DOE/ER/45518--T1

Final Report

Theoretical Studies of Magnetic Systems

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August 1, 1994 - November 30, 1997

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DE-FG05-94ER45518

I. During the grant period we have studied five areas of research, 1) low dimensional ferrimagnets, 2) lattice effects in the mixed valence problem, 3) spin compensation in the one dimensional Kondo lattice, 4) the interaction of quasi particles in short coherence length superconductors, and 5) novel effects in angle resolved photoemission spectra from nearly antiferromagnetic materials.

1) Under the topic of "Low-Dimensional Ferrimagnets", two d=2 square lattice classical spin models for ferrimagnets were studied. They both have atoms with spin 1/2 on one sublattice and spin 1 or spin 2 on the other sublattice. Both were studied using the non-perturbative computer techniques of Monte Carlo simulations, numerical transfer-matrix calculations, finite-size scaling, and exact ground-state analysis.

The work for the spin 1/2 - spin 1 ferrimagnet was first reported in a conference proceeding entitled "Computer Study of a d=2 Mixed Ising Ferrimagnet" by G.M. Buendía, M.A. Novotny, and J. Zhang and published in "Computer Simulations in Condensed Matter Physics VII", edited by D.P. Landau, K.K. Mon, and H.-B. Schüttler, (Springer Verlag, Heidelberg, 1994), page 223-227. A larger paper by G.M. Buendía and M.A. Novotny entitled "Numerical Study of a Mixed Ising Ferrimagnet System" was published in J. Phys.: Condens. Matter, 9, (1997), page 5951-5964. This work was also presented by M.A. Novotny at the 1995 March Meeting of the American Physical Society (the abstract is published in the Bulletin of the American Physical Society, Vol. 40, page 213, 1995) These computer studies found that *contrary to previous mean-field analysis* of the same nearest-neighbor (nn) model, the nn model does not have a tricritical point (TCP) or a compensation point (CP). It is only when a certain type of next-nearest neighbor interactions are present in the model that a CP exists, and even then a TCP is not present. These studies are relevant to low-dimensional ferrimagnetic materials that are currently being synthesized and analyzed by a number of groups (such as the Miller/Epstein group - see the Bulletin of the American Physical Society, Vol.40, p.328 for molecular magnets based on metalloporphyrin-tetracyanoethylene; a preprint by Peter Day and collaborators for ferrimagnetic mixed valency and mixed metal Tris(oxalato)FeIII compounds; or a preprint by C. Landee and collaborators). The Miller/Epstein group has also observed a CP in the V(TCNE) x solvent family of molecular magnets.

The work on the other model, for the spin 1/2 - spin 2 ferrimagnet has been published in a conference proceeding entitled "Critical Behavior of a Mixed Ising Ferrimagnet" by G.M. Buendía

and M.A. Novotny was presented by G.M. Buendía and published in J. Phys. IV France, Colloque Cl, Supplement au Journal de Physique III de mars 1997, **7**, (1997), page Cl-175 - C1-176.

2) An attempt is made to improve the common approach to Mixed Valence(MV) phenomenon by a more careful account of the lattice degrees of freedom. The MV problem is usually formulated in terms of fluctuating occupation of the 4f-/5f-shells for the atomic orbitals. Thus, it is difficult to understand the origin of rather small energy scales of order of lO-lOOK, typical for the heavy fermion and mixed valence physics. We assume that fluctuating configurations are formed with some essential involvement of lattice deformations, which would then produce a characteristic time scale of order of inverse phonon frequency, at least.

To realize such an idea, a polaronic model is adopted in[1] to describe one of the two configurations. Polaronic displacements in this model lowers the level's energy for one of the configurations in such a manner that the adiabatic potential decreases and touches the chemical potential of conducting electrons. In this range of deformations calculations of the adiabatic potential reduce to solution of an Anderson model with an effective on-site interaction which depends on the deformation itself. It is known (see, e.g.,[2]) that polaronic effects may dramatically reduce the hybridization width of the level in the Anderson model. In[1] a simple classical model is considered to demonstrate that at a proper choice of parameters the local level of the effective Anderson model may also become pinned in close vicinity of the chemical potential of electrons in the conduction sea. Therefore, the smallness of energy scales in heavy fermion and mixed valence phenomena might be ascribed to renormalization of bare parameters by polaronic effects of the lattice

References:
1. L.P.Gor'kov, “Phase Transitions in Mixed Valence Systems", Physica B 223-245, (1996).
2. D.Sherrington and S.von Molnar, Solid State Comm.**16**,1347(1975)

3) The physical origin of spin compensation in the periodic Kondo lattice is conventionally ascribed to the Nozieres exhaustion principle. In this approach a small fraction of the electrons, T_K/T_F, where T_K and T_F are the Kondo and Fermi temperatures, compensate all the localized spins by a local spin zero Kondo state resonating between sites forming an overall spin singlet. We propose an alternative view in which the electrons provide an interaction between the localized spins and the localized spins compensate each other due to this interaction. We have studied this problem using the Mandelstam bozonization scheme. We find that the ground state is a spin singlet with a gap to the first excited state. Further, we find that the spins are correlated in a manner which supports the view that the conduction electrons play the role of providing an interaction between localized spins. This work was reported at the APS meeting, March, 1996: Bull.APS 41, 362 (1996), Ju Kim and J. R. Schrieffer.

4) We have studied the interaction between quasi particles in superconductors with short coherence length. In these materials, the energy gap 2Δ is strongly depressed in the vicinity of each quasi particle if the coupling between electrons is strong. This depression arises as a competition between the quasi particle energy being lowered proportional to Δ as Δ is reduced from its equilibrium value Δ_o, but the condensation energy $-N(o)(\Delta-\Delta_o)^2/2$ is raised. This leads to a Δ - polaron, where the pairing field Δ plays the role of the phonon field in the conventional polaron. We find that two of these objects attract and form a bound state of energy inside the conventional gap Δ_o. Furthermore, when many quasi particles are added, a many body bound

state can occur in which the quasi particles form a domain wall with the order parameter Δ changing sign across the wall. The quasi particles are bound to the domain wall. We have carried out self consistent solutions of the Bogoliukov-de Gennes equations which exhibit these novel properties. M. I. Salkola and J. R. Schrieffer, submitted for publication.

5) We have studied the physical origin of two effects in the ARPES spectrum of strongly correlated electron systems, shadow bands and three peak spectra. Shadow bands are due to exchange Bragg scattering from strong antiferromagnetic spin fluctuation which persist into the paramagnetic phase of strongly correlated materials. Three peak spectra arise as a superposition of the antiferromagnitic split bands smeared by the finite correlation length of the spin fluctuations plus the residual peak of the Landau quasi particle. The presence of the Landau peak is due to time averaging of the exchange scattering potential for low energy excitations. This effect leads to anomalous dispersion of the self energy for energies smaller than the characteristic spin fluctuation energy. This work lead to the papers A. P. Kampf and J. R. Schrieffer, J. Phys. Chem. Sol. 56, 12, 1673 (1995) and Proceedings of Physical Phenomena in High Magnetic Fields II, P. 609 (1996) World Scientific.

II. Other Current Federal Support

M. A. Novotny - NSF CARM-95 program (Computational Aspects of Real Materials) "Computational Studies of Dynamical Phenomena in Nanoscale Ferromagnets" (with Per Arne Rikvold) $434,000.00 for August 1995-August 1998. (FY96 for $217,000.00)

J. R. Schrieffer - NSF DMR96-29987, "Theory of Strongly Correlated Electron Systems" $405,000, 7/1/96 - 6/30/99

III. Personnel associated with the grant:

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IV. Funds Unexpended $ 5,236