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Technical Progress Report

Grant: DE-FG05-91ER45443 entitled "Heavy fermions and other highly correlated electron systems".

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The work performed during the above mentioned award period is a continuation of our efforts (see Final Technical Report of grant DE-FG02-87ER45333) to gain a microscopic understanding of the magnetic and electronic properties of heavy-fermion and related highly correlated systems. In view of the short period since the beginning of this award I am going to report on work carried out since the expiration of the previous grant (December 1990). During this period P.D. Sacramento completed is dissertation (at Temple Univ.) and two students at FSU started to work on this project. I am presently profiting from the collaboration of V. Dorin as a postdoctoral associate.

Below I give a brief summary of the achievements grouped under three main headings, namely (1) heavy-fermion, mixed-valence and Kondo systems, (2) the n-channel Kondo problem and applications, and (3) one-dimensional conductors and antiferromagnets. The list of published papers and preprints is attached to the report, as well as a list of abstracts submitted to Conferences. All these papers are new in the sense that none of them was listed in the final technical report of grant DE-FG02-87ER45333.

1) <u>Heavy-fermion, mixed-valence and Kondo systems</u>

The main effort of the research was concentrated on topics of heavy fermion and Kondo alloys and compounds. For the sake of clarity I have subdivided the research activities into three topics, which are briefly described below. In addition I have been co-editor of two conference proceedings books, which are listed at the end of the report.

1a) **Kondo insulators and Kondo holes** [5,13]

The Kondo hole is an isolated nonmagnetic impurity in a heavy fermion lattice. Experimentally the Kondo hole can be realized by

La or Th atoms replacing a Ce ion in a stoichiometric Ce-compound or Th substituting for U in a U-compound. The Kondo hole breaks the translational invariance of the lattice and with increasing impurity concentration the coherent heavy fermion state is destroyed. Perturbations of the coherent state can be studied in the f-electron density of states. We consider a dispersionless orbitally nondegenerate f-band locally hybridized with one tight binding conduction band with nearest neighbor hopping on a simple cubic lattice. The Kondo hole is introduced by a large local f-level energy, which suppresses the occupation of the f-state at that site. We have studied the effects of the scattering off the impurity on the local density of f-states in the neighborhood of the Kondo hole. The scattering can be described in terms of one scattering phase shift. The correlations within the f-band are introduced via a selfenergy, evaluated to second order perturbation in U, using the leading order in the 1/d expansion, in which the tedious **k** integrations are properly carried out, but the **k** dependence of the selfenergy is neglected.

For a Kondo insulator we find a δ-function-like boundstate in the gap. The spectral weight of the boundstate decreases rapidly with increasing distance from the impurity for all values of the f-level energy. In the metallic case we obtain a resonance of finite width in the pseudogap of the lattice, which again is localized in the neighborhood of the Kondo hole. These localized states appear only in the coherent phase and disappear in the continuum at higher temperatures ($T > T_K$).

Although Kondo holes are also important in heavy fermion metals, their effects are more dramatic in Kondo insulators. In view of the very narrow gap Kondo hole defects are almost unavoidable in Kondo insulators. The recent discovery of new Kondo insulators, e.g. CeNiSn, $Ce_3Bi_4Pt_3$, YbB_{12} and UNiSn, has renewed the experimental interest in these compounds. Isolated Kondo holes in insulators are magnetic (Curie susceptibility and Schottky anomaly in a magnetic field) and could be detected by EPR. A larger concentration of Kondo holes should be observable by infrared spectroscopy.

An impurity band [13] develops in the gap of insulators with finite concentrations of Kondo holes. This impurity band gradually smears the hybridization gap. For a low density of Kondo holes the width and the height of this band depend nonanalytically on the impurity concentration. The Fermi level is pinned within this band. As a consequence of the finite width of the impurity band there is a small low temperature regime with a specific heat proportional to T. The γ coefficient is strongly enhanced. The susceptibility does no longer diverge as $T \to 0$, as for the isolated Kondo hole, but follows a Curie-Weiss-like behavior with an antiferromagnetic Weiss-temperature. We have also studied the Korringa relation associated with the NMR relaxation rate.

1b) **The two-impurity Kondo problem** [11]

At low T heavy fermion compounds may order antiferromagnetically or display anomalous superconducting properties or just remain a Pauli paramagnet of electrons with strongly enhanced mass. In order to understand such nonuniversal behavior it is necessary to invoke at least two competing energy scales, one of them being the Kondo temperature. The simplest model showing the competition between two energy scales is the two impurity Kondo model. The two energy scales are T_K and the RKKY-interaction, whose $k_F R$-dependence yields the desired nonuniversal behavior.

The single impurity Kondo problem can be mapped onto a resonant level of spinless fermions with an attractive interaction between the localized and extended states (Falicov-Kimball interaction). We consider two such impurities at sites $\mathbf{R}_1$ and $\mathbf{R}_2$ interacting with each other via a hopping matrix element t and an interaction G between the localized fermions. The interactions t and G resemble the RKKY-interaction between the impurities. The physics of the model is most conveniently discussed in terms of even and odd parity states with respect to the point $(\mathbf{R}_1+\mathbf{R}_2)/2$. We obtain the k-space renormalization group equations for the model, which are integrated and discussed in terms of Ward-cancellations. Finally, approximate expressions for the static and dynamical susceptibilities for the response to a homogeneous and staggered field are obtained. No dramatic anomalies are found, probably as a consequence of the broken spin-rotational invariance of the model.

1c) **$YbPd_2Si_2$: Comparison of theory and experiment** [12]

This work is a continuation of my efforts to obtain a detailed quantitative comparison between theory and experiment for Kondo systems. The theoretical basis for this comparison is the exact Bethe-ansatz solution of the degenerate Anderson model.

The available data for the specific heat, magnetic susceptibility, magnetization , valence, NMR Knight shift and relaxation rate, and the quadrupolar moment of $YbPd_2Si_2$ have been examined within the framework of the single-ion Anderson model. Previous similar analysis were successful for numerous light heavy-fermion compounds, where crystalline fields do not play a dominant role (e.g. $CeSn_3$, $(Ce,La)Pb_3$, YbCuAl, $YbCu_2Si_2$ and $YbCu_4Ag$). For $YbPd_2Si_2$ substantial crystalline field splittings difficult a quantitative comparison with existing exact solutions of the Anderson model. Inconsistencies with a previously proposed interpretation that a nearly degenerate ground-quadruplet determines the low-temperature thermodynamics are pointed out [12]. It is concluded that at least three of the four Kramers doublets participate in the low T properties. These three doublets should have an overall splitting of the order of T_K, i.e. about 100K. We also propose a simple resonant level model to parametrize the NMR relaxation rate at low T. Finally, we suggest hydrostatic pressure experiments to study the nature of the faint ordered phase at very low temperatures.

2) The n-channel Kondo problem and applications

The n-channel Kondo problem was originally proposed to describe the interaction of S-state ions with conduction electrons in a simple metal. For a given spin S the model has two parameters, namely the Kondo temperature and the number of channels n. For $n = 2S$ the conduction spins can exactly compensate the impurity spin at low T, giving rise to Fermi-liquid properties. This situation is experimentally realized for instance with Fe and Cr impurities in a noble metal like Cu. If $S > n/2$ (undercompensated spin) the combined spin-density of the conduction electrons at the impurity site is not large enough to completely screen the impurity spin. The remaining degeneracy, $S - n/2$, is then lifted by the magnetic field giving rise to a Schottky anomaly. Finally, if $S < n/2$ (overcompensated spin) there are more conduction electron spin-degrees of freedom than needed to screen the impurity spin S. The consequence is critical behavior, i.e. power laws in the susceptibility and specific heat as T and H tend to zero. Most of the work described below refers to this overcompensated situation.

2a) **Electron assisted tunneling of an atom in a double-well potential** [1,6]

We considered an atom in a double-well potential (parametrized by a two-level system (TLS)) interacting with screened conduction electrons. The tunneling of the TLS is assisted by the Fermi gas, the scattering giving rise to logarithmic infrared singularities. We derived and analyzed the renormalization group equations for an arbitrary number of relevant orbital channels. As discussed previously by Zawadowski et al. two situations have to distinguished: (i) the commutative model, in which the invariant coupling is not renormalized, and (ii) the noncommutative model, which scales into a strong coupling fixed point. We have shown that close to this strong coupling fixed point the model is equivalent to the n-channel Kondo problem with $S = 1/2$ (the TLS) and an effective number of channels that depends on the initial conditions of the renormalization procedure. The Zeeman splitting in the Kondo problem represents the energy difference between the two positions of the tunneling atom (asymmetry of the well). In general this then corresponds to the overcompensated situation, so that the atom is not localized at one of the potential minima. The susceptibility (to an asymmetry in the well) diverges as $H \rightarrow 0$ and $T \rightarrow 0$, indicating that the symmetric TLS is unstable to a local lattice deformation via coupling to phonons. The lattice distortion disappears above a critical temperature T_c. The groundstate equilibrium situation of the TLS corresponds to $H \neq 0$ and a Fermi liquid picture applies. The specific heat γ-values become giant as $H \rightarrow 0$. For small fields the specific heat shows a double peak structure which is particularly pronounced for $n = 2$. There is a very close relationship between this model and the quadrupolar

Kondo effect.

2b) **Impurity-induced critical behavior in antiferromagnetic Heisenberg chains** [3,4,6]

The purpose of this work is the construction of an antiferromagnetic Heisenberg chain with similar properties as the n-channel Kondo problem. We considered an integrable SU(2)-invariant model consisting of the Heisenberg chain of arbitrary spin S (Takhtajan-Babujian model) interacting with an impurity of spin S'. The impurity is assumed to be located on the m-th link of the chain and interacts only with both nearest neighbor sites. Our starting point is a set of commuting transfer matrices, whose local weights satisfy the triangular Yang-Baxter relations. The diagonalization of the transfer matrices leads to the Bethe ansatz equations for the model. The Hamiltonian can be derived from the diagonalized transfer matrix. The thermodynamics of the system has been studied. As in the n-channel Kondo problem three situations have to be distinguished: (i) If $S' = S$ the impurity just corresponds to one more site in the chain. (ii) If $S' > S$ the impurity spin is only partially compensated at $T = 0$, leaving an effective spin of $(S'-S)$ (undercompensated impurity). (iii) $S' < S$ the entropy has an essential singularity at $T = H = 0$, giving rise to critical behavior as H and T tend to zero. As a consequence a two-peak structure arises in the specific heat in a small but finite field and giant γ-values are obtained. These properties are in close analogy to those of the n-channel Kondo problem. This relation is stressed in [6].

2c) **Thermodynamics of the n-channel Kondo model for general n and impurity spin S in a magnetic field** [7]

We completed our study of the thermodynamic Bethe ansatz equations of the n-channel Kondo problem. Results were obtained both analytically and numerically; this work constitutes the central part of P.D. Sacramento's Ph.D. thesis. The thermodynamics of the impurity was obtained as a function of temperature, external field, impurity spin S and the number of channels. Several numerical procedures had to be employed to obtain satisfactory results for the entire parameter range. The main difficulty we had to confront was that the problem requires a substantial increase in the numerical precision compared to similar efforts for the Kondo and Coqblin-Schrieffer models. This is in particular the case for situations where properties vary on a logarithmic scale or diverge resembling critical behavior. We have for the first time looked into the field-dependence of the thermodynamics of these non-Fermi-liquid-like (and nontrivial) cases. This study involves all three cases; (i) the perfectly compensated impurity ($n = 2S$), and the (ii) undercompensated and (iii) overcompensated situations. Physical applications have been presented in [6] and in the final technical report of the preceding grant.

3) <u>One-dimensional conductors and antiferromagnets</u>

One-dimensional conductors and quantum magnetic systems are highly correlated, since as a consequence of the reduced phase space the quantum fluctuations play a fundamental role. These systems are related to other subjects investigated here in two ways: (i) the same mathematical techniques are employed (e.g., Bethe ansatz, renormalization groups) and (ii) they have common physical aspects with high-T_c superconductivity.

3a) **Hubbard chain with an attractive interaction** [2]

Two types of states play a role in the groundstate properties of the Hubbard chain with an attractive interaction; (i) spin-singlet boundstates of the Cooper-pair type and (ii) states of unpaired electrons. From the symmetry of the wavefunction and their spin the "Cooper pairs" are bosons, while unpaired electrons are fermions. These bosons are hard-core bosons, i.e., they all must have different quantum numbers. Hence, the states are occupied according to the Fermi distribution, rather than the Bose-Einstein one. These bosons have a "Fermi surface" and do not undergo a condensation (analogous to spin waves in the antiferromagnetic Heisenberg chain), i.e., the system has no long-range order.

In the ground state for a less-than-half-filled band and zero magnetic field, all the electrons are paired in spin-singlet Cooper-pairs. A magnetic field H larger than a critical value H_c is needed to overcome the binding energy of the Cooper pairs. In other words, there is no response to a field smaller than H_c. The depaired electrons for $H > H_c$ occupy the unpaired-electron band and give rise to a magnetization, which just above H_c is proportional to $(H - H_c)^{½}$ in analogy to a Prokovsky-Talapov transition. This point was questioned by Woynarovich and in our Comment we provide the mathematical proof for this nonanalytical behavior.

3b) **Metal-insulator transition in the one-dimensional Hubbard model with degeneracy** [10]

The starting point for this calculation is the SU(N) generalization of Lieb and Wu's Bethe ansatz solution of the standard one-dimensional Hubbard model to N spin degrees of freedom. This model is integrable and has several unusual properties at low temperatures, one of them being a metal-insulator transition at a finite U. The Bethe-ansatz equations at $T = 0$ were analyzed in the thermodynamic limit in the absence of external fields. As usual spin and charge degrees of freedom decouple in one dimension. Using the Bethe-ansatz equations we derived the phase shift for the scattering between charges and obtained their effective interaction potential. In the continuum limit this effective interaction corresponds to a potential of the form $[\mathrm{Sinh}(ax)]^{-2}$, where x is the distance between the particles involved and a is an inverse length scale. In the limit $N \rightarrow \infty$ and in the continuum limit the charges reduce to a Bose gas interacting via a δ-function potential. We further have addressed the properties of the charge degrees of freedom for a band-filling close to one electron per site. The charge excitations obey Fermi statistics. We found a Mott metal-insulator transition at a critical value U_c of the Coulomb repulsion. For $U < U_c$ the system is metallic, while for $U > U_c$ it is insulating. U_c depends on N ($U_c = 0$ for $N = 2$). A qualitative change in the charge rapidity distribution is found at U_c. The Fermi velocity is finite for $U < U_c$, diverges as $U \rightarrow U_c$ and vanishes for $U > U_c$. Such a metal insulator transition is also predicted by mean-field theories, which should hold for sufficiently large N, independently of the dimension.

3c) **Universal properties of one-dimensional systems with SU(N)-symmetry** [8,9]

We have shown that quite generally the zero-temperature susceptibility to a field breaking the SU(N)-invariance of the internal degrees of freedom of an integrable one-dimensional system has logarithmic singularities as the field tends to zero. The logarithms arise from the interference of the two "Fermi points" of the spin wave spectrum. As a consequence of these logarithms the specific heat coefficient γ behaves singularly as $H \rightarrow 0$ and $T \rightarrow 0$. The spin wave velocity is shown to be inversely proportional to the zero-field susceptibility. These properties hold for a large variety of models, e.g., the SU(N)-invariant Heisenberg chain of arbitrary spin [9] including the Babujian-Takhtajan model, the N-component supersymmetric t-J model in one dimension, the Gross-Neveu model, and the SU(N) generalization of the Hubbard chain.

PUBLICATIONS

[1] P.D. Sacramento and P. Schlottmann, Low-temperature properties of a two-level system interacting with conduction electrons, Phys. Rev. B **43**, 13294 (1991).

[2] P. Schlottmann, Reply to Comment on: Low-temperature properties of the Hubbard chain with an attractive interaction, Phys. Rev. B **43**, 11451 (1991).

[3] P. Schlottmann, Impurity induced critical behavior in antiferromagnetic Heisenberg chains, J. Phys. Cond. Matt. **3**, 6617 (1991).

[4] P. Schlottmann, Overcompensated impurities in antiferromagnetic Heisenberg chains, J. Appl. Phys. **70**, 6071 (1991).

[5] R. Sollie and P. Schlottmann, Local density of states in the vicinity of a Kondo hole, J. Appl. Phys. **70**, 5803 (1991).

[6] P.D. Sacramento and P. Schlottmann, Applications of the overcompensated n-channel Kondo problem, J. Appl. Phys. **70**, 5806 (1991).

[7] P.D. Sacramento and P. Schlottmann, Thermodynamics of the n-channel Kondo model for general n and impurity spin S in a magnetic field, J. Phys. Cond. Matt. , in print.

[8] P. Schlottmann, Some universal properties of one-dimensional systems with SU(N)-symmetry, in Physical Phenomena at High Magnetic Fields, eds. E. Manousakis et al. (Addison-Wesley, 1991), p.502.

[9] P. Schlottmann, Logarithmic singularities in the susceptibility of the antiferromagnetic Heisenberg model, preprint.

[10] P. Schlottmann, Metal-insulator transition in an Hubbard-like model with degeneracy in one-dimension, preprint.

[11] P. Schlottmann and J.W. Rasul, Two interacting magnetic impurities in a metal: Renormalization group treatment of a simple model, preprint.

[12] P. Schlottmann, $YbPd_2Si_2$: An N = 4 Kondo compound at low T ?, preprint.

[13] P. Schlottmann, Impurity bands in Kondo insulators, preprint.

BOOKS EDITED

[1] G.E. Barberis, M.E. Foglio, J.E. Crow and P. Schlottmann, Proceedings of the 6th International Conference on VALENCE FLUCTUATIONS, Rio de Janeiro, Brazil, July 1990; Physica B**171**, 1991.

[2] E. Manousakis, P. Schlottmann, P. Kumar, K.S. Bedell and F.M. Mueller, Proceedings of the Conference on PHYSICAL PHENOMENA AT HIGH MAGNETIC FIELDS, Tallahassee, May 1991, Addison-Wesley, 1991.

OTHER ACTIVITIES

[1] Short Course at the Naval Coastal Research Center, Panama City, June 1991; P. Schlottmann and P. Wise, lecturers.
Superconductivity and applications.

[2] Invited participant at the workshop on Novel Superconductors: Concepts, Models and Methods; Institute for Scientific Interchange Foundation, Turin, Italy, November 1991.
Invited talk: Some applications of the n-channel Kondo problem.

[3] Member of the Local Organizing and Program Committees of the Conference on PHYSICAL PHENOMENA at HIGH MAGNETIC FIELDS, Tallahassee, May 1991.

Abstracts submitted to Conferences

March 1991 Meeting of the American Physical Society, Cincinnati

1) Low temperature properties of a two level system interacting with conduction electrons, P.D. Sacramento and P. Schlottmann.

2) Influence of potential scattering on the diffusion of a heavy charged particle in a metal, P. Schlottmann and J.W. Rasul.

3) A simple theory of the Kondo hole, R. Sollie and P. Schlottmann.

4) Isolated ferromagnetic bonds in the two dimensional spin 1/2 Heisenberg antiferromagnet, K. Lee and P. Schlottmann.

5) Thermal conductivity of impurity doped high T_c superconductors, S.T. Ting, P. Pernambuco-Wise, J.E. Crow and P. Schlottmann.

The 5th Joint MMM-Intermag Conference, Pittsburgh, June, 1991

6) Local density of states in the vicinity of a Kondo hole, R. Sollie and P. Schlottmann.

7) Low temperature properties of a two level system interacting with conduction electrons, P.D. Sacramento and P. Schlottmann.

8) Impurity induced critical behavior in antiferromagnetic Heisenberg chains, P. Schlottmann.

Conference on Physical Phenomena at High Magnetic Fields, Tallahassee, 1991.

9) Some universal properties of one-dimensional systems with SU(N) symmetry, P. Schlottmann.

Workshop on Novel Superconductors: Concepts, Models and Methods, Fall 1991.

10) Some applications of the n-channel Kondo problem, P. Schlottmann.

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