Universal low-temperature properties of normal heavy-fermion systems (invited)

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We present a microscopic derivation of the Fermi-liquid properties of the Anderson lattice. Our calculations suggest that the low-temperature state of the *normal* heavy Fermi liquid has a number of universal features, for which there is good experimental evidence. Using the Kondo-boson $1/N$ expansion, we find the Fermi liquid is characterized by the mean-field "bare" particles (which are heavy) and their respective interactions. The latter are mediated by fluctuations in the f-level position and valence-conduction electron hybridization. Our calculations lead to the following experimental predictions: (i) the low-temperature specific heat behaves as $C=\gamma T \propto T/T_K$ with corrections $\Delta C=(T/T_K)^3 \ln(T/T_K)$, (ii) the zero-temperature spin susceptibility $\chi \propto 1/T_K$, and (iii) the resistivity $\rho \propto (T/T_K)^2$. These results all contain a unique energy scale T_K which is proportional to the inverse effective mass. Experimental support for these predictions is provided by evidence of systematic scaling of χ and ρ with γ throughout the entire class of heavy-fermion compounds. In addition we analyze recent pressure-dependent specific-heat measurements on UPt_3 combined with χ and ρ data to confirm the scaling of these quantities with a single strongly pressure-dependent energy scale. This analysis provides evidence against current ferromagnetic spin-fluctuation theories.

Theoretical studies of heavy-fermion metals have been rather diverse in style. Phenomenological approaches are for the most part based on the description of Fermi-liquid theory.[1,2] The microscopic picture underlying this Fermi liquid has been assumed[2] to be very similar to that of liquid ^{3}He. The dominant interaction between the quasiparticles is taken to be through the exchange of ferromagnetic spin fluctuations. The strongest support for this analogy is apparently the observation[3] of a $T^3 \ln T$ term in the specific heat C in UPt_3. At the opposite extreme are theoretical approaches which are more microscopically based.[4] There the lattice has been viewed as a collection of independent Kondo impurities. In this latter viewpoint the connection to Fermi-liquid theory is not obvious since coherence effects in the solid are clearly ignored.

The purpose of this paper is to describe our own approach to heavy-fermion systems, which represents (i) an extension of the Kondo impurity theory to include effects of the lattice and (ii) a merger of the Kondo lattice microscopics with the language of Fermi-liquid theory. In this way the two rather disparate viewpoints outlined above are combined. Our theory of the Kondo lattice is based on the $1/N$ expansion[5] which has been successfully applied to the impurity case. Here N corresponds to the degeneracy of the localized f levels in the Anderson Hamiltonian. Our emphasis is on *normal*-state properties which can be directly measured experimentally. It is our contention[6,7] that many properties of the Fermi-liquid state of heavy fermions are universal. This observation, which can be made purely on the basis of an analysis of the data, is an important consequence of the theory which we will present below. It is clear that phase transitions to superconducting or magnetically ordered states are nonuniversal features of these heavy Fermi liquids. However, our concern here is with the universal behavior of the *normal* Fermi liquid.

There are three types of measurements which give, perhaps, the strongest evidence for universal behavior. These are measurements of (i) the ratio of susceptibility χ to the linear specific-heat coefficient γ, (ii) the temperature dependence of C/T at low T, and (iii) the T^2 coefficient in the low-temperature resistivity as a function of γ. In Fig. 1 the linear coefficient of the specific heat is plotted versus the magnetic susceptibility χ for a variety of heavy-fermion systems. The data are taken from Ref. 8. There are a number of key conclusions which should be drawn from the data. It should be noted that χ and γ are both strongly enhanced but that their ratio is comparable to the free-electron value (for spin $\frac{1}{2}$) which is shown by the solid line. This ratio can be interpreted in the language of Fermi-liquid theory. In the absence of complications associated with contributions to χ other than those deriving from the Zeeman term or renormalizations of the free-electron magnetic moment, the ratio χ/γ is given in dimensionless units by

$$\chi/\gamma = 1 - A_0^a , \tag{1}$$

where

$$A_l^{s,a} = F_l^{s,a}/(1+F_l^{s,a}) . \tag{2}$$

Here $A_l^{s,a}$ and $F_l^{s,a}$ are the Landau scattering amplitudes in the standard notation.[9] Thus it follows from Fig. 1 that A_0^a is systematically negative but not large. The general physical

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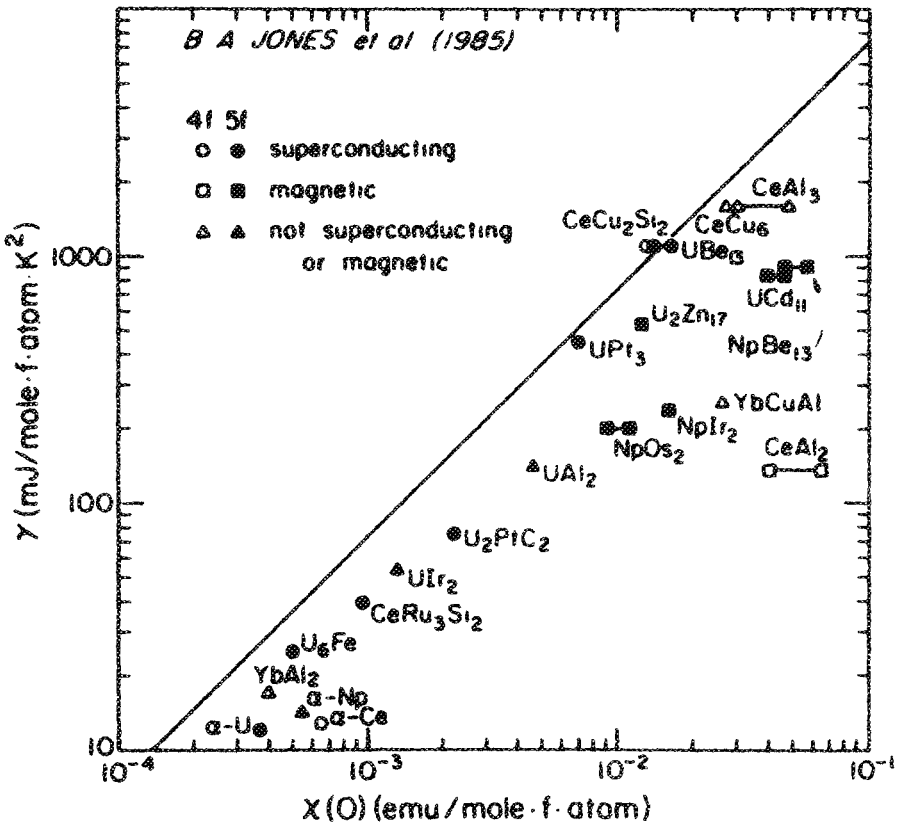

FIG. 1. Specific-heat coefficient γ vs the zero-temperature susceptibility $\chi(0)$ for some heavy-electron systems. From Ref. 8. The straight line corresponds to results for noninteracting electrons for $N=2$ (spin $\frac{1}{2}$).

picture that one derives from this figure is that the Fermi liquid is composed of heavy quasiparticles but that the parameter A_0^a is not strongly enhanced.

Additional evidence for universality is shown in Fig. 2. Figure 2(a) plots the specific heat divided by temperature in $CeCu_2Si_2$ and UBe_{13} as a function of T^2. This same plot is shown for UPt_3 in Fig. 2(b). The data for the Ce compound corresponds to samples which do not become superconducting at low temperatures. Both figures are from Ref. 3. In UPt_3 this specific-heat behavior has been fitted to a $T^3 \ln T$ dependence over a wide range of temperatures. As can seen, all three heavy-fermion systems exhibit a rapid upturn in C/T at low T. However, the scale of this upturn varies from system to system. Similar behavior is observed in UAl_2 and to a lesser extent in $CeCu_6$ and USn_3. It should be noted that the best low-temperature measurements[10] in $CeAl_3$ do *not* show this behavior. Based on a simple analysis of the data, the temperature range over which C/T increases rapidly with decreasing T is correlated with the size of γ. Interestingly enough, the two systems shown in Fig. 2(b) have essentially the same γ values and the C/T ratios appear to scale together over the entire temperature region shown. Both Figs. 2(a) and 2(b) suggest that the low-temperature behavior of C/T is similar throughout the heavy fermions. On this basis one may expect that the $T^3 \ln T$ law applies to a large number of heavy-fermion systems.[11]

What is important to stress is that the observation that the specific heat varies as $T^3 \ln T$ is characteristic of Fermi-liquid theories, in general.[12] The temperature dependence is set by the characteristic energies of the system. Thus in paramagnon or spin-fluctuation theories the energy scale is related to the spin-fluctuation energy; for electron-phonon systems the scale is set by the Debye frequency. In the absence of any other lower energy scale, the Fermi energy itself characterizes the $T^3 \ln T$ behavior. The temperature dependence of the specific heat contains important information about the boson which is exchanged by the interacting electrons. More precisely, this behavior arises formally when the interaction between the quasiparticles is mediated by a screened boson with propagator $D(q,\omega)$ which depends on $(\omega/T_0)(k_0/q)$. Here T_0 and k_0 are the characteristic energy and wave number of the interaction.

Additional evidence for universal behavior is the Kadowaki and Woods[13] plot of the coefficient of the T^2 term in the resistivity, called A, as a function of γ^2. Their rather remarkable plot illustrated in Fig. 3 shows that for a large number of heavy-fermion systems the T^2 coefficient varies as γ^2. The coefficient of proportionality appears to be relatively insensitive to the details of the system. The existence of a T^2 term in the resistivity is a signature of strong electron-electron interactions. One may presume that these same interactions are responsible for the $T^3 \ln T$ term in the specific heat. This same resistivity behavior is seen in paramagnon systems where this anomalous low-temperature specific heat is also observed.[14] However, there is no reason to assume that the underlying microscopic mechanism for the interaction between electrons in heavy-fermion systems can be described by the simple paramagnon model.

With these experimental insights we now review the theory of the Anderson lattice Hamiltonian which serves as a microscopic basis for our Fermi-liquid theory of heavy-fermion metals. We have shown elsewhere[6,7] that this Fermi-liquid theory has the universal features plotted in Figs. 1–3. While the temperature dependencies in the specific heat and

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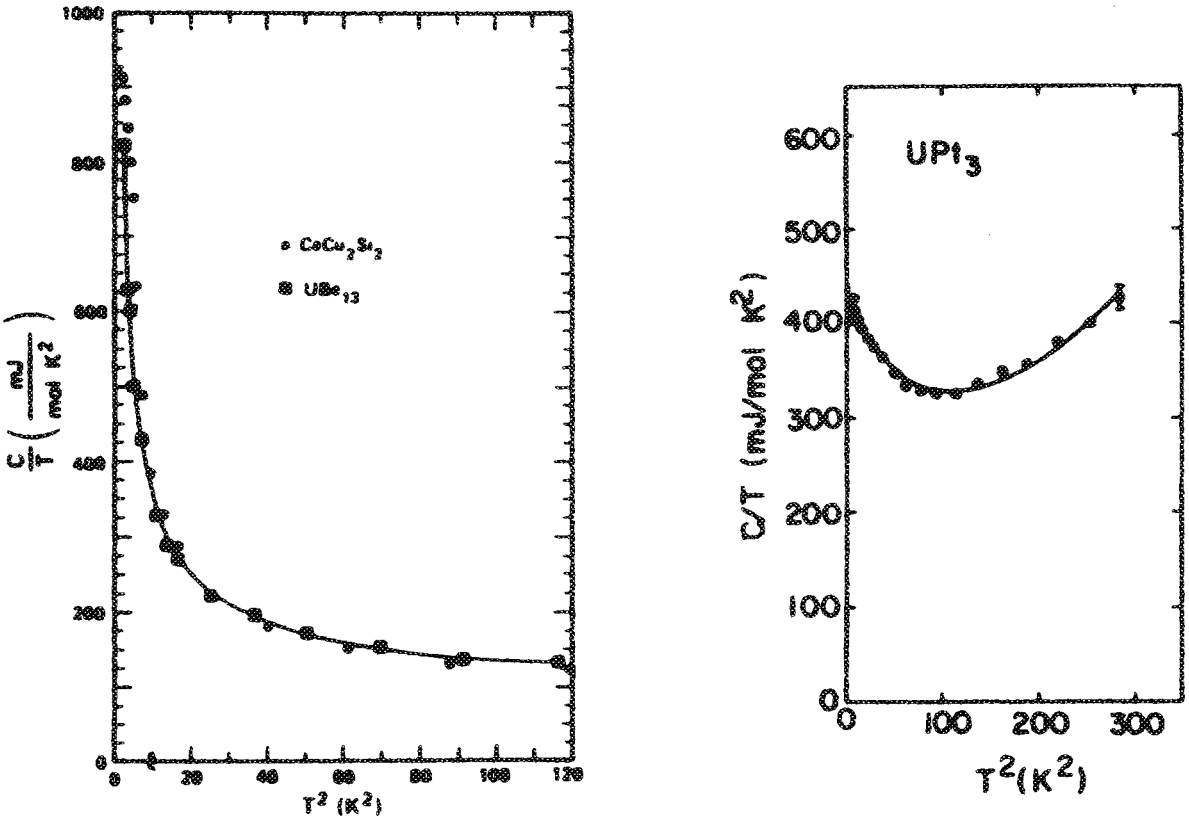

FIG. 2. Temperature dependence of the specific heat C divided by T for various heavy-electron systems in the normal state. Solid lines are guides to the eye. The data are from Ref. 3.

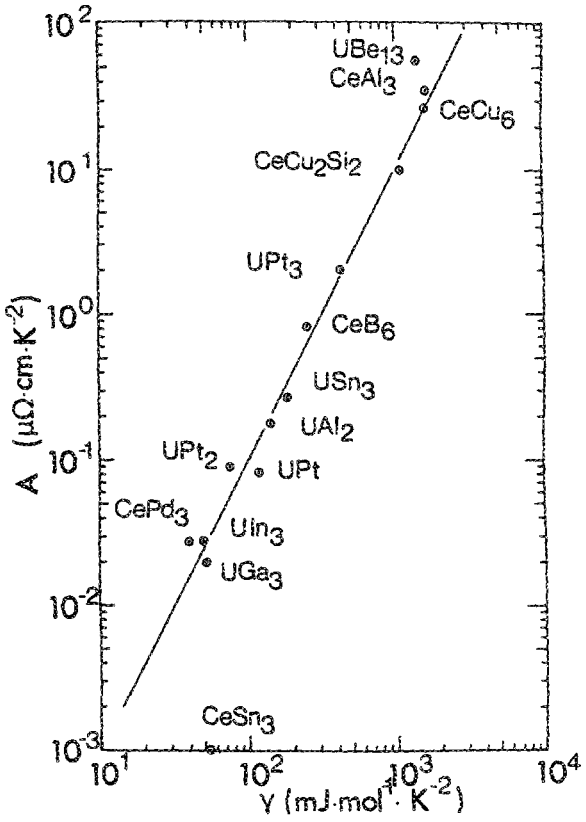

FIG. 3. Coefficient of the T^2 contribution to the resistivity, $\rho = AT^2$, for various heavy-fermion systems as a function of γ. The straight line corresponds to $A \sim \gamma^2$. Data are from Ref. 13.

resistivity are rather similar to paramagnons, our treatment of the Anderson or Kondo Hamiltonian makes it clear that the electron-electron interactions do not derive from exchange of simple spin fluctuations as in paramagnon systems. The Anderson Hamiltonian on a lattice is given by

$$H = \sum_{km} \epsilon(k) c^{\dagger}_{km} c_{km} + \sum_{im} \epsilon_f f^{\dagger}_{im} f_{im} + \sum_{im} V(c^{\dagger}_{im} f_{im} + \text{c.c.}) + U \sum_{imm'} f^{\dagger}_{im} f_{im} f^{\dagger}_{im'} f_{im'} . \quad (3)$$

Here V represents the constant hybridization matrix element and U is the Coulomb potential which is taken to be infinite, compared to all other energies in the system. The index m corresponds to one of N different spin channels and N is assumed to be large. We may assume that we are in the "Kondo" limit so that the dimensionless exchange parameter

$$\rho_0 J \equiv V^2 \rho_0 / (\mu - \epsilon_f) < 1 , \quad (4)$$

and the number of f electrons at a site is close to unity. Here ρ_0 is the conduction-electron density of states. The infinite-U limit has been successfully treated for the single-impurity case by the introduction of the "Kondo boson," which imposes the constraint that the number of f electrons at a site never exceeds unity. With the introduction of this boson the Hamiltonian can be simply written as

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$$H = \sum_{km} \epsilon(k) c_{km}^{\dagger} c_{km} + \sum_{im} \epsilon_f f_{im}^{\dagger} f_{im} + \sum_{im} V(c_{im}^{\dagger} f_{im} b_i^{\dagger} + \text{c.c.}) + \sum_{im} \lambda_i \left(f_{im}^{\dagger} f_{im} + \frac{1}{N} b_i^{\dagger} b_i - Q_0 \right), \quad (5)$$

where b_i is the boson destruction operator at site i. The parameter λ_i is introduced so as to constrain the local number of f electrons to be less than 1. (In actuality, in order to be consistent[5] one replaces unity by the parameter NQ_0 in the constraint condition. At the end of the calculation Q_0 is taken to be $1/N$). The effects of this boson are quite physical if one applies the notions of mean-field theory.[15] Then b_i can be replaced by a constant c-number $\bar{b}$ and the Lagrange multiplier λ_i is also taken to be a constant λ. The effects of infinite U are as expected. There is a large reduction in the effective hybridization matrix element because large U inhibits hybridization. Similarly it causes a shift in the position of the local f level. In order to accomodate no more than one f electron at a site, the f level is moved upwards from the low lying "bare" level position to slightly above the Fermi level. In a mean-field decoupling scheme the Hamiltonian is given by

$$H^{\mathrm{MF}} = \sum_{km} \epsilon(k) c_{km}^{\dagger} c_{km} + \sum_{im} \bar{\epsilon}_f f_{im}^{\dagger} f_{im} + \sum_{km} \bar{V}(c_{im} f_{im}^{\dagger} + \text{c.c.}) + \lambda(|\bar{b}|^2 - 1), \quad (6)$$

where the renormalized f-level position and hybridization are given by

$$\bar{\epsilon}_f = \epsilon_f + \lambda, \quad \bar{V} = V\bar{b}. \quad (7)$$

These two renormalized parameters can then be obtained from the variational conditions

$$\frac{\partial F}{\partial \bar{b}} = \frac{\partial F}{\partial \bar{\epsilon}_f} = 0, \quad (8)$$

where F is the mean-field free energy. The resulting Hamiltonian in Eq. (6) thus describes noninteracting electrons in a hybridized band structure given in terms of the renormalized parameters as

$$E^{\pm}(k) = \{[\epsilon(k) + \bar{\epsilon}_f]/2\} \pm \tfrac{1}{2}\sqrt{[\bar{\epsilon}_f - \epsilon(k)]^2 + 4\bar{V}^2}. \quad (9)$$

A key parameter in the theory is T_K, which sets the scale for coherence effects as we will see shortly. T_K also determines the degree of enhancement of the conduction electron density of states: $N(0) \sim Q_0 \rho_0 / T_K$. Here $N(0)$ and ρ_0 are the density of states at the Fermi energy for the mean field renormalized band structure and the conduction-electron component, respectively, and

$$T_K = \bar{\epsilon}_f - \mu = \mu_0 \exp(-1/\rho_0 J) \ll 1. \quad (10)$$

Thus $N(0)$ is strongly enhanced relative to the conduction electron contribution ρ_0. Here μ_0 is the chemical potential of the conduction electrons in the absence of f electrons. That such a mean-field approach makes sense at all can be argued on the basis of experimental observations. This approach has a number of successes. It explains why the ratio χ/γ is close to the free electron value as shown in Fig. 1. Because the density of states at the Fermi energy is enhanced by a factor of T_K^{-1} in this renormalized band theory one can understand the large enhancements in both χ and γ. Finally it can be seen that γ which varies as T_K^{-1} is expected to be strongly pressure dependent since T_K depends exponentially on the parameters of the theory. Presumably any small change in these bare parameters under pressure will be greatly magnified in the exponential. This strong pressure dependence in γ in seen experimentally. For example,[16] in UPt_3 $\partial \ln \gamma / \partial \ln V \simeq 57$.

Despite these successes this mean-field approach is clearly insufficient. (i) It cannot explain the $T^3 \ln T$ dependence observed in the low-temperature specific heat in a variety of heavy-fermion systems. (ii) It will not give rise to a T^2 dependence of the resistivity, since in mean-field theory there are no residual electron-electron interactions. (iii) Finally, it cannot explain why the Landau parameter $A_0^a = 1 - \chi/\gamma$ is nonvanishing, and in particular systematically negative.

Because of the inadequacies of mean-field theory, we have studied the leading fluctuation or correction terms. This can be done in a systematic fashion within the context of the $1/N$ expansion, from which mean-field theory is derived at the leading order. The general scheme is to write

$$H = H^{\mathrm{MF}} + (H - H^{\mathrm{MF}}) \equiv H^{\mathrm{MF}} + \delta H \quad (11)$$

and treat δH as in the random-phase approximation (RPA) as in electron-phonon or paramagnon theory. It is important to stress that this RPA-like theory is formally justified on the basis of the $1/N$ expansion. The Kondo boson which plays the role of the phonon or paramagnon in analogous theories is described by the propagator $D(q,\omega)$ which is a 2×2 matrix. *Physically this boson can be viewed as coherent fluctuations in the effective hybridization and renormalized f-level position.*

An important insight into the treatment of the fluctuation corrections for the single impurity case was made by Read and Newns.[5] These authors noted that there can be no divergences in physical observables resulting from Goldstone bosons in the Anderson Hamiltonian. The mean field prescription $b_i \to \bar{b}$ corresponds to breaking a *local* gauge symmetry. This forbidden "broken" symmetry must be restored by the fluctuations. By applying a local time-dependent gauge transformation

$$b_i \to b_i' = b_i e^{i\theta_i}, \quad f_i \to f_i' = f_i e^{i\theta_i} \quad (12)$$

the phase of the boson θ_i can be absorbed by that of the valence electrons and the constraint field at each site. The price one pays for this gauge transformation is that the transformed Hamiltonian contains a time-dependent constraint field arising from $\dot{\theta}_i$. All these features can be readily handled by a functional integral formulation similar to that of Ref. 5 where the single-impurity case is treated.

The description of the Fermi liquid is straightforward. The "bare" parameters are defined at the mean-field level. These bare particles are those linear combinations of the c and f states which diagonalize H^{MF} in Eq. (6) or more physically correspond to the renormalized band structure. The bare particles interact by exchange of a single boson (or

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hybridization fluctuation). The usual Fermi-liquid identities are given with respect to the mean-field reference values by, for example,

$$\chi/\chi^{MF} = [1 + (\delta m/m)](1 - A_0^a), \tag{13}$$

where δm is the relatively small mass enhancement that arises from the self-energy correction due to quasiparticle interactions. In Eq. (13) χ^{MF} is the "bare" particle susceptibility which is given by the mean-field result. Following standard many-body theory[9] the Landau parameters $A_l^{s,a}$ can be computed directly from the interaction term or vertex function

$$A_{mm'}(\hat{k}_F, \hat{k}'_F) = \lim_{|q|\to 0} \lim_{\omega/|q|\to 0} \Gamma_{mm'}(\hat{k}_F \hat{k}'_F q)$$
$$= D(0) - \delta_{mm'} D(\hat{k}_F - \hat{k}'_F), \tag{14}$$

where, as above, m, m' correspond to the generalized spin index. The parameters $A_l^{s,a}$ can be obtained by Legendre expansions of $D(\hat{k}_F - \hat{k}'_F)$. We find for $l = 0$

$$A_0^s \cong 1,$$

$$A_0^a = -\frac{1}{N} + \frac{0.08}{N}\left(\frac{Q_0}{\mu_0 \rho_0}\right). \tag{15}$$

Thus A_0^a is small and negative and since $A_0^s \cong 1$, it follows from Fermi-liquid identities that $\partial n/\partial \mu$ is approximately the same as that for the noninteracting system. Both these observations are consistent with experiment.

What is particularly satisfying about this Landau theory is that one can also *derive* the Landau identities such as that in Eq. (13). In particular, a direct calculation[7] of χ using $\chi = \partial^2 F/\partial H^2$ yields the same answer as that obtained from Eq. (13), using Eq. (14) for A_0^a. This represents an important microscopic check on the Landau theory. That such a consistent Landau theory can be constructed is a consequence of our controlled approximation scheme. Furthermore, because they are microscopically derived the Landau parameters A_l automatically satisfy the forward scattering sum rule (which can be readily generalized to the case $N \neq 2$).

Because this RPA theory is formally similar to paramagnon theory one can follow the paramagnon formalism[17] to deduce the finite temperature contributions to $C - \gamma T$ and the resistivity ρ. It follows that

$$C \sim \gamma T + (T/T_K)^3 \ln(T/T_K) + O(T^3) \tag{16a}$$

and

$$\rho \sim T^2/T_K^2. \tag{16b}$$

T_K can be viewed as the "coherence" energy scale. Note that the temperature dependence of C in Eq. (16a) corresponds to a *decrease* in C/T with increasing T as is observed experimentally in the examples shown in Fig. 2. Equation (16a) is not compatible with experimental results in $CeAl_3$, however.

Despite all the formal similarities with paramagnon theory the differences are important and should be emphasized. In Table I we contrast the general characteristics of paramagnon theory and our Fermi-liquid theory of the Kondo lattice. This table emphasizes the fact that in the Kondo lattice case there is a single energy scale γ whereas in the case of spin fluctuations there are two characteristic energies T_F and T_{SF}. These correspond to the Fermi energy and spin-fluctuation temperature, respectively. Thus while T_{SF} sets the scale for the T^2 contributions to ρ and the $T^3 \ln T$ term in C, there is no simple dependence of these quantities on γ, as there is in the Kondo lattice case.

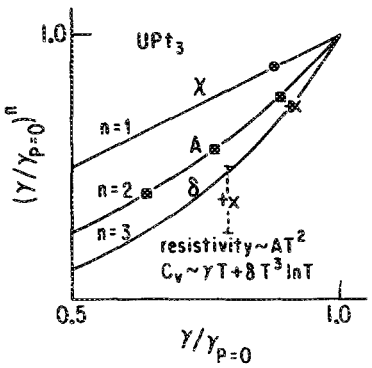

FIG. 4. Scaling of thermodynamic and transport coefficients with pressure dependent γ. For the latter see Ref. 16. χ data are from Ref. 17. Resistivity data are from Ref. 20. The symbols + and × correspond, respectively, to the coefficient γ of $T^3 \ln T$ term in C and the coefficient ϵ of T^3 in C (from Ref. 16). The data points are ratios of the coefficients with respect to their value at ambient pressure.

An important means of determining the microscopic mechanism for the interactions in the Fermi liquid comes from pressure dependent studies in UPt_3. In Fig. 4 are plotted the dependence of χ and $A = \rho/T^2$ and δ, the coefficient of the $T^3 \ln T$ term, as a function of γ which is varied under pressure.[18] The χ, A, and δ measurements are from Refs. 19, 20, and 18, respectively. The solid lines represent the theoretically predicted dependence on γ as shown in Table I, for the three pressure-dependent quantities, χ, A, and δ normalized by their ambient pressure values. As can be seen the data points fall on the theoretical curves with the exception of δ at the largest pressure values. The position of this last data point is rather uncertain so that the deviation from the curve may not be meaningful. It should be stressed that good agreement with experiment would not obtain for a spin-fluctuation model where ρ, C, and χ do not depend on simple powers of γ.

Additional evidence against the paramagnon description of UPt_3 comes from inelastic neutron experiments which show a tendency towards antiferromagnetic ordering.[21] Furthermore the data summarized in both Figs. 1 and 3 shows clearly that the so-called "ferromagnetic spin fluctuators" UPt_3, UAl_2, and USn_3 all lie on the universal curves. They do not appear to be particularly distinct from other heavy-fermion systems. We maintain that because

TABLE I. Comparison of paramagnon and Kondo lattice theories.

Paramagnon systems	Kondo lattices
$\lvert A_0^a \rvert$ large, $\chi \gg \gamma$	$\lvert A_0^a \rvert$ small, $\chi \sim \gamma$
$\gamma \sim (\ln T_{SF}) T_F^{-1}$; $\frac{d \ln T_F}{d \ln V} \sim O(1)$	$\gamma \sim T_K^{-1}$; $\frac{d \ln T_K}{d \ln V} \sim 10$–$10^2$
$\rho \sim T^2/T_{SF}^2 \neq \gamma^2 T^2$	$\rho \sim \gamma^2 T^2$
$C_v - \gamma T \sim (T/T_{SF})^3 \ln T$ $\neq \gamma^3 T^3 \ln T$	$C_v - \gamma T \sim \gamma^3 T^3 \ln T$

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these three compounds have intermediate values of γ they are optimal for observing the $T^3 \ln T$ contributions in the specific heat over a wide range of temperatures.

In summary we have presented a microscopic basis for Fermi-liquid theory in heavy-fermion systems. We use the $1/N$ theory of the Anderson lattice as a basis for this Fermi-liquid description. The leading $1/N$ contribution corresponds to a mean-field description.[15] Mean-field theory defines the heavy "bare particles" of the Fermi liquid. Basically these correspond to the eigenstates of a renormalized band structure of noninteracting c and (localized) f electrons which hybridize weakly with each other. The corrections to mean-field theory arising from coherent hybridization and f-level fluctuations are important and formally resemble RPA theories of the electron-phonon and electron-paramagnon type. The hybridization and f-level fluctuations lead to interactions between the bare particles which can be represented by the Landau parameters $\{A_l^{s,a}\}$. Landau identities such as the relation between χ and A_0^a can be derived in this theory because it represents a controlled expansion in a small parameter $1/N$. As in paramagnon theories a $T^3 \ln T$ contribution to C and a T^2 term in the resistivity all derive from the fluctuation term. Their energy scale is set by γ, unlike their counterparts in paramagnon theory.

This microscopic Fermi-liquid theory appears to be in semiquantitative agreement with experiment. More importantly it suggests that in terms of the linear specific-heat coefficient γ many properties of heavy-fermion systems are universal. Indeed the relations $\chi \sim \gamma$, $C - \gamma T \sim (\gamma T)^3 \ln(T\gamma)$, and $\rho \sim \gamma^2 T^2$ appear to be satisfied for a wide class of materials and within a single system (UPt_3) as a function of pressure. Although N is probably not particularly large (the data for χ/γ suggest $N = 2$) the qualitative features of this theory are presumably more general.

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. (14) were found to be attractive. A simplistic deduction[22] 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 ^{3}He, since it uses a spherical Fermi surface and it assumes that the frequency cutoff scale in Γ is much smaller than the characteristic variations in the electronic energies. In the present theory both relevant frequency scales appear to be of order T_K.

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