Quantum Monte Carlo calculation of reduced density matrices

LUCAS WAGNER, University of Illinois at Urbana-Champaign — Quantum Monte Carlo(QMC) methods offer an efficient way to approximate the interacting ground state and some excited states of realistic model Hamiltonians based on the fundamental Coulomb interaction between electrons and nuclei. Many highly accurate results have been obtained using this method; however, it is often a challenge to extract the important correlations that the QMC wave function contains. I will describe some new results using the reduced density matrices(RDM's) to understand the electron correlation in the many-body wave function. The RDM's have both informative usage for describing correlation and pragmatic uses in further improving the variational wave function.

Lucas Wagner
University of Illinois at Urbana-Champaign