QUEST: QUantum Electron Simulation Toolbox

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Abstract. 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 paper, we show how QUEST is capable of treating lattices of unprecedentedly large sizes and how this can be fruitful in the study of the physics of trapped fermionic system, in the development of more efficient solvers for Dynamical Mean Field Theory (DMFT) and as a tool to test and, in the future, improve diagrammatic approaches such as the Parquet approximation. 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. The work reported here is a key step forward in achieving the goals of our SciDAC project.

1. Introduction

QUEST is a Fortran 90/95 package that implements the determinant quantum Monte Carlo (DQMC) method for the finite temperature simulation of system of fermions [1]. This method has two highly attractive features: a computational time that scales linearly with inverse temperature and a sign problem milder than that of other stochastic approaches. One of its numerical kernels, a long multiplicative chain of ill-conditioned matrices, is however numerically unstable and prevents a simple implementation of the method. However, thanks to a deeper understanding of the origin of these numerical problems, it has become possible to extend the domain of applicability of this method to systems containing several hundreds of fermions. At the software level, our development of QUEST serves then three purposes. (1) To improve simulation performance by using new algorithms, like delayed update, and

[10] Part of this work was completed while this author was a postdoctoral scholar at the Department of Computer Science, University of California, Davis.

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. At the application level, the use of QUEST has provided several important new insights into the physics of correlated quantum systems. QUEST has been used to treat lattices of unprecedentedly large sizes to allows us for accurate extraction of the interaction dependence of the antiferromagnetic order parameter (using finite-size scaling) to map its evolution from the weak to the strong coupling Heisenberg limit [8].

2. Simulation of confined strongly-interacting gases

The possibility of trapping rarefied atomic gases using magnetic fields and the ensuing possibility of studying their properties is one of the most active areas of research in atomic and condensed matter physics. The further use of standing electromagnetic waves causes the atoms to experience the presence of a periodic potential and allows the experimental realization of systems that are described by formally simple Hamiltonians. The interest in these systems relies on the fact that these same Hamiltonians have been studied in the condensed matter community for decades and, through simulations, helped understand many important materials properties. However, these Hamiltonians have resisted both an exact solution and robust numerical solution over the full parameter range of interest.

Optical lattices are then envisioned as simulators of these simple models, free of the limitation of numerical and analytical techniques. These experiments face, however, different challenges. Chief amongst them is the presence of the magnetic confining potential that causes the density to vary across the lattice, at odds with the homogeneous situation that one would like to emulate. In Ref.[3], we have employed QUEST to study the Hubbard model in the presence of a confining potential to address the effect of the latter on some selected short range properties and to investigate their evolution as a function of the interaction potential. The DQMC method allows the treatment of temperatures that are comparable or lower than those presently achievable in experiments, and QUEST can manage large enough systems that both magnetic and paired phases can be detected in the same simulation.

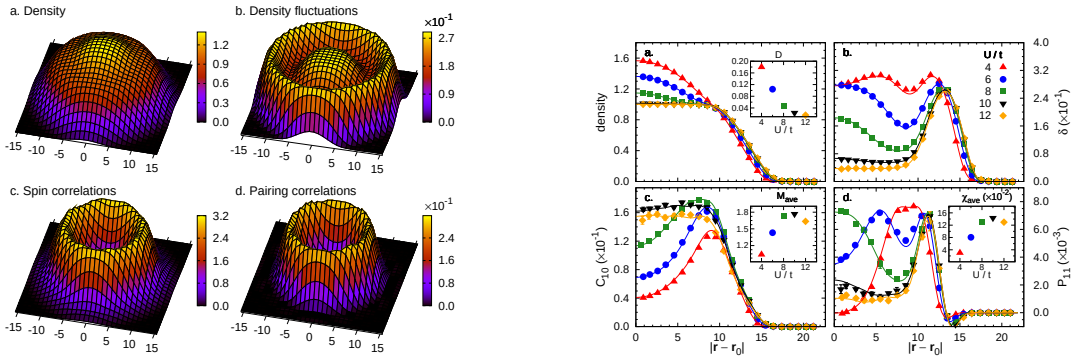

Figure 1. Properties of 560 fermions confined by an harmonic trap. $U/t = 6$ and $T/t \simeq 0.32$ (left) and evolution of properties as a function of U/t at $T/t \simeq 0.5$ (right).

The left of Figure 1 is the typical outcome of such a simulation. Panel (A) displays the density profile. Because of the presence of interaction, this profile shows a plateau when the density goes through one. This feature represents one of the most direct signatures of the presence of a Mott insulator phase. The origin of the plateau is easily explained considering that this phase is incompressible (an infinitesimal variation of the density costs a finite amount

of energy) and, as such, resistant to the density variation that would be naturally caused by the underlying trap. Panel (B) strengthens this observation by showing a dip in the density fluctuation in precise correspondence of the same region. Panel (C) and (D) are measures of magnetic and pairing order, both of which appear to peak in the same, half-filled region.

This last observation is a bit surprising since one would think that pairing correlations (intimately linked to superfluidity in fermionic systems) should appear away from the insulating regime. This is an entirely correct observation and points to the fact that a global measure of order, as that reported on the left of Figure 1, may not be appropriate at high temperature. The right of Figure 1 shows instead the nearest-neighbor correlation for spin and next-nearest-neighbor correlation for pairing (panel (C) and (D)). One can see that pairing is enhanced around the Mott insulator region as expected and in agreement with experiments done on the cuprate materials for which the Hubbard model is supposed to be qualitatively correct.

The right of Figure 1 reports the dependence on interaction strength of the same properties reported on the left of Figure 1 (with the modification for panel (C) and (D) detailed in the previous paragraph). Due to the kind of probes available in optical lattice experiments, it is of particular importance to determine the optimal interaction strength for the observation of magnetism and pairing. The right of Figure 1 makes clear that a value of $U/t = 8$ is optimal for the observation of anti-ferromagnetic correlations while pairing is, in this respect, more robust and can be "optimally" observed for any U/t larger than 8.

3. DMFT cluster 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 strongly correlated systems. It is a kind of mean-field theory where the fields, in contrast to ordinary static mean-field theory, depend on (imaginary) time and can describe quantum fluctuations. The DMFT approach finds a natural practical implementation in a quantum Monte Carlo algorithm due to Hirsch and Fye that allows the possibility of specifying the time dependence of the fields arbitrarily (albeit on a discrete grid). This method however scales as the cube of the inverse temperature and the question naturally arises on whether one can use DQMC, which scales linearly with inverse temperature, to address the same issues. The answer to this question is positive and in Ref.[7], we have developed a method of comparable accuracy which exhibits linear scaling in inverse temperature and which is entirely based on DQMC.

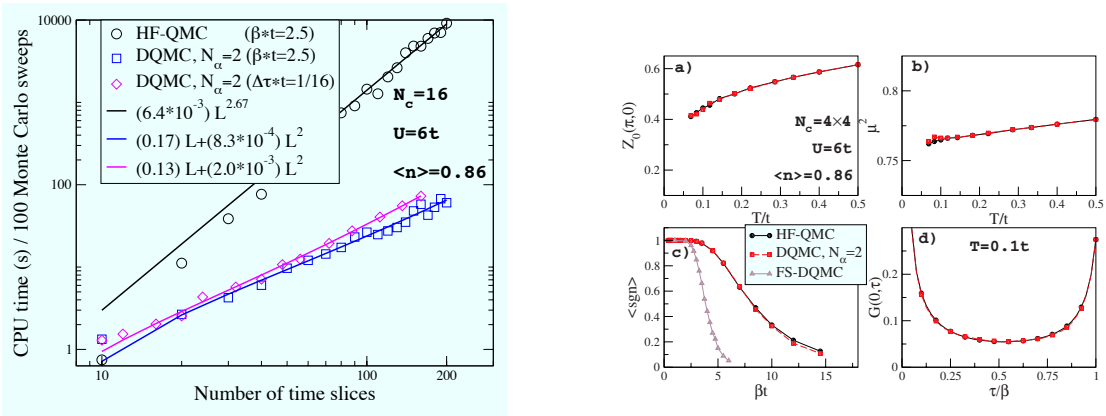

Figure 2. Comparison of CPU time for DQMC and HFQMC (left) and comparison of properties computed with DQMC and HFQMC (right). The agreement of the latter and the better performance makes DQMC an ideal solver for DMFT.

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 is shown in the left of Figure 2 for simulations with identical parameters. In DQMC one needs to "supplement" the cluster with additional sites where fermions can hop without interacting. The answer will of course depend on the number of supplementary sites (N_α) used although we have shown that an average of two supplementary sites per site of the original cluster is enough to obtain a converged answer.

The left of Figure 2 shows a clear improvement in performance: the scaling goes from cubic to linear and the prefactor is such that DQMC is always advantageous with respect to HFQMC even for the highest temperature. As an example of the comparable accuracy of the technique we also report a set of quantities computed in the right of Figure 2. As one can see there is no appreciable difference and both techniques outperform the canonical DQMC (without the bath of external fields) as far as the average sign is concerned. This last aspect has been crucial for the success of DMFT and it is a highly desirable result that this property is preserved by the DQMC solver.

4. Numerical solution of the Parquet equations

QUEST has also been used to test the accuracy of the Parquet approximation (PA). The PA is a conserving diagrammatic approach which is self-consistent at the one and two particle level. Given the exact, fully irreducible, interaction vertex the PA specifies a set of non-linear equation that suffices to determine the thermodynamic and transport property of the system. In Ref.[9], we have solved the PA approximating the fully irreducible vertex with the bare interaction and we used QUEST to check how the PA and other diagrammatic approaches compare for properties of a 4×4 Hubbard cluster where DQMC gives an essentially exact answer. We found that, already at this level, the PA performs significantly better than other diagrammatic approaches (see Figure 3). Since the PA becomes exact when the vertex is exact, we plan to further improve this approximation by using DQMC and QUEST as a way of obtaining a more accurate approximation for the fully irreducible vertex.

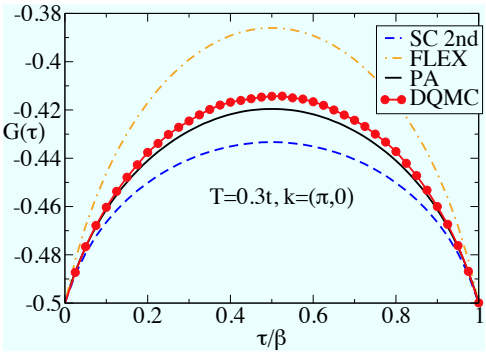

Figure 3. Comparison of the Green's function at $k = (0, \pi)$ with different diagrammatic approximation against the exact DQMC result.

5. Robust and stable matrix algorithms

A critical computational kernel of the DQMC is to stably repeatedly compute the Greens functions G_ℓ, which involving a long chain multiplication of matrices B_i and the explicit inversion. The time-fluctuating matrix entries of B_i incorporate energy scales and the block and sparsity structures reflect the multiple length scales. For example, an equal-time Greens function is of the form $G_\ell = (I + B_{\ell-1}B_{\ell-2}\cdots B_1 B_L B_{L-1}\cdots B_\ell)^{-1}$. Based on the previous

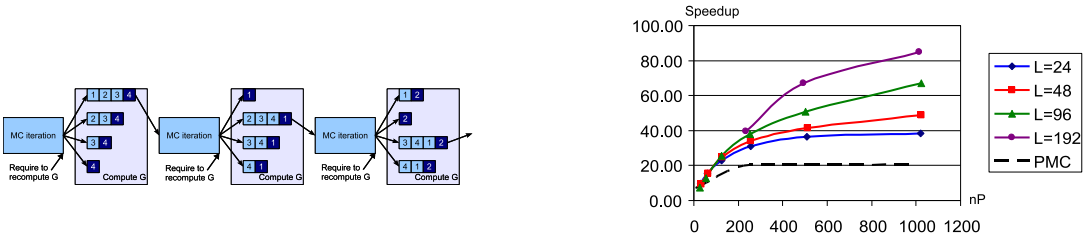

Figure 4. Parallel rolling feeder algorithm for computing Green's functions (left) and speedup for various L (right).

work of Loh Jr.*et al* [5, 6], we have conducted a range of synergistic efforts on the development and analysis of stable and robust linear algebra solvers specifically designed to greatly expand the length scales of the DQMC simulation in QUEST. For example, in [2], we show that the computed solution $\widehat{x}$ of the Greens linear system of equations $(I + B_L B_{L-1} \cdots B_1)x = b$ is *weakly backward* and satisfies a structurally nearby Greens linear system:

$$[I + (B_L + \Delta B_L)(B_{L-1} + \Delta B_{L-1}) \cdots (B_1 + \Delta B_1)]\,\widehat{x} = b.$$

where $\|\Delta B_i\| = O(\epsilon_{\mathrm{M}}\|B_i\|)$, ϵ_{M} is the machine precision.

6. Parallelization

Parallelization of the DQMC simulation is extremely challenging due to the serial nature of underlying Markov chain and numerical stability issues. In [4], we developed a hybrid granularity parallelization (HGP) scheme that combines algorithm and implementation techniques to explores the parallelism on different levels of DQMC simulation, such as parallel Markov chain method, task decomposition, communication and computation overlapping, message compression and load balancing. The left of Figure 4 shows the parallel rolling feeder algorithm for computing Green's functions G_ℓ for $\ell = 1, 2, \ldots, L$. Unlike the parallel scan method, the response time of compute G_ℓ by rolling feeder algorithm is independent of L. The right of Figure 4 shows the speedup for various L with equal-time measurements on an IBM Blue Gene/P system. As we can see that with 1024 computational processors, the parallel QUEST obtained a factor of 80 speedup.

Acknowledgement

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