Report on MERIT Long-term Overseas Dispatch

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Place:	Eidgenössische Technische Hochschule Zürich
Group to Visit	Manfred Sigrist's Group
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Research Project:	Anomalous Nernst Effect Involving Magnetism and Topology: Toward a Giant Thermoelectric Effect with Magnon Drag and Rashba Effect

Abstract

I conducted research on the anomalous Nernst effect under the supervision of Professor Manfred Sigrist at the Swiss Federal Institute of Technology in Zurich (Eidgenössische Technische Hochschule Zürich, ETH) in Switzerland. Two systems were used for the study: one with Rashba-type interactions and another where magnon and s-d interactions coexist.

For systems with the Rashba interaction, we found that a significant Nernst coefficient occurs near the band edge when the magnetic parameter is sufficiently large, causing the band to split. This Nernst coefficient surpasses that of conventional ferromagnets. We also provide a general proof that this large Nernst coefficient arises from the momentum dependence of the Rashba interaction.

Regarding the anomalous Nernst effect due to Magnons, our model shows that the substantial anomalous Nernst conductivity observed in MnBi can be reproduced. Furthermore, we confirmed that our model shows the anisotropy similar to what has been experimentally observed.

Results for the Rashba System

We examined a system introducing z-axis ferromagnetism and a Rashba spin-orbit interaction, whose Hamiltonian is

$$\hat{\mathcal{H}} = \sum_{\boldsymbol{k}} \hat{\boldsymbol{c}}_{\boldsymbol{k}}^{\dagger} \left(\varepsilon_{\boldsymbol{k}}^{0} + \alpha (\hat{\boldsymbol{\sigma}} \times \boldsymbol{v}_{\boldsymbol{k}}) + h \hat{\sigma}_z + V^{\mathrm{imp}} \right) \hat{\boldsymbol{c}}_{\boldsymbol{k}}. \tag{1}$$

This model is more general than previous models that are used for research of anomalous Hall effect in Rashba systems, extending beyond the conventional free electron-like energy dispersion.

We performed numerical calculations of the anomalous Nernst effect for this setup as follows: First, we calculated the system's self-energy using the Born approximation and solved the Dyson equation self-consistently. Next, we computed the current operator. To take into account the vertex correction of impurities, we have to introduce correction terms for the current operator proportional to the Pauli matrix, which we also solved self-consistently. Finally, using these self-energies and operators, we calculated the conductivity spectrum for each energy through numerical integration.

We applied these calculations to a cos-type band that corresponds to the energy dispersion of a tight-binding model. We found that the Nernst coefficients cannot be significant without band splitting due to ferromagnetism. However, large coefficients emerged near the band edge when band splitting occurred, several times larger than those of common ferromagnets.

This phenomenon can be explained as follows: Assuming the Sommerfeld-Bethe relation holds, we can introduce the spectrum for longitudinal conductivity σ, and the spectrum for transverse conductivity η. Let us treat $(-f')\sigma$ and $(-f')\eta$ as "probability density functions," where f is the Fermi distribution function. Then, we can prove that the Nernst coefficient is proportional to the difference in expected energy values under the densities $(-f')\sigma$ and $(-f')\eta$. In conventional magnetic materials, this difference is very small because the momentum dependence of the current operators for longitudinal and transverse conductivities coincides. However, with the Rashba interaction, the momentum dependence of the current operator from the Rashba term differs significantly from that of the velocity operator, resulting in a large Nernst coefficient in systems with the Rashba interaction.

Results for the Magnon System

We have calculated how Magnons in ferromagnets affect the anomalous Nernst effect. Using perturbation theory, we derived a general formula for the thermoelectric coefficients due to Magnon drag. The method is following: First, we assume that the Hamiltonian is a sum of the unperturbed Hamiltonian whose the Bloch eigenstates can be obtained, magnon interactions, and s-d interactions. The s-d interaction is then rewritten in terms of these Bloch eigenstates. For the lowest-order perturbation contribution, we use the correlation between the electron current operator and the magnon heat current operator, as depicted in the Feynman diagrams. We consider intra-band and inter-band current operators separately to discuss each contribution individually.

For a specific numerical calculation of MnBi using this formula, we adopted the Bi model for the electron system's Hamiltonian and introduced parameters corresponding to ferromagnetism such as

$$\hat{\mathcal{H}} = \sum_{\boldsymbol{k}\sigma} \begin{pmatrix} c^\dagger_{+\downarrow} & c^\dagger_{+\uparrow} & c^\dagger_{-\uparrow} & c^\dagger_{-\downarrow} \end{pmatrix} \begin{pmatrix} \Delta\sigma_0 + h\sigma_z & i\hbar\gamma\boldsymbol{k}\cdot\boldsymbol{\sigma} \\ -i\hbar\gamma\boldsymbol{k}\cdot\boldsymbol{\sigma} & -\Delta\sigma_0 + h\sigma_z \end{pmatrix} \begin{pmatrix} c^\dagger_{+\downarrow} \\ c^\dagger_{+\uparrow} \\ c^\dagger_{-\uparrow} \\ c^\dagger_{-\downarrow} \end{pmatrix}. \tag{2}$$

This model replicates the scenario where itinerant electrons move through Bi sites and are influenced by Mn's magnetism. However, some difficulties lied in adopting this model because the Bloch eigenstates in this model are not diagonal with respect to spin. To overcome this difficulty, we extended our theory and developed a method to calculate the thermal conduction coefficients using the spin components of the Bloch eigenstates.

After that, we performed numerical calculations based on this extended theory, and it showed behavior consistent with experimental data. Specifically, we confirmed the presence of large Nernst conductivity and anisotropy, validating our calculations.

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