Mark Jarrell Memorial Symposium on Computational Condensed Matter Physics

A Celebration of life and work of Mark Jarrell (1960-2019)

The LSU Center for Computation & Technology, LSU Department of Physics & Astronomy, and the LSU College of Science are organizing this Symposium to honor and remember our colleague Mark Jarrell, who passed away on July 20, 2019. Professor Jarrell, one of the foremost experts in computational many-body physics, made a career of lending deep insights into some of the most challenging questions in the field of condensed matter physics. Let us gather together to honor the many ways he has contributed to science, our research, and our lives.

February 28 - March 1, 2020
Digital Media Center Theatre and Student Union - Castilian Room
Louisiana State University

Invited Speakers

- Fakher Assaad, Wuerzburg University
- Arun Bansil, Northeastern University
- Daniel Cox, University of California-Davis
- John Deisz, California Lutheran University
- Randy S. Fishman, Oak Ridge National Laboratory
- Herbert Fotso,University at Albany
- James Freericks, Georgetown University
- Jong Han, State University of New York at Buffalo
- Vaclav Janis, Institute of Physics, Czech Academy of Sciences, Prague
- Helmut Katzgraber, Microsoft Quantum
- Ehsan Khatami, San Jose State University
- H. R. Krishnamurthy, Indian Institute of Science, Bangalore
- Thomas Maier, Oak Ridge National Laboratory
- Muhammad Aziz Majidi, Universitas Indonesia, Jakarta
- Samuel Moukouri, Ben-Gurion University of the Negev
- Mark A. Novotny, Mississippi State University
- Frank Pinski, University of Cincinnati
- Richard Scalettar, University of California-Davis
- Leigh Smith, University of Cincinnati
- Ka-Ming Tam, Louisiana State University
- Hanna Terletska, Middle Tennesse State University
- N. S. Vidhyadhiraja, Jawaharlal Nehru Centre, Bangalore
- Dieter Vollhardt, University of Augsburg
- Yang Wang, Carnegie Mellon University

Visit https://www.cct.lsu.edu/Memorial_Jarrell for full schedule and details.

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Louisiana State University, Baton Rouge, LA, U.S.A.

February 28^{th} to March 1^{st}, 2020

Friday, February 28^{th}, 2020

Student Union, Castilian Room (304)

8:00	Registration & Coffee, pastries
8:30-8:45	Opening remarks by Cynthia Peterson (Dean, LSU College of Science), Ram Ramanujam (Director, LSU Center for Computation & Technology), John DiTusa (Chair, LSU Department of Physics & Astronomy), and Jane Ellen Jarrell

Session 1	**Chair: Juana Moreno** (Louisiana State University)
8:45-9:25	**Daniel Cox** (University of California, Davis), *Mark, the Early Years: a Scientific and Personal Remembrance*
9:25-10:05	**Thomas Maier** (Oak Ridge National Laboratory), *Revisiting Mark's Interest in Lifshitz Transitions: Disappearance of Superconductivity in the Overdoped Cuprates*
10:05-10:45	**Dieter Vollhardt** (University of Augsburg), *Dynamical Mean-Field Theory: A Status Report*
10:45-11:10	Coffee break
11:10-11:50	**James Freericks** (Georgetown University), *Mark Jarrell, Thomas Pruschke and Me: The Early Days of Dynamical Mean-Field Theory*
11:50-12:30	**Ka-Ming Tam** (Louisiana State University), *Beyond Quantum Cluster Methods*
12:30-1:30	Lunch break

Session 2	**Chair: Daniel Cox** (Univ. of California, Davis)
1:30-2:10	**Richard Scalettar** (Univ. of California, Davis), *Charge Density Wave and Superconductivity in the Disordered Holstein Model*
2:10-2:50	**Hanna Terletska** (Middle Tennessee State University), *Typical Medium Quantum Cluster Method for Disordered Electron Systems*
2:50-3:15	Coffee break
3:15-3:55	**Randy S. Fishman** (Oak Ridge National Laboratory), *Model for the Spin Dynamics of the Multiferroic* $(NH_4)_2FeCl_5(H_2O)$
3:55-4:35	**N. S. Vidhyadhiraja** (Jawaharlal Nehru Centre, Bangalore), *Emergent non-Fermi Liquid Behaviour in Disordered, Strongly Correlated Electron Systems*
4:35-5:15	**Mark A. Novotny** (Mississippi State University), *Order amidst Disorder' in 2D, 3D, and 2D+3D Quantum Nanodevices*

Saturday, February 29^{th}, 2020

Digital Media Center Theater

8:00-8:30	Coffee & pastries

Session 3	**Chair: Hanna Terletska** (Middle Tennessee State University)
8:30-9:10	**John Deisz** (California Lutheran University), *Modeling of Superconducting Sr_2RuO_4 using Dynamical Mean Field Theory and Self-consistent Perturbation Theory*
9:10-9:50	**H. R. Krishnamurthy** (Indian Institute of Science, Bangalore), *Correlation Induced Metallic, Half-metallic and Superconducting Phases in Strongly Correlated Band Insulators*
9:50-10:15	Coffee break
10:15-10:55	**Fakher Assaad** (Würzburg University), *Kondo Nano-Structures and Lattices*
10:55-11:35	**Arun Bansil** (Northeastern University), *Mark Jarrell: Friend and a Scholar*
11:35-12:15	**Leigh Smith** (University of Cincinnati), *Oh, The Places We Went! Mark and I as young Faculty in Cincinnati*
12:15-1:30	Lunch break

Session 4	**Chair: Ka-Ming Tam** (Louisiana State University)
1:30-2:10	**Helmut Katzgraber** (Microsoft Quantum), *Quantum-driven Classical Optimization*
2:10-2:50	**Herbert Fotso** (University at Albany), *Making Better Qubits out of Spectrally Noisy Solid State Quantum Emitters*
2:50-3:15	Coffee break
3:15-3:55	**Ehsan Khatami** (San Jose State University), *Uncovering the Many Faces of a Non-Fermi Liquid with AI*
3:55-4:35	**Yang Wang** (Carnegie Mellon University), *Multiple Scattering Theory Approach to the Ab-initio Investigation of Disordered Structures*
4:35-5:15	**Muhammad Aziz Majidi** (Universitas Indonesia, Jakarta), *Understanding Unconventional Plasmons in Mott-like Insulators and Nanoparticle Systems*

6:00-8:00	**Banquet**, The Club at Louisiana State University

Sunday, March 1st, 2020

Digital Media Center Theater

8:00-8:30	Coffee & pastries

Session 5	**Chair: Randy Fishman** (Oak Ridge National Laboratory)
8:30-9:10	**Samuel Moukouri** (Ben-Gurion University of the Negev), *An Experimental Test of the Geodesic Rule Proposition for the Non-cyclic Geometric Phase*
9:10-9:50	**Jong Han** (State Univ. of New York at Buffalo), *Issues and Prospects in Understanding of Nonequilibrium in Solids*
9:50-10:15	Coffee break
10:15-10:55	**Václav Janiš** (Acad. Sciences, Czech Republic), *Genesis of the Curie-Weiss Law in Strongly Correlated Electron Systems*
10:55-11:35	**F. J. Pinski** (University of Cincinnati), *Infinite Dimensions and Singular Limits*
11:35-11:45	Closing remarks by Juana Moreno (Louisiana State University) and Jane Ellen Jarrell
11:45	Lunch (boxed sandwiches)

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Fakher Assaad (Würzburg University), *Kondo Nano-Structures and Lattices.*
How do various spin system interact with a metallic host? Is the coupling relevant? And if so, does it lead to novel states of matter? In this talk I will show that it is possible to simulate a large class of spin models coupled to conduction electrons without encountering the notorious negative sign problem inherent to quantum Monte Carlo simulations. We will then discuss various setups and provide insight into the aforementioned questions. In particular we will consider i) nano-magnets on metallic surfaces ii) the crossover from Kondo impurity to Kondo lattice physics, iii) partial Kondo screening resulting from frustration and finally the phase diagram of the SU(N) Kondo lattice model.

Arun Bansil (Northeastern University), *Mark Jarrell: Friend and a Scholar.*
I had the privilege of knowing Mark in a number of different roles over the years. In these interactions I not only came to appreciate the depth of Mark's understanding of the many-body physics of materials but also his wonderful human side and his interest in all things important around him. Mark was my go-to person for QMC related questions as an authority in the field and as someone from whom I was sure to get a straight answer. He was also very interested in first-principles approaches. In this connection, I will discuss some very recent advances that have enabled parameter-free (no U) modeling of the electronic structure of cuprate superconductors and other complex materials [Y. Zhang et al., Proc. National Academy of Sciences, 10.1073/pnas.1910411116 (2019)], which I think Mark would have enjoyed.

Daniel Cox (University of California, Davis), *Mark, the Early Years: a Scientific and Personal Remembrance.*
In this talk, I will share my scientific and personal remembrances of our friend Mark Jarrell beginning from the time we met at the Woodstock of Physics when he was a bright eyed graduate student and I was a young assistant professor through his early days as an assistant professor himself. Mark was remarkable for his drive, his simultaneous ability to focus on a problem intensely while conversing about 4 or 5 separate things in one sitting, and his deep commitment to teaching and mentoring, which extended to several of my students. In that compressed frame of time, Mark contributed on collaborations enhancing our understanding of impurities in superconductors, theories of orbitally driven superconductivity, the maximum entropy approach to analytic continuation for extracting dynamics from quantum Monte Carlo simulations, and the first calculations for the Hubbard model in dynamical mean field theory, and I will reflect on the science and his remarkable process in that work.

John Deisz California Lutheran University), *Modeling of Superconducting Sr_2RuO_4 using Dynamical Mean Field Theory and Self-consistent Perturbation Theory.*
The dynamical cluster approximation extends dynamical mean-field theory to capture nonlocal correlations such as those driven by antiferromagnetic spin fluctuations. With the dynamic cluster approximation one can investigate the significance of the momentum dependence in the electron self-energy and the possibility of correlation-driven superconducting transitions to non-s-wave pairing states. We apply the dynamical cluster approximation to weak coupling models for Sr_2RuO_4, a material for which decades of experiments have failed to resolve unambiguously the nature of the pairing state. Results show that the self-energy has a strong momentum dependence near a van Hove singularity that is a focus of recent T_c vs strain experiments.

Randy S. Fishman (Oak Ridge National Laboratory), *Model for the Spin Dynamics of the Multiferroic $(NH_4)_2FeCl_5(H_2O)$.*
The multiferroic behavior of any material sensitively depends on the microscopic interactions between the spins. We evaluate the magnetic interactions in the multiferroic erythrodsiderite $(NH_4)_2FeCl_5(H_2O)$ by comparing inelastic neutron scattering spectra of a single crystal sample with a simple Heisenberg model containing five exchange interactions and an easy-plane anisotropy. The cycloidal spin state in every bc plane is produced by two competing exchange interactions. Using the observed wavevector of this cycloidal spin state is used as a constraint, excellent agreement is found between the observed and predicted spectra. The resulting exchange and anisotropy parameters are compared with the predictions of first-principle calculations.

Herbert Fotso (University at Albany), *Making Better Qubits out of Spectrally Noisy Solid State Quantum Emitters.*
Many of the systems that are promising qubits for quantum information processing are solid state quantum emitters. Most of these systems are subject to spectral diffusion: the random drift of the emission/absorption spectrum away from a set target frequency. This uncontrolled dynamics is due to the fluctuations (strain, charge or spin) in the surrounding bath and negatively affects many fundamental operations for scalable quantum information processing platforms. In particular, the ability to entangle distant quantum nodes is essential for the construction of quantum networks and for quantum information processing. For solid-state quantum emitters entanglement generation can be achieved by photon interference. When the emitter is subject to spectral diffusion, this process that relies on photons from respective qubits being indistinguishable can become highly inefficient, impeding the achievement of scalable quantum technologies. Solutions to this challenge from the device manufacturing point of view remains a formidable task. We study optical properties of quantum emitters in dynamic environments when they are driven by external fields and show that the emission/absorption spectrum can be kept fixed despite the influence of the environment. Furthermore, we show that photon indistinguishability assessed through two-photon interference in the context of a Hong-Ou-Mandel (HOM)-type experiment for two separate quantum emitters can be greatly enhanced by suitable pulse control protocols.

James Freericks (Georgetown University), *Mark Jarrell, Thomas Pruschke and Me: The Early Days of Dynamical Mean-Field Theory.*
In this talk I will discuss much of the history of the early days of dynamical mean-field theory including the major role played by Mark in much of this development. When I started as a postdoctoral fellow at the ITP in Santa Barbara (before it had a "K"), Doug Scalapino introduced me to Mark and this began a seven year-long collaboration, where we worked through a number of joint projects in these early days. Mark was clearly the leader of this effort and much of this work remains important today. During this time period, I became a Professor at Georgetown, secured external funding for my work, and launched my career. Mark was a critical mentor to me during that time; he even was a member of my wedding party in 1999. After this intense period of work, our interests separated and we moved in different directions. He focused on cluster extensions to DMFT and I worked on inhomogeneous DMFT in multilayers and on nonequilibrium DMFT. Mark was a critically important friend and mentor during this formative part of my career. I will always remember his powerful influence on me. In this talk, I will give you a flavor of what the "grand old days" were like.

Jong Han (State Univ. of New York at Buffalo), *Issues and Prospects in Understanding of Nonequilibrium in Solids.*
Strong nonequilibrium physics in solid-state physics can be considered as old as mankind's control of electricity. Although some nonequilibrium phenomena such as sudden change of resistive state on application of strong electric field have been well-known, the understanding of their microscopic mechanism has remained very limited. Recent works of high-field and ultra-fast-probe experiments have begun to unlock the mechanisms of symmetry breaking in nonequilibrium-driven phase transitions in solids. Despite the intense effort with computational theories to understand the correlated behaviors near switching induced by an electric field, the fundamental role of the electric field on the electronic structure has not been well understood. In particular the discrepancy between theories and measurements on the switching condition is of many orders of magnitude. To build a qualitative understanding of the nonequilibrium in solids, model studies in driven-dissipative solids are presented. We review the theoretical efforts for understanding electronic transport in the charge-density-wave and resistive switching phenomena in transition-metal oxides and chalcogenides. We develop an analytic method of one-dimensional fermion model to propose a new framework of how to approach nonequilibrium effects in metallic solids. Through a bosonized theory of one-dimensional metallic fermion system, we show that the effect of a uniform electric field is absorbed by the bosonic zero-mode (BZM) which has largely been ignored in condensed matter applications. The generation of the BZM becomes macroscopic with its statistical spectrum giving the field-induced effective temperature and the electric current. In the insulating limit, we analyze the electronic excitations in gapped systems which result in a realistic description of switching behavior in vanadium oxides, and resolves some of the long-standing issues.

Václav Janiš (Acad. Sciences, Czech Republic), *Genesis of the Curie-Weiss Law in Strongly Correlated Electron Systems.*
The Curie-Weiss behavior of the magnetic susceptibility is universally observed in ferromagnetic materials and is connected with the existence of local magnetic moments in the paramagnetic phase. It has been a long-term enigma how the Curie-Weiss susceptibility can emerge in itinerant magnetic systems where Pauli behavior and Fermi liquid are expected at low temperatures. We show that a renormalization of the bare interaction strength is essential for the generation of the Curie-Weiss low-temperature behavior in the strongly correlated electron systems. We use a renormalized perturbation expansion for the vertex functions of the Hubbard model in the mean-field (local) approximation. The basis of our approach are the parquet equations. Their complexity is reduced in the critical region of the magnetic transition via decoupling of convolutions of Matsubara frequencies so that a static self-consistent approximation for the irreducible vertex in the electron-hole scattering channel (effective interaction) is reached [V. Janiš, P. Zalom, V. Pokorný, and A. Klíč, Phys. Rev B 100, 195114 (2019)]. The temperature dependence of the effective interaction of the Anderson impurity model is obtained from which we determine the behavior of the local magnetic susceptibility. We show that there is crossover behavior around the Kondo temperature in the magnetic susceptibility in the strong-coupling regime. The susceptibility follows the Curie-Weis law above the Kondo temperature and goes over to the Pauli one in the Fermi-liquid regime when approaching zero temperature [V. Janiš and A. Klíč, arXiv:1909.02292 (2019)]. A Stoner-like criterion for the existence of the Curie-Weiss magnetic response is set.

Helmut Katzgraber (Microsoft Quantum), *Quantum-driven Classical Optimization.*
The advent of the first useful quantum computing devices has resulted in an arms race with classical algorithms on traditional computing hardware. While near-term quantum devices might revolutionize, e.g., optimization and quantum chemistry, tackling many applications will directly depend on either hybrid or purely classical computing techniques. Inspired by these recent exciting developments, a variety of new classical algorithms have emerged. In this talk an overview on quantum inspired methods and their applications is given.

Ehsan Khatami (San Jose State University), *Uncovering the Many Faces of a Non-Fermi Liquid with AI.*
Quantum gas microscopes for ultracold atoms in optical lattices have transformed quantum simulations of many-body Hamiltonians. Analysis of atomic snapshots using conventional order parameters or correlation functions have led to new discoveries for the Fermi-Hubbard model in two dimensions. Here, we enlist the help of artificial intelligence to go beyond this paradigm and allow snapshots of particles shape our knowledge about the correlations in less well-understood phases of matter, where no microscopic theory is available. We employ our technique to extract relevant spin and charge fluctuations in the mysterious non-Fermi liquid region of the repulsive Hubbard model around 18% hole doping.

H. R. Krishnamurthy (Indian Institute of Science, Bangalore), *Correlation Induced Metallic, Half-metallic and Superconducting Phases in Strongly Correlated Band Insulators.*
While experimental and theoretical studies of strongly correlated band metals (i.e., systems

that should be metals according to band theory) have occupied center-stage in condensed matter physics in recent decades, not that much attention has been paid to strong correlation effects in band insulators (i.e., systems that should be insulating as per band theory). In this talk I given an overview of theoretical work, including our own*, that suggests that there are interesting possibilities here as well. Specifically I discuss the physics of what is perhaps the simplest model of such materials, namely, the Ionic Hubbard Model with a strong on-site Coulomb repulsion energy, using approximations such as Hartree-Fock approximation, Dynamical Mean-Field Theory, slave-particle mean filed theories, Gutzwiller approximation, etc. In the paramagnetic regime which can persist down to low temperatures in models with frustration, a metallic phase is induced by strong correlations! Among the magnetically ordered phases are an antiferromagnetic insulating phase with different band gaps for the up and down, a half-metallic antiferromagnet where one of the spin gaps vanish, and a ferrimagnetic metal. Possibilities exist for superconducting phases as well. [*Work done in collaboration with Arti Garg, Soumen Bag and Anwesha Chattopadhyay]

Thomas Maier (Oak Ridge National Laboratory), *Revisiting Mark's Interest in Lifshitz Transitions: Disappearance of Superconductivity in the Overdoped Cuprates.*
The abrupt disappearance of superconductivity in the overdoped cuprates challenges theories of high-temperature superconductivity. ARPES experiments on some of these materials find that the overdoped end of the Tc dome is near a Lifshitz transition where the Fermi surface changes from hole-like to electron-like. Here I will discuss dynamic cluster quantum Monte Carlo calculations for the Hubbard model that were motivated by these experiments and by Mark's previous work on Lifshitz transitions. Specifically, I will describe how these calculations can provide a framework for understanding this end point behavior.

Muhammad Aziz Majidi (Universitas Indonesia, Jakarta), *Understanding Unconventional Plasmons in Mott-like Insulators and Nanoparticle Systems.* Plasmonics, a research field that exploits interactions between photons and plasmons in a material, has become important for the development of information technology today. In conventional picture, plasmon is understood as the quantum view of a collective oscillatory motion of free electrons, normally existing in metals. There are three kinds of plasmons widely known so far, namely bulk and surface plasmons in bulk size metals, and localized surface plasmons (LSP) in metal nanoparticles. Recent experimental study on family, supported by a classical oscillator model, has revealed a new kind of plasmons occurring in the Mott-like insulating phase, arising due to confinement and Coulomb correlation effects. Unlike conventional bulk plasmons in metals, these plasmons are readily excitable via photon absorption, appear with multiple peaks in the absorption spectra which coincide with those in the loss function spectra, and have low energy loss. Here we present a theoretical explanation of such plasmons based on a modified Hubbard model. Our results give good qualitative agreement with the experimental data as well as the classical oscillator model, and provide more physical insight of the microscopic mechanism underlying the phenomenon. In addition, motivated by our current experimental study on optical responses of gold nanoparticles, whereby the samples behave in many respects like insulator, here we attempt to provide a theoretical explanation for such a system. We construct a finite-size tight- binding-based Hamiltonian incorporating

s-d hybridization and on-site Coulomb repulsion on the d orbital. Our results qualitatively agree with the experimental data and suggest that noble metals such as gold behave as regular metal showing conventional plasmonic behavior when in bulk, but become correlated insulator exhibiting unconventional plasmonic behavior in nanoscale size. The unconventional plasmonic energy may be controlled by tuning the nanoparticle size or by the choice of material with suitable hybridization and on-site Coulomb interaction strength.

Samuel Moukouri (Ben-Gurion University of the Negev), *An Experimental Test of the Geodesic Rule Proposition for the Non-cyclic Geometric Phase.*
The geometric phase due to the evolution of the Hamiltonian is a central concept in quantum physics, and may become advantageous for quantum technology. In non-cyclic evolutions, a proposition relates the geometric phase to the area bounded by the phase-space trajectory and the shortest geodesic connecting its end points. The experimental demonstration of this geodesic rule proposition in different systems is of great interest, especially due to the potential use in quantum technology. Here, we report a novel experimental confirmation of the geodesic rule for a non-cyclic geometric phase by means of a spatial SU(2) matter-wave interferometer, demonstrating, with high precision, the predicted phase sign change and π jumps. We show the connection between our results and the Pancharatnam phase.

Mark A. Novotny (Mississippi State University), *Order amidst Disorder' in 2D, 3D, and 2D+3D Quantum Nanodevices.*
Quantum effects in nanodevices can lead to unexpected physical properties. The electrical conductance of a nanodevice connected to leads, according to Landauer, is a function of the electron transmission T(E) at energy E, obtained from the solution of the appropriate Schrödinger equation. If a nanodevice has complete electron transmission T(E)=1 for all energies E of the incoming electron, the electrical conductance is infinite in four-probe measurements, and equal to the quantum of conductance, G_0, in two-probe measurements. Pure systems (no disorder) which have T(E)=1 are said to exhibit ballistic transport, and this quantum property is utilized in graphene-based devices from FETs to qubits. Devices with strong disorder with T(E)=1 we call quantum dragons [[M.A. Novotny, Energy-independent total quantum transmission of electrons through nanodevices with correlated disorder, Physical Review B **90**, 165103 (2014)]. We show for carbon-based nanodevices with strong disorder, as well as for other disordered 2D, 3D, and 2D+3D nanodevices, it is possible to have T(E)=1 for all E. Furthermore, even with only short-range correlations these strongly disordered devices have at least one non-localized state, demonstrating 'order amidst disorder'. Carbon-based quantum dragons can have very strange shapes, be very disordered, be very tatty, and still exhibit 'order amidst disorder'. A number of both carbon-based and other quantum dragon nanodevices will be described, as well as instances where small deviations cause related nanosystems to be almost quantum dragon nanodevices.

F. J. Pinski (University of Cincinnati), *Infinite Dimensions and Singular Limits.*
In many instances, it is important to understand events that rarely happen. For example, chemical transitions where an energy barrier limits the reaction rate. To this end, it is instructive to examine the Brownian dynamics of a particle moving in an external potential,

and consider "paths" that are constrained to begin and end in different free-energy basins. In such a classical path integral approach, the probability of such double-ended paths is described by the analog of the single particle propagator using Feynman path integrals (with the Wick rotation). However, in the classical case, the continuous time limit is singular. In this talk, I will illustrate the relevant issues using very simple examples.

Richard Scalettar (Univ. of California, Davis), *Charge Density Wave and Superconductivity in the Disordered Holstein Model.*
The interplay between electron-electron correlations and disorder has been a central theme of condensed matter physics over the last several decades, with particular interest in the possibility that interactions might cause delocalization of an Anderson insulator into a metallic state, and the disrupting effects of randomness on magnetic order and the Mott phase. Here we extend this physics to explore *electron-phonon* interactions and show, via exact quantum Monte Carlo simulations, that the suppression of the charge density wave correlations in the half-filled Holstein model by disorder can stabilize a superconducting phase. We discuss the relationship of our work to studies of the disorder quenching of the charge ordered phase in $ZrTe_3$ through Se doping, and the interplay with the observed superconductivity in that material, reproducing the qualitative features of the phase diagram in the temperature-disorder strength plane.

Leigh Smith (University of Cincinnati), *Oh, The Places We Went! Mark and I as young Faculty in Cincinnati.*
Mark Jarrell and I arrived as newly minted untenured Assistant Professors at the University of Cincinnati in the Summer of 1990. This is a bit of a rememberance of those times when we were young and sometimes stupid and pushed the envelope at every point. We really enjoyed feeding off each other, pushing each other, and most of all complaining about the powers that be at the University. It was probably the most fun I had in my life, and I would not take any of it back. Unfortunately, our research areas really did not overlap strongly, but Mark was always willing to talk about anything and his advice was invaluable, particularly the political nature of the beast of getting funding. What is very funny and at the same time sad, is that what I am doing now in my research finally is approaching the point where Mark would have actually been interested and we could have actually collaborated! If time permits, I will end by giving a short description of my group's recent work on the mid-infrared optical spectroscopy of Weyl semimetals.

Ka-Ming Tam (Louisiana State University), *Beyond Quantum Cluster Methods.*
The effect of strong correlations in electronic systems is believed to be the key to understand a plethora of unusual properties of materials. Classic examples include high temperature superconducting cuprates, heavy fermion systems, and organic superconductors. The dynamical mean field theory tackles the strong correlations by suppressing the spatial fluctuations. Its extensions–quantum cluster methods–provide a systematic framework for recouping spatial fluctuations albeit at the cost of solving a cluster of quantum impurities. Even with the substantial improvements of numerical impurity solvers over the years, quantum cluster methods still face an insurmountable barrier. An alternative proposed by Mark Jarrell and his col-

laborators was to introduce an extra intermediate length scale or an expansion on top of the solution from the dynamical mean field theory or dynamical cluster approximation. This was originally coined as the Multi Scale Many Body Method. In this talk, we will discuss the developments in this direction over the last decade. Methods including the parquet approximation, dynamical vertex approximation, dual fermion approximation, and functional renormalization group will be discussed.

Hanna Terletska (Middle Tennessee State University), *Typical Medium Quantum Cluster Method for Disordered Electron Systems.*
Disorder is ubiquitous in many materials and can dramatically affect their structural, magnetic, and electric properties. One of the most notable effects of disorder is electron localization, associated with a disorder-driven conductor to insulator transition. Having a proper numerical tool to treat disorder effects is necessary for better understanding and control of the properties of real materials. Recently, we have developed a typical medium DCA (TMDCA) method [1], which has been used to properly described the electron localization in disordered systems. In this talk, I will discuss the TMDCA method, which we has applied to study disorder effect in multiple model Hamiltonian systems. This includes systems with the off-diagonal disorder, multi-orbital materials, as well as disordered interacting systems. Examples of TMDCA analysis in combinations with ab-initio calculations will also be discussed. [1] H. Terletska, Yi Zhang, K. M. Tam, T. Berlijn, L. Chioncel, N. S. Vidhyahiraja, and M. Jarrell, "Systematic Quantum Cluster Typical Medium Method For the Study of Localization in Strongly Disordered Electronic Systems", Appl. Sci. 8(12), 2401 (2018).

N. S. Vidhyadhiraja (Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore), *Emergent non-Fermi Liquid Behaviour in Disordered, Strongly Correlated Electron Systems.*
We provide strong evidence for a quantum critical point (QCP) associated with the destruction of Kondo screening in the Anderson-Hubbard model for interacting electrons with quenched disorder. The evidence comprises three elements: (a) the identification of an energy scale, ω, that delineates infrared Fermi-liquid damping from higher frequency non-Fermi liquid (nFL) dynamics; (b) the finding that this crossover scale ω appears to vanish with increasing disorder; and (c) the concomitant appearance of a finite intercept in a broad distribution of Kondo scales. Our findings indicate a Kondo destruction scenario, albeit distinct from the local QCP picture. The nFL behavior is shown to stem from an interplay of strong electron-electron interactions and the systematic inclusion of short-range dynamical fluctuations induced by the underlying random potential. The results have been obtained through a computational framework based on the typical medium dynamical cluster approximation.

Dieter Vollhardt (University of Augsburg), *Dynamical Mean-Field Theory: A Status Report.*
Dynamical mean-field theory (DMFT) is the generic mean-field theory of correlated electron systems and has shaped our present understanding of electronic correlations in solids. In particular, the combination of DMFT with methods to compute electronic band structures provides a conceptually new framework for the realistic study of correlated materials. This

approach is applicable to bulk systems (homogeneous and inhomogeneous) and even to topological states of matter. The inclusion of non-local correlations into DMFT makes it possible to explore unconventional superconductivity and the critical behavior at thermal or quantum phase transitions. By generalizing DMFT to nonequilibrium states the real-time dynamics of correlated systems can also be investigated. In my talk I will review the current status of DMFT.

Yang Wang (Carnegie Mellon University), *Multiple Scattering Theory Approach to the Ab-initio Investigation of Disordered Structures.*
Ab initio electronic structure calculation based on density functional theory is a widely used powerful tool for the computational study of physical and chemical properties of materials. A major computational task in the ab initio calculations is to solve the Kohn-Sham equation, which is a Schrodinger equation (or a Dirac equation in relativistic case) for one electron moving in an effective potential in the local density approximation. In this presentation, I will introduce MuST, an NSF funded project for which Prof. Mark Jarrell had devoted his final days and energies. This project aims to implementing multiple scattering theory, also known as Korringa-Kohn-Rostoker (KKR) method, for the solution of the Kohn-Sham equation and applying the method to the ab initio investigation of disorder effects in solid state materials. I will give an overview of the multiple scattering theory, and discuss the potential applications and computational challenges of the multiple scattering theory based ab initio methods at the dawn of exascale computing era.

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