Institute for Materials Science

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IMS Rapid Response 2016 * Phase I Recipient Seminar

Dr. Jian-Xin Zhu
Los Alamos National Laboratory
T-4: Physics of Condensed Matter and Complex Systems

Gutzwiller Variational Wavefunction Approach to Electronic Correlation and Lattice Dynamics in Multi-Orbital Models

Monday, May 16, 2016
2:00 - 3:00pm
MSL Auditorium (TA-03 - Bldg 1698 - Room A103)

Abstract: Electronic correlation effects in complex materials give rise to emergent phenomena including Mott insulators, magnetism, heavy fermions, and unconventional superconductivity. These phenomena defy the description of density functional theory (DFT) within local density approximation (LDA), which has been successful in describing electronic and structural properties of good metals and several semiconductors. The inadequacy of the LDA method for strongly correlated electron materials can be partly cured by including a direct treatment of quantum fluctuation effects by such quantum many-body approaches like the dynamical mean-field theory (DMFT). Together with its success in describing key physical observables in many strongly correlated electron materials (SCEMs), however, the LDA+DMFT with non-perturbative impurity solvers is computationally expensive and in practice limited to solid state systems with high crystalline symmetry, making it time consuming to describe the structural relaxation problems.

Recently, the Gutzwiller approximation to the determination of a project wavefunction has proven to be important tools to study strongly correlated electron systems. When it is combined with the LDA, realistic SCEMs can be simulated much more efficiently, which opens the door to perform the quantum molecular dynamics for the structure stability in these materials. In this first lecture, I will present an overview on the basics of the Gutzwiller approximation. Its applications to simpler models including single-band Hubbard model and Anderson lattice model will be discussed on the electronic correlation effects. Our current progress on the project will also be briefed.

Bio: Dr. Zhu's research interest includes the impurity problem of strongly correlated electron systems, quantum phase transitions in heavy-fermion systems, and LDA+DMFT electronic structure calculations of strongly correlated electron materials. Dr. Zhu is a staff scientist in the Theoretical Division at the Los Alamos National Laboratory. He obtained his Ph.D from the University of Hong Kong in 1997. Prior to joining LANL in 2001, he spent four years as a postdoctoral fellow and then as a research assistant professor at the Texas Center for Superconductivity, University of Houston.

For general information contact Caryll Blount, IMS Administrator
caryll@lanl.gov * 665-3950

Hosted by Alexander Balatsky * Director of the Institute for Materials Science

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