REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	2. REPORT TYPE	3. DATES COVERED *(From - To)*
17-12-2007	Final	21-10-2004--30-09-2007

4. TITLE AND SUBTITLE Theoretical modeling of 10K and 30K Josephson junctions	**5a. CONTRACT NUMBER**
	5b. GRANT NUMBER N00014-05-1-0078
	5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S) James K. Freericks	**5d. PROJECT NUMBER**
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Georgetown University 37th and O Sts. NW Washington, Dc 20057	**8. PERFORMING ORGANIZATION REPORT NUMBER**
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) Office of Naval Research 875 N. Randolph St. Arlington, VA 22203-1995	**10. SPONSOR/MONITOR'S ACRONYM(S)** ONR
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release; distribution is unlimited.

20071226039

13. SUPPLEMENTARY NOTES

14. ABSTRACT

This is the final report for grant N000140510078. Work was completed on a number of projects including developing a multiband multilayered inhomogeneous dynamical mean-field theory code for analyzing properties of magnesium diboride junctions. In addition, work was completed on how one can use a generalized Thouless energy to describe properties of Josephson junctions, and on the nonlinear response of strongly correlated materials to large electric fields. The PI was also involved in two successful CAP projects with the HPCMO. Finally, a textbook entitled Transport in multilayered nanostructures: the dynamical mean-field theory approach was published by Imperial College Press.

15. SUBJECT TERMS

Josephson junctions, magnesium diboride, nonlinear response, electric field, strongly correlated materials, metal-insulator transition

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			James Freericks
U	U	U	UU	6	19b. TELEPHONE NUMBER *(Include area code)* 703-807-0776

Final report on theoretical modeling of 10K and 30K Josephson junctions

Grant number N000140510078

J. K. Freericks, Department of Physics, Georgetown University, Washington, DC

Executive Summary

Work on MgB_2 junctions completed a general multiband JJ code for the supercurrent as a function of the phase difference across the junction. This code takes into account the correct geometry and sp-hybridized bands of the material and also includes the superconducting two-gap structure. This work is still in the production stage for the running of the code; a paper is expected to be completed in the Winter of 2008. In addition, we finished work on a series of projects. We have published a paper that summarizes all we have learned about how to employ the Thouless energy to describe transport in both the normal and the superconducting states when the barrier is tuned to lie close to a metal-insulator transition. Our work demonstrates clearly why the quasiclassical approach works so well, and it shows specifically how the quasiclassical approach breaks down as the barrier undergoes a metal-insulator transition. We have also finished work on understanding nonequilibrium transport for materials close to the metal-insulator transition. This effort is important because it allows one to uncover the nonlinear response of devices, and it is often the nonlinear response which determines the overall device performance. In addition, military applications usually operate in extreme environments, where the electric fields over the devices can be large. In this regime nonlinearities also play a critical role. We have utilized significant high performance computing resources for this project; we successfully completed a Capabilities Application Project Phase II award from the HPCMP office which included finding and reporting bugs in the operating system. The ERDC computer center has published an article on the success of this project for their newsletter, and Cray has made a marketing poster highlighting these results. We have one article on this work published in Phys. Rev. Lett. one under review at Phys. Rev. B and one being planned for submission to Nature Physics. We also have a scientific outreach project, as the PI has written a graduate level textbook on the theoretical description of multilayered nanostructures from the dynamical mean-field theory perspective with Imperial College Press. The book was published in the winter of 2006. The book has one chapter on the Thouless energy work and one chapter on Josephson junctions, which highlights work completed under ONR support over the past five years. It also used research pictures from the labs of Nate Newman, Bob Buhrman, and X-X. Xi, which further highlight the program's activities.

Summary of work completed

We developed a multiband Josephson junction code to calculate the critical current carried in a MgB_2 device. We finished work on using the Thouless energy to understand transport in superconducting Josephson junction with barriers tuned to lie close to a metal-insulator transition (MIT) and on solving the formalism to examine nonequilibrium dynamical mean-field theory and the nonlinear response of systems that lie close to a MIT. Work was also completed on studying properties of tantalum deficient TaN as a barrier for a Josephson junction. Finally, a graduate level textbook has been completed that highlights much work supported by the ONR superconducting electronics program, including the theoretical treatment of JJs with barriers near the MIT and some experimental work of Newman, Buhrman, and Xi.

The main ongoing work that we have been engaged in is developing a multiband model for transport in Josephson junctions made of MgB_2. We developed a code to evaluate the supercurrent as a function of the phase difference across the junction. This work required significant modifications of our old codes to take into account the geometry and symmetry of the different orbitals, and is now complete. We were selected to run in a Phase I CAP project, but were not selected for Phase II production, so we are trying to find sufficient computer time to finish the project; we anticipate this to be done by the Winter of 2008. In the code, we include the s-p hybridized bands of the boron atoms, since these are the orbitals close to the Fermi energy. The hexagonal plane unit cell requires a basis of two atoms, so the electronic band structure has eight active bands. The superconducting interaction is chosen to reproduce the two-gap structure---a large gap on the two-dimensional planar bands and a small gap on the bands that primarily transport between the planes. Since the planar bands do have some direct overlap between neighboring planes, there are actually two sources of current within the Josephson junction, arising from each of the bands. Our codes calculate the current flowing through each of these bands, so we can separately determine the contribution from each to the total current. This will eventually allow us to examine what properties are most likely to reduce the current from the large gap states, or, if possible, how to enhance that current. An example of results from this code appear in Fig. 1. Note how the portion of the current that arises from the two-d band (and hence from the large gap) is sizeable, even larger than the portion that arises from the three-d band with the small gap, even though the junction is a c-axis junction. This is already a surprising result, which can be seen only through this kind of theoretical modeling. What it potentially implies is that the c-axis junctions may be able to achieve large currents even though the current flows perpendicular to the planes. We will also examine more physically realistic cases, as described below.

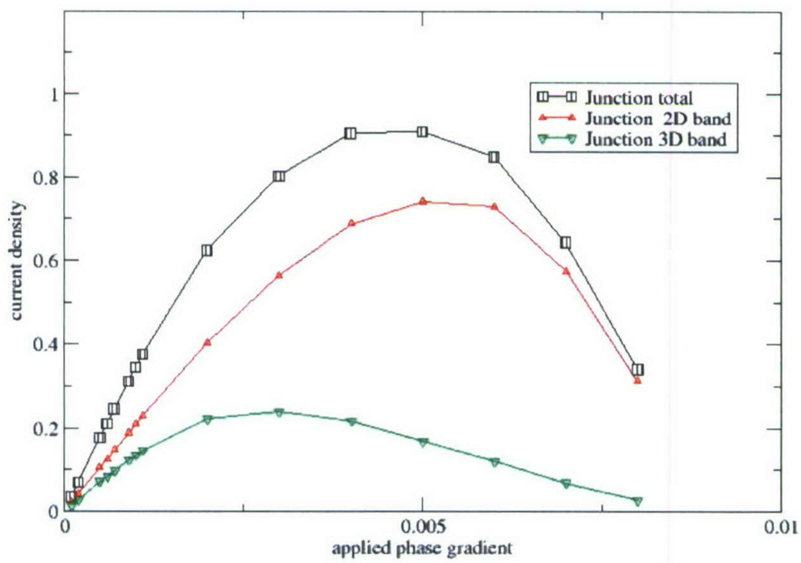

Figure 1. *Current versus the phase gradient in the leads for an artificial test-case junction that is made of MgB_2 everywhere, but has the superconducting pairing turned off in the barrier (black curve). The current density is compared to that of bulk MgB_2 (blue curve), and it is separated into the components coming from the large gap (red curve) and the small gap (green curve). Note how the majority of the current is carried by the large gap, even though this is a c-axis junction; this is especially true near the critical current through the junction.*

We finished our work on using the Thouless energy to describe transport in strongly correlated Josephson junctions. The main focus of this work, which was published as an ASC conference proceedings and as a Phys. Rev. B regular article (J. K. Freericks, A. N. Tahvildar-Zadeh, and B. K. Nikolic, *"Use of a generalized Thouless energy in describing the transport properties of Josephson junctions"*, IEEE Trans. Appl. Supercond. **15**, 896—899 (2005) and A. N. Tahvildar-Zadeh, J. K. Freericks, and B. K. Nikolic, *"Thouless energy as a unifying concept for Josephson junctions tuned through a the Mott metal-insulator transition"*, Phys. Rev. B **73**, 184515-1—10 (2006) and Virtual Journal of Applications of Superconductivity, **10,** Issue 10 (2006)), was to find a unifying means to describe barriers independent of whether they are described as metals or insulators. Our criterion is fairly simple to use, and we hope it will be adopted by experimentalists. Some of the results from this work, and from some previously completed work, appear in Figure 2, where we show a false color plot of the electronic DOS for the strongly correlated device, illustrating the Friedel-like oscillations induced by the nanoscale inhomogenity, and a plot of the figure-of-merit for the Josephson junction, which indicates how the quasiclassical approach breaks down as the barrier becomes more insulating. What is remarkable is that, when expressed in terms of the Thouless energy, the figure-of-merit is described by the quasiclassical approach well outside of its putative realm of validity. This helps explain why the quasiclassical approach works for so many different devices. The phenomenon is similar to a universality relation, but, since it does not involve a diverging length scale around a critical temperature, such a language is not normally used.

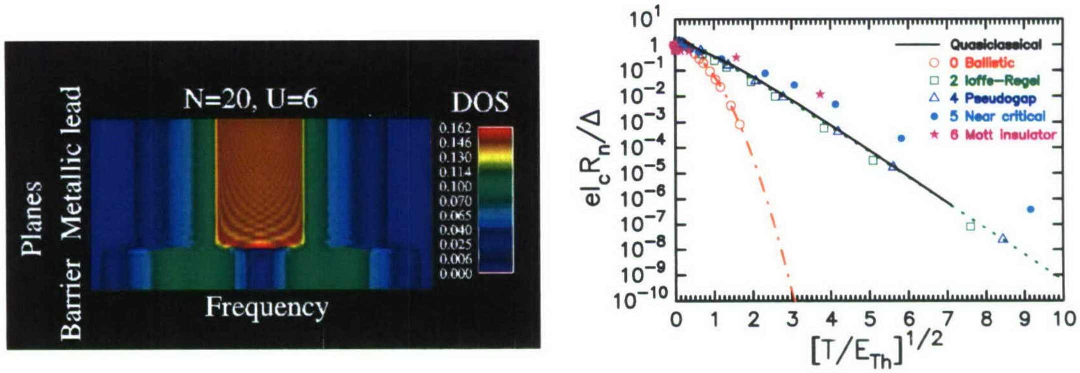

Figure 2. *The left panel shows the many-body DOS of an N=20 thick barrier embedded in a metallic-lead sandwich (only half of the junction is shown). Note the Friedel oscillations in the metal, and the mismatch of the bands due to the insulating behavior in the barrier. The right panel shows a plot of the JJ figure of merit divided by the superconducting gap, versus the square root of the ratio of the temperature to the Thouless energy. This formulation provides a clear distinction between the ballistic case (lowest curve), the diffusive case (middle curves with the quasiclassical approach in the solid black line) and the correlated insulator case (uppermost curves).*

The Thouless energy work shows a remarkable similarity in the behavior of the Josephson-junction figure-of-merit for a diffusive barrier and for a barrier on the insulating side of the MIT which undergoes a tunneling-incoherent transport crossover as a function of thickness. We use this observation to explain and understand how the quasiclassical approach to JJ's begins to fail as the barrier becomes more insulating.

Our work on nonequilibrium problems has finally reached fruition with the solving of two significant research problems. The first one, which is actually an equilibrium problem solved with the nonequilibrium formalism, is to determine the spectral function of the localized electron in the Falicov-Kimball model. This problem is nontrivial, because the conduction electron hops onto and off of the local site as a function of time, and the f electron feels the presence of the conduction electron via the on-site Coulomb interaction. We have had three papers published on this topic, two conference proceedings (HPC Users group conference, 2004, where we had an oral presentation, and SCES'04, where we had a poster), and one regular PRB article [*Parallelizing the Keldysh formalism for strongly correlated electrons*, in Proceedings of the Users Group Conference Williamsburg, VA, June 7--11, 2004 (IEEE Computer Society, Los Alamitos, CA, 2004), p. 7—16; *F-electron spectral function near a quantum critical point*, (proceedings of the Strongly Correlated Electron Systems conference, Karlsruhe, Germany), Physica **359--361C**, 684--686 (2005); and *F-electron spectral function of the Falicov-Kimball model in infinite dimensions: The half-filled case*, Phys. Rev. B **71**, 115111--1-12 (2005)]. Results are summarized in the two figures, where the f-electron DOS develops a sharp peak (much sharper than the conduction DOS) when the system is metallic (left), and where it develops a gap (similar to the conduction DOS) when the system is a Mott insulator. These calculations employed significant HPC resources. After our work was completed, a German group re-analyzed our work using a numerical renormalization group approach. They find that the DOS actually has a divergence as a power law at T=0 when in the metallic phase, and it goes to zero in the insulating phase. This was then followed up by some Chinese work which provided analytic support for such a scenario. This divergence is identical to the behavior in the X-ray edge problem.

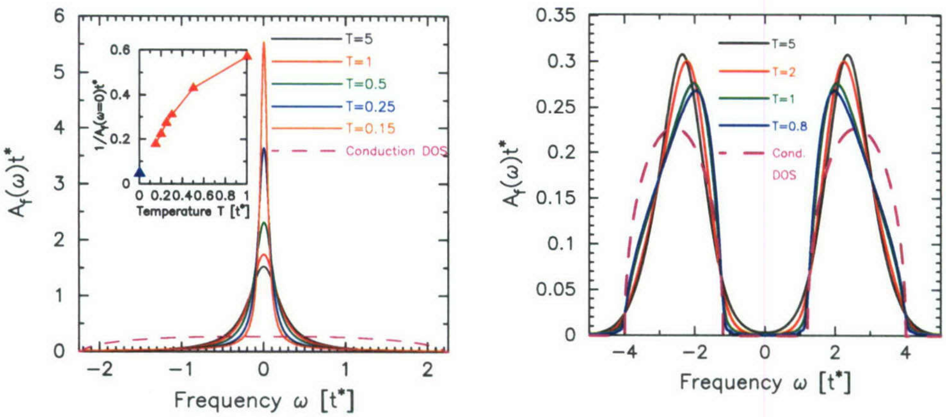

Figure 3. *F-electron DOS for the FK model on a Bethe lattice with U=1 (left) and U=5 (right). The conduction electron DOS is given by the dashed magenta curve. Note the sharp peak in the left panel, and the gap opening in the right. The curves are for different temperatures. These results were checked against a number of different moment sum rules and spectral formulas, and our error estimates are on the order of a few percent (pointwise). Inset in the left panel is a plot of the inverse DOS at zero frequency versus temperature, indicating a peak height of about 20 at T=0. We cannot rule out a divergence of the peak though, which has been verified by numerical renormalization group calculation.*

In the second problem, we perform calculations by turning on an electric field at time t=0, and watching how the system evolves. For noninteracting electrons, it is well known that in the limit of large time, the system approaches a steady state characterized by a Wannier-Stark ladder, where the DOS is a series of delta functions spaced at multiples of eaE/ħ, the current driven through the material oscillates at the Bloch oscillation frequency (similar in many respects to the *ac* Josephson effect). In our calculations, we restrict ourselves to a finite time interval, so we cannot reach the large-time steady state with our computer resources. We have shown how the initial response is similar to the Bloch oscillation, and then decays as the oscillations are damped. We find the behavior remains fairly regular, with the Bloch period essentially preserved for all metals, but when we enter the Bloch insulating regime, the current develops a very irregular pattern, and all remnants of the Bloch oscillations seem to disappear (see Fig. 4). This work was made possible by a Capabilities Application Project which was allocated about 600,000 cpu-hours for the Phase II part of the work. We were one of the few groups able to successfully use the new Cray XT3 computer; the ERDC has published an article about this work for their newsletter [J. K. Freericks, *"Nonlinear response of materials to large electric field: a capabilities application project on the Cray XT3"*, ERDC MSRC Resource, Spring, 2006, 10—12], and Cray has developed a marketing poster highlighting this work. We also participated in a CAP phase II project with this work on the ARSC Midnight Sun computer, where the large memory capabilities of that machine were employed to solve the largest problems we tried to tackle.

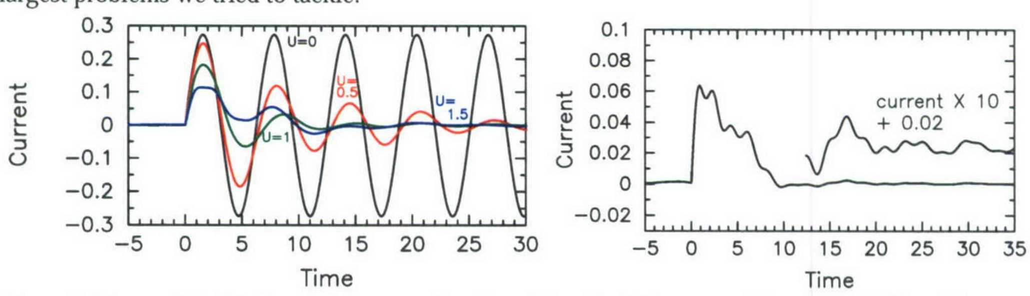

Figure 4. *Decay of the Bloch oscillations as a function of time for different metallic systems (left) and for a small-gap Mott insulator (right). Note how the increase of scattering quenches the oscillations more rapidly, but that the calculations have not yet reached the steady state. In the insulator, the current has a much more irregular behavior that is difficult to describe via any form of regular oscillations.*

In solving this problem, we have developed a real-time formalism that discretizes the continuous matrix operators (Green's functions and self-energies) on the Kadanoff-Baym-Keldysh contour and makes them into discrete matrices. We have given an oral presentation at the 2006 User's Group Conference of the HPCMP office, and have submitted a conference proceedings ["*Nonlinear response of strongly correlated electrons to large electric fields*", in Proceedings of the Users Group Conference Denver, CO, June 27--30, 2065 (IEEE Computer Society, Los Alamitos, CA, 2006), submitted]. We have published a conference proceedings for an invited talk we gave at an International Workshop on Nonequilibrium Physics III in Kiel, Germany in the end of August, 2005 [the work is entitled "*Nonequilibrium dynamical mean field theory and the quantum Boltzmann equation*"; J. Phys.: Confer. Ser. **35,** 39—52 (2006)]. That work develops the quantum Boltzmann equation for DMFT and explicitly proves the equivalence of the Kubo formula with the nonequilibrium results in linear response. We also published an article on spectral moment sum rules for nonequilibrium problems, which showed that many of these sum rules are essentially unchanged in the presence of a field, and they can be used in benchmarking calculations for accuracy. Indeed, we used them to verify that our calculations had accuracies on the order of 1% or better for most cases we examined. The reference is V. M. Turkowski and J. K. Freericks, "*Spectral moment sum rules for strongly correlated electrons in time-dependent electric fields,*" Phys. Rev. B **73**, 075108-1—15 (2006); Erratum: Phys. Rev. B **73,** 209902-1--1 (2006). We also published the article J. K. Freericks, V. M. Turkowski, and V. Zlatic', "*Nonequilibrium dynamical mean-field theory,*" Phys. Rev. Lett. **97**, 266408-1--4 (2006), and have submitted the article J. K. Freericks, "*Quenching Bloch oscillations in a strongly correlated material,*" to Phys. Rev. B. We are planning a possible *Nature Physics* article submission on the nonequilibrium electron distribution functions (see Fig. 5) and how they evolve after the electric field is turned on.

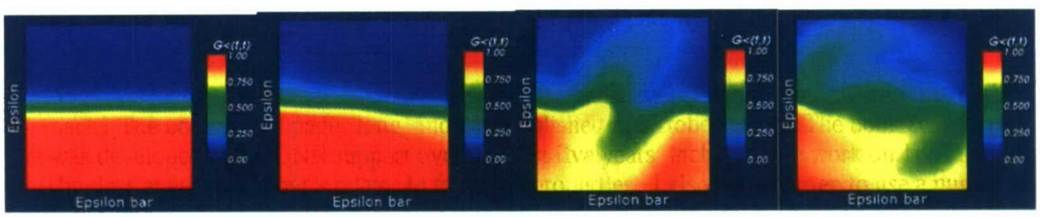

Figure 5. *Distribution function of electrons in a strong electric field as a function of time, starting on the left before the field is turned on, and increasing in units of time equal to about one third of the Bloch period for each time step. Note how the distribution of electrons gets mixed with a swirling motion as the time increases, and how the occupation of states becomes more evened out as time increases.*

We also spent a significant amount of time trying to model the MIT in Ta_xN with the Falicov-Kimball model. While we find at any fixed temperature, we can easily model all of the resistivity data, we are unable to produce the same level of T dependence of the resistivity in the data. We received some samples from Nate Newman's group that a student took with him to Croatia to study the thermopower and resistivity as functions of temperature. The measurements completed their indicated that the transport was dominated by the two-dimensional grain structure, and hence could not be used to predict the c-axis transport when Ta_xN is utilized as a barrier for a JJ.

Our final project has been the writing of a textbook on multilayered nanostructures from the DMFT approach. The book is 329 pages long, and was published in October, 2006. The book covers much work that was developed under ONR support over the past five years, including the work on JJ's and the work on the Thouless energy and how it relates to transport properties. I also have chosen to use a number of ONR supported researchers (Newman, Buhrman, and Xi) as resources for photographs and diagrams that are used in the book, which provides some additional exposure of the superconducting electronics work to a broader community.