Effect of Matrix Elements on the Pairing Kernel in Exchange Mediated Superconductors

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A method is derived for calculating the pairing kernel in exchange mediated superconductors including matrix element effects. Various models for the interaction vertex are considered, including spin exchange, orbital exchange, and quadrupolar exchange. As an example, this formalism is applied to $UPt_3$ using relativistic wavefunctions from a local density band calculation.

PACS numbers: 74.20.-z, 74.70.Tx
Much work has been done over the past decade in trying to understand the microscopic basis for superconductivity in heavy fermion metals, and more recently in the copper oxides. In the heavy fermion case particularly, a large body of experimental data points to the presence of a non-trivial order parameter reminiscent of $^3He$. Because of this, many theorists working on this subject, including the author, have borrowed techniques successful for $^3He$ and applied them to the heavy fermion problem. In particular, a favorite mechanism being explored is pairing due to spin fluctuations. In the calculations performed, one uses some model for the dynamic susceptibility and solves a gap equation. The solution is determined by the $k$ dependence of the susceptibility and the Fermi surface$^{1,2,3,4}$. Similar calculations have been recently performed on copper oxide materials$^5$.

The deficiency of this approach is obvious. It ignores matrix element effects, that is, the $k$ dependence enters only through the energy dispersion and not from the wavefunctions. In the analogous magnetic problem, the magnetism would be determined solely by nesting effects. Given the commensurate nature of the magnetic order in heavy fermions, nesting is an unlikely determinator for magnetism, and thus, one would suspect, for superconductivity also. This was realized from the beginning of theoretical work on this subject$^6$. Despite this, little work has been done along these lines, a noticable exception being a paper by Appel and Hertel$^7$, where a real space approach to pairing in heavy fermions is advocated.

In this paper, following the spirit of Refs. 6 and 7, the author develops a formalism for calculating the pairing kernel in exchange mediated superconductors including relativistic matrix elements determined from band structure calculations. Various models for the pairing interaction are considered, including spin, orbital, and quadrupolar exchange. As an example, this method is applied to the case of $UPt_3$, the best studied of the heavy fermion superconductors.

The pairing kernel to be evaluated is of the form $<k, -k|V|k', -k'>$ where $V$ is the
pairing interaction (note that the band index is implicitly included in the definition of \(k\)).

This form reduces to those considered in Refs. 1-5 if \(|k>\) is taken to be a free electron plane wave and \(V\) a function of \(r-r'\). In this paper, a different approach is taken by using the results of local density band calculations for \(|k>\). Moreover, since it is assumed that the physics is primarily determined by the \(f\) electrons, an approximation is made of assuming that \(V\) acts only on the \(J=5/2\) \(f\) states on the \(f\) atom site. \(V\) is further approximated by assuming it has just three values corresponding to whether the two electrons are on the same site (U), on near neighbor sites (J), and on next near neighbor sites (JN). Finally, the dependence on orbital quantum number, \(\mu\) (where \(\mu\) ranges from -5/2 to 5/2), is taken into account by the exchange process, which is denoted by \(X\), with \(V\) taking the form \(V_{RR'}^{ij}X_iX_j\) where \(i,j\) represent Cartesian indices (x,y,z), \(R,R'\) denote the positions of \(f\) atom sites, and \(X\) will be some appropriate analogue of the Pauli spin matrix, \(\sigma\). Given this, the pairing kernel is now of the form

\[
\sum_{R,R',i,j} V_{RR'}^{ij} < k|X_i|k'>_R < -k|X_j|-k'>_{R'}
\]  

(1)

where \(< | >_R\) denotes an integral over a Wigner-Seitz sphere centered at \(R\). To evaluate this, note that the band structure wavefunction is of the form

\[
|k> = \sum_{\mu,R} a_{\mu,k,R}|\mu >_R
\]  

(2)

where \(|\mu>\) is the appropriate combination of spherical harmonics and spinors times the \(f\) electron radial function. Since \(X\) has no dependence on radial coordinate, the radial integrals factor out of the problem, except that since an LMTO band method is used, the wavefunction has a radial term and its energy derivative as expansion functions. For notational convenience, this complication is ignored, but is taken into account when evaluating the matrix elements. In a band calculation, \(|k>\) is just generated in one irreducible wedge of the zone and only on the sites inside the primitive cell. The rest of the information for
$|k>$ can be obtained by use of Bloch’s theorem plus by application of the group operations on $|k>$. This is somewhat complicated for $UPt_3$ since the space group is non-symmorphic with two U atoms in the primitive cell. This means that some group operations must be followed by non-primitive translations and others lead to the interchange of the two U sites. The effect of group operations on $|\mu>$ is well known, for $UPt_3$ they transform as $\Gamma_7, \Gamma_8$, and $\Gamma_9$. This has been tabulated in Ref. 7, for instance, but the author rederived all relations used in the programs as a safety check. Finally, in the approximation used in this paper, Bloch’s theorem will appear by factors of the form $e^{ikR}$ in the matrix elements where R is the site position of a U ion. These cancel one another for the on-site case, but must be carefully kept track of for near neighbor and next near neighbor terms.

The nature of the operator X will now be discussed. In the $^3He$ problem, it is taken to be the Pauli spin matrix. The simplest generalization for the current case is to replace $\sigma$ by the pseudo-spin matrix $\tau$, where $\tau$ has the same effect on k, $PTk$ (or $P_k$, $Tk$) that $\sigma$ has on up and down spinors. Note that P is the parity operator, and T the time reversal operator. Further generalizations can be made by replacing $\tau$ by $J$, the total angular momentum operator. Further, if one is interested in quadrupolar interactions, thought by some to be of fundamental significance in the heavy fermion problem$^8$, then one can in turn replace $J$ by $O_2^0 = [3J_z^2 - J(J + 1)]/\sqrt{3}$, $O_2^1 = [J_z(J_+ + J_-) + (J_+ + J_-)J_z]/2$, or $O_2^2 = [J_+^2 + J_-^2]/2$.

To determine the appropriate symmetry of the gap function, one must project the pairing kernel onto each group representation. For $UPt_3$ these are $\Gamma_1$ through $\Gamma_6$, equivalent to the more common ”chemical” notation of $A_1, A_2, B_1, B_2, E_2, E_1$. Moreover, a projection must also be done on odd and even parity. For even parity, the pair function notation $|k, -k>$ is replaced by $|k, Tk> = -|PTk, Pk>$. The odd parity case involves a three component vector. An assumption will be made in this case. Experimentally, it appears from neutron scattering data$^9$ that the moments in $UPt_3$ are confined to the basal plane.
If a similar effect occurs for the Cooper pair moments, then one expects only the "\( d_z \)" component of the odd parity order parameter vector to survive. Such an order parameter is consistent with a recent analysis of \( H_{c2} \) anisotropy in \( UPt_3 \). This projection automatically occurs in the \( \tau \) model if one assumes that \( V^{xx} = V^{yy} \) with the rest of the \( V^{ij} \) equal to zero. For the other models, mixing will occur. It is assumed, though, that there is some term in the pairing Hamiltonian which also acts in these cases to project onto \( d_z \). For the relativistic case, \( d_z = |k, Tk > + |PTk, Pk > \).

To summarize, the following pair interactions will be explored: \( \tau_x \tau_x + \tau_y \tau_y, J_x J_x + J_y J_y, O_0^0 O_2^0, O_2^1 O_1^1, O_2^2 O_2^2 \). \( |k, -k > \) will be taken to be \( |k, Tk > \mp |PTk, Pk > \) where the upper sign is for even parity and the lower one for \( d_z \) odd parity. The weak-coupling gap equation to be solved is

\[
\Delta_k = \lambda^{-1} \sum_{k'} V_{k,k'} \Delta_{k'}
\]

where \( V_{k,k'} \) is the pairing kernel discussed above and \( \lambda^{-1} \), the inverse coupling constant, is \( \ln(1.13 \omega_c / T_c) \) with \( T_c \) the transition temperature and \( \omega_c \) some cut-off energy. The sum is carried out over all \( k \) vectors on the Fermi surface. For \( UPt_3 \), a 137 \( k \) vector mesh is used on the Fermi surface in the irreducible wedge, noting that there are 24 group operations in this case. The \( k \) vectors are weighted by the appropriate density of states factors derived from a tetrahedron decomposition of the Brillouin zone.

In Table 1, the results of the above formalism for \( UPt_3 \) are summarized. In column 2, an on-site interaction of unit value is looked at. The sign in each case is chosen opposite to that which would yield a nodeless \( A_{1g} \) (s-wave) solution. This sign is positive for the \( \tau \), \( J \), and \( O_2^2 \) cases, but is negative for the \( O_2^0 \) and \( O_2^1 \) cases. Despite the "repulsive" value of the sign, solutions are indeed found, due to the momentum dependence of the matrix elements. The solution with the largest coupling constant either has \( A_{1g} \) symmetry or is odd parity (for the \( \tau \) case, the interaction is repulsive for all even parity states). Addition
of a repulsive momentum independent constant to the gap equation did not suppress the $A_{1g}$ solution since this solution already has a complicated nodal structure. In fact, the stability of the $A_{1g}$ solution over all other even parity solutions is most likely due to this complicated nodal structure, since the nodal structure of the other representations is fixed by symmetry and therefore not free to adjust itself to minimize the free energy.

In the final four columns, results for ferromagnetic (positive) and antiferromagnetic (negative) unit values of $J$ (near neighbor) and $JN$ (next near neighbor) interactions are tabulated. Again, the solution with the largest coupling constant either has $A_{1g}$ symmetry or is odd parity. An interesting point to remark on is that for the $\tau$ and $J$ cases, one finds that the ferromagnetic sign supports odd parity solutions whereas the antiferromagnetic sign supports even parity (for the $\tau$ case, the ferro case is repulsive for all even parity states and the antiferro case is repulsive for all odd parity states). This is in accord with earlier wisdom on this subject\(^1\) but did not occur for realistic calculations on $UPt_3$ which ignored matrix element effects\(^2\). This illustrates the crucial importance of matrix elements when evaluating the pairing kernel. Another interesting point is that quadrupolar interactions prefer $A_{1g}$, regardless of the sign, in ten of twelve cases.

The most favored explanation for the large body of experimental data on $UPt_3$ is that the order parameter is from a two-dimensional group representation with line nodes orientated perpendicular to the c axis\(^1^1\). In the current context, this could be realized by $E_{1g}$ or $E_{2u}$, the latter being consistent with the $H_{c2}$ anisotropy analysis\(^1^0\). Neither state is favored by any of the pair interactions analyzed in the current paper (the same was found for earlier work which ignored matrix element effects\(^2\)). The most favored two dimensional rep in the current work is $E_{1u}$. This solution has point nodes. On the other hand, arguments have been put forth that the observed line node structure in $UPt_3$ may not be due to the symmetry of the order parameter, but rather to gaplessness due to the normal state self-energy\(^1^2\). More work will certainly be necessary before the actual form
of the order parameter is unambiguously determined.

An alternate explanation of the data would be a near degeneracy of two different representations\textsuperscript{13}. This picture is certainly supported by the current work, which indicates several such cases which involve one single dimensional rep and one two dimensional rep. The picture advocated by Machida and co-workers\textsuperscript{14} which assumes a near degeneracy of the three components of an odd parity solution is not consistent with the treatment of this paper where strong spin-orbit effects prohibit such a degeneracy.

The author concludes with some remarks on strong coupling effects. The author has performed calculations on $UPt_3$ including the full momentum and frequency dependence of the pairing interaction and treating all $k$ vectors and $f$ bands (instead of restricting to the Fermi surface) as recently advocated by Monthoux and Pines\textsuperscript{5}, but ignoring matrix element effects. Although this treatment leads to a renormalization of the value of $T_c$, no change in the ordering of the solutions with respect to coupling constant was seen. For that reason, one would suspect that strong coupling effects would not alter the ordering of solutions seen here, although it is conceivable that variation of the matrix elements when going off the Fermi surface could alter the results. The author plans to test such effects in the future if the effort seems warranted. An alternate strong coupling effect to consider is feedback to the pair potential caused by changes induced when the metal enters the superconducting phase. These effects are crucial in the case of $^3He$, but for the heavy fermion case, there has been little evidence for a change in the dynamic susceptibility below $T_c$. Until such changes are identified, it would be premature to invoke such effects in the current formalism.

As a final thought, the author would like to emphasize the generality of the above method. Currently, this has been applied to a phenomenological and very simple interaction vertex for $UPt_3$ as an example. Once a more microscopic theory is available, then the resulting calculation for properly testing such a theory must follow a similar formalism as
expounded in this paper. This statement will most likely apply to other cases which might involve exchange mediated interactions, such as the copper oxide materials.

In summary, a new method is derived for evaluating the pairing kernel in exchange mediated superconductors utilizing matrix elements determined from relativistic band structure calculations. As an example, several models for the pairing interaction for $U\text{Pt}_3$ were considered, yielding a rich variety of solutions. Further work, both experimental and theoretical, will be necessary before it can be determined what relevance the determined solutions have to the experimental situation.

This work was supported by U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. W-31-109-ENG-38.
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Table 1. Pairing coupling constants for various group representations for $UPt_3$. U represents an on-site interaction of unit value, with the sign chosen opposite that which would give a nodeless s-wave solution. N and NN represent near neighbor and next near neighbor interactions of unit value with either a positive sign (F) or negative sign (AF). The interaction vertex is denoted by $\tau$ for $\tau_x \tau_x + \tau_y \tau_y$, $J$ for $J_x J_x + J_y J_y$, $O^0_2$ for $O^0_2 O^0_2$, $O^1_2$ for $O^1_2 O^1_2$, and $O^2_2$ for $O^2_2 O^2_2$. Listed are the group representations with the largest coupling constants (with the coupling constant in parenthesis).

| Case | U         | F-N      | AF-N     | F-NN     | AF-NN    |
|------|-----------|----------|----------|----------|----------|
| $\tau$ | $B_{1u}(0.015)$ | $E_{1u}(0.040)$ | $A_{1g}(0.064)$ | $B_{1u}(0.047)$ | $A_{1g}(0.164)$ |
|      | $A_{2u}(0.009)$ | $B_{1u}(0.036)$ | $E_{2g}(0.047)$ | $E_{1u}(0.046)$ | $E_{2g}(0.070)$ |
| $J$ | $A_{1g}(0.058)$ | $E_{1u}(0.188)$ | $A_{1g}(0.209)$ | $B_{1u}(0.280)$ | $A_{1g}(0.728)$ |
|      | $B_{1u}(0.047)$ | $B_{1u}(0.169)$ | $E_{2g}(0.172)$ | $E_{1u}(0.236)$ | $E_{2g}(0.397)$ |
|      |            |          |          |          | $A_{1g}(0.207)$ |
| $O^0_2$ | $A_{2u}(0.247)$ | $A_{1g}(0.838)$ | $A_{1g}(1.33 )$ | $A_{1g}(2.32 )$ | $A_{2u}(0.484)$ |
|      | $E_{1u}(0.171)$ | $A_{2u}(0.699)$ | $E_{2g}(0.600)$ | $E_{1u}(0.635)$ | $B_{1u}(0.334)$ |
|      | $E_{2g}(0.161)$ | $E_{1u}(0.392)$ | $E_{1u}(0.413)$ | $B_{1u}(0.629)$ | $A_{1g}(0.328)$ |
|      |            |          |          |          | $E_{1u}(0.323)$ |
| $O^1_2$ | $A_{1g}(0.157)$ | $A_{1g}(0.438)$ | $A_{1g}(0.361)$ | $A_{1g}(1.60 )$ | $A_{1g}(0.547)$ |
|      | $B_{1u}(0.121)$ | $A_{2u}(0.216)$ | $E_{2g}(0.227)$ | $E_{2g}(0.486)$ | $E_{1u}(0.323)$ |
|      | $E_{2g}(0.102)$ | $B_{1u}(0.215)$ | $A_{2u}(0.186)$ |            | $B_{1u}(0.272)$ |
|      |            |          |          |          |            |
| $O^2_2$ | $A_{1g}(0.145)$ | $A_{1g}(0.374)$ | $A_{1g}(0.236)$ | $A_{1g}(0.381)$ | $A_{1g}(1.05 )$ |
|      | $B_{1u}(0.141)$ | $E_{1g}(0.100)$ | $E_{1u}(0.235)$ | $E_{2g}(0.174)$ | $E_{2g}(0.571)$ |
|      |            |          |          |          | $E_{2g}(0.166)$ | $B_{1u}(0.163)$ |
|      |            |          |          |          |            | $B_{1u}(0.392)$ |