One-Component Fermi-Liquid Theory and the Properties of UPt_3

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A simple one-component version of Fermi-liquid theory is applied to measurements of the specific heat of UPt_3 and shown to suggest that UPt_3 is an odd-parity superconductor of purely electronic origin. The calculated transition temperature as a function of pressure is found to be in quantitative agreement with experiment.

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Stewart, Fisk, Willis, and Smith[1] have shown that the specific heat of UPt_3 at zero pressure can be fitted by an expression of the form

$$C=\gamma T+\delta T^3\ln T+\beta T^3 \tag{1}$$

over a temperature range $0.5\ \mathrm{K}<T<18\ \mathrm{K}$, while Brodale *et al.*[2] show that the specific heat under pressure takes a similar form. Since the existence of $T^3\ln T$ contributions to the specific heat is an unavoidable consequence of Fermi-liquid theory,[3] and hence is to be regarded as a general property of normal Fermi liquids, it is tempting to analyze the experimental information on UPt_3 in terms of Fermi-liquid theory. Although UPt_3 (and other heavy-fermion systems) exhibits significant anisotropy, here we shall consider only quantities averaged over directions, and explore the consequences of assuming that these may be described in terms of the properties of a spin-$\frac{1}{2}$ Fermi liquid with a spherical Fermi surface. We shall not, however, assume that the liquid is Galilean invariant, and therefore contributions from band structure to the effective mass can be allowed for.

The $T^3\ln T$ contributions to the specific heat are particularly large if one of the Landau parameters is close to the value at which the Fermi liquid would become unstable with respect to distortions of the Fermi surface.[4] In this Letter we pursue the consequences of the assumption that it is an $l=0$ channel which is responsible for the large value of δ. We show below that, for a given choice of the Fermi-surface radius k_F, it enables us to obtain the Fermi-liquid parameter F_0^a as a function of pressure. We combine this parameter with sum-rule arguments and an elementary expression for the superconducting transition temperature[5] to show that simple Fermi-liquid theory leads to the conclusion that UPt_3 is an odd-parity superconductor of purely electronic origin. We calculate the transition temperature of UPt_3 as a function of pressure and find that for a limited range of values of k_F one can obtain quantitative agreement with the experimentally measured results.[6] We consider as well the relationship between thermal expansion[7] and the specific-heat measurements of Brodale *et al.*[2] and compare our approach with previous applications of Fermi-liquid theory to heavy-fermion systems.[8,9]

Pethick and Carneiro[3] use the concept of statistical quasiparticles and show that Fermi-liquid theory enables one to obtain the relationship

$$\delta=-(3\pi^2/10)\gamma(B^s/T_F^2), \tag{2}$$

where $\gamma=(\pi^2/3)k_B^2N(0)$ is the usual linear coefficient in the specific heat. $N(0)=m^*k_F/\pi^2$ is the interacting density of states per unit energy, m^* is the effective mass of particles at the equivalent spherical Fermi surface of radius k_F, and $T_F=k_F^2/2m^*$. If Landau parameters with $l>1$ are neglected, B^s may be expressed in terms of the Landau scattering amplitudes as

$$B^s=-\tfrac{1}{2}\sum_{\lambda=s,a}\omega_\lambda[(A_0^\lambda)^2(1+A_1^\lambda-\tfrac{1}{12}\pi^2A_0^\lambda)+(A_1^\lambda)^2(1-\tfrac{1}{48}\pi^2A_1^\lambda)-2A_0^\lambda A_1^\lambda], \tag{3}$$

where s and a refer to symmetric and antisymmetric terms, $\omega_s=1$, $\omega_a=3$, and the Landau scattering amplitudes are $A_l^\lambda=F_l^\lambda[1+F_l^\lambda/(2l+1)]^{-1}$.

If one considers for the moment only the $l=0$ contributions to B^s, one has

$$B^s=\tfrac{1}{8}\pi^2(A_0^a)^3-\tfrac{3}{2}(A_0^a)^2+\tfrac{1}{24}\pi^2(A_0^s)^3-\tfrac{1}{2}(A_0^s)^2. \tag{4}$$

TABLE I. Fermi-liquid parameters relevant to the $T^3 \ln T$ terms in the specific heat of UPt_3. The corresponding parameters for UAl_2 are given for the purpose of comparison.

System	Pressure (kbar)	γ (mJ/mole-K^2)	δ (mJ/mole-K^4)	k_F (Å^{-1})	m^*	T_F (K)	F_0^s	A_0^s	T_c^{theory} (K)	$T_c^{\text{expt.}}$ (K)
UPt_3	0	429	1.90	1.08	178	289	−0.811	−4.29	0.48	0.48
	3.8	378	0.97	1.08	157	328	−0.794	−3.85	0.41	0.43
	8.9	332	0.46	1.08	138	375	−0.773	−3.41	0.32	0.36
UAl_2	0	142	1.4	1.15	55	1054	−0.93	−13.8		

For electron systems,[10] $A_0^s = 1$; hence an appreciable $T^3 \ln T$ term in the specific heat requires a large negative value of A_0^a. From the experimental results of Brodale *et al.* for γ and δ as functions of pressure, one obtains the corresponding values of B^s/T_F^2. To go further, a value of k_F is needed. If we adopt the value $k_F = 1.08$ Å at zero pressure which was obtained by Chen *et al.*[11] by assuming that each uranium atom contributes three electrons to the Fermi sphere, we obtain the results given in Table I for A_0^a and F_0^a. (We consider below the sensitivity of our results to the choice of k_F.)

To examine the possible transition to the superconducting state, we use the approximate expression of Patton and Zaringhalam,[5] and the s-p approximation expression of Dy and Pethick.[12] For electron systems, since $A_0^s = 1$, the forward-scattering sum rule in the s-p approximation reads

$$A_1^s + A_1^a = -(1 + A_0^a) \tag{5}$$

on neglect of possible phonon contributions to the scattering amplitudes. For the large negative values of A_0^a obtained here, it is readily seen from Eq. (5) that p-state pairing is preferred.

The transition temperature for our model calculation of triplet pairing is given by

$$T_c = T^* \exp(1/g_1) = \alpha T_F \exp[6/(1 + A_0^a)], \tag{6}$$

where $T^* = \alpha T_F$ is a cutoff (analogous to the Debye cutoff introduced in BCS theory) which reflects the fact that the interactions we consider are highly frequency dependent, and the expression used for the effective interaction is valid only for a restricted range of energies T^* in the immediate vicinity of the Fermi surface. On substituting the values we have obtained for A_0^a and F_0^a into Eq. (6), on choosing the cutoff α ($= 0.0103$) so as to get the correct value of T_c at zero pressure, and on *assuming* that α does not vary with pressure, we obtain the results shown in Table I. Given the approximate nature of our calculations, the agreement with experiment is gratifying. For this choice of k_F, inclusion of the $l = 1$ contributions to B^s changes these results by less than 1%.

That we are able to obtain a negative slope for $\partial T_c/\partial \rho$ (ρ is the system density), despite the substantial positive slope of $\partial T_F/\partial \rho$, is not an accident. To see this, consider the logarithmic derivative of T_c, which takes the form

$$\frac{1}{T_c}\frac{\partial T_c}{\partial \rho} = -\frac{1}{\gamma}\frac{\partial \gamma}{\partial \rho} - \frac{6}{(1 + A_0^a)^2}\frac{\partial A_0^a}{\partial \rho}. \tag{7}$$

Our derived positive slope of A_0^a more than compensates for the negative slope in γ. It should be noted that since A_0^a, the value of A_0^a we extract from experiment, approximately scales with k_F^2, $\partial T_c/\partial \rho$ is sensitive to the choice of k_F. Thus a 20% decrease in k_F increases the magnitude of the second term on the right-hand side of Eq. (7) substantially, with the result that the negative slope of $\partial T_c/\partial \rho$ is markedly increased.

Thermodynamics provides a connection between measurements of thermal expansion and the pressure dependence of the specific heat. The volume coefficient of thermal expansion is $\alpha_v = -(\partial s/\partial P)T$, where s is the entropy per unit volume, from which we find for the average linear coefficient of thermal expansion

$$\alpha \equiv \alpha_v/3 = \gamma_\alpha T + \delta_\alpha T^3 \ln T + O(T^3), \tag{8}$$

where $\gamma_\alpha = -\frac{1}{3}\partial\gamma/\partial P$ and $\delta\alpha = \frac{1}{9}\partial\delta/\partial P$.

As may be seen in Fig. 1, the experimental results of de Visser, Franse, and Menovsky[7] for the thermal expansion of UPt_3 may be fitted by an expression of the form of Eq. (8). Our fit to the *thermal expansion* yields the values $\gamma_\alpha = 1.12 \times 10^{-6}$ K^{-2} and $\delta_\alpha = 0.765 \times 10^{-8}$ K^{-4}; these coefficients are in excellent agreement with the values we calculate from a quadratic fit to the *specific-heat* experimental results of Brodale *et al.*,[2] $\gamma_\alpha = 1.05 \times 10^{-6}$ K^{-2} and $\delta_\alpha = 0.8 \times 10^{-8}$ K^{-4}. The internal consistency of the two experiments is thereby demonstrated.

We call the attention of the reader to the ways in which our approach differs from those of previous attempts to apply Fermi-liquid theory or paramagnon theory to UPt_3. Comparatively large negative values of F_0^a have been calculated previously by Bedell and Quader,[8] using an induced-interaction approach, and by Valls and Tesanović,[9] using a Gutzwiller approach;

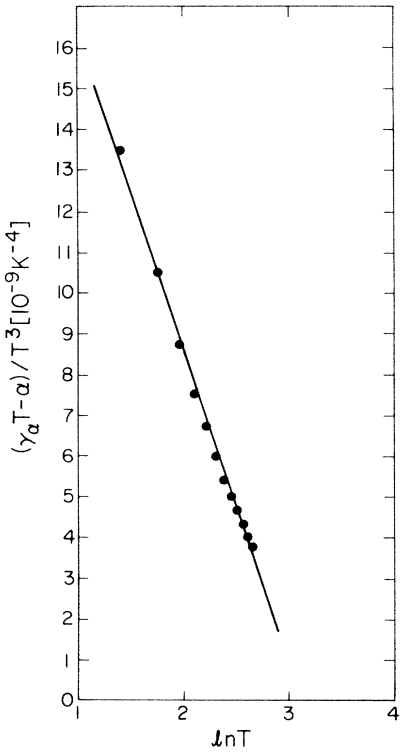

FIG. 1. Plot to exhibit $T^3\ln T$ terms in the thermal-expansion coefficient.

here we derive F_0^a directly from experiment. We make no assumptions concerning the origin of the quasiparticle effective mass, and use the electron liquid result, $A_0^s = 1$, rather than appealing to a Gutzwiller or ^{3}He analogy. The experimentally observed decreases of F_0^a, m^*, and T_c with pressure are in contradiction with a straightforward application of the Gutzwiller approach for liquid ^{3}He to heavy fermions.[9] As to the application of paramagnon theory to heavy fermions, we note that paramagnon calculations are model dependent (since one must make an assumption about the physical origin of the effective mass) and, as Pethick and Carneiro long ago pointed out,[3] can easily lead to an overestimate of the spin-fluctuation contribution to the $T^3\ln T$ term by a factor as large as 3.

The alert reader may wonder what our theory would lead us to conclude concerning UAl_2, which also exhibits a pronounced $T^3\ln T$ term in the specific heat. We find that the corresponding value of F_0^a is -0.93, so that in this metal one is very close to a ferromagnetic instability—so close indeed that any application of Fermi-liquid theory to calculations of transport properties or the superconducting transition temperature must necessarily involve quasiparticle interactions in many different l channels. (Note that experiment implies a value of $A_0^a = -13.8$, so that the forward-scattering sum rule tells one of the importance of a number of different channels.)

The simple one-component Fermi-liquid theory we have described above has also been used to calculate the quasiparticle contribution to the spin-fluctuation spectrum and the normal-state transport properties of UPt_3 in the very low-temperature limit. However, since in heavy-fermion systems the magnetic moment is not a conserved quantity, both the spin-fluctuation spectrum and the magnetic susceptibility will contain contributions which cannot be expressed solely in terms of heavy-electron quasiparticles, and which may be thought of as associated with polarization of the compensated local moments on lattice sites.

In neutron-scattering experiments, which measure the spin-fluctuation excitation spectrum, one would therefore expect to see long-wavelength excitations of two sorts, those associated with itinerant heavy electron-hole pairs, whose frequency vanishes in the long-wavelength limit, and those from the compensated moments of the f electrons at magnetic sites, whose frequency remains finite in the long-wavelength limit.

A calculation of the quasiparticle contribution to the spin-spin correlation function at finite wave vectors and energies, analogous to that of Aldrich, Pethick, and Pines[13] for liquid ^{3}He, yields, with $F_0^a = -0.811$, $k_F = 1.08$ Å^{-1}, a spectrum at $q = 1.0$ Å^{-1} which peaks at ~ 9 meV and thus agrees with the results at this wave vector obtained in spin-polarized neutron-scattering experiments on polycrystalline UPt_3.[14] However, this agreement does not provide a conclusive test of the model, since the scattering from compensated local moments has not been taken into account. Indeed, the recent neutron-scattering experiments of Aeppli, Bucher, and Shirane[15] on single crystals of UPt_3 provide strong evidence for substantial scattering from compensated local moments which exhibit antiferromagnetic correlations.

A further consequence of the lack of magnetization conservation is that no direct information on quasiparticle interactions can be obtained from the ratio of the experimental values of the spin susceptibility and the specific heat (as done in liquid ^{3}He), since neither the effective quasiparticle magnetic moment[16] nor the nonquasiparticle contribution to the spin susceptibility is known. However, given a set of values of F_0^a, such as those deduced here from the specific-heat experiments, one can obtain an upper bound on the heavy-electron magnetic moment from experimental measurements of χ.

Hess[17] has used the scattering amplitudes we have deduced from the specific-heat measurements to estimate the T^2 contributions (produced by electron-electron scattering) to the transport coefficients of UPt_3, and obtains with $k_F = 1.08$ Å semiquantitative agreement with experiment for both the thermal and electrical resistivities.

The above essentially represented our views at the time the manuscript was originally submitted. Very recently, Taillefer *et al.*[18] have carried out de Haas–van Alphen measurements of UPt_3. They find direct evidence for the existence of multiple sheets of the Fermi surface characterized by substantially smaller values of k_F, m^*, and T_F than those considered here, and consequently the agreement with experiment found above may prove to be fortuitous. Clearly it would be worthwhile to extend the Fermi-liquid description to take into account the multisheet character of the Fermi surface.

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