Supplementary Information: Measuring all compatible operators in one series of single-qubit measurements using unitary transformations

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Hamiltonian Generation

**H\textsubscript{2} molecule:** One- and two-electron integrals in the canonical restricted Hartree–Fock (RHF) molecular orbitals basis for $R$(H-H)=1.5 \textdegree{Å}, were used in the Bravyi–Kitaev (BK) transformation to produce the corresponding qubit Hamiltonian. Spin-orbitals were alternating in the order $\alpha$, $\beta$, $\alpha$, ...,

**LiH molecule:** Using the parity transformation for the LiH molecule at $R$(Li – H) = 3.2 \textdegree{Å}, a 6-qubit Hamiltonian containing 118 Pauli words was generated. Spin-orbitals were arranged as “first all $\alpha$ then all $\beta$” in the fermionic form; since there are 3 active molecular orbitals in the problem, this leads to 6-qubit Hamiltonian. This qubit Hamiltonian has 3\textsuperscript{rd} and 6\textsuperscript{th} stationary qubits, which allowed us to replace the corresponding $\hat{z}$ operators by their eigenvalues, $\pm1$, thus defining the different “sectors” of the original Hamiltonian. Each of
these sectors is characterized by its own 4-qubit effective Hamiltonian. The ground state lies in the $z_3 = -1$, $z_6 = 1$ sector; the corresponding 4-qubit effective Hamiltonian ($\hat{H}_{LiH}$) has 100 Pauli words.

**H$_2$O molecule:** 6- and 26-qubit Hamiltonians were generated for this system in the 6-31G basis, and the 14-qubit Hamiltonian was generated using the STO-3G basis. The geometry for all Hamiltonians was chosen to be $R(O - H) = 0.75$ Å and $\angle HOH = 107.6^\circ$. The 14- and 26-qubit Hamiltonians were obtained in OpenFermion using both JW and BK transformations without any modifications, while for the 6-qubit Hamiltonian we used several qubit reduction techniques detailed below.

Complete active space (4, 4) electronic Hamiltonian was converted to the qubit form using the BK transformation grouping spin-orbitals as “first all alpha than all beta”. The resulting 8-qubit Hamiltonian contained 185 Pauli terms. 4$^{th}$ and 8$^{th}$ qubits were found to be stationary; the ground state solution is located in the $z_3 = 1$, $z_7 = 1$ subspace. By integrating out $z_3$ and $z_7$, the 6-qubit reduced Hamiltonian with 165 terms was derived.

**N$_2$, BeH$_2$, and NH$_3$ molecules:** The BK and JW transformations of the electronic Hamiltonian in the 6-31G and STO-3G bases produced qubit Hamiltonians by OpenFermion. The nuclear geometry was fixed at $R(N - N) = 1.1$ Å($N_2$); $R(\text{Be} - H) = 1.4$ Å, collinear geometry (BeH$_2$); $\angle HNH = 107^\circ$ and $R(N - H) = 1.0$ Å(NH$_3$).