Genuine multipartite spin entanglement from many-electron systems

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Abstract: We show that a high degree of genuine multipartite entanglement can be extracted from a variety of closed-shell fermionic states, including the ground states of atomistic Hamiltonians and of archetypal models in solid-state physics (arXiv:2410.11314).

Estimation of entanglement in atomistic systems requires a combination of advanced ab initio calculations - to account for the effect of the electron-electron interaction - and rigorous quantum-informational theoretical analyses. This combination is a challenging task that has not been tackled so far to investigate genuine multipartite entanglement (GME) in materials. Here we show that, contrary to conventional wisdom, a high degree of GME can be extracted from closed-shell states - even in the non-interacting limit (single-configuration states). Close to maximal values of the GME concurrence are also obtained from the ground state of an archetypal fermionic model (Hubbard) and of an atomistic molecular Hamiltonians. The comparative analysis of the above fermionic states allow us to highlight the role played by symmetry and the interplay between GME and spin-pair entanglement. Because the relevant states fulfill the super-selection rules, the generated entanglement may in principle represent also a physical resource.

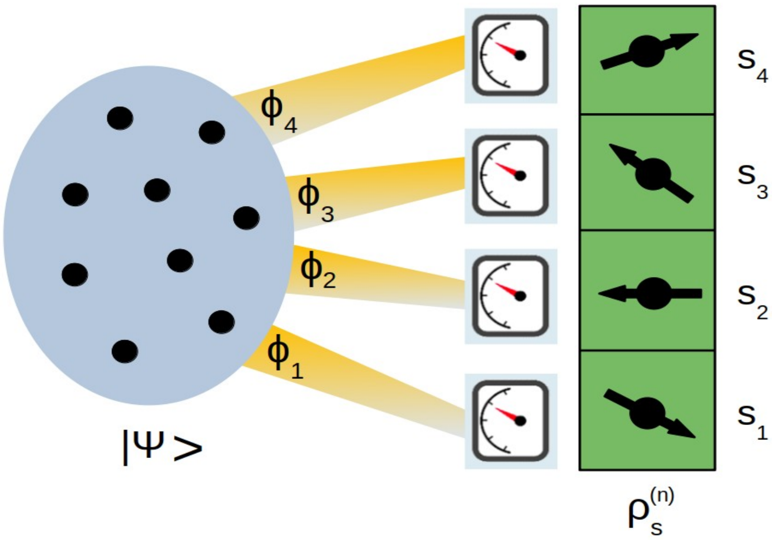

Fig. 1 Schematic representation of the considered procedure: from an N-electron system in a state $|\Psi>$, one extracts an n-spin state ($n \leq N$ in general, N=9 and n=4 in the example). Each of the n spins s_i is labelled by the respective orbital Φ_i.

References

[1] F. Troiani, C. Angeli, A. Secchi, and S. Pittalis, *Genuine multipartite entanglement from many-electron systems*, arXiv:2410.11314 (2024).