Possible microscopic model for superconductivity in UPt_3

M. R. Norman
Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439
(Received 2 August 1990; revised manuscript received 2 October 1990)

Currently, microscopic models based on spin-fluctuation-mediated pairing are at odds with phenomenological theories as regards the symmetry of the order parameter for the heavy-electron superconductor UPt_3. The author shows that this discrepancy can be resolved for high-frequency spin fluctuations by including a weak ferromagnetic coupling between next-nearest-neighbor U atoms.

I. INTRODUCTION

Over the past two years, great progress has been made in understanding the nature of the superconducting ground state of UPt_3 by an interplay between various experiments and phenomenological Ginzburg-Landau theories. These theories propose an E_1 order parameter for UPt_3 (Refs. 1–10) to explain the results of longitudinal ultrasound,[11,2,12] specific heat,[13,14] torsional oscillator,[15] upper critical field,[16,17,14] lower critical field,[17,14] and neutron scattering[18] data which indicate multiple superconducting phases. The multiple phases are conjectured to be due to the lifting of the degeneracy of the two-dimensional group representation caused by the presence of weak magnetic ordering in UPt_3 (Ref. 18) which reduces the crystal symmetry from hexagonal to orthorhombic. Moreover, a number of measurements including specific heat,[19,13] transverse ultrasound,[20] and penetration depth[21] indicate that the gap function has nodes, which is consistent with order parameters of E_1 symmetry. Complementing this were microscopic spin fluctuation calculations which indicated an E_{1g} order parameter as the stable superconducting state;[22] so it would appear that the nature of the superconducting state was well understood from both a microscopic and phenomenological viewpoint.

Not all data, though, are consistent with an even-parity order parameter. Measurements of the Knight shift indicate no change below T_c, which is in support of an odd-parity state.[23,6] Recently, Choi and Sauls have shown that the large anisotropy of H_{c2} for different field directions can be explained if the order parameter is an odd-parity state with d vector orientated along the c axis.[24] On the theoretical side, the microscopic calculations of Ref. 22 are in error for the same reason that earlier calculations of the author[25] are. The assumption of these calculations was that the pair potential has the same momentum dependence as the susceptibility.[26,25,22] This is all right for a simple Bravais lattice, but UPt_3 is an hcp lattice with two U atoms per cell with the inversion site in between the atoms. Thus, the susceptibility does not have the periodicity of the reciprocal lattice, and when used in a gap equation, it leads to solutions which are not properly periodic in reciprocal-lattice space. Correcting for this leads to solutions which do not have E_1 symmetry.[27,28]

In this paper a brief review of the microscopic calculations is given. The author further shows that for high-frequency spin fluctuations with antiferromagnetic coupling between the planes, the addition of a weak ferromagnetic coupling within the planes is sufficient to stabilize an order parameter of E_{1u} symmetry.

II. MICROSCOPIC THEORY

The general assumption of the microscopic theory based on spin fluctuation pairing is that the pair potential is related to the dynamic magnetic susceptibility, and thus its momentum dependence reflects the momentum dependence of the susceptibility.[22,25–30] Most of the calculations were based on the results of earlier neutron scattering data which indicate antiferromagnetic correlations between near neighbors separated in planes stacked along the c axis with a characteristic energy of 5 meV.[31] The susceptibility can be fit by an on-site repulsion term, U, which is momentum independent, and an intersite exchange term, J, whose momentum dependence is given by the Fourier transform $\mathrm{Re}[\phi(\mathbf{q})]=\sum e^{i\mathbf{q}\cdot\mathbf{R}}$ where $\mathbf{R}$ is a near neighbor vector, with $\phi(\mathbf{q})$ or its conjugate obtained if one restricts to just one site in the unit cell. This function has a periodicity of two reciprocal lattice vectors along c and three reciprocal lattice vectors in the basal plane. Thus, when used in the gap equation, this susceptibility leads to gap functions which are not lattice periodic. The norm of the full complex function $\phi(\mathbf{q})$ is properly lattice periodic, as first pointed out by Konno and Ueda.[30] This in turn leads to a resolution of the periodicity problem. If one treats the pair interaction as a 2×2 matrix in site space, one gets a bare interaction of the following form:[28,32] $I_{11}(\mathbf{q})=I_{22}(\mathbf{q})=U$, $I_{12}(\mathbf{q})=I_{21}(\mathbf{q})^*=J\phi(\mathbf{q})$. Diagonalizing this, one obtains two bare interactions, $I_\pm=U\pm J|\phi(\mathbf{q})|$, each of which is properly periodic in reciprocal space (i.e., there are two pair eigenvalues for the same reason there are two energy bands per orbital, because of the two sites per primitive cell). The full pair potential is then obtained by summing an RPA series involving the bare interaction. Finally, one assumes that since the spins are confined to the basal

plane, the pair interaction is multiplied by $S_xS_x+S_yS_y$ where **S** is a spin vector, with a constant assumed multiplying the S_zS_z term since no antiferromagnetic correlations are observed for fields directed along the c axis. Using such a pair potential, one obtains an odd-parity solution of the form $k_z\mathbf{z}$.[28] An odd-parity solution is obtained since the susceptibility peaks at a reciprocal lattice vector, as opposed to peaking at the zone boundary which one would obtain for a simple Bravais lattice. Moreover, the d vector is along the c axis, which confines the spin of the Cooper pair to be orthogonal to the c axis, as assumed when constructing the spin part of the pair potential. Note that an odd-parity solution with a d vector along the c axis is what is needed to fit the H_{c2} data.[24] Despite this, the above solution does not have the correct group symmetry.

This motivated the author to look at pairing via low-frequency fluctuations, which are known to have a large spectral weight.[32] They have a characteristic energy of order 0.3 meV. The momentum dependence of the pair potential is primarily determined by antiferromagnetic coupling between next-nearest neighbors separated by a lattice constant in the basal plane. The spin part of the pair interaction has to be generalized to allow three different terms involving S_xS_x, S_yS_y, and S_xS_y to explain the anisotropy of the magnetic moment, which prefers to lie along the x direction in the basal plane. This basal-plane anisotropy allows new odd-parity solutions with d vectors in the basal plane, and in fact the most stable superconducting state is predicted to be of the form $k_x\mathbf{x}+k_y\mathbf{y}$.[29] This solution has both the wrong symmetry and the wrong d-vector orientation to be consistent with current phenomenological models. Moreover, it has been argued that low-frequency spin fluctuations would act much like static magnetic impurities, and thus would be detrimental for pairing.[29] In fact, by using the arguments in Ref. 29 assuming a high-frequency energy scale of 5 meV, one would expect pair breaking for energies up to about 0.3 meV, which is the characteristic energy for the observed low-frequency fluctuations.

This leads one to look again at pairing via high-frequency spin fluctuations. Note from Ref. 28 that although the largest coupling constant was for A_{1u}, the second highest was for E_{1u}. This leads to the question of whether an E_{1u} solution could be stabilized by an appropriate change in parameters. In Ref. 28, it was assumed that there was only antiferromagnetic coupling between atoms in neighboring planes (this leads to an induced ferromagnetic alignment between atoms in the plane). This was sufficient to fit the data, which has relatively large error bars.[31] On the other hand, when one heats the sample, the antiferromagnetic coupling is lost, but the ferromagnetic alignment in the planes persist.[31] This indicates that there is a weak ferromagnetic interaction in the plane independent of the induced alignment from the antiferromagnetic coupling between planes. This coupling is included in the above formalism by replacing U by $U+J_{\mathrm{NNN}}\phi_{\mathrm{NNN}}(\mathbf{q})$ where J_{NNN} is the in-plane exchange coupling and $\phi_{\mathrm{NNN}}(\mathbf{q})$ is the Fourier transform of the in-plane distance vectors.

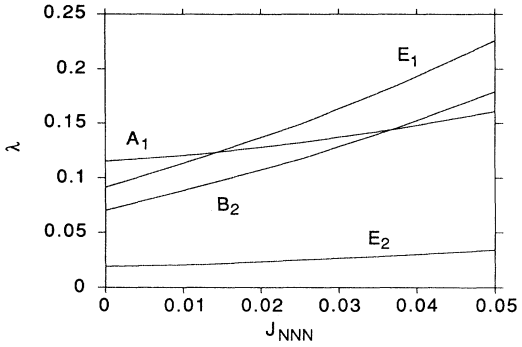

FIG. 1. Coupling constants for odd-parity representations as a function of J_{NNN} with $U=0.3$ and $J=-0.1$ in units of Γ (5 meV).

In Fig. 1 the coupling constants as a function of J_{NNN} are shown using the same parameter as in Ref. 28 ($U=0.3$ and $J=-0.1$ in units of Γ). The **k**-point grid was truncated to 24 points in the irreducible wedge so as to accelerate the calculations (the results for $J_{\mathrm{NNN}}=0$ are comparable to those of Ref. 28 which used a 137-point grid). One can see that only a small in-plane coupling is needed to stabilize E_{1u}. In fact, for an in-plane coupling of about 15% of the out-of-plane coupling, A_{1u} and E_{1u} are degenerate. This is of interest, since a recent phenomenological model by Joynt *et al.*[33] indicates that such a scenario can explain the observed phase diagram without invoking coupling to the weak antiferromagnetic order parameter. Finally, it should be remarked that the E_{1u} solution is of the form $(k_x\pm ik_y)\mathbf{z}$. Such a gap has point nodes along the c axis. Most fits to thermodynamic data indicate line nodes perpendicular to c, but some fits indicate point nodes, so it remains to be seen whether the nodal structure of this gap is consistent with experiment or not.

III. CONCLUSION

The author has shown that including a weak ferromagnetic coupling within the planes in the pair potential for high-frequency spin fluctuations leads to an E_{1u} gap consistent with current phenomenological theories for UPt_3. Whether this is indeed the solution to the microscopic problem of superconductivity in UPt_3 remains to be seen by further experimental and theoretical work.

ACKNOWLEDGMENTS

The author would like to thank Jim Sauls for a copy of Ref. 24 prior to publication. This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. W-31-109-ENG-38.

[1]G. E. Volovik, J. Phys. C **21**, L221 (1988).
[2]A. Schenstrom, M-F. Xu, Y. Hong, D. Bein, M. Levy, B. K. Sarma, S. Adenwalla, Z. Zhao, T. Tokuyasu, D. W. Hess, J. B. Ketterson, J. A. Sauls, and D. G. Hinks, Phys. Rev. Lett. **62**, 332 (1989).
[3]R. Joynt, Superconductor Sci. Tech. **1**, 210 (1988).
[4]M. E. Zhitomikskii, Pis'ma Zh. Eksp. Teor. Fiz. **49**, 333 (1989) [JETP Lett. **49**, 379 (1989)].
[5]D. W. Hess, T. A. Tokuyasu, and J. A. Sauls, J. Phys. Condens. Matter **1**, 8135 (1989).
[6]K. Machida and M. Ozaki, J. Phys. Soc. Jpn. **58**, 2244 (1989); K. Machida, M. Ozaki, and T. Ohmi, *ibid.* **58**, 4116 (1989).
[7]S. K. Sundaram and R. Joynt, Phys. Rev. B **40**, 8780 (1989).
[8]T. A. Tokuyasu, D. W. Hess, and J. A. Sauls, Phys. Rev. B **41**, 8891 (1990).
[9]E. I. Blount, C. M. Varma, and G. Aeppli, Phys. Rev. Lett. **64**, 3074 (1990).
[10]R. Joynt, J. Phys. Condens. Matter **2**, 3415 (1990).
[11]V. Muller, Ch. Roth, D. Maurer, E. W. Scheidt, K. Luders, E. Bucher, and H. E. Bommel, Phys. Rev. Lett. **58**, 1224 (1987); Y. J. Qian, M-F. Xu, A. Schenstrom, H-P. Baum, J. B. Ketterson, D. Hinks, M. Levy, and B. K. Sarma, Solid State Commun. **63**, 599 (1987).
[12]S. Adenwalla, S. W. Lin, Q. Z. Ran, Z. Zhao, J. B. Ketterson, J. A. Sauls, L. Taillefer, D. G. Hinks, M. Levy, and B. K. Sarma, Phys. Rev. Lett. **65**, 2298 (1990).
[13]R. A. Fisher, S. Kim, B. F. Woodfield, N. E. Phillips, L. Taillefer, K. Hasselbach, J. Flouquet, A. L. Giorgi, and J. L. Smith, Phys. Rev. Lett. **62**, 1411 (1989); K. Hasselbach, L. Taillefer, and J. Flouquet, *ibid.* **63**, 93 (1989).
[14]L. Taillefer, Physica B **163**, 278 (1990).
[15]R. N. Kleiman, P. L. Gammel, E. Bucher, and D. J. Bishop, Phys. Rev. Lett. **63**, 328 (1989).
[16]U. Rauchschwalbe, Physica B **147**, 1 (1987); B. S. Shivaram, T. F. Rosenbaum, and D. G. Hinks, Phys. Rev. Lett. **57**, 1259 (1986); L. Taillefer, F. Piquemal, and J. Flouquet, Physica C **153-155**, 451 (1988).
[17]B. S. Shivaram, J. J. Gannon, Jr., and D. G. Hinks, Phys. Rev. Lett. **63**, 1723 (1989); Z. Zhao, F. Behroozi, J. B. Ketterson, Y. Guan, B. K. Sarma, and D. G. Hinks, Physica B **165-166**, 345 (1990).
[18]G. Aeppli, E. Bucher, C. Broholm, J. K. Kjems, J. Baumann, and J. Hufnagl, Phys. Rev. Lett. **60**, 615 (1988); G. Aeppli, D. Bishop, C. Broholm, E. Bucher, K. Siemensmeyer, M. Steiner, and N. Stusser, *ibid.* **63**, 676 (1989).
[19]A. Sulpice, P. Gandit, J. Chaussy, J. Floquet, D. Jaccard, P. Lejay, and J. L. Tholence, J. Low Temp. Phys. **62**, 39 (1986).
[20]B. S. Shivaram, Y. H. Jeong, T. F. Rosenbaum, and D. G. Hinks, Phys. Rev. Lett. **56**, 1078 (1986); S. Schmitt-Rink, K. Miyake, and C. M. Varma, Phys. Rev. Lett. **57**, 2575 (1986).
[21]J. J. Gannon, Jr., B. S. Shivaram, and D. G. Hinks, Europhys. Lett. **13**, 459 (1990); W. O. Putikka, P. J. Hirschfeld, and P. Wolfle, Phys. Rev. B **41**, 7285 (1990).
[22]W. Putikka and R. Joynt, Phys. Rev. B **37**, 2372 (1988); **39**, 701 (1989).
[23]Y. Kohori, T. Kohara, H. Shibai, Y. Oda, T. Kaneko, Y. Kitaoka, and K. Asayama, J. Phys. Soc. Jpn. **56**, 2263 (1987).
[24]C. H. Choi and J. A. Sauls (unpublished).
[25]M. R. Norman, Phys. Rev. Lett. **59**, 232 (1987); Phys. Rev. B **37**, 4987 (1988).
[26]K. Miyake, S. Schmitt-Rink, and C. M. Varma, Phys. Rev. B **34**, 6554 (1986).
[27]M. R. Norman, Phys. Rev. B **39**, 7305 (1989); H. Monien and C. J. Pethick (unpublished).
[28]M. R. Norman, Phys. Rev. B **41**, 170 (1990); Physica B **163**, 733 (1990).
[29]A. J. Millis, S. Sachdev, and C. M. Varma, Phys. Rev. B **37**, 4975 (1988).
[30]R. Konno and K. Ueda, Phys. Rev. B **40**, 4329 (1989).
[31]G. Aeppli, A. Goldman, G. Shirane, E. Bucher, and M.-Ch. Lux-Steiner, Phys. Rev. Lett. **58**, 808 (1987); A. I. Goldman, G. Shirane, G. Aeppli, E. Bucher, and J. Hufnagl, Phys. Rev. B **36**, 8523 (1987).
[32]C. Broholm, Ph.D. thesis, Riso National Laboratory, 1988.
[33]R. Joynt, V. P. Mineev, G. E. Volovik, and M. E. Zhitomirsky, Phys. Rev. B **42**, 2014 (1990).