UC Davis Final Report on DOE SciDAC project on "Next Generation of Multi-Scale Quantum Simulation Software for Strongly Correlated Materials"

DE-FC-02-06ER25793

Zhaojun Bai
Department of Computer Science
University of California, Davis
bai@cs.ucdavis.edu

Sergey Savrasov and Richard Scalettar
Department of Physics
University of California, Davis
savrasov@physics.ucdavis.edu
scalettar@physics.ucdavis.edu

Original version July, 2012, Revised July 2014

Contents

1 Introduction

This report summarizes the accomplishments of the University of California Davis team which is part of a larger SciDAC collaboration including Mark Jarrell of Louisiana State University, Karen Tomko of the Ohio Supercomputer Center, and Eduardo F. D'Azevedo and Thomas A. Maier of Oak Ridge National Laboratory. In this report, we focus on the major UCD accomplishments. As the paper authorship list emphasizes, much of our work is the result of a tightly integrated effort; hence this compendium of UCD efforts of necessity contains some overlap with the work at our partner institutions.

2 Major accomplishments and milestones

2.1 Software package and public availability

1. QUEST (Quantum Electron Simulation Toolbox), `http://quest.ucdavis.edu`, is a Fortran 90/95 package that implements the Determinant Quantum Monte Carlo method for simulation of magnetic, superconducting, and metal-insulator transitions in model Hamiltonians. The code is extensively documented, and complete downloading, installation, and release notes are provided, as well as sample input and output results. UCD and LSU investigators have developed a modification of QUEST which can serve as a cluster solver for DMFA, DCA and the MSMB calculations. This approach scales linearly in the inverse temperature rather than as the cube of the inverse temperature. The latter scaling is characteristic of all previous QMC embedded cluster solvers and was the primary computational bottleneck in most applications. QUEST had a very large impact on our project.

2. SE-LDA is a Fortran 90 based package of programs that implements electronic structure calculations using a combination of local density approximation (LDA) and externally given k- and frequency-dependent self-energy. It is based on the extension of the LDA code LMTART which implements linear muffin tin orbital (LMTO) method. The prototype of this code which includes the source files, the manual and some example files is available together with the user friendly interface MINDLab which runs under the Windows operating system and is designed specifically for students and non-experts in the field.

2.2 Research achievements

These codes have been extensively tested against problems whose solutions have already been established via other methodologies, or on smaller systems that existing computational approaches were previously capable of simulating. They have then been applied to several research areas to validate their ability to push forward the frontier of correlated electron physics.

1. QUEST was used to evaluate the interaction dependence of the antiferromagnetic order parameter and Fermi surface topology of the Hubbard model. This requires finite size scaling and momentum resolution which had been beyond the capability of existing DQMC codes.

2. The Parquet- and $\Gamma-$ based diagrammatic codes have been compared with the results of these QMC programs, and shown to reproduce the exact QMC at weak to intermediate couplings. They are now poised to be integrated with DQMC in our full multiscale technique.

3. The electronic and magnetic properties of the LaFeAsO superconductors have been extensively studied using dynamical mean field theory (DMFT) and a first principles linear response theory, adding important new insight into the superconductivity mechanism. The evaluation of the magnetic exchange interactions in this effort has provided important feedback into QMC work on these materials. Work has also begun on integrating our new cluster solver, which has much improved scaling in inverse temperature, and the diagrammatic codes, which should work well for these moderately correlated materials, into LDA+DMFT codes. This integration will allow the next step in exploring interaction effects in these materials.

2.3 UCD publications, awards, and invited talks

Seven publications describing these UCD SciDAC research accomplishments have appeared in refereed journals or refereed conference proceedings, including two in Physical Review Letters. An additional six manuscripts have been submitted for publication, and several more are in preparation. Significantly, a majority of these papers have authorship lists which include researchers at two or more of the institutions supported by this SciDAC grant. We also have several papers co-authored with members of another SciDAC team led by Giulia Galli, reflecting coordination of our efforts on multiscale many-body physics and their focus on quantum simulations of materials and nanostructures.

The UCD PIs, postdoctoral researchers and graduate students, have given 18 invited presentations decribing this project. These include talks at prominent international conferences in Italy, Germany, and China, as well as the March Meeting of the American Physical Society, the Aspen Institute for Physics, and the Kavli Institute for Theoretical Physics.

2.4 Connections to milestones

The majority of the UCD milestones in our original proposal have been accomplished. Of course, some modifications of our plans have emerged as work has progressed: We have addressed higher profile topics (both in code development and applications) as they emerged and the primary development location of some of the milestones has changed. Some of the frontier algorithmic development has proven very challenging. In our previous project progress reports we have described the limitations we have encountered in a few of the project goals and how we have adjusted our efforts to account for them.

Development of many-body codes was the central theme of our early UCD milestones. The SE-LDA and QUEST DQMC programs have been released to the web as open source software. The Parquet code has been released early, in the second year rather than the third. , and the Gamma based code will be released in the near future.

The DQMC multiscale effort is one area where we encountered significant obstacles. While the algorithm formally is linear in the number of particles N, that scaling is predicated on the assumption that the number of iterations involved in conjugate gradient computation of the matrix inverse on a vector does not grow with system size. Despite very significant efforts at constructing an efficient preconditioner, we were unable to achieve this goal. Fortunately, the computational improvements to QUEST (an order N^3 method) to a large extent eliminated the need for the linear scaling code. That is, we are able to achieve our targeted system sizes through dramatic improvements in QUEST despite its order N^3 scaling.

This progress with the QUEST DQMC code has allowed us to proceed with the software interface between DQMC and the parquet and Gamma codes, accomplishing the milestone earlier than

anticipated.

2.5 Development of human resources

At UC Davis, three postdoctoral researchers have worked with our SciDAC team. Dr. Cherung Lee has taken a position as an assistant professor in the Computer Science Department at the National TsingHua University, Taiwan. Dr. Nikolai Zarevich is a researcher in the Materials Science and Engineering Department at the University of Maryland. Dr. Andres Tomas has taken a position in Universidad Politécnica de Valencia, Spain.

Graduate student Ichitaro Yamazaki was supported by this grant. He graduated in September 2008. After finished his post-doctoral research at Lawrence Berkeley Lab working on the another SciDAC COMPASS project, he now is a research scientist at Innovative Computing Laboratory, University of Tennessee, Knoxville. Graduate student Chris Varney at UC Davis has also worked with this SciDAC project and finished his thesis in September 2009. He is now an assistant professor at University of West Florida.

2.6 Supercomputing time leverage

Over the course of the project, our team has successfully been awarded a large number of core hours for this project. At UC Davis, we mostly used the allocation at DOE NERSC ERCAP awards.

3 Detailed research and code development results

In this section we provide a detailed look at our specific UCD project accomplishments. The SciDAC supported individuals and institutions involved are indicated. Our SciDAC goals envisioned a multi-scale integration of Quantum Monte Carlo, diagrammatic, and mean field approaches to the many body correlated electron problem. We have completed the majority of our UCD milestones involving the development of robust foundational codes for each of these length scales, as well as made substantial initial progress towards their integration. We will not provide a comprehensive bibliography, but focus only on the SciDAC publications resulting from the UCD team's work.

3.1 Determinant quantum Monte Carlo code development and applications

A fundamental step in building a multi-scale many body approach is to extend current Quantum Monte Carlo (QMC) technologies to lattice sizes and temperatures which can be matched onto the diagrammatic approaches at the next length and energy scale. We have successfully achieved this objective, extending our QMC capability from order 10^2 to order 10^3 electrons. This is a necessary and crucial advance in building a multiscale many-body approach. We have also significantly generalized the lattice geometries and orbital structures which can be simulated, an important advance for applications.

More specifically, we have developed QUantum Electron Simulation Toolbox (QUEST), a Fortran 90/95 package that implements Determinant Quantum Monte Carlo (DQMC) methods. In the multi-scale quantum simulation scheme, this software provides a faster QMC cluster solver for short length scale simulations. In addition, it also serves as a verification tool for diagrammatic methods in certain intermediate length scale simulations, because larger simulations now can be made in a more affordable time. The benchmark problems have demonstrated that the sequential version is 7 to 8 times faster than the original QMC solver; and the current parallel QUEST has

a speedup of 15 compared to the sequential version. Thus, together, our code has more than two orders of magnitude performance improvement over earlier simulation codes.

Several efforts have made those improvements possible. Sequential QUEST optimizes the original QMC solver by using modern numerical libraries, BLAS/LAPACK, and by introducing new algorithms, such as delayed update and checkerboard methods. The parallel version accelerates the simulation both with coarse grain parallelization schemes that come naturally from the Monte Carlo method, and also fine grain parallelization techniques, which have better scalability with larger simulations. For example, the rolling feeder algorithm, which pipelines the calculation and delivers the result in turn, reduces the response time of Green's function calculation from $O(N^3L)$ to $O(N^3)$, where N is the number of sites and L is the number of time slices. QUEST is descibed in detail in the first publication listed in Sec. 4.1.

The new QUEST software, and its antecedents, has been applied to a number of initial projects. The next two papers in Sec. 4.1 used an early version, and hence studied lattice sizes not so different from past work. They were undertaken both because of their intrinsic interest and also to test the new code. The final project, explores systems of up to 600 electrons.

We first studied the 'dynamic Hubbard Hamiltonian' in which the usual static on-site Hubbard repulsion is generalized to an interaction form which can vary in time. It had been suggested that such a term would give rise to superconductivity at elevated temperatures, and also explain the particle-hole asymmetry present in the transition temperatures of the cuprates. This work is described in [Phys. Rev. B77, 014516 (2008)].

A second application was to a bilayer Hubbard model in which one layer is electron doped and one layer is hole doped. We showed that the Hamiltonian can be studied to lower temperatures than a single sheet, and exhibits an interesting signal of d-wave pairing. The results of our simulations bear resemblance to a recent report on the magnetic and superconducting properties of $Ba_2Ca_3Cu_4O_8F_2$ which contains both electron and hole doped CuO_2 planes. We also explored the phase diagram of bilayer models in which each sheet is at half-filling. The paper [Phys. Rev. B77, 144527 (2008)] describes our work.

A final application has been a high precision Quantum Monte Carlo study of the 2D fermion Hubbard Model at half-Filling. This work was motivated not only by traditional questions concerning magnetic properties and metal-insulator transitions in strongly correlated materials, but also by new work on ultracold atomic gases which offers the prospect of using "optical lattice emulators" for precise comparison of experimental and theoretical phase diagrams. The development of the QUEST code under this SciDAC grant has allowed us to get unprecedented momentum resolution from these Quantum Monte Carlo simulations which is vital for experimental comparisons. Figure 1 shows results for the Fermi surface contained in [Phy.Rev.B.075116,2009].

A second DQMC code-development project involved a new method for use as the cluster solver in Dynamical Mean Field Theory and its cluster extensions. These techniques provide a very useful approach to examining quantum phase transitions in model Hamiltonians, and, in combination with electronic structure theory, constitute powerful methods to treat strongly correlated materials. Their key advantage is that, unlike competing real space methods, the sign problem is well controlled in the Hirsch-Fye (HF) Quantum Monte Carlo used as an exact cluster solver. However, an important computational bottleneck remains; the HF method scales as the cube of the inverse temperature β. This often makes simulations at low temperature extremely challenging. We developed a new method based on DQMC which scales linearly in β, and demonstrated that the sign problem is identical to HF. Fig. 2 shows a two order of magnitude improvement of our new approach (squares) over the Hirsch-Fye impurity algorithm (circles). More complete results are presented in [Phys. Rev. E81, 056703 (2010)] We have especially high hopes for the usefulness

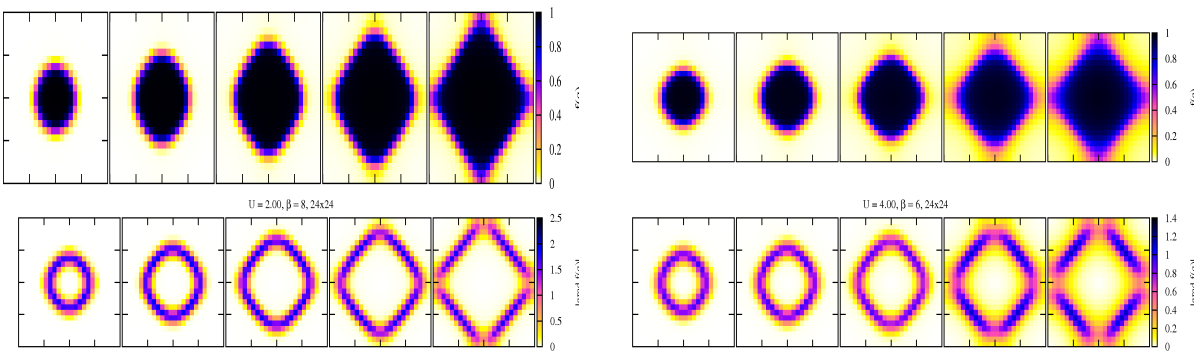

Figure 1: (color online). Color contour plot depiction of the Fermi function $n(\mathbf{k})$ and its gradient $\nabla n(\mathbf{k})$. Top panel, left to right, $n(\mathbf{k})$ at weak coupling $U = 2$ and fillings $\rho = 0.23, 0.41, 0.61, 0.79$, and 1.0. Second panel, $\nabla n(\mathbf{k})$ for the same parameters. Third and fourth panels, intermediate coupling $U = 4$. The increased breadth of the Fermi surface with interaction strength is evident. In all cases the lattice size $= 24 \times 24$ and the inverse temperature $\beta = 8$.

of this new code in integration with the LDA+MSMB approaches.

3.2 Dynamic cluster approximation and Parquet code development and application

This aspect of our SciDAC project has been led by the LSU, OSC, and ORNL teams and is extensively described in the Consolidated Project Report. The main UCD contribution was to provide DQMC data to validate the Parquet codes.

3.3 Applications to strongly correlated materials

We have being studying electronic properties of novel LaFeAsO family of superconductors which displays remarkably high temperature superconductivity with Tc up to 55 K. We found that its most energetically stable antiferromagnetic (AFM) phase is comprised of tetragonal-symmetry breaking alternating chains of aligned spins, there exists a deep pseudogap in the Fe 3d states centered at the Fermi energy arising from light carriers, and very strong magnetophonon coupling is uncovered. Doping (of either sign) results in heavy carriers per Fe with a large Fermi surface. With additional insight from a tight-binding representation, dynamical mean field theory, and linear response theory, we have extensively investigated the magnetic interactions of nine ferropnictides representing three different structural classes. The calculated magnetic interactions are found to be short range, and the nearest and next-nearest exchange constants follow the universal trend of J_{1a}=2J_2, despite their itinerant origin and extreme sensitivity to the z position of As. The calculated spin-wave dispersions show strong magnetic anisotropy in the Fe plane, in contrast to the cuprates. We also investigated electronic structure and magnetic properties of $Fe_{1+x}Te$ using first–principles density functional calculations. While the undoped FeTe has the same Fermi surface nested at (π,π) as in Fe arsenides, doping by 0.5 electrons reveals a novel square–type Fermi surface showing a strong (π, 0) nesting and leading to a different magnetic structure. Our result strongly supports the same mechanism of superconductivity in chalcogenides as in the arsenides, reconciling theory to existing experiments. Calculated magnetic interactions are found to be critically dependent on doping and notably different from the arsenides. This research is a collaboration between members of two

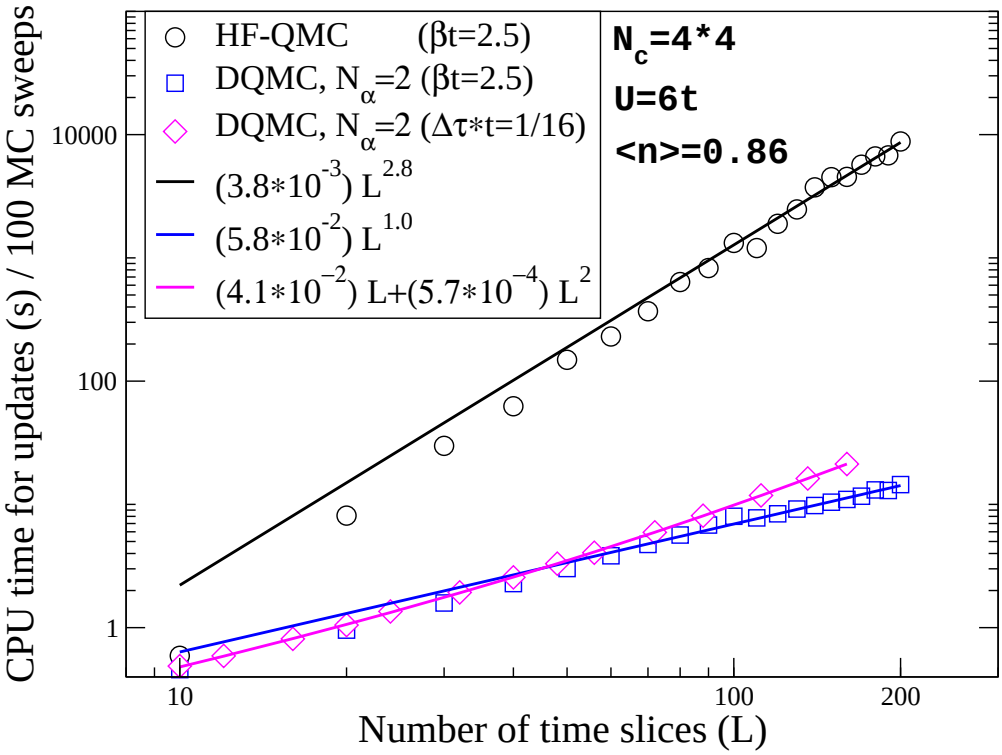

Figure 2: The CPU time required for the updating part of the HF-QMC and DQMC algorithms versus the number of time slices on a 4 x 4 cluster. All other quantities are kept constant. The solid lines show the power-law fits of the data. The diamond symbols show the CPU time in DQMC with a constant $\Delta\tau$ (changing temperature) where orthogonalization is performed to stabilize the matrix multiplications.

SCIDAC teams, Grants No. SE-FC02-06ER25793 and No. DEFC02-06ER25794. Two papers have been published in Physical Review Letters.

Using a first principles linear response approach, two members of our SciDAC team studied the magnetic exchange interactions J for a series of superconducting cuprates. We reproduced the observed spin-wave dispersions together with other experimental trends, and show that different cuprates have similar J's regardless of their T_c. The nearest neighbor J is not sensitive to the hole-doping, which agrees with recent experiments. For the undoped cuprates, the second nearest neighbor J is ferromagnetic, but changes its sign with hole-doping. We also find that, in contrast to the hopping integral, the exchange interaction is not sensitive to the position of apical oxygen. To see the effect of the long–range nature of the exchange on the superconducting T_c, we study the dynamical spin susceptibility $\chi(q,\omega)$ within the $t-J$ model using a dynamical cluster approximation.

We published the paper [1] on Weyl metal states and Fermi arcs in pyrochlore iridates which is receiveing many hits these days. In the paper, we propose a novel phase of matter, a topological semimetal, which is a three-dimensional analog of graphene with linearly dispersing excitations (see Fig. 6). This provides a condensed-matter realization of Weyl fermions of particle physics that

[1] Xiangang Wan, Ari Turner, Ashvin Vishwanath, Sergey Y. Savrasov Topological semimetal and Fermi-arc surface states in the electronic structure of pyrochlore iridates Physical Review B 83, 205101 (2011).

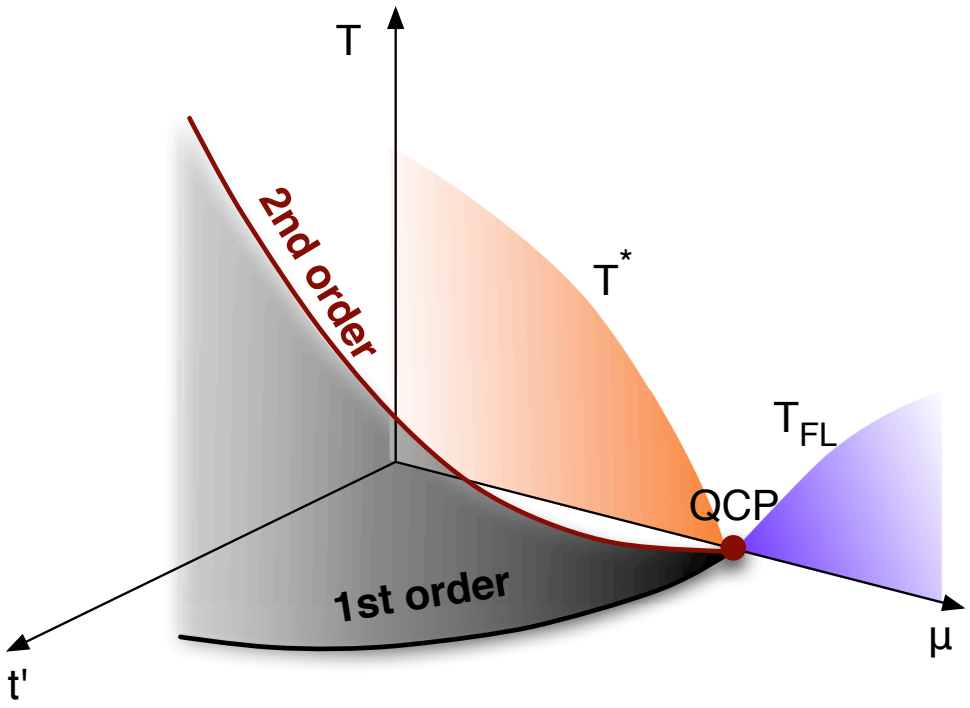

Figure 3: The journal reference is [Phy. Rev. B.81.201101 (2010)]. The figure shows the phase diagram of the Hubbard Hamiltonian, a model often used to describe strongly interacting material like high temperature superconductors, magnetic materials, and heavy fermions. The axes are temperature T, chemical potential mu (controls electron density) and next nearest neighbor hopping t'. When t'=0 there is a Pseudogap (PG) phase separated from a Fermi Liquid (FL) phase by a Quantum Critical Point. What we showed was that this QCP appears at the end of a line of transition points havingto do with phase separation which extend out when t' is made non-zero.

obeys a two-component Dirac equation. It emerges from the interplay of electron correlations and strong spin-orbit interactions and we argue that it may be realized in a class of pyrochlore iridates (such as Y2Ir2O7) based on the large-scale computer simulations using electronic structure based LDA+U method. The paper was ranked as the most cited Physical Review B article for the year 2011.

This state exhibits remarkable topological properties manifested by surface states in the form of Fermi arcs, which are impossible to realize in purely two-dimensional band structures (see Fig. 7). Fermi arcs have appeared before in experimental studies of high-temperature cuprate superconductors. However, in that context they are driven by correlations which open pseudogaps at some Fermi surface momenta. Otherwise they would be prohibited by topology since the Fermi surface is by definition the boundary between occupied and unoccupied states, and if it terminates then one could go "around" the termination point and smoothly change from one to another, which is impossible at zero temperature. At a surface, this paradox is avoided because the surface states may unbind into the bulk when going around the end of a Fermi arc.

Let me know if you want me to elaborate more on this and whether you need more pictures for the highlight.

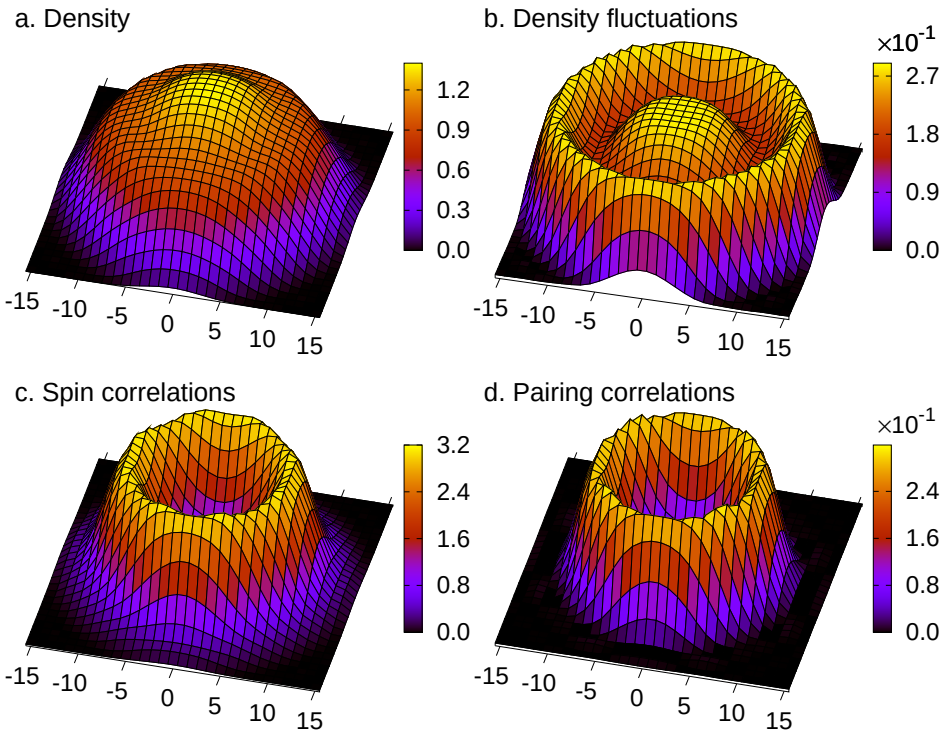

Figure 4: Journal reference [Phys. Rev. Lett. 106, 035301 (2011)]. The figure shows various properties of a cloud of trapped fermions as one moves away from the cloud center. Panel [a] is the density. Panel [b] are the density fluctuations- the ring of depressed values is a signature of a Mott insulating region. Panel [c] shows that spin correlations are large in the Mott region. Panel [d] shows the region of enhanced superconducting order.

3.4 Coordination with supercomputer initiatives

Access to supercomputer time has been critical for the success of this project, where single runs of the Parquet solver for problem sizes of interest (Nt=6400) are projected to consume 800,000 core hours, and Quantum Monte Carlo simulations on very large lattices can be equally time consuming. During the first half of this project we have submitted several large computer allocation requests as listed below. As a result of these requests we have secured 17.4 million core hours for this project. We list here all the time allocated by the entire SciDAC team, since in general these resources are shared across institutions. These include:

1. Early Access allocation for Science-at-scale, DOE NCCS, Jaguar XT5 system, 15,000,000 core hours, 12/31/2008, Mark Jarrell (PI).

2. Discovory Grant, Ohio Supercomputer Center, Glenn Opteron Cluster, 100,000 RUs (1,000,000 core hours), 01/30/2008, Mark Jarrell (PI).

3. Louisiana Optical network Initiative, Queenbee Dell Xeon cluster, 1,000,000 core hours, 09/01/2008, J. Moreno (PI)

4. ERCAP Request, DOE NERSC, Franklin Cray XT4 system, 400,000 core hours, 12/12/08, Mark Jarrell (PI).

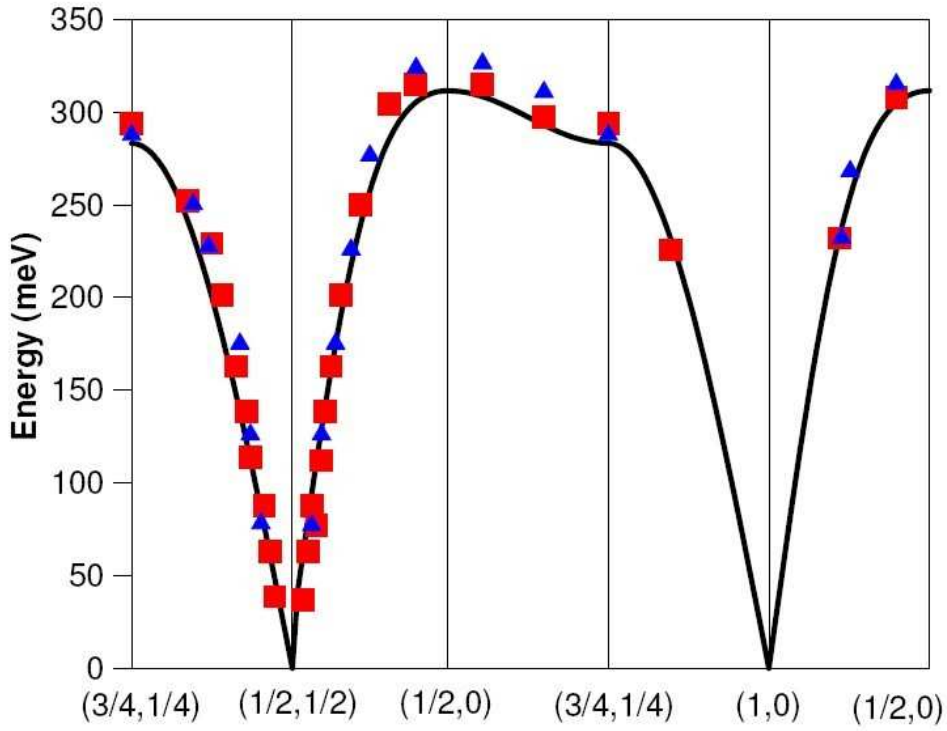

Figure 5: Comparison between calculated (solid lines) and experimental (symbols) spin-wave dispersions for La2CuO4. The triangles and squares are the experimential results.

5. ERCAP request, 50,000 Cray XT4-equivalent MPP hours, 12//08–present, Z. Bai (PI).

4 UCD publications

Here we list papers and presentations involving UCD team members. Many of the manuscripts are co-authored with our SciDAC collaborators at other institutions.

1. "Robust and Efficient Numerical Linear Algebra Solvers and Applications in Quantum Mechanical Simulations," Z. Bai, W. Chen, R. Scalettar, and I. Yamazaki, Proceedings of the 4th International Congress of Chinese Mathematician (ICCM), Edited by L. Ji, K. Liu, L. Yang, S.-T. Yau, Vol.III, pp.253–268, Higher Education Press, 2007.

2. "Sign change of the extended s-wave pairing vertex in the dynamic Hubbard model: A quantum Monte Carlo study," K. Bouadim, M. Enjalran, F. Hébert, G.G. Batrouni, and R.T. Scalettar, Phys. Rev. B77, 014516 (2008).

3. "Superfluid and Mott Insulator Phases of one dimensional Bose-Fermi Mixtures", A. Zujev, A. Baldwin, R.T. Scalettar, V.G. Rousseau, P.J.H. Denteneer, and M. Rigol, Phys. Rev. A78, 033619 (2008)

4. "Magnetic and transport properties of a coupled Hubbard bilayer with electron and hole doping," K. Bouadim, G.G. Batrouni, F. Hébert, and R.T. Scalettar, Phys. Rev. B77,

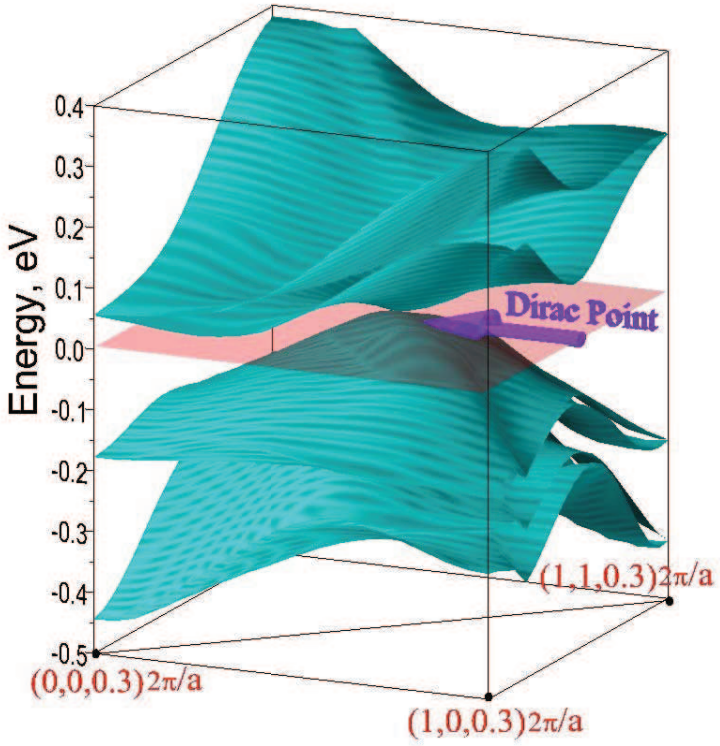

Figure 6: A topological semimental, a three-dimensional analog of graphene with linearly dispersing excitations.

144527 (2008).

5. "Electron-Hole Symmetry and Magnetic Coupling in Antiferromagnetic LaFeAsO," Z. P. Yin, S. Lebegue, M. J. Han, B. P. Neal, S.Y. Savrasov, and W.E. Pickett, Phys. Rev. Lett. 101, 047001 (2008).

6. "Anisotropy, Itineracy, and Magnetic Frustration in High-TC Iron Pnictides," M. J. Han, Q. Yin, W. E. Pickett, and S. Y. Savrasov, Phys. Rev. Lett. 102, 107003 (2009).

7. "Calculated Magnetic Exchange Interactions in High-Temperature Superconductors," X. Wan, T. A. Maier, S. Y. Savrasov, Phys. Rev. B79, 155114 (2009).

8. "Doping Driven (π, 0) Nesting and Magnetic Properties of $Fe_{1+x}Te$ Superconductors," M. J. Han and S. Y. Savrasov, Phys. Rev. Lett. 103, 067001 (2009).

9. "Quantum Monte Carlo Study of the Two-dimensional Fermion Hubbard Model", C.N. Varney, C.R. Lee, Z.J. Bai, S. Chiesa, M. Jarrell, and R. T. Scalettar, Phys. Rev. B80, 075116 (2009).

10. "Cluster Solver for Dynamical Mean Field Theory with Linear Scaling in Inverse Temperature", E. Khatami, C.R. Lee, Z.J. Bai, R.T. Scalettar, and M. Jarrell, Phys. Rev. E81, 056703 (2010).

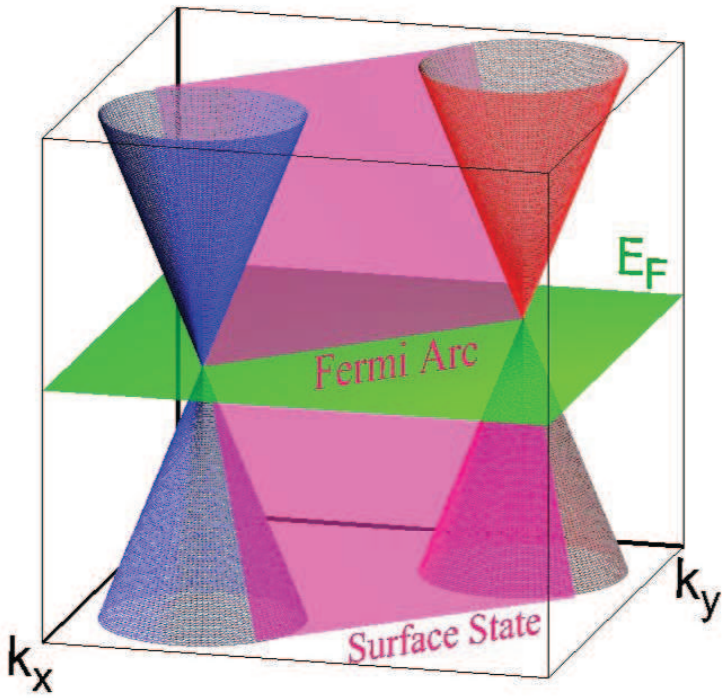

Figure 7: Topological properties manifested by surface states in the form of Fermi arcs, which are impossible to realize in purely two-dimensional band structures

11. "Parallelization of Determinant Quantum Monte Carlo Simulation of Strongly Correlated Electron Systems", R.-C. Lee, I.H. Chung, Z. Bai, in the Proceedings of 24th IEEE International Parallel and Distributed Processing Symposium (IPDPS 2010), Atlanta, USA, April 2010.

12. "A high-quality preconditioning technique for multi-length-scale symmetric positive definite linear systems," I. Yamazaki, Z. Bai, W. Chen and R. Scalettar, Numer. Math. Theor. Meth. Appl. Vol.2, No.4, pp.469-484, 2009.

13. "Sign change of the extended s-wave pairing vertex in the dynamic Hubbard model: A quantum Monte Carlo study," K. Bouadim, M. Enjalran, F. Hébert, G.G. Batrouni, and R.T. Scalettar, Phys. Rev. B77, 014516 (2008).

14. "Superfluid and Mott Insulator Phases of one dimensional Bose-Fermi Mixtures", A. Zujev, A. Baldwin, R.T. Scalettar, V.G. Rousseau, P.J.H. Denteneer, and M. Rigol, Phys. Rev. A78, 033619 (2008).

15. "Magnetic and transport properties of a coupled Hubbard bilayer with electron and hole doping," K. Bouadim, G.G. Batrouni, F. Hébert, and R.T. Scalettar, Phys. Rev. B77, 144527 (2008).

16. "A High Quality Preconditioning Technique for Multi-Length-Scale Symmetric Positive Definite Linear Systems", I. Yamazaki, Z. Bai, W. Chen, and R. Scalettar, Numerical Mathematics: Theory, Methods and Applications 2, 469 (2009).

17. "High Precision Quantum Monte Carlo Study of the 2D Fermion Hubbard Model at Half-Filling", C.N. Varney, C.R. Lee, Z.J. Bai, S. Chiesa, M. Jarrell, and R. T. Scalettar, Phys. Rev. B80, 075116 (2009).

18. "Dynamical Mean Field Theory Cluster Solver with Linear Scaling in Inverse Temperature", E. Khatami, C.R. Lee, Z.J. Bai, R.T. Scalettar, and M. Jarrell, Phys. Rev. E81, 056703 (2009).

19. "Parquet approximation for the 4x4 Hubbard cluster," S. X. Yang, H. Fotso, J. Liu, T. A. Maier, K. Tomko, E. F. D'Azevedo, R. T. Scalettar, T. Pruschke, and M. Jarrell, Phys. Rev. E80, 046706 (2009).

20. "The screening of $4f$ moments and delocalization in the compressed light rare earths", A.K. McMahan, R.T. Scalettar, and M. Jarrell, Phys. Rev. B80, 235105 (2009).

21. "Effect of strong correlations on the high energy anomaly in hole- and electron-doped high-T_c superconductors," B. Moritz, F. Schmitt, W. Meevasana, S. Johnston, E.M. Motoyama, M. Greven, D.H. Lu, C. Kim, R.T. Scalettar, Z.-X. Shen, and T.P. Devereaux, New J. Physics 11 093020 (2009).

22. "Quantum Criticality Due to Incipient Phase Separation in the 2D Hubbard Model," E. Khatami, K. Mikelsons, D. Galanakis, A. Macridin, J. Moreno, R.T. Scalettar, and M. Jarrell, Phys. Rev. B81, 201101 (2010).

23. "Magnetism and pairing of two-dimensional trapped fermions," Simone Chiesa, Richard T. Scalettar, Christopher N. Varney and Marcos Rigol, Phys. Rev. Lett. 106, 035301 (2011).

24. "The response to dynamical modulation of the optical lattice for fermions in the Hubbard model," Z. Xu, S. Chiesa, S. Yang, S-Q. Su, D.E. Sheehy, J. Moreno, R.T. Scalettar, and M. Jarrell, Phys. Rev. A84, 021607 (2011).

25. "Magnetism and pairing of two-dimensional trapped fermions," Simone Chiesa, Richard T. Scalettar, Christopher N. Varney and Marcos Rigol, Phys. Rev. Lett. 106, 035301 (2011).

26. "Redesign of higher-level matrix algorithms for multicore and hybrid architectures and applications in quantum Monte Carlo simulation", R.-C. Lee and Z. Bai, in Proceedings of 25th IEEE International Parallel and Distributed Processing Symposium (IPDPS 2011)

27. "Advancing large scale many-body QMC simulations on GPU accelerated multicore systems", A. Tomas, C.-C. Chang, R. Scalettar and Z. Bai, in Proceedings of 26th IEEE International Parallel and Distributed Processing Symposium (IPDPS 2012)

28. "Optimized Confinement of Fermions in Two Dimensions," J.D. Cone, S. Chiesa, V.R. Rousseau, G.G. Batrouni, and R.T. Scalettar, Phys. Rev. B85, 075418 (2012).

29. "Phase Stability in the Two dimensional Anisotropic Boson Hubbard Hamiltonian", T. Ying, G.G. Batrouni, V.G. Rousseau, M. Jarrell, J. Moreno, X.D. Sun, and R.T. Scalettar, Phys. Rev. B87, 195142 (2013).

30. "Electronic structure and magnetic properties of NaOsO3," Yongping Du, Xiangang Wan, Li Sheng, Jinming Dong, and Sergey Y. Savrasov, Phys. Rev. B85, 174424 (2012).

31. "Ferroelectricity induced by interatomic magnetic exchange interaction," Xiangang Wan, Hang-Chen Ding, Sergey Y. Savrasov, Chun-Gang Duan, arXiv:1202.3381. presented at APS March Meeting, March 19, 2013

32. "Exchange constants and spin waves of the orbital ordered, non-collinear spinel MnV_2O_4," R. Nanguneri, S. Y. Savrasov, Phys. Rev. B86, 085138 (2012).

33. "Computational Design of Axion Insulators Based on 5d Spinels Compounds" Xiangang Wan, Ashvin Vishwanath, Sergey Y. Savrasov, Phys. Rev Lett. 108, 146601 (2012).

34. "Topological semimetal and Fermi-arc surface states in the electronic structure of pyrochlore iridates," Xiangang Wan, Ari Turner, Ashvin Vishwanath, Sergey Y. Savrasov, Physical Review B83, 205101 (2011).

35. "Self consistent GW determination of the interaction strength: application to the iron arsenide superconductors," A. Kutepov, K. Haule, S.Y. Savrasov, G. Kotliar, Phys. Rev. B82, 045105 (2010).

36. "First Principle Simulations of Heavy Fermion Cerium Compounds Based on the Kondo Lattice," Munehisa Matsumoto, Myung Joon Han, Junya Otsuki, Sergey Y. Savrasov, Phys. Rev. Lett. 103, 096403 (2009).

37. "Doping Driven (pi, 0) Nesting and Magnetic Properties in Iron Chalcogenide Superconductors," Myung Joon Han, Sergey Y. Savrasov, Phys. Rev. Lett. 103, 067001 (2009).

38. "Anisotropy, Itineracy, and Magnetic Frustration in High-TC Iron Pnictides," Myung Joon Han, Quan Yin, Warren E. Pickett, and Sergey Y. Savrasov, Phys. Rev. Lett. 102, 107003 (2009).

39. "Calculated Magnetic Exchange Interactions in High-Temeprature Superconductors," Xiangang Wan, Thomas A. Maier, Sergej Y. Savrasov Phys. Rev. B79, 155114 (2009).

40. "Topological semimetal and Fermi-arc surface states in the electronic structure of pyrochlore iridates" Xiangang Wan, Ari Turner, Ashvin Vishwanath, Sergey Y. Savrasov Phys. Rev. B83, 205101 (2011).