Mass Renormalizations and Superconductivity in Heavy-Fermion UPt_3

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The Eliashberg equations for magnetic fluctuations are solved for the case of UPt_3. As input, the neutron data of Aeppli *et al.* are used for the spectral function, and the results of band-structure calculations are used to model the Fermi surface. The results indicate a mass-renormalization factor of about 16, a value confirmed by comparisons of band calculations to de Haas–van Alphen data. Moreover, a superconducting transition temperature of the order of 0.1–0.2 K is calculated (due to the momentum dependence of the susceptibility) with polar gaps in parts of the zone.

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The possibility of superconductivity in heavy-fermion metals due to a nonphonon mechanism has been recognized for some time.[1] In the case of UPt_3, a normal phonon mechanism was proposed.[2] Further work involving solutions of the Eliashberg equations revealed that for the parameters appropriate to UPt_3, normal superconductivity is not possible.[3,4] The reason for this is that the large mass renormalizations have a frequency range which is much larger than the estimated value of the critical temperature, and thus strongly suppress the superconductivity, leading to a renormalized critical temperature of the order of 10^{-23} K.

There have been several other proposed mechanisms which might be responsible for the observed superconductivity which are reviewed by Lee *et al.*[5] The particular mechanism focused on here came about when neutron data on UPt_3 indicated antiferromagnetic correlations.[6] Two groups showed the possibility of an attractive superconducting pairing interaction coming from these correlations.[7,8] The purpose of this paper is to put these ideas on a quantitative basis.

We start with the Eliashberg equations for spin fluctuations of Berk and Schrieffer.[9] We look at the normal self-energy as given in Eq. (2.14) of Stamp[10]

$$\Sigma(p,z) = -\frac{3}{2} I^2 \sum_q \int_{-B}^{B} d\epsilon\, \delta(\epsilon - \epsilon_{p-q}) \int_0^\infty \frac{d\Omega}{2\pi} \mathrm{Im}\chi(q,\Omega) \left[\frac{f(\epsilon)+n(\Omega)}{z-\epsilon+\Omega} + \frac{1-f(\epsilon)+n(\Omega)}{z-\epsilon-\Omega} \right], \tag{1}$$

where I is the contact interaction, χ the susceptibility, f the Fermi function, n the Bose function, and $2B$ the bandwidth. In most cases, χ is approximated by the Lindhard function and a simple sphere is used for the Fermi surface. This leads to a mass renormalization which scales as $\log(S)$,[11] where S is the Stoner factor, $(1-IN)^{-1}$ (N is the density of states). I will not make that approximation here. Instead, we look at what is needed to solve this equation realistically. First, one needs to calculate the full interacting susceptibility. This is extremely difficult to do, and only recently has been solved with the use of density-functional techniques for Pd and V.[12] Instead, we note that this is known in a crude sense from the neutron data. In fact, Aeppli *et al.*[6] find that their data are reasonably well fitted with the following form for the imaginary part of χ:

$$\mathrm{Im}\chi = -\chi(q)\Gamma\omega/(\Gamma^2+\omega^2), \tag{2}$$

where $\chi(q)$ is the static susceptibility and Γ is the neutron linewidth (about 5 meV in the case of UPt_3). Both I and N can be extracted from band-structure calculations. In fact, it is now clear that angle-dependent de Haas–van Alphen data[13] on UPt_3 predict the same Fermi surface as local-density band-structure calculations[2,14]; thus we know the Fermi surface to input into the equations. I is obtained from S, which is the ratio of the experimental susceptibility to the noninteracting band susceptibility.

We first solve Eq. (1) by ignoring the q dependence of χ and the energy dependence of N. In this case we can analytically integrate. We solve at zero temperature and thus ignore $n(\Omega)$. The frequency integral is of the form given on page 300 in Gradshteyn and Ryzhik.[15] The remaining energy integral is trivial at $T=0$, and we obtain

$$\Sigma = -\tfrac{3}{8} I^2 N \Gamma \chi \tan^{-1}(z/\Gamma). \tag{3}$$

The ratio of the quasiparticle mass to the band mass at the Fermi surface is given by $1 - d\Sigma/dz$ evaluated at $z=0$. This is

$$m^*/m_b = 1 + \tfrac{3}{8} I^2 N \chi = Z. \tag{4}$$

We note that the mass renormalization no longer scales as $\log(S)$, but as S itself. In other words, the specific heat coefficient γ scales with χ, which is experimentally observed.[16] We note that the linewidth, Γ, determines the frequency range over which the mass renormalizations exist. To test Eq. (4) for UPt_3, we note that $\chi(0)$ is about 0.26 state/meV,[16] and N is about 0.0089

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state/meV from the band calculations.[2,14] This implies that I is about 109 meV, which yields a mass renormalization factor of 11.3. The neutron data, though, indicate that χ peaks at $(\pi/c)(0,0,2)$ (twice the zone boundary), at which point it is approximately twice the value at $q=0$.[6] With use of this value, Z is 21.6. I thus expect that the average value of Z is about 16.5, which is what is found when comparing the de Haas–van Alphen results to band-structure calculations.[14]

At this point, it would be wise to test another case to see whether this theory holds. In the case of mixed-valent $CeSn_3$, de Haas–van Alphen data agree with results of band-structure calculations modulo a Z of about 5.[17] Neutron data[18] on $CeSn_3$ indicate a frequency dependence of χ similar to UPt_3 with a linewidth of about 11 meV. In the case of $CeSn_3$, we have $N=0.0053$ state/meV,[17] $\chi=0.062$ state/meV,[19] and thus $I=172$ meV. This yields a Z of 4.7, again consistent with experiment.

Having seen that the observed mass renormalizations are consistent with self-energy corrections due to magnetic fluctuations, we turn to the pairing self-energy.

The pairing equation is given in Ref. 9. With use of a form given by McMillan,[20] it is

$$\Delta_p(z)=-\frac{1}{Z_p(z)}\frac{3}{2}I^2\sum_q\int_{-\omega_c}^{\omega_c}\frac{d\epsilon}{\epsilon}\,\mathrm{Re}[\Delta_{p-q}(\epsilon)]\delta(\epsilon-\epsilon_{p-q})D[\Omega], \tag{5}$$

where Δ is the gap, ω_c a cutoff energy, and D the same frequency integral as in Eq. (1). The frequency integration is performed as in the previous section, and we obtain

$$\Delta_p(z)=-\frac{1}{Z_p(z)}\frac{3}{8}I^2\sum_q\int_{-\omega_c}^{\omega_c}\frac{d\epsilon}{\epsilon}\,\mathrm{Re}[\Delta_{p-q}(\epsilon)]\delta(\epsilon-\epsilon_{p-q})\frac{\Gamma^2\chi(q)}{\Gamma^2+(z-\epsilon)^2}\tanh\left[\frac{\epsilon}{2kT}\right]. \tag{6}$$

To solve the energy integral, I ignore the energy dependence of N (a fairly safe approximation[14]), and assume a step function for the gap, $\Delta(\omega)=\Delta$, $\omega<\omega_c$, and zero otherwise. (The latter approximation will be remedied later.) To integrate over the energy, I set $z=0$ and separate the integral into two parts, an integral from 0 to $6T_c$ (where T_c is the critical temperature), and one from $6T_c$ to ω_c. In the first integral, we can replace the factor $(\Gamma^2+\epsilon^2)$ by Γ^2 and get the standard tanh integral. In the second integral, we can replace tanh by 1, and we are left with a standard integral (see page 69 of Ref. 15). The result is

$$\Delta_p=-\frac{1}{Z_p}\frac{3}{4}I^2\ln\left[\frac{\Gamma}{0.88T_c}\right]\sum_q\Delta_{p-q}\delta(\epsilon-\epsilon_{p-q})\chi(q), \tag{7}$$

which is our transition-temperature equation (note that the cutoff energy drops out approximately). We also see that since Z scales as $I^2N\chi$, the mass renormalization drops out for large Z.

It can easily be seen that if $\chi(q)$ is independent of q, then Eq. (7) leads to a repulsive contribution to superconductivity. It is the q dependence of χ which can lead to an attractive interaction.[7,8] For the case of UPt_3, we know that χ peaks at $(\pi/c)(0,0,2)$, corresponding to antiferromagnetic correlations between the two equivalent U atoms in the unit cell. This implies that the gap is antiferromagnetically ordered, which in real space means that the gap function changes sign from one atom to the next.[21]

To solve this problem, we wish to first know what the gap structure is like at zero temperature. In this case, tanh = 1 and Eq. (6) is easily solved (the integral is from Δ to ω_c this time) and we obtain

$$\Delta_p=-\frac{1}{Z_p}\frac{3}{4}I^2\sum_q\Delta_{p-q}\delta(\epsilon-\epsilon_{p-q})\chi(q)\ln\left[\frac{2\Gamma}{\Delta_{p-q}}\right]. \tag{8}$$

To go further, we have to perform numerical integrals over the Fermi surface. The primary contributions to the density of states in UPt_3 are a distorted ellipsoid centered at Γ and a disk centered at A which is interconnected to other disks by arms.[2,14] [Γ is the zone center; A is the zone boundary, $(\pi/c)(0,0,1)$.] We thus approximate the Fermi surface by an ellipsoid at Γ, and a flattened ellipsoid at A. The advantage here is we only have two Fermi surfaces, and the integrals over the ellipsoids reduce to one-dimensional form (I assume some average band mass, m_b). We solve Eq. (8) for various forms of χ, and various values for a and c (a and c are the ellipsoid radii in the basal and z directions). The adjustment of a and c reflect attempts to take into account (1) possible necking between the piece centered at Γ and a smaller piece centered at K, and (2) the arms attached to the A-centered disk. We solve Eq. (8) by a simple iterative procedure, with a mixing factor of 20% used to stabilize convergence. For a particular set of parameters, I found that Eq. (8) converged to the same solution regardless of the starting values.

To calculate the critical temperature, invert Eq. (7). I now assume that the ratio of the gaps is independent of temperature, and substitute Eq. (8) for Δ and get

$$T_c=(\Gamma/0.88)\exp[-\textstyle\sum_q\Delta_{p-q}\delta(\epsilon-\epsilon_{p-q})\chi(q)\ln(2\Gamma/\Delta_{p-q})/\sum_q\Delta_{p-q}\delta(\epsilon-\epsilon_{p-q})\chi(q)]. \tag{9}$$

I assume that the actual T_c is the maximum value in Eq. (9). The anisotropy in Z is taken into account by performing a similar Fermi-surface integral in Eq. (4).

At this point, we might note that for χ functions which depend on r (the distance in the reciprocal basal plane), there is a ϕ integration which has to be performed (ϕ is the angle in the basal plane). By the assumption of a cylindrical symmetry for χ, there is no ϕ dependence in the gap function; but for the more realistic hexagonal case, such a dependence is possible. The advantage of assuming cylindrical symmetry is that we can integrate χ analytically with respect to ϕ, thus keeping the Fermi-surface integrals in one-dimensional form.

In Table I, the results for various runs are presented. The predicted transition temperatures are of the order of 0.1–0.2 K, not too far from the experimental value of 0.5 K.[16] Moreover, we find a polar gap on the Γ-centered surfaces. The A-centered surfaces have roughly constant gaps. The reason for the peculiar gap structure lies in the functional form of χ, which drives an antiferromagnetic structure in the gap. The gaps change sign when one translates by $(\pi/c)(0,0,2)$. The gaps also change sign when one inverts through the $z=0$ plane, and thus the Γ-centered pieces have lines of nodes, whereas the A-centered pieces do not. In the case where χ is taken to peak at $(\pi/c)(0,0,1)$, the Γ-centered surface has two lines of nodes.

We also see in Table I that the transition temperature is fairly sensitive to the dimensions of the Fermi surface and the choice of χ. The highest T_c is found for that solution where the density of states is largest on the A-centered piece. This is easy to understand since that piece has constant gap, and the angular integrals over such a gap are not reduced as they are for a polar-gap case. As for χ, the largest transition temperature is for the case where χ is a function of z only. This is easy to understand since such a χ has oscillatory behavior over a larger region of the zone than in those cases where there is a dropoff of χ with r. We also see that T_c is quite sensitive to the degree of r dependence; the larger the dropoff with r, the lower the T_c. Experimentally, there is a dropoff with r,[22] but one expects the dropoff to be weaker in the r direction than in the z one. Therefore, I feel that the fourth solution in the table ($T_c=0.15$ K) is the most realistic one, as it (1) crudely takes into account the disk arms of the A piece and the possible necking between the Γ and K pieces, and (2) has a weaker dropoff with r than with z.

TABLE I. Solutions of the Eliashberg equations for various choices of $\chi(q)$ and Fermi-surface dimensions. In all cases the Γ-centered surface has a line of nodes in the $z=0$ plane, and the A-centered surface has a roughly constant gap, except in the last case where there are two lines of nodes on the Γ surface. The first column contains the type of $\chi(q)$ used (types listed below the table); the next columns have the Fermi-surface radii in the basal (π/a units) and z (π/c units) directions for the Γ surface (column 2) and the A surface (column 3). In the fourth column, the range of Z over the zone is listed, and in the fifth column, the estimated superconducting transition temperature. For the $\chi(q)$ types, $|z|\leq 2$ is assumed except for the last case. [I consider that the fourth case ($T_c=0.15$) is probably the most realistic.]

$\chi(q)$[a]	Γ coord.	A coord.	Z range	T_c
Type 1	0.55,0.75	0.65,0.15	16.5–16.5	0.146
Type 2	0.55,0.75	0.65,0.15	13.9–14.5	0.102
Type 2	0.55,0.75	1.00,0.15	13.8–14.5	0.189
Type 2	1.00,0.75	1.00,0.15	13.8–14.4	0.146
Type 2	1.00,0.75	0.65,0.15	13.9–14.3	0.080
Type 3	0.55,0.75	1.00,0.15	15.4–15.6	0.124
Type 4	0.55,0.75	1.00,0.15	13.2–13.8	0.042
Type 5	0.55,0.75	1.00,0.15	14.8–18.2	0.339

[a]Type 1, $\chi(q)=1+z/2$; type 2, $\chi(q)=1+z^2/16[(1-r)^2+3]$; type 3, $\chi(q)=1+z/8[(1-r)^2+3]$; type 4, $\chi(q)=1+z^2/8[(1-r)^2+1]$; type 5, $\chi(q)=1+z$ ($|z|\leq 1$).

At this point, a discussion of the various approximations used are in order. The frequency dependence of the gap has been ignored up to now. The author has iterated the fourth solution with respect to frequency (approximately). The result was to replace the factor of 0.88 by 1.1 in Eq. (9). This leads to a T_c reduction of about 20%. Next, we used cylindrical symmetry to simplify the problem. The inclusion of hexagonal symmetry will lead to a ϕ dependence of the gap. Whether such a dependence will further induce nodes is not known. A more likely source for inducing nodes is additional structure in $\chi(q)$. Certainly, the q dependence is known only crudely at present. In fact, since we know that Th-doped UPt_3 orders with a $\mathbf{q}$ vector[23] of (0.5,0,1) as opposed to the (0,0,2) vector considered here, it is highly important that the full q dependence of χ be mapped out. Once this is known, it will then be worth the effort to put the full band-structure Fermi surface into the problem. Finally, the effect of interband matrix elements is probably crucial. Reduction of the interband terms by 75% is sufficient to boost the T_c of the fourth solution up to 0.5 K.

In summary, using band-structure information and neutron data, I have been able to show that a superconducting transition in the temperature range found for UPt_3 can be induced by magnetic fluctuations. The appropriate solutions are derived by solving the resultant Eliashberg equations, and show polar-type gaps on some surfaces in the zone. More importantly, this approach is quite general and provides a quantitative tool for looking at anisotropic superconductivity in general.

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