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Magnetism and Fermi surfaces of UGe_2

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Abstract

A self-consistent calculation of the ground-state electronic structure and magnetic properties of the ferromagnetic superconductor UGe_2 is performed using a Dirac-type relativistic spin-polarized linearized augmented-plane-wave (LAPW) method within a local spin-density approximation. The total energy oriented along the (100) direction of magnetization gives a minimum compared with the other directions, in agreement with the fact that the easy axis is along the (100) direction. In addition, the orbital moment is comparable to recent neutron scattering measurements. The ferromagnetic Fermi surfaces are composed mainly of the 5f-majority spin state with some nesting structures.

A great deal of attention has been attracted recently to the uranium ferromagnet UGe_2, since the appearance of a non-conventional superconductivity induced by pressure in the ferromagnetic phase was announced [1]. At ambient pressure UGe_2 orders ferromagnetically with a Curie temperature (T_C) of 52 K [2]. In resistivity measurements, superconductivity (SC) was found to occur, at pressures between 1.0 and 1.6 GPa, below the superconducting critical temperature (T_{sc}) of 0.8 K [1, 3].

Another interesting feature is that a transition, for which the characteristic temperature is defined as T^*, is observed in the ferromagnetic state [4]. The transition shows a meta-magnetic-like behaviour [5] and a maximum value of T_{sc} exists just at the critical pressure where T^* disappears. Thus the transition at T^* is closely related to the appearance of SC [3] and a possible pair-symmetry in the superconducting state is theoretically indicated to be the nonunitary triplet state [6].

UGe_2 crystallizes in a c-based-centred-orthorhombic (CBCO) $ThGe_2$-type structure with $Cmmm$ crystal symmetry [7] and the magnetization indicates it to be strongly anisotropic with the easy axis along the a-axis [2]. Along the b- and c-axes, the reductions of magnetization are less then 15% even under a high field of 21 T, and the saturated magnetization along the a-axis was estimated to be 1.43 μ_B/U. The same anisotropy is observed in the resistivity and susceptibility.

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Table 1. Total energies (mRyd/fu) in ferromagnetic orderings along the *a*-, *b*- and *c*-axes. The total energies are measured from the ground-state total energy for the *a*-axis.

Magnetization	*a*-axis	*b*-axis	*c*-axis
RSPLAPW (LSDA)	0.00	0.31	0.46
FLAPW (LDA + *U*)	0.00	0.55	0.67

Table 2. Spin (μ_S), orbital (μ_L) and total magnetic ($\mu_T = \mu_S + \mu_L$) moments at the U site for the three directions of magnetization. The units of all the moments are μ_B.

	RSPLAPW/LSDA			FLAPW/LDA + *U*			Experiment	
	a-axis	*b*-axis	*c*-axis	*a*-axis	*b*-axis	*c*-axis	U^{+3}	U^{+4}
μ_S	−1.36	−1.34	−1.35	−1.52	−1.62	−1.41	−1.17	−0.91
μ_L	2.56	2.51	2.51	2.98	3.18	2.85	2.62	2.37
μ_T	1.20	1.17	1.16	1.46	1.43	1.56	1.45	1.46

For a theoretical investigation of the magnetism and Fermi surfaces of UGe_2, self-consistent band calculations are performed using a Dirac-type relativistic spin-polarized linearized augmented-plane-wave (RSPLAPW) method [8] with local spin-density approximation (LSDA) [9] and muffin-tin (MT) approximations. The basis functions, expressed in the MT spheres, are numerically solved by the spin-polarized coupled Dirac (SPCD) equation with a magnetic interaction between the $j = \ell \pm 1/2$ states. A starting valence-electron configuration is set as $6p^6$, $5f^3$, $6d^1$ and $7s^2$ for the U atom and $3d^{10}$, $4s^2$ and $4p^2$ for the Ge atom. In the self-consistent procedure the core states are calculated by solving SPCD equations under the boundary condition of atoms. The lattice constants $a = 4.099$ Å, $b = 15.089$ Å and $c = 4.095$ Å are used.

First let us turn to the magnetic properties of UGe_2. Table 1 shows the RSPLAPW total energies obtained from the self-consistent calculations in the case of the ferromagnetic ordering along the *a*-, *b*- and *c*-axes, together with the FLAPW total energies with the LDA+*U* method [10]. The units are mRyd/fu and the origin of energy is set as the total energy obtained along the *a*-axis. The directions of local magnetic moments in the calculation are oriented using the relativistic spin-rotation matrices [11]. As a result the ferromagnetic state ordered along the *a*-axis is the ground-state of the ferromagnet UGe_2 and it is in agreement with the experimental result that the easy axis is along the *a*-axis. Both band theories suggest the same sequence for the *a*-, *b*- and *c*-total energies, though the absolute values of the RSPLAPW total energies are smaller than those of the FLAPW total energies in the *b*- and *c*-axes.

The spin–orbit interaction is known to produce a magnetocrystalline anisotropy and large orbital moment at the U site through the spin polarization by a local exchange field. Table 2 shows the calculated and experimental values of the spin, orbital and total magnetic moments at the U site, where the *a*-, *b*- and *c*-axes of RSPLAPW and FLAPW magnetic moments are ordered directions in the calculations and U^{+3} and U^{+4} denote an assumed valence of ions in the fitting of neutron scattering data [12]. The RSPLAPW calculations with only the LSDA suggest that the orbital moments thus obtained are comparable to the experimental ones, but that the total magnetic moments would be improved by a decrease of spin moments of $\sim 0.2\ \mu_B$/U compared with the enhancement of both spin and orbital moments by the LDA + *U* method.

In the electronic structure near the Fermi energy (E_F) the U-5f bands, split into two sub-bands of $j = 5/2$ and $7/2$ states separated by about 60 mRyd, are hybridized with the dispersive U-6d and Ge-4p bands. Since E_F exists in the middle of the 5f sub-bands with state

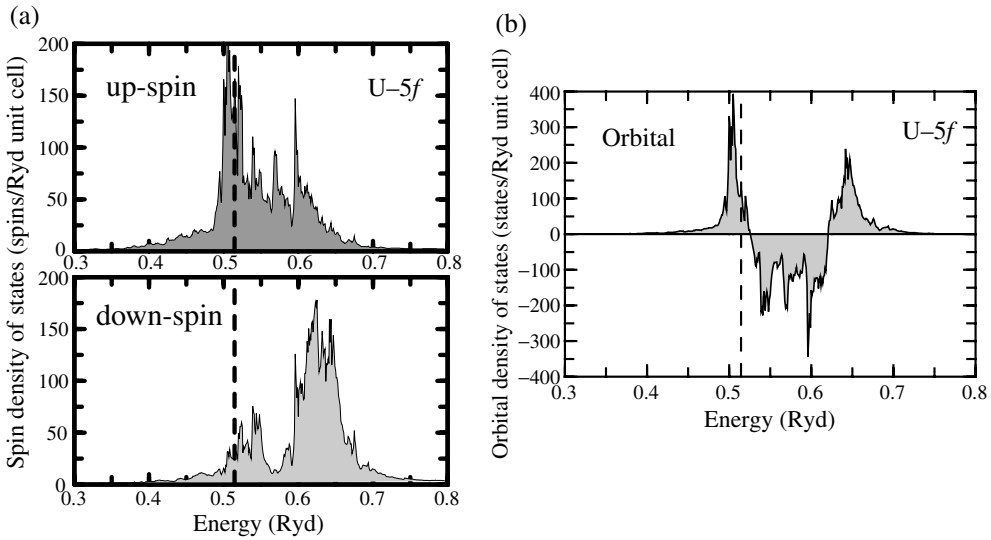

Figure 1. (a) U-5f up- and down-spin and (b) orbital density of states in ferromagnetic UGe_2.

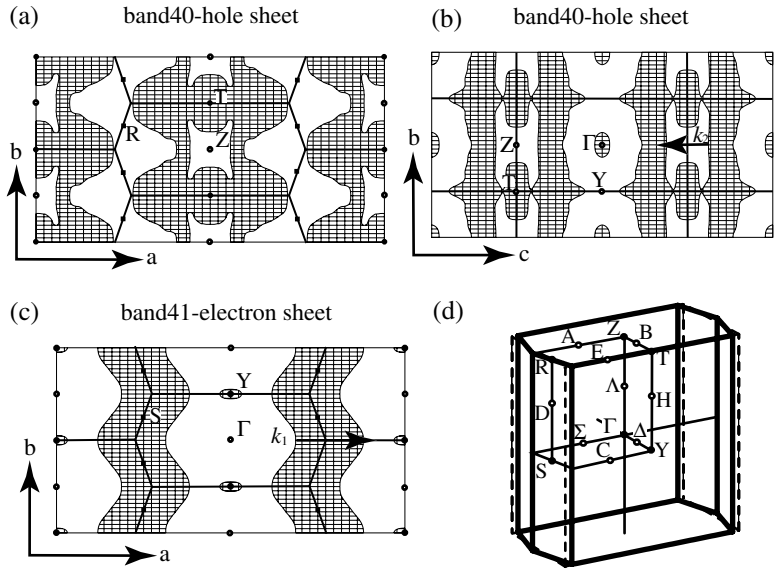

Figure 2. Cross sections of the Fermi surfaces in ferromagnetic UGe_2.

$j = 5/2$, the theoretical electronic specific heat coefficient (γ_b) has a relatively large value of 19.50 mJ K^{-2} mol^{-1}, thus being comparable with the experimental one (γ_{exp}) at ambient pressure of 35 mJ K^{-2} mol^{-1}. The Fermi surfaces are made up of the 39th, 40th, 41st and 42nd bands; the 39th and 40th bands form the hole Fermi surfaces and the 41st and 42nd bands compose the electron Fermi surfaces [13].

In the Dirac-type relativistic band theory, the up-spin density of states (DOS) ($N_\uparrow(\varepsilon)$) and down-spin DOS ($N_\downarrow(\varepsilon)$) can be projected from the total DOS ($N(\varepsilon)$) and the magnetization DOS ($M(\varepsilon)$) by using the relationship of $N_\uparrow(\varepsilon) = (N(\varepsilon) + M(\varepsilon))/2$ and $N_\downarrow(\varepsilon) = (N(\varepsilon) - M(\varepsilon))/2$. Figure 1(a) shows the up-spin and down-spin DOS in the U-5f site of UGe_2.

The up-spin DOS has a peak near E_F, while the largest distribution of down-DOS appears at an energy higher by $\sim$0.15 Ryd. The down-spin 5f states are almost unoccupied. As shown in figure 1(b), moreover, the orbital DOS is small near E_F, so that the angular momentum is almost quenched on the Fermi surface. Such a magnetic feature supports the possibility of magnetically-mediated p-wave triplet superconducting pairing.

Finally let us attempt to consider the transition characterized as T^* from the viewpoint of the Fermi surface of UGe_2. The resistivity measurements show that T^* decreases with pressure and disappears at a pressure close to the area of strongest SC. This transition is quite similar to that observed in α-uranium, which structurally resembles UGe_2. For α-uranium, there is direct evidence that the anomalies are due to the formation of a charge density wave (CDW), resulting from nesting at the Fermi surface. The band structure calculations made clear that there is a possibilibity of nesting with the appearance of a similar CDW. Therefore it is suggested that T^* is theoretically interpreted by the CDW/SDW (spin density wave) transition [14].

Figure 2 shows the cross sectional area of band40-hole and band41-electron sheets on planes normal to a symmetry axis in order to reveal where the nesting vectors are in the (100)-ferromagnetically-ordered Fermi surfaces of UGe_2. It turns out that some possible nesting vectors exist on the cross sections in figure 2, though they cannot be indicated in detail here for lack of space. The relationship between T^* and the nesting mechanism still remains to be tested in experiment.

Acknowledgments

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References

[1] Saxena S S *et al* 2000 *Nature* **406** 587
[2] Ōnuki Y *et al* 1992 *J. Phys. Soc. Japan* **61** 293
[3] Huxley A *et al* 2001 *Phys. Rev.* B **63** 144519
[4] Oomi G, Kagayama T and Ōnuki Y 1998 *J. Alloys Compounds* **271–273** 482
[5] Tateiwa N *et al* 2001 *J. Phys.: Condens. Matter* **13** L17
[6] Machida K and Ohmi T 2001 *Phys. Rev. Lett.* **86** 850
[7] Oikawa K *et al* 1996 *J. Phys. Soc. Japan* **65** 3229
[8] Yamagami H 1998 *J. Phys. Soc. Japan* **67** 3176
[9] Barth U von and Hedin L 1972 *J. Phys. C: Solid State Phys.* **5** 1629
[10] Shick A B and Pickett W E 2001 *Phys. Rev. Lett.* **86** 300
[11] Yamagami H 2000 *Phys. Rev.* B **61** 6246
[12] Kernavanois N *et al* 2001 *Phys. Rev.* B **64** 174509
[13] Settai R *et al* 2002 *J. Phys.: Condens. Matter* **14** L29
[14] Watanabe S and Miyake K 2001 *Physica* B **312/313** 115