Refutation of an adaptive algorithm for molecular simulation on quantum computers

Abstract: We evaluate "a unitary variant of coupled cluster theory (UCCSD) [as] defined by replacing the excitation operators with an anti-Hermitian sum of excitation and de-excitation operators". It is *not* tautologous, hence refuting the subsequent sections for the ADAPT-VQE algorithm, molecular dissociation simulation results, and dependence of convergence on operator ordering. The conjecture of the paper is refuted from its abstract as: "an arbitrarily accurate variational algorithm that instead of fixing an ansatz upfront, … grows it systematically one operator at a time in a way dictated by the molecule being simulated … [to] highlight the potential of our adaptive algorithm for exact simulations with present-day and near-term quantum hardware."
These equations form a *non* tautologous fragment of the universal logic VŁ4.

We assume the method and apparatus of Meth8/VŁ4 with Tautology as the designated proof value, **F** as contradiction, N as truthity (non-contingency), and C as falsity (contingency). The 16-valued truth table is row-major and horizontal, or repeating fragments of 128-tables, sometimes with table counts, for more variables. (See ersatz-systems.com.)

LET ~ Not, ¬ ; + Or, ∨, ∪, ⊔ ; - Not Or; & And, ∧, ∩, ⊓ , · , ⊗ ; \ Not And;
> Imply, greater than, →, ⇒ , ↦, ≻, ⊃, ↠ ; < Not Imply, less than, ∈, ≺, ⊂, ⊬, ⊭, ↞, ≲ ;
= Equivalent, ≡, :=, ⇔, ↔, ≙, ≈, ≃ ; @ Not Equivalent, ≠, ⊕;
% possibility, for one or some, ∃, ◊, M; # necessity, for every or all, ∀, □, L;
(z=z) T as tautology, ⊤, ordinal 3; (z@z) **F** as contradiction, Ø, Null, ⊥ , zero;
(%z>#z) N as non-contingency, Δ, ordinal 1; (%z<#z) C as contingency, ∇, ordinal 2;
~(y < x) (x ≤ y), (x ⊆ y), (x ⊑ y); (A=B) (A~B).
Note for clarity, we usually distribute quantifiers onto each designated variable.

From: Grimsley, H.R.; Economou, S.E.; Barnes, E.; Mayhall, N.J. (2019). An adaptive variational algorithm for exact molecular simulations on a quantum computer. arxiv.org/pdf/1812.11173.pdf

II. Results
A. Specification of the adopted notation

… In this context, a unitary variant of coupled cluster theory (UCCSD) was defined by replacing the excitation operators with an anti-Hermitian sum of excitation and de-excitation operators:

$$\hat{t}_{ij}^{ab} \rightarrow \hat{t}_{ij}^{ab} - \hat{t}_{ab}^{ij} = \hat{\tau}_{ij}^{ab}. \qquad (4)$$

We write the snippet (4) above as (4.1) below:

t^ab_ij → t^ab_ij − t^ ij_ab = ^τ ab_ij . (4.1)

LET p, q, r, s: t^, ^τ, ab_ij, ij_ab.

(p&r)>(((p&r)-(p&s))=(q&r)) ;
TTTT TTT**F** TTTT TTT**F** (4.2)

Remark 4.2: Eq. 4.2 as rendered is *not* tautologous, hence refuting the subsequent sections for the ADAPT-VQE algorithm, molecular dissociation simulation results, and dependence of convergence on operator ordering.

The conjecture of the paper is refuted from its abstract as: “an arbitrarily accurate variational algorithm that instead of fixing an ansatz upfront, … grows it systematically one operator at a time in a way dictated by the molecule being simulated … [to] highlight the potential of our adaptive algorithm for exact simulations with present-day and near-term quantum hardware.”