Density Matrix Entanglement Embedding for Strongly Correlated Electronic Structure

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Self-consistent quantum embedding forms a route to bridge local descriptions of electronic structure methods and the electronic structure of very large systems and condensed phases. Existing examples of quantum embedding methods include the density functional embedding of Cortona, Wesolowski and Warshel, based on the single-particle density and Carter, and the dynamical mean-field theory, based on the single-particle Greens function. In this talk, however, I will describe a new formalism for quantum embedding that is based on the single-particle density matrix, and which is based on a self-consistent approximation to the exact entanglement embedding of a subsystem in an environment. Unlike density functional embedding, this formalism can practically describe strongly correlated systems, and unlike dynamical mean-field theory, it is easily combined with traditional ground-state electronic structure methods, such as quantum chemical wavefunction methods and projector and variational Monte Carlo approaches. I will demonstrate the performance of the method on the phase diagram of the 1D and 2D Hubbard models and discuss applications to ab-initio systems.

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