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THE ANDERSON LATTICE AND UNIVERSAL PROPERTIES OF HEAVY FERMION SYSTEMS

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ABSTRACT

Using the Kondo Boson - 1/N expansion, we solve for the Fermi liquid properties of the Anderson lattice at low temperatures. The Kondo limit of this model is shown to necessarily induce large mass enhancements $m^*/m \gg 1$, and generate a low lying energy scale $\overline{T}_K \propto (m^*/m)^{-1}$, which dominates the dynamics of this heavy Fermi liquid. In particular, our calculation leads to the following predictions: (1) The specific heat $C_V = \gamma T \propto T/\overline{T}_K$ with corrections $\Delta C_V = (T/\overline{T}_K)^3 \log(T/\overline{T}_K)$ (2) The zero temperature spin susceptibility $\chi \propto 1/\overline{T}_K$, and (3) the resistivity $\rho \propto (T/\overline{T}_K)^2$. We analyze recent pressure dependent C_V, χ and ρ/T^2 measurements on UPt_3 to confirm the scaling of these quantities with a single strongly pressure dependent energy scale. The universality of these relations is supported by evidence of systematic trends throughout the entire class of heavy fermion compounds.

The class of heavy electron materials poses a new challenge for condensed matter theorists, where traditional "tools of the trade" seem unable to provide a link between the underlying microscopic physics and the Fermi liquid phenomena seen in experiments[1]. Strong two-body interactions U between valence electrons, are present at the rare-earth sites. When U is large these cannot simply be treated by standard perturbative expansions, and complications reminiscent of those of the Kondo impurity problem arise.

It is the purpose of this paper to explain the origin of Fermi liquid properties in the heavy fermion compounds. We use a simple microscopic model, and 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 heavy fermions from the Anderson lattice model (AL). Although no unambigous *ab-initio* calculation of the parameters of the AL has yet been provided, it is based on an intuitive real-space picture which seems to capture the important underlying physics. This model is the translationally invariant generalization of the Anderson impurity model which has successfully been used to explain the Kondo effect.

The Anderson lattice (AL) hamiltonian in second quantized notation is given by:

$$H^{AL} = \sum_{\mathbf{k},m} \varepsilon_{\mathbf{k}} c^{+}_{\mathbf{k},m} c_{\mathbf{k},m} + \varepsilon^0_f \sum_{\mathbf{k},m} f^{+}_{\mathbf{k},m} f_{\mathbf{k},m} + \frac{V}{\sqrt{N}} \sum_{i,m} (f^{+}_{im} c_{im} + c^{+}_{im} f_{im}) + U \sum_{imm'} f^{+}_{im} f_{im} f^{+}_{im'} f_{im'} \quad , \tag{1}$$

where $\varepsilon_{\mathbf{k}}$ and ε^0_f are the conduction and dispersionless valence band energies respectively. The label i denotes the Wannier state at site $\mathbf{r}_i$. The N-fold degeneracy of both bands is labelled by

m, $|m|\leq(N-1)/2$. V is the local hybridization matrix element which in this simplified version is taken to be independent of $\mathbf{k},m$. The large local Coulomb repulsion is parametrized by U. The band structure $\varepsilon_{\mathbf{k}}$ defines the bare density of states ρ_c, and the fermi surface at $\varepsilon_{\mathbf{k}}=\mu_0$. The bare chemical potential μ_0 is determined by the total (valence plus conduction) electron density

$$N_e=\int_{-\infty}^{\mu_0} d\varepsilon\rho_c(\varepsilon)\ .$$

In the case of large U, i.e $U\gg\varepsilon_f^0, \mu_0$, we can proceed by introducing the Kondo-Boson (KB) fields of Coleman at each lattice site[2], and replacing 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)

$$Z_{AL} = \int D\,\lambda b^* bc^* cf^* f \exp\left[-\int_0^\beta d\tau\ (L_{AL}(\tau)+i\sum_{im}\lambda_i(f^*_{im}f_{im}+\frac{1}{N}b_i^*b_i-Q_0))\right]\ , \qquad (2a)$$

where,

$$L_{AL} = \sum_{\mathbf{k}m}\{\ c^*_{\mathbf{k}m}(\partial_\tau+\varepsilon_{\mathbf{k}})c_{\mathbf{k}m}+f^*_{\mathbf{k}m}(\partial_\tau+\varepsilon_f^0)f_{\mathbf{k}m}\} +\sum_i b_i^*\partial_\tau b_i$$

$$+ \frac{V}{\sqrt{N}}\sum_{im}\{c^*_{im}f_{im}b_i^* + b_i f^*_{im}c_{im}\}\ , \qquad (2b)$$

Here, c_{im} and f_{im} are grassman variables, and b_i are the KB complex fields. 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 mean field theory N=∞ of the AL has already been amply discussed in the literature[3]. It bears close resemblence to the Hartree approximation in other many-body problems such as the Coulomb gas and the Hubbard model. As a variational estimate of the ground state, the same theory has been also derived using other approaches such as a generalized Gutzwiller approximation of Rice and Ueda[4], for which the relation to the KB theory has been recently explored[5]. In essence, the Bose fields are replaced by their expectation values and an effective single particle band theory is obtained. The mean field parameters r_0=$\langle b\rangle$ and $\varepsilon_f=\varepsilon_f^0+i\langle\lambda\rangle$, 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 $J\equiv\rho_c V^2/(\varepsilon_f-\varepsilon_f^0)\ll 1$. The mean field variational equations extremize the free energy with respect to r_0 and ε_f. In the

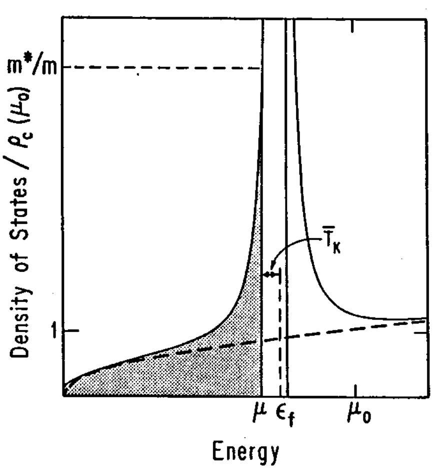

Fig. 1: The spherical band AL model, mean field N=∞ level. The dashed line in the bare conduction band density of states. The solid lines is the renormalized mean field band structure. Shaded area is the occupied Fermi sea at zero temperature.

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. In Fig. 1 we plot the density of states for a heavy fermion system with a spherical conduction band. The large peak of the renormalized density of states at the Fermi level is a direct consequence of the local f-charge constraint, and it confirms the idea (supported by the "dense Kondo system" approaches[1]) that the individual Kondo resonances overlap and form a narrow band of mostly f-character.

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 it is necessary to allow for fluctuations in the bose fields. This was carried out by the authors using a functional integral formalism[6] and applying the Read and Newns[7] radial gauge transformation on the Bose fields. The analogous calculation in the cartesian coordinates has been carried out by Millis and Lee[8], 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 $\{A_l^{s,a}\}$ following the microscopic prescription of Ref.9. Here, "s" and "a" denote the generalized symmetric and antisymmetric channels respectively. We find that the l=0,1 parameters are (up to relative corrections of $O(1/N, m^*/m^{-1})$:

$$A_0^a = \frac{-1.000}{N} + \frac{0.08}{N}(Q_0/\mu_0) \; ; \; A_0^s = 1.000 \; ; \; A_1^s = A_1^a = \frac{-.12}{N}(Q_0/\mu_0) \; . \qquad (3)$$

Also, it follows that the susceptibility and specific heat are renormalized such that

$$\chi = \chi^0(1+\delta m^*/m - A_0^a + O(1/N^2)) \; , \qquad (4)$$

and simililarly:

$$\gamma = \gamma^0(1+\delta m^*/m + O(1/N^2)) \; . \qquad (5)$$

These are known Fermi liquid identities related to spin and charge conservation. $\delta m^*/m$ is given in terms of the derivatives of the O(1/N) self energy.

In addition to the correction to γ, there exists a specific heat correction ΔC_V analogous to the paramagnon $T^3 \log T$ contribution in liquid ^{3}He. Our analysis followed Ref. 10, where the Kondo boson propagator replaced the RPA susceptibility that mediates the spin fluctuations. We found:

$$\Delta C_V = \delta \, T^3 \log \left[\frac{T}{\bar{T}_K}\right] + O((T/\bar{T}_K)^3) \; , \; ; \delta = a \left[\frac{T}{\bar{T}_K}\right]^3 \; , \qquad (6)$$

where a is a positive number close to unity. The contributions to C_v from higher powers of temperature are dominated by the variation of the mean field parameters r_0, ε_f, and μ, with characteristic energy scale $\bar{T}_K$.

Using this approach we were also able to estimate the T^2 coefficient of the low temperature resistivity $\rho = AT^2$. We follow the analogous paramagnon calculation[11]. The result is:

$$\rho = A \; T^2 + O(T^3) \; ; A = \rho_{max} (1/\lambda \bar{T}_K)^2 \; , \qquad (7)$$

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

Our results in Eqs. (4), (5), (6) and (7), can best be summarized by the simple proportionality relations which are obtained between γ, χ, A and δ.

$$\chi \propto \gamma \; ; \; A \propto \gamma^2 \; ; \; \delta \propto \gamma^3 \; . \qquad (8)$$

The pressure dependence is a useful probe to the relations (8). In UPt_3, γ can vary under pressure by 40%. As shown in Fig. 2, our predictions appear to be well confirmed by experiments. This analysis of the data raises doubts about the validity of paramagnon models, for which

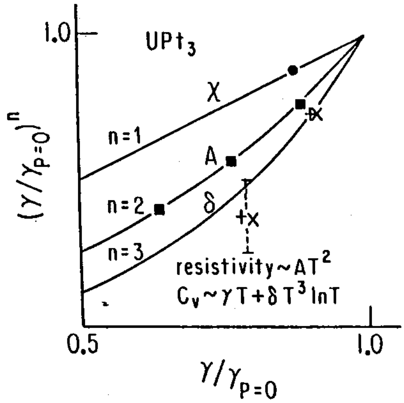

Fig. 2: Scaling of thermodynamic and transport coefficients with pressure dependent γ. (For the latter see Ref. 12). χ are from Ref. 13, resistivity from Ref. 14. The symbols + and x correspond respectively to the coeffient δ of $T^3 \ln T$ term in C_V and the coefficient ε of T^3 term in C_v (from Ref. 12). The solid lines are theoretical results summarized in Eq. (8).

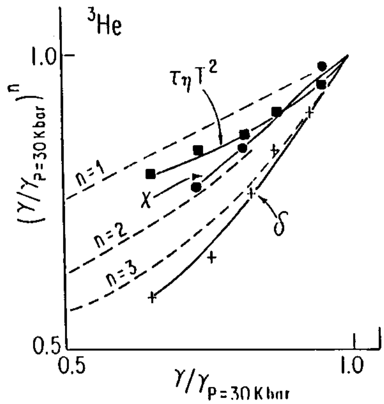

Fig. 3: Scaling of χ, δ, and $A=\tau_\eta T^2$ with pressure dependent γ in liquid ^3He. Data taken from Ref. 15. Here, τ_η is the quasiparticle lifetime as measured by the viscosity. In contrast to Fig. 2., it is evident that the relations (8) are not applicable to this Fermi liquid, in which ferromagnetic spin fluctuations are assumed to be important.

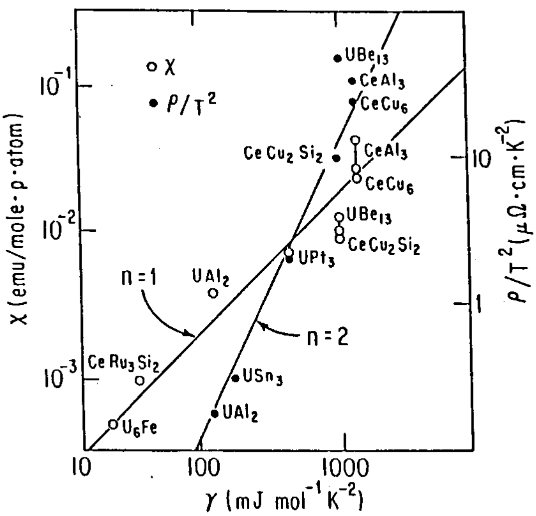

Fig. 4: Universal ratios in the heavy Fermion compounds. χ/γ data are from Ref. 1 and $A = \rho/T^2$ data are from Ref. 16. The solid lines are theoretical results summarized in Eq. (8).

relations (8) are not expected to be valid as happens in liquid ^3He. In fact, large deviations from these relations are found for the analogous experimental measurements in ^3He. These are plotted in Fig. 3. Also, as demonstrated in Fig. 4., universal relations between γ, χ and A for many different heavy fermions seem to correlate remarkably well with Eq. (8), We can therefore use the data to rule out theories which invoke different energy scales for γ^{-1} and e.g. $A^{-1/2}$. For example the so called "single Kondo" and the "intersite coherence" temperatures were used to characterize these quantities respectively in several heavy fermion materials. However such theories would be hard pressed to explain Fig. 4, where the coefficients in materials with completely different chemical composition and lattice structure seem to obey the same relations.

There is widespread evidence for antiferromagnetic correlations[17], in the heavy fermion materials. Because these fluctuations sometimes lead to spin density wave instabilities, this raises questions about the relation between the two instabilities and their implications on the symmetry of the order parameter. The present O(1/N) level of course is insufficient to provide answers related to multiple scattering of quasiparticles which thus requires an infinite resummation scheme. We are currently investigating such schemes in relation to both channels of instability. The analogy to theories of itinerant antiferromagnetism suggests that the KB interaction, with sufficient Fermi surface nesting, is sufficient to produce such an instability. To provide a detailed understanding of different materials it is necessary of course to generalize the spherical band AL model and include a realistic band structure with the correct crystal symmetries.

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