Beyond the "Standard Model" for Superconductivity

James K. Freericks

October 18, 1999

Summary:

This grant has supported four people: the PI Jim Freericks, and three postdoctoral fellows Woonki Chung (30 months), Paul Miller (24 months), and Romuald Lemanski (6 months). Work was completed on a number of different problems in superconductivity ranging from examining the effects of vertex corrections in real materials to anharmonicity in model systems to perturbative approaches for strongly coupled superconductors. In addition, much work was completed on examining materials near the metal-insulator transition which are likely to be the optimal barrier materials for Josephson junctions. Finally models that exhibit the basic physics behind phase separation and stripe formation in strongly correlated systems were analyzed and solved in detail. A number of other miscellaneous projects were also completed.

1 Summary of technical projects completed

1.1 Electron-phonon based superconductivity

An initial study of the vertex-corrected tunneling inversion of Pb was completed with Elisabeth Nicol, Amy Liu, and Andrew Quong. The tunneling data of Rowell and McMillan for Pb was inverted including the effect of the vertex corrections. Even though the Migdal parameter is 0.0007 for Pb, the effect on $\alpha^2F(\Omega)$ is about a 1% effect (λ changing from 1.54 to 1.56). The vertex corrections enhanced both phonon peaks, and suppressed the spectral weight in the region beyond 9 mev which is the maximum phonon frequency in bulk Pb. The formalism is in place to analyze other materials where the vertex corrections will be stronger, but no high-quality tunneling data is yet available to analyze and invert in materials like K_3C_{60} or $Ba_{1-x}K_xBiO_3$.

Effects of anharmonicity on the electron-phonon interaction were examined in detail for a model system in collaboration with Jerry Mahan, Mark Jarrell, and Veljko Zlatić. We examined both perturbative approaches and exact solutions via quantum Monte Carlo simulation and other techniques. We discovered a remarkable scaling law of the transition temperature with the wavefunction renormalization parameter. Systems with vastly different coupling strengths and anharmonicity are mapped onto the same universal curve, helping to explain why anharmonic effects can be ignored in most real materials.

Two projects on examining how weak-coupling perturbation theory can be extended into the strong-coupling regime were completed (in collaboration with Veljko Zlatić and Paul Miller). Our motivation was to examine how far perturbation theory could be pushed before it breaks down. Unfortunately, we found that all schemes broke down at approximately the same coupling strength regardless of how the self-consistency was incorporated, or how the diagrammatic analysis was truncated. We also studied whether or not one could mimic the effects of vertex corrections with a Coulomb pseudopotential, or if there was a definitive experiment that could show the effects of vertex corrections in a real material. We discovered that reconciling tunneling data (for α^2F) with the transition temperature and the isotope effect was the most sensitive way to test for effects of vertex corrections.

1.2 Josephson-junction barrier materials near the metal-insulator transition

Work was completed in three different areas. The first involved an examination of the periodic Anderson model away from the symmetric limit in collaboration with Alireza Tahvildar-Zadeh and Mark Jarrell. This is a two band model consisting of localized electrons that are correlated and hybridize with otherwise uncorrelated conduction electrons. We examined the regime where the f-electrons have nearly unit occupancy, and varied the d-electron occupancy, which corresponds to the most physical case of a narrow band located near, but just below the Fermi energy. This is the regime of heavy-Fermion physics, and we discovered a number of novel results. The photoemission of heavy Fermions has a much weaker dependence on temperature than the single-impurity model does. This conclusion has been verified by Al Arko and his coworkers. Furthermore, because of this weak temperature dependence Kondo physics effects can be seen at temperatures much higher than the Kondo temperature, because the Kondo effect evolves over a much wider temperature range. We examined magnetic properties, discovered a novel Kondo-effect induced ferromagnetism, and examined optical conductivity and discovered that contrary to conventional expectations, the Drude weight decreases as temperature is lowered and a mid-IR peak develops, which is seen in nearly all heavy Fermion compounds.

We performed a number of detailed studies of the Falicov-Kimball model, examining the first-order metal-insulator transition, and intermediate valence phenomena (in collaboration with Woonki Chung). This is a model just like the periodic Anderson model except the f and conduction electrons do not hybridize and the Coulomb interaction between the f and conduction electrons is included. By solving this problem exactly, we were able to settle a number of long-standing controversies about the model. We established that the system is able to display first-order metal-insulator transitions as a function of temperature. We also discovered that intermediate valence phenomena is suppressed due to phase separation or a direct metal-insulator transition.

I completed a project with Veljko Zlatić on the anomalous magnetic properties of the intermediate-valence compound $YbInCu_4$ and am in the process of finishing up a second paper. In this work, we developed a new model for explaining the properties of this system which include a strong peak in the magnetic susceptibility as a function of temperature. We find that the Falicov-Kimball model applies here in the high-temperature phase where it can cause a large redistribution of spectral weight including the generation of a correlation induced gap in the density of states. Kondo-effect physics can be neglected in this regime because there are no states at the Fermi level to hybridize with. As the temperature is lowered, the density of states rises, until there is a first-order transition into an intermediate moderately heavy-Fermion state at low temperatures.

Since the most interesting and most difficult to understand barrier regions in a Josephson junction are those that border between a metal and an insulator, this work will be incorporated into a new ONR project that will examine how to optimize the properties of a Josephson junction by varying the properties of the barrier material. We have a number of interesting materials that can be tuned through a variety of different metal-insulator transitions, or can live in an intermediate-valence state which can produce new phenomena in or optimize properties of Josephson junctions.

1.3 Phase separation and stripe physics

Work has been performed on trying to understand just how strong-correlation effects can lead to phase separation and how that can then be linked to stripe formation. This work was completed in collaboration with Christian Gruber, Romuald Lemanski, and Nicolas Macris. We examined the simplest possible model for this phase separation: the spinless Falicov-Kimball model. We found when the interaction strength is infinite, the system always phase separates into regions with different total charge densities. Since this model neglects the long-range Coulomb interaction, any real material that has a tendency toward such a phase separation will reorganize its charge in some long-range pattern, which could become the charge stripes seen in high T_c materials. We have completed the work in the infinite interaction strength limit, and are currently writing up results for the case of finite interaction strength to see how pervasive this phenomena is.

1.4 Miscellaneous projects

A collaboration with Hartmut Monien and Matthias Niemeyer has been completed on the dirty Boson problem in a magnetic field. Granular superconductors can sometimes be thought of as a system of Cooper pairs that live in each of the grains, which can gain or lose global phase coherence, and hence have a superconductor-insulator phase transition. Many experiments have been performed in a magnetic field to tune through the transition, but little theoretical work has addressed this problem in a magnetic field because of a number of theoretical difficulties. We examined this problem perturbatively and found remarkable agreement with experiments performed by Mooij's group on one-dimensional arrays of Josephson junctions which can also be described by such a model.

A collaboration with Christian Gurber and Nicolas Macris has examined higher-period ordered charge-density-wave phases on the Bethe lattice. We found very interesting results, including the fact that high-period order does exist, and the transitions to this ordered phase are first-order. A paper on these results is currently in preparation.

2 Relevance to Superconducting Electronics

The most relevant work completed in this project involved the development of a formalism that will allow for a microscopic modelling of the Josephson junction, including a variety of different barrier materials that can all be tuned through the metal-insulator transition to see whether or not properties of the Josephson junction can be optimized by a theoretical analysis. This project is part of an ongoing effort supported by a current ONR grant with interaction between two other experimental groups who are also working on this problem: John Price and Chuck Rodgers at University of Colorado and Laura Greene at University of Illinois. Both groups are looking at creating Josephson junctions from Niobium and semiconducting barrier materials ranging from Nb-doped strontium titanate to indium arsenide. From the theoretical side, we have in place a study of many different metal-insulator transitions, all which can serve as barrier materials, and have partially in place a formalism to study the different relevant superconducting phases (with the remaining work on d-wave superconductivity currently being undertaken by Mark Jarrell).

The second most relevant piece of work is the study of phase separation in strongly correlated systems. We find that strong correlation naturally leads to a tendency to phase separate, which we believe is the underlying physics behind stripe formation in the cuprates, and is driven by a competition between phase separation and the long-range Coulomb interaction, which does not allow charges to spatially separate by too large of an amount. This is the scenario needed by Kivelson and Emery for their model of fluctuating stripe superconductivity. Work on measuring these stripes will be completed by Seamus Davis at the University of California, Berkeley, and there may be an opportunity for theoretical input into those results.

3 Publications

- "Vertex-corrected tunneling inversion in superconductors", J. K. Freericks, E. J. Nicol, A. Y. Liu, and A. A. Quong, Czechoslovak Journal of Physics **46**, Supplement S2, 603 (1996).
- "Vertex-corrected tunneling inversion in superconductors: Pb", J. K. Freericks, E. J. Nicol, A. Y. Liu, and A. A. Quong, Phys. Rev. **B**, 11651–11658 (1997).
- "Magnetic phase diagram of the Hubbard model in three dimensions: the second-order local approximation," A. N. Tahvildar-Zadeh, J. K. Freericks, and M. Jarrell, Phys. Rev. B **55**, 942–946 (1997).
- "Protracted screening in the periodic Anderson model," A. N. Tahvildar-Zadeh, M. Jarrell, and J. K. Freericks, Phys. Rev. B **55**, 3332–3335 (1997) (Rapid Communication).
- "Low-temperature coherence in the periodic Anderson model: Predictions for photoemission of heavy Fermions," A. N. Tahvildar-Zadeh, M. Jarrell, and J. K. Freericks, Phys. Rev. Lett. **80**, 5168–5171 (1998).
- "Charge-transfer metal-insulator transitions in the spin-one-half Falicov-Kimball model," Woonki Chung and J. K. Freericks, Phys. Rev. B **57**, 11955–11961 (1998).
- "Anomalous magnetic response of the spin-one-half Falicov-Kimball model," J. K. Freericks and V. Zlatić, Phys. Rev. B **58**, 322–329 (1998).
- "Vertex-corrected perturbation theory for the electron-phonon problem with non-constant density of states," J. K. Freericks, V. Zlatić, Woonki Chung, and M. Jarrell, Phys. Rev. B **58**, 11613–11623 (1998).
- "Possible experimentally observable effects of vertex corrections in superconductors," P. Miller, J. K. Freericks, and E. J. Nicol, Phys. Rev. B **58**, 14498–14510 (1998).
- "Phase separation and the segregation principle in the infinite-U spinless Falicov-Kimball model," J. K. Freericks, Ch. Gruber, and N. Macris, Phys. Rev. B **60**, 1617–1626 (1999).
- "Strong-coupling perturbation theory for the two-dimensional Bose-Hubbard model in a magnetic field," M. Niemeyer, J. K. Freericks, and H. Monien, Phys. Rev. B **60**, 2357–2362 (1999).
- "Evidence for exhaustion in the conductivity of the infinite-dimensional periodic Anderson model," A. N. Tahvildar-Zadeh, M. Jarrell, Th. Pruschke, and J. K. Freericks, Phys. Rev. B **61**, XXX (1999).
- "Approximate scaling relation for the anharmonic electron-phonon problem," J. K. Freericks, V. Zlatić, and M. Jarrell, submitted to Phys. Rev. B (Rapid Communication).
- "Competition between phase separation and "classical" intermediate valence in an exactly solved model," Woonki Chung and J. K. Freericks, submitted to Phys. Rev. Lett.

4 Invited Talks

- "Do we really understand low-temperature superconductors?" delivered at Old Dominion University (Sept. 20, 1996), Virginia Commonwealth University (Feb. 14, 1997), Institute of Physics, Zagreb, Croatia (May 8, 1997), and Josef-Stefan Institute, Ljubljana, Slovenia (May 15, 1997).

- "Ground-state quantum numbers of superconductors," delivered at the University of California, Santa Barbara (Jan. 14, 1997).

- "How does the Pauli principle lead to crystallization: studies of the one-dimensional Falicov-Kimball model," invited talk delivered at the Middle European Cooperation in Statistical Physics, Wroclaw, Poland, (April 4, 1997).

- "The quantum world around us: teaching quantum mechanics and solid state physics to nonscientists," Institute of Physics, Zagreb, Croatia (May 12, 1997), University of Split, Split, Croatia (May 26, 1997).

- "The quantum world around us: sample lecture," Institute of Physics, Zagreb, Croatia (May 13, 1997), University of Split, Split, Croatia (May 27, 1997).

- "The quantum world around us: Teaching quantum and solid-state physics to nonscientists," University of Maryland (Sept. 25, 1997) and University of Cincinnati (April 9, 1998).

- "Does exchange of a phonon always produce pairing of electrons?" Institute of Low Temperature and Structure Research, Polish Academy of Science, Wroclaw, Poland (May 29, 1998).

- "Intermediate-valence and metal-insulator transitions in the Falicov-Kimball model," presented at the University of Fribourg (June 7, 1999) and the Ecole Polytechnique Fédérale de Lausanne (June 24, 1999).

- "Modeling the anomalous thermodynamic and transport properties of Yterbium intermetallic compounds," Concepts in Electron Correlations, Hvar, Croatia, (September 29, 1999).

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*: 21-10-1999
2. REPORT DATE: Final Technical report
3. DATES COVERED *(From - To)*: 06-01-1996 - 08-31-1999

4. TITLE AND SUBTITLE:
Final Technical Report for
Beyond the "standard model" for Superconductivity

5a. CONTRACT NUMBER:
5b. GRANT NUMBER: N00014-96-1-0828
5c. PROGRAM ELEMENT NUMBER:
5d. PROJECT NUMBER:
5e. TASK NUMBER:
5f. WORK UNIT NUMBER:

6. AUTHOR(S):
Freericks, James K.

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES):
Department of Physics
Georgetown University
Washington, DC 20057

8. PERFORMING ORGANIZATION REPORT NUMBER:

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES):
Office of Naval Research
800 North Quincy St.
Arlington, VA 22217-5660

10. SPONSOR/MONITOR'S ACRONYM(S): ONR

11. SPONSORING/MONITORING AGENCY REPORT NUMBER:

12. DISTRIBUTION AVAILABILITY STATEMENT:
Approved for public release; distribution unlimited

13. SUPPLEMENTARY NOTES:

14. ABSTRACT
Final technical report for James Freericks Young Investigator Program grant. Work was completed on a number of different problems in superconductivity ranging from vertex corrections in real materials, anharmonicity in model systems, and perturbation theory for strongly coupled superconductors. In addition much work was completed on understanding Josephson Junction barrier materials near the metal insulator transition, and understanding how strong correlation leads to phase separation and possibly stripe formation.

15. SUBJECT TERMS
Superconductivity, metal-insulator phase transition, phase separation.

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON	19b. TELEPONE NUMBER *(Include area code)*
U	U	U	UU	5	James Freericks	202-687-6159

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI-Std Z39-18