# Theory of superconductivity coexisting with the antiferromagnetic state in $UPd_2Al_3$



2003 J. Phys.: Condens. Matter 15 S2247

(http://iopscience.iop.org/0953-8984/15/28/361)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **15** (2003) S2247–S2250 PII: S0953-8984(03)62844-4

# Theory of superconductivity coexisting with the antiferromagnetic state in $UPd_2Al_3$

**H Ikeda**

Department of Physics, Kyoto University, Sakyo-ku, Kyoto 606-8502, Japan

Received 12 November 2002
Published 4 July 2003
Online at stacks.iop.org/JPhysCM/15/S2247

**Abstract**
We investigate the superconductivity (SC) coexisting with the antiferromagnetic (AF) state observed in $UPd_2Al_3$. Referring to the band calculation, we consider the band structure with a dual nature, that is, localized electrons, which mainly construct the AF state, and itinerant electrons, which form the heavy fermion state and the unconventional SC at lower temperatures. Within the random-phase approximation (RPA), we estimate the AF transition temperature $T_N$, and calculate the dynamical spin susceptibility. It possesses a collective spin wave around $\boldsymbol{Q} = (0, 0, 0.5)$ below $T_N$. In this situation, we evaluate the Eliashberg equation for the remaining itinerant band within the RPA. The most favourable even-parity pairing symmetry is $\cos(k_x + 2k_y) - \cos(k_x - 2k_y)$ modulated by a $\cos(k_z)$-like function. This is the symmetry $d_{xy}$ which, in addition, possesses a tiny gap around the AF zone boundary.

## 1. Introduction

In strongly correlated electron systems, the coexistence of the magnetic state and the superconductivity (SC) is one of the most fascinating problems. Recently, in the Ce115 family, the coexistence around the boundary between the antiferromagnetic (AF) state and the SC has been reported, and vigorously investigated. However, there are a variety of such coexistence phenomena in U compounds. Among them, experimental investigations in $UPd_2Al_3$ have made good progress and provide us with clear data. $UPd_2Al_3$ is an AF metal with the wavevector $\boldsymbol{Q} = (0, 0, 0.5)$ below $T_N = 14.5$ K [1] and coexists with the singlet SC with line nodes below $T_c = 2$ K [2]. The AF state possesses relatively large ordered moments 0.85 $\mu_B$/U and the transition seems to be that of the localized f-electron system. For $T_c < T \ll T_N$, it exhibits the typical behaviour of heavy fermion systems; a large enhanced coefficient of electronic specific heat $\gamma = 140$ mJ K$^{-2}$ mol$^{-1}$ and $T^2$-behaviour in the resistivity with a large coefficient [2]. Thus, in $UPd_2Al_3$ two separated subsystems, a localized part leading to the AF long-range order and an itinerant part forming the heavy fermion state, seem to coexist in momentum space. This dual nature and the sizable interaction between these subsystems have been stressed by Sato, Miyake and co-workers [3] from the inelastic ('resonance') peak observed at the AF zone centre $\boldsymbol{Q} = (0, 0, 0.5)$ in the SC by neutron scattering measurements [4]. Furthermore, they have proposed that the dispersive magnetic exciton by localized 5f electrons is responsible for the unconventional SC. This has symmetry $A_{1g}$ with the horizontal line nodes on the antiferromagnetic zone boundary (AFZB). However, it has been recently shown by Thalmeier that this mechanism favours an odd-parity state [5]. In addition, it is questionable whether such an indirect interaction as mediated by magnetic excitons dominates the on-site Coulomb repulsion, which directly acts between itinerant quasi-particles. On the other hand, if the two subsystems are decoupled, or weakly coupled as discussed at first, it is natural that the itinerant quasi-particles themselves lead to the unconventional SC by their own on-site Coulomb interaction. In this case, the shape of the Fermi surfaces (FSs) and the dispersion near the Fermi level are very important for the SC. In $UPd_2Al_3$, the de Haas–van Alphen effect in the AF phase is well explained by the FSs evaluated by the band calculation [6]. The two FSs ('party hat' and 'column') are the dominant FS with heavy cyclotron mass and the quasi-two-dimensional FS. These FSs will favour the unconventional SC with the vertical line nodes, if the itinerant quasi-particles construct the pairing state by the on-site Coulomb repulsion. This is another probable candidate for the unconventional SC discussed by Nisikawa and Yamada [7]. Thus, in the coexistence phase of the AF and the SC in $UPd_2Al_3$, the direction of line nodes and the mechanism of the SC is not yet consistently understood. In this paper, we investigate the SC coexisting with the AF properties within the random-phase approximation (RPA).

## 2. Formulation and results

We here consider the two-band Hubbard model, reflecting the dual nature of the antiferromagnetism and the SC. For simplicity, we assume that one band (band B) dominantly contributing to the antiferromagnetism possesses the perfect nesting at $\boldsymbol{Q} = (0, 0, 0.5)$ and another band (band A) is the quasi-two-dimensional band structure leading to the two FSs of 'party hat' and 'column' type under the AF background. In fact, the band calculation in the paramagnetic state indicates the existence of two bands with such properties [8]. Thus, we consider the following Hamiltonian,

$$H = H_A + H_B + V_{AB}, \tag{1}$$

$$H_\mu = \sum_{\boldsymbol{k}} \xi^\mu_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\mu\sigma} c_{\boldsymbol{k}\mu\sigma} + U_\mu \sum_i n^\mu_{i\uparrow} n^\mu_{i\downarrow}, \tag{2}$$

$$V_{AB} = U_{AB} \sum_{i\sigma} n^A_{i\sigma} n^B_{i\bar{\sigma}} - U_{AB} \sum_i (S^+_{iA} S^-_{iB} + S^-_{iA} S^+_{iB}), \tag{3}$$

with $\xi^A_{\boldsymbol{k}} = -2t_A\bar{\epsilon}_{\boldsymbol{k}} - 2t^z_A \cos(k_z) + \epsilon_A - \mu$, $\xi^B_{\boldsymbol{k}} = -2(t_B\bar{\epsilon}_{\boldsymbol{k}} + t^z_B)\cos(k_z) - \mu$, where $n^\mu_{i\sigma} = c^\dagger_{i\mu\sigma} c_{i\mu\sigma}$, $S^\pm_{i\mu} = c^\dagger_{i\mu\alpha}\sigma^\pm_{\alpha\beta} c_{i\mu\beta}$ with Pauli matrices $\sigma^\pm_{\alpha\beta} = (\sigma^x_{\alpha\beta} \pm \mathrm{i}\sigma^y_{\alpha\beta})/2$ and a band index $\mu = A, B$. The two dispersions possess the triangular lattice structure in the plane $\bar{\epsilon}_{\boldsymbol{k}} = \cos(k_x + 2k_y) + \cos(k_x - 2k_y) + \cos(2k_x)$, reflecting the structure on the $c$-plane in $UPd_2Al_3$. For simplicity, we hereafter assume $U_A = U_B = U_{AB} = U = 1.3$. Referring to the band calculation, we set $t_A = 1$, $t^z_A = 0.3$, $t_B = 0.5$ and $t^z_B = 0.4$. This is the case where the coupling between band A and band B is strong. In addition, we set the site energy $\epsilon_A = -0.805$ and the total electron number per spin $n = 1.00$ to reconstruct the two FSs in the AF state, although we do not consider distortion into the c-base-centred orthorhombic structure.

Let us proceed to the study of the SC coexisting with the antiferromagnetism. First of all, we calculate the AF transition temperature $T_N$ and the staggered field $h_s$ at the nesting vector $\boldsymbol{Q} = (0, 0, 0.5)$ within the mean field theory. In the AF phase, the dynamical spin susceptibility within the RPA is given by

$$\chi_z(q) = 2\chi_z^0(q)/(1 - U\chi_z^0(q)), \tag{4}$$

$$\hat{\chi}_\perp(q) = \begin{pmatrix} \chi_{uu}(q) & \chi_{us}(q) \\ \chi_{su}(q) & \chi_{ss}(q) \end{pmatrix}, \tag{5}$$

$$\chi_{uu}(q) = ((1 - U\chi_{ss}^0)\chi_{uu}^0 + U\chi_{us}^0\chi_{su}^0)/D(q), \tag{6}$$

$$\chi_{us}(q) = ((1 - U\chi_{ss}^0)\chi_{us}^0 + U\chi_{us}^0\chi_{ss}^0)/D(q), \tag{7}$$

$$\chi_{ss}(\boldsymbol{q}, \nu_n) = \chi_{uu}(\boldsymbol{q} + \boldsymbol{Q}, \nu_n), \tag{8}$$

$$\chi_{su}(\boldsymbol{q}, \nu_n) = \chi_{us}(\boldsymbol{q} + \boldsymbol{Q}, \nu_n) = \chi_{us}(\boldsymbol{q}, \nu_n), \tag{9}$$

$$D(q) = (1 - U\chi_{uu}^0)(1 - U\chi_{ss}^0) - U^2\chi_{us}^0\chi_{su}^0, \tag{10}$$

with

$$\chi_z^0(q) = -\sum_{k\mu}[\mathcal{G}_\mu(k)\mathcal{G}_\mu(k+q) + h_\mu(k)h_\mu(k+q)], \tag{11}$$

$$\chi_{uu}^0(q) = -\sum_{k\mu}[\mathcal{G}_\mu(k)\mathcal{G}_\mu(k+q) - h_\mu(k)h_\mu(k+q)], \tag{12}$$

$$\chi_{us}^0(q) = -\sum_{k\mu}[h_\mu(k)\mathcal{G}_\mu(k+q) - \mathcal{G}_\mu(k)h_\mu(k+q)], \tag{13}$$

where $\mathcal{G}_\mu(k) = -\langle\langle c_{\boldsymbol{k}\mu\sigma}c^\dagger_{\boldsymbol{k}\mu\sigma}\rangle\rangle = -\int_0^\beta \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau}\langle T_\tau c_{\boldsymbol{k}\mu\sigma}(\tau)c^\dagger_{\boldsymbol{k}\mu\sigma}(0)\rangle$ and $h_{\mu\sigma}(k) = \sigma h_\mu(k) = -\langle\langle c_{\boldsymbol{k}\mu\sigma}c^\dagger_{\boldsymbol{k}+\boldsymbol{Q}\mu\sigma}\rangle\rangle$, respectively, represent the diagonal and off-diagonal parts of one-particle Green functions under the AF phase with $k = (\boldsymbol{k}, \omega_n)$. In the AF phase, band A yields the quasi-two-dimensional two FSs, corresponding to the 'party hat' and the 'column' types, and band B becomes fully gapped. The poles of the transverse component $\hat{\chi}_\perp(q)$ provide the spin-wave dispersion around $\boldsymbol{Q} = (0, 0, 0.5)$.

We next evaluate the Eliashberg equation under the AF background. In the AF state, the spin label is not a good quantum number and the two-fold degeneracy of the quasi-particle band is linked by time-reversal and successively translational operations between the magnetic ions. In this case, the pairing symmetry is separated into parity even and odd, not spin singlet and triplet. We hereafter consider only even-parity pairing states. Since band B is fully gapped, we concentrate on the SC of quasi-particles on band A. If, for simplicity, neglecting the staggered pairing $\langle a_{\boldsymbol{k}\uparrow}a_{-\boldsymbol{k}+\boldsymbol{Q}\downarrow}\rangle$, the linearized-gap equation is represented by

$$\lambda\Delta(k) = U\sum_{k'}\mathcal{F}(k') + \sum_{k'}\left[U^2\chi_{uu}(k-k') + \frac{U^3}{2}\chi_z(k-k')\right]\mathcal{F}(k'), \tag{14}$$

where $\mathcal{F}(k) = -\Delta(k)|\mathcal{G}(k)|^2 - \Delta(k+\boldsymbol{Q})|h(k)|^2$ is the linearized anomalous Green function $-\langle\langle a_{\boldsymbol{k}\uparrow}a_{-\boldsymbol{k}\downarrow}\rangle\rangle$ and $\lambda$ is the eigenvalue. The pairing interaction in this equation includes both contributions of the collective spin-wave poles and the Coulomb repulsion on band A itself through the dynamical spin susceptibilities.

At temperatures ($T = 0.04$, $h_s = 0.6$) sufficient low enough to observe the spin wave, the most favourable pairing state ($\lambda = 0.166$) is $\cos(k_x + 2k_y) - \cos(k_x - 2k_y)$ modulated by the $\cos(k_z)$-like function shown in figure 1(a). This indicates the symmetry $\mathrm{d}_{xy}$ with vertical line nodes in the plane and, in addition, possesses a tiny gap around the AFZB. $\Delta(\boldsymbol{Q}/2)$ does not vanish exactly. A more detailed examination is needed to decide whether the line node avoids the FS and passes through the gap in the AFZB. The second stable solution ($\lambda = 0.151$) shown in figure 1(b) is a higher-harmonics one transformed from $(\sin(k_x+2k_y)-\sin(k_x-2k_y))\sin(k_z)$ with symmetry $\mathrm{d}_{yz}$. Both these solutions possess vertical line nodes and the $A_{1g}$ mode like $\cos(k_z)$ does not have a positive eigenvalue in this case. Since $\lambda$ of the two solutions evaluated

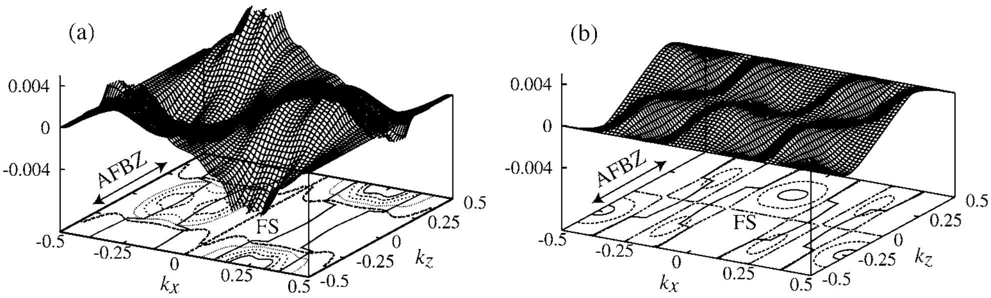


**Figure 1.** Two possible $\Delta(\boldsymbol{k}, \pi T)$ in the $k_x$–$k_z$ plane at $k_y = 1/8$ in $2\pi$. Only negative values are illustrated by contour plots. Four lines along the $k_z$-axis with a step at AFBZ $k_z = \pm 0.25$ show the FSs. The period of AF Brillouin zone (AFBZ) is $k_z = 0.5$.

here is close, these solutions might be exchanged by a change of input parameters and the introduction of staggered pairing. In order to obtain a realistic $T_c/T_N$, we must consider the AF fluctuation beyond the RPA. These are problems to be studied in the future.

## Acknowledgments

The author thanks Professor H Yamagami for the band calculation, and Professors K Yamada, M Ozaki, N K Sato and K Miyake for useful discussions.

## References

[1] Krimmel A *et al* 1992 *Z. Phys.* B **86** 161
[2] Geibel C *et al* 1991 *Z. Phys.* B **84** 1
[3] Sato N *et al* 2001 *Nature* **410** 340 and references therein
Miyake K and Sato N K 2001 *Phys. Rev.* B **63** 052508
[4] Metoki N *et al* 1997 *J. Phys. Soc. Japan* **66** 2560
Bernhoeft N *et al* 1998 *Phys. Rev. Lett.* **81** 4244
[5] Thalmeier P 2002 *Eur. J. Phys.* B **27** 29
[6] Inada Y *et al* 1999 *J. Phys. Soc. Japan* **68** 3643
[7] Nisikawa Y and Yamada K 2002 *J. Phys. Soc. Japan* **71** 237
[8] Yamagami H 2002 private communications