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Many Body Theory Program

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Abstract

This is the final report of a two-year, Laboratory-Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). We have obtained a description of symmetry of the order parameter and pairing state in high-T_c superconductors. We developed a theory of ferromagnetic instability of Fermi-liquid. We have conducted an experimental investigation of the intermetallic compounds and Zintl-type compound. We investigated the properties of Cu-O ladders. We have developed the theory of Lifshitz tails in superconductors. We have conducted number of summer workshops.

Background and Research Objectives

The foundations of the theory of metals and superconductors have been shaken by a number of discoveries over the last fifteen years. These include the Quantum Hall effect, heavy-fermions, low dimensional conductors and the high temperature superconductors (HTS). The standard theory of metals is the Landau Fermi liquid theory and for superconductors it is the s-wave, phonon mediated pairing of Bardeen, Cooper, and Schrieffer (BCS). While many of the traditional metals and superconductors can be understood in terms of these theories, many of the new materials exhibit behaviors that do not fall within these standard models. The newer classes of materials have a number of properties that favor a much richer spectrum of ground and excited states. This includes strong electronic and lattice correlations, reduced dimensionality, restricted geometry, disorder, and non-linearity. The competition and interplay between these various properties leads to the rich variety of ground states observed in these strongly correlated materials. This includes unconventional superconductivity in heavy-fermion and possibly HTS superconductors, the field induced metal insulator transition expected in some of the heavy-fermion insulators (Kondo insulators), Luttinger liquid and non-Fermi liquid behavior in HTS and heavy-fermion materials.

The development of microscopic theories to describe and understand the behavior of these materials is one of the biggest challenges in condensed matter theory today. What makes this even more exciting is that the novel characteristics of these materials will make them likely candidates for new electronic applications in the future. To best design materials for specific applications we must understand the relationship between the underlying microscopic interactions and the other parameters that restrict the electrons motion, for example, reduced dimensionality, disorder, and magnetic fields. There is a considerable activity at Los Alamos to understand and harness the properties of the strongly correlated electronic materials for applications. This includes the use of Kondo insulators

for cyro-cooler applications, colossal magnetoresistive materials for read heads in magnetic storage devices, and HTS for infrared detectors and superconducting tapes and wires, to name a few. Many of the properties of the materials used in these applications arise from the unusual many-body correlations that are present in most of them and it is this underlying thread that ties these various research activities together.

There are a number of research activities at LANL in which an understanding of the many-body physics is crucial. Some examples are: the pairing mechanisms in high temperature superconductors, physical phenomena in high magnetic fields (this includes the fractional quantum Hall effect, many-body effects in high magnetic fields, and field induced metal-insulator transitions), non-Fermi liquid behavior in heavy-fermion and HTS compounds, and inelastic resonant tunneling in quantum well structures. There are a number of groups and centers actively involved in these research projects, they include T-11, MST-10, the CMS, the STC, LANSCE, and the NHMFL. The CMS over the years has played a crucial role in the development of these research activities through the theory programs it has supported. The past programs that have contributed to the LANL activities in many-body physics were the Advanced Studies Program in High Temperature Superconductivity (ASP) directed by J. R. Schrieffer (Florida State University) and the Correlated Electron Theory Program directed by K. Bedell (T-11). This program in the CMS, the Many-Body Theory Program (MBTP), provided a link between the internal programs and a number of University researchers actively involved in this area of physics. The recent CAM initiative, started by D. Pines and Z. Fisk is naturally connected to the MBTP.

Importance to LANL's Science and Technology Base and National R&D Needs

Los Alamos has a broad spectrum of technical competencies in the many-body physics of correlated electronic materials. The interactions with the participants of the MBTP enhanced the research of these Laboratory capabilities. The largest impact is on the theory effort in T-11. The theory effort in T-11 is funded, in part, by an LDRD/IP proposal and a DOE/OBES proposal. In addition to this, there is funding for microscopic HTS research in T-11 coming from LDRD/PD. The research activities was enhanced by interactions between the MBTP participants and LANL staff.

There are other programs that were impacted by the MBTP. This includes the experimental efforts in MST-10 as well as those in the CMS and STC. These encompass the characterization efforts in HTS, heavy fermions and colossal magnetoresistive materials. There is a close connection between the MBTP effort and the research conducted at the NHMFL. Recent effort to bring together different parts of the Lab under CAM initiative started after Z. Fisk and D. Pines, who are program fellows, suggested it.

Scientific Approach and Accomplishments

The R&D approach to the MBTP is in part administrative and part scientific. The science side has to do with the development and application of many-body techniques to a class of strongly correlated materials. Some of the materials we focus on have real potential for applications in electronic devices. These include the HTS materials, Kondo insulators, and colossal magnetoresistive materials (CMR) to name a few. There are other problems that were studied that do not have any immediate applications. This includes the field induced metal-insulator transition in the Kondo insulators, the fractional quantum Hall effect and lower dimensional materials as possible examples. The physical phenomena studied in these materials are relevant to the more device oriented materials, however, the interesting physics takes place in some range of the parameter space that is not readily available to small scale electronic devices. For example the field induced metal-insulator transition in the Kondo insulator $\text{Ce}_3\text{Bi}_4\text{Pt}_3$ is expected to occur at low temperature, T of the order of 10K, and high magnetic fields, B of the order of 100 Tesla. This of course is not

the kind of parameter range needed in a real head in a magnetic storage device! However, the physical phenomena are similar, a large change in the resistivity due to a change in the magnetic correlations in the presence of a magnetic field.

These are some of the scientific issues we have investigated. The other aspect of this program is its administrative side. The program was structured around three key components:

i) As with the previous programs we brought into the research efforts of Los Alamos in many-body theory some of the leading experts in the field. The three key participants will be J. R. Schrieffer (Florida State University and the NHMFL), D. Scalapino (UCSB) and D. Pines (University of Illinois). Each participated and helped to coordinate activities in a number of areas. Professor Schrieffer was involved in research activities in the theory of HTS and in research involving physical phenomena in high magnetic fields. He also played an important role in developing research ties between Los Alamos and the two Florida campuses involved in the research program of the NHMFL. Professor Scalapino was involved in the development of many-body techniques with an emphasis on numerical methods for strongly correlated electronic materials. This includes the HTS materials, the metal-insulator transition, and lower dimensional materials. He also played an active role in promoting collaborations between Los Alamos and the UC campuses. Professor Pines participated in research activities in the theory of the HTS. In particular he was involved in research to determine the pairing state of the HTS materials and the physical realization of that state. These research activities will couple very strongly with the research directions in T-11, MST-10, the CMS, LANSCE, and the STC.

ii) The activities of visitors to the MBTP during these years was mostly focused around specific areas of research. See section 5 for some of the programs. The idea was to bring into Los Alamos a number of experts in a specific research area for collaborations.

iii) The third component to the program was the summer workshops. During this time we brought together theorists and experimentalists to discuss in an informal setting the current issues in many-body physics in strongly correlated systems. The research areas discussed in this workshop was related to the research activities during the year. We also brought some of the leading theorists in the many-body theory of strongly correlated electronic materials together during this time.

Below is the list of the specific projects:

Zack Fisk (Florida State University) during his summer visits had a number of successful projects finished, [1-24].

- 1) Discovered two new series of rare earth intermetallics: $\text{RE}_3\text{Pt}_4\text{In}_{13}$ cubic stannide-type phases and RERhIn_5 and REIrIn_5 , and measured their properties.
- 2) Studied the ferromagnetism of CeAlSi , a Zintl-type low carrier material.
- 3) Showed that the impurity system $\text{Ca}_{1-x}\text{Sm}_x\text{B}_6$ (which is one dilute limit of the Kondo insulator SmB_6) has a Kondo compensated quartet ground state at low concentration, $x=0.03$.
- 4) Started studies of other dilute rare earths in CaB_6 and SrB_6 . This has led to the discovery of a weak ferromagnetism for $x < 0.01$. This ferromagnetism is present to at least 350K, where are magnetometer measures to.
- 5) Studies the ferromagnetism in single crystals of YbInNi_4 , and studied the evolution of properties as Ni is substituted with Cu.

Kevin Bedell (Boston College) had worked on two major projects [33, 34]:

The first was on the properties of one dimensional, 1D, metals. It has been argued that the properties of the high temperature superconductors, High-T_c, in the normal state are like those of a 1D Luttinger liquid. One of the important properties of a metal is the Fermi surface. A theorem first derived by Luttinger was the property that the volume of this surface in 2D and 3D was conserved as the interactions were turned on. It was argued by Anderson and Haldane that in 1D there was as well a Luttinger theorem.

Another program was the behavior of the weak ferromagnets close to a quantum critical point. This is a topic of much interest since the limit of weak ferromagnetism is a regime of strong correlations. He also found that several new instabilities are possible in the neighborhood of small magnetic moments. In particular there is a possibility of an s-wave superconducting instability in the presence of ferromagnetism. There is as well as phase separation instability at the point where the ferromagnetic to paramagnetic transition occurs. These results are exact in leading order in the small parameter, T_c/E_f , where T_c is the Curie temperature and E_f is the Fermi energy. The possibility of an s-wave instability in the presence of ferromagnetism was unexpected.

John Wilkins (Ohio State University) worked on low dimensional systems [25-32]:

The effects of strong electron-electron interactions in systems of restricted dimensionality has been explored in laser-excited quantum dots, two-layer systems, and far-infrared cascade lasers. More generally, strong interactions effects have been explored in heat transport in dirty metals and in the conductivity of charge density systems. Finally, massive electronic computations, using object-oriented programming, has revealed the nature of extended defect structures in silicon.

Doug Scalapino (University of California, Santa Barbara) worked on [60-66]:

To study the n -leg t - J and Hubbard models because we believe that they can provide important new insight into the high-temperature superconducting cuprate puzzle.

He developed a local description of pairing in the presence of short-range antiferromagnetic interactions and studied the effects of retardation. We have also carried out Monte Carlo and diagrammatic calculations to study the nature of the effective pairing interaction.

He is presently working with Rich Martin to understand the effect of possible chemical substitutions (e.g. S for O , Ni^{+1} for Cu^{+2}) in determining t and J in cluster models. He also continues to interact with M. Salkola regarding the coexistence of stripes and d -wave pairing.

J.R. Schrieffer [35-59] worked on the physics involved in the large volume changes in the phase diagram of Pu. In collaboration with Abrahams, he proposed a model in which the f electrons are in tightly bound atomic orbitals or in extended orbitals which mix with extended orbitals from neighboring atoms forming a bonding f -bond. This scheme can be mapped onto a periodic Anderson model with the lattice spacing a parameter of the system. One finds within the mean field approximation that the low temperature phase is a strongly bound solid with a small lattice spacing while the high temperature phase has large volume and large entropy due to the weaker elastic constants resulting from the absence of f -electron bonding as is observed. We are attempting to generalize the model by including directionality of the f -orbitals and the crystal structure of the solid.

A.V. Balatsky worked on impurity states in unconventional superconductors [67].

In the process of working on this project, participants were acknowledged with a number of awards:

A. Balatsky, Achievement Award, T-Division

J.R. Schrieffer University Eminent Scholar Professor The Florida State University System, 1996-Present; Member Advisory Board, Asia Pacific Center for Theoretical Physics, 1996-Present.

Guggenheim Foundation Awards Committee, 1996-Present President's Committee on the National Medal of Science, 1996-present.

President American Physical Society, 1996; Past President, 1997.

D. Pines, Ulam Scholar, 1996-1997.

Z. Fisk, National Academy of Sciences member, 1996.

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