**QUEST: QuAntum Electron Simulation Toolbox**

(Par t of Project on Next Generation Multi-Scale Quantum Simulation Software for Strongly Correlated Materials)


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**Introduction**

- QUEST is a Fortran 90/95 package that implements the Determinant Quantum Monte Carlo (DQMC) method for quantum electron simulations.
- QUEST serves three purposes: (1) To improve simulation performance by using new algorithms, like delayed update, and by integrating modern numerical kernels. (2) To integrate existing programs by modularizing their computational components. (3) To assist new simulations development with, for example, the ability of creating new Hamiltonians.
- QUEST is a part of SciDAC project PETMAT for developing multi-scale many body codes, in which short length scales treated explicitly with DMC, intermediate length scales treated diagrammatically using vertices obtained from the QMC, long length scales treated in the mean field.
- The development of QUEST has been the key to study a new class of physical system: trapped fermionic atoms in optical lattices. These systems are characterized by the presence of a trapping potential that causes the system to become inhomogeneous and imposes the study clusters that would not have been manageable by legacy DQMC codes.

The 2-Dimensional Hubbard Model

QUEST allows the treatment of clusters of unprecedentedly large size. This allows for an accurate extraction of the interaction dependence of the antiferromagnetic order parameter (using finite-size scaling), so that one can map its evolution from the spin-liquid to the spin-Peierls limit. The lattice, provide improved resolution of the Green’s function in momentum space, that will allow a more quantitative comparison with time-of-flight optical lattice experiments.

**Evolution of the Momentum distribution**

- Color contour plot depiction of the momentum distribution $n(k)$ and its gradient, (a) and (b) : Left to right, $n(k)$ and its gradient at weak couplings. $W = 0, 0.25, 0.5$ and $1.6$, for fillings $n=0.23, 0.41, 0.61, 0.79$ and 1.0. (c) and (d) : same quantities at intermediate coupling $W=1$ and fillings $n=0.21, 0.41, 0.59, 0.79$ and 1.0. The increased breadth of the Fermi surface with interaction strength is evident. Calculations are performed on 24 by 24 clusters at temperature $T=8$. (Published: C.-R. Lee, C.-H. Lee, Z. Lin, S. Chiesa, M. Jarrell and R. T. Scalettar: Quantum Monte Carlo study of the two-dimensional Hubbard model. Phys. Rev. B 81 (2010) 16.)

**Parquet Approximation and QUEST**

QUEST has been used to test the accuracy of the Parquet approximation (PA). In the PA the fully irreducible vertex has been approximated by the bare interaction. Already at this level the PA performs significantly better than other diagrammatic approaches and we plan to further improve it by using the fully irreducible vertex computed in QUEST.

**Comparison of Green’s function**

- Single-particle Green function for a 4 by 4 Hubbard cluster and U=2 computed using three diagrammatic approaches and DMC at half-filling. For the temperature reported in the figure the PA result is very close to the DMC one as confirmed by self-consistent second-order perturbation theory and the Fluctuation-Exchange approximation.


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**Simulation of Ultracold Gases in a Trap**

We employed QUEST to study the emergence of local phases in a trapped two-component Fermi gas in an optical lattice. QUEST 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.

**Optimal interaction strength for the observation of strong correlation physics**

- The (A) density, (B) density fluctuations, (C) nearest-neighbor spin correlations, and (D) next-nearest-neighbor d-wave pairing are shown for interaction strengths $U = 4, 6, 1.8, 1, 10$ and $12$ at $T=0.5$ for 560 fermions. The inset of panel A is the double occupancy normalized by the number of particles, and the insets of panels B and C are the lattice averages of the local staggered magnetization and the d-wave pairing. An interaction strength of $U=3$ causes the largest enhancement in spin-correlation and produces regions with insipient superfluid order that surround the magnetic domain.

(Submitted: S. Chiesa, Christoph N. Varney, Marcus Rapol, Richard T. Scalettar: Magnitudes and pairing of two-dimensional trapped fermions. arXiv:0912.1921v1 [cond-mat].)

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**Cluster DMFT Solver with Linear Scaling in Inverse Temperature**

Dynamical Mean Field Theory (DMFT) is a powerful approach to study magnetism, superconductivity, and metal-insulator transitions in solids. The approach has traditionally relied on the Hirsch-Fye algorithm (HF-DMFT) that scales as the cube of the interacting temperature. We developed a method of comparable accuracy which exhibits linear scaling (see figure) using ideas from determinant Quantum Monte Carlo (DQMC).

**Performance improvement.** The CPU time required for updating and measuring in the Hirsch-Fye-QMC and DQMC algorithms versus the number of time slices on a 4 by 4 cluster. All other quantities are kept constant. The lines show power-law fits of the data. The diamond symbols show the CPU time in DQMC with a constant time step (decreasing temperature) where orthogonalization is performed to stabilize the matrix multiplications.


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**High Performance Computing**

- **Parallelization of the DQMC simulation.** We have been conducting a range of synergistic activities on the development of stable and robust linear algebra solvers specifically designed to greatly expand the length scales of the DQMC simulation in QUEST. For example, mathematically, we show that the numerical solution of the Green’s linear system of equations is weakly backward of a nearby Green’s linear system: $\dot{\Phi} = (1 + B_1 B_2 \ldots B_3)^{-1}$

- **Agreement of properties computed using DQMC**

- **High Performance Computing**

- **Parallel Markers chain for DQMC simulation**

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**Interdisciplinary Team Members**

**Physics and Material Science**

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