Research Statement

My current research focuses in the area of strongly correlated electron systems. In an effort to understand the physics of strongly correlated electron materials, I was able to develop computational tools, derive analytical formalisms and work on phenomenological theories. I have experience with standard analytical techniques (mean field theory, diagrammatic methods, renormalization group calculations, $1/N$ expansions) and also strong computational skills. I worked both individually and also in collaboration with other students and I have experience in advising them. As part of my postdoc I also collaborated in the preparation of proposals. For my future research I would be interested to investigate different directions in theoretical condensed matter physics, most notably strongly correlated electron materials, high-T_c superconductivity, spintronics, topological insulators, quantum computing, emerging states of matter. I am not tied to a particular technique and I am interested both in analytical and computational calculations.

In this document, I provide a summary of the accomblished research, a statement for future directions and a detailed description of the accomblished research.

Summary of present and past research

As a PhD student I worked with Professor P. Phillips in the University of Illinois at Urbana-Champaign. Originally we worked on deriving low energy effective theories for the Hubbard model, using appropriate similarity transformations. We found that well known perturbative schemes such as the Brilluin-Wigner perturbation theory, the canonical transformation method and the resolvent method, which seemingly give different effective Hamiltonians, are in fact connected to one another via a well defined rotation. This line of research concluded by showing that the high energy scale of the Mott insulators is essential in strongly correlated electron physics. The quasiparticle weight at the thermodynamic limit vanishes if this scale is retained, but it remains finite if this scale is integrated out. I have also worked on the physics of the cobaltates, Na_xCoO_2, a class of materials that superconduct when hydrated, exhibit a metal to insulator transition at $x = 0.5$ and exhibits strongly correlated behavior in finite doping. We proposed a phenomenological form for the $x = 0.5$ insulating state and in the framework of the extended Hubbard model we demonstrated that it is energetically stable and captures the temperature behavior of the Hall coefficient and the resistivity. We also investigated the normal state properties numerically in the context of the Hubbard model on the triangular lattice for various fillings. For this I implemented from scratch a numerical scheme based on cluster dynamical mean field theory, using the non-crossing approximation as the impurity solver. We obtained a spectrum with features similar to the experiements including the presence of a dispersionless band.

For my first postdoc, I am working in collaboration to Mark Jarrell's and Juana Moreno's group. Using highly sophisticated codes, based on the Dynam-

ical Cluster Approximation, we investigate the phase diagram of the Hubbard model. Our main focus is the presence of quantum criticality at a finite doping. We have established the existence of a quantum critical point, based on the fact that the entropy S, exhibits a peak at a critical filling ($n_c = 0.85$ for a Coulomb repulsion $U = 6t$ and next nearest hoping $t' = 0$). Around this critical filling we found the energy, the chemical potential and the double occupancy, all have a $T^2 \ln T$ temperature dependence, characteristic of a Marginal Fermi Liquid. Furthermore we observed that when $t' > 0$ the quantum critical point is "lifted" to finite temperature and it becomes a classical critical point. This classical point is the terminal critical point of a line of first order transitions, associated with charge separation. Those findings may give an insight about the origin of the quantum critical fluctuations.

I have also worked in collaboration to Stefanos Papanikolaou, from Cornell University. In one project we developed a phenomenological theory to understand the features of the local density of states obtained in Scanning Tunneling Microscopy experiments. We proposed a model in which a $d-$wave superconductor is coupled to an $s-$ wave order parameter which fluctuates spatially following anisotropic checkerboard patterns. Because of this coupling the local density of states is anisotropic with features that closely mimic the one observed by the experiments. On another project we did an exact diagonalization of a supersymmetric lattice model of hard-core fermions proposed by Fendley el. al. The low energy physics of this model is controlled by zero energy ground states. For a particular zero energy state for a 42 site cluster in the triangular lattice, we found that in the dominant configurations the fermion motion is confined in non overlapping regions. Even though we haven't fully understood this behavior this is the first observation of such patterns in this model.

Finally, recently I have developed an intense interest in the physics of cold atoms and in particular the physics of imbalanced Fermi gases. Under certain conditions, the minority atoms create a cloud of particle-hole excitations which behave as a quasiparticle, called polaron, which is experimentally detectable[2]. The physics of isolated polarons, as evidenced from experiements and numerical simulations, seems to be captured quite well from a wave function proposed by Chevy [3]. However the interaction between those polarons is not understood very well. In collaboration with Daniel Sheehy I am currently working on a diagrammatic and numerical scheme that may allow us to determine if there is an interaction between the polarons and may give rise to a phenomenological theory of their collective behavior.

Future directions

In the future I would be happy to continue working in the area of strongly correlated physics, but I would also be extremely interested to investigate different directions. I would like to understand better the phase diagram of the Hubbard model and its relevance to the physics of the cuprates, numerically and phenomenologically. The origin of quantum criticality and the nature of the corresponding quantum fluctuations is of great importance and they could

accessible numerically using cluster computational schemes. I would also like to better understand the local density of states of the cuprates using a more refined version of our model, for example by introducing dynamics in the $s-$wave order parameter. On a different direction I would like to investigate the physics in other materials such as the cobaltates and the pnictides ($FeAs$) and graphene. The insulating state of the cobaltates using more sophisticated numerical techniques and compare its excitations with the ones predicted by phenomenological theories. Recently I became particularly interested in the physics of topological insulators. This is an expanding field, with a lot of potential applications and open issues, such as the physics of interfaces between topological insulators and superconductors, which are very relevant to topological quantum computing. Other areas of interest are disordered systems, quantum phase transitions, non-equilibrium dynamics and heavy fermions.

Research accomplished

Phase diagram of the Hubbard model using Dynamical Cluster Approximation

The phase diagram of the Hubbard model has been an object of intense study and controversy for the last couple of decades. It's structure is considered to be of utmost importance in the understanding of the physics that drives the intricate behavior of the cuprate superconductors. Several analytical and numerical results suggest that close to half filling the system is in a pseudogap state whereas away from half filling it behaves like a Fermi liquid. It has been proposed that the two states are connected by a Quantum critical point (QCP), but due to the complexity of the problem this suggestion hasn't been confirmed rigorously. In two recent publications we study the phase diagram of the Hubbard model in the region between the pseudogap and the Fermi liquid state, using the Dynamical Cluster Approximation (DCA) with various quantum impurity solvers.

First using Dynamical Cluster Approximation (DCA) with Continuous Time Monte Carlo (CTQMC) as the impurity solver, which is devoid of the $\Delta\tau$ error, we performed an extremely accurate calculation of the entropy S as a function of doping and temperature. We found that S/T as a function of doping demonstrates a clear peak at a particular filling ($n_c = 0.85$ for $U = 6t$), which is considered as one of the "smoking guns" of quantum criticality. Furthermore, right at this critical filling we were able to demonstrate from the behavior of various thermodynamic quantities, such as the energy $E(T)$, that the system is consistent to a Marginal Fermi Liquid with a $T^2 \ln T$ temperature dependence of the energy, whereas in the Fermi liquid side it's the usual T^2 behavior. We interpret our findings as thermodynamic evidence for the existence of a QCP separating the two regimes.

Second and most importantly, we investigated the phase diagram with the next-nearest-neighbor hoping t', using DCA, with Determinantal Quantum monte carlo (DQMC) and Hirsh-Fye quantum monte carlo (HFQMC). We found that when t' is switched on, the quantum critical point is "lifted" to non-zero temperature. This is consistent with previous results according to which for positive t' there is a charge separation first order transition at temperatures below a particular critical temperature $T_c(t')$ and at a critical filling $n_c(t')$. We found that the second order terminal point $(T_c(t'), n_c(t'))$ is moved to higher temperatures and fillings closer to half filling as t' increases. The line of second order terminus points seems to be continuously connected the the QCP observed before of t'. We believe that those results, are very strong evidence for the existence of a QCP, but also they suggest that charge fluctuations may dominate the physics in it's vicinity.

Pairing disorder in d-wave superconductors

The features of the local density of states (LDOS) of the cuprates as observed by Scanning Tunneling Microscopy (STM) experiments have been studied extensively in the recent years. Such features are the checkerboard oscillations, strong nanoscale gap inhomogeneities, and the rotational anisotropies. Even though it is currently unclear whether those features have purely electronic origin or driven by disorder or lattice distortions, they may well affect the properties of the cuprates, such as the magnitude of T_c. Therefore finding a phenomenological model that can explain those features may lead to a deeper understanding of superconductivity and strongly correlated physics. In a very recent publication, we proposed a model of pairing disorder. In this model an itinerant d-wave superconductor is coupled to an s-wave order parameter, Δ_s, which fluctuates spatially following a checkerboard pattern which is slightly distorted. This model is solved in the context of mean field theory in a finite lattice. We find that the resulting LDOS is rotationally anisotropic at high frequencies and isotropic for frequencies $\omega < 1/\Delta_s$. The behavior of the resulting anisotropy compares very well with the experimental observations. We have also investigated the case of pairing disorder in the d-wave channel, and we found that it cannot account for the same anisotropies in any frequency. Therefore we believe that the model we proposed is a good starting point in order to understand the anisotropies in the LDOS.

Supersymmetric model of strong correlations using exact diagonalization

In this line of work we have investigate a strongly interacting fermion system introduced by Fendley *el. al.* [1]. The system consists of hard-core fermions that can hope on a lattice. When the hoping element and the interaction are equal the Hamiltonian obtains the exact form $H = \left\{Q^\dagger, Q\right\}$ which constitutes a supersymmetric non-relativistic model. As a consequence of this symmetry the system has a large number of zero energy states which dominate it's low energy behavior. This system has been studied extensive in the square lattice using Bethe-Ansatz and cohomology as well as numerically. We have also performed numerical calculations on the square lattice using exact diagonalization on small clusters. From the energy as a function of doping we find tendency for phase separation at large doping. However our most interesting result came from studying the system in a 42 site cluster in the triangular lattice. There we observed that for $n = 10$ particles, there is a single zero energy state. In this states the cluster is broken into dimers and 6 site coupled rotors. The fermions chose to only hope inside those rotors. We think that this observation may give some insight in the structure of the zero energy eigenstates in the triangular lattice.

Mott transition on a triangular lattice using Cellular Dynamical Mean Field Theory

We study the paramagnetic side of the phase diagram of the cobaltates, Na_xCoO_2, using an implementation of the cellular dynamical mean-field theory with a non-crossing approximation impurity solver for the one-band Hubbard model on a triangular lattice. At low doping we find that the low-energy physics is dominated by a quasi-dispersionless band generated by strong correlation physics. At half filling, we find a metal-insulator transition at a critical value of the on-site interaction $U_c = 5.6 \pm 0.15t$ which depends weakly on the cluster size. The onset of the metallic state occurs through the growth of a coherence peak at the chemical potential. Away from half filling, in the electron-doped regime, the system is metallic with a large continuous Fermi surface as seen experimentally. Upon hole doping, a quasi-non-dispersing band emerges at the top of the lower Hubbard band and controls the low-energy physics. This band is a clear signature of non-Fermi-liquid behavior and cannot be captured by any weakly coupled approach. This quasi-dispersionless band, which persists in a certain range of dopings, has been observed experimentally. We also investigate the pseudogap phenomenon in the context of a triangular lattice and propose a general framework for discussing the pseudogap problem. This framework involves a momentum-dependent characterization of the low-energy physics and links the appearance of the pseudogap to a reconstruction of the Fermi surface without invoking any long-range order or symmetry breaking. Within this framework we predict the existence of a pseudogap for the two-dimensional Hubbard model on a triangular lattice in the weakly hole-doped regime.

Phenomenology for the insulating state of the cobaltates

One of the most intriguing properties of the cobaltates is a novel insulating state at a filling of 1.5. Understanding the mechanism of this insulating state is still an open issue and a lot of research has been done. Along with members of my research group I investigated a possible phenomenological explanation based on a sodium induced, electron charge-ordering scenario. In particular we have demonstrated that in the extended Hubbard model a hexatic insulating state is energetically stable. This state is composed of two tetragonal sublattices, one at half filling and one maximum filling ($n = 2$). By using a phenomenological argument we showed that the half filled lattice has antiferromagnetic correlations described by an effective exchange interaction. We showed that this state has a charge gap and we were able to explain qualitatively and quantitatively the correct temperature dependence for the Hall coefficient, including it's sign change at a finite temperature, the temperature dependence of the resistivity and the persistence of the antiferromagnetism above the insulating state.

Higher order perturbative techniques

One plausible approach to strongly correlated electron physics is to derive a low energy theory. As in all fields of physics, low energy theories offer the enormous advantage of an exponentially small Hilbert space which is of course much easier to conceptualize. Most efforts for deriving a low energy theory were based on transforming a standard strong coupling Hamiltonian such as the Hubbard model using the Brilluin-Wigner perturbation theory, the canonical transformation method and the resolvent method. Those methods result in the t-J model with the addition of extra "exchange" terms that differ from one method to the other. My contribution was to point out that all those methods are connected in a fundamental way through an additional and well defined similarity transformation.

Cluster computational schemes

Computational techniques have a long history of being employed for the understanding of strongly correlated systems. Dynamical Mean Field Theory (DMFT) represents one major step forward in our attempt to understand strong electronic correlation. It treats a single site as an impurity in an effective medium determined self-consistently. It is a non-perturbative technique which has been successful in describing the Mott transition and is exact in infinite dimensions. However in finite dimensions it suffers from a serious limitation that it ignores spatial fluctuations. Its natural extension, cluster DFMT, where the single site is replaced by a cluster of sites, restores spatial fluctuations and is considered to be a valuable tool in elucidating strongly correlated electron physics. As part of my PhD thesis I have constructed a geometry-independent and generic CDMFT based algorithm which solves the cluster using the non-crossing approximation (NCA). While NCA has a limited regime of validity, it is a good first approximation since it offers state-by-state information, it can give some deep insight in the involved mechanisms. I have used this algorithm specifically on the triangular lattice with a variety of clusters, in a attempt to understand the physics of the cobaltates.

References

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