Supporting Information: Reducing Quantum Circuit Depth for Noise-Resilient Quantum Chemistry using the Transcorrelated Method and Adaptive Ansätze

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CONTENTS

I. ROBUSTNESS OF THE ALGORITHM

We investigate the algorithm's robustness by adjusting how operators are appended in TC-AVQITE for the H_4 system with a bond length 1.23 Å. We tested two parameters: $i_{\max}$, the maximum amount of added operators per iteration, and d, the minimum amount of iterations before adding additional operators.

Figure 1 shows that modifying the parameters $i_{\max}$ and d influences the total parameter count, however, it does so equally between TC-AVQITE and AVQITE. This result suggests that these parameters can simply be treated as any other parameter – an appropriate setting for a desired quality of simulation will not favour either method unfairly. One unexpected result arises at the point $(d, i_{\max}) = (5, 0)$, where, for some unclear reason, the AVQITE simulation converges with fewer parameters than TC-AVQITE. This behaviour is, however, only observed once.

In general, increasing the number of iterations, d, before adding new operators naturally slows down the simulation in imaginary time, i.e., more steps are required to reach convergence. However, as there appears to be no clear benefit of doing so, the parameters d and $i_{\max}$ can safely be ignored. In all simulations other than this test, we use the values (0,7) of the parameters $(d, i_{\max})$.

Furthermore, parameters such as the imaginary time step $\Delta\tau$, and the McLachlan distance cutoff L_{cut} were adjusted to see if it unfairly affected simulation quality of TC-AVQITE and AVQITE. As no trend difference was observed, we conclude that TC-AVQITE is robust w.r.t these parameters. For all simulations other than the test, we use the values $\Delta\tau = 0.05$ and $L_{\text{cut}} = 1 \times 10^{-5}$.

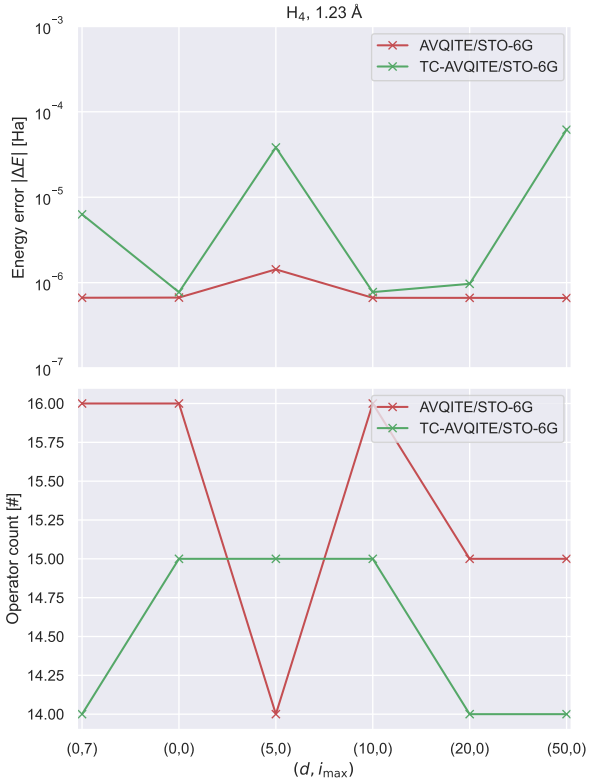

FIG. 1: The effect of the parameters $i_{\max}$ and d for H_4 at bond length 1.23 Å. Each point represents a different run with parameter settings $(d, i_{\max})$.

II. TABLE OF CONVERGED RESULTS

Table I summarises the final values of all (TC-) AVQITE trajectories.

III. (TC-)AVQITE TRAJECTORIES

Figures 2-15 show all individual (TC-)AVQITE trajectories.

IV. BETTER CONVERGENCE BY CUTTING CIRCUIT DEPTH

In the main results, TC-AVQITE outperforms AVQITE in the number of appended operators and final energy. Previous findings for ADAPT-VQE suggest that the en-

TABLE I: A summary of the final values of all (TC-)AVQITE trajectories. Every entry in this table corresponds to a point in Fig. 6 in the main results. Energies are given in Hartrees.

System[a]	Bonding regime	Final energy	$\lvert\Delta E\rvert$ to STO-6G/ FCI or ED[b]	$\lvert\Delta E\rvert$ to CBS/FCI	# operators
H_4, 1.0 Å	Repulsive	−1.781 25	1.514×10^{-1}	3.256×10^{-1}	17
H_4, 1.0 Å, TC	Repulsive	−1.997 98	7.529×10^{-7}	1.089×10^{-1}	15
H_4, 1.23 Å	Bonding	−1.985 60	6.657×10^{-7}	1.343×10^{-1}	16
H_4, 1.23 Å, TC	Bonding	−2.056 75	6.298×10^{-6}	6.311×10^{-2}	14
H_4, 2.0 Å	Half-broken	−1.915 44	9.078×10^{-5}	1.324×10^{-1}	15
H_4, 2.0 Å, TC	Half-broken	−2.014 37	2.167×10^{-6}	3.349×10^{-2}	15
H_4, 3.0 Å	Broken	−1.883 81	1.501×10^{-3}	1.198×10^{-1}	18
H_4, 3.0 Å, TC	Broken	−1.990 37	6.199×10^{-4}	1.329×10^{-2}	14
LiH, 1.6 Å	Bonding	−7.972 25	4.533×10^{-6}	9.812×10^{-2}	115
LiH, 1.6 Å, TC	Bonding	−8.054 44	1.309×10^{-5}	1.593×10^{-2}	54
LiH, 2.25 Å	Half-broken	−7.930 92	4.056×10^{-6}	1.141×10^{-1}	105
LiH, 2.25 Å, TC	Half-broken	−8.024 26	9.487×10^{-6}	2.077×10^{-2}	66
LiH, 3.0 Å	Broken	−7.887 51	3.781×10^{-6}	1.203×10^{-1}	109
LiH, 3.0 Å, TC	Broken	−7.988 03	1.661×10^{-5}	1.974×10^{-2}	68
H_2O, 0.96 Å	Bonding	−75.714 67	2.490×10^{-6}	6.583×10^{-1}	143
H_2O, 0.96 Å, TC	Bonding	−76.036 28	3.076×10^{-6}	3.366×10^{-1}	106
H_2O, 1.5 Å	Half-broken	−75.590 79	2.082×10^{-6}	5.898×10^{-1}	190
H_2O, 1.5 Å, TC	Half-broken	−75.920 23	3.041×10^{-6}	2.603×10^{-1}	174
H_2O, 2.5 Å	Broken	−75.461 76	9.917×10^{-2}	5.283×10^{-1}	119
H_2O, 2.5 Å, TC	Broken	−75.923 01	5.563×10^{-4}	6.705×10^{-2}	142

[a] Syntax: Molecule, bond length. TC-AVQITE trajectories are marked TC, and AVQITE trajectories are unmarked.
[b] If Absolute energy error to basis set is lower than 1×10^{-3} Ha, we have achieved "computational accuracy".

TABLE II: Comparison of TC-AVQITE and TC-VarQITE, i.e. with and without the adaptive ansätze. Energies in Hartrees. Bold font indicates the result with a lower error.

System[a]	Operator count	$\lvert\Delta E\rvert$ to basis set[b]
H_4, 1.0 Å, TC-VarQITE	149	9.174×10^{-5}
H_4, 1.0 Å, TC-AVQITE	15	7.529×10^{-7}
H_4, 1.23 Å, TC-VarQITE	149	2.158×10^{-4}
H_4, 1.23 Å, TC-AVQITE	14	6.298×10^{-6}
H_4, 2.0 Å, TC-VarQITE	149	1.026×10^{-3}
H_4, 2.0 Å, TC-AVQITE	15	2.167×10^{-6}
H_4, 3.0 Å, TC-VarQITE	149	3.502×10^{-4}
H_4, 3.0 Å, TC-AVQITE	14	6.199×10^{-4}

[a] Syntax: Molecule, bond length, method. [b] If Absolute energy error to basis set is lower than 1×10^{-3} Ha, we have achieved "computational accuracy".

ergy difference could also partly be caused by using adaptive ansätze.[1] To evaluate if this holds for TC-AVQITE, we compare it with the TC method using a full UCCSD ansatz (TC-VarQITE), i.e., without an adaptive approach for H_4 at all four studied bond distances (Figs. 12-15). We summarize the result from this comparison in Table II.

The results show that TC-AVQITE is usually more accurate w.r.t. the basis set ED – TC energy than the TC UCCSD calculation (except for the broken-bond regime, where both perform roughly equivalent). This finding suggests that similar to ADAPT-VQE findings,[1] adaptive ansätze improves convergence within a TC setting.

[1] H. R. Grimsley, S. E. Economou, E. Barnes, and N. J. Mayhall, Nature Communications **10** (2019), 10.1038/s41467-019-10988-2, publisher: Springer Science and Business Media LLC.

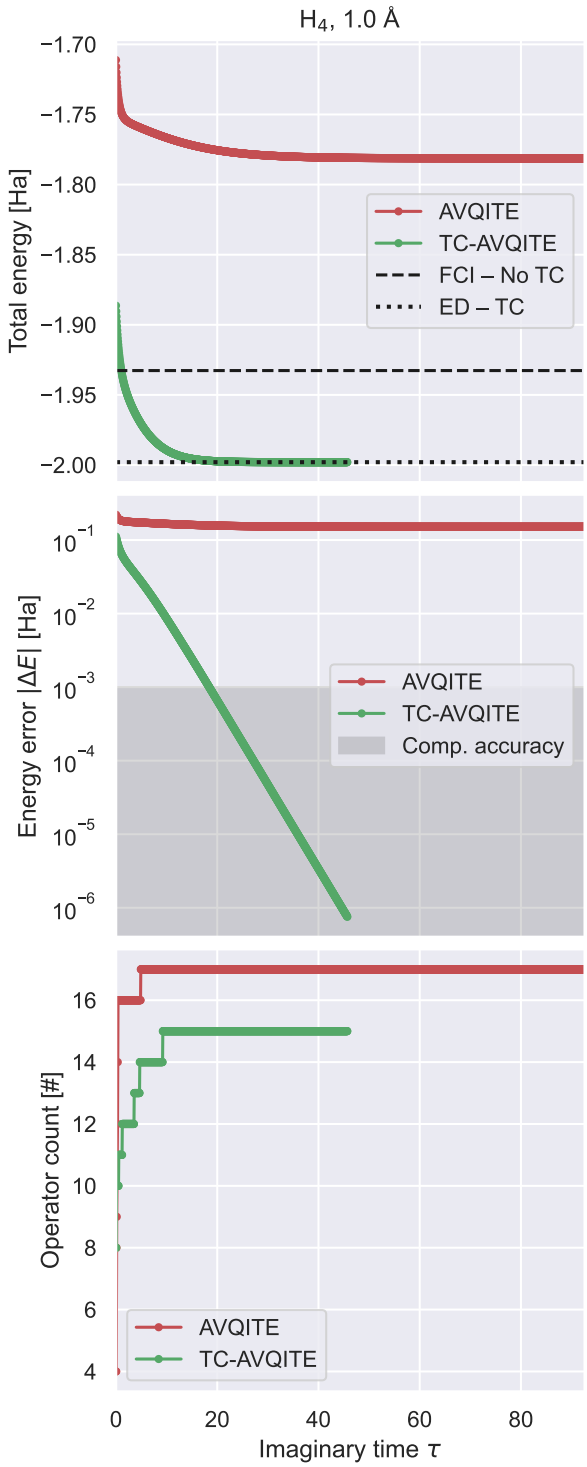

FIG. 2: A comparison between TC-AVQITE and AVQITE for H_4 with bond length 1.0 Å, corresponding to rows 1 and 2 in Table I.

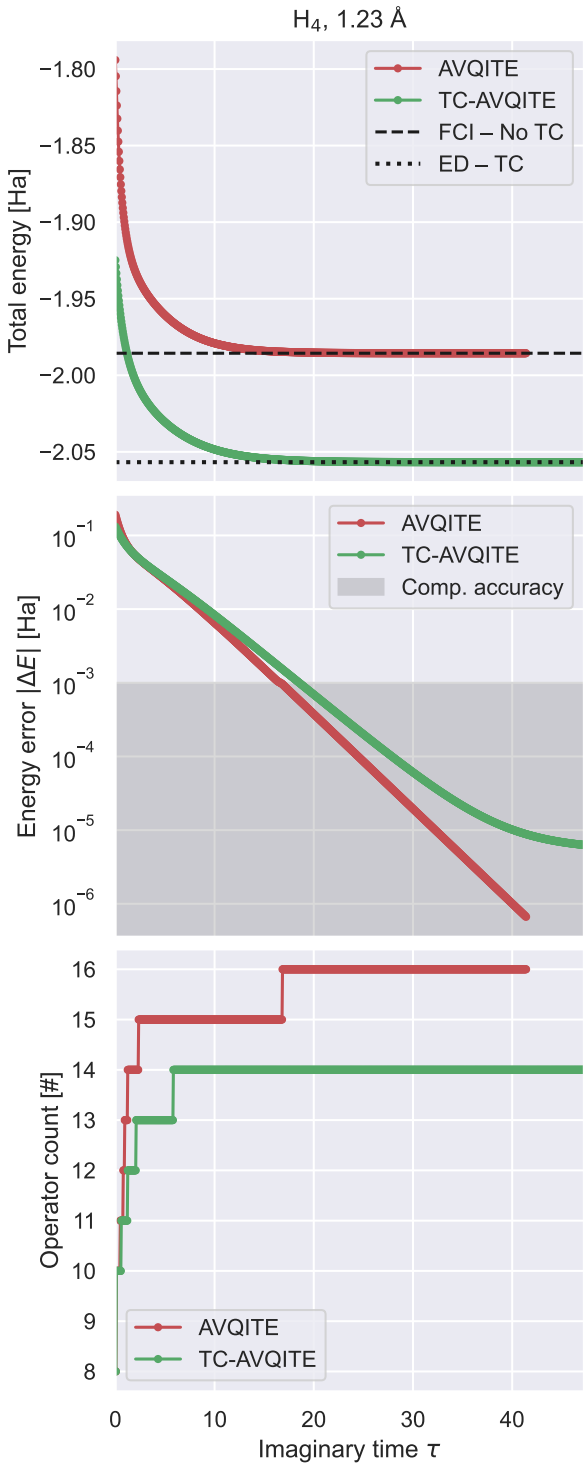

FIG. 3: A comparison between TC-AVQITE and AVQITE for H_4 with bond length 1.23 Å, corresponding to rows 3 and 4 in Table I.

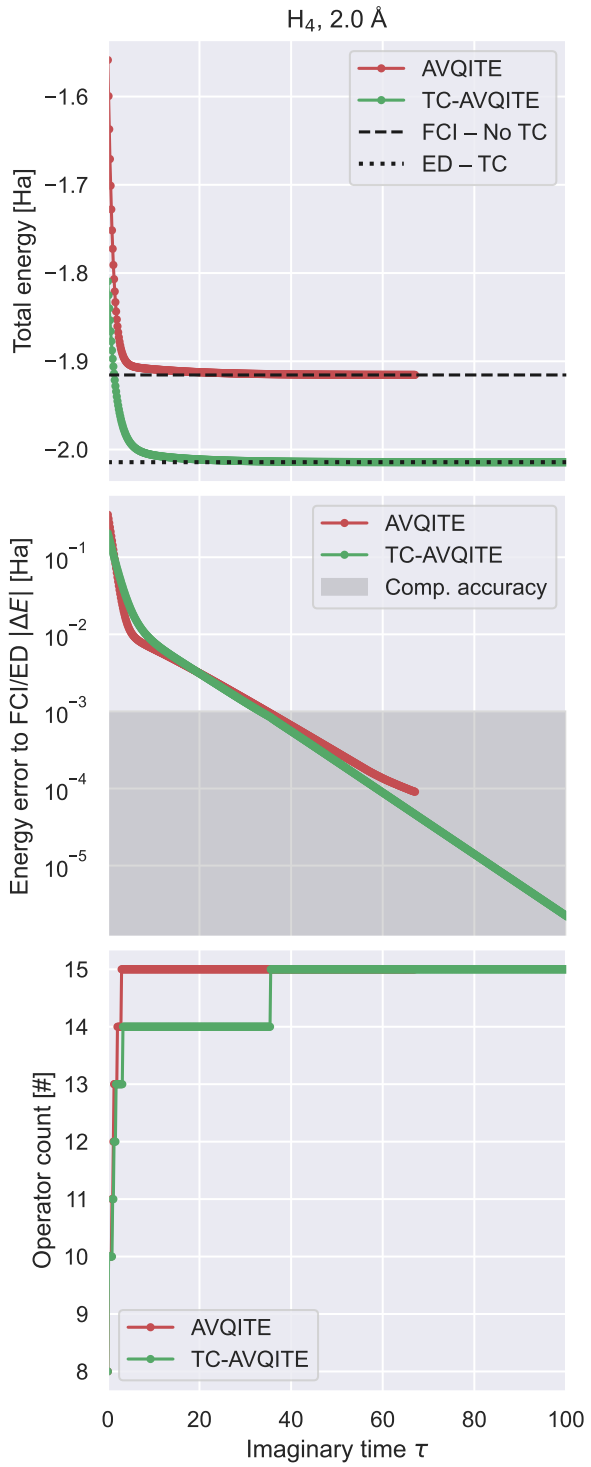

FIG. 4: A comparison between TC-AVQITE and AVQITE for H_4 with bond length 2.0 Å, corresponding to rows 5 and 6 in Table I.

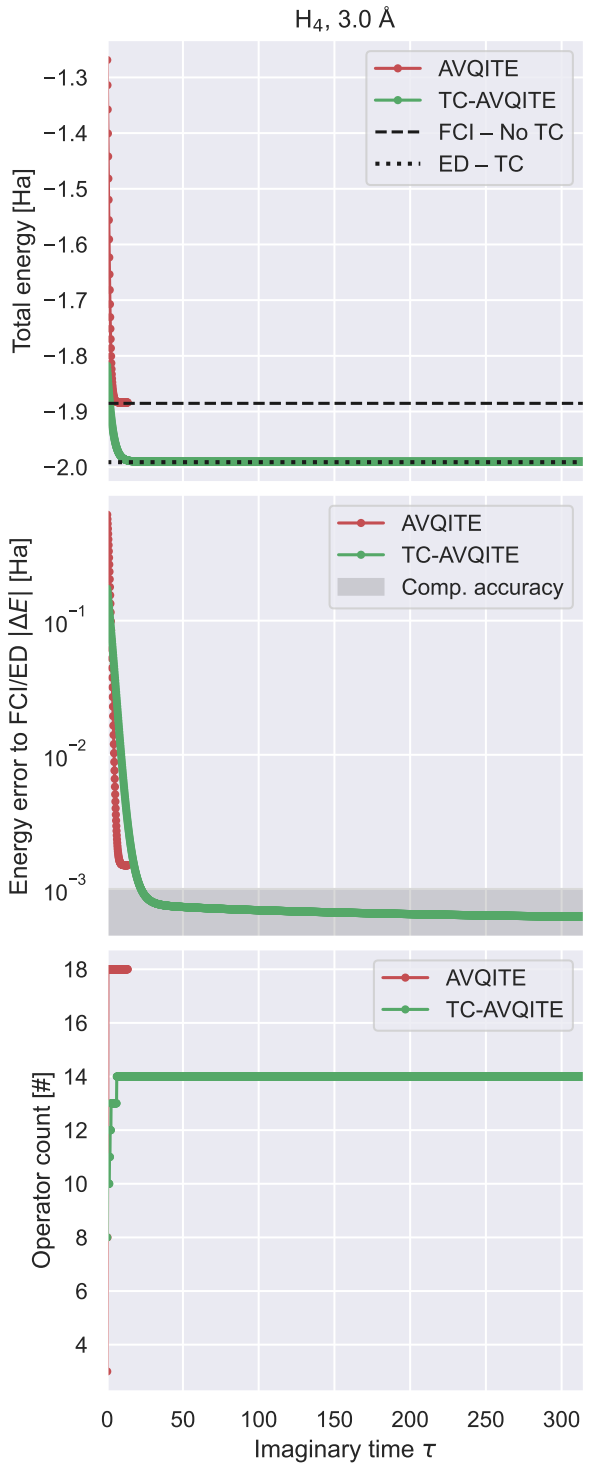

FIG. 5: A comparison between TC-AVQITE and AVQITE for H_4 with bond length 3.0 Å, corresponding to rows 7 and 8 in Table I.

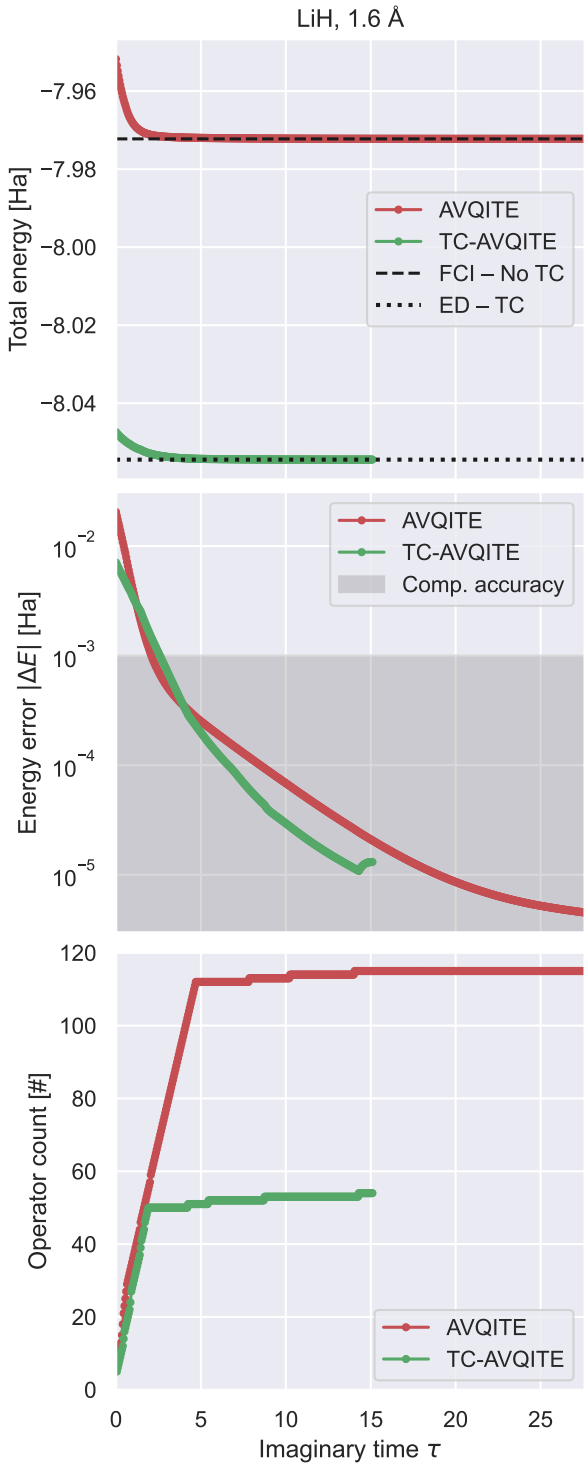

FIG. 6: A comparison between TC-AVQITE and AVQITE for LiH with bond length 1.6 Å, corresponding to rows 9 and 10 in Table I.

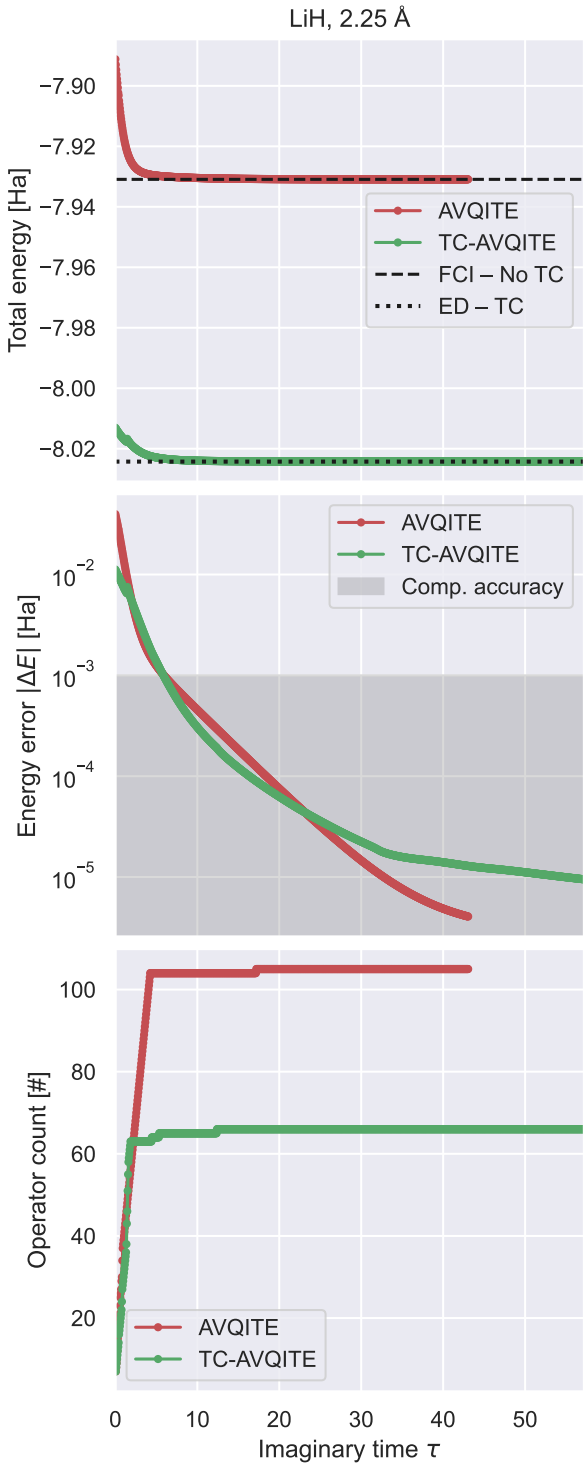

FIG. 7: A comparison between TC-AVQITE and AVQITE for LiH with bond length 2.25 Å, corresponding to rows 11 and 12 in Table I.

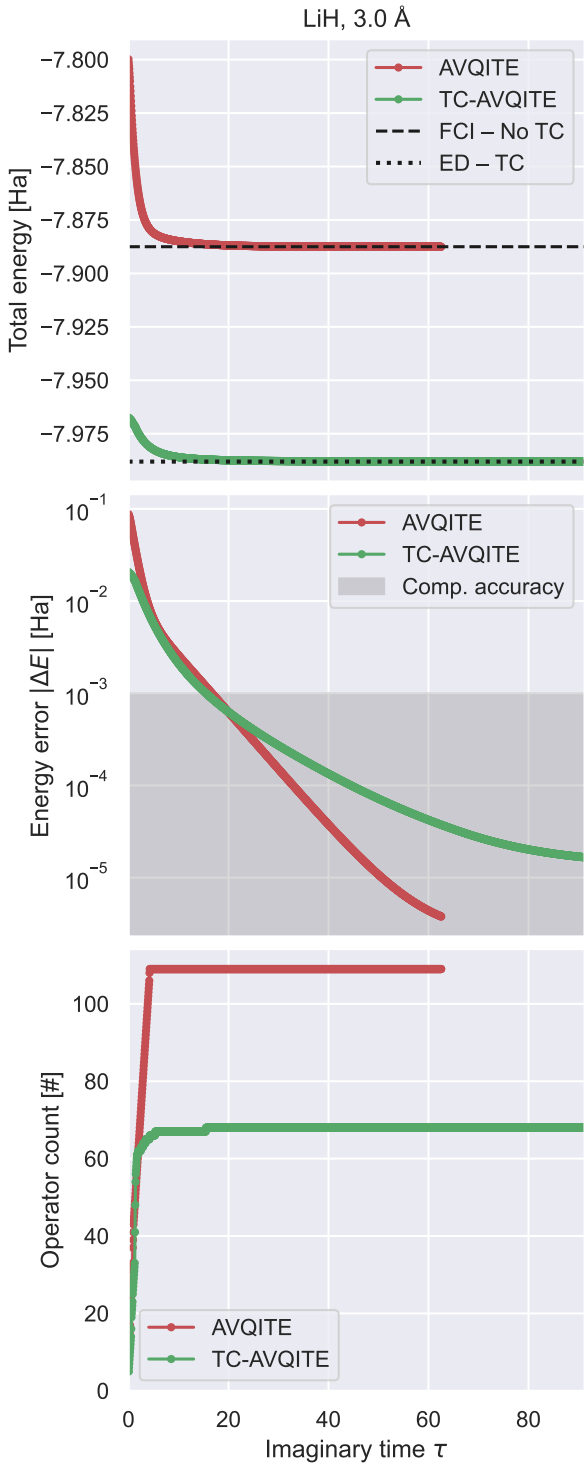

FIG. 8: A comparison between TC-AVQITE and AVQITE for LiH with bond length 3.0 Å, corresponding to rows 13 and 14 in Table I.

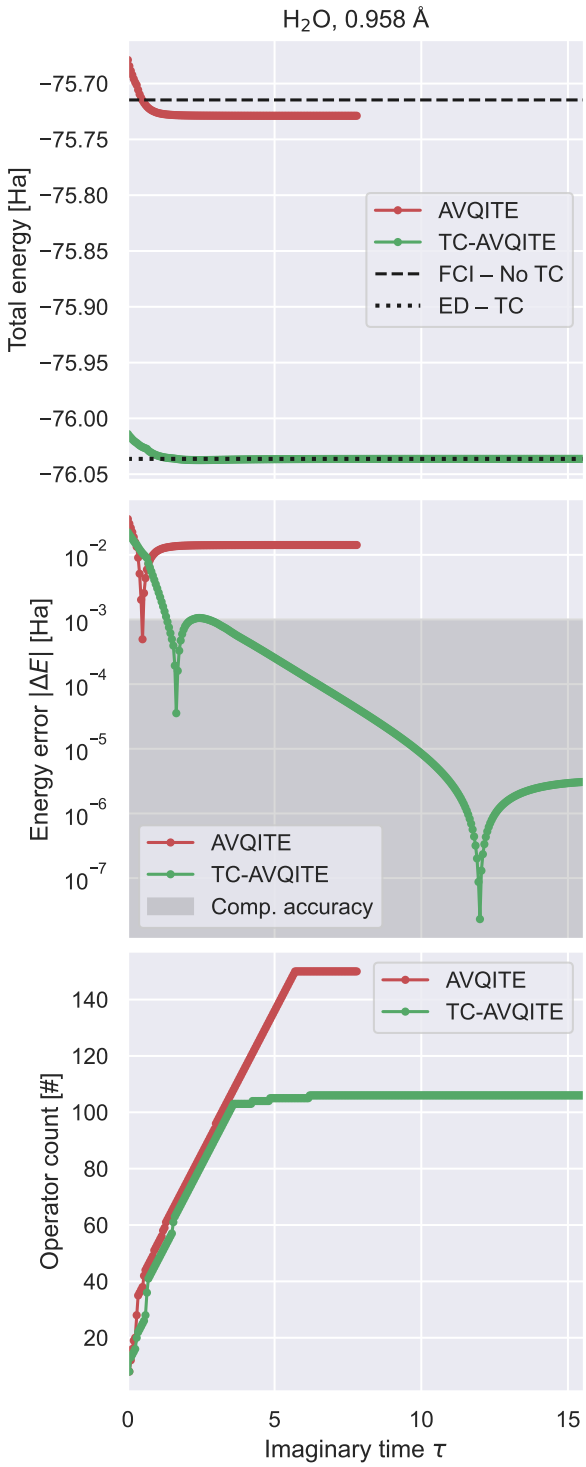

FIG. 9: A comparison between TC-AVQITE and AVQITE for H_2O with bond length 0.958 Å, corresponding to rows 15 and 16 in Table I.

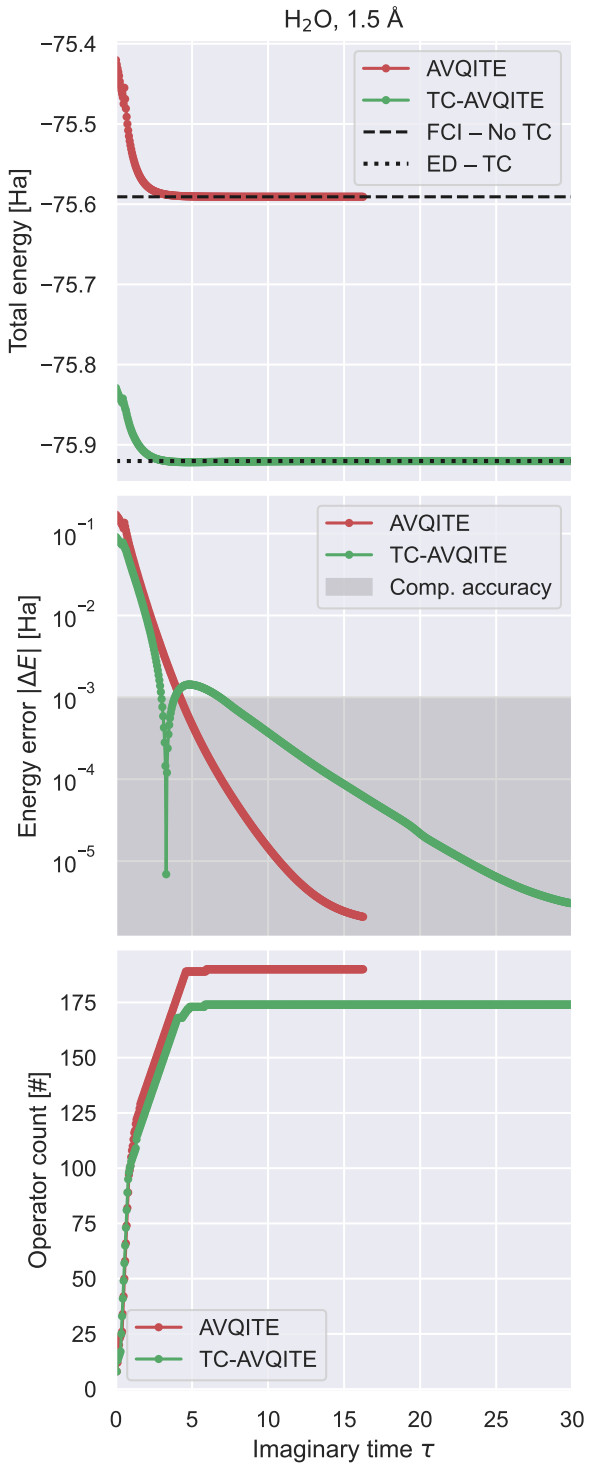

FIG. 10: A comparison between TC-AVQITE and AVQITE for H_2O with bond length 1.5 Å, corresponding to rows 17 and 18 in Table I.

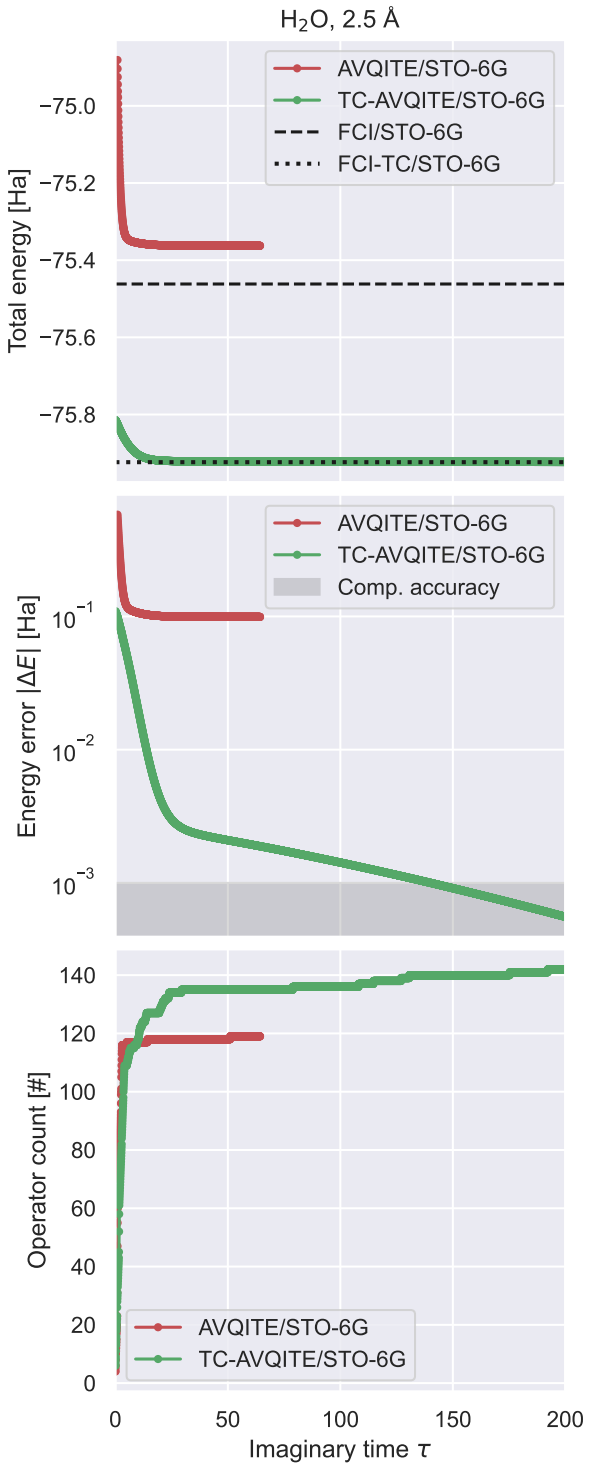

FIG. 11: A comparison between TC-AVQITE and AVQITE for H_2O with bond length 2.5 Å, corresponding to rows 19 and 20 in Table I.

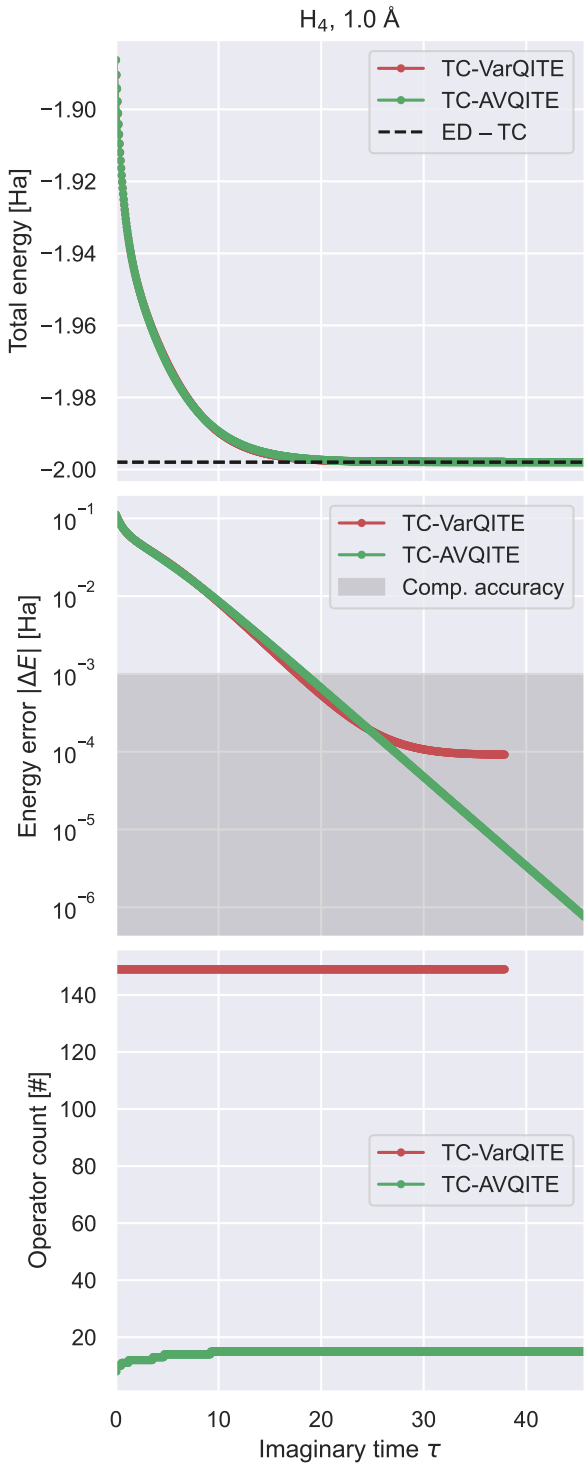

FIG. 12: A comparison between TC-AVQITE and TC-VarQITE for H_4 with bond length 1.0 Å, corresponding to rows 1 and 2 in Table II.

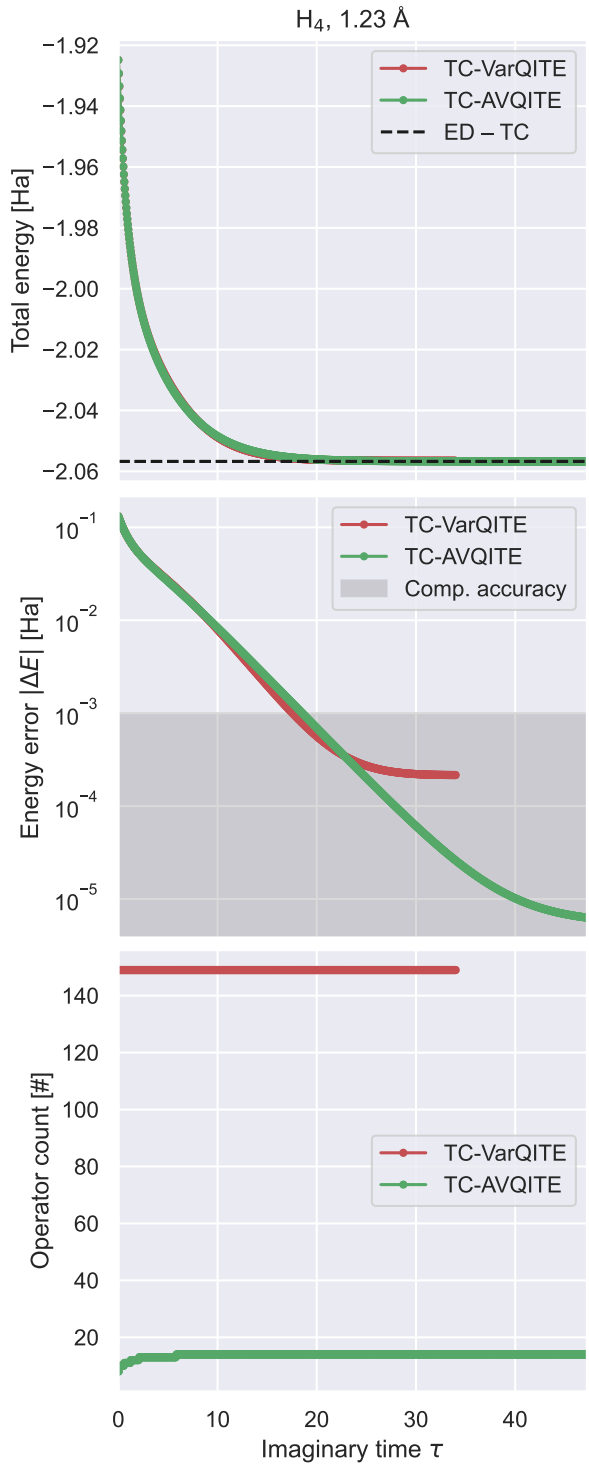

FIG. 13: A comparison between TC-AVQITE and TC-VarQITE for H_4 with bond length 1.23 Å, corresponding to rows 3 and 4 in Table II.

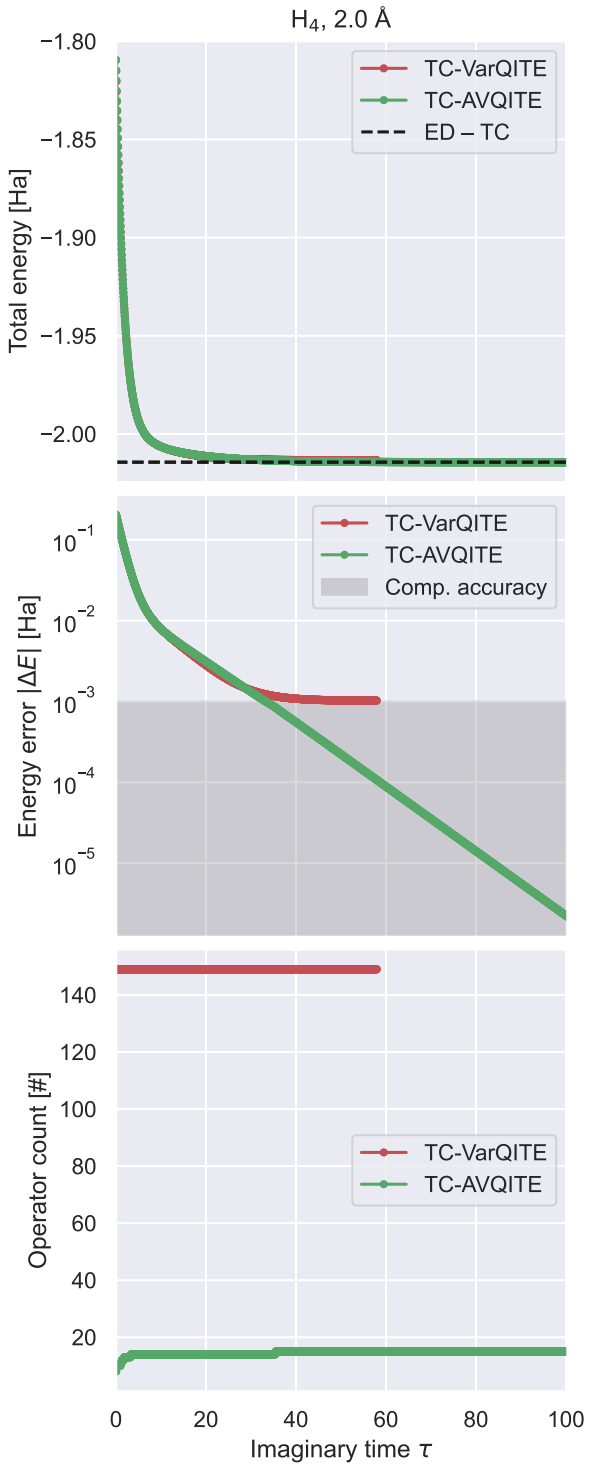

FIG. 14: A comparison between TC-AVQITE and TC-VarQITE for H_4 with bond length 2.0 Å, corresponding to rows 5 and 6 in Table II.

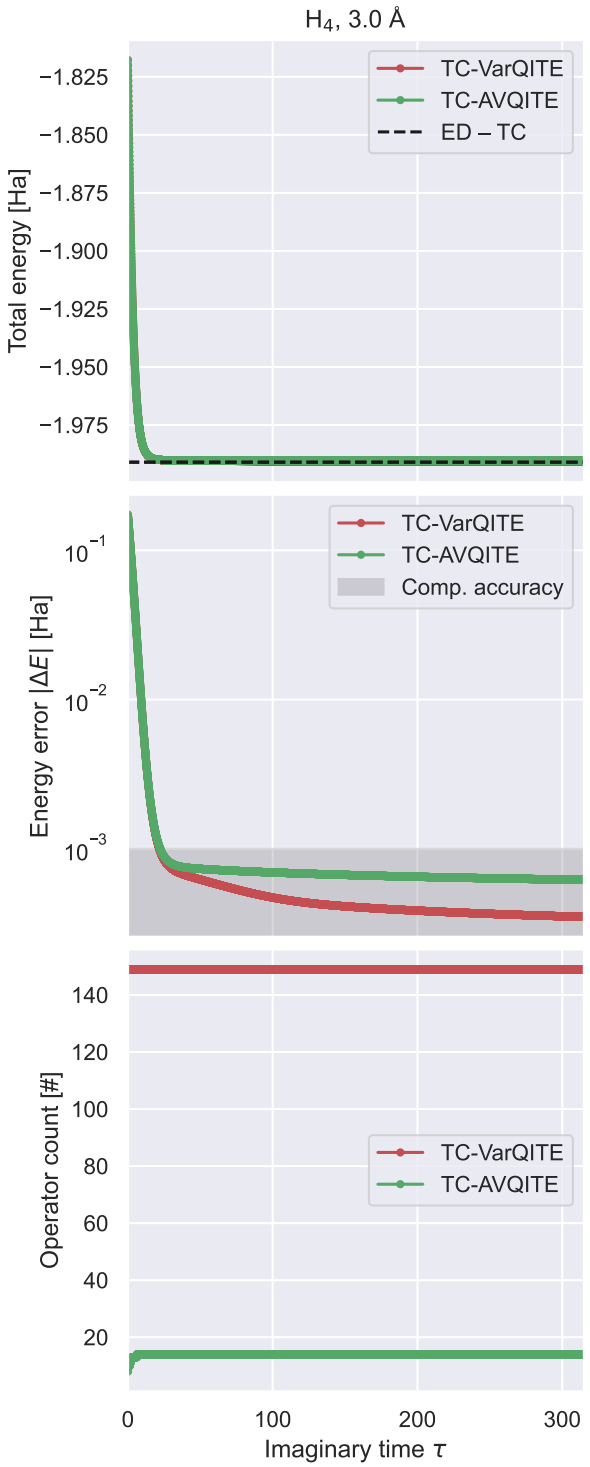

FIG. 15: A comparison between TC-AVQITE and TC-VarQITE for H_4 with bond length 3.0 Å, corresponding to rows 7 and 8 in Table II.