Journal of Physics: Conference Series **592** (2015) 012040 doi:10.1088/1742-6596/592/1/012040

The spin directions of the Parity violated spin-splitting states in non-centrosymmetric compounds

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Abstract. The spin-directions and orientations are calculated for the Fermi surfaces of non-centrosymmetric compounds. Even in non-centrosymmetric compounds, each electron state is doubly degenerate by time reversal symmetry, but has the opposite spin-direction in the state with opposite sign of $\boldsymbol{k}$-vector as its Kramers pair. For the states with high symmetry $\boldsymbol{k}$-vector, the spin direction is determined by the symmetry, but not the orientation of the vector. Generally, to know the direction and the orientation of the spin, band structure calculations should be performed. The results are not as expected from so-called Rashba type spin-structure for the tetragonal $CePt_3Si$. In $TaSi_2$, the origin of anomalous magnetic breakdown effect might be related to its spin structure.

1. Introduction

Electronic states are at least doubly degenerate in paramagnetic materials with space inversion symmetry, because time reversal symmetry changes the sign of both the spin σ and the wavevector $\boldsymbol{k}$ and the space inversion symmetry changes only the sign of the wavevector $\boldsymbol{k}$. Therefore, the degeneracy is connected with the spin degree of freedom. Once the inversion symmetry is violated, electronic states are no longer degenerate in general, so the splitting is often called "spin-splitting", like Zeeman-type spin splitting under magnetic fields. The splitting originates in the parity violation (lack of space inversion symmetry), so it might be called parity violation splitting. Actually, it can be shown that the magnitude of the splitting mainly depends on the inter-site parity-mixing transfer [1]. Such the splitting has been already known as a consequence due to the anti-symmetric coupling between the spin σ and the wave vector $\boldsymbol{k}$. Such a kind of anti-symmetric couplings are called as Rashba type in two-dimensional case with lack of the mirror symmetry, or Dresselhaus type in crystals without inversion center.

Even in three-dimensional cases, the splitting is often discussed based on the Rashba type coupling when the crystal lost the mirror symmetry like $LaTGe_3$ (T: Transition Metal) [2], where the de Haas-van Alphen (dHvA) effect has revealed the magnitude of the splitting. Besides, band structure calculations have succeeded in reproducing the observed Fermi surface splitting in such the non-centrosymmetric compounds.

In this paper, not only the spin directions but also the orientations have been calculated in non-centrosymmetric $CePt_3Si$ and $TaSi_2$. Then it is realized that the spin orientations are not so simple as expected from the Rashba type coupling, even in the symmetry planes in the Brillouin

Zone. It tells us the importance of understanding the mechanism of the parity violation splitting in such crystals. The calculated spin structures of the Fermi surfaces would bring us a hint to explain the anomalous magnetic breakdown effect observed in chiral crystal $TaSi_2$ [3, 4].

2. Method of calculation

Band structure calculations are performed based on an FLAPW (full potential augmented plane wave) method with a local density approximation. The relativistic effect is considered by using the technique proposed by Koelling and Harmon [5]. The spin-orbit interaction is included based on the second variational procedure for valence electrons.

In the energy band structure for non-centrosymmetric compounds the spin-degeneracy is lifted in general, which is called parity violation splitting [6]. By using the method, split Fermi surfaces are calculated for many compounds, i.e. Yb_4Sb_3 [7], $LaPt_3Si$ [8, 9] $LaTGe_3$(T =Co, Rh, Ir) [2], $LaRhSi_3$ [10], $LaNiC_2$ [11], VSi_2 [4, 12], $NbSi_2$ [4] and $TaSi_2$ [3, 4]. In these compounds, the dHvA measurements clearly show the splitting of the Fermi surfaces. Then the magnitudes of the splitting are well reproduced by the calculations.

In the above calculations, each state except the high symmetry points, has certain spin direction and the orientation, though such information is not used for constructing a charge density, as we take a sum of Kramers pairs. In this paper, the direction and the orientation of each spin has been drawn in some cross sections for the Fermi surface of $CePt_3Si$ and $TaSi_2$.

3. The calculated spin structures

3.1. $CePt_3Si$

In $CePt_3Si$, superconductivity is realized in the long-range antiferromagnetic ordering. The Néel temperature is 2.2 K, while the superconducting transition temperature is 0.75 K [13]. The crystal structure of $CePt_3Si$ is tetragonal, the space group $P4mm$ (# 99, C_{4v}^1), in which there are two mirror planes, but no inversion symmetry.

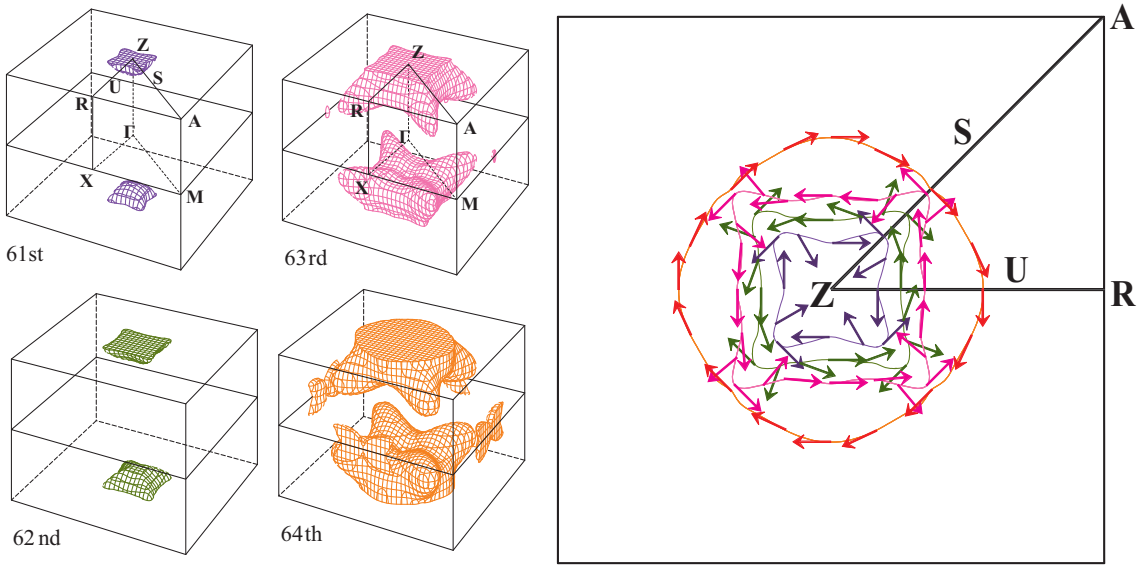

Figure 1. The calculated Fermi surfaces of $CePt_3Si$ (left) and the spin structure in the $k_z = \pi$ plane (right). Note that there are Kramers pairs, i.e., $E(\boldsymbol{k}, \sigma) = E(-\boldsymbol{k}, -\sigma)$ by the time reversal symmetry.

The Fermi surfaces for paramagnetic $CePt_3Si$ have been calculated [8]. There appear 6 Fermi surfaces, then 4 of them are shown in Fig. 1 (left). In this space group, there are two mirror planes including the c-axis and the Z-R line (U axis) or the Z-A line (S axis) in the Brillouin Zone. Therefore, along the Z-R line (U axis) or the Z-A line (S axis), the spin directions are perpendicular to the direction of the wave vector $\boldsymbol{k}$, as shown in Fig. 1 (right). The spins of the 63rd and the 64th Fermi surfaces rotate as anticlockwise and clockwise, respectively. However, the spin structure of the 61st and the 62nd Fermi surfaces are not so simple, rotating much more than the $\boldsymbol{k}$ directions. Such the spin structures are not expected from the simple anti-symmetric Rashba type coupling. This is because the Rashba type coupling is only appropriate for the small $\boldsymbol{k}$, and the real orientations of spins are determined by the atomic spin-orbit coupling, the on-site parity mixing of wave functions due to odd-order potential terms, and the inter-site parity-mixing transfer [1]. The detailed analysis of the origin will be discussed in a separate paper.

3.2. $TaSi_2$

$TaSi_2$ belongs to the space group $P6_422$ (# 181, D_6^5), in which there is no mirror symmetry, so it is called a chiral structure. The properties of the Fermi surfaces have been revealed by both the dHvA measurements and the band structure calculations [3, 4]. Anomalous magnetic breakdown effect is realized in the dHvA measurements [3].

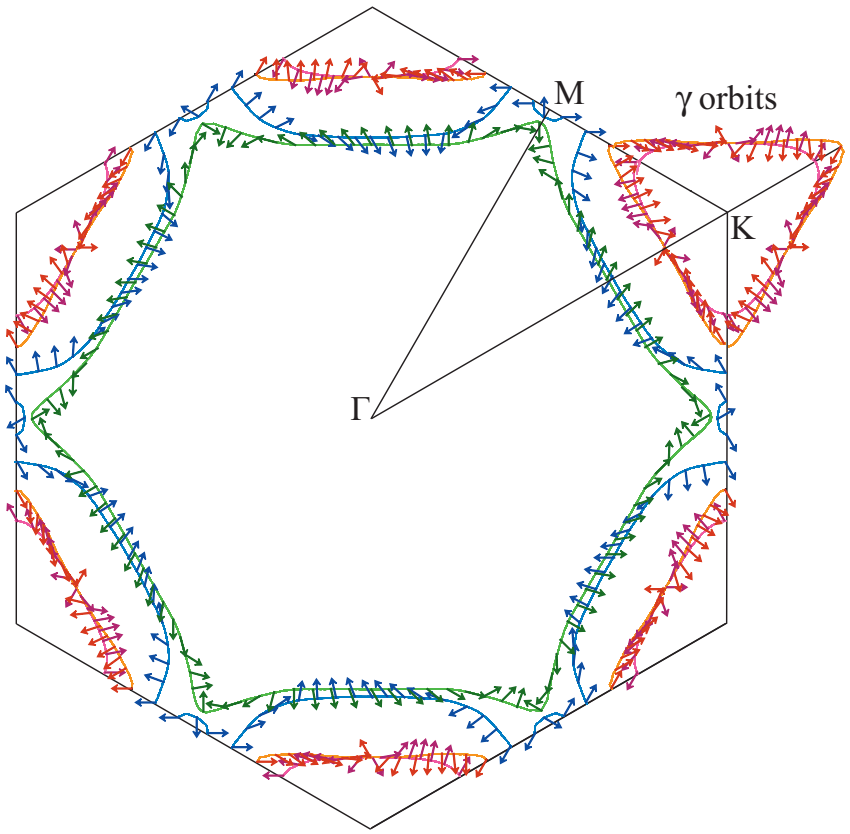

Figure 2. The cross sections and the spin structure in the $k_z = 0$ plane calculated for the Fermi surfaces of $TaSi_2$. The spin directions are restricted only on the plane, and show six fold rotational symmetry. Note that two closed orbits around the K point are not degenerate, but the spin orientations are exchanged near the nearly degenerate parts.

The spin structures in the $k_z = 0$ plane are shown in Fig. 2. There is only 6-fold rotational symmetry, so spin orientations cannot be determined in any $\boldsymbol{k}$-direction on the plane. We focus on two γ orbits, which look triangle shape centered at the K points, originating in the 103rd and 104th hole Fermi surfaces. They are not degenerate even in the $k_z = 0$ plane, but there are four dHvA signals are observed [3]. It can be attributed to magnetic breakdown effect, in which the cyclotron orbit gets through from one Fermi surface to the other one. However, the intensities for the breakdown orbits are found to be enormously large, although penetration probability is usually expected to be very small due to an energy gap between two Fermi surfaces [14].

As shown in Fig. 2, the spin structures for the γ orbits show three-fold symmetry around the K points. It is found that the spin orientations are exchanged each other near the three parts with a very small energy gap. The probability of the magnetic breakdown has been discussed not only for spin-degenerate cases, but also for the spin-splitting case [15]. In the paper, the spin-dependent magnetic breakdown effect has been discussed for simple Fermi surface model, though the model is too specific to directly applied to the realistic case in Fig. 2. The penetration probability in the magnetic breakdown effect in spin-splitting Fermi surfaces should be generally studied to understand anomalous magnetic breakdown effect realized in $TaSi_2$. We would expect the spin conserved magnetic breakdown orbits is preferable.

4. Summary

This article is our first report for the spin structures calculated for $CePt_3Si$ and $TaSi_2$. In the tetragonal $CePt_3Si$, the spin structure on the $k_z = \pi$ plane shows four-fold symmetry. Some of them are simply clockwise and anticlockwise, like so-called Rashba type, but the others are not. In $TaSi_2$, we have found the spin orientation exchanged at the nearly degenerate parts. It might be related to the anomalous magnetic breakdown effect observed in this compounds.

Acknowledgments

HH is grateful to Y. Yanase for valuable discussions and useful comments, and to Y. Ōnuki and his colleagues for the collaboration on the Fermi surface studies. This work was supported by JSPS KAKENHI Grant Number 25400342.

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