Electronic Entanglement in Strongly Correlated Materials

Patrik Thunström
Material Theory group at Uppsala University

Entanglement is a fundamental aspect of quantum mechanics, responsible for a large range of complex phenomena not present in a classical setting.[1] Most research has been directed toward the entanglement of distinguishable two-level states (qubits) in the context of quantum information theory, where entanglement is treated as a resource. The entanglement of the electrons in a material has received less explicit attention, but it has been indirectly studied in both the quantum chemistry and condensed matter communities. The description of the electronic structure as a pure separable state, represented as a single Slater determinant, is at the very heart of many modern computational approaches, and the inability to do so is known under the term *correlation*. The term encompasses however both classical and quantum correlations, where the former corresponds to statistically mixed states and the latter electronically entangled states.

In this talk I will first give an introduction to the concept of entanglement between indistinguishable fermions, and how it necessarily differs from the treatment of distinguishable particles. One key point is the distinction of two different forms of entanglement, where the first form focuses on the bipartition of a fixed one-particle basis (orbital entanglement) while the second form is basis independent and instead focuses directly on the full many-body state of the electrons (electronic entanglement). The second part of the talk will focus on the electronic entanglement in the late transition monoxides[2] – MnO, FeO, CoO, and NiO – and the Topological Kondo Insulator SmB_6[3] using Exact Diagonalization within the Density Functional Theory+Dynamical Mean Field Theory scheme. The final part of the talk I will briefly discuss the still open question of how to probe the electronic entanglement in the ground state of a strongly correlated material in an experiment.

[1] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. 80, 517 (2008).
[2] P. Thunström, I. Di Marco, and O. Eriksson, Phys. Rev. Lett. 109, 186401 (2012).
[3] P. Thunström and K. Held, to be published.