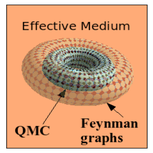
QUEST: QUantum Electron Simulation Toolbox

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

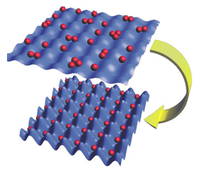
C.-R. Lee, S. Chiesa, E. Khatami, C.N. Varney, Z. Bai, E. D'Azevedo, M. Jarrell, Th. Maier, S. Savrasov, R. T. Scalettar, K. Tomko

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 lattice geometries.
- http://www.cs.ucdavis.edu/~bai/PETAMAT
- QUEST is a part of SciDAC project PETMAT for developing multi-scale many body codes, in which short length scales treated explicitly with QMC, intermediate length scales treated diagrammatically using vertices obtained from the QMC, long length scales treated in the mean field.

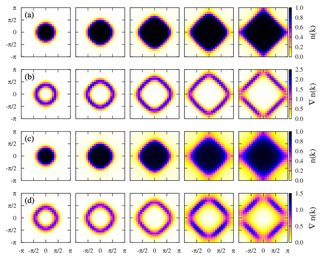


- The development of QUEST has been the key to study a new class of physical system: trapped fermionic atoms in optical lattices. These systems are characterized by the presence of a trapping potential that causes the system to become inhomogeneous and imposes the study clusters that would not have been 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 weak to the strong coupling Heisenberg limit. The lattices 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.



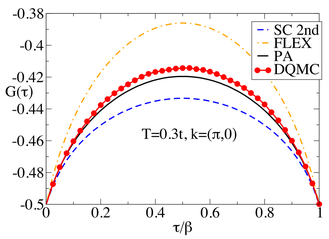
Evolution of the Momentum distribution . Color contour plot depiction of the momentum distribution n(k) and its gradient. (a) and (b) : Left to right, n(k) and its gradient at weak-coupling U=2t and fillings n=0.23, 0.41, 0.61, 0.79, and 1.0. (c) and (d) : same quantities at intermediate coupling U=4t 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=t/8.

Publication: C. N. Varney, C.-R. Lee, Z. Bai, S. Chiesa, M. Jarrell and R. T. Scalettar, ***Quantum Monte Carlo study of the two-dimensional fermion Hubbard model.*** *Phys. Rev. B. 80, 075116, (2009)*

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=2t computed using three diagrammatic approaches and DQMC at half-filling. For the temperature reported in the figure the PA result is very close to the DQMC one as compared to self-consistent second-order perturbation theory and to the FLuctuation-EXchange approximation.

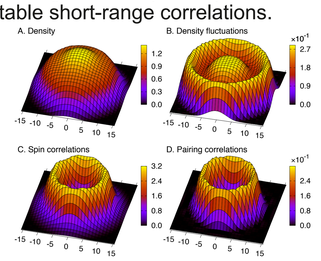


Publication: S. X. Yang, H. Fotso, J. Liu, T. A. Maier, K. Tomko, E. F. D'Azevedo, R. T. Scalettar, T. Pruschke, M. Jarrell, ***Parquet approximation for the 4x4 Hubbard cluster.*** *arXiv:0906.4736*

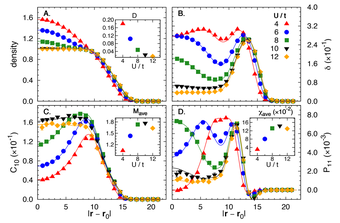
Simulation of Ultracold Gases in a Trap

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.

Emergence of strong correlation effects in the simulation of optical lattices. The system is confined by a harmonic potential that causes the density to vary and leads to the development of local phases. A Mott insulating domain is emerging in the density profile of panel A, in the form of a half-filled ring 6-10 lattice spacings from the trap center. The density fluctuations are minimized in this region while staggered magnetization and the d-wave pairing show a pronounced maximum.



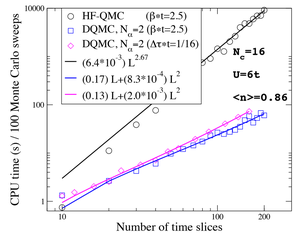
Optimal interaction strength for the observation of strong correlation physics. The (A) density, (B) density fluctuations, (C) nearest-neighbor spin correlations, and (D) next-nearest-neighbor d-wave pairing are shown for interaction strengths U = 4 t, 6 t, 8 t, 10 t and 12 t at T = 0.5 t, for 560 fermions.The 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 = 8t causes the largest enhancement in spin correlation and produces regions with incipient superfluid order that surround the magnetic domain.



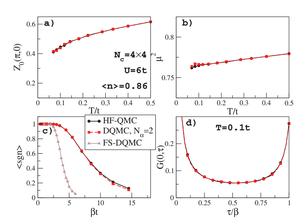
Publication: Simone Chiesa, Christopher N. Varney, Marcos Rigol, Richard T. Scalettar ***Magnetism and pairing of two-dimensional trapped fermions*** *arXiv:1004.0970, 2010*

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-QMC) that scales as the cube of the inverse temperature. We have developed a method of comparable accuracy which exhbits linear scaling (see figure) using ideas from determinant Quantum Monte Carlo (DQMC).



Performance improvemnent. 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.



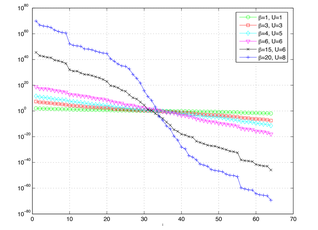
Agreement of properties computed using DQMC and Hirsch-Fye-QMC. a) the Matsubara frequency quasiparticle fraction versus temperature, b) the unscreened moment versus temperature, c) the average sign versus inverse temperature, d) the Green's function at a low temperature versus imaginary time. Panel c) includes the sign for a simulation where the cluster is not coupled with the infinite mean-field medium and shows how the coupling helps in reaching significantly lower temperatures.

Publication: E. Khatami, C. R. Lee, Z. J. Bai, R. T. Scalettar, and M. Jarrell. ***Cluster solver for dynamical mean field theory with linear scaling in inverse temperature.*** *Phys. Rev. E 81, 056703 (2010)*

Stable and Robust Matrix Algorithms

A critical computational kernel of the DQMC is to stably repeatedly compute the Green's function G, which involving a long chain of matrix multiplications and the inversion of matrices whose time-fluctuating entries incorporate energy scales and the block and sparsity structures reflect the multiple length scales. For example, an equal-time Green's function is of the form

$$G = (I + B_L B_{L-1} \dots B_2 B_1)^{-1}$$



Singular value distributions of Green's functions

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 x of the Green's linear system of equations is weakly backward of a nearby Green's linear system:

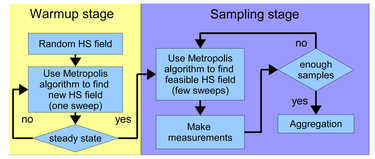
$$[I + (B_L + \Delta B_L)(B_{L-1} + \Delta B_{L-1}) \dots (B_1 + \Delta B_1)]\hat{x} = b$$

Publication: Z. Bai, C.-R. Lee, R.-C. Li and S. Xu, ***Stable solutions of linear systems involving long chain of matrix multiplications.*** *To appear in Linear Algebra and its Applications, 2010*

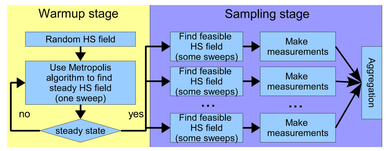
High Performance Computing

- Parallelization of the DQMC simulation is extremely challenging due to the serial nature of underlying Markov chain and numerical stability issues.
- We developed a hybrid granularity parallelization (HGP) scheme that combines algorithm and implementation techniques to explores the parallelism on different levels, such as parallel Markov chain and task decomposition, communication and computation overlapping, message compression and load balancing.
- Performance on an IBM Blue Gene/P system with 1014 computational processors have shown over a factor of 80 speedup.

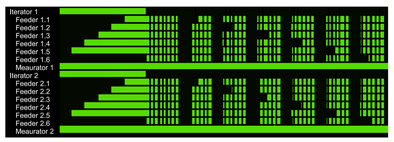
Sequential DQMC simulation

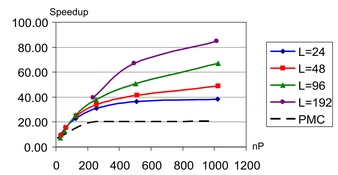


Parallel Markov chain for DQMC simulation



Communication patterns for iterators, feeders and M-servers:





Publication: C.-R. Lee, I-H. Chung, Z. Bai, ***Parallelization of DQMC Simulation for Strongly Correlated Electron Systems.*** *In Proceedings of 24th IEEE International Parallel and Distributed Processing Symposium (IPDPS 201). April 2010*

Interdisciplinary Team Members

Physics and Material Science
- Mark Jarrell, LSU
- Thomas Maier, ORNL
- Sergey Savrasov, UCD
- Richard Scalettar, UCD
- Chris Varney, Georgetown Univ.
- Simone Chiesa, UCD
- E. Khatami, Georgetown Univ.

Applied Math./Computer Science
- Zhaojun Bai, UCD
- Che-Rung Lee, NTHU, Taiwan
- Edward D'Azevedo, ORNL.
- Karen Tomko, Ohio Supercomputer Center

Office of Science U.S. DEPARTMENT OF ENERGY
SciDAC Scientific Discovery through Advanced Computing
LSU
UC DAVIS UNIVERSITY OF CALIFORNIA
OAK RIDGE NATIONAL LABORATORY