Title: Natural Orbitals Renormalization Group and Its Application

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Abstract: The quantum renormalization group (RG) procedure is one of the most important and accurate approaches for studying interacting many-electron correlated systems, upon which we propose a concept in the framework of natural orbitals so that we can generalize the RG into general orbital space, namely natural orbitals renormalization group (NORG). We show that for a quantum impurity model the NORG takes a polynomial (cubic power) rather than exponential computational cost in the number of electron bath sites to solve its low-energy states. Moreover, the NORG can work on a quantum impurity model with any lattice topological structure. Actually, the effectiveness of the NORG is basically irrespective of a model's topological structure. Thus, the NORG is naturally appropriate for studying quantum impurity model, especially with multi-orbital/site degrees. This makes the NORG be a natural impurity solver to dynamical mean field theory (DMFT). Recently we have accomplished the DFT+DMFT software package and applied it to study correlated materials.