MANY-BODY EFFECTS IN HEAVY FERMION COMPOUNDS

Final Technical Report

for Period September 1984 – January 2001

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May 2002

Prepared for the US Department of Energy
AWARD NO. DE-FG02-84ER45127

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6.26.02
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The DOE award resulted in 75 papers that were published in professional scientific Journals. A list of papers made possible by the grant is included as supplemental material. The technical results are presented under three major headings; Photo-emission, heavy fermion semi-conductors and transition metal heavy fermion compounds.

PHOTOEMISSION SPECTRA

In this period a number of models for the Photo-emission and Inverse Photo-emission spectra of Heavy Fermion and Cerium systems and other strongly correlated materials were developed.

- (A) The role of the electrostatic interactions, which lead to electrical neutrality and the Friedel sum rule, were investigated. These interactions do produce satellites peaks in the spectra corresponding to poorly screened and well-screened peaks. In addition, it was found that the Coulomb interactions result in the production of electron-hole pairs, so that even if the satellite has negligible intensity the spread in energies caused by the continuum of electron-hole pair excitations causes the spectral widths to be strongly renormalized.
- (B) It was also shown that the photoemission spectra of the normal state of the high temperature superconductors is consistent with a strongly interacting Fermi-liquid. The large strength of the Coulomb interaction can produce a strong reduction in the temperature where the cross-over to the Fermi-liquid starts forming. At low temperatures, the small temperature window of Fermi-liquid behavior is mirrored by a small energy region in which the imaginary part of the self-energy shows a E^2 variation. However, for higher energies the imaginary part of the self-energy shows a linear variation with E , which is consistent with the observed energy dependence of the Angle resolved photo-emission and also with the linear T dependence of the electrical resistivity.
- (C) The interpretation of photoemission spectra lead to the development of models of photoemission based on the single impurity Anderson model, in which the effects of spin-orbit coupling and the crystalline electric field were included. Although the model has proven difficult to calculate, a number of simple approximations based on the limit of large orbital degeneracy do lead to reliable results. The model was treated by a variational $1/N$ method and later a Non-Crossing Approximation (N.C.A.) code was developed. This research resulted in a highly successful interaction with the experimental group of Al Arko at Los Alamos National Labs. . This work resulted in over 10 collaborative publications in scientific Journals.

HEAVY FERMION SEMICONDUCTORS

A break through in our understanding of heavy fermion systems was made possible by the discovery of $\text{Ce}_3\text{Bi}_4\text{Pt}_3$ by the work of Zachary Fisk and Joe Thompson at Los Alamos. The heavy fermion semi-conductors show the existence of local magnetic moments interacting with itinerant conduction electrons at high temperatures, but at low temperatures show a cross-over between the metallic state to semi-conducting state at low temperatures. The effects of the strong many body interactions show up in a renormalization of the semi-conducting gap to extremely small values, of the order of a few 10's of degrees Kelvin, in contrast to 10,000 K found in pure Si. While there are many heavy fermion semi-conductors, $\text{Ce}_3\text{Bi}_4\text{Pt}_3$ is special as the value of the gap is sufficiently large that impurity effects do not dominate the low temperature behavior. Motivated by the discovery, a theory was developed that described the low temperature properties of the heavy fermion semi-conductors. In the mean field approximation, it was discovered that the low temperature gap had an unusual temperature dependence, and vanished at sufficiently high temperatures leading to the metallic state. The temperature dependence of the gap was subsequently confirmed by transport measurements performed by Joe Thompson's group at Los Alamos and also by inelastic neutron scattering experiments. This work led to an experimental-theoretical collaboration and lead to a number of joint publications. It was predicted that the unusual temperature dependence should also show up in infra-red absorption measurements. At low temperatures, the optical conductivity should show the development of a gap. The gap was then observed in the low temperature optical conductivity. The theory predicted that the spectral weight removed from the energy region where the gap appears should reappear at higher energies. Experimentally, it was determined that the spectral weight did not re-appear at energies below 1 eV and lead to speculations about the failure of the optical sum rule, or occurrence of super-conductivity. Later measurements on better materials did show the missing spectral weight does reappear at higher energies.

The theory was subsequently developed further, by investigating the effects of processes of higher order in $1/N$, where N is the degeneracy of the f shell. The photo-emission spectrum was calculated and it was found that the semi-conductors showed significantly rapid temperature dependencies than the metallic heavy fermion systems. This was independently confirmed by both the FLEX calculations of Hess and by the quantum Monte-Carlo calculations of Jarrell. This result has impact upon the "Exhaustion Principle" formulated by Nozieres, which argues that the physics of the single impurity Kondo model can not be applied to concentrated heavy fermion compounds.

The theoretical work on the dynamical susceptibility revealed an exciting possibility, namely, that there can be a branch of collective magnetic excitations with threshold energies lower than the gap. It was predicted that these modes should only develop at low temperatures and have a dispersion relation with a minimum at the Brillouin zone boundary. Although the original inelastic neutron scattering measurements of Thompson and Severing failed to show evidence of these magnetic exciton modes, neutron scattering experiments on SmB_6 and YbB_{12} , which are also heavy fermion semi-conductors have shown the existence of modes in the gap, which do have the expected dispersion relation and also only appear at low temperatures. Furthermore, these modes

also appear in Raman scattering and thus have well defined selection rules that attest to their magnetic character.

HEAVY FERMION TRANSITION METAL COMPOUNDS

It was discovered that LiV_2O_3 is a metallic system that exhibits a large linear T coefficient in the specific heat and is reminiscent of actinide or lanthanide based heavy fermion systems. We were the first group that calculated the electronic structure of LiV_2O_3 , and confirmed its metallic character. Our calculations also revealed that the mechanism behind the formation of the heavy mass was probably not the same as the Kondo-effect, as the bands in the vicinity of the Fermi-energy have comparable width. However, the large T^2 coefficient in the electrical resistivity does provide strong supporting evidence that the large mass has a contribution that originates from strong electron-electron interactions. Our calculations indicate that the system is highly frustrated and speculated that it is the frustration in the system which provides an alternate route to large quasi-particle mass enhancements.

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