Projective purification of correlated reduced density matrices

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Non-equilibrium Green's function methods are among the most successful methods for describing time-dependent systems beyond the mean-field level. However, they typically suffer from nonlinear scaling with the number of time steps. Conversely, methods that amount to equal-time limits of non-equilibrium Green's function methods — that is, methods that use reduced density matrices instead of Green's functions — have linear scaling with time, but they often suffer from instabilities related to the N-representability problem. In this talk, I will present a method to overcome these instabilities through an a posteriori purification of the reduced density matrices. I will present an algorithm that can restore a given set of N-representability conditions while maintaining contraction consistency between successive orders of reduced density matrices and preserving all conserved quantities. I will demonstrate how the purification algorithm outperforms previous algorithms in the context of the time-dependent two-particle reduced density matrix method applied to the quench dynamics of the Fermi-Hubbard model.