Quantum Information Perspective on the Ground State Problem: What is Electron Correlation?

Christian Schilling, Lexin Ding

Arnold Sommerfeld Centre for Theoretical Physics, LMU Munich

Describing strongly interacting electrons is one of the crucial challenges of modern quantum physics. A comprehensive solution to this electron correlation problem would simultaneously exploit *both* the pairwise interaction and its spatial decay. By taking a quantum information perspective, we explain how this structure of realistic Hamiltonians gives rise to two conceptually different notions of correlation and entanglement. The first one describes correlations between *orbitals* while the second one refers more to the *particle* picture. We illustrate those two concepts of orbital and particle correlation and present measures thereof. Our results for different molecular systems reveal that the total correlation between molecular orbitals is mainly classical, raising questions about the general significance of entanglement in chemical bonding. Finally, we also speculate on a promising relation between orbital and particle correlation and explain why this may replace the obscure but widely used concept of static and dynamic correlation.

[1] C.Schilling, R.Schilling, Phys. Rev. Lett. 122, 013001 (2019)

[2] L.Ding, C.Schilling, J. Chem. Theory Comput. 16, 7, 4159 (2020)

[3] L.Ding, S.Mardazad, S.Das, S.Szalay, U.Schollwoeck, Z.Zimboras, C.Schilling, J. Chem. Theory Comput. 17, 1, 79 (2021)

[4] S.Szalay, Z.Zimborás, M.Máté, G.Barcza, C.Schilling, O.Legeza, J. Phys. A: Math. Theor. 54, 39, 393001 (2021)

[5] L.Ding, Z.Zimboras, C.Schilling, arXiv:2207.03377

[6] L.Ding, S.Knecht, Z.Zimborás, C.Schilling, Quantum Sci. Technol. 8, 1, 015015 (2023)

[7] L.Ding, G.Duennweber, C.Schilling, Quantum Sci. Technol. 9, 1, 015005 (2023)

[8] L.Ding, S.Knecht, C.Schilling, J. Phys. Chem. Lett. 14, 11022 (2023)