Long-range Coulomb interactions and the specific heat of the large-degeneracy version of the lattice Anderson model

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The Fermi-liquid interactions between elementary excitations in the large-degeneracy (large-N) auxiliary-boson version of the lattice Anderson model and the concomitant $T^3\ln T$ term in the specific heat are studied to leading nontrivial order in $1/N$. The previously neglected but physically necessary long-range part of the Coulomb interaction is included. To this order, the interaction is shown to arise entirely from exchange of virtual density fluctuations between quasiparticles; interactions arising from exchange of virtual spin fluctuations are not included to this order. The coefficient of the $T^3\ln T$ term in the specific heat is computed, and its observability in heavy-fermion materials is discussed. The theory predicts a $T^3\ln T$ coefficient more than 100 times smaller than the coefficient observed in UPt_3. Possible explanations for the discrepancy are discussed.

I. INTRODUCTION

This paper is concerned with the contribution of long-wavelength, low-energy fluctuations to the thermodynamic properties of the auxiliary-boson large-N version of the $U=\infty$ lattice Anderson model, with how this contribution changes when the long-range part of the interelectron Coulomb interaction is incorporated into the auxiliary-boson model, and with the relevance of the model to heavy-fermion materials. The $U=\infty$ lattice Anderson model is believed to contain the essential physics of the currently interesting heavy-fermion metals.[1] It describes a structureless band of conduction (c) electrons hybridizing with a dispersionless band of f electrons which are at an energy far below the Fermi level (we measure all energies with respect to the chemical potential, which we take to be zero) and are subject to the constraint that the number of f electrons on a site i, $n_{fi}\leq 1$. The low-temperature properties of this model have not been amenable to study by conventional techniques. To gain insight several groups[2–6] have applied to this model the auxiliary-boson large-N technique originally developed[7–9] for the single-impurity Anderson model. In this technique one introduces a new Bose field b, which represents an unoccupied f site, and studies a new model of electrons coupled to bosons in which $n_{bi}+n_{fi}=1$. Here n_{bi} is the number of bosons on site i. If one makes the additional, unphysical assumption that both c and f electrons are characterized by a conserved, N-fold-degenerate "spin" quantum number N,[3–6] then the model may be studied by a $1/N$ expansion about a mean-field theory of electrons moving in a "renormalized band structure." Corrections to the mean-field theory come from electron-boson interactions. These may be treated analogously to the familiar electron-phonon interaction.[3] The coupling constant for this interaction is $1/N$.

Many physical quantities have been computed within this formalism, including the coefficient of the linear term in the specific heat,[2,3,5,6] the magnetic susceptibility,[2,3,5,6] the Kondo spin compensation cloud,[3] the temperature-[3,5] and frequency[3]-dependent conductivities, and the superconducting instability of the model.[4] The results are, in general, in qualitative agreement with experiments.

A key insight into the model came from Auerbach and Levin,[5] who related the model to conventional Fermi-liquid theory by identifying the diagram in which two electrons exchange a boson with the Landau interaction amplitude Γ. They also asserted that the auxiliary-boson-mediated interaction leads to a $T^3\ln T$ term in the specific heat, qualitatively similar to that observed in the heavy-fermion material UPt_3.

However, several issues have been, so far, left obscure, including the physical interpretation of the auxiliary-boson and of the boson-mediated interaction between electrons, and the qualitative importance of the (previously neglected) effects of the long-range part of the Coulomb interaction, and also the quantitative applicability of the model to real heavy-fermion materials.

Therefore, in this paper we study further the long-wavelength, low-frequency modes of the system and their contribution to the specific heat. We also extend the model to include the long-range part of the Coulomb interaction, and we study the Fermi-liquid properties of the extended model. We work to leading nontrivial order in $1/N$ and restrict attention to low temperatures T. A study of other "Fermi-liquid" properties of the auxiliary-boson model, including collective mode and plasmon effects, will be published separately.[10]

We show that (to leading nontrivial order in $1/N$) the $T^3\ln T$ term in the specific heat, and, indeed, the Fermi-liquid interaction parameters in general, come from an interaction mediated by exchange of virtual density fluctuations between quasiparticles (as, in the paramagnon model of ^{3}He, the interactions come from exchange of virtual spin fluctuations). Contributions to the interactions from virtual spin fluctuations would only appear in higher orders in $1/N$. Proper treatment of these terms requires at least a two-loop calculation which has not, to our knowledge, been performed.

Phenomena involving density fluctuations in metals are drastically altered by the long-range part of the Coulomb interaction. We therefore extend the Anderson model to include this. We show that the $T^3 \ln T$ term due to auxiliary-boson mediated interactions disappears. However, the Coulomb interaction alone is shown to lead to a $T^3 \ln T$ term in the specific heat which is of the same sign and essentially the same magnitude as the auxiliary-boson $T^3 \ln T$ term. We give Fermi-liquid arguments to explain why this is so.

$T^3 \ln T$ contributions to the specific heat of the Anderson lattice without Coulomb interactions have been previously derived.[5,6] The expressions given here are similar to (although differing in a few respects from) the previous ones, but the connection with Landau parameters, the physical origin of the term, the discussion of the relevance of this term to heavy-fermion materials, and of course, the effects of the long-range part of the Coulomb interaction have not, to the author's knowledge, appeared in the literature before. The relation of this work to the previous work is discussed in more detail at the end of Sec. III.

The rest of the paper is organized as follows. In Sec. II we write down and explain the models to be studied, and we give a convenient expression for the contribution of electron–auxiliary-boson interactions to the free energy. In Sec. III we study the boson propagator, density-density correlation function, and $T^3 \ln T$ term for the model without long-range Coulomb interactions. In Sec. IV we do the same for the model with long-range Coulomb interactions.

Readers uninterested in the details of the calculation may turn directly to Sec. V, which contains a summary of the previous three sections and a discussion of the applicability of these results (and the auxiliary-boson method in general) to real heavy-fermion materials. The effect of impurity scattering is briefly considered. The coefficient of the $T^3 \ln T$ term in the specific heat is compared with experimental data for UPt_3 and found to be too small by a factor of more than 10^2. Possible explanations for the discrepancy are discussed. Large (and so far unobserved) variations in the Fermi velocity over the Fermi surface could explain the difference, as could strong antiferromagnetic spin fluctuations, which the auxiliary-boson $1/N$ method does not correctly treat.

II. MODELS

In this section we write down and explain the models to be analyzed and give a convenient expression for the free energy F in terms of a coupling constant integral over the auxiliary-boson propagator. In this expression the contribution to F from electron-auxiliary-boson interactions is separated from other contributions to F, such as that coming from the Coulomb interaction.

As discussed above, we are interested in asymptotically low temperatures and in long-wavelength phenomena. In what follows we retain only leading order temperature and momentum dependences. In particular, we neglect terms of relative order q/p_F, where p_F is the Fermi momentum.

We use the radial gauge formulation of the "auxiliary-boson," large N version of the Anderson model, to which we add a term accounting for the long-range part of the Coulomb interaction. We briefly outline the formulation here; for more detailed discussions see Refs. 1, 3, and 7–9. The $U=\infty$ lattice Anderson model describes a band of conduction (c) electrons with energy ε_k hybridizing with a set of localized f orbitals at energy E_0, via a hybridization matrix element V (conventionally assumed to be structureless) and subject to the constraint that the number of electrons on the f orbital on site i, n_{fi}, is less than or equal to one. All energies are measured from the chemical potential, which we take to be zero. We are interested in the Kondo limit, in which $-E_0/\rho_0 V^2 \gg 1$, where $\rho_0 \sim dk/d\varepsilon_k$ is a typical value of the c-electron density of states. In the auxiliary-boson method one introduces a new Bose field $b_i^\dagger$ which creates a hole on the f orbitals on site i, rewrites the hybridization as $(Vc_i^\dagger f_i b_i^\dagger + \text{H.c.})$ and replaces the constraint by $n_{fi}+n_{bi}=1$, where n_{bi} is the number of bosons on site i. To apply the $1/N$ expansion method to the lattice one assumes[3–6] that both c and f electrons are characterized by an N-fold degenerate spin quantum number, m, which is conserved in hybridization and c-electron propagation, and one replaces the constraint by $n_{fi}+n_{bi}=q_0 N$. To obtain a sensible $1/N$ expansion one must treat q_0 as a parameter independent of N.[11] One may regain contact with the original Anderson model by setting $q_0=1/N$.[3] The calculations in this paper are performed for arbitrary q_0 to leading nontrivial order in $1/N$.

To obtain the $1/N$ expansion one splits the Bose fields into static and fluctuating parts. Retaining only the static parts leads to a mean-field theory in which the c electrons hybridize, by a renormalized hybridization $\sigma_0 \ll V$, with a dispersionless band of quasi f electrons at an energy ε_f which is just above the Fermi energy. Corrections to the mean-field theory may be thought of as coming from interactions between the fluctuating parts of the Bose fields and electrons moving in the renormalized band structure. The coupling constant for this interaction is $1/N$.

After some algebra the auxiliary-boson version of the Anderson model may be written in functional integral form with Lagrangian L given by

$$L = L_F + L_B + L_I + L_{\text{rest}} , \tag{2.1}$$

where

$$L_F = \sum_{k,m} d_{2km}^\dagger [\partial_\tau + \varepsilon_2(k)] d_{2km} + d_{1km}^\dagger [\partial_\tau + \varepsilon_1(k)] d_{1km} , \tag{2.2a}$$

$$L_B = \frac{N}{2V^2} \sum_q \sigma_q [\varepsilon_f - E_0] \sigma_{-q} + i\sigma_0(\sigma_q \lambda_{-q} + \lambda_q \sigma_{-q}) , \tag{2.2b}$$

$$L_I = \sum_{k,q,m} \sigma_q [2u_k v_k (d^\dagger_{1km} d_{1,k+q,m} - d^\dagger_{2km} d_{2,k+q,m}) + (u_k^2 - v_k^2)(d^\dagger_{2km} d_{1,k+q,m} + d^\dagger_{1km} d_{2,k+q,m})] ,$$
$$+ i\lambda_q [(u_k^2 d^\dagger_{1km} d_{1,k+q,m} + v_k^2 d^\dagger_{2km} d_{2,k+q,m}) - u_k v_k (d^\dagger_{2km} d_{1,k+q,m} + d^\dagger_{1km} d_{2,k+q,m})] . \tag{2.2c}$$

Here $\varepsilon_2(k)$ and $\varepsilon_1(k)$ are the dispersion relations and $d_2^\dagger$ and $d_1^\dagger$ the creation operators for the upper and lower bands of the renormalized band structure. They are related to the c and f operators via[3]

$$d_{2km} = -v_k f_{km} + u_k c_{km} , \tag{2.3a}$$

$$d_{1km} = u_k f_{km} + v_k c_{km} , \tag{2.3b}$$

where

$$\varepsilon_2(k) = \tfrac{1}{2}(\varepsilon_k + \varepsilon_f) + \tfrac{1}{2}E_k , \tag{2.4a}$$

$$\varepsilon_1(k) = \tfrac{1}{2}(\varepsilon_k + \varepsilon_f) - \tfrac{1}{2}E_k , \tag{2.4b}$$

$$E_k = [(\varepsilon_k - \varepsilon_f)^2 + 4\sigma_0^2]^{1/2} , \tag{2.4c}$$

and

$$u_k^2 = \tfrac{1}{2}[1 + (\varepsilon_k - \varepsilon_f)/E_k] , \tag{2.5a}$$

$$v_k^2 = \tfrac{1}{2}[1 - (\varepsilon_k - \varepsilon_p)/E_k] , \tag{2.5b}$$

$$u_k v_k = \sigma_0 / E_k . \tag{2.5c}$$

The operators σ and λ are Bose operators. $\sigma = Vr$, where r is the magnitude of the original Bose field b. σ has been split into mean-field (σ_0) and fluctuating (σ_q) parts. λ is a new field made up from a Lagrange multiplier field (introduced to enforce the constraint $n_{fi} + n_{bi} = q_0 N$) and the "imaginary time" derivative of the phase of the original Bose field. It too has been split into mean-field (ε_f) and fluctuating (λ_q) parts.

L_I describes interactions between electrons and the fluctuating parts of the Bose fields. In Eq. (2.2c) we have written only the leading order terms. There are other terms of relative order q/p_F (k_F is the Fermi momentum) which we have not written.

The remaining terms in the Lagrangian, which we have denoted L_{rest} and not explicitly written, are of two sorts. There are multiboson interaction terms, which do not contribute, to the order in $1/N$ to which we work, and there are "anomalous" terms containing only one Bose operator and no fermion operators. Requiring that these do not contribute to physical quantities[3] or, equivalently, requiring that the free energy computed from L be an extremum under variations of ε_f and σ_0,[8] fixes the values of ε_f and σ_0. To leading order in $1/N$ one finds

$$\varepsilon_f = D \exp(E_0/\rho_0 V^2) , \tag{2.6a}$$

$$\sigma_0^2 = q_0 V^2 (1 - n_f) . \tag{2.6b}$$

Here D is an energy of order the c-electron bandwidth, $n_f = \sum_{k<k_F} u_k^2$ and $\rho_0 = dk/d\varepsilon_k$ evaluated at $\varepsilon_k = 0$. Explicit expressions for D and n_f to leading order in $1/N$ and leading[2] and next to leading[3] order in q_0 have been calculated.

In this paper we are primarily interested in the Kondo limit, in which $-E_0/\rho_0 V^2 \gg 1$. In this limit $\varepsilon_f \ll D$. In addition, $1 - n_f \cong \varepsilon_f / \rho_0 V^2 \ll 1$ (Refs. 3 and 8) thus $\sigma_0 \ll V$. We assume the Fermi level lies in the lower band $\varepsilon = \varepsilon_1(k)$. The Fermi surface is defined by $\varepsilon_1(k_F) = 0$. The density of states at the Fermi surface, ρ, is given by

$$\rho = dk/d\varepsilon_1(k_F) = (m^*/m) dk/d\varepsilon_k , \tag{2.7}$$

where the mass enhancement m^*/m (m is the c-electron mass) is given by

$$m^*/m = d\varepsilon_k / d\varepsilon_1(k) = 1/v_k^2 . \tag{2.8}$$

In the Kondo limit, $m^*/m = \sigma_0^2/\varepsilon_f^2 \gg 1$. In this case the low-energy electronic excitations of the band structure determined by L_F are heavy fermions. The effective Fermi temperature for the heavy fermions is ε_f.[3]

We now extend the model to include the long-range part of the Coulomb interaction. We consider a new Lagrangian L_E, where

$$L_E = L + L_C , \tag{2.9}$$

L was defined in Eq. (2.1), and

$$L_C = \sum_q \frac{4\pi e^2}{N q^2} n_q n_{-q} . \tag{2.10}$$

Here n_q is the electron-density operator. The electron density is of order N; the explicit factor of N renders L_C of order N, as is L. In terms of the c-f operators one has

$$n_q = \sum_{k,m} c^\dagger_{k+q,m} c_{km} + f^\dagger_{k+q,m} f_{km} \tag{2.11a}$$

or, using Eqs. (2.3) and (2.5) and dropping terms of order q/k_F;

$$n_q = \sum_{k,m} d^\dagger_{2,k+q,m} d_{2km} + d^\dagger_{1,k+q,m} d_{1km}$$
$$+ \mathbf{P}_k \cdot \mathbf{q} (d^\dagger_{2,k+q,m} d_{1km} + d^\dagger_{1,k+q,m} d_{2km}) . \tag{2.11b}$$

Here $\mathbf{P}_k$ is the dipole operator which gives interband transitions:

$$\mathbf{P}_k = \frac{\mathbf{k}}{m} \frac{u_k v_k}{E_k} + O((q/k_F)^2) . \tag{2.12}$$

Note that L_C includes intra-f Coulomb interactions. The large-q part of this interaction is already included in the Anderson model; it produces the "infinite U" repulsion between f electrons at the same site, which leads to the constraint $n_{fi} \leq 1$. However, the $q \to 0$ part is not included, as can be seen from a Gedanken experiment in which one removes a few f electrons from one region of space and distributes them over another, holding the remaining charges fixed. It is physically obvious that in this case a long-range electric field must be present. Such a field is accounted for by L_C, but would not appear in the original Anderson model. The short-range part of the Coulomb interaction is included in L. To avoid doubling counting interactions one must cut off the sum on q in Eq. (2.10) at some $q_c \ll k_F$. Specifying q_c would be difficult; however, we are interested in small q phenomena and our results will be independent of q_c.

We conclude this section by deriving, via a coupling constant integration, a convenient expression for the contribution to the free energy F from the electron-boson interactions described by L_I. The expression we derive is of order $1/N$ relative to the mean-field terms, and gives correctly the leading-order (in $1/N$) contribution to the $T^3\ln T$ contribution to the specific heat C. Our expression does not include contributions to the free energy arising from $1/N$ and finite temperature corrections to the mean-field parameters ε_f and σ_0; however, we show in Appendix A that these do not affect the coefficient of the $T^3\ln T$ term. Our derivation parallels the textbook derivation of the free energy of the electron-phonon system;[12] it applies to both the models with and without Coulomb interactions. We consider a new Lagrangian L', where

$$L' = L_F + L_B + gL_I(+L_c) . \tag{2.13}$$

Then we differentiate a formal expression for F with respect to g, reexpress the result in terms of the exact boson Green function D, and integrate over g. The derivation is notationally more complicated than in the electron-phonon problem because there are two boson fields, σ and λ. D is thus a 2×2 matrix, which we write as

$$D(q,\tau) = \begin{bmatrix} D_{\sigma\sigma}(q,\tau) & D_{\sigma\lambda}(q,\tau) \\ D_{\lambda\sigma}(q,\tau) & D_{\lambda\lambda}(q,\tau) \end{bmatrix} , \tag{2.14}$$

where τ is imaginary time and $D_{\sigma\sigma} = \langle T_\tau[\sigma(q,\tau),\sigma(q,0)]\rangle$, etc.

When $g=0$, the boson propagator is given by its bare value D_0, where

$$D_0^{-1}(q,\tau) = \frac{N}{2V^2} \begin{bmatrix} \partial_\tau + (\varepsilon_f - E_0) & i\sigma_0 \\ i\sigma_0 & 0 \end{bmatrix} . \tag{2.15}$$

Now following the standard arguments it is easy to show

$$F = F_0 + \int_0^1 \frac{dg}{g} T \sum_\nu \int \frac{d^3q}{(2\pi)^2} \mathrm{Tr}[\Sigma_g D_g] . \tag{2.16}$$

Here the boson self-energy matrix Σ_g is given by

$$\Sigma_g = D_g^{-1} - D_0^{-1} \tag{2.17}$$

and D_g is the exact boson Green function for coupling constant g. Note that the derivation of (2.16) applies whether or not the model includes the long-range part of the Coulomb interaction. In each case F_0 is the free energy of the model with $g=0$.

In Sec. III we shall show that to leading order in $1/N$, $\Sigma_g \sim g^2$, so that

$$\frac{1}{g}\mathrm{Tr}\Sigma_g D_g = \frac{-1}{2}\frac{d}{dg}\ln D_g^{-1} .$$

Then one has

$$F = F_0 - \tfrac{1}{2} T \sum_\nu \int \frac{d^3q}{(2\pi)^3} \mathrm{Tr}\,\ln D^{-1}(q,i\nu) .$$

The sum over Matsubara frequencies may be handled in the usual way, yielding

$$F = F_0 - \int \frac{d\Omega}{2\pi} \int \frac{d^3q}{(2\pi)^3} n(\Omega)\,\mathrm{Im}\,\mathrm{Tr}\,\ln D^{-1}(q,\Omega+i\delta) . \tag{2.18}$$

Here $n(\Omega)$ is the usual Bose distribution function,

$$n(\Omega) = [\exp(\beta\Omega) - 1]^{-1} .$$

We note that (2.18) contains only the small-q contributions to the thermodynamics. It has sometimes been argued[13] that $T^3\ln T$ contributions can arise from processes where $q \sim 2k_F$, although this conclusion has been questioned.[14] However, $q \sim 2k_F$ processes would, in the present formalism, involve "crossed ladders" of boson propagators, and so would be smaller in powers of $1/N$, than the terms in (3.8).

III. MODEL WITHOUT COULOMB INTERACTIONS

In this section we study the auxiliary-boson model without Coulomb interactions. We compute, to leading nontrivial order in $1/N$, the long-wavelength, low-frequency, and temperature expressions for the density-density correlation function and boson propagator, and also the coefficient of the $T^3\ln T$ term in the specific heat.

We begin with the boson propagator, which satisfies the usual Dyson equation,

$$D^{-1}(q,\Omega+i\delta) = D_0^{-1}(q,\Omega+i\delta) - \Sigma(q,\Omega+i\delta) . \tag{3.1}$$

Here Ω is a real frequency. By Eq. (2.15), D_0^{-1} is of order N. The only order N contributions to Σ are simple fermion bubbles. Thus $\Sigma \sim g^2$, where g is the electron-boson coupling constant. We assume temperature $T \ll \sigma_0 = \min_k\{\varepsilon_2(k) - \varepsilon_1(k)\}$, where $\varepsilon_{1,2}(k)$ are defined in Eqs. (2.4). There are then generically two kinds of contributions to Σ: an interband bubble and an intraband bubble. For small (q,Ω,T) the interband bubble tends to a constant, while the intraband bubble is proportional to χ_0, the familiar particle hole bubble from Fermi-liquid theory. One finds

$$\rho\chi_0(q,\Omega+i\delta) = \rho\left[1 + \frac{1}{2}s\ln\left|\frac{1-s}{1+s}\right| + \frac{i\pi}{2}s\Theta(1-|s|)\right] , \tag{3.2}$$

where $s = \Omega/v^*q$. Here ρ is the quasiparticle density of states and v^* is the quasiparticle velocity; both were defined in Sec. II.

The details of the computation of Σ are given in Appendix B. We find for the components of D (up to terms of order m/m^*)

$$D_{\lambda\lambda}=N\left[\rho_0-\frac{m}{m^*}\rho\chi_0\right]\Big/\det D^{-1}\ , \tag{3.3a}$$

$$\begin{aligned}D_{\sigma\lambda}&=D_{\lambda\sigma}\\&=-iN\left[\frac{\sigma_0}{2V^2}+\frac{1}{2}\left[\frac{m}{m^*}\right]^{1/2}(\rho\chi_0+\rho_0)\right]\Big/\det D^{-1}\ ,\end{aligned} \tag{3.3b}$$

$$D_{\sigma\sigma}=\tfrac{1}{4}N[\rho\chi_0+\rho_0]\ , \tag{3.3c}$$

where

$$\det D^{-1}(q,\Omega+i\delta)=\tfrac{1}{4}N^2A\rho_0[\rho\chi_0(q,\Omega+i\delta)+B\rho_0]\ , \tag{3.4a}$$

$$A=\left[1+\frac{m}{m^*}+\left[\frac{m}{m^*}\right]^{1/2}\frac{\sigma_0}{\rho_0V^2}\right]=1+O(m/m^*)\ , \tag{3.4b}$$

$$B=1+\frac{\sigma_0^2}{4V^4\rho_0^2A}=1+(1-n_f)^2+O(m/m^*)\ . \tag{3.4c}$$

We note that one may calculate D^{-1} for arbitrary values of m^*/m (although the algebra is lengthy and certain integrals cannot be performed analytically), and that an expression of the form (3.4a) for $\det D^{-1}$ always results, with A and B still of order 1 but given by more complicated expressions than (3.4b) and (3.4c).

The imaginary part of D^{-1} (which one may think of as the spectral weight for boson excitations) is nonzero in two regions of the (Ω,q) plane: one is the familiar particle-hole continuum $\Omega<v^*q$, where $\mathrm{Im}\chi_0\neq0$; the other is specified by $\det D^{-1}(q,\Omega)=0$. From (3.4a) and (3.2) this is found to be

$$\Omega=cq\ , \tag{3.5a}$$

where

$$c^2=\tfrac{1}{3}(\rho/\rho_0B)(v^*)^2\ . \tag{3.5b}$$

Along the line (3.5a) the system has a propagating undamped boson mode.

Proceeding similarly, one may compute the density-density correlation function $S(q,\Omega)$. Details of the calculation will be given elsewhere;[10] the result is that $S(q,\Omega)$ has the familiar Landau form

$$S(q,\Omega)=\frac{\rho\chi_0(q,\Omega)}{1+F_0^S\rho\chi_0(q,\Omega)}\ , \tag{3.6}$$

where

$$F_0^S=\frac{\rho}{\rho_0B}[1+O(m/m^*)] \tag{3.7}$$

(note $F_0^S\sim m^*/m\gg1$). This is a reflection of the $U=\infty$ constraint built into the Anderson model. It is well known that in the limit $F_0^S\gg1$, a neutral Fermi liquid supports a zero sound mode with dispersion $\Omega=cq$, where $c^2=\frac{1}{3}F_0^S(v^*)^2$; this is precisely the Eq. (3.5) that determines the propagating part of the boson. We therefore identify physically the auxiliary boson with a density fluctuation of the system. This identification will be confirmed in Sec. IV, where it will be shown that the addition of the long-range part of the Coulomb interaction which is known to eliminate the zero sound mode, also eliminates the singularity in the boson propagator, in the Fermi-liquid regime $\Omega\ll T_K$.

Note that the Landau A parameters for this mode are to leading order in $1/N$ obtained[5] from averages over the $\omega=0$, finite q boson propagators. Because the boson propagator is a density fluctuation, the leading-order (in $1/N$) expressions for Landau parameters must represent the effects of exchange of virtual density fluctuations only.

We now use Eqs. (2.18) and (3.4) to write the contribution of the electron-boson interactions to the free energy F_B as

$$F_B=-\int\frac{d\Omega}{2\pi}\frac{d^3q}{(2\pi)^3}n(\Omega)\tan^{-1}\left[\frac{\mathrm{Im}\rho\chi_0(q,\Omega)}{B\rho_0+\mathrm{Re}\rho\chi_0(q,\Omega)}\right]\ . \tag{3.8}$$

We now compute the $T^3\ln T$ contribution to this entropy S by differentiating (3.8) with respect to temperature. There are in principle two sources of temperature dependence: that of χ_0 and that of the Bose function $n(\Omega)$. However, we show in Appendix C that as far as the $T^3\ln T$ contribution to S is concerned, one may neglect the temperature dependence of χ_0. This point seems to have been missed in the earlier paramagnon literature,[15,16] where the contributions to S arising from the temperature dependence of χ_0 were divided into two parts (which give contributions to the $T^3\ln T$ term in S which sum to zero) and then combined with other contributions before being evaluated.

In any event, retaining only the temperature dependence of the Bose function and evaluating the resulting expression in the standard way one finds:

$$\Delta S_B=\frac{-dF_B}{dT}=\frac{\pi^2}{15}\frac{1}{(v^*)^3}(A_0^S)^2\left[1-\frac{\pi^2}{12}A_0^S\right]T^3\ln T\ , \tag{3.9}$$

where A_0^S is the standard density-channel Landau parameter; $A_0^S=F_0^S/(1+F_0^S)$. Differentiating (3.9) leads to an expression for the specific heat. Assuming a spherical Fermi surface, and defining

$$T^*=k_F^2/2m^*\ , \tag{3.10a}$$

$$n=Nk_F^3/6\pi^2\ , \tag{3.10b}$$

as the Fermi temperature and density (summed over spin directions) one finds

$$\Delta C_B = \frac{1}{N}\frac{3\pi^4}{20} n\,(A_0^S)^2 \left[1-\frac{\pi^2}{12}A_0^S\right]\left[\frac{T}{T^*}\right]^3 \ln T \ . \quad (3.11)$$

Equation (3.11) agrees with the general expression of Pethick and Cerneiro[17] for the $T^3\ln T$ term in the specific heat for a Fermi-liquid theory in which only A_0^S is non-negligible. This is the situation in the auxiliary-boson large-N model, where $A_0^S \sim 1$ and all other A's are $O(1/N)$.[3,5] The factor of N is the spin degeneracy, and would be 2 in the case of ^{3}He.

Note that the $T^3\ln T$ contributions come from performing the integrals in (3.8) over the region $\Omega < v^x q \ll T_K$. For this reason it is clear that they are not produced by the zero-sound mode, which contributes significantly to the sum in (3.8) only along the line $\Omega = cq$, where c^2 was defined in Eq. (3.5b). It is easy to show that the zero-sound mode gives a T^3 contribution to ΔC, as would any boson mode with a linear dispersion.

The $T^3\ln T$ term in the specific heat of the auxiliary-boson model was first pointed out by Auerbach and Levin.[5] They worked in the limit $m^*/m \to \infty$, so that $A_0^S = 1$, and chose a density of electrons such that (in our language) $n = N$. Their coefficient is a factor of 3 less than the one obtained here. Also, their characteristic temperature T^* was stated to be the quantity $q_0\varepsilon_f$.[5] In general,[3] $q_0\varepsilon_f \neq k_F^2/2m^*$. In the limit $q_0 \to 0$, $\varepsilon_f \sim q_0 n_f k_f^2/2m^*$. Because $q_0 < \frac{1}{2}$ the temperature scale found by Auerbach and Lewin is much smaller than the one found here. The source of this discrepancy is not clear.

A $T^3\ln T$ contribution to C has also been obtained by Rasul and Desgranges.[6] Their result coincides with our result (3.11) if the limit $q_0 \to 0$ is taken and terms of relative order m/m^* are dropped. In this limit,[3] $A_0^S = 1-(1-n_f)^2$ and $q_0 n_f T^* = \varepsilon_f$. [Note that there is a sign error in Eq. (24) of Ref. 6, which is inconsistent with both Eq. (23) of Ref. 6 and our Eq. (3.11).]

Note that the $T^3\ln T$ term has been shown to arise from small-q density fluctuations since only the Landau parameter A_0^S is involved. Phenomena involving long-wavelength density fluctuations in metals can be crucially altered by the presence of the long-range Coulomb interaction.[18] Hence we turn to Sec. IV to a study of Coulomb effects in our model, before returning to the question of the comparison of our results with experiment.

IV. MODEL WITH LONG-RANGE COULOMB INTERACTIONS

In this section we consider the long-wavelength properties of the Anderson model extended to include the long-range part of the Coulomb interaction; this model is given by Eq. (2.9). The discussion follows that in Sec. III.

We begin with the boson propagator D which as before satisfies the Dyson equation

$$D^{-1}(q,\Omega+i\delta) = D_0^{-1}(q,\Omega+i\delta) - \Sigma(q,\Omega+i\delta) \ . \quad (4.1)$$

Previously, the leading contributions to Σ were interband and intraband fermion bubbles. However, in the present case chains of fermion bubbles linked by the Coulomb interaction can also contribute. However, from Eqs. (2.11b) and (2.2c) one sees that the Coulomb interaction couples to the interband bubble via a vector coupling while the auxiliary bosons couple to the interband bubble via a scalar coupling. Any interband fermion bubble coupled at one vertex to a boson and at the other vertex to the Coulomb interaction therefore vanishes by symmetry, and terms in Σ proportional to an interband bubble are identical to those computed in Sec. III. Proceeding as in Sec. III one obtains (denoting the intraband contribution to Σ by $\Sigma_{\rm intra}$)

$$\Sigma_{\rm intra} \sim h(s,q) = \rho\chi_0(s)/1+V_s\rho\chi_0(s) \ . \quad (4.2)$$

As before, $s = \Omega/v^* q$, while V_s is the effective Coulomb interaction between lower-band quasiparticles; V_s is reduced from its "bare" value, $V_C = 4\pi e^2/Nq^2$ because the medium is polarizable via virtual interband transitions. Explicitly, one finds[10] $V_s = V_C/\varepsilon$ with

$$\varepsilon = 1 + V_C P_1(\varepsilon, i\nu=0) \quad (4.3a)$$

and

$$P_1(q,i\nu) = -\sum_{k,\omega} (\mathbf{P}_k\cdot\mathbf{q})^2 [\,G_2(k+q,i\omega+i\nu)G_1(k,i\omega) + G_1(k+q,i\omega+i\nu)G_2(k,i\omega)] \ . \quad (4.3b)$$

Here $\mathbf{P}_k$ was defined in Eq. (2.12) and $G_{1,2}$ are the Green functions for electrons in the lower and upper bands of L_F, Eq. (2.2c). $P_1(q)$ may be easily evaluated in the small (q,ν) limit, and so one finds

$$\varepsilon = 1 + \tfrac{2}{3}\omega_{pc}^2/\sigma_0^2 + O(m/m^*) \ , \quad (4.4)$$

where ω_{pc}, the plasma frequency of the c-electrons, is given by

$$\omega_{pc}^2 = 4\pi e^2 n_c/mN \ , \quad (4.5)$$

where n_c is the density of conduction electrons. In a model with a spherical Fermi surface, $n_c = Nk_h^3/6\pi^2$, where $\epsilon(k_h)=0$. The factor of N in (4.5) comes from the form of the Coulomb interaction, Eq. (2.10).

Combining these various results we may write for the boson propagator in the presence of the Coulomb interactions D_C,

$$D_{C\sigma\sigma}(q,\Omega) = \tfrac{1}{4}N[\rho_0 + h(s,q)]/\det D_C^{-1} \ , \quad (4.6a)$$

$$D_{C\sigma\lambda} = D_{C\lambda\sigma} = -iN\left[\frac{\sigma_0}{2V^2} + \frac{1}{2}\left[\frac{m}{m^*}\right]^{1/2}[h(s,q)-\rho_0]\right]\Big/\det D_C^{-1} \ , \quad (4.6b)$$

$$D_{C\lambda\lambda}=N\left[\rho_0-\frac{m}{m^*}h(s,q)\right]\Big/\det D_C^{-1}\ , \tag{4.6c}$$

while

$$\det D_C^{-1}(q,\Omega)=N^2A\rho_0[h(s,q)+B\rho_0]\ . \tag{4.7}$$

Note, however, that for small q and $\omega<\varepsilon_f$, $h(s,q)\sim q^2$; $\det D^{-1}(q,\Omega)$ therefore never vanishes in the "Fermi-liquid" region $\Omega,q\to 0$. We conclude that Coulomb effects destroy the "soft mode" in the boson propagator. This is physically reasonable, as the auxiliary boson represents a density fluctuation and it is clear that Coulomb effects will convert the soft zero-sound density fluctuation mode of a neutral Fermi liquid into the plasmon mode of a Coulomb gas.[18] This paper is concerned with low-frequency properties; in another paper[10] plasmon effects in this model are discussed.

It is worth contrasting this situation with the more familiar electron-phonon problem. In this latter case the soft mode in the "boson" (i.e., phonon) propagator is not destroyed by Coulomb interactions. The physical reason is that there are two kinds of charge in the system (electrons and ions); a long-wavelength phonon then represents a mode of the system in which the electrons and ions oscillate with respect to each other in such a way that the total charge density at any point is constant. There is also a symmetry (translation of the electrically neutral electron plus ion system) which guarantees that this mode is soft as $q\to 0$. In the electron–auxiliary-boson problem the auxiliary bosons do not represent a physical excitation of the system; a relative oscillation of the two sorts of charges (c and f) in the system costs a finite hybridization energy ($\sim\sigma_0$) even as $q\to 0$, and the long range of the Coulomb interaction means that one cannot apply the translational invariance argument to a motion of the electron gas alone.

We now consider the $T^3\ln T$ term in the specific heat. Substituting (4.7) into (2.18) and differentiating once with respect to temperature, one finds for the entropy, $S=S_0+S_B$. Here $S_0=-dF_0/dT$ [F_0 was defined after Eq. (2.17)] and the boson contribution S_B is given by

$$S_B=\int\frac{d\Omega}{2\pi}\frac{d^3q}{(2\pi)^2}\frac{dn(\Omega)}{dT}\tan^{-1}\left[\frac{\operatorname{Im}h(s,q)}{\operatorname{Re}h(s,q)+B\rho_0}\right]\ . \tag{4.8}$$

However, from (4.2),

$$h(s,q)=\frac{\varepsilon q^2}{4\pi e^2}\left[1+\frac{q^2\varepsilon}{4\pi e^2}(\rho\chi_0)^{-1}\right]^{-1} \tag{4.9}$$

and so to obtain a logarithmic divergence from the q integral one must expand χ_0 at least to order s^7 [note that the $B\rho_0$ term dominates the denominator in (4.5) for small q]. This leads to a term proportional to $T^7\ln T$, a contribution to S which is negligible compared to the $O(T^3)$ terms which have not been computed. Therefore, when the long-range part of the Coulomb interactions is correctly included, the electron–auxiliary-boson interaction does not give a $T^3\ln T$ contribution to the entropy to leading nontrivial order in $1/N$. However, the term F_0, which represents the entropy of a system of electrons moving in the renormalized band structure described by Eq. (2.1a) and interacting via the Coulomb interaction, does give rise to a $T^3\ln T$ contribution to S. To compute F_0 to leading nontrivial order in $1/N$ one uses the same coupling-constant integration technique which led to Eq. (2.18). One then finds that

$$F_0=F_T+F_C\ , \tag{4.10a}$$

where F_T is the "trivial" free energy of noninteracting fermions moving in the renormalized band structure and

$$F_C=-\int\frac{d\Omega}{2\pi}\frac{d^3q}{(2\pi)^2}n(\Omega)\operatorname{Im}\ln A^{-1}(q,\Omega+iS)\ . \tag{4.10b}$$

Here A is the Coulomb interaction dressed with interband and intraband bubbles. By the same Dyson-equation arguments that led to Eq. (4.2) one finds

$$A^{-1}(q,\Omega+iS)=\rho\chi_0+O(q^2)\ . \tag{4.11}$$

The manipulations that led to Eq. (3.9) then yield for the specific heat an expression identical to (3.9) with A_0^S set equal to unity, i.e.,

$$\Delta C=\frac{3\pi^2}{15}\frac{1}{(v^*)^3}\left[1-\frac{\pi^2}{12}\right]T^3\ln T\ . \tag{4.12}$$

This expression can be simply understood in terms of Fermi-liquid theory if all Landau parameters except A_0^S are negligible. The $T^3\ln T$ term comes from repeated scattering of a quasiparticle quasihole pair in the limit that the energy transfer Ω is less than the "momentum" transfer v^*q, but both are small. In this limit, the interaction between quasiparticles is the statically screened Coulomb interaction, which must, in our model, lead to a Landau parameter $A_0^S=1$. (The fact that the other Landau parameters are negligible is an artifact of the $1/N$ method.) The relation $A_0^S=1$ (which implies $F_0^S=\infty$) is the signature of an incompressible Fermi liquid, since the compressibility $dn/d\mu=\rho/(1+F_0^S)$. Our model involves an electron gas in a uniform positive background, but we consider only fluctuations of the electrons; these leave the positive background unchanged. The long-ranged Couloub interactions then guarantee that the system is incompressible. We note that in the model without long-ranged Coulomb interactions, $F_0^S\sim m^*/m\gg 1$ because the "infinite U" constraint on f occupancy ensures that f-density fluctuations do not contribute to the thermodynamics, so the compressibility is essentially that of the light "c" electrons, and does not involve the mass enhancement factor m^*/m. For this reason the numerical value of the coefficient of the $T^3\ln T$ term in (4.12) is close to that of the $T^3\ln T$ term in (3.12), but the interactions which produce the $T^3\ln T$ term in the two models are very different.

V. SUMMARY AND CONCLUSIONS

In this section we recapitulate the results of the previous sections, outline their implications for the physical interpretation of the auxiliary-boson model, and discuss their experimental relevance for heavy fermions in general and UPt_3 in particular. The expression for the coefficient of the $T^3\ln T$ term in UPt_3 is computed and found to be incorrect by a factor of $\gtrsim 10^2$. It is argued that the discrepancy with experiment for UPt_3 occurs because the auxiliary-boson $1/N$ method omits an important aspect of the physics of heavy fermions, namely, interactions in the spin channel due to exchange of antiferromagnetic spin fluctuations, although another possible explanation, a large (more than factor of 10) variation of the Fermi velocity over the Fermi surface cannot be ruled out until more complete de Haas–van Alphen data are available.

The auxiliary-boson large degeneracy (N) lattice Anderson model and the same model extended to include the long-range part of the Coulomb interaction have been studied to leading nontrivial order in $1/N$, in the long-wavelength, low-frequency, low-temperature limit. The model without Coulomb interactions possesses an undamped collective mode (the zero-sound mode) which appears as a singularity in both the density-density correlation function and the auxiliary-boson propagator. The model also possesses a $T^3\ln T$ term in the specific heat due to electron–auxiliary-boson interactions. This term has been calculated by differentiating an expression for the free energy. The calculation is similar to the paramagnon-model calculation of δ, the coefficient of the $T^3\ln T$ term in the specific heat of ^3He.[16] As a by product, the calculation of δ in exchange models (such as paramagnon and auxiliary boson) has been simplified. A set of contributions to δ previously believed to be important has been shown on general grounds to sum to zero.

The expression for the $T^3\ln T$ term found in this work agrees with the general Fermi-liquid expression of Pethick and Carneiro[17] if one uses in their expression the Landau parameters appropriate to our model [$A_0^S=(1+\rho_0/\rho)^{-1}$, all other $A\sim 1/N$]. The value of A_0^S is read off from the density-density correlation function, which is explicitly evaluated in a separate paper[10] and shown to have the form required by Landau Fermi-liquid theory with a value of F_0^S corresponding to the quoted value of A_0^S.

When the physically necessary long-ranged Coulomb interactions are included, the zero-sound mode, the singularity in the boson propagator and the contribution from electron-boson interactions to the $T^3\ln T$ term in the specific heat all disappear. The $T^3\ln T$ term in this case is shown to come entirely from the screened Coulomb interaction.

These results show that the auxiliary boson is—to leading order in $1/N$—an electron-density fluctuation and in contrast to a phonon not a distinct physical excitation of the system. The boson-mediated interactions between quasiparticles are to leading order in $1/N$ entirely due to exchange of virtual density fluctuations.

The fact that the auxiliary boson is a density fluctuation may be easily understood. The bosons were introduced to enforce a constraint on f occupancy; the boson field b represents a hole on an f site. The leading effect of the electron-boson interactions is to cancel out of the mean-field theory those contributions which involve intermediate states which violate the constraint on f occupancy. Thus in the mean-field theory the static compressibility $dn/d\mu$ is enhanced by a factor of m^*/m over a typical light-electron compressibility, but after electron-boson interactions are included, the compressibility is found to have the light-electron value. Thus the fact that the boson is a density fluctuation is related to the fact that in the Anderson model the charge fluctuations are suppressed by the f-occupancy constraint. The effect of electron-boson interactions upon spin fluctuations is much weaker; for example, the deviation of the Wilson ratio R ($R=\chi/\gamma$, where χ is the static magnetic susceptibility and γ the specific-heat coefficient) from unity measures the degree to which ferromagnetic spin fluctuations are enhanced. In the auxiliary-boson $1/N$ method, $R-1\sim 1/N$.

We note also that the large effective mass m^* comes from the spin entropy of the electrons on the f sites, as first pointed out by Varma.[19] The auxiliary-boson method includes spin fluctuation effects in this sense, as it produces a large m^*. Also, if the theory could be solved to all orders in $1/N$, it would presumably include all spin-fluctuation effects. What is shown in this work is that to leading order in $1/N$, the heavy quasiparticles interact via exchange of density fluctuations only, and not via exchange of spin fluctuations.

Because N is not believed to be large in real heavy-fermion materials, and because interactions via exchange of spin fluctuations are not included, and because an oversimplified c-electron band structure and c-f hybridization are used to simplify computations, the auxiliary-boson method can give results which are at best only qualitatively applicable to experiments. Nevertheless, it is of interest to compare the results obtained so far with experimental data on real heavy-fermion materials. Because all real heavy-fermion materials involve electrons, the long-range Coulomb effects must be included. We thus consider applying Eq. (4.12) to experimental data.

We note first that real materials have always some impurities, and that in the presence of impurities the quasiparticles acquire a lifetime τ related to the mean free path l by $l/v_F=\tau$. For temperatures $T<1/\tau$, the $T^3\ln T$ temperature dependence goes over to a $T^{3/2}$ dependence, with coefficient determined by the diffusion constant D.[20] Furthermore, to observe a $T^3\ln T$ term, the temperature must be low enough (relative to the Fermi temperature T_F of the heavy fermions) that inelastic scattering (from e.g., electron-electron interactions) can be neglected. Thus one must have

$$1/\tau < T \ll T_F$$

for the $T^3\ln T$ term to be observable. Many heavy-fermion systems have rather low characteristic temperatures T_F and, even at low temperatures, rather large resistivities, which indicates that either inelastic or impurity effects are important. If inelastic effects are important, the specific heat should not have a simple temperature dependence. There is no rigorous theory for auxiliary bosons in a disordered lattice but it would be interesting to look for a $T^{3/2}$ dependence in the specific heat of heavy-fermion materials in the limit $T<1/\tau$.

For the heavy-fermion material UPt_3, however, cyclotron resonance experiments[21] have determined the quasiparticle velocity v^* and have shown that (at least for the sample studied) the scattering rate, in temperature units, is much less than the superconducting transition temperature T_c. The Fermi surface was observed to be a complicated multisheeted structure, but defining a Fermi temperature by $k_F^2/2m^*$ for a typical sheet gives tempertures of order 50 K, much greater than the superconducting T_c. There should therefore be an appreciable range of temperature $T_c<T\ll T_F$ over which a $T^3\ln T$ term is observable in UPt_3.

Of course, since UPt_3 has a complicated Fermi surface, the relevance of the calculations in the previous sections is unclear (even assuming the auxiliary-boson $1/N$ method adequately represents the physics of heavy fermions), since in the previous sections a simple spherical Fermi surface was implicitly assumed. However, one may argue that as the $T^3\ln T$ term comes from repeated small-angle scattering of a quasiparticle quasihole pair of nearly parallel momenta, scattering from one sheet of the Fermi surface to another (a large momentum-transfer process) will be unimportant. In this case the polarization bubbles which "dress" the Coulomb interaction may be written as a sum, over sheets, of a contribution from each sheet. If one further assumes that over each sheet the velocity v^* and density of states is essentially constant, then for a given sheet the polarization contribution may be written as the product of the area of the sheet and the function χ_0 evaluated using the velocity v^* on the sheet. Experimentally,[21] the velocity v^* (defined as k_0/m^*, where k_0 is a typical k value for the sheet) ranges from $4-5\times10^5$ cm/sec sheet to sheet. (The values of k_0 and m^* are taken from Table I of Ref. 21.) Assuming v^* is the same for every sheet, one finds that up to a constant factor the polarization bubble is proportional to χ_0. The factor of proportionality does not enter into the $T^3\ln T$ term, and Eq. (4.12) may therefore be used. Now in the large-N model, the specific-heat coefficient γ is given[3] (to leading order in $1/N$) by

$$\gamma=\frac{N}{24\pi}\sum_S A_S/v_S^* \ . \tag{5.1}$$

Here N is the spin degeneracy, the 24π comes from a combination of thermal and phase space factors, S indexes the sheets, A_S is the area, and v_S^* the velocity of sheet S.

Then, assuming v_S^* is constant from sheet to sheet, one has for the ratio of linear specific-heat coefficient (γ) to $T^3\ln T$ coefficient (δ),

$$\gamma/\delta=\frac{N}{24\pi^3(1-\pi^2/12)}\left[\frac{\hbar}{k_B}\right]^2(v^*)^2\sum_S A_S \tag{5.2}$$

(we have restored the previously suppressed factors of $\hbar$ and k_B). We may now use the experimentally measured[21] values of $v^*\cong4\times10^5$ cm/sec and $N\sum_S A_S$ (from γ and v^*) to compute

$$\gamma/\delta\sim6\times10^4\ \mathrm{K}^{+2}\ . \tag{5.3}$$

The experimental value[22] is closer to $10^2\ \mathrm{K}^{+2}$.

There are several possible explanations for the factor of 600 discrepancy. One is that the simple model used here is simply inapplicable to a multiply sheeted Fermi surface. Another possibility is that the velocity is more than 10 times smaller than the observed value in some regions of the Fermi surface not observed in the de Haas–van Alphen experiments[21] (and also more than ten times larger in other regions, so the agreement with the specific-heat data is not destroyed). We note that published data for UPt_3 gives velocities only in certain symmetry directions, so different velocities in other directions are not ruled out. An experiment for $CeCu_6$ yields velocities varying by a factor of ~3 over the Fermi surface.[23]

An alternative explanation is that the auxiliary-boson $1/N$ method omits some important interaction which leads to a large value of some Landau A parameter. One Fermi-liquid analysis[24] has indicated a value of $A_0^a\sim-4$ (in contrast to the value $1/N$ given by the auxiliary-boson method): such a value of A_0^a indicates that *ferromagnetic* spin fluctuations are important. Because the coefficient of the $T^3\ln T$ term $\sim(A_0^S)^3$ (if $A_0^S\gg1$) this could help to resolve the discrepancy. However, such a large value of A_0^S is inconsistent with the observed[25] Wilson ration $R=1-A_0^S\sim1$. Various neutron scattering experiments have concluded that *antiferromagnetic* spin fluctuations are important in UPt_3.[26] A recent Fermi-liquid analysis[27] indicates that strong antiferromagnetic fluctuations lead via crossing symmetry to large values of an $l=2$ Landau parameter; this accounts for the coefficient of the $T^3\ln T$ term. Note that the $l=2$ Landau parameters are predicted to be of order q_0/N in the simple auxiliary-boson models so far considered.[4] The Fermi-liquid analysis is however open to criticism because it assumes a simple spherical Fermi surface and treats only Landau parameters with $l\le2$.

The reason for the discrepancy between the calculated and observed $T^3\ln T$ coefficient deserves further study. More complete de Haas–van Alphen data could decide whether variation in the Fermi velocity is a viable explanation. It seems more likely (although it is not proven) that the leading order (in $1/N$) approximation to the auxiliary-boson version of the Anderson model, although it has been very useful in providing qualitative understanding of some aspects of heavy-fermion physics, omits an interaction (most likely involving exchange of antiferromagnetic spin fluctuations) which is important for the thermodynamics of UPt_3.

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APPENDIX A

In this Appendix we show that the coefficient of the $T^3\ln T$ term in the specific heat may be expressed in terms of the $T=0$ values of ε_f and σ_0, whereas the T^3 term cannot be.

On general grounds one may write the free energy F as

$$F=\alpha+\beta T^2+\delta T^4\ln T+\varepsilon T^4+\cdots \ . \tag{A1}$$

The coefficients $\alpha,\beta,\ldots$ depend on ε_f,σ_0 and the other parameters of the problem. They depend on T implicitly via the dependence of ε_f,σ_0 on T. We now show that the T dependence of ε_f does not contribute to the $T^3\ln T$ term in S. The argument for the T dependence of σ_0 is identical.

At any temperature T, ε_f is fixed by the equation

$$\partial F/\partial\varepsilon_f=0 \ . \tag{A2}$$

By combining (A1) and (A2) and expanding in powers of T we obtain

$$\varepsilon_f=\lambda_0+\lambda_1 T^2+\lambda_2 T^4\ln T+\cdots \ . \tag{A3}$$

Here the λ's are determined by derivatives of $\alpha,\beta,\ldots$ with respect to ε_f and σ_0, and are independent of T.

The specific heat C is given as usual by

$$C=T\frac{d^2}{dT^2}F \ . \tag{A4}$$

The derivatives in (A4) are total derivatives. Using (A2) and the chain rule one finds:

$$C=T\left[\frac{\partial^2 F}{\partial T^2}+\frac{\partial^2 F}{\partial\varepsilon_f^2}\left[\frac{\partial\varepsilon_f}{\partial T}\right]^2+\cdots\right] . \tag{A5}$$

Here the ellipsis denotes terms involving derivatives with respect to σ_0, which we have not written explicitly. By combining (A2), (A3), and (A5) we find

$$C=2\beta T+12\delta T^3\ln T+O(T^3) \ . \tag{A6}$$

From (A3) we see that

$$\beta(T)=\beta(T=0)+\lambda_1\frac{\partial\beta}{\partial\varepsilon_f}T^2+\cdots$$

so that

$$C=2\beta(T=0)+12\delta(T=0)T^3\ln T+O(T^3) \ . \tag{A7}$$

This is what was to be proved.

APPENDIX B

In this Appendix we give some details of the computation of the self-energies of the boson propagators, in the small q and Ω limit. More details can be found in Ref. 10. There are four self-energies: $\Sigma_{\sigma\sigma}$, $\Sigma_{\sigma\lambda}=\Sigma_{\lambda\sigma}$, and $\Sigma_{\lambda\lambda}$. We give details of the calculation of $\Sigma_{\sigma\sigma}$; the others may be computed similarly.

By use of Eqs. (2.2) we may write the interband and intraband contributions to $\Sigma_{\sigma\sigma}$ as

$$\Sigma_{\sigma\sigma}^{\rm intra}(q,i\Omega_n)=-\tfrac{1}{4}\sum_{k,\omega_n}\frac{M^{11}_{p,p+q}}{[i\omega_n-\varepsilon_1(0)][i(\omega_n+\Omega_n)-\varepsilon_1(p+q)]} , \tag{B1a}$$

$$\Sigma_{\sigma\sigma}^{\rm inter}(q,i\Omega_n)=-\tfrac{1}{4}\sum_{p,\omega_n}M^{12}_{p,p+q}\left[\frac{1}{[i\omega_n-\varepsilon_1(p)][i(\omega_n+\Omega_n)-\varepsilon_2(p+q)]}+\frac{1}{[i\omega_n-\varepsilon_2(p)][i(\omega_n+\Omega_n)-\varepsilon_1(p+q)]}\right] . \tag{B1b}$$

Here we use the Matsurbara formalism. ω_n and Ω_n are Fermi and Bose frequencies respectively. The $-\frac{1}{4}$ is a symmetry factor. $\varepsilon_{1,2}(p)$ were defined in Eqs. (2.4). The matrix elements are given by

$$M^{11}_{p,p+q}=u^2_{p+q}v^2_p+v^2_{p+q}u^2_p+2\sigma_0^2/E_pE_{p+q} \ , \tag{B2a}$$

$$M^{12}_{p,p+q}=u^2_{p+q}u^2_p+v^2_{p+q}v^2_p-2\sigma_0^2/E_pE_{p+q} \ . \tag{B2b}$$

The various quantities in Eqs. (B2) were defined in Eqs. (2.5). Performing the Matsubara sum in the usual way, analytically continuing $\Omega_n\to\Omega+i\delta$, taking the small (q,Ω) limit, using Eq. (2.5c) and defining

$$\rho\chi_0(q,\Omega+i\delta)=\sum_p\frac{f(\varepsilon_1(p))-f(\varepsilon_1(p+q))}{\Omega-v^*\hat{p}\cdot q+i\delta} \ , \tag{B3}$$

yields $[v^*=\partial\varepsilon_1(p)/\partial p\,|_{p=p_F}]$,

$$\Sigma_{\sigma\sigma}(q,\Omega+i\delta)=-2\frac{\sigma_0^2}{E_{kF}^2}\chi_0(q,\Omega+i\delta)-\tfrac{1}{2}\sum_{p<p_F}\frac{1}{E_p}+2\sum_{p<p_F}\frac{\sigma_0^2}{E_p^3} \ . \tag{B4}$$

The second term in Eq. (B4) is, by the mean-field equations, equal to $-(\varepsilon_f-E_0)$.[3] In the limit $m^*/m\gg 1$, by use of Eq. (2.4c) one sees that the integral in the last term is sharply peaked about $k=k_h$ (where k_h is the point where the original conduction-band energy equals the chemical potential, i.e., $\varepsilon_{k_h}=0$), because $\sigma_0\ll\varepsilon_{k_F}$. Thus up to corrections of order $(\sigma_0/\varepsilon_{k_F})^2\sim m/m^*$, the third term is $2\rho_0$, where

$\rho_0 = dk/d\varepsilon_k|_{k=k_h}$, and so using $\sigma_0^2/E_{k_F}^2 = m/m^* + O((m/m^*)^2)$,

$$\Sigma_{\sigma\sigma}(q,\Omega+i\delta) = -\tfrac{1}{2}(\varepsilon_f - E_0) - \left[\frac{m}{m^*}\right]\chi_0(q,\Omega+i\delta) + \rho_0 \; . \tag{B5}$$

APPENDIX C

In this Appendix we evaluate the temperature dependence of the polarization bubble $\chi_0(q,\Omega)$. We show that the temperature dependence of χ_0 does not contribute to the $T^3\ln T$ term in the entropy.

The derivative of χ_0 with respect to temperature, for small q and for $T \ll T_K$ may be written as

$$\frac{d\chi_0(q,\Omega)}{dT} = -\frac{N}{v^* q}\int \frac{d\varepsilon_1 d\mu}{4\pi^2}\rho \frac{df(\varepsilon_1)/dT - df(\varepsilon_1 + v^* q\mu)/dT}{\mu - (\Omega/v^* q) - i\delta} \; . \tag{C1}$$

Here μ is the angle between p and q and ρ is the density of states at the Fermi surface. By changing variables from ε_1 to $\varepsilon_1 + v^* q\mu$ in the second term one shows that this expression vanishes (since one may extend the range of the ε_1 integration to $\pm\infty$ with errors exponentially small in T/T_k). The leading term in an expansion of χ_0 with respect to q is thus independent of temperature up to terms exponentially small in T/T_k (we ignore the temperature dependence of the mean field parameters), regardless of the value of the ratio $\Omega/v^* q$, and thus cannot contribute to the temperature dependence of the free energy in Eq. (3.8).

One may extend the calculation to higher order in q by expanding $\varepsilon_1(p+q)$ further. (Note that the terms generated in this expansion involve second or higher derivatives of the energy with respect to momentum, so they cannot be expressed in terms of Fermi-liquid quantities such as m^*, v^*, and the Landau parameters.) As long as it is permissible to approximate the density of states, velocity, etc. by their values at the Fermi surface, one may still make a change of variables, showing that (C1) still vanishes (up to exponentially small terms in T/T_k).

One must therefore extend the calculation yet further by considering the variation of ρ and v^* away from the Fermi surface writing, e.g., $\rho \to \rho + \varepsilon(d\rho/d\varepsilon)$. This would lead to a contribution to $d\chi_0/dT$ proportional to $(T/T_K)g(\Omega/v^* q)$ [the factor of T comes from integrating $\int d\varepsilon\, \varepsilon df(\varepsilon)/dT$, $g(x)$ is some function of x analytic near $x=0$, and one expects $d\rho/d\varepsilon \sim \rho/T_K$]. To obtain a logarithm from the sum over q in (3.8) one must expand g to order $(\Omega/v^* q)^3$; the three factors of Ω and the factor T/T_K then ensure that the contribution to the entropy is at least of order $T^4\ln T$.

Clearly, higher-order terms in the expansion away from the Fermi surface will give even higher-order contributions. Thus, the temperature dependence of χ_0 need not be considered in the evaluation of the $T^3\ln T$ term in the entropy from Eq. (3.8).

In the paramagnon literature[15,16] the temperature dependence of the polarization bubbles occurring in an expression analogous to Eq. (3.8) is evaluated by writing χ_0 explicitly, differentiating the Fermi functions explicitly with respect to temperature, and then using an identity to rewrite these terms as a "Fermi" contribution proportional to the temperature derivative of the Fermi function and a "Bose" contribution proportional to the temperature derivative of the Bose function. For the model considered in Sec. III of this paper, one finds (similar equations hold in the paramagnon case)

$$\Delta S_{\text{Bose}} = \int \frac{d\Omega}{2\pi}\frac{d^3q}{(2\pi)^3}\frac{d^3p}{(2\pi)^3}\frac{dn(\Omega)}{dT}[\mathrm{Re}1/(\rho\chi_0+\rho_0)]\pi\delta(\Omega+\varepsilon_1(p)-\varepsilon_1(p+q))[f(\varepsilon_1(p+q))-f(\varepsilon_1(p))] \; , \tag{C2a}$$

$$\Delta S_{\text{Fermi}} = \int \frac{d^3}{(2\pi)^3}\frac{df(\varepsilon_1(p))}{dT}\Sigma(\varepsilon_1(p)) \; , \tag{C2b}$$

$$\Sigma(\varepsilon_1(p)) = \int \frac{d\Omega}{2\pi}\frac{d^3q}{(2\pi)^3}\left[[1-2f(\varepsilon_1(p)+\Omega)]\mathrm{Re}[\rho\chi_0+\rho_0]^{-1}\pi\delta(\Omega+\varepsilon_1(p)-\varepsilon_1(p+q)) + n(\Omega)\mathrm{Im}[\rho\chi_0+\rho_0]^{-1}\frac{2[\varepsilon_1(p+q)-\varepsilon_1(p)]}{\Omega^2-[\varepsilon_1(p+q)-\varepsilon(p)]^2}\right] . \tag{C2c}$$

In the paramagnon literature the contribution ΔS_{Bose} in Eq. (C2a) is combined with the "Bose" term arising from differentiation of the explicit $n(\Omega)$ factor in Eq. (3.8) before being evaluated. However, the $T^3\ln T$ contributions to S arising from Eqs. (C2a) and (C2b) may be explicitly calculated in the usual way. They precisely cancel, in this model and in the paramagnon model.

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