QUEST: Quantum Electron Simulation Toolbox

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QUEST is a part of the SciDAC project on next generation multi-scale quantum simulation software for strongly correlated materials. It is a Fortran 90/95 package that implements the determinant quantum Monte Carlo (DQMC) method for simulation of magnetic, superconducting, and metal-insulator transitions in model Hamiltonians.

In this poster, we show that QUEST is able to treat lattices of unprecedentedly large sizes. This allows for accurate extraction of the interaction dependence of the antiferromagnetic order parameter (using finite-size scaling) so that one can map its evolution from the weak to the strong coupling Heisenberg limit. QUEST has been used to study the emergence of local phases in a trapped two-component Femi gas in an optimal lattice. It allows the treatment of temperatures that are comparable or lower than those presently achievable in experiments and large enough systems that both magnetic and paired phases can be detected by inspection of the behavior of suitable short-range correlations. In addition, QUEST has also been used to test the accuracy of the Parquet diagrammatic approximation, and to develop a method of comparable accuracy, which exhibits linear scaling Dynamical Mean Field Theory (DMFT).

We will also present a range of synergistic activities on the development of stable and robust numerical algorithms and hybrid granularity parallelization scheme that combines algorithmic and implementation techniques to high-performance DQMC simulation.