

Center for Quantum Science and Engineering (CQSE)

Weekly Seminar
Nov. 19, 2010 (Friday)

TIME Nov. 19, 14:30 ~ 15:30
TITLE QUEST: QUAntum Electron Simulation Toolbox
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PLACE Rm716, CCMS & New Physics Building, NTU

Abstract

Originated by Richard Scalettar and modernized later, QUAntum Electron Simulation Toolbox (QUEST) is a Fortran 90/95 package that implements the Determinant Quantum Monte Carlo (DQMC) methods for quantum electron simulations. QUEST possesses three features.

1. The performance of QUEST is improved by new algorithms, such as delayed update, and by modern numerical kernels, such as BLAS/LAPACK.
2. QUEST modularizes the frequently used kernels and integrates several simulations. Most simulations can be configured by parameters.
3. QUEST provides not only the programmed simulations, but a modularized toolbox that can be used and expanded for new simulations.

In this talk, I will introduce the physics model, numerical methods, and program structure of QUEST. Its applicability and limitations will be illustrated as well. Some published results that employed QUEST and future work will be mentioned if time permits.

