Proc. 18th Int. Conf. on Low Temperature Physics, Kyoto, 1987
Japanese Journal of Applied Physics, Vol. 26 (1987) Supplement 26-3

Theory of the Coherent Heavy Fermion State: Universal Behavior, Pressure Dependence and Neutron Scattering Cross Section

Assa AUERBACH and K. LEVIN
The James Franck Institute, The University of Chicago, Chicago, IL 60637

We discuss a solution of the Anderson lattice Hamiltonian within a 1/N expansion framework which provides a well controlled microscopically based description of the coherent heavy fermion state and associated Landau parameters. This theory has been previously used to explain systematic scaling with γ (the linear coefficient of the specific heat) of the T^2 contribution to the resistivity and $T^3 \ln T$ term in the specific heat. Here it is also extended to discuss recent neutron experiments. Antiferromagnetic peaks in the neutron cross section which correspond to zone boundary wave vectors and frequencies of the order of T_K arise naturally as a consequence of transitions across the hybridization gap. Finite frequency structure at low wave vectors derives from f-spin non conserving processes which occur at the 1/N level when a realistic c-f hybridization to a local crystal field doublet is included in the Anderson lattice.

It is the purpose of this paper to review our results in the 1/N expansion of the Anderson Lattice (AL) model, and compare them to recent experiments in various heavy fermion compounds. We show that the AL model predict universal features which are common to most of the materials for which large mass enhancement m^*/m values are observed. We derive a consistent Fermi liquid theory for the coherent state including the quasiparticle interactions. We argue that correlations observed in the the inelastic neutron data can be understood within the leading order approximation.

In the case of large on-site Coulomb repulsion U between f-electrons we can introduce the Kondo-Boson (KB) fields of Coleman at each lattice site[1], and replace the 4-fermion term by a constraint on the total f-electron and KB occupation. This results in the following path integral representation of the AL partition function:($\hbar$=1,β=1/T)

$$Z_{AL} = \int D\,\lambda b^* bc^* cf^* f \exp\left[-\int_0^\beta d\tau\, (L_{AL}(\tau)+ \right. \qquad (1a)$$

$$\left. i\sum_{im}\lambda_i (f^*_{im} f_{im} + \frac{1}{N} b^*_i b_i - Q_0)\right)$$

where,

$$L_{AL} = \sum_k \{ c^*_{ks}(\partial_\tau + \varepsilon_k) c_{ks} + f^*_{km}(\partial_\tau + \varepsilon^0_f) f_{km} \} +$$

$$\sum_i b^*_i \partial_\tau b_i + \frac{V}{\sqrt{N}} \sum_{k,q,s,m} \{ u_{s,m}(k) c^*_{k,s} f_{k+q,m} b^*_q + [h.c] \}, \qquad (1b)$$

where ε_k and ε^0_f are the conduction and dispersionless valence band energies respectively. The band structure ε_k defines the bare density of states ρ_c, and the fermi surface at $\varepsilon_k = \mu_0$. The bare chemical potential μ_0 is determined by the total (valence plus conduction) electron density Here, c_{is} and f_{im} are grassman variables of Wannier states, and b_i are the KB complex fields. Both spin indices run over N values. We shall use that expansion to describe the physical system for which N=2. The integrations over the Lagrange multiplier fields $\lambda_i(\tau)$ impose the local constraints of $n_f + n_b = Q_0$ at all times and sites, where n_α denotes the number operator of particle α. Q_0 is kept as a fixed parameter (instead of $Q_0 = 1/N$) in order to define a true N-independent mean field theory. The pseudo-spin matrices $u_{s,m}(k)$, represent the correct scattering amplitude of a $s=\frac{1}{2}$ conduction electron from a local f-crystal-field doublet. The anisotropy of the magnetic moment operator in k-space leads to substantial modification from the spin conserving model $u \propto \delta_{s,m}$. We shall later demonstrate why these matrices are important to understand the forward scattering rate of neutrons in the low temperature regime.

The mean field theory $N=\infty$ of the AL has already been amply discussed in the literature[2]. In essence, the Bose fields are replaced by their expectation values and an effective single particle band theory is obtained. The variationally determined mean field parameters $r_0 = \langle b \rangle$ and $\varepsilon_f = \varepsilon^0_f + i\langle\lambda\rangle$, represent the effective c-f hybridization and renormalized f-level respectively. They determine the two renormalized bands, which are separated by a gap at ε_f. In heavy fermion systems we are interested in a specific limit of the AL model, the Kondo limit, where $J \equiv \rho_c V^2/(\varepsilon_f - \varepsilon^0_f) \ll 1$. In the Kondo limit the density of states enhancement at the Fermi level is $m^*/m \propto \exp(1/J) \gg 1$, and the characteristic energy scale of the renormalized band structure $\bar{T}_K \propto \mu_0 \exp(-1/J)$. Also the AL model reduces to the Coqblin-Schrieffer (Kondo, for N=2) lattice since the f-charge fluctuations are greatly suppressed. For large m^*/m, the Kondo lattice temperature $\bar{T}_K$ emerges as the smallest energy scale in the Fermi liquid and thus dominates its low temperature properties.

The results of the mean field theory thus allow us to understand the large mass enhancements as observed in the specific heat and susceptibility. However the Wilson ratio at this level is unity and the resistivity vanishes at all temperatures since no interactions between quasiparticles have yet been included.

In order to obtain information about the interactions in the Fermi liquid it is necessary to allow for fluctuations in the bose fields. This was carried out by the authors using a functional integral formalism[3] and applying the Read and Newns[4] radial gauge transformation on the Bose fields. The analogous calculation in the cartesian coordinates has been carried out by Millis and Lee[5], who arrived independently at the same results. The steepest descents evaluation of the free energy amounts to a 1/N expansion, with which we have extracted the leading orders in the vertex function and quasiparticle self energy. Interactions are mediated by an RPA-like Kondo boson propagator which represents simultaneous fluctuations of the c-f hybridization matrix elements and the renormalized f-level energies. We have obtained the Landau scattering amplitudes $\{A^{s,a}_l\}$ following the microscopic prescription of Ref. 6. Our main results are that the Wilson ratio $\chi/(\gamma g^2) = 1 - A^a_0 = 1 + 1/N + O(Q_0/N)$ and all the Landau parameters are independent of $\bar{T}_K$. Charge fluctuations $1 - A^s_s = O(m/m^*)$ are largely suppressed, as expected from the microscopic constraint on the f-charge. These results are expected to survive also in the non spin conserving generalization of the AL model.

There exists a specific heat correction ΔC_V analogous to the paramagnon $T^3 \log T$ contribution in liquid ^{3}He:

$$\Delta C_V = \delta\, T^3 \log\left[\frac{T}{\bar{T}_K}\right] + O((T/T_K)^3) \ , \qquad (2)$$

$$\delta = a \left[\frac{T}{\bar{T}_K}\right]^3 \ ,$$

where a is a positive number close to unity, and the resistivity goes as:

$$\rho = A\ T^2 + O(T^3)\ ; \qquad (3)$$

$$A = \rho_{max}\ (1/\lambda \bar{T}_K)^2\ ,$$

where $\rho_{max} = h/(e^2 k_f N^2) = 100\text{–}300\mu\Omega\text{cm}$ and where λ is a Fermi surface geometric factor of order unity.

Our results can best be summarized by the simple scaling relations relations which are obtained between γ, χ, A and δ.

$$\chi \propto \gamma\ ;\ A \propto \gamma^2\ ;$$

$$\delta \propto \gamma^3\ . \qquad (4)$$

The pressure dependence is a useful probe to the relations (8). *In other words the dominant interactions and temperature dependence in the fermi liquid have a single energy scale $\bar{T}_K$.* In UPt_3, γ can vary under pressure by 40%. As we have shown in Ref. 3, predictions appear to be well confirmed by experiments[7,8,9]. This analysis of the data raises doubts about the validity of paramagnon models, or any models involving RKKY derived interactions with a different energy scale than $\bar{T}_K$, for which relations (4) are not expected to be valid. Large deviations from these relations are found for the analogous experimental measurements in ^3He which is a Fermi liquid that is not expected to obey the Kondo lattice scaling behavior.

Recent neutron experiments have yielded evidence for antiferromagnetic correlations in a variety of heavy fermion systems[10,11]. Two features of the neutron data are most striking: (1) A maximum in the magnetic diffuse scattering at the Brillouin zone edge, which occurs at extremely low energies (of order meV); (2) A non-vanishing contribution at the zone center (low q), at the same energy scale. Both these features were interpreted in terms of antiferromagnetic interactions between local f-spins, derived from renormalized RKKY interactions. Here, however, we suggest that these features could be understood in the context of the leading order 1/N expansion of the Anderson model, including realistic hybridization to the cystal field f-level. (1) arises naturally at the mean-field level (non interacting renormalized band structure). The enhancements of the imaginary susceptibility at the zone edge corresponds to interband transitions across the narrow hybridization gap. These inealstic processes dominate the neutron cross section because both initial and final states have large densities of states. This explanation of the inelastic antiferromagnetic correlations has been provided previously in the context of mixed valence systems[12]. (2): The small q feature in the data suggests important relaxation processes of the f-electron spins[13]. It is known that the Kondo interaction with the conduction electrons leads to sizeable relaxation of the f-electron spin in the Kondo impurity systems. However, in the coherent Fermi liquid state of the Kondo lattice, quasiparticles on the Fermi surface are long lived excitations (as opposed to resonances), and therefore by feature (2) one must conclude that the Fermi liquid interactions do not conserve the spin quantum numbers. It is clear however that the rare earth ion which is in a crystal field doublet at low temperatures, hybridizes with a conduction band state k via a non spin conserving interaction $u_{s,m}(k)$, such as was introduced in Eq. (1). $u_{s,m}$ can be diagonalized in a pseudo-spin basis, which is not the eigenstate representation of the magnetic moment operator. We can show that if indeed the magnetic moment operator $\mu_{s,s'}(k) = u^+(k) <m\,|J_f \cdot \hat{q}\,|m'> u(k)$ varies on the Fermi surface, the O(1/N) corrections to $\text{Im}\chi$ do not vanish at q=0, and yield

$$\text{Im}\chi(q=0,\omega) = \sum_{q,rr'} \bar{\Pi}_{r,r'}(q,\omega) D_{rr'}(q)\ , \qquad (5a)$$

where $D_{r,r'}$ is the Kondo Boson propagator[3], and

$$\bar{\Pi} = \sum_k \text{Tr}\ \{[\mu_k \mu_k - \mu_{k+q}\mu_k]\ c^r_{k,k+q} c^{r'}_{k+q,k}\ G_k G_{k+q+\omega} \qquad (5b)$$

Numerical evaluation of the resulting sum yields the results shown in Fig. 1, which can be seen to be in qualitative agreement with the neutron data.

This work was supported by NSF DMR-84-20187 and MRL grant NSF-DMR-82-6892.

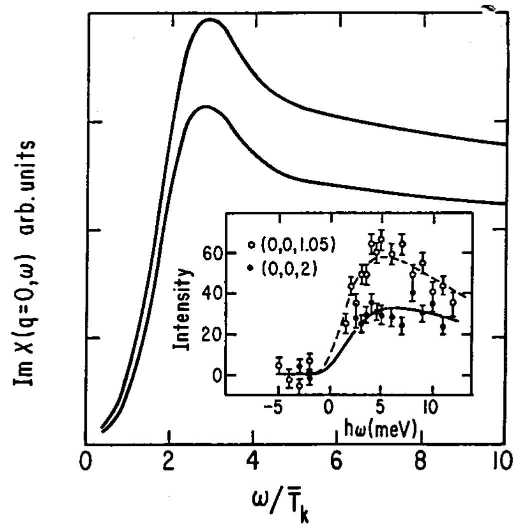

Fig. 1: Imaginary susceptibility at the zone center. Upper and lower curves are computed by Eq. 5 using different k-dependence of magnetic moment operator. Inset: UPt_3 data from Ref. 10, for two values of q. Solid dots are at the "effective" zone center, circles - zone boundary for a doubly large Brillouin zone. (There are 2 uranium atoms per unit cell at approximately half a lattice vector apart).

References

1. P. Coleman, Phys. Rev. B **29**, 3035 (1985); Proc. 8 Tanaguchi Symp. on Mixed Valence, S. St. Phys. **62**, Springer-Verlag (1985).
2. C. Lacroix and M. Cyrot, Phys. Rev. B **20**, 1969 (1979). P.F. de-Chatel, Sol. St. Comm. **41**, 853 (1982). N. Read and D.M. Newns, Sol. St. Comm. **52**, 993 (1984). T.M. Rice and K. Ueda, Phys. Rev. B (in press); D. Baeriswyl, C. Gros and T.M. Rice, ETH-Hongerberg preprint. B.H Brandow, Phys. Rev. B **33**, 215 (1986).
3. A. Auerbach and K. Levin, Phys. Rev. Lett. **57**, 877 (1986); A. Auerbach and K. Levin, Phys. Rev. **B34**, 3524 (1986).
4. N. Read and D.M.Newns, J. Phys. **C16**, 3273 (1983); N. Read, J. Phys. **C18**, 2651 (1985).
5. A.J. Millis and P.A. Lee, Phys. Rev. B, to be published.
6. A.A. Abrikosov, L.P. Gorkov and I.E. Dzyaloshinski, "Methods of Quantum Field Theory in Statistical Physics", Dover N.Y. (1975).
7. G.E. Brodale, R.A. Fisher, Norman E. Phillips, G.R. Stewart and A.L. Giorgi Phys. Rev. Lett. **57**, 234 (1986).
8. J.J. M. Franse, P.H. Frings, A. Menovsky and A. de Visser, Physica **130B**, 180 (1985).
9. J.O. Willis, J.D. Thompson, Z. Fisk, A. deVisser, J.J.M. Franse and A. Menovsky, Phys. Rev. B **31**, 1654 (1985).
10. G. Aeppli et al. Phys. Rev. Lett. **58**, 808 (1987);
11. G. Aeppli et al. Phys. Rev. Lett. **57** 122 (1986).
12. S. M. Shapiro and B. H. Grier, Phys. Rev. B, **25**, 1457 (1982); A.J. Fedro and S.K. Sinha, "Valence Fluctuations In Solids", edited by L.M. Falikov, W. Hanke, M.B. Maple, North Holland, New York, (1981); Also recently B.H. Brandow, Los Alamos preprint,submitted to Phys. Rev. B.
13. If the total magnetization commutes with the Hamiltonian, the f-sum rule guarantees the vanishing of the integrated inelastic cross section as q^2 for small q. We thank David Pines and Tony Legget for illuminating to us the generality of this theorem. See also C.E.T Goncalves da-Silva, Phys. Rev. Lett. **42**, 1305 (1979).