Supplementary information for 'Simple Fermionic backflow states via a systematically improvable tensor decomposition'

Massimo Bortone[1*], Yannic Rath[1,2] and George H. Booth[1*]

[1]Department of Physics and Thomas Young Centre, King's College London, Strand, London, WC2R 2LS, United Kingdom.
[2]National Physical Laboratory, Teddington, TW11 0LW, United Kingdom.

*Corresponding author(s). E-mail(s): massimo.bortone@kcl.ac.uk; george.booth@kcl.ac.uk;
Contributing authors: yannic.rath@npl.co.uk;

1 Supplementary Note 1: Spin-spin Correlations

For a pair of atoms a and b, we define the instantaneous spin-spin correlation function as

$$\left\langle \hat{S}^z_{\vec{r}_a} \hat{S}^z_{\vec{r}_b} \right\rangle = \frac{1}{4} \sum_{ijkl} P^a_{ij} P^b_{kl} \left(\Gamma^{\alpha\alpha}_{ijkl} - \Gamma^{\alpha\beta}_{ijkl} - \Gamma^{\beta\alpha}_{ijkl} + \Gamma^{\beta\beta}_{ijkl} \right) + \frac{1}{4} \sum_{ijk} P^a_{ik} P^b_{jk} \left(\gamma^{\alpha}_{ij} + \gamma^{\beta}_{ij} \right), \tag{1}$$

where P^a and P^b are projectors onto the orbital subspaces of atom a and b, the indices i, j, k, l are orbital labels, and γ^{σ}_{ij} and $\Gamma^{\sigma\tau}_{ijkl}$ are spinned one- and two-body reduced density matrices (RDMs), respectively.

During the evaluation of the local energy, the spin-free one- and two-body RDMs, γ_{ij} and Γ_{ijkl}, are computed, so that it pays off to express the previous equation in terms of these quantities. This can be done using the following identities [1, 2]:

$$\gamma^{\alpha}_{ij} = \gamma^{\beta}_{ij} = \gamma_{ij} \tag{2}$$

$$\Gamma^{\alpha\alpha}_{ijkl} = \Gamma^{\beta\beta}_{ijkl} = \frac{1}{6} \left(\Gamma_{ijkl} - \Gamma_{kjil} \right) \tag{3}$$

$$\Gamma^{\alpha\beta}_{ijkl} = \Gamma^{\beta\alpha}_{ijkl} = \frac{1}{6} \left(2\Gamma_{ijkl} + \Gamma_{kjil} \right). \tag{4}$$

Then, Eq. 1 can be written as

$$\left\langle \hat{S}^z_{\vec{r}_a} \hat{S}^z_{\vec{r}_b} \right\rangle = -\frac{1}{2} \sum_{ijkl} P^a_{ij} P^b_{kl} \left(\frac{\Gamma_{ijkl}}{6} + \frac{\Gamma_{kjil}}{3} \right) + \frac{1}{4} \sum_{ijk} P^a_{ik} P^b_{jk} \left(\gamma_{ij} \right). \tag{5}$$

Since the 6×6 hydrogen lattice results of the main text are obtained in a minimal basis of localized orthogonal orbitals, P^a projects exactly onto one local orbital used in the sampling basis of the VMC and can thus be written as

$$P^a_{ij} = \begin{cases} 1 & \text{if } i = a \text{ and } j = a, \\ 0 & \text{otherwise.} \end{cases} \tag{6}$$

For a given a variational state $|\psi\rangle$, the one- and two-body RDMs are estimated via Monte Carlo estimation of local operators

$$\gamma^{loc}_{ij} = \frac{\langle \mathbf{n}|\hat{c}^\dagger_i \hat{c}_j|\psi\rangle}{\langle \mathbf{n}|\psi\rangle}, \tag{7}$$

$$\Gamma^{loc}_{ijkl} = \frac{\langle \mathbf{n}|\hat{c}^\dagger_i \hat{c}^\dagger_j \hat{c}_k \hat{c}_l|\psi\rangle}{\langle \mathbf{n}|\psi\rangle}, \tag{8}$$

Evaluating these local operators involves finding all the connected Fock configurations $\mathbf{n}'$ for a given $\mathbf{n}$ sampled from $|\psi\rangle$ according to the corresponding Born distribution $|\psi(\mathbf{n})|^2$. In the case of the one-body RDM, connected configurations are obtained by moving one electron from orbital j to orbital i, while for the two-body RDM, they are obtained by a two-electron move. The Fermionic commutation relations then imply that a sign is picked up for every electron that is passed during the move, within the pre-established orbital ordering. This can be accounted for by computing a parity factor $P_{\mathbf{nn}'}$ for each pair of configurations $\mathbf{n}$ and $\mathbf{n}'$.

Supplementary References

[1] Jan-Niklas Boyn and David A. Mazziotti. Accurate singlet–triplet gaps in biradicals via the spin averaged anti-Hermitian contracted Schrödinger equation. *The Journal of Chemical Physics*, 154(13):134103, April 2021.

[2] Sujun Yun, Werner Dobrautz, Hongjun Luo, Vamshi Katukuri, Niklas Liebermann, and Ali Alavi. Ferromagnetic domains in the large-U Hubbard model with a few holes: A full configuration interaction quantum Monte Carlo study. *Physical Review B*, 107(6):064405, February 2023.