

From: CONDENSED MATTER THEORIES, Vol. 2
Edited by P. Vashishta, Rajiv K. Kalia,
and R.F. Bishop
(Plenum Publishing Corporation, 1987)

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 $\bar{T}_K \propto (m^*/m)^{-1}$, which dominates the dynamics of this heavy Fermi liquid. In particular, our calculation leads to the following predictions: (1) The specific heat $C_V \propto T \propto T/\bar{T}_K$ with corrections $\Delta C_V = (T/\bar{T}_K)^3 \log(T/\bar{T}_K)$ (2) The zero temperature spin susceptibility $\chi \propto 1/\bar{T}_K$; and (3) the resistivity $\rho \propto (T/\bar{T}_K)^2$. 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.

1. INTRODUCTION

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 experiments¹. 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. In particular, difficulties are encountered in applying e.g. the local density approximation², an important and cherished tool of band structure calculations. Crude estimates of the scale of U in uranium and cerium show it to be of order electron-volts, which necessarily implies that the independent valence and conduction electron picture is a doubtful zeroth order approximation for these materials.

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 m^*/m values are observed. We derive a consistent Fermi liquid theory for heavy fermions from the Anderson lattice model (AL). Although no unambiguous *ab-initio* calculation of the parameters of the AL has yet been provided², 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 (AI) model which has successfully been used to explain the Kondo effect.

Experimentally, heavy fermions exhibit the following properties³:

The high temperature (T) regime, where the susceptibility follows a $1/T$ Curie-Weiss law, has the signatures of localized and uncompensated valence spins fluctuating at the rare-earth sites, which weakly interact with the conduction electrons. The low temperature phase, on the other hand, exhibits coherent compensation of the spins and becomes a paramagnetic Fermi liquid of

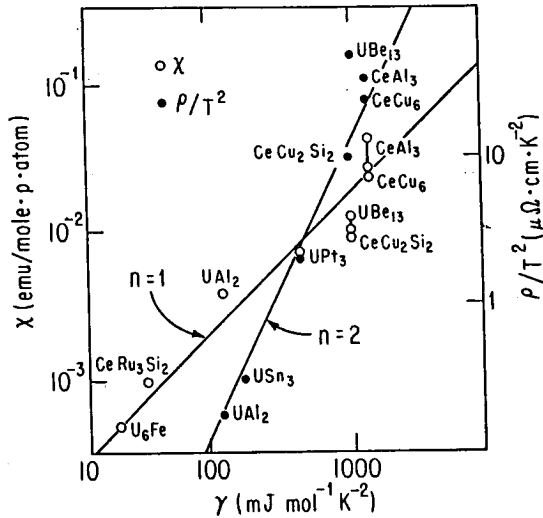


Fig. 2. Universal ratios in the heavy Fermion compounds. χ/γ data are from Ref. 1 and $A = \rho/T^2$ data are from Ref. 14. The solid lines are theoretical results summarized in Eq. (5.1).

class (Fig.2.), and detailed pressure dependences in UPt_3 (Fig. 4.). By comparison, we show that such scaling does not occur in liquid ^3He , by compiling the pressure dependence of the respective coefficients in Fig. 5.

In section 2 we introduce the large- U AL model and discuss its bare input parameters. The Kondo limit of the AL is defined. Since, unfortunately, no exact solutions are available for the AL problem (in contrast to the AI problem), we resort to the asymptotic approximation of the Kondo-boson (KB) $1/N$ expansion, where N is the valence degeneracy⁶. The interaction term in the limit of $U \rightarrow \infty$ is handled by introducing Coleman's Kondo-Boson (KB) fields⁷ (alias "Slave-Bosons"), and a functional integral formalism developed by Read and Newns⁸ is applied to enforce the local constraints on the KB and valence occupation. The analogous expansion has been recently studied in the AI problem and compared to exact results⁹. It proved to be successful in calculating the Wilson ratio, as well as continuously interpolating between the "asymptotically free" local moment phase and the "local Fermi liquid" ground state. Our analysis is separated into two levels: the $O(1)$ - "mean field theory", and the $O(1/N)$ - "fluctuations" respectively.

In section 3 we discuss the mean field theory. Here, the saddle-point variational equations are presented and solved, which results in an effective non-interacting renormalized band structure for the fermion quasiparticles. The KB fields are static (c-numbers) and constant in space. An important consequence of the mean field solution is the emergence of a new energy scale which is exponentially dependent on the parameters of the AL. We define the Kondo limit and show that it necessarily yields a large mass enhancement $m^*/m \gg 1$. The other consequence of this limit is that the average valence occupation becomes very close to an integer, and its fluctuations are greatly suppressed. Most of the so-called many body effects on γ and χ are already included at this level. The mean field solution thus allows us to replace some of the bare AL input parameters by the experimentally observed mass enhancement. The density of states structure at the Fermi level defines the Kondo-lattice temperature \bar{T}_K , which for heavy fermions is of order 5 - 50K. Since the Debye temperature and other "non universal" features such as the valence charge fluctuation energies and crystal field splittings are typically at much higher energy scales, the Fermi liquid behavior in the absence of incipient instabilities is predicted to be dominated by \bar{T}_K .

The mean field theory, however, does not include the quasiparticle interactions. Therefore, to proceed it is necessary to calculate the gaussian fluctuations of the KB fields, that is to say the Kondo-Boson propagator $D(\mathbf{q}, \omega)$. In section 4 we perform this calculation in the "radial gauge" of Read and Newns⁸. This allows us to obtain the leading order vertex function and self energy, and the correction to the Wilson ratio. Using the microscopic prescription of Ref. 10 the Landau parameters are determined. Physically, the interactions are mediated by coherent hybridization fluctuations screened by quasiparticle-hole excitations, with characteristic frequency scale of \bar{T}_K . The KB thus gives rise to a large $(T/\bar{T}_K)^2$ term in the dc resistivity, and a $(T/\bar{T}_K)^3 \log(T/\bar{T}_K)$ contribution to the specific heat. The Fermi liquid properties 1 - 3 are thus derived.

In section 5 we summarize our main results, and show that they agree with recently measured pressure dependence in^{11,12} γ , χ , and the resistivity¹³ data, and also explain the remarkable universal behavior throughout the heavy fermion class¹⁴. The data also serves to exclude alternate interpretations such as that of ferromagnetic spin fluctuations.

We conclude with a brief discussion of the role a more realistic band structure plays in producing antiferromagnetic spin fluctuations, and the nature of superconducting instability. Both of them invoke resummation of our $O(1/N)$ theory.

2. THE ANDERSON LATTICE MODEL

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

$$H^{AL} = \sum_{\mathbf{k}, m} \epsilon_{\mathbf{k}} c_{\mathbf{k}, m}^\dagger c_{\mathbf{k}, m} + \epsilon_f^0 \sum_{\mathbf{k}, m} f_{\mathbf{k}, m}^\dagger f_{\mathbf{k}, m} + \frac{V}{\sqrt{N}} \sum_{i, m} (f_{im}^\dagger c_{im} + c_{im}^\dagger f_{im}) + U \sum_{im} f_{im}^\dagger f_{im} f_{im'}^\dagger f_{im'} \quad (2.1)$$

where $\epsilon_{\mathbf{k}}$ and ϵ_f^0 are the conduction and dispersionless valence band energies respectively. The label i denotes the Wannier state at site 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 $\epsilon_{\mathbf{k}}$ defines the bare density of states ρ_c , and the fermi surface at $\epsilon_{\mathbf{k}} = \mu_0$. The bare chemical potential μ_0 is determined by the total (valence plus conduction) electron density

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

In the case of large U , i.e $U \gg \epsilon_f^0, \mu_0$, we can proceed by introducing the Kondo-Boson (KB) fields of Coleman at each lattice site⁷, 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: ($\beta=1, \beta=1/T$)

$$Z_{AL} = \int D \lambda b^* b c^* c f^* f \exp \left[- \int_0^\beta d\tau (L_{AL}(\tau) + i \sum_{im} \lambda_i (f_{im}^* f_{im} + \frac{1}{N} b_i^* b_i - Q_0)) \right] \quad (2.2a)$$

where,

$$L_{AL} = \sum_{\mathbf{k}m} \{ c_{\mathbf{k}m}^* (\partial_\tau + \epsilon_{\mathbf{k}}) c_{\mathbf{k}m} + f_{\mathbf{k}m}^* (\partial_\tau + \epsilon_f^0) f_{\mathbf{k}m} \} + \sum_i b_i^* \partial_\tau b_i + \frac{V}{\sqrt{N}} \sum_{im} (c_{im}^* f_{im} b_i^* + b_i f_{im}^* c_{im}) \quad (2.2b)$$

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.

At this stage we find it useful to apply the Read and Newns⁸ (RN) time dependent local gauge transformation which acts simultaneously on the Bose field $b_i = r_i \exp(i\phi_i)$ and the fields f_i :

$$f_i \rightarrow f_i' = e^{-i\phi_i} f_i \quad ; \quad \lambda_i \rightarrow \lambda_i' + \dot{\phi}_i \quad (2.3a)$$

Let us rescale the radial coordinate by

$$r_i \rightarrow r_i' = \frac{V}{\sqrt{N}} r_i. \quad (2.3b)$$

Rewriting the lagrangian in terms of the primed coordinates and using the Bose periodicity condition of $\phi(\beta) = \phi(0)$ we are left with two real fields r' and λ' , and the zero mode ϕ is made redundant as it contributes only to an overall constant of Z . The RN transformation thus eliminates infrared divergencies which are known to plague perturbation theory and $1/N$ expansions. Price is paid, however, since the KB in the radial gauge loses its physical meaning as a particle operator and becomes a "noise field" in the functional integral formalism. Henceforth we shall drop the primes on the f' , λ' , and r' fields.

Since the lagrangian is bilinear in the fermion fields, it is possible to integrate them out exactly and arrive at a Bose path integral with an effective action S :

$$Z_{AL} = \exp[-\beta F] = \int D r^2 \lambda \exp \left[-N \beta S((r), [\lambda]) \right] \quad (2.4a)$$

$$S = -\frac{1}{2\beta N} \text{Tr}_k \log \det \begin{pmatrix} (ik_0 - \epsilon_k) \delta_{kk'} & r_q \delta_{kk+q} \\ r_q \delta_{kk+q} & (ik_0 - \epsilon_f^j) \delta_{kk'} + i \lambda_q \delta_{k, k+q} \end{pmatrix} \\ + i \sum_{kq} \frac{\lambda_q}{V^2} r_k r_{k-q} - Q_0 \lambda_q \delta_{q0}. \quad (2.4b)$$

Here, k and q denote the usual Fermi and Bose four-vectors (implicitly including the label m for the fermions). The zeroth components k_0 , q_0 , are the Matsubara frequencies $(2n+1)\pi T$, and $2n\pi T$ respectively.

Eq. (2.4a) is used to generate an asymptotic expansion for the free energy F , using $1/N$ as the small parameter (analogous to \hbar of the semiclassical approximation). By adding source terms to the lagrangian in the form $j_{kk'} \alpha_k^* \alpha_{k'}$ for $\alpha_k = (c_k f_k)$, the electronic correlation functions are determined as functional derivatives of $F[j]$. At low temperatures Eq. (2.4a) is dominated by a non trivial saddle point $\bar{r}, \bar{\lambda} \neq 0$, which constitutes the parameters of the mean field theory discussed in the next section. By expanding Eq. (2.4b) around the saddle point and performing the gaussian integration, we generate the higher order terms in $1/N$.

3. MEAN FIELD THEORY

The mean field theory $N \rightarrow \infty$ of the AL has already been amply discussed in the literature¹⁵⁻¹⁸. It bears close resemblance 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^{17,4}, for which the relation to the KB theory has been recently explored¹⁹. In essence, the Bose fields are replaced by their expectation values and an effective single particle band theory is obtained. Here we shall define the mean field parameters and band structure in terms of the saddle point KB fields given by the variational equations:

$$\frac{\delta S}{\delta r} \Big|_{r=\bar{r}} = 0 \quad (3.1)$$

where $r \equiv (r, \lambda)$ is a vector notation for the two real KB fields. By expanding the logarithm in Eq. (4), it is easy to verify that (in the absence of source currents) $\bar{r} \propto \delta_{q,0}$, i.e. the saddle point fields are constants in space-time. The mean field parameters $r_0 = \bar{r}$ and $\epsilon_f = \epsilon_f^j + i \bar{\lambda}$, represent the effective c-f hybridization and renormalized f-level respectively. They determine the renormalized bands E^\pm , which are separated by a gap at ϵ_f .

$$E_k^\pm = \frac{\epsilon_k + \epsilon_f}{2} \pm \sqrt{\left(\frac{\epsilon_k - \epsilon_f}{2}\right)^2 + r_0^2} \equiv \epsilon_f \pm r_0 \text{ctg} \theta(\epsilon_k)^{\pm 1}, \quad (3.2)$$

which defines the function $\theta(\epsilon) = \theta_{E^\pm}$. The quasiparticles α^\pm of these bands are given by the θ dependent coherence factors:

$$\alpha_{k,m}^+ = \cos \theta f_{k,m} + \sin \theta c_{k,m} \\ \alpha_{k,m}^- = -\sin \theta f_{k,m} + \cos \theta c_{k,m} \quad (3.3)$$

The Fermi level at $T=0$ lies on the bottom band and equals $\mu = E^-(\mu_0)$. The mass enhancement at the Fermi level is $m^*/m = \sin^{-2}\theta_\mu$. The mean field parameters are determined by the implicit equations

$$\frac{dS}{dr_0} = 2r_0 \left\{ \int_{\tan\theta_0}^{\tan\theta_\mu} d\tan\theta \rho_c / \tan\theta + \frac{\epsilon_f - \epsilon_f^0}{V^2} \right\} = 0, \quad (3.4a)$$

$$\frac{dS}{d\epsilon_f} = -r_0 \int_{\tan\theta_0}^{\tan\theta_\mu} d\tan\theta \rho_c / (\tan\theta)^2 - Q_0 \langle n_f \rangle = 0, \quad (3.4b)$$

where,

$$\langle n_f \rangle = 1 - r_0^2 / (Q_0 V^2). \quad (3.4c)$$

In heavy fermion systems we are interested in a specific limit of the AL model, the Kondo limit, where $J \equiv \rho_c V^2 / (\epsilon_f - \epsilon_f^0) \ll 1$. For small Q_0 the slow variations of $\rho_c(\epsilon)$ away from the Fermi surface at $\epsilon = \mu_0$ can be ignored. Eqs.(3.4) to leading order in $(m^*/m)^{-1}$ and Q_0 yield:

$$m^*/m \approx \frac{r_0^2}{(\mu_0 - \epsilon_f)^2} = \frac{Q_0 \langle n_f \rangle}{\rho_c \mu_0} \exp[1/J] \gg 1, \quad (3.5a)$$

and

$$\bar{T}_K \equiv \epsilon_f - \mu \approx \frac{Q_0 \langle n_f \rangle}{\rho_c} (m^*/m)^{-1}. \quad (3.5b)$$

\bar{T}_K is the Kondo Lattice energy scale which measures the width of the renormalized density of states structure and characterizes the heavy Fermi liquid. Since it is exponentially dependent on $(-1/J)$, \bar{T}_K is expected to be much smaller than any bare energy scale (e.g. μ_0 , ρ_c^{-1} , V), and thus for small J :

$$1 - \langle n_f \rangle \approx \bar{T}_K / (\rho_c V^2) \ll 1. \quad (3.6)$$

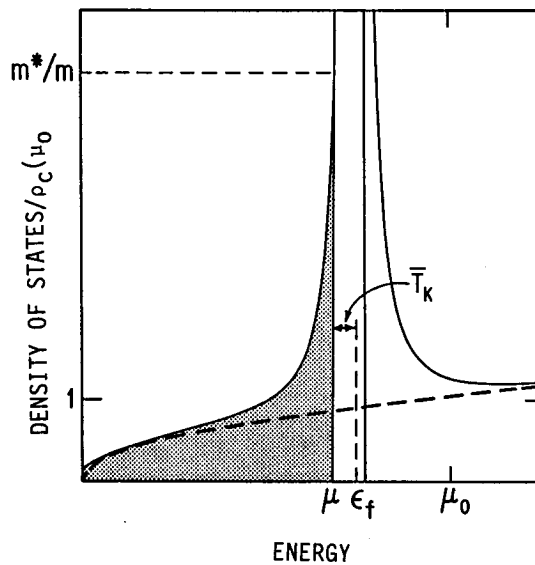


Fig. 3: The spherical band AL model, mean field $N \rightarrow \infty$ level. The dashed line in the bare conduction band density of states. The solid lines is the renormalized mean field band structure. Shaded area is the occupied Fermi sea at zero temperature.

Eqs. (3.5) and (3.6) prove that the mean field large mass enhancement is necessarily correlated with the near integer valence occupation, and, as will later be shown, suppression of f-charge fluctuations. In Fig. 3 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" approaches¹⁾ that that the individual Kondo resonances overlap and form a narrow band of mostly f-character.

The mean field theory of the AL replaces two bare parameters ϵ_f^0 and V , by the renormalized ones r_0 and ϵ_f . These, in turn, can be replaced by the more physical parameters m^*/m and $\langle n_f \rangle$. In the Kondo limit, one parameter, namely $\langle n_f \rangle$, drops out.

In the presence of a magnetic field h , the mean field free energy is given by

$$F^0 = \frac{1}{(2\beta)} \text{Tr} \log G^0(h), \quad (3.7a)$$

where the z-component of the spin is coupled with a magnetic moment g to the static magnetic field. The mean field Greens function is given by:

$$G^0(h) = \left[ik_0 - E_k^\alpha - hgm \right]^{-1} \delta_{km\alpha, k'm'\alpha'}. \quad (3.7b)$$

The linear temperature coefficient of the specific heat $\gamma^0 = -d^2F^0/dT^2|_{T=0}$ and the zero temperature susceptibility $\chi^0 = -d^2F^0/dh^2|_{h=0}$ are readily determined:

$$\gamma^0 = \frac{\pi^2 N}{3} (m^*/m) \rho_c; \quad \chi^0 = g^2 N \frac{(N^2-1)}{12} (m^*/m) \rho_c. \quad (3.8)$$

It can be shown that field and temperature variations of the saddle point parameters r_0, ϵ_f , and μ only contribute to higher F^0 derivatives of even order. The Wilson ratio R at the mean field level is thus:

$$R = (2\pi/g)^2 / (N^2-1) \chi^0 / \gamma^0 = 1. \quad (3.9)$$

which is expected of course, since no interactions between quasiparticles have yet been included.

4. FLUCTUATIONS AND INTERACTIONS

We expand the effective action S (Eq. 2.4b) of the partition function in the presence of source currents, to second order in the Bose fields, and obtain (up to overall constants⁸⁾:

$$Z[j] = e^{(-\beta F^0[j])} \int D \delta r \exp \left[-\frac{N\beta}{2} \sum_{qq'} \frac{\delta^2 S}{\delta r_q \delta r_{q'}} \Big|_{r=r_j} \delta r_q \delta r_{q'} + O(\delta r^3) \right]. \quad (4.1)$$

r_j satisfies Eq. (3.1) in the presence of an arbitrary source current j . Performing the gaussian integration in (4.1) yields

$$F^{(2)}[j] = -\frac{1}{\beta} \log Z^{(2)}$$

$$= \frac{1}{(2\beta)} \text{Tr}_k \log G(j, r_j) - \frac{1}{(2\beta)} \text{Tr}_q \log \det D(j, r_j) + O(1/N) \quad (4.2)$$

where G^0 is the mean field Greens function (with the source term as the self energy) and $D_{r,r'}$ is the KB propagator $\langle \delta r_r \delta r_{r'} \rangle$. $D_{r,r'}$ is given by the RPA sum of bubble diagrams, such that

$$D(q) = \frac{-1}{N} (\Pi(q) + \Pi^0)^{-1}; \quad \Pi^0 = 2 \begin{bmatrix} 1/J & \sqrt{\lambda_c} \\ \sqrt{\lambda_c} & 0 \end{bmatrix}, \quad (4.3a)$$

where Π^0 is the "unscreened vertex" in which $\lambda_c \equiv [(1-\langle n_f \rangle) Q_0 / r_0]^2$. λ_c can be shown to represent the f-charge fluctuations at the gaussian level, and following the discussion of the previous section, it is seen to vanish in the Kondo limit of large m^*/m . The bubble diagram Π is given by:

$$\Pi_{r,r'} = -\beta^{-1} \sum_{k, \alpha\alpha'} C_r^{\alpha\alpha'}(\theta_k, \theta_{k+q}) C_{r'}^{\alpha'\alpha}(\theta_{k+q}, \theta_k) G_{k,\alpha}^0 G_{k+q,\alpha}^0. \quad (4.3b)$$

The C 's are the quasiparticle-boson vertices arising from the orthogonal transformation from the (c, f) basis to the $(+, -)$ bands:

$$\begin{aligned} C_1^- &= \sin(\theta_k + \theta_{k+q}) & C_1^+ &= \cos(\theta_k + \theta_{k+q}) & C_1^{++} &= C_1^- \\ C_2^- &= i \cos \theta_k \cos \theta_{k+q} & C_2^+ &= -i \cos \theta_k \sin \theta_{k+q} & C_2^{++} &= i \sin \theta_k \sin \theta_{k+q} \end{aligned} \quad (4.3c)$$

For $j=0$, the functions in Π contain interband and intraband terms, the latter being very similar in their low (q, ω) behavior to the familiar Lindhard functions or polarization insertions in the electron gas. It can also be verified that $\lim_{q, \omega \rightarrow 0} \det(-D)$ and $\lim_{q, \omega \rightarrow 0} \text{Tr}(-D)$ are positive, which ensures the stability of the mean field solution¹⁹. The explicit factor of $1/N$ in Eq. (4.3a) provides us with the small parameter of the RPA or gaussian approximation, since all the corrections either involve higher powers of D , or do not contain the maximal number of internal bubbles which reduces their contribution by factors of $1/N$.

We can now derive the electronic response and correlation function, to leading order in $1/N$, by functionally differentiating $F^{(2)}[j]$ in Eq. (4.2). In particular it is straightforward to read off the quasiparticle self energy Σ and irreducible vertex function Γ from the first and second derivatives respectively²⁰. The quasi particles interact via the exchange of a Kondo Boson propagator. This propagator can be physically interpreted as an effective hybridization fluctuation which is strongly screened by the quasiparticle density response Π . The effective mass correction is given by $d\Sigma/dE_{\bar{k}}$ at $T=0$:

$$\begin{aligned} \frac{\delta m^*}{m} &= -\frac{d}{dE_{\bar{k}}} \sum_{q, r, r'} \int_0^\infty \frac{d\omega}{\pi} D_{rr'}^{im}(q, \omega) C_r^{-\alpha}(\theta_k, \theta_{k+q}) C_{r'}^{\alpha}(-\theta_{k+q}, \theta_k) \\ &\quad \times \left[\frac{1 + \Theta(\mu - E_{k+q}^\alpha)}{E_{\bar{k}}^- - E_{k+q}^\alpha - \omega} - \frac{\Theta(\mu - E_{k+q}^\alpha)}{E_{\bar{k}}^- - E_{k+q}^\alpha + \omega} \right]_{E_{\bar{k}} = \mu} \end{aligned} \quad (4.4)$$

where $D^{im} = \lim_{\eta \rightarrow 0} [D(\omega + i\eta) - D(\omega - i\eta)]$. Γ contains two contributions to the leading order in $1/N$:

$$\begin{aligned} \Gamma^{\alpha\beta; \alpha'\beta'}(k, m, k+q, m; k', m', k'-q, m') &= \sum_{r, r'} C_r^{\alpha\beta}(\theta_k, \theta_{k+q}) C_{r'}^{\alpha'\beta'}(\theta_{k'}, \theta_{k'-q}) D_{r, r'}(q) \left[\equiv \Gamma^{dir} \right] \\ &\quad - \delta_{m, m'} \sum_{r, r'} C_r^{\alpha\alpha'}(\theta_k, \theta_{k'-q}) C_{r'}^{\beta\beta'}(\theta_{k+q}, \theta_{k'}) D_{r, r'}(k' - k - q) \left[\equiv -\Gamma^{exch} \right] + O(1/N^2) \end{aligned} \quad (4.5)$$

We can obtain the Landau scattering amplitudes $\{A_l^{f, a}\}$ following the microscopic prescription of Ref.¹⁰. Here, "s" and "a" denote the generalized symmetric and antisymmetric channels respectively. One considers the $\omega \rightarrow 0$ limit of Γ evaluated on the spherical Fermi surface i.e. ($E_k = E_{k'} = \mu$), and projects it onto Legendre polynomials, P_l , such that:

$$\begin{aligned} A_l^s &= \rho_c (m^*/m) N \delta_{l,0} \lim_{|q|, \frac{\omega}{|q|} \rightarrow 0} \Gamma^{dir} + A_l^f \\ A_l^a &= -\rho_c (m^*/m) (2l+1)/2k_f^2 \int_0^{2k_f} d\kappa \Gamma^{exch}(\kappa, 0) P_l(1 - \kappa^2/2k_f^2) \kappa \end{aligned} \quad (4.6)$$

where k_f is the Fermi wave vector ($\epsilon_{k_f} = \mu_0$). Eq. (4.5) guarantees that the forward scattering sum rule is automatically satisfied. To leading order in $1/N$ there are no renormalization factors or other corrections to Eqs. (4.4) and (4.5). It should be stressed that in this Fermi liquid theory the "bare" particles are the heavy mean field quasiparticles, and thus $\delta m^*/m$ in Eq. (5) is *not* large. Using Eqs. (4.5) and (4.6) we computed the $\{A_l^{f, a}\}$ numerically. We found that $D(q, 0)$ is slowly varying, and higher moments decrease rapidly with l . Considerable simplification arises when a parabolic band structure is used for $\epsilon(k) \propto |k|^2$ since angular integrations may then be done analytically, leaving us with just a 1-dimensional numerical integration. Here we neglect Umklapp processes and set $\chi_c = 0$. We find that the $l=0, 1$ parameters are (up to relative corrections of $O(1/N, m^*/m^{-1})$):

$$A_0^a = \frac{-1.000}{N} + \frac{0.08}{N} (Q_0/\mu_0) ; A_0^s = 1.000 ; A_1^s = A_1^f = \frac{-12}{N} (Q_0/\mu_0) . \quad (4.7)$$

A direct differentiation of the free energy in Eq. (4.2) with respect to temperature and magnetic field yields χ and γ . The mean field contributions of the first term were calculated in Eqs. (3.8) and (3.9). The $1/N$ corrections arise from the term $\text{Tr} \ln \det D$. After some algebra it follows that the susceptibility and specific heat are renormalized such that

$$\chi = \chi^0(1 + \delta m^*/m - A_0^2 + O(1/N^2)), \quad (4.8)$$

and similarly:

$$\gamma = \gamma^0(1 + \delta m^*/m + O(1/N^2)). \quad (4.9)$$

These are known Fermi liquid identities related to spin and charge conservation. Their direct verification lends further support to our assignment of Landau parameters in Eq. (4.6). The result for A_0^2 is intimately related to the constraint imposed on the f-charge fluctuations by setting $\chi_c = 0$. It is important to note that this theory is not galilean invariant (because of hybridization between bands of largely different curvature or "masses"). Therefore the relation $1 + \delta m^*/m = (1 - A_1^2/3)^{-1}$ is incorrect as could be checked against Eq. (4.4). These observations are consistent with Fermi liquid properties listed under point 2 in the introduction.

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 ^3He . Our analysis follows Ref. 21, where D_{rr} replaces the RPA susceptibility that mediates the spin fluctuations. We find:

$$\Delta C_V = \delta T^3 \log \left[\frac{T}{\bar{T}_K} \right] + O((T/\bar{T}_K)^3), \quad ; \quad \delta = a \left[\frac{T}{\bar{T}_K} \right]^3, \quad (4.10)$$

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 are also able to estimate the T^2 coefficient of the low temperature resistivity $\rho = AT^2$. We follow the analogous paramagnon calculation¹⁴, and determine A by evaluating $\partial D^{im}/\partial \omega$, at $\omega=0$. The result is:

$$\rho = A T^2 + O(T^3); \quad A = \rho_{\max} (1/\lambda \bar{T}_K)^2, \quad (4.11)$$

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

5. SUMMARY AND DISCUSSION

In heavy fermion materials where crystal field splittings are larger than $\bar{T}_K \approx 5 - 50 K$, the valence degeneracy is not large ($N=2$ and $Q_0=1/2$). The present $1/N$ expansion, while it may not be quantitatively accurate in detail, is nevertheless a viable systematic description of the Fermi liquid properties which has many satisfying features including:

- 1) The local f-charge constraint is imposed at each order, and Fermi liquid identities and sum rules are satisfied.
- 2) The model we have used is generic and depends on a minimal set of microscopic parameters. These are the bare band structure, and the Kondo lattice temperature \bar{T}_K .
- 3) Translational invariance is ab-initio built into the theory. This is in contrast to "interacting impurities" approaches where more sophisticated resummation schemes are needed to recover coherence effects.

We find that the Fermi liquid parameters in Eq. (4.7) for a spherical band structure are given by $A_0^2 \approx 1/N$ and $A_0^2 = 1$, and the higher moments are smaller than $1/N$. Also a $\delta T^3 \log T$ contribution to the specific heat and a AT^2 resistivity term are calculated. These last two effects are similarly obtained in paramagnon theories. For this reason paramagnon models have been extensively used to explain both the normal state and the superconductivity in UPt_3 in analogy to ^3He . However, the degree of independent evidence for an incipient ferromagnetic instability in UPt_3 remains controversial⁵. The origin of the $T^3 \log T$ behavior in this KB theory is the non analytic low ($|\mathbf{q}|, \omega$) behavior of Π via the ratio $\omega/|\mathbf{q}|$. The presence of such a term is not surprising, since it is a general property of theories with an RPA-like boson mediating the interactions. On the other hand, it should be stressed that unlike the paramagnon mechanism, this behavior does not derive solely from the spin fluctuation channel, as seen by the relative magnitudes of A_0^2 and A_0^2 .

Our results in Eqs. (4.8), (4.9), (4.10) and (4.11), can best be summarized by the simple proportionality relations which are obtained between γ, χ, A and δ .

$$\chi \propto \gamma; \quad A \propto \gamma^2; \quad \delta \propto \gamma^3. \quad (5.1)$$

In Eq.(3.5) we observe that m^*/m strongly depends on the value of the Kondo coupling J , which is expected to increase with pressure. This implies that \bar{T}_K should dramatically increase with applied pressure, and thus explains why the Gruneisen parameter $\Gamma_\gamma = d \log \gamma / d \log V$ is observed to be anomalously large in comparison to typical non heavy metals ($\Gamma_\gamma \approx 57$ in $^{11}\text{UPt}_3$). Thus, the pressure dependence is a useful probe to the relations (5.1). In UPt_3 , γ can vary under pressure by 40%. As shown in Fig. 4, our predictions appear to be well confirmed by experiments. Also universal relations between γ , χ and A for many different heavy fermions seem to correlate remarkably well with Eq. (5.1). This analysis of the data raises doubts about the validity of paramagnon models, for which relations (5.1) 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. 5.

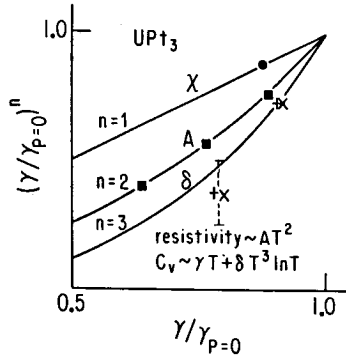


Fig. 4. Scaling of thermodynamic and transport coefficients with pressure dependent γ . (For the latter see Ref. 11). χ are from Ref. 12, resistivity from Ref. 13. The symbols + and x correspond respectively to the coefficient δ of $T^3 \ln T$ term in C_V and the coefficient ϵ of T^3 term in C_V (from Ref. 11). The solid lines are theoretical results summarized in Eq. (5.1).

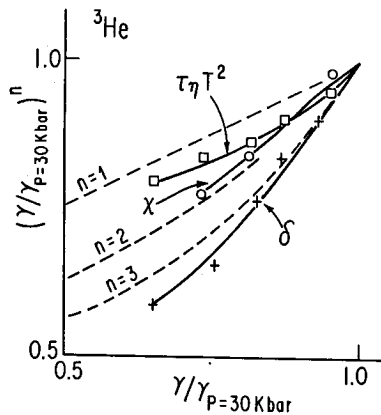


Fig. 5. Scaling of χ , δ , and $A = \tau_\eta T^2$ with pressure dependent γ in liquid ^3He . Here, τ_η is the quasiparticle lifetime as measured by the viscosity. In contrast to Fig. 2., it is evident that the relations (5.1) are not applicable to this Fermi liquid, in which ferromagnetic spin fluctuations are assumed to be important.

It is worth mentioning at this point that the mechanism leading to superconductivity at e.g. $T_c \approx 5K$ in UPt_3 is still unresolved. The participation of the heavy quasiparticles in the formation of Cooper pairs is inferred from the large specific heat jump at T_c . The possibility that Kondo-Boson mediated pairing drives the superconductivity in some of the heavy fermion compounds may be the most interesting extension of this theory. The $l=2$ Landau parameters in Eq. (4.6) were found to be attractive. A simplistic deduction^{22,23} of the transition temperature and order parameter symmetry from the Landau ($\omega=0$) limit of the vertex function would yield d -wave pairing. However, it might not be applicable as in 3He , since it uses a spherical Fermi surface and it assumes that the frequency cut-off scale in Γ is much smaller than the characteristic variations in the electronic energies. In the KB theory both relevant frequency scales appear to be of order T_K .

There is widespread evidence for antiferromagnetic correlations²⁴, 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.

We thank P. Coleman, G. Crabtree, R. Dunlap, G.S. Grest, G. Mazenko, P. Schlottmann and S. Shenker for useful discussions. This work was supported by NSF DMR-84-20187 and MRL grant NSF-DMR-82-6892. K.L. also thanks Argonne National Laboratory for their support and hospitality.

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