Sandeep Pathak, PhD

Contact Information

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Employment

Louisiana State University, Baton Rouge, LA

PostDoc Fellow, Department of Physics & Astronomy, Aug 2010-Present

- Research Focus: *Quantum Criticality in the Hubbard model, Multi-scale Many Body Approach*
- Advisors: Prof. Mark Jarrell & Prof. Juana Moreno

Education

Indian Institute of Science, Bangalore, India

PhD, Materials Research Centre, 2006-2010

- Thesis Topic: *Ground State Studies of Strongly Correlated 2D Systems*

M.S., Materials Research Centre , 2004-2006

Indian Institute of Technology, Kanpur, India

B.Tech., Mechanical Engineering, 2000-2004

Research Interests

Unconventional Superconductivity
Quantum Criticality
Cold Atoms Physics
Metal-Insulator Transition
Computational Methods for Strongly Correlated Systems

Research Skills

- *Techniques of quantum condensed matter physics*: diagrammatic perturbation theory, two-particle field theories (e.g. Dual Fermions method, Parquet formalism), renormalization group, slave particle mean field theories.
- *Computational techniques*: Dynamical Mean Field Theory, Dynamical Cluster Approximation, Variational Monte Carlo, Molecular Dynamics.
- *High Performance Computing*: Experience in Large scale code development on parallel platforms. Currently, I am leading a GPU (Graphical Processing Unit) team to develop an efficient Variational Monte Carlo (VMC) code.

Grants & Supports

July 2011 - July 2012, *"Simulations of Strongly Correlated Systems"*, PI: J. Moreno, Co-PIs: H. Fotso, M. Jarrell, **S. Pathak**, V. Rousseau, D. E. Sheehy, K.-M. Tam, S. Yang, Z. Bai, C.-C. Chang, S. Chiesa, R. Scalettar, A. Tomas, K. Tomko, D. Galanakis and F. F. Assaad, 10 million SUs (service units) in Kraken and 1.2 million SUs in Trestles at the Teragrid funded by the National Science Foundation.

Publications

Peer Reviewed

1. S. Y. Chang, **S. Pathak** and N. Trivedi, Repulsive fermions in optical lattices: Phase separation versus coexistence of antiferromagnetism and d-wave superfluidity, *Physical Review A*, **85**, 013625 (2012)

2. K.-S. Chen, **S. Pathak**, S.-X. Yang, S.-Q. Su, D. Galanakis, K. Mikelsons, M. Jarrell and J. Moreno, Role of the van Hove Singularity in the Quantum Criticality of the Hubbard Model, *Physical Review B*, **84**, 245107 (2011)

3. **S. Pathak**, V. B. Shenoy and G. Baskaran, Possible high-temperature superconducting state with a $d + id$ pairing symmetry in doped graphene, *Physical Review B*, **81**, 085431 (2010)

4. **S. Pathak**, V. B. Shenoy, M. Randeria and N. Trivedi, Competition between antiferromagnetic and superconducting states, electron-hole doping asymmetry, and Fermi Surface topology in high temperature superconductors, *Physical Review Letters*, **102**, 027002 (2009)

5. **S. Pathak** and V. B. Shenoy, Size Dependence of Thermal Expansion of Nanostructures, *Physical Review B*, **72**, (2005), 113404

Submitted/To be submitted

6. **S. Pathak**, S.-X. Yang, Z.Y. Meng, M. Jarrell and J. Moreno, Application of the Dual Fermion-Dynamical Cluster Approach to the Falicov-Kimball Model (Under Preparation)

7. Z.Y. Meng, S.-X. Yang, **S. Pathak**, H. Terletska, J. Moreno and M. Jarrell, Dynamical mean-field embedding of the dual fermion dynamical cluster approach for strongly correlated systems (Under Preparation)

8. **S. Pathak** and V. B. Shenoy, A General Variational Approach to Strongly Correlated Spin Singlet States (Under Preparation)

9. **S. Pathak**, V. B. Shenoy and H. R. Krishnamurthy, *"Modeling of carbon nanotube FETs"*, (Preprint)

Book Chapters

10. H. Fotso, S. Yang, K. Chen, **S. Pathak**, J. Moreno, M. Jarrell, K. Mikelsons, E. Khatami and D. Galanakis, Dynamical Cluster Approximation in *Theoretical Methods for Strongly Correlated Systems*, edited by A. Avella and F. Mancini (Springer Series in Solid-State Sciences, 171, 2011)

Conference/Symposium Proceedings

1. C.W. Moore, D.Z. Poliakoff, J. Caprino, S. Abu Asal, K.R. Rajagopalan, S.-X. Yang, E.C. Ekuma, S. Feng, Y. Fang, K.-M. Tam, **S. Pathak**, B. Thakur, K. Tomko, J. Moreno, R. Hall and M. Jarrell, GP-GPU Computing: Massively Parallel Accelerated Science, *Proceedings of Louisiana EPSCoR RII LA-SiGMA 2011 Symposium*, p.57

Talks

1. *"Role of the van Hove Singularity in the Quantum Criticality of the Hubbard model"* at the Department of Physics, Northeastern University (Boston, MA) (June 22, 2011)

2. *"Repulsive Fermions in the Optical Lattices: Phase separation or Coexistence of Antiferromagnetism and d-Superfluidity?"* at *APS March Meeting 2011* at Dallas, TX (March 21-25, 2011) URL

3. *"Role of the van Hove Singularity in the Quantum Criticality of the Hubbard model"* at *APS March Meeting 2011* at Dallas, TX (March 21-25, 2011) URL

4. *"Transport Properties near Quantum Critical Point in 2D Hubbard Model"* at *APS March Meeting 2011* at Dallas, TX (March 21-25, 2011) URL

5. *"Competition between antiferromagnetism and superconductivity, electron-hole doping asymmetry and Fermi Surface topology in cuprates"* at *APS March Meeting 2009* at Pittsburgh, PA (March 16-20, 2009) URL

6. *"Ground State Studies of Strongly Correlated Superconductors"* at The Institute of Mathematical Sciences (IMSc) (Chennai, India) (Aug 14, 2008)

Posters

1. "*Variational Monte Carlo on GPGPU*" in the *LA-SiGMA All Hands Meeting*, Baton Rouge, LA (Aug 05, 2011). URL

2. "*Competition between antiferromagnetic and superconducting states, electron-hole doping asymmetry, and "Fermi Surface" topology in high temperature superconductors*" in the conference *Recent Progress in Many Body Theories* at the Ohio State University, Columbus, OH (July 27-31, 2009). URL

Awards & Honors

- Selected for *India-U.S. Student Visitation Program 2009* awarded by Indo-U.S. Science and Technology Forum (IUSSTF) & American Physical Society (APS). Visited the department of Physics at Ohio State University under the program.

- Graduate assistantship, Indian Institute of Science, Bangalore, India, 2006-2010

Journal Refereed

Pramana

Academic Experience

Louisiana State University, Baton Rouge, LA

- (2010 - Present) Mentoring a GPU team consisting of three graduate students, Niladri Sengupta, Sameer Abu Asal and Kaushik Rajagopalan developing an efficient Variational Monte Carlo (VMC) code.

- (Jun 2011 - Aug 2011) Mentored an undergraduate student, Sharae Williams under *Research Experiences for Undergraduates* (REU) program.

- (2010 - 2011) Mentored a graduate student, K.-S. Chen.

Indian Institute of Science, Bangalore, India

Teaching Assistant **(Aug 2005 to Dec 2005)**

- *Concepts in Materials Science*.
- Instructor: Prof. Vijay B. Shenoy

Teaching Assistant **(Jan 2008 to May 2008)**

- *Quantum Statistical Field Theory*.
- Instructor: Prof. Vijay B. Shenoy

Teaching Assistant **(Aug 2008 to Dec 2008)**

- *Advanced Condensed Matter Theory*
- Instructor: Prof. Chandan Dasgupta

Outreach Activities

Participated in *NanoDays* at Louisiana Arts and Science Museum on April 02, 2011. NanoDays is a nationwide festival celebrating the science of ultra small matter. LA-SiGMA (Louisiana Alliance for Simulation-Guided Materials Applications) faculty members gave lectures and graduate students led demonstrations to 288 guests at the Louisiana Arts and Science Museum.

References

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2. **Prof. Juana Moreno**
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3. **Prof. Vijay B. Shenoy**
   Centre for Condensed Matter Theory
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4. **Prof. G. Baskaran**
   Perimeter Institute for Theoretical Physics
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5. **Prof. H. R. Krishnamurthy**
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Detailed Research Statement

Sandeep Pathak (spathak@phys.lsu.edu)

My research interests lie in the area of theoretical condensed matter physics, particularly in strongly correlated electrons. In what follows, I describe some of my research accomplishments, as well as future research plans. I am not strictly restricted to the areas of my present study but also keen to work in other research areas such as *Topological Insulators, Spin Liquids, Graphene*, etc.

1 Present Research

1.1 Role of the van Hove singularity in the Quantum Criticality of the Hubbard model

A quantum critical point (QCP), separating the non-Fermi liquid region from the Fermi liquid, exists in the phase diagram of the 2D Hubbard model (Phys. Rev. Lett. 102, 206407 (2009)). Near the QCP, the real part of the bare d-wave particle-particle susceptibility, χ'_{0d} exhibits algebraic divergence with decreasing temperature, replacing the logarithmic divergence found in a Fermi liquid (Phys. Rev. Lett. 106, 047004 (2011)). Also, a van Hove singularity (vHS) in the single particle dispersion crosses the Fermi level near the quantum critical filling. We explore the role played by this crossing in the quantum criticality of the Hubbard model.

In this project, my major contribution was to perform analytical calculations along with a graduate student, K.-S. Chen who performed Quantum Monte Carlo simulations. We found that non-interacting models with vHS at Fermi level cannot completely describe the critical algebraic behavior of χ'_{0d}. We also found that a negative next-near-neighbor hopping t' increases the doping region with marginal Fermi liquid character by studying the transport properties.

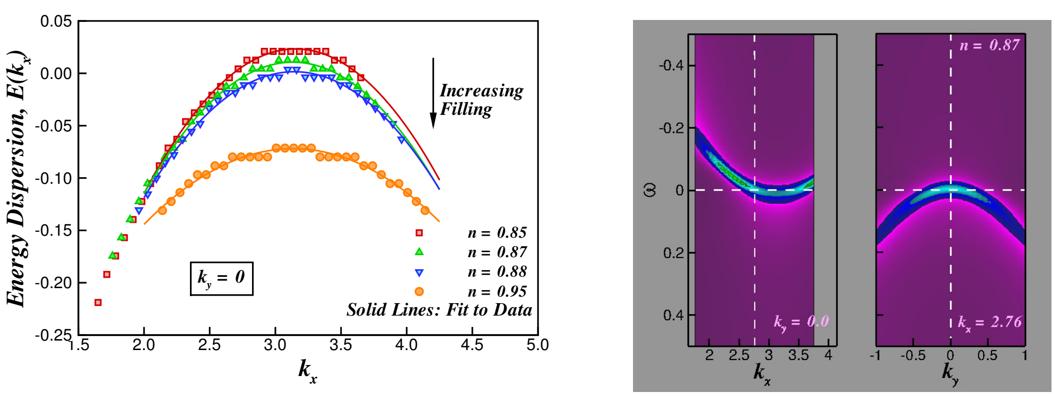

Figure 1: (left) Single particle dispersion around the Fermi energy taken along the anti-nodal direction ($k_y = 0$), (right) Energy dispersion obtained from the peaks of the spectral function $A(\boldsymbol{k}, \omega)$ around the Fermi vector $\boldsymbol{k}_F$ along the anti-nodal direction for $n = 0.87$, $t' = 0$, $U = 6t$, $4t = 1$, $N_c = 16$ and $\beta = 58$. The dispersion along the k_x direction is explored by fixing $k_y = 0$ and along the k_y direction by fixing $k_x = k_{Fx}$. Note that the vHS (flat region in the dispersion) crosses the Fermi level *away from half-filling*.

1.2 Development of an efficient Variational Monte Carlo (VMC) scheme

Often, there is a need for studying ground state wavefunctions having a large number of variational parameters. In order to optimize energy for such wavefunctions, we require optimization methods that rely on derivative information. The optimization scheme that I developed enables very efficient calculation of derivatives of energy and it wouldn't be possible to find the optimal values of the variational parameters without such a scheme. This scheme could be used to optimize wavefunctions involving a large number of variational parameters (~ 100). It was used in the VMC study of extended t-t'-t''-J model on square lattice (Phys. Rev. Lett. 102 ,027002 (2009)) and Hubbard model on honeycomb lattice (Phys. Rev. B 81, 085431 (2010)).

1.3 A General Variational Approach to Strongly Correlated Spin Singlet States

I have developed a general variational approach to study the strongly correlated systems which are believed to have spin singlet ground states. In this approach, the many-body spin singlet zero momentum state is written as a linear combination over two body spin singlet states. The singlet wavefunction $\varphi(\boldsymbol{r})$ serves as a variational parameter and the system has the freedom to choose $\varphi(\boldsymbol{r})$ rather than assuming an apriori form. Thus, this wavefunction can describe a superconductor, spin density wave, Fermi liquid, non-Fermi liquid etc. These wavefunctions are written in terms of singlet pairs but the approach can be systematically improved further by having 4 body terms, 6 body terms etc. to generate a hierarchy of wavefunctions.

2 Ongoing Projects

2.1 Application of the Dual Fermion-Dynamical Cluster approach to 1D Falicov Kimball model

The Falicov Kimball model is the simplest model for correlated electrons, introduced to study metal-insulator transitions. In one dimension, it is known to possess a charge density wave (CDW) instability at zero transition temperature (T_c). However, finite cluster methods like Dynamical Mean Field Theory (DMFT), Dynamical Cluster Approximation (DCA), Cellular Dynamical Mean Field Theory (CDMFT) , etc. show finite temperature CDW transition. In this work, we have investigated the model using the recently developed Dual Fermion-Dynamical Cluster approach (Phys. Rev. B 84, 155106 (2011)) that takes into account large length scale correlations through the auxiliary particles known as dual Fermions. We find that T_c obtained from this method is lower than that obtained from the cluster methods. In particular, we focus on the scaling behavior of T_c with the linear cluster size.

2.2 Multi-scale Many-Body approach

In this work, we extend the recently developed Dual Fermion-Dynamical Cluster approach to a multi-scale many-body technique that treats the short length scales explicitly by the dynamical cluster approach, intermediate length scales diagrammatically with the dual fermions, and the largest length scales at a dynamical mean-field level. We aim at obtaining iterative self-consistent solution that preserves causality on all the three length scales. To illustrate the implementation and applicability of this method, we are studying the 1D and 2D Falicov-Kimball model with this approach.

2.3 Possibility of the QCP in the Hubbard model (A VMC study)

The Dynamical cluster method suggests that there is a QCP in the Hubbard model at $T = 0$, but this is inferred by extrapolating finite temperature data to zero temperature as it is exponentially hard to perform QMC calculations at low temperatures due to the minus sign problem. Motivated by the physics intuition obtained from the cluster methods, we aim at studying a *normal state* resonating valence bond (RVB) wavefunction with enhanced antiferromagnetic correlations at $T = 0$ as a function of doping using the method described in 1.3. Currently, I am leading a team comprising of physicists and computer scientists to develop a massively efficient VMC code for this project on the *Graphical Processing Units (GPUs)* platform.

3 Future Projects

3.1 Lifshitz Transition in the Hubbard model

There is a change in Fermi surface topology from hole-like to electron-like associated with the vHS crossing the Fermi level. This change in Fermi surface topology can introduce *Lifshitz* singularities in the free energy. We are working on developing a mean-field theory to study such transition based on the physics intuition obtained from the cluster studies.

3.2 Dual Fermion study of strongly correlated disordered systems

I am currently collaborating on a project that aims at extending the Dual Fermion approach towards the disordered systems to study the correlation effects in the disordered systems.