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Magnetic pairing in a lattice of Kondo ions: Application to UPt_3

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Recently, several groups have calculated possible superconducting solutions for UPt_3 from magnetic fluctuation pairing by utilizing the band-structure Fermi surface and experimental dynamic susceptibility as input. The resulting solutions do not have proper periodicity in reciprocal-lattice space, though. In this paper, a more fundamental derivation of the pairing interaction is given by treating a lattice of interacting Kondo ions. Proper inclusion of umklapp processes leads to odd-parity solutions for UPt_3, with order parameters of A_{1u} or E_{1u} symmetry preferred.

I. INTRODUCTION

Several years ago it was suggested that antiferromagnetic spin fluctuations could be mediating the superconductivity seen in some heavy-electron metals,[1] and this viewpoint has become increasingly favored.[2,3] The author showed that Fermi-surface information from band-structure calculations along with dynamic susceptibility information from neutron scattering could be used to determine realistic superconducting solutions.[4] This formalism treated the frequency dependence of the interaction so as to estimate transition temperatures, but treated the susceptibility and Fermi surface in an axial approximation, leading to anisotropic s-wave solutions for UPt_3. Recently, Putikka and Joynt[5] solved the gap equations using the simpler formalism of Ref. 1, but included the dependence of the susceptibility in the basal direction as recently determined by Goldman *et al.*,[6] and found d-wave solutions for UPt_3.

The reason for the above difference involves the momentum dependence of the susceptibility. Experimentally, the susceptibility χ peaks at the first reciprocal lattice vector in both the basal and k_z directions, reflecting antiferromagnetic correlations between the two U atoms in the unit cell.[6,7] In the earlier work of Ref. 4, only the k_z dependence was treated, and it was assumed that the susceptibility had a periodicity of two reciprocal-lattice vectors in this direction. In Ref. 5, the basal dependence was included, causing an additional assumed periodicity of three reciprocal lattice vectors in the basal direction. The difference in the symmetry of the solutions is due to the fact that in Ref. 5 the k-vector sum was confined to the first zone, whereas in Ref. 4 the sum was done over a double zone in the k_z direction and thus covered the assumed periodic range of χ.

In reality, the solutions of both Refs. 4 and 5 are incorrect due to the fact that they are not invariant under translation by a reciprocal-lattice vector. (This can be seen by noting that the gap functions in both references have the same periodicity as χ.) This in turn implies that the gap equations should be altered so as to project from the pairing interaction a lattice periodic part. Moreover, the pairing interaction itself is suspect since it is not damped at large k vectors. This indicates that a more careful derivation of the pairing interaction is in order.

In Sec. II a new pairing interaction is constructed by considering a simple model involving a lattice of interacting Kondo ions, with the parameters being determined by fitting to neutron scattering data. This interaction has the advantage of being damped at large k vectors. In Sec. III, the resulting gap equations are introduced, numerical methods for solving them outlined, and the various solutions and their nodal structures discussed. Finally, in Sec. IV, various improvements to this simple model are suggested, with some conclusions being rendered in Sec. V.

II. THE MODEL

A simple model of a lattice of interacting Kondo ions has been successfully used to explain neutron scattering data.[8] In this model, the dynamical susceptibility of a bare Kondo ion is characterized by a frequency Γ, with interactions between the ions being described by the function $I(k)$. This leads to the following formula for the $\chi(k,\omega)$:

$$\chi(k,\omega)=\chi_0\Gamma/[\Gamma(k)-i\omega]\,, \tag{1}$$

where χ_0 is the bare ion susceptibility, and $\Gamma(k)=\Gamma[1-I(k)\chi_0]$. $I(k)$ can be determined by Fourier transforming $I(r,r')$. A standard approximation is to set $I(r,r')$ equal to a constant U if r and r' refer to the same site, and equal to a constant J if r and r' refer to nearneighbor sites. This, in fact, has already been done in Ref. 5 [the function is identified there as $\chi(k)$, but it is actually $I(k)$]. The result for the UPt_3 lattice is

$$I_0(k)=U+J\cos(k_zc/2)\times[\cos(k_xa/\sqrt{3})+2\cos(k_xa/\sqrt{12})\cos(k_ya/2)]\,. \tag{2}$$

This function has the property mentioned in the introduction that it peaks at the first reciprocal lattice vectors in both the k_z and basal directions (if J is negative), and has a periodicity of two reciprocal vectors in the k_z direction, and three in the basal direction.

A better approximation is to include the spatial dependence of the f electrons[9] by multiplying U and J by $\phi(r)\phi(r')$ where ϕ is the wave function for the local f

TABLE I. Values of $I(k)$ and $S(k)=1/[1-I(k)\chi_0]$ for various k values derived from Eqs. (1)–(3) with $U=0.5\Gamma$ and $J=-0.1\Gamma$. $I(k)$ is in units of Γ. Units are $4\pi/\sqrt{3}a$ for k_x and $2\pi/c$ for k_z.

k	$I(k)$	$S(k)$
0,0,0	0.20	1.25
0,0,1	0.70	3.29
0,0,2	0.13	1.14
0,0,3	0.29	1.40
1,0,0	0.58	2.40
0.5,0,1	0.47	1.90

state. This has the effect of changing Eq. (2) to

$$I(k)=I_0(k)f^2(k)\,, \tag{3}$$

where f is the form factor of the uranium ion. This function has been experimentally determined for UPt_3 by Stassis *et al.*,[10] and is in agreement with theoretical calculations for either an f^2 or f^3 ion.[11] Such a function is rapidly damped in momentum space, as desired.

We now describe a fit of this function to neutron scattering data for UPt_3. Experimentally, one measures the imaginary part of $\chi(k,\omega)$ multiplied by $f^2(k)$. As noted in Ref. 6, if one extracts $f^2(k)$ out by using the data of Ref. 10, then the measured $\chi(k)$ increases with increasing k. This is due to multiphonon contamination in the data, so one must be careful about which data points one uses to fit to. First, the parameter U can be fitted theoretically by noting that with J set to zero one has a lattice of noninteracting Kondo ions. Assuming a Wilson ratio of two for such a case, then from Eq. (1) we see that U must be $\Gamma/2$ (in units where χ_0 is equal to $1/\Gamma$). To determine J, we need to compare data at two k points. We choose these points such that (i) there is substantial k dependence of χ between them, (ii) they are close together in k space such as to avoid differences in multiphonon contamination, and (iii) they are away from phonon peaks in the data. Two such points from Ref. 6 are $k=(0.5,0,1)$ and $k=(0,0,1)$ with k_x being in units of $4\pi/\sqrt{3}a$ and k_z in units of $2\pi/c$. From Ref. 10, $f^2(0.5,0,1)$ is about 0.85, and $f^2(0,0,1)$ about 0.87 [with $f(0,0,0)=1$], whereas from Ref. 6, $\chi(0,0,1)/\chi(0.5,0,1)$ is about 1.74 (using again the above form factor values). Combining this information with that of Eqs. (1)–(3), one easily derives that J is about -0.1Γ.

In Table I, $I(k)$ and $S(k)=1/[1-I(k)\chi_0]$ are shown for various k values. One sees peaks at $k=(0,0,1)$ and $k=(1,0,0)$ as expected. Moreover, the variation with k is consistent with the data of Ref. 6. Finally, we can estimate Γ itself. From the data of Ref. 7, $\Gamma(0,0,1)$ is about 5 meV. From Table I, we see that $\Gamma(0,0,1)$ is about 0.3Γ, therefore, Γ is about 190 K.

III. GAP EQUATIONS AND THEIR SOLUTIONS FOR UPt_3

From the work of Ref. 4, the gap equation at T_c is

$$\Delta(k)=-\ln(1.13\omega_c/T_c)\sum W(k')V(k-k'-Q)\Delta(k')\,, \tag{4}$$

with the sum being over k' and Q where k' is in the first zone and Q is the set of reciprocal lattice vectors. $W(k')$ is the density-of-states (DOS) weighting and $V(k)$ is the pairing potential, with ω_c being equal to $\Gamma(k-k'-Q)$. In the case considered here, one obtains equivalent numerical results by using just Γ for ω_c. The gap equation is invariant under the replacement of k by $k+Q$ as long as the k-k' part of the argument of V is translated back to the first zone. Finally, there should be a factor of g^2 in Eq. (4), where g is the vertex for the scattering of a quasiparticle from state k to state k' from a local moment fluctuation. This factor will be discussed in Sec. IV.

To solve Eq. (4), we perform the zone sum using the tetrahedron method,[12] with the calculated band structure of Ref. 13 being used for the Fermi surface of UPt_3. As was shown in Ref. 14, this Fermi surface is in good agreement with de Haas–van Alphen data. The number of tetrahedra used is 4608 in the first zone (3912 of which contain the Fermi surface), with the function $W(k')$ being the contribution from each tetrahedron. Actually, the DOS in Eq. (4) is the quasiparticle DOS $N(0)$, which is larger by about a factor of 17 than the band DOS, so the actual $W(k')$ used in Eq. (4) are normalized such that their sum over the zone is $N(0)$. The product $V(k-k'-Q)\Delta(k')$ is evaluated at the center of mass of the Fermi surface inside each tetrahedron.[12] For computational purposes, we approximate the form factor by $\cos(\pi k/10)$ where k is the length of the vector in reciprocal units, and keep all Q vectors in Eq. (4) such that the magnitude of Q is less than or equal to some cutoff. One can solve Eq. (4) in each irreducible representation (there are six of these for a hexagonal crystal).

Note that Eq. (4) is not separable in k and k', so one must solve the problem numerically. To do this, one takes advantage of the fact that the effect of a group operation is to multiply the gap function by a constant (in the case of the two-dimensional representations, certain operations will also cause a complex conjugation of the gap function). For a hexagonal crystal, these effects are tabulated in Table I of Ref. 15. One can then write Eq. (4) in the following form:[16]

$$\sum M_{kk'}\Delta_{k'}=0\,, \tag{5}$$

where k and k' are in the irreducible wedge of the zone and the sum is over k'. T_c is then defined to be where the first eigenvalue of M crosses zero. The resulting eigenvector is the gap function. We solved Eq. (5) using standard EISPACK routines. For the case of the one-dimensional representations, M is a real symmetric matrix of order 163 for the Fermi surface grid considered. For the two-dimensional representations, one has two equations for the real and imaginary parts of the gap function, and M reduces to a real symmetric matrix of order 326.

We first looked at the even-parity case. Two forms for the pairing potential were considered. The first case assumes that $V(k)=I(k)$, which is the first term in a ladder series. The second case assumes that $V(k)=I(k)/[1-I(k)\chi_0]$, an ansatz for the full ladder sum.[3] (Note that there is no formal justification for this expression, unlike in the case where I is k independent.) The results are shown in Table II. Tabulated is the coupling

TABLE II. Coupling constants for the even-parity representations. $V1$ is the pairing potential $V(k)=I(k)$, and $V2$ is the pairing potential $V(k)=I(k)/[1-I(k)\chi_0]$. The cutoff for reciprocal lattice vectors was set to three (139 reciprocal vectors).

	$V1$	$V2$
A_{1g}	0.0276	0.0155
E_{1g}	0.0250	0.0028
E_{2g}	0.0194	0.0058
B_{2g}	0.0169	0.0018

constant λ for each representation, where $\lambda^{-1}=N(0)\Gamma \ln(1.13\omega_c/T_c)$ with $N(0)\Gamma$ about 3.0 for UPt_3. Only results for four of the representations are shown, as the λ's for the other two representations are in general small. (Note in the separable case of Ref. 5, only four representations occur.) As seen, the λ's are small, and furthermore, those from the full ladder sum are smaller than those gotten from just using $V(k)=I(k)$. This result indicates that even-parity pairing is suppressed, despite the presence of antiferromagnetic correlations. To understand this, note that $V(k)$ peaks at a reciprocal lattice vector. This is equivalent to umklapp scattering from $k=0$. Therefore, the effective pairing potential (the sum over umklapps of V) actually peaks at $k=0$, implying odd-parity pairing.

For the odd-parity case, we used $V(k)=-I^2(k)\chi_0/[1-I^2(k)\chi_0^2]$, an ansatz for the sum over odd bubble diagrams. The odd-parity case is complicated in the presence of spin-orbit coupling since the order parameter vector is locked to the lattice.[17] For a general direction, the order parameter is a sum of x, y, and z components. In the case of UPt_3, the moments are locked to the x-axis direction[18] because of spin-orbit effects.[13] We believe that a similar effect happens for the order parameter vector (that is, that the order parameter is locked to either the x, y, or z axis). We will thus label the representations assuming that the order parameter is pointing along the z axis (the other two directions will simply relabel the representations). Note that the assumption of a unique direction implies that nodal lines are possible.[17] The appropriate matrix elements under group operations can be obtained from those of Ref. 15, Table I by applying a sign change for every operation involving a sign change in z.

In Table III, the results for UPt_3 are shown for the odd parity case for two cutoffs for the magnitude of Q. Again, only four representations are shown since the coupling constants are small for the other two. We note that the coupling constants are an order of magnitude larger than those in Table II. The one-dimensional A_{1u} solution has the largest λ, with the two-dimensional E_{1u} solution having the next largest.

TABLE III. Coupling constants for the odd-parity representations (the representation labeling assumes that the order-parameter vector points along the z axis). The cutoff for reciprocal lattice vectors was set to three (first column, 139 reciprocal vectors) and four (second column, 321 reciprocal vectors).

	$Q3$	$Q4$
A_{1u}	0.444	0.481
E_{1u}	0.330	0.357
E_{2u}	0.098	0.112
B_{2u}	0.253	0.276

A point to consider now is how well the most obvious basis functions do in reproducing the numerical solution. These are tabulated in Table IV for the odd parity case, and are lattice periodic versions of those listed in Ref. 5. Comparisons show that only the E_{2u} basis function is a good approximation to the numerical gap functions, indicating the need for several terms in the basis function expansion.

We now analyze the nodal structures for the four odd-parity representations (remembering the assumption here that the order parameter vector points along a unique symmetry axis). The E_{1u} solution has point nodes along the k_z axis. The B_{2u} solution has line nodes in the $k_y=0$ (and hexagonal equivalent) planes. The E_{2u} solution has point nodes along the k_z axis, and line nodes in the $k_z=0$ and $k_z=\pi/c$ planes, with the A_{1u} solution having the same line nodes. Transverse ultrasound reveals that most likely, each major Fermi surface sheet has a nodal line perpendicular to the k_z axis.[19] This is consistent with both the A_{1u} and E_{2u} representations. More recently, high-frequency rf susceptibility measurements reveal an axial state,[20] consistent with the E_{1u} representation. An advantage of E_{1u} is that it is two dimensional, which can be used to explain a second phase transition seen in superconducting UPt_3 as due to a rotation in the two-dimensional order parameter space.[21] Alternately, this second transition may simply be due to a change in the weak spin-density-wave ordering recently observed in UPt_3.[22] More experimental work will be needed to clarify this matter.

TABLE IV. Basis functions for the odd-parity representations. Units are π/c for k_z and $2\pi/\sqrt{3}a$ for k_x and k_y. $f(x)$ is $a+b\cos(x)$, and a and b are arbitrary constants.

A_{1u}	$a\sin(\pi k_z)[\cos(2\pi k_y/\sqrt{3})+2\cos(\pi k_y/\sqrt{3})\cos(\pi k_x)]/\sqrt{3}+b\sin(\pi k_z)$
B_{2u}	$f(\pi k_z)[\sin(2\pi k_y/\sqrt{3})-2\sin(\pi k_y/\sqrt{3})\cos(\pi k_x)]/\sqrt{3}$
E_{2u}	$2\sin(\pi k_z)[\cos(2\pi k_y/\sqrt{3})-\cos(\pi k_y/\sqrt{3})\cos(\pi k_x)]/\sqrt{6}$ $+2i\sin(\pi k_z)\sin(\pi k_y/\sqrt{3})\sin(\pi k_x)/\sqrt{2}$
E_{1u}	$2f(\pi k_z)[\sin(2\pi k_y/\sqrt{3})+\sin(\pi k_y/\sqrt{3})\cos(\pi k_x)]/\sqrt{6}$ $+2if(\pi k_z)\cos(\pi k_y/\sqrt{3})\sin(\pi k_x)/\sqrt{2}$

IV. DISCUSSION

An obvious question to ask is, "Where do we go from here?" Some important physics is still missing from the model discussed in Secs. II and III. First, $I(k)$ is an exchange integral, and the form-factor approximation used in this paper may be inadequate. Anisotropy in the form factor itself has been ignored in this paper as no experimental knowledge of it is known at this time. Second, the pairing potential considered in this paper is essentially that due to local moment fluctuations. One would expect that there are two additional contributions: one due to the weak spin-density-wave state and the other due to quasiparticle terms. The contribution of these terms to the dynamic susceptibility appear to be small,[7,22] but it is possible that they could qualitatively change the results presented here.

The most important piece of physics which needs to be explored is the vertex $g_{nn'}(q,\omega)$ which represents scattering of a quasiparticle state ψ_{nk} to a state $\psi_{n'k'}$ caused by a local moment fluctuation, where $q=k-k'+Q$. This function not only includes the effects of spin-orbit scattering, but also differentiates between intraband and interband scattering. g would essentially be a matrix element involving the two quasiparticle wave functions, the local moment fluctuation (presumably a local f^2 state in a $^3H_4$ configuration), appropriate combinations of moment operators, and factors such as $e^{iq\cdot r}$. The machinery for evaluating such matrix elements already exists,[13] so when an appropriate theoretical evaluation of this quantity is made available such effects could be included. Note that a factor of g^2 enters into the gap equation. Comparisons of T_c's extracted from the tables to experiment would indicate that the average g has a value less than one, an encouraging finding.

Finally, we note that recently, a new fixed point for antiferromagnetic couplings was discovered for the problem of two Kondo impurities.[23] This fixed point would be characterized by a strong increase in the momentum dependent part of the interaction given in Eq. (2), and thus such a fixed point would mean an enhancement of the superconducting instability discussed in the present paper. Inclusion of such effects would therefore also be desirable in the context of the current model.

V. CONCLUSIONS

In this paper, an approximate form of the pairing interaction was derived from a simple model of a lattice of interacting Kondo ions, with the parameters being evaluated from neutron scattering data. The resulting gap equations were solved numerically for UPt_3 utilizing the Fermi surface from band-structure calculations, with the odd-parity solutions of A_{1u} and E_{1u} symmetry having the highest T_c. A more complete theory, which would include the scattering vertex g, is necessary before more definitive conclusions can be rendered.

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