Kondo Bosons and the Kondo Lattice: Microscopic Basis for the Heavy Fermi Liquid

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A consistent Fermi-liquid theory of heavy-electron compounds at low temperatures is microscopically derived from the Kondo-lattice model. Interactions between the heavy quasiparticles are mediated by fluctuations of effective valence-conduction hybridization parameters. The computed values of the Wilson ratio, the $T^3 \ln T$ term in the specific heat, and the T^2 coefficient of the low-temperature resistivity are in agreement with systematic experimental trends.

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Heavy-electron systems exhibit a rich variety of low-temperature (T) behavior.[1,2] In general the low-T state is a Fermi liquid with a highly enhanced density of states. In many cases it may further undergo a transition at lower temperature to superconductivity or magnetic ordering. The following strikingly systematic features in the data are noted: (i) The measured dimensionless Wilson ratio R of linear coefficient of the specific heat $\gamma \equiv \lim_{T\to 0} C_v/T$ and the susceptibility χ is close to, but always greater than, unity.[2] (ii) A large number of systems[1] exhibit a rapid decrease in C_v/T with increasing T. (iii) The resistivity in relatively clean samples varies as $\rho \approx AT^2$ at low T, where A appears[3] to scale with γ^2.

Mean-field theories, which incorporate the large on-site Coulomb repulsion U between f electrons of the rare-earth ions, have been formulated in several approaches.[1,4] Among these are the Gutzwiller approximation and the large-N limit of the Kondo lattice (where N is the degeneracy of the fractionally occupied f levels). They lead to a renormalized band-structure scheme which yields the "heavy" quasiparticles and can explain the large enhancements of C_v and χ, as well as the fact that $R \approx 1$. However, the fluctuation corrections to mean-field theory and the quasiparticle dynamical interactions have not yet been systematically determined from a microscopic model. The above observations (i), (ii), and (iii) suggest that such interactions do play an important role in both thermodynamic and transport data.

It is the purpose of the present paper to derive a consistent and systematic Fermi-liquid description of the Kondo lattice with the $1/N$-Kondo-boson (KB) approach as the microscopic basis. Our goals are threefold: (a) to demonstrate the analytic structure of the corrections of leading order in $1/N$ to the Kondo-lattice mean-field theory, (b) to compute the Landau parameters and associated vertex functions and relate them to R, χ, C_v, and ρ, and (c) to show that our results may explain the experimental observations (i)–(iii), and thus provide insight into some universal features of these systems.

For simplicity we study the Coqblin-Schrieffer lattice (CSL) which is a Kondo limit of the large-U Fano-Anderson lattice, in which the f electrons have vanishingly small charge fluctuations. It was already shown[5,6] that the same Lagrangean describes the lattice model away from that limit, provided one includes the finite f-charge susceptibility χ_c in Eq. (4a).

The partition function is given by ($h = 1$)

$$Z_{\mathrm{CSL}} = \int D \prod_{i,m} \lambda c^* c f^* f \exp\{ -\int_0^\beta d\tau [L(\tau) + i \textstyle\sum_{i,m} \lambda_i (f^*_{i,m} f_{i,m} - Q_0)] \},$$
$$L = \textstyle\sum_{\mathbf{k},m} c^*_{\mathbf{k}m} (\partial_\tau + \epsilon_{\mathbf{k}}) c_{\mathbf{k}m} + f^*_{\mathbf{k}m} \partial_\tau f_{\mathbf{k}m} + (J/N) \sum_{i,m,m'} c^*_{i,m} f^*_{i,m'} f_{i,m} c_{i,m'}, \quad (1)$$

where $c_{i,m}$ and $f_{i,m}$ are Grassmann variables of an electron at site $\mathbf{r}_i$ and magnetic quantum number m, $|m| \leq (N-1)/2$, in the conduction band (of dispersion $\epsilon_{\mathbf{k}}$) and the dispersionless f band, respectively. J is the antiferromagnetic Kondo interaction energy. The integration over $\lambda_i(\tau)$ imposes the local constraint of the f-charge conservation, $n_f = Q_0$, at all times and sites. 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.[6] The Bose fields $b_i(\tau) = r_i e^{i\theta_i}$ are introduced by a Hubbard-Stratonovich transformation which allows us to integrate out the fermions and evaluate Z_{CSL} by steepest descents.[5,6] The saddle point $r_q = r_0 \delta_{q,0}$, $i\lambda_q = \epsilon_f \delta_{q,0}$, is given by the variational mean-field equations, where r_0 is the effective hybridization constant and ϵ_f the renormalized f-level renormalized energy. For lack of space, we omit a full discussion of the mean-field equations and their detailed solutions, which have already been presented in the literature.[4] The mean-field theory, that is, the order $O((1/N)^0)$ of this model, in general corresponds to a renormalized band structure given by

$$E^{\pm}_{\mathbf{k}} = \tfrac{1}{2}(\epsilon_{\mathbf{k}} + \epsilon_f) \pm \{ [\tfrac{1}{2}(\epsilon_{\mathbf{k}} - \epsilon_f)]^2 + r_0^2 \}^{1/2} \equiv \epsilon_f \pm r_0 \cot\theta(\epsilon_{\mathbf{k}})^{\pm 1}, \quad (2)$$

which defines the function $\theta(\epsilon)$. We choose our units of energy so that the bare, single-spin, conduction-electron density of states (or inverse bandwidth) ρ_0 in a unit-cell volume satisfies $1/\rho_0(\mu_0)=1$, where μ_0 is defined in terms of the total number of electrons per unit cell, $N_e=\int_0^{\mu_0} d\epsilon\,\rho_0(\epsilon)$. The paramagnetic state possesses an exponentially large (in $1/J$) value of the renormalized density of states ρ at the Fermi level μ which lies in the lower band, $\mu=E_{\mathbf{k}}^{-}(\mu_0)$. We choose to define the dimensionless Kondo lattice temperature T_K as the inverse of the mass enhancement factor, $\rho(\mu)^{-1}=T_K=\sin^2\theta(\mu_0)\ll 1$.

To go beyond mean-field theory we follow the single-impurity analysis of Read and Newns[5] and introduce a time-dependent local gauge transformation which acts simultaneously on the Bose field b_i and the fields f_i, and removes the redundant phase of the Bose fields $\theta_i(\tau)$. The Read-Newns transformation elegantly bypasses the familiar complications of infrared divergences associated with unphysical Goldstone bosons. This leads to a 2×2-matrix description of the boson propagator $D_{rr'}$, where the index $r=1$ corresponds to the fluctuations of the local KB amplitude r_q, and $r=2$ to the constraint field λ_q.

Performing the Gaussian integration of the fields r and λ, we find the free energy to be given by

$$F=-(1/\beta)\ln Z=NS^0+(1/2\beta)\sum_q \mathrm{Tr}\ln\det D(q)+O(1/N), \tag{3}$$

where $S_0=-(2\beta)^{-1}\sum_{k,\alpha}\mathrm{Tr}\ln G_k^{\alpha}$ and $G=(ik_0-E_{\mathbf{k}}^{\alpha})^{-1}$ are the single-spin mean-field free energy and Green's function, respectively. Here k and q denote the usual Fermi and Bose four-vector Fourier components, respectively. $D_{r,r'}(q)$ is the KB propagator, given by the random-phase-approximation (RPA) sum of bubble diagrams, such that

$$D(q)=-(1/N)[\Pi(q)+\Pi^0]^{-1},\quad \Pi^0=2\begin{pmatrix}1/J & \sqrt{\hat{\chi}_c}\\ \sqrt{\hat{\chi}_c} & 0\end{pmatrix}, \tag{4a}$$

where Π^0 is the "unscreened vertex" in which $\hat{\chi}_c$ is set equal to zero for the CSL, and the bubble diagram Π is given by

$$\Pi_{r,r'}=-\beta^{-1}\sum_{k,\alpha\alpha'=\pm} C_r^{\alpha\alpha'}(\theta_{\mathbf{k}},\theta_{\mathbf{k}+\mathbf{q}})\,C_{r'}^{\alpha'\alpha}(\theta_{\mathbf{k}+\mathbf{q}},\theta_{\mathbf{k}})\,G_k^{\alpha}G_{k+q}^{\alpha'}. \tag{4b}$$

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

$$\begin{aligned}&C_1^{--}=\sin(\theta_{\mathbf{k}}+\theta_{\mathbf{k}+\mathbf{q}}),\quad C_1^{-+}=\cos(\theta_{\mathbf{k}}+\theta_{\mathbf{k}+\mathbf{q}}),\quad C_1^{++}=C_1^{--},\\ &C_2^{--}=i\cos\theta_{\mathbf{k}}\cos\theta_{\mathbf{k}+\mathbf{q}},\quad C_2^{-+}=-i\cos\theta_{\mathbf{k}}\sin\theta_{\mathbf{k}+\mathbf{q}},\quad C_2^{++}=i\sin\theta_{\mathbf{k}}\sin\theta_{\mathbf{k}+\mathbf{q}}.\end{aligned} \tag{4c}$$

The functions in Π contain interband and intraband terms, the latter being very similar in their low-$(\mathbf{q},\omega)$ behavior to the familiar Lindhard functions or polarization insertions in the electron gas. It can also be verified that $\lim_{\mathbf{q},\omega\to 0}\det(-D)$ and $\lim_{\mathbf{q},\omega\to 0}\mathrm{Tr}(-D)$ are positive, which ensures the stability of the mean-field solution.[7] The explicit factor of $1/N$ in Eq. (4a) 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 quasiparticle self-energy Σ and vertex function Γ to leading order in $1/N$ by functionally differentiating Z_{CSL} with respect to source currents.[8] The quasiparticles interact via the exchange of a single Kondo-boson propagator (see Fig. 1). 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 the usual $T=0$ expression expanded for small $\Sigma\propto 1/N$:

$$\frac{\delta m}{m}=-\frac{d}{dE_{\mathbf{k}}^{-}}\sum_{\mathbf{q},rr',\alpha}\int_0^{\infty}\frac{d\omega}{\pi}D_{rr'}^{\mathrm{im}}(\mathbf{q},\omega)\,C_r^{-\alpha}(\theta_{\mathbf{k}},\theta_{\mathbf{k}+\mathbf{q}})\,C_{r'}^{\alpha-}(\theta_{\mathbf{k}+\mathbf{q}},\theta_{\mathbf{k}})\times\left[\frac{1+\Theta(\mu-E_{\mathbf{k}+\mathbf{q}}^{\alpha})}{E_{\mathbf{k}}^{-}-E_{\mathbf{k}+\mathbf{q}}^{\alpha}-\omega}-\frac{\Theta(\mu-E_{\mathbf{k}+\mathbf{q}}^{\alpha})}{E_{\mathbf{k}}^{-}-E_{\mathbf{k}+\mathbf{q}}^{\alpha}+\omega}\right]_{E_{\mathbf{k}}^{-}=\mu}, \tag{5}$$

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

$$\begin{aligned}&\Gamma^{\alpha\beta;\alpha'\beta'}(km,k+q\,m;k'm',k'-q\,m')\\ &\quad=\sum_{r,r'}C_r^{\alpha\beta}(\theta_{\mathbf{k}},\theta_{\mathbf{k}+\mathbf{q}})\,C_{r'}^{\alpha'\beta'}(\theta_{\mathbf{k}'},\theta_{\mathbf{k}'-\mathbf{q}})\,D_{r,r'}(q)\ (\equiv\Gamma^{\mathrm{dir}})\\ &\qquad-\delta_{m,m'}\sum_{r,r'}C_r^{\alpha\alpha'}(\theta_{\mathbf{k}},\theta_{\mathbf{k}'-\mathbf{q}})\,C_{r'}^{\beta\beta'}(\theta_{\mathbf{k}+\mathbf{q}},\theta_{\mathbf{k}'})\,D_{r,r'}(k'-k-q)\ (\equiv-\Gamma^{\mathrm{exch}})+O(1/N^2).\end{aligned} \tag{6}$$

We can obtain the Landau scattering amplitudes $\{A_l^{s,a}\}$ following the usual microscopic prescription[9,10]: One considers the $\omega \to 0$ limit of Γ evaluated on the Fermi surface, i.e., $E_{\mathbf{k}} = E_{\mathbf{k}'} = \mu$, and projects it onto Legendre polynomials, P_l, such that

$$A_l^s = T_K^{-1} N \delta_{l,0} \lim_{|\mathbf{q}|,\omega/|\mathbf{q}| \to 0} \Gamma^{\mathrm{dir}} + A_l^a, \quad A_l^a = -T_K^{-1} \frac{2l+1}{2k_F^2} \int_0^{2k_F} d\kappa\, \Gamma^{\mathrm{exch}}(\kappa,0) P_l\left(1 - \frac{\kappa^2}{2k_F^2}\right)\kappa, \tag{7}$$

where k_F is the Fermi wave vector ($\epsilon_F = \mu_0$), and, as defined earlier, T_K^{-1} is the Fermi-level density of states. Equation (6) 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. (7). 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. (6) and (7) we computed the $\{A^{s,a}\}$ numerically. We found that $D(\mathbf{q},0)$ is slowly varying, and higher moments decrease rapidly with l. Considerable simplification arises when a parabolic band structure is used for $\epsilon(\mathbf{k}) \propto |\mathbf{k}|^2$ since angular integrations may then be done analytically, leaving us with just a one-dimensional numerical integration. Here we neglect umklapp processes. For this case the $l = 0, 1$ parameters are (up to corrections of order T_K)

$$A_0^s = \frac{-1.000}{N} + \frac{0.08}{N}\frac{Q_0}{\mu_0}, \quad A_0^s = 1.000 + A_0^a,$$
$$A_1^s = A_1^a = \frac{-0.12}{N}\frac{Q_0}{\mu_0}. \tag{8}$$

In the Landau theory of an SU(N)-invariant Fermi liquid, the phenomenological parameter A_0^a is related to the Wilson ratio by $R = [g^{-2} 4\pi^2/(N^2-1)]\chi/\gamma = 1 - A_0^a$. Here, $K_B = 1$ and g is the electron magnetic moment. With allowance for some uncertainty in the effective moments, the result $0 \leq R - 1 < 1$ appears to be consistent with the experimentally observed systematic trend[2] noted earlier.

A direct differentiation of the free energy in Eq. (3) with respect to temperature and magnetic field yields χ and C_v. The mean-field contributions are $\chi^0 = g^2 N(N^2-1)/12T_K$ and $C_v^0 = \pi^2 NT/3T_K = \gamma^0 T$. The $1/N$ corrections arise from the term $\mathrm{Tr}\ln\det D$. After some algebra it follows that the susceptibility and specific heat are renormalized such that $\chi = \chi^0[1 + \delta m/m - A_0^a + O(1/N^2)]$, and similarly $\gamma = \gamma^0[1 + \delta m/m + O(1/N^2)]$. These are known Fermi-liquid identities related to Ward identities of spin and charge conservation. Their direct verification lends further support to our assignment of Landau parameters in Eq. (7). At this point 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 Galilean relation $1 + \delta m/m = (1 - A_1^s/3)^{-1}$ is incorrect as could be checked against Eq. (5).

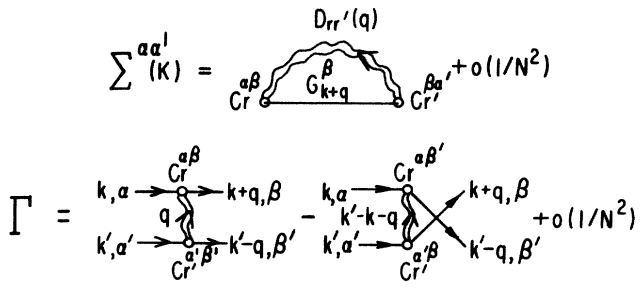

FIG. 1. The self-energy Σ and vertex function Γ [Eq. (6)] to leading order in $1/N$, which involve a single Kondo-boson (wavy line) exchange.

In addition to the correction to γ, there exists a specific-heat correction ΔC_v analogous to the paramagnon $T^3 \ln T$ contribution in liquid ^{3}He. Our analysis follows Engelsberg and co-workers and Riedel[11], where $D_{rr'}$ replaces the RPA susceptibility that mediates the spin fluctuations. We find

$$\Delta C_v = 0.85(T/\bar{T}_K)^3 \ln(T/\bar{T}_K) + O(T^3),$$
$$\bar{T}_K = Q_0 T_K. \tag{9}$$

It is important to note that this behavior has been experimentally observed[1] in, e.g., UPt_3 with $\bar{T}_K \approx 20$–30 K, *and it may also be the source of the rapid temperature dependence of $C_v T$ observed in a wide class of heavy-fermion systems.*[1] By analogy to liquid ^{3}He, it has been previously attrributed in UPt_3 to paramagnons. However, the degree of independent evidence for an incipient ferromagnetic instability in UPt_3 remains controversial.[12] The origin of the $T^3 \ln T$ behavior in this KB theory is the nonanalytic 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, it does not derive solely from the spin-fluctuation channel, as seen by the relative magnitudes of A_0^a and A_0^s. The contributions to C_v from higher powers of temperature are much harder to calculate since the temperature dependence of the variational parameters r_0, ϵ_f, and μ must also be considered in the T^3 order and above.

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 calculation,[13] and determine A by evaluating $\partial D^{\rm im}/\partial\omega$, at $\omega = 0$. The result is

$$\rho = \rho_{\rm max}(T/\lambda \bar{T}_{\rm K})^2 + O(T^3), \tag{10}$$

where $\rho_{\rm max} = h/e^2 k_{\rm F} N^2 = 100$–$300\ \mu\Omega$ cm and where λ is a factor of order unity. This result is qualitatively consistent with the remarkable universal scaling[3] of A and γ^2. *It should be emphasized that Q_0 emerges as a key parameter which determines the $l \geq 0$ Landau parameters, and the coherence energy scale $\bar{T}_{\rm K}$ which appears in both C_v/T and ρ [Eqs. (9)–(10)].* Our analysis[12] of recent pressure-dependent data on UPt_3, as well as universal trends throughout the heavy-fermion materials, lends experimental support to the existence of this universal coherence scale $\bar{T}_{\rm K}$.

Although in many heavy-fermion systems N is not really large ($=2$), the present $1/N$ expansion is a systematic description of the quasiparticle interactions. It has many satisfying features including the following: (1) There is dependence on a minimal set of predetermined microscopic parameters. These are the bare band structure and the Kondo lattice temperature $T_{\rm K}$. (2) 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. (3) It yields the full vertex function [Eq. (6)]. Realistic band structure, umklapp processes, and phonon interactions[14] must be also considered in any further application to real materials.

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. (7) were found to be attractive. A simplistic deduction[10,15] 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 it is in ^{3}He, since it assumes that the frequency cutoff 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 $T_{\rm K}$. The detailed spectral behavior of the full vertex function is clearly important and may ultimately provide a better understanding of this important issue.[8]

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Note added.—Recently we received a preprint from A. Millis and P. A. Lee which applied a similar technique to the Anderson lattice model using, however, the Cartesian Kondo-boson coordinates.

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