Computational design and optimization of nanoscale spintronic and thermoelectric devices

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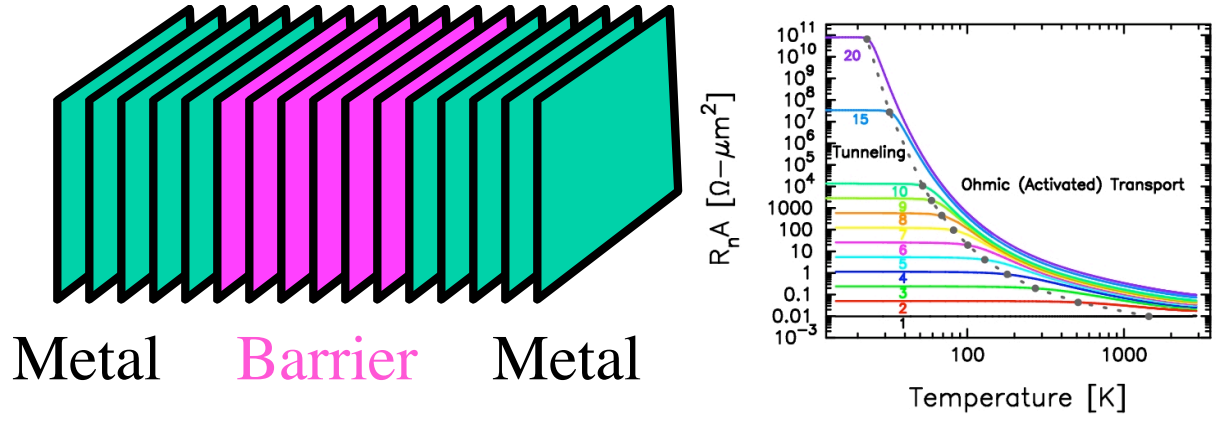
PIs: **J. K. Freericks[a], A. Y. Liu[a], and B. A. Jones[b]**
[a]Georgetown University and [b]IBM, Almaden Research Center

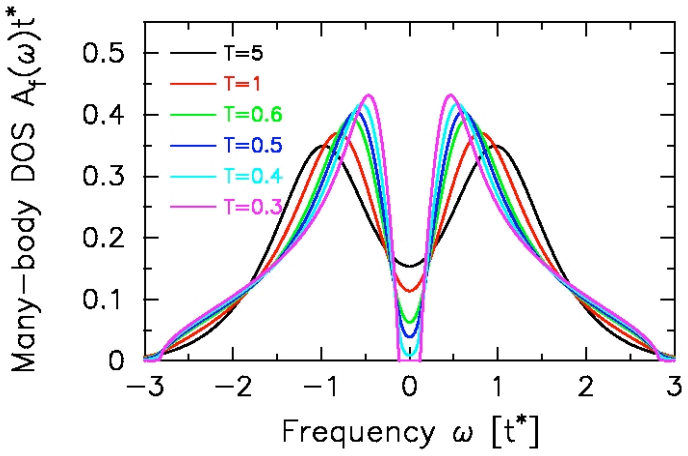
The electronic devices of the future will have smaller and smaller functional sizes on the nanoscale. While creation of electronic devices, with all dimensions of the circuitry on the nanoscale is still many years off, a number of important devices are already in use that have layers that are only nanometers thick. One class of such devices is tunnel junctions, where metallic leads are separated by a thin insulating layer. Our project focuses on these kinds of devices, but with the barriers constructed out of correlated materials, which can have their metallicity tuned to lie close to the metal-insulator boundary, and where the thickness is tens to hundreds of atomic layers rather than the few layers of an ultrathin tunnel junctions [1]. The fundamental questions we want to answer are how do electrons conduct charge and heat through these devices? What happens to many-body correlations when squeezed on the nanoscale? Can device perfomance be improved by using correlated materials in the barrier? Can we design useful spintronic or thermoelectric materials using these ideas? Can new experimental probes like inelastic x-ray scattering investigate local charge and magnetic excitations in these devices?

We use an inhomogeneous version of the dynamical mean field approximation, coupled with density functional theory calculations to model the properties of different nanoscale devices. The dynamical mean field theory is a well controlled technique for including many-body correlations into equilibrium and nonequilibrium problems. Our strategy is to use density functional theory to determine microscopic parameters of the interfaces (electronic screening length, spin-polarization, electrical polarizability, etc.) and then input these parameters into a simplified many-body physics transport code. We perform equilibrium calculations to determine the linear-response regime of these systems (junction resistance, junction capacitance, thermopower, thermal resistance, etc.) and then use nonequilibrium calculations to examine nonlinear response effects such as current-voltage characteristics, heat flow, switching speeds, etc.



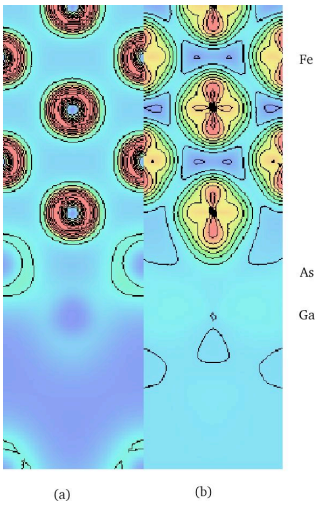
During the first year we have focused on first developing a series of equilibrium codes that can calculate the transport properties. To date, we are able to determine the many-body density of

states (to examine localized interface states, the exponential decays of the electronic wavefunctions as they move into the barrier, and so on), the electrical resistance, thermopower, and thermal resistance for junctions that do not have Schottky-like rearrangements of charge or spin polarizations. Using these codes, we observed the crossover from tunneling-like behavior of a junction to incoherent (thermally-activated) Ohmic transport as functions of the barrier thickness and the temperature. In so doing, we discovered a generalization of the Thouless energy to the case where the barrier is an insulator which can be easily employed as a diagnostic to predict (or even engineer) where the crossover from tunneling to incoherent transport takes place [2].



We also have spent a significant amount of time working on developing the nonequilibrium formalism. For this problem, one must integrate the electronic path integral over a Keldysh contour, and determine electronic Green's functions that depend on two time variables. We have tested this formalism by performing the analytic continuation of a bulk equilibrium problem, which evolves in a nontrivial time-dependent field, and cannot be solved by any other technique. This test case is nearly complete, and future work will focus on developing codes for true nonequilibrium problems and for the inhomogeneous systems. We include a figure of the temperature dependent density of states and how a gap opens as the temperature is lowered (due to the strong correlations).

Our computer algorithms have the benefit that they are easy to parallelize, and that they tend to scale linearly with the number of processors. Hence we are able to get good throughput on massively parallel computational platforms when we do production runs.



Our first-principles studies of interfaces have focused on lattice-matched Fe/GaAs and Co/GaAs structures. It has been noted that different surface reconstructions and atomic relaxations can exhibit significantly different properties. The calculated charge and spin densities for the structurally relaxed As-terminated Fe/GaAs(001) interface are shown in the figure to the left. A significant distortion of the spin density can be seen at the interface. Using the method of macroscopic averaging, we obtain Schottky barrier heights, potential, charge, and magnetization profiles across the interface. Preliminary results for the barrier heights are in good agreement with available experimental data.

On a different project, we have been studying the electronic and magnetic properties of dicyanomide molecule-based magnets ($M[N(CN)_2]_2$, with M=Mn, Fe, Co, Ni, and Cu). In moving across the series, the magnetic ordering varies from a canted antiferromagnet to a ferromagnet. Our calculations indicate differences in the angle of the superexchange pathway are less important than the occupation of the d-shell in determining the type of magnetic order [3].

We have also been investigating the current-induced magnetization reversal in magnetic domains of nanopillars, building upon earlier work on current-induced reversal in multilayered pillars constructed out of magnetic/nonmagnetic/magnetic materials. Our work is focusing on the generalization of the Gilbert equations appropriate for the domain-wall system. We find that the majority of the scattering occurs at the metallic lead interface, not at the domain-wall boundaries and the proper evolution of the spins requires one to consider the full spatial profile of the magnetization, not just the Slonczewski-like terms.

Finally, we have invested some effort on continuing to investigate resonant effects in Raman and inelastic x-ray scattering [4], with the hope of constructing a theory of resonant x-ray scattering that can be used as a high precision probe of correlated nanostructures.

Part of our project involves developing a mini network with European researchers interested in similar problems. Dr. Veljko Zlatic from Croatia has visited Georgetown University during the first year of the grant and he is actively working on the nonequilibrium project. A trip to visit the Steglich group in Dresden is planned for next summer, and we are currently trying to recruit an undergraduate researcher to work part of the summer in Zlatic's labs in Croatia.

The Department of Physics at Georgetown University has developed a graduate program designed to train Ph.D.'s who desire to work in industry. One requirement of the program is a year-long apprenticeship at an industrial site. This past year, Ling Chen was sent to IBM's Almaden Research Center to work with Barbara Jones on the current-induced magnetization reversal in magnetic nanopillars. We also teach a Materials Science and quantum mechanics course for nonscientists that employs techniques like the tutorial system developed at the University of Washington to foster conceptual-based learning. We are currently planning to start a case-study to document the long-term learning that takes place in the course.

References

[1] For further information about this project email **freericks@physics.georgetown.edu, liu@physics.georgetown.edu, or bajones@almaden.research.ibm.com .**
[2] Submitted to Applied Physics Letters (2003).
[3] Submitted to Phys. Rev. B.
[4] Submitted to Phys. Rev. Lett.