Final Report for Period: 08/2006 - 07/2007 **Submitted on:** 10/17/2007

Principal Investigator: Freericks, James K. **Award ID:** 0210717

Organization: Georgetown University

Title:

NIRT: Computational Design and Optimization of Nanoscale Spintronic and Thermoelectric Devices

Project Participants

Senior Personnel

Name: Freericks, James

Worked for more than 160 Hours: Yes

Contribution to Project:

Name: Jones, Barbara

Worked for more than 160 Hours: Yes

Contribution to Project:

Name: Liu, Amy

Worked for more than 160 Hours: Yes

Contribution to Project:

Post-doc

Name: Demchenko, Denis

Worked for more than 160 Hours: Yes

Contribution to Project:

Denis performed density-functional theory calculations on ferromagnetic/semiconductor interfaces and performed modeling of bulk thermal transport in materials close to the correlated metal-insulator transition. He is currently a postdoctoral fellow at Lawrence Berkeley Laboratories.

Name: Turkowski, Volodomyr

Worked for more than 160 Hours: Yes

Contribution to Project:

Dr. Turkowski is working on developing the nonequilibrium formalism. His first project has been to calculate the f-electron spectral function of the Falicov-Kimball model. He identified a number of subtle numerical issues with this calculation and completed this project. he helped develop the formalism for nonequilibrium transport of conduction electrons in the bulk, including an exact DMFT treatment, perturbative approaches, and exact moment sum rules. He left in 2006 for a postdoctoral fellowship at the University of Missouri.

Name: Park, Kyungwha

Worked for more than 160 Hours: Yes

Contribution to Project:

Name: Schnell, Ilan

Worked for more than 160 Hours: Yes

Contribution to Project:

Ilan Schnell worked on developing calculations in DFT for superconductivity related phenomena. Some in the bulk and some for multilayered structures using supercells. He left in the spring of 2006 to pursue employment in the private sector.

Name: Zenia, Hand

Worked for more than 160 Hours: Yes

Contribution to Project:

Hand was supported as a postdoctoral fellow on this grant for three months in 2007. He worked on transport properties of MgB2-based Josephson junctions.

Graduate Student

Name: Joura, Alexander

Worked for more than 160 Hours: Yes

Contribution to Project:

Sasha examined problems in thermal transport in the bulk, spent one year at IBM on an apprenticeship where he focused on the quantum corals work in Don Eigler's group, and he has since focused on developing a steady-state nonequilibrium formulation of the many-body problem within the DMFT framework.

Name: Chen, Ling

Worked for more than 160 Hours: Yes

Contribution to Project:

Ling had a one-year apprenticeship at IBM where he worked on current-induced switching in magnetic nanostructures. he completed a publication on electronic charge reconstruction of doped Mott insulators, and is currently on leave from the University.

Name: Hale, Simon

Worked for more than 160 Hours: Yes

Contribution to Project:

Simon is currently on an apprenticeship at IBM, Almaden (under the guidance of Barbara Jones) and is supported by the grant. He is working on new technologies based on magnetic storage in tape media and has been closely involved in some new patent work that will increase the density of storage on the tapes.

Name: Wang, Peng

Worked for more than 160 Hours: Yes

Contribution to Project:

Peng has been working on computational based projects in DFT that are related to the grant goals.

Undergraduate Student

Name: Huntington, Craig

Worked for more than 160 Hours: No

Contribution to Project:

Name: Stimmel, Ron

Worked for more than 160 Hours: No

Contribution to Project:

Name: Nelson, Greg

Worked for more than 160 Hours: Yes

Contribution to Project:

During the summer of 2005, Greg traveled to the Institute of Physics, Zagreb, Croatia to perform research in the lab of Miroslav Ocko. He took with him a set of samples of tantalum-deficient tantalum nitride and measured the resistivity and thermopower at low temperatures. Then, after returning to Georgetown, he worked on modeling the data with the Falicov-Kimball model.

Name: Boocock, Sean

Worked for more than 160 Hours: No

Contribution to Project:

Sean spent the Spring 2006 semester working on learning how to image complex scienbtific data using paraview to create false color images od the DOS of strongly correlated barrier devices. The goal was to find a way to image small oscillations that lay on top of large amplitude data. He found a subtraction technique, and used methods of playing with the color maps to be able to bring out this behavior in a clear way.

In the Spring of 2007, he continued the visualization work by analyzing large data sets on the distribution functions of electrons driven by a large external electric field as they approach the steady state. He has been aiding with the creation of movie animations of how those distribution functions evolve over time.

Technician, Programmer

Other Participant

Research Experience for Undergraduates

Organizational Partners

IBM Almaden Research Center

Year long student exchanges and shorter term senior personnel exchanges have taken place and will continue throughout the collaborative grant

Institute of Physics, Zagreb, Croatia

Veljko Zlatic, of the IFS is involved in collaborative research and in visits/exchanges both to the US and to Croatia

Other Collaborators or Contacts

Veljko Zlatic, Institute of Physics, Zagreb Croatia
Tom Devereaux, University of Waterloo, Toronto, Canada
Andrij Shvaika, Institute for Condensed Matter Physics, Lviv, Ukraine
Stamatis Vokos, Seattle Pacific University
Alex Hewson, Imperial College, London
Thomas Pruschke, University of Goettingen
Frank Steglich, Max Planck Institute for the chemical physics of solids

Activities and Findings

Research and Education Activities:

We have been developing computer codes to describe transport through nanoscale heterostructures using many-body theory. In conjunction with this, we have also been carrying out first-principles calculations to characterize electronic and magnetic properties of interfaces in heterostructures, with a focus on the influence of atomic structure at the interface. Systems of interest include ferromagnetic/semiconducting and superconducting/insulating junctions.

We have been investigating novel probes for nanostructures such as inelastic light scattering. We have discovered a new sum rule for Raman and inelastic x-ray scattering, and verified its existence in SmB6.

We are currently developing nonequilibrium dynamical mean field theory in both the steady state and in the transient response region. In particular, we have solved the problem of how Bloch oscillations are damped as the system moves through a metal-insulator (Mott) transition.

We developed the formalism for thermal transport in nanostructures which is significantly more complex than charge transport because there is no thermal current conservation. We also examined a number of new thermoelectric properties of heavy Fermion materials including an examination of the ratio of the specific heat coefficient to the thermopower.

We are currently working on adapting NRG calculations to nanostructures to examine the Hubbard and periodic Anderson models.

Using density-functional calculations, we have been studying structural, magnetic, and electronic properties of molecule-based magnetic materials. We have also been investigating dispersion interactions between large molecules. In addition to the usual electronic dispersion interaction arising from fluctuating dipoles dues to motion of electrons, we are considering vibrational contributions due to atomic displacements. We have developed efficient computational formalisms for calculating both contributions within density functional theory.

Freericks has written a graduate-level textbook on the dynamical mean-field theory of multilayered nanostructures, which is designed to be accessible to graduate students who have completed a first-year quantum mechanics course. Advanced undergraduates might be able to understand this work as well. The manuscript was published in the Fall of 2006.

We have started a long-term case study to assess learning in the Quantum World Around Us, a course in materials science for non-science students.

We have integrated research in an industrial setting with graduate-student training as part of the Industrial Leadership in Physics program. With IBM as a partner, we are arranging for graduate students to spend one year at the Almaden Research Center during their PhD training. Ling Chen spent one year at IBM under the direction of Barbara Jones. He has published one paper on work started there and has a second in progress. Alexander Joura completed his one year internship at IBM in May 2005. He worked with Barbara Jones on analyzing quantum mirage STM images of a magnetic ion in a elliptical quantum corral. He also worked on an analogy between current-induced domain-wall switching and the Josephson effect, where the analogy helps explain the presence of steps in the current voltage characteristic similar to the Shapiro steps of a Josephson junction.
Currently, Simon Hale is working on magnetic storage problems in determining how to switch ultrasmall domains and increase storage density on magnetic tape storage. He has written an extensive computer code to calculate the magnetic properties of platelette-shaped disks, including dipole fields, with parameters set by experimental values of the systems studied at IBM. His code can calculate magnetic reversal paths as a function of time, for magnetic fields of various frequencies, and his work has revealed regions of reversal parameter space which can be used for unusual switching designs. He is working closely with the magetic tape experimental group at IBM Almaden, and is preparing a user-friendly version of the code which can be used by experimentalists and other theorists. At least one publication is planned on these results.

Research talks:

Invited talks:

[1] ``Inelastic Light Scattering and the Correlated Metal-Insulator Transition'' given at the NATO Advanced Research Workshop and School on Correlated Electronic Systems in Hvar, Croatia (Freericks, 2002)

[2] ``A simplified explanation of the Mott insulator-superfluid transition in the Bose Hubbard model,'' an atomic physics seminar at the National Institute of Standards and Technology (Gaithersberg) (Freericks, 2002).

[3] ``Multigap superconductivity in magnesium diboride,'' XI International Materials Research Congress, Cancun, Mexico (Liu, 2002)

[4] ``The Industrial leadership in Physics program at Georgetown

University," a seminar given at ENSCO, a technology company in Springfield, VA (Freericks, 2003)

[5] ``Inelastic light scattering and the correlated metal-insulator transition," at the Advanced Photon Source colloquium, Argonne National Laboratory (Freericks, 2003)

[6] ``Computational design and optimization of nanoscale spintronic and thermoelectric devices" given at the Nanotechnology interdisciplinary research team grantees conference at the National Science Foundation (Freericks, 2003)

[7] ``Strongly correlated multilayered nanostructures near the Mott transition" 28th International conference on nano and macro systems, Ustron, Poland (Freericks, 2004).

[8] ``Nanoscience at Georgetown," Meeting of the Nanotechnology Committee of the Northern Virginia Technology Council (Liu, with three other Georgetown faculty members, 2004).

[9] ``Electronic & Magnetic Structure of Transition-Metal Dicyanamide Molecule-Based Magnets," Annual Meeting of the Southeastern Section of the American Physical Society, Oak Ridge, TN (Liu, 2004).

[10] 'Nonequilibrium dynamical mean field theory,' Progress in Nonequilibrium Field Theory III, Kiel, Germany, (Freericks, 2005).

[11] ``Nonlinear response of a Mott insulator", Dynamical Mean-Field Theory for Correlated Electrons: Applications to Real Materials, Extensions and Perspectives, Trieste, Italy (Freericks, 2005).

[12] ``Optical sum rules for inelastic light scattering that relate to the potential energy of strongly correlated materials", Strongly Correlated Electrons Conference, Vienna, Austria (Freericks, 2005).

[13] ``The particle-hole asymmetric Mott transition", March meeting of the American Physical Society, Los Angeles, CA (Demchenko, 2005).

[14] ``Inelastic light scattering of a Mott insulator", seminar at the Oak Ridge National Laboratory, Oak Ridge, TN (Freericks, 2005).

[15] ``Thermal transport in strongly correlated nanostructures", Workshop on Strongly Correlated Thermoelectrics, and International Institute for Complex Adaptive Matter Workshop held in Hvar, Croatia, (Freericks, 2005).

[16] ``Sum Rules in Inelastic Light Scattering", Imperial College, London (Freericks, 2005).

[17] ``Electronic structure and schottky barrier formation in Fe/GaAs junctions: effects of interface structure," International Materials Research Congress, Cancun, Mexico (Liu, 2005).

[18] ``Nonequilibrium dynamical mean field theory of strongly correlated electrons," Rutgers University (Turkowski, 2006).

[19] ``Sum rules in inelastic Raman scattering", Resonant X-ray scattering workshop at the University of British Columbia, (Freericks, 2006).

[20] ``Nonlinear response of strongly correlated materials to a large electric field", 2006

User's Group Conference (DOD) in Denver, CO, (Freericks, 2006).

[21] ``Transport in multilayered nanostructures: the dynamical mean-field theory approach," 2006 Oxide thin-film workshop in Goettingen, Germany, (Freericks, 2006).

[22] ``Enhanced thermal transport in strongly correlated multilayered nanostructures," 30th international conference on nano and macro systems, Ustron, Poland, (Freericks, 2006).

[23] ``Enhanced thermal transport in strongly correlated multilayered nanostructures," Workshop on thermoelectric power generators for transportation, Oak Ridge National Laboratory (Freericks, 2006).

[24] ``Transient response of strongly correlated materials to a large electric field", 2007 User's Group Conference in Pittsburg, PA (DOD), (Freericks, 2007).

[25] ``Many body physics issues with the core hole propagator and resonant inelastic X-ray scattering", CMSN planning meeting, Argonne National Laboratory, (Freericks, 2007).

[26] ``Enhanced thermal transport in multilayered devices arising from electronic charge reconstruction", Materials Research Society, Spring Meeting, (Freericks, 2007).

[27] ``Nonlinear dynamical mean-field theory," March meeting of the American Physical Society, (Freericks, 2007).

[28] ``Inhomogeneous dynamical mean-field theory: transport in multilayered nanostructures", University of Augsburg, Germany (Freericks, 2007).

[29] ``Nonequilibrium dynamical mean-field theory: from strongly correlated electrons to ultracold atoms", University of Augsburg, Germany (Freericks, 2007).

[30] ``Nonequilibrium dynamical mean-field theory: from strongly correlated materials to ultracold atoms", APCTP and MPI-PKS Workshop on Strongly Correlated Electron Systems, Pohang, S. Korea, (Freericks, 2007).

[31] ``The electron-phonon interaction in LiB," Workshop on Ab Initio Approaches to Electron-Phonon Coupling, San Sebastian, Spain (Liu, 2007).

Contributed talks:

[1] ``Crossover from tunneling to bulk scaling limit in correlated nanostructures" given at the Fall meeting of the Materials Research Society in Boston, Massachusetts (Freericks, 2003)

[2] ``Effects of electron correlations on bulk thermal transport" given at the March meeting of the APS, Montreal, CA (Joura, 2004)

[3] ``Effects of the Particle-Hole Asymmetry on the Mott-Hubbard Metal-Insulator Transition" given at the March meeting of the APS, Montreal, CA (Demchenko, 2004).

[4] ``Electronic and Magnetic Structure of Transition-Metal Dicyanamide Molecule-based Magnets" given at the March meeting of the APS, Montreal, CA (Demchenko, 2004).

[5] ``Crossover from tunneling to Ohmic (incoherent) transport in a correlated nanostructure" given at the March meeting of the APS, Montreal, CA (Freericks, 2004).

[6] ``F-electron spectral function near a quantum critical point" Strongly Correlated Electron Conference, Karlsruhe, Germany (Freericks, 2004).

[7] ``Parallelizing the Keldysh formalism for strongly correlated electrons" 2004 Users group conference (HPCMO), Williamsburg, Virginia (Freericks, 2004).

[8] ``Electronic structure and Schottky barier formation in Fe/GaAs magnetic junctions, March meeting of the American Physical Society, Los Angeles, CA (Demchenko, 2005).

[9] 'Analytic properties of the insulating solution of the half-filled Hubbard model', March Meeting of the American Physical Society, Los Angeles, CA (Joura, 2005).

[10] 'Nonequilibrium properties of a Mott insulator in an external electric field', March Meeting of the American Physical Society, Los Angeles, CA (Turkowski, 2005).

[11] ``Thermal transport in strongly correlated multilayered nanostructures", March meeting of the American Physical Society, Baltimore, MD (Freericks, 2006).

[12] 'Nonlinear response of a Mott insulator', March Meeting of the American Physical Society, Baltimore, MD (Turkowski, 2006).

[13] ``Combining advantages of superconducting MgB2 and CaC6: suggestions from first-principles calculations," March Meeting of the American Physical Society, Denver, CO (Liu, 2007).

Findings:

We have found some interesting features in the transport through nanostructures. In particular we have observed directly the crossover from an exponential scaling (tunneling) regime for the resistance to a bulk ``ohmic" linear scaling regime as functions of thickness and interaction strength. We discovered that this crossover is determined by a generalized Thouless energy, which can provide simple diagnostics for real systems. This work is important for the design of tunnel-based devices (nonvolatile memory, Josephson junctions, etc.) In addition, we discovered novel features of the Mott insulator when it is confined on the nanoscale between two semi-infinite metallic leads. We have discovered an interesting enhancement of thermal transport (figure of merit ZT>1) at low temperature near the metal-insulator transition. We have also made significant progress in understanding the principles of inelastic light scattering in correlated materials, laying the groundwork for a future study on scattering from nanostructures. We have also discovered a new sum rule for inelastic light scattering (Raman and x-ray). We have fully developed the many-body formalism for nonequilibrium dynamical mean field theory in both the steady state and in the transient response regime. Our results show how Bloch oscillations are quenched in a strongly correlated material in a large field. We also determined a series of spectral moment sum rules for the nonequilibrium problem, which turn out to be independent of the time-dependence of the electric field (in many cases).

In our study of Fe/GaAs and Co/GaAs interfaces, we find good agreement between calculated Schottky barrier heights and recent values measured on very clean interfaces. The calculated barriers display a moderate dependence on interface structure, consistent with discrepancies in measured barrier heights reported in the literature. In Fe/GaAs, we find that minority-spin Fe interface states induce states within the semiconductor gap, providing an additional channel for tunneling of minority spins. The proximity of these interface states to the Fermi level, which affects the magnitude and possibly the sign of the spin polarization of the tunneling current, is found to vary significantly with interface structure.

In our investigation of the 3d-transition-metal dicyanamide molecular magnets, we have found that structural differences in the superexchange pathway are not sufficient to account for changes in magnetic order across the series. Instead, the occupation of the 3d orbitals is the dominant factor.

A simple model, loosely based on the unconventional superconductor Sr_2Ru_O4, was used to investigate the possibility of phonon-induced non-s-wave superconductivity. The model includes an electron-phonon interaction and a spin-fluctuation-induced pairing interaction. Separately, each interaction favors singlet pairing, but in combination, we find a variety of singlet and triplet pairing symmetries that are not ground states of the individual interactions. Our results suggest that the interplay between the spin and phonon pairing interactions could be key to understanding the order-parameter symmetry in Sr_2RuO_4, and possibly in other unconventional superconductors.

Training and Development:

Denis Demchenko, whose graduate training was in electronic structure and magnetism, has broadened his research skills by learning about many-body theory and superconductivity (he has already completed three publications in many-body physics). He also benefited greatly from attending the 2003 Boulder Summer School on Frontiers of Magnetism.

Alexander Joura, Ling Chen, Simon Hale and Peng Wang are graduate students who have worked on the grant. Ling Chen spent one year at IBM's Almaden Research Center (under the direction of Barbara Jones), and is now back at Georgetown working on understanding electronic charge reconstruction of strongly correlated nanostructures. Alexander Joura finished a one year apprenticeship at IBM in May of 2005. He is now studying the steady-state nonequilibrium response of a Mott insulator. Simon Hale is currently on an apprenticeship at IBM working on magnetic storage. These apprenticeships are an integral part of our graduate program 'Industrial Leadership in Physics' which aims to prepare graduate students for careers in industry.

We also worked with a Georgetown undergraduate, Ron Stimmel, to develop the assessment case study (supported by internal Georgetown funds). He is learning about physics education research, and how to create unbiased questionnaires and interviews.

We sent a sophomore undergraduate (Greg Nelson) to Velko Zlatic's group in Zagreb, Croatia in the summer of 2005 to work on measuring the thermopower and charge transport in different samples of tantalum deficient tantalum nitride that we will obtain from Nate Newman's group at Arizona State University. He also carried out some modeling of the results.

A sophomore physics major, Sean Boocock, learned about visualization of complex datasets. He successfully produced images of oscillations in the DOS of strongly correlated nanostructures. He also worked on imaging the distribution functions of strongly correlated electrons placed in an electric field.

Outreach Activities:

We are participating in discussions with other colleagues at Georgetown who are working in nanoscience on jointly organizing activities such as seminars, public lectures, and an educational web site on nanotechnology. In conjunction with this initiative, a group of us spoke about Georgetown's nanoscience research and education programs at a meeting of the Northern Virginia Tech Council.

We have developed a website for our NIRT project that summarizes all of our research activities and products including publications and presentations. We are working on developing descriptions of our work suitable for nontechnical audiences.

Journal Publications

T. P. Devereaux, G. E. D. McCormack and J. K. Freericks, " Inelastic x-ray scattering in correlated (Mott) insulators", Physical Review letters, p. 067402, vol. 90, (2003). Published,

J. K. Freericks, T. P. Devereaux, R. Bulla, and Th. Pruschke, "Nonresonant inelastic light scattering in the Hubbard model", Physical Review B, p. 155102, vol. 67, (2003). Published,

A. M. Shvaika and J. K. Freericks, "Equivalence of the Falicov-Kimball and Brandt-Mielsch forms for the free energy of the infinite-dimensional Falicov-Kimball model", Physical Review B, p. 153103, vol. 67, (2003). Published,

J. K. Freericks and V. Zlatic, "Exact dynamical mean field theory of the Falicov-Kimball model", Reviews of Modern Physics, p. 1333, vol. 75, (2003). Published,

J. K. Freericks, D. Demchenko, A. Joura, and V. Zlatic, "Optimizing thermal transport in the Falicov-Kimball model: binary-alloy picture", Physical Review B, p. 195120, vol. 68, (2003). Published,

V. Zlatic' and J. K. Freericks, "DMFT solution of the Falicov-Kimball model with an internal structure", Acta Physica Polonica B, p. 931, vol. 34, (2003). Published,

J. K. Freericks, T. P. Devereaux, and R. Bulla, "Inelastic light scattering and the correlated metal-insulator transition", Proceedings NATO ARW on Electron Correlations, p. 115, vol. 110, (2003). Published,

V. Zlatic' and J. K. Freericks,, "Describing the valence-change transition by the DMFT solution of the Falicov-Kimball model", Proceedings of the NATO ARW on Electron Correlations, p. 287, vol. 110, (2003). Published,

T. P. Devereaux, G. E. D. McCormack and J. K. Freericks, " Inelastic x-ray scattering as a probe of electronic correlations", Physical Review B, p. 075105, vol. 68, (2003). Published,

R. Lemanski, J.K. Freericks and G. Banach, "Charge stripes due to electron correlations in the two-dimensional spinless Falicov-Kimball model", Journal of Statistical Physics, p. 699, vol. 116, (2004). Published,

Ling Chen, B. A. Jones, and J. K. Freericks, "Charge-density-wave order parameter of the Falicov-Kimball model in infinite dimensions", Physical Review B, p. 153102, vol. 68, (2003). Published,

J. K. Freericks, "Crossover from tunneling to incoherent (bulk) transport in a correlated nanostructure", Applied Physics Letters, p. 1383, vol. 84, (2004). Published,

A. V. Joura, D. Demchencko, and J. K. Freericks, "Thermal transport in the Falicov-Kimball model on a Bethe lattice", Physical Review B, p. 165105, vol. 69, (2004). Published,

A. M. Shvaika, O. Vorobyov, J. K. Freericks, and T. P. Devereaux, "Resonant Enhancement of Inelastic Light Scattering in Strongly Correlated Materials", Physical Review Letters, p. 137402, vol. 93, (2004). Published,

D.O. Demchenko, A.V. Joura, and J.K. Freericks, "Effect of particle-hole asymmetry on the Mott-Hubbard metal-insulator transition", Physical Review Letters, p. 216401, vol. 92, (2004). Published,

D. O. Demchenko, A. Y. Liu, E. Z. Kurmaev, L. D. Finkelstein, V. R. Galakhov, A. Moewes, S. G. Chiuzbaian, M. Neumann, C. R. Kmety, and K. L. Stevenson, "Electronic Structure of Transition-Metal Dicyanamides Me[N(CN)2]2 (Me=Mn, Fe, Co, Ni, Cu)", Physical Review B, p. 205105, vol. 69, (2004). Published,

J. K. Freericks, "Dynamical mean field theory for strongly correlated inhomogeneous multilayered nanostructures", Physical Review B, p. 195342, vol. 70, (2004). Published,

J. K. Freericks, "Strongly correlated multilayered nanostructures near the Mott transition", physica status solidi b, p. 189, vol. 242, (2005). Published,

A. M. Shvaika, O. Vorobyov, J. K. Freericks, and T. P. Devereaux, "Electronic Raman scattering in correlated materials: A treatment of nonresonant, mixed, and resonant scattering with dynamical mean field theory Materials,", Physical Review B, p. 045120, vol. 71, (2005). Published,

J. K. Freericks, V. Turkowski, and V. Zlatic', "F-electron spectral function of the Falicov-Kimball model in infinite dimensions: The half-filled case", Physical Review B, p. 115111, vol. 2005, (71). Published,

V. Turkowski and J. K. Freericks, "Nonlinear response of Bloch electrons in infinite dimensions", Physical Review B, p. 085104, vol. 71, (2005). Published,

J.K. Freericks, T.P. Devereaux, M. Moraghebi, and S.L. Cooper, "Optical sum rules that relate to the potential energy of strongly correlated systems", Physical Review Letters, p. , vol. 94, (2005). Published,

J. K. Freericks, V. O. Turkowski, and V. Zlatic', "F-electron spectral function near a quantum critical point", Physica C, p. 684, vol. 359-361, (2005). Published,

A. M. Shvaika, O. Vorobyov, J. K. Freericks, and T. P. Devereaux, "Resonant electronic Raman scattering near a quantum critical point", Physica C, p. 705, vol. 359-361, (2005). Published,

A. M. Shvaika, O. Vorobyov, J. K. Freericks, and T. P. Devereaux, "Resonant Enhancement of Electronic Raman Scattering", Journal of the Physics and Chemistry of Solids, p. 336, vol. 67, (2006). Published,

V. M. Loktev and V. Turkowski, "On the theory of pseudogap anisotropy in the cuprate superconductors", International Journal of Modern Physics B, p. 2035, vol. 18, (2004). Published,

K. Park, E.-C. Yang, and D.N. Hendrickson, "Electronic structure and magnetic anisotropy for nickel-based molecular magnets", J. Appl. Phys., p. 10M522, vol. 97, (2005). Published,

A. N. Tahvildar-Zadeh, J. K. Freericks, and B. K. Nikolic', "Thouless energy as a unifying concept for Josephson junctions tuned through the Mott metal-insulator transition", Phys. Rev. B, p. 184515, vol. 73, (2006). Published,

J. K. Freericks and V. M. Turkowski, "Steady-state nonequilibrium dynamical mean-field theory and the quantum Boltzmann equation", J. Phys.: Conf. Ser., p. 39, vol. 35, (2006). Published,

V. Zlatic', R. Monnier, and J. K. Freericks, "Thermoelectricity of EuCu$_2$(Ge$_{1-x}$Si$_x$)$_2$ intermetallics", Physica B, p. 661, vol. 378--38, (2006). Published,

V. M. Turkowski and J. K. Freericks, "Spectral moment sum rules for strongly correlated electrons in time-dependent electric fields", Phys. Rev. B, p. 075108, vol. 73, (2006). Published,

V. Zlatic', R. Monnier, J. K. Freericks, and K. Becker, "Relationship between the thermopower and entropy of strongly correlated electron systems
electron systems", Phys. Rev. B, p. 085122, vol. 76, (2007). Published, 10.1103/PhysRevB.76.085122

J. K. Freericks and V. Zlatic', "Nonlinear Peltier effect and the nonequilibrium Jonson-Mahan theorem", Special issue of Cond. Matter Phys. on Green's functions, p. , vol. 9, (2006). Published,

K. Park et al., "Electronic structure and vibrational spectra of C_2B_10-based clusters and films", Phys. Rev. B, p. 035109, vol. 73, (2006). Published,

D. O. Demchenko and A. Y. Liu, "Influence of interface structure on electronic properties and Schottky barriers in Fe/GaAs magnetic junctions", Phys. Rev. B, p. 115332, vol. 73, (2006). Published,

K. Park, M. R. Pederson, and A. Y. Liu, "Comparison of vibrational and electronic contributions to van der Waals interactions
", Phys. Rev. B, p. 205116, vol. 73, (2006). Published,

I. Schnell, I. I. Mazin, and A. Y. Liu, "Unconventional superconducting pairing symmetry induced by phonons", Phys. Rev. B, p. 184503, vol. 74, (2006). Published,

Freericks, JK; Devereaux, TP, "Sum rules for inelastic light scattering in the Hubbard model", PHYSICA B-CONDENSED MATTER, p. 650, vol. 378-80, (2006). Published, 10.1016/j.physb.2006.01.18

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Chen, L; Freericks, JK, "Electronic charge reconstruction of doped Mott insulators in multilayered nanostructures", PHYSICAL REVIEW B, p. , vol. 75, (2007). Published, 10.1103/PhysRevB.75.12511

Freericks, JK; Zlatic, V; Shvaika, AM, "Electronic thermal transport in strongly correlated multilayered nanostructures", PHYSICAL REVIEW B, p. , vol. 75, (2007). Published, 10.1103/PhysRevB.75.03513

Freericks, JK; Turkowski, VM; Zlatic, V, "Nonequilibrium dynamical mean-field theory", PHYSICAL REVIEW LETTERS, p. , vol. 97, (2006). Published, 10.1103/PhysRevLett.97.26640

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Web/Internet Site

URL(s):
http://physics.georgetown.edu/~jkf/nirt.html
Description:
This site presents all research results from the NIRT grant.

Other Specific Products

Contributions

Contributions within Discipline:

We are developing new ways of calculating the transport in devices that have correlated materials in them. This technique, based on dynamical mean field theory, goes beyond the conventional quasiclassical approach and can be applied to many different kinds of devices. Of recent interest is the ability to examine the crossover from a tunneling regime to an ``Ohm's'' law regime.
We have also been calculating effects of charge transfer at interfaces (Schottky-like effects) and have been generalizing the transport codes to examine thermal transport. A graduate-level text has been completed on this subject. Ling Chen spent one year working with Barbara Jones on spin transport, namely current-driven magnetic-domain wall reversal in nanopillars being investigated in Stuart Parkin's laboratory. That work has not yet led to a publication. Alexander Joura also spent one year working with Barbara Jones on electrons in quantum corrals and on current-induced domain wall motion. Simon Hale spent one year working with Barbara Jones on magnetic storage problems.
We also have been calculating properties associated with inelastic light scattering. We have investigated the nonresonant case for x-ray scattering and the resonant case for Raman scattering.
A long review article in Reviews of Modern Physics summarizes a decade's worth of work on correlated systems, with a novel formalism based on path integrals in Matsubara frequency space. We have also completed significant work on the nonequilibrium many-body problem, including a first exact solution of the nonlinear response of a Mott insulator, and the derivation of sum rules for spectral functions. Our materials-specific studies of magnetic junctions suggests that details of interfacial structure can significantly influence spin transport across these junctions. Our work on the dicyanamides helps settle a debate in the literature on the role of small structural differences in determining the magnetic ground state.

Contributions to Other Disciplines:

We have determined new optical sum rules for Raman scattering that relate to the potential energy (similar to the optical sum rule, which relates to the kinetic energy). These new sum rules may have an impact into a wide number of disciplines, as sum rules are generically one of the most important theoretical discoveries in spectroscopy. These results have been published in Physical Review Letters.

We developed the formalism for nonequilibrium dynamical mean field theory, which, being perhaps the only exactly solvable many-body nonequilibrium problem, is likely to have impact in other fields where nonequilibrium physics in the presence of strong electron correlations is important (techniques could be applied to cold atom systems or to quantum-dot/mesoscopic systems). In addition, we have developed a series of sum rules here too.This work was awarded a national leadership in computing grant by Nasa for 900,000 hours on their supercomputer Columbia. It is the only physics project chosen during the 2006 competition.

Contributions to Human Resource Development:

We are training students for research in physics and exposing them to both academic and industrial environments. We have helped post-doctoral fellows broaden their perspective on condensed-matter physics and strengthen their computational and theoretical research skills. We are sending undergraduate students on research experiences in Europe to help develop their appreciation for the international and collaborative nature of science research.

We have completed a graduate level textbook on mutilayered nanostructures and dynamical mean-field theory. It was published in 2006.

Contributions to Resources for Research and Education:

We have begun a multi-year case study in collaboration with Stamatis Vokos (Seattle Pacific University) to assess the long-term learning of students who take 'The Quantum World Around Us,' a materials science course we designed for nonscientists. In the project, former students A are asked to read a Scientific American article (Quantum Seeing in the Dark). They are then interviewed to assess their understanding. This work involves undergraduate researchers (Ron Stimmel) in the development and implementation of the survey, and draws upon the expertise of Georgetown's Center for New Designs in Learning. Currently, five undergraduate alumni of the quantum mechanics course have been interviewed.

Contributions Beyond Science and Engineering:

Categories for which nothing is reported:

Any Product

Contributions: To Any Beyond Science and Engineering