Spin Hall effect in $\text{Sr}_2\text{RuO}_4$ and transition metals (Nb, Ta)

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We study the intrinsic spin Hall conductivity (SHC) and the $d$-orbital Hall conductivity (OHC) in metallic $d$-electron systems based on the multiorbital tight-binding model. The obtained Hall conductivities are much larger than that in $p$-type semiconductors. The origin of these huge Hall effects is the “effective Aharonov-Bohm phase” induced by the signs of inter-orbital hopping integrals as well as atomic spin-orbit interaction. Huge SHC and OHC due to this mechanism is ubiquitous in multiorbital transition metals.

1. Introduction

Transport phenomena give us significant information on the manybody electronic states and help us to understand the electronic properties in the superconducting state. Multiorbital effect is significant in many superconductors (SC). For example, superconducting state in $\text{Sr}_2\text{RuO}_4$ shows a prominent orbital dependent SC [1]. Multiorbital effect is also important in transport phenomena. Spin Hall effect (SHE) and anomalous Hall effect (AHE) are significant examples which arise from the multiorbital effect.

Recent experiments declared the existence of sizable SHC in various compounds. Especially, the SHC in Pt reaches $240 \mu \text{e}^{-1}\Omega^{-1}\text{cm}^{-1}$ at room temperature, which is $10^4$ times larger than that in semiconductors [2]. Now SHC in various transition metals attracts great attention. However, simple electron gas models cannot explain this experimental facts. In ref. [3], we presented the first report on the theoretical study of the SHE in transition metals: They have shown that the anomalous velocity due to the atomic degrees of freedom gives rise to the large SHC comparable to the experimental values. Therefore, analyses based on the multiorbital tight-binding model are indispensable to elucidate the origin of the huge SHC in transition metals. Later, refs. [4,5] reproduced the SHC in Pt theoretically.

In this paper, we study the intrinsic spin Hall effect (SHE) and $d$-orbital Hall effect (OHE) based on a realistic tight-binding model. We first discuss the SHE in $\text{Sr}_2\text{RuO}_4$, which is a famous triplet superconductor at $T_c=1.5$. Next, we discuss the SHE in Nb and Ta, which are superconductors at $T_c=9.23$ for Nb and $T_c=4.39$ for Ta. The magnitude of obtained SHC are comparable to that in Pt. The theoretical technique developed in this study will serve to elucidate the origin of large SHC in other $d$-electron systems.

2. SHE in $\text{Sr}_2\text{RuO}_4$

In this section, we study the SHE in $\text{Sr}_2\text{RuO}_4$, where the metalicity appears in two-dimensional $\text{RuO}_2$ planes, and the Fermi surface is composed mainly of $t_{2g}$ ($d_{xz}, d_{yz}, d_{xy}$) orbitals. The tight-binding model for $\text{Sr}_2\text{RuO}_4$, which we call the $t_{2g}$-model, is introduced in ref. [1].

Hereafter, we denote $xz=1$, $yz=2$, $xy=3$. Using this presentation, the matrix element of the Hamiltonian without spin-orbit (SO) interaction is given by

$$
\hat{H}_0 = \begin{pmatrix}
\xi_1(k) & g(k) & 0 \\
g(k) & \xi_2(k) & 0 \\
0 & 0 & \xi_3(k)
\end{pmatrix},
$$

(1)

where the first, the second and the third row (column) correspond to $xz$, $yz$ and $xy$, respectively. $\xi_1 = -2t \cos k_x$, $\xi_2 = -2t \cos k_y$, and $\xi_3 = -2t (\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y + \xi_3^0$ are in-
traorbital kinetic energies; $t$ is the nearest neighbor $d_{xz}-d_{xz}$ ($d_{yz}-d_{yz}$) hopping along $x$ ($y$)-axis, and $t_3, t_3'$ are the nearest and the second nearest neighbor $d_{xy}-d_{xy}$ hoppings, respectively. Here, a constant $\xi_0$ is included in $\xi^3$ to adjust the number of electrons $n_l$ on $l$-orbital. We note that the interorbital kinetic energy $g = -4t'\sin k_x \sin k_y$, which breaks the mirror symmetry with respect to $k_x$ and $k_y$-axes, causes the large anomalous velocity $|e|/2\pi a$. This is the origin of huge SHE. Next, we consider the SO interaction $H_{SO} = \sum_l \lambda_l t_l s_l$. Since the SO interaction mixes electrons with different spins, $H_{SO}$ is given by $6 \times 6$ matrix:

$$H_{SO} = \frac{\lambda \hbar^2}{2} \begin{pmatrix} 0 & -i & 0 & 0 & 0 & i \\ +i & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -i & 1 & 0 \\ 0 & 0 & i & 0 & i & 0 \\ 0 & 0 & 1 & -i & 0 & 0 \\ -i & -1 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad (2)$$

where the first three rows (columns) correspond to $xz \uparrow, yz \uparrow$ and $xy \uparrow$, and the second three rows (columns) correspond to $xz \downarrow, yz \downarrow$ and $xy \downarrow$, respectively. As a result, the total Hamiltonian $H_{tot} = H_0 + H_{SO}$ is given by $6 \times 6$ matrix. According to ref. [1], we put $t = 1$, $t' = 0.1$, $t_3 = 0.8$, $t_3' = 0.35$, and assume that $t \approx 0.2eV$ and $\lambda \sim 0.2t$.

Here, charge current operator for $\mu$-direction ($\mu = x, y$) is given by [2]

$$j_\mu^C = -e \frac{\partial H}{\partial k_\mu} = -e \begin{pmatrix} v_x & v_x^a & 0 \\ v_x^a & 0 & 0 \\ 0 & 0 & v_x^z \end{pmatrix}, \quad (3)$$

where $v_x = \partial \xi_1 / \partial k_x$ and $v_x^z = \partial \xi_3 / \partial k_x$. The interorbital velocity $v_x^z = \partial g / \partial k_x = -4t'\sin k_y \cos k_x$ is called the “anomalous velocity”, which is the origin of the Hall effects [3,6]. Since $v_x^z$ has the same symmetry as $k_y$, $\langle v_x^z v_y \rangle$ can remain finite after the $k$-summations. Next, the $\sigma_z$-spin current and the $l_z$-orbital current are given by $j_\mu^S = \{j_\mu^C, s_\mu \}/2$ and $j_\mu^O = \{j_\mu^C, l_z \}/2$, respectively [3]. In the present model, current operators are also given by $6 \times 6$ matrix.

Now, we show the numerical results. We calculate the intrinsic SHC and OHC in the presence of local impurities using linear response theory. According to the linear response theory [7], the SHC and OHC is composed of the “Fermi surface term (I)” and “Fermi sea term (II)”.

![Figure 1](image-url)  

Figure 1 shows the $\lambda$-dependence of the (top) SHC and (bottom) OHC in $t_2g$-model for Sr$_2$RuO$_4$ $[n=4]$. A typical value of $\lambda$ for Ru$^{4+}$-ion corresponds to 0.4.
corresponds to ≈ 670 [ℏ/|e|]Ω^{-1}cm^{-1} if we put the interlayer distance of Sr$_2$RO$_4$; a ≈ 6Å. The obtained SHC and OHC for a typical values of λ ≈ 0.2 are much larger than values in semiconductors, because of the large Fermi surfaces and the large SO interaction in transition metal atoms.

3. SHE in transition metals

In this section, we study the SHE in Nb and Ta. They have a body-centered cubic (bcc) structure with lattice constant a = 3.3Å. To describe the electronic structure in Nb and Ta, we use the Naval Research Laboratory tight-binding (NRL-TB) model [8] within nine orbitals: 5s, 5p, 4d for Nb and 6s, 6p, 5d orbitals for Ta. In the presence of SO interaction λ \sum l \cdot s for d electrons, the total Hamiltonian is given by

$$\hat{H} = \begin{pmatrix} \hat{H}_0 + \lambda \hat{l}_z/2 & \lambda(\hat{l}_x - i\hat{l}_y)/2 \\ \lambda(\hat{l}_x + i\hat{l}_y)/2 & \hat{H}_0 - \lambda \hat{l}_z/2 \end{pmatrix}$$

where \(\hat{H}_0\) is a 9 × 9 matrix given by NRL-TB model. The matrix elements of \(l\) are given in ref. [4]. We set the SO coupling constant λ by use of ref. [9]: λ=0.006 Ry for 4d electron in Nb, and 0.023 Ry for 5d electron in Ta. We verified that the obtained band structures agree well with the results of a relativistic first-principles calculation near the Fermi level.

Now, we perform the numerical calculations for the SHC and OHC. Fig. 3 shows the resistivity (ρ) dependence of SHC and OHC in Nb and Ta. We find that the SHCs take large negative values in Nb and Ta. Note that the SHC in Pt is opposite in sign [15]. In usual, intrinsic SHC is independent of resistivity in the low resistive regime (ρ ≤ 50µΩcm), whereas it decreases approximately in proportional to ρ^{-2} in the high resistive regime [6]. We see that this coherent-incoherent crossover takes place in Nb. However, the obtained SHC in Ta decreases as ρ decreases even in the low resistive regime. We find that this anomalous behavior arises when accidental degenerate points exist slightly away from the Fermi level [10].

4. Summary

In summary, we studied the SHE and OHE in Sr$_2$RuO$_4$ and transition metals such as Nb and Ta. We found that huge SHE and OHE originate from the “effective Aharonov-Bohm phase” induced by the angular momentum of the atomic orbitals. The present study strongly suggests that “giant SHE and OHE” are ubiquitous in multi-
orbital $d, f$-electron systems with atomic orbital degrees of freedom. In near future, the novel field of SHE and OHE will be extended to wide variety of materials.

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