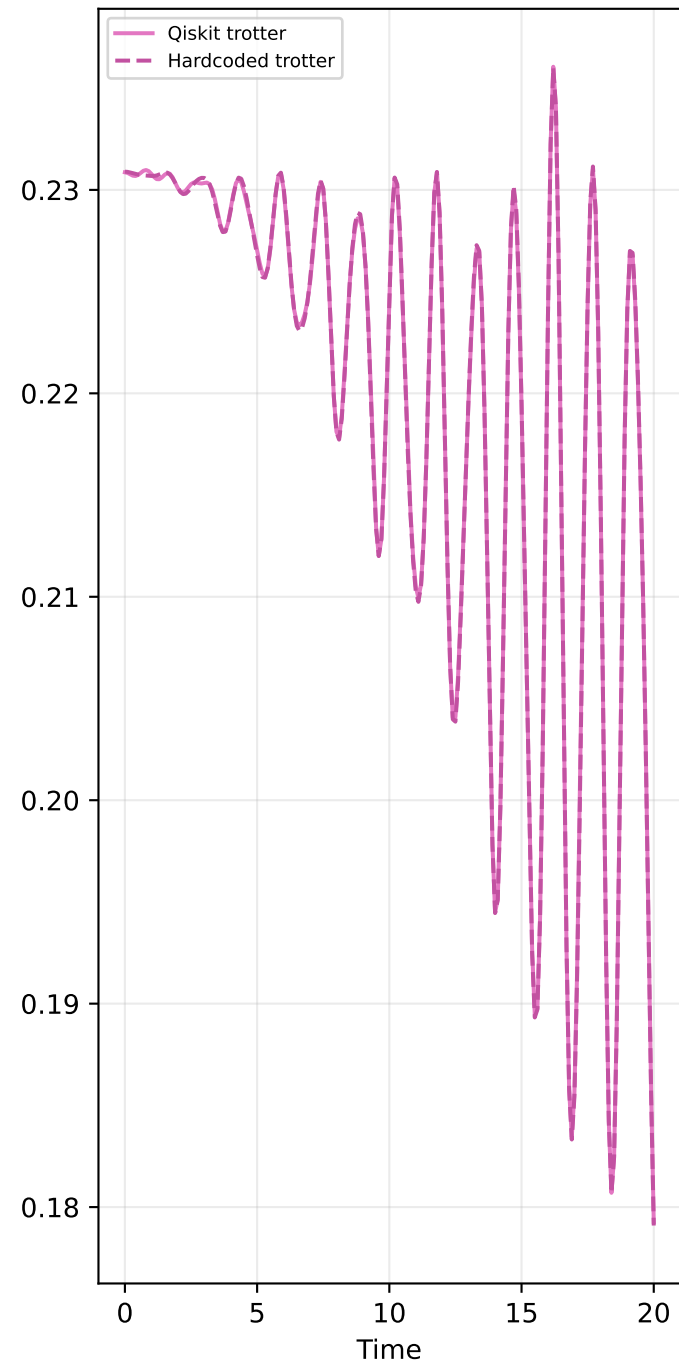
L=3 Site-0 n_{up}



L=3 Site-0 n_{dn}



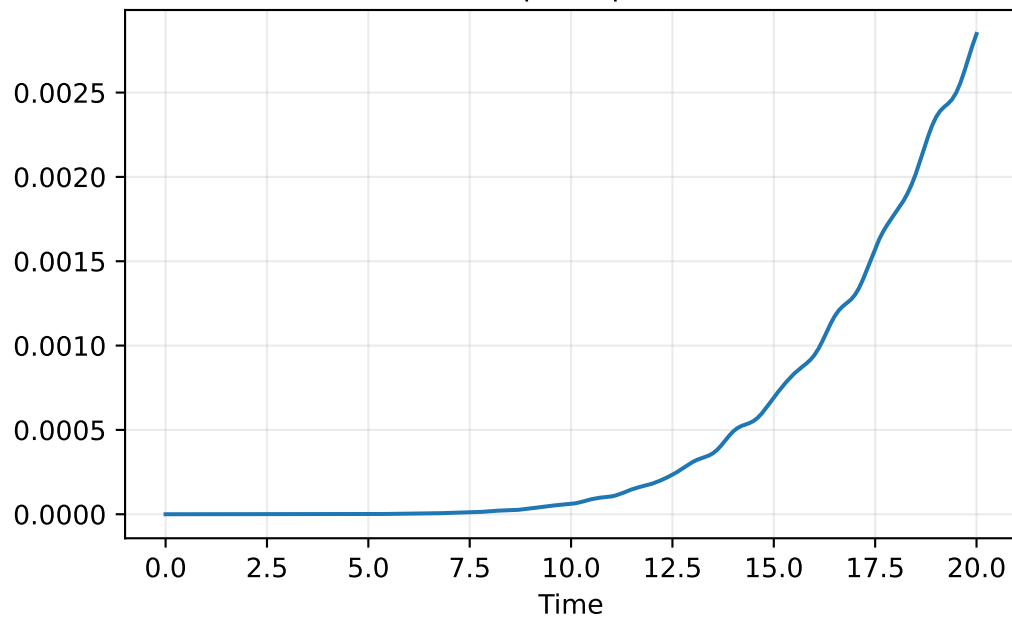
L=3 Doublon



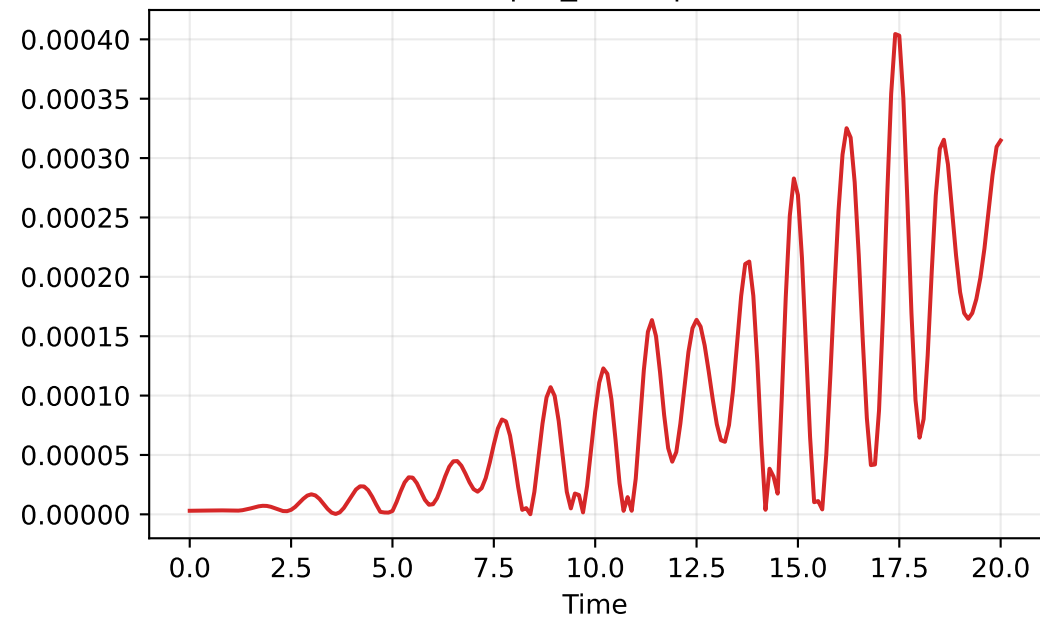
Bundle Delta Diagnostics L=3

$$\Delta X(t) = |X_{hc}(t) - X_{qk}(t)|$$

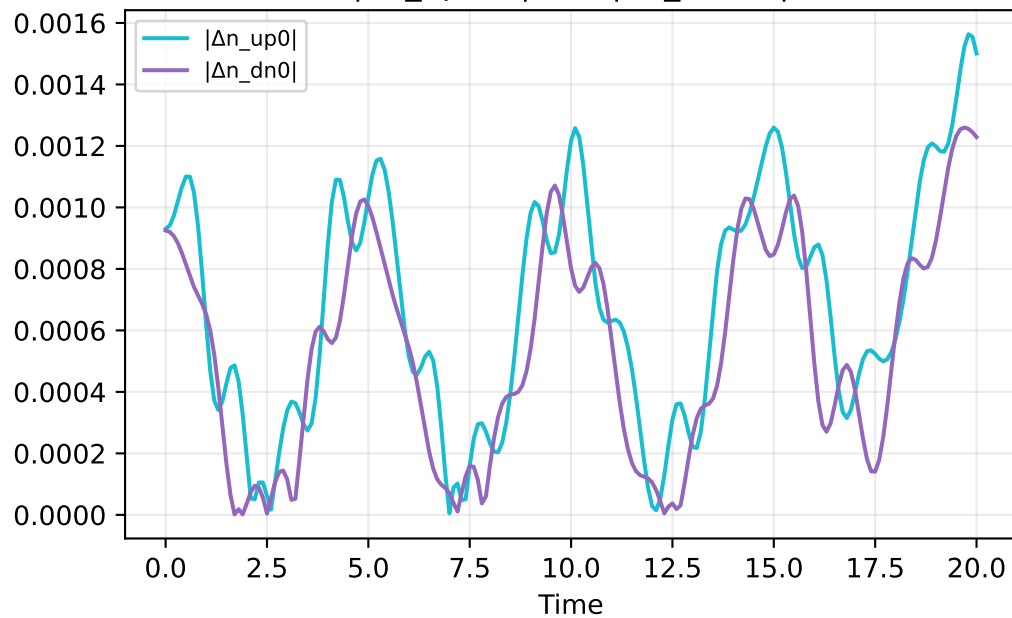
$|\Delta F(t)|$



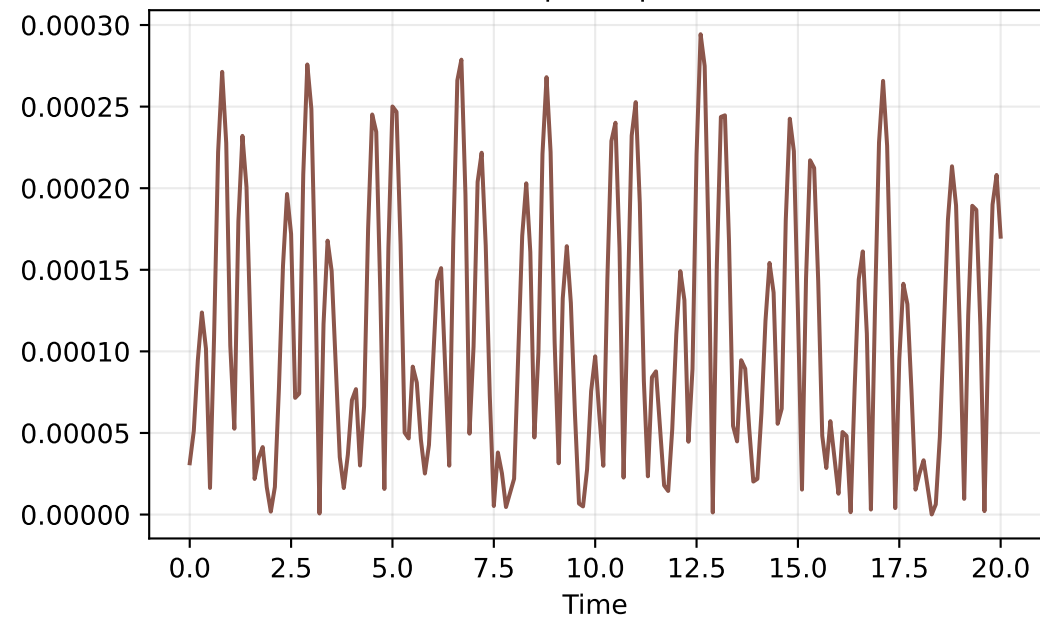
$|\Delta E_{\text{trot}}(t)|$



$|\Delta n_{\text{up}0}(t)|$ and $|\Delta n_{\text{dn}0}(t)|$



$|\Delta D(t)|$



Bundle metrics page L=3

```
ground_state_energy_abs_delta = 0.0
fidelity max/mean/final = 0.0028472181418830456 / 0.0004863150217258033 / 0.0028472181418830456
energy_trotter max/mean/final = 0.00040448998847808504 / 8.782021618988957e-05 / 0.00031480678318551725
n_up_site0_trotter max/mean/final = 0.001563395558948688 / 0.0006754864255162744 / 0.0015008393939485165
n_dn_site0_trotter max/mean/final = 0.0012600920797239956 / 0.0005352107584712608 / 0.0012287359904210593
doublon_trotter max/mean/final = 0.00029437047651986736 / 0.00011316375758190726 / 0.00017030616756291694
```

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