Berry phase and thermal transport coefficients in magnon systems

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Abstract. We theoretically calculate transverse thermal transport coefficients of the magnon system in the clean limit by the linear response theory in analogy with the electron. We find that there are additional correction terms to what are calculated by the usual Kubo formula. These correction terms arise because external fields change not only the distribution function but also the current operators in thermal transport. We show that the total thermal transport coefficients are expressed by the Berry curvature in momentum space; therefore the thermal Hall effect of magnon is totally due to the property of the magnon band structure.

1. Introduction
Linear response theory is one of the most useful and general formalisms to calculate various coefficients. For example, an electrical conductivity can be calculated as the linear response of the system to an external electric field, and then one obtains the general expression for the electrical conductivity expressed by the correlation functions; this is called the Kubo formula [1]. Such derivation is often called as a “mechanical” approach because Hamiltonian of both the system and the interaction with the external fields are well-defined. However, to consider the thermal transport, one cannot use this formula as such, because the thermal gradient cannot be taken into the Hamiltonian as an external field. To put it another way, the thermal gradient is not a dynamical force which exerts force to particles directly, but a statistical force which affects only through the distribution function of particles. To get rid of this difficulty, Luttinger [2] introduced a gravitational potential whose space- or time-variation produces an energy current (or a heat current), and it can be easily incorporated into the Hamiltonian as a perturbation. Replacement of the thermal gradient with this gravitational potential allows us to use the Kubo formula to calculate the thermal transport coefficients. In this way, Smrčka and Středa [3] obtained thermal coefficients in the electron system with the linear response theory, and Oji and Středa [4] obtained more general expressions by including the interactions of electrons.

In this paper, we calculate transverse thermal transport coefficients in a boson system, e.g., a magnon system, in the same manner as in a fermion system. We derive simple expressions of the thermal coefficients, using the Bloch wave function. In this expression, we show that the thermal coefficients and thermal Hall conductivity are described as a Berry curvature in momentum space; therefore we find that the thermal Hall effect of magnon in the clean limit [5, 6] is purely
due to the magnon band structure. This calculation gives a theoretical basis for understanding of dynamics of magnon wavepackets in ferromagnets [7].

2. Electron system

First we review the Smrčka and Středa’s work [3, 4] for the electron systems. The relation of both the electric current and the energy current to the fields can be written as

\[
\begin{align*}
J &= (LF)_{11} \left[ E + \frac{e}{c} \nabla \left( \frac{\psi}{c} \right) \right] + (LF)_{12} \left[ T \nabla \left( \frac{\psi}{c} \right) - \frac{\psi^2}{2c} \right], \\
J_E &= (LF)_{12} \left[ E + \frac{e}{c} \nabla \left( \frac{\psi}{c} \right) \right] + (LF)_{22} \left[ T \nabla \left( \frac{\psi}{c} \right) - \frac{\psi^2}{2c} \right],
\end{align*}
\]

where we label the thermal coefficients with superscript “F”, meaning a fermion, \( E \) is an electric field, \(-e (e > 0) \) is the electron charge, \( \mu \) is the chemical potential, \( T \) is the temperature, \((LF)_{ij}\) is the transport coefficients \((i, j = 1, 2)\), \( c \) is the speed of light and \( \psi \) is the gravitational field. In the presence of these fields, the electric and heat current operators, which are defined by the equation of continuity, acquire additional terms. These additional terms also produce correction terms to the thermal transport coefficients. Thus the thermal transport coefficients \((LF)_{ij}^{\alpha\beta}\), which are expressed as \((LF)_{ij}^{\alpha\beta} = (SF)_{ij}^{\beta\alpha} + (MF)_{ij}^{\alpha\beta} (\alpha, \beta = x, y, z)\), can be obtained as the followings:

\[
\begin{align*}
(SF)_{ij}^{\alpha\beta} &= \frac{i\hbar}{V} \int f(\eta) \text{Tr} \left( j^{\alpha}_i \frac{dG^+}{d\eta} j^{\beta}_j \delta(\eta - H) - j^{\beta}_j \delta(\eta - H) j^{\alpha}_i \frac{dG^-}{d\eta} \right) d\eta, \\
(MF)_{ij}^{\alpha\beta} &= \frac{e}{2V} \int f(\eta) \text{Tr} \delta(\eta - H) (\epsilon^{\alpha\beta} v^\alpha - \epsilon^{\beta\alpha} v^\beta) d\eta, \\
(SF)_{ij}^{\alpha\beta} &= \frac{1}{V} \int \eta f(\eta) \text{Tr} \delta(\eta - H) (\epsilon^{\alpha\beta} v^\alpha - \epsilon^{\beta\alpha} v^\beta) d\eta + \frac{i\hbar}{4V} \int f(\eta) \text{Tr} \delta(\eta - H) [\epsilon^\alpha, \epsilon^\beta] d\eta.
\end{align*}
\]

Here \( H \) is the unperturbed Hamiltonian of the system, \( V \) is a volume of the system, \( f(\eta) = (e^{(\eta - \mu)/k_BT} + 1)^{-1} \) is the Fermi distribution function, \( G^\pm \) is the Green’s function \( G^\pm(\eta) = (\eta - H \pm i\epsilon)^{-1} \), \( j^{\alpha}_i = -e v_i \), \( j^{\beta}_j = \frac{1}{i} (H v_j - v_j H) \), and \( v \) is the velocity. \((SF)_{ij}^{\alpha\beta}\) represent results from the usual Kubo formula since the equation (3) is indeed the Kubo formula itself; \((MF)_{ij}^{\alpha\beta}\) represent the correction terms [3, 4].

From these results derived by Smrčka and Středa, we derive some useful equations which are applicable for generic systems including magnon systems. First, we find that \((SF)_{ij}^{\alpha\beta}\) is expressed in terms of Berry phase by taking the trace. For example, we can write \((SF)_{12}^{\alpha\beta}\) as follows:

\[
(SF)_{12}^{\alpha\beta} = -\frac{e}{\hbar V} \text{Im} \sum_{\lambda} \left( f(\varepsilon_\lambda) \left( \frac{\partial u_{\lambda\alpha}}{\partial k_\alpha} \right| (H + \varepsilon_\lambda) \left( \frac{\partial u_{\lambda\beta}}{\partial k_\beta} \right) \right).
\]

Here the indices \( \lambda, \nu \) denote both the band index \( n \) and wave number \( k \), and \( u \) is the periodic part of the Bloch wave function. Second, at zero temperature, \((MF)_{12}^{\alpha\beta}\) and \((SF)_{12}^{\alpha\beta}\) is written as \((MF)_{12}^{\alpha\beta} = \mu e (LF)_{11}^{\alpha\beta} = -2e\mu \sum_\lambda \Theta(\mu - \varepsilon_\lambda) \text{Im} \left( \frac{\partial u_{\lambda\alpha}}{\partial k_\alpha} \right| \frac{\partial u_{\lambda\beta}}{\partial k_\beta} \right), \) and \((SF)_{12}^{\alpha\beta} = -2e\mu \text{Im} \sum_\lambda \Theta(\mu - \varepsilon_\lambda) \left( \frac{\partial u_{\lambda\alpha}}{\partial k_\alpha} \right| \frac{\partial u_{\lambda\beta}}{\partial k_\beta} \right). \) We note that the Fermi distribution function \( f(\eta) \) becomes the step function \( \Theta(\mu - \eta) \) at zero temperature. Using the relation \((MF)_{12}^{\alpha\beta} = (SF)_{12}^{\alpha\beta} + (MF)_{12}^{\alpha\beta}\) and equation (4) in the zero temperature limit, we obtain the following relation:

\[
\text{Tr}[\delta(\mu - H)(\epsilon^{\alpha\beta} v^\alpha - \epsilon^{\beta\alpha} v^\beta)] = \frac{d}{d\mu} \int_{-\infty}^{\mu} \text{Tr}[\delta(\eta - H)(\epsilon^{\alpha\beta} v^\alpha - \epsilon^{\beta\alpha} v^\beta)] d\eta = \frac{2V}{-e} \frac{d}{d\mu} \left( MF_{12}^{\alpha\beta} \right)_{T \to 0} = -2\frac{d}{\hbar} \sum_\lambda \Theta(\mu - \varepsilon_\lambda) \text{Im} \left( \frac{\partial u_{\lambda\alpha}}{\partial k_\alpha} \right| (H + \varepsilon_\lambda - 2\mu) \left( \frac{\partial u_{\lambda\beta}}{\partial k_\beta} \right).
\]
This equation is useful for the later calculation in the next section. We note that the l.h.s. of equation (7) corresponds to the orbital angular momentum. Hence by following the theories in [8, 9, 10, 11, 12], one can also derive equation (7) directly. It turns out that equation (7) holds whichever the particle is boson or fermion. Therefore we can apply this equation (7) to the magnon system as well.

3. Magnon system

Next we apply these formalisms to the magnon system. Since the magnon has no charge, the electron charge \(-e\) is dropped and the electric field \(E\) is replaced by a gradient of a confining potential \(-\nabla U(r)\) [7]. The equation (3)-(5) can be recast to

\[
(S^B)^{\alpha\beta}_{ij} = \frac{i\hbar}{V} \int \rho(\eta) \text{Tr} \left( j_i^\alpha \frac{dG^+}{d\eta} j_j^\beta (\eta - H) - j_j^\beta \delta(\eta - H) j_i^\alpha \frac{dG^-}{d\eta} \right) d\eta, \tag{8}
\]

\[
(M^B)^{\alpha\beta}_{11} = 0, \quad (M^B)^{\alpha\beta}_{12} = \frac{1}{2V} \int \rho(\eta) \text{Tr} \delta(\eta - H)(r^\alpha v^\beta - r^\beta v^\alpha) d\eta, \tag{9}
\]

\[
(M^B)^{\alpha\beta}_{22} = \frac{1}{V} \int \eta \rho(\eta) \text{Tr} \delta(\eta - H)(r^\alpha v^\beta - r^\beta v^\alpha) d\eta + \frac{i\hbar}{4} \int \rho(\eta) \text{Tr} \delta(\eta - H)[v^\alpha, v^\beta] d\eta, \tag{10}
\]

where \(j_1 = v\), and \(j_2 = \frac{1}{2}(Hv + \nu H)\), \(\rho(\eta) = (e^{(\eta - \mu)/k_B T} - 1)^{-1}\) is the Bose distribution function, and we labeled the thermal coefficients in the magnon system with superscript “B”, meaning a boson. As equation (6), we can similarly express \((S^B)^{\alpha\beta}_{ij}\) with the Bloch wave function. The calculation of correction terms \((M^B)^{\alpha\beta}_{12}\) and \((M^B)^{\alpha\beta}_{22}\) in terms of Berry phase is technical, because the expectation value of the position operator \(r^\alpha\) is not well-defined in the Bloch representation. To calculate these terms, we apply equation (7) to equation (9) and (10). For example, \((M^B)^{\alpha\beta}_{12}\) is calculated as the following:

\[
(M^B)^{\alpha\beta}_{12} = \frac{1}{2V} \int_{-\infty}^{\infty} \rho(\eta) \left( -\frac{2}{\hbar} \frac{d}{d\eta} \sum_\lambda \Theta(\eta - \varepsilon_\lambda) \text{Im} \left\langle \frac{\partial u_\lambda}{\partial k_\alpha} (H + \varepsilon_\lambda - 2\eta) \left| \frac{\partial u_\lambda}{\partial k_\beta} \right| \right\rangle \right) d\eta
\]

\[
= \frac{1}{\hbar V} \sum_\lambda \int_{\varepsilon_\lambda}^{\infty} \frac{d\rho(\eta)}{d\eta} \left( \text{Im} \left\langle \frac{\partial u_\lambda}{\partial k_\alpha} (H + \varepsilon_\lambda - 2\mu) \left| \frac{\partial u_\lambda}{\partial k_\beta} \right| \right\rangle - 2(\eta - \mu) \text{Im} \left\langle \frac{\partial u_\lambda}{\partial k_\alpha} \left| \frac{\partial u_\lambda}{\partial k_\beta} \right| \right\rangle \right) d\eta
\]

\[
= \frac{1}{\hbar V} \sum_\lambda \left( c_0(\rho(\varepsilon_\lambda)) \text{Im} \left\langle \frac{\partial u_\lambda}{\partial k_\alpha} (H + \varepsilon_\lambda - 2\mu) \left| \frac{\partial u_\lambda}{\partial k_\beta} \right| \right\rangle + 2c_1(\rho(\varepsilon_\lambda)) k_BT \text{Im} \left\langle \frac{\partial u_\lambda}{\partial k_\alpha} \left| \frac{\partial u_\lambda}{\partial k_\beta} \right| \right\rangle \right), \tag{11}
\]

where \(c_q(\rho) = \int_{\varepsilon_{nk}}^{\infty} d\varepsilon (\beta\varepsilon)^q \left( -\frac{d\rho}{d\varepsilon} \right)_{\mu=0} = \int_0^\mu \left( \log(1 + t^{-1}) \right)^q dt. For example, c_0(\rho) = \rho, c_1(\rho) = (1 + \rho) \log(1 + \rho) - \rho \log \rho, c_2(\rho) = (1 + \rho) \left( \log \frac{1+\rho}{\rho} \right)^2 - (\log \rho)^2 - 2L_2(-\rho), and L_2(z) is the polylogarithm function.

Similarly we obtain the convenient expressions of equation (8)-(10),

\[
(S^B)^{\alpha\beta}_{ij} = \frac{2}{\hbar V} \text{Im} \sum_{n,k} \rho_n \left\langle \frac{\partial u_n}{\partial k_\alpha} \left| \frac{H + \varepsilon_{nk}}{2} \right| \frac{\partial u_n}{\partial k_\beta} \right\rangle, \tag{12}
\]

\[
(M^B)^{\alpha\beta}_{11} = 0, \quad (M^B)^{\alpha\beta}_{12} = -\frac{2}{\hbar V} \text{Im} \sum_{n,k} \left( \mu \rho_n + k_BT c_1(\rho_n) \right) \left\langle \frac{\partial u_n}{\partial k_\alpha} \left| \frac{\partial u_n}{\partial k_\beta} \right| \right\rangle, \tag{13}
\]

\[
(M^B)^{\alpha\beta}_{22} = -\frac{2}{\hbar V} \text{Im} \sum_{n,k} \left( \mu^2 \rho_n + 2\mu k_BT c_1(\rho_n) + (k_BT)^2 c_2(\rho_n) \right) \left\langle \frac{\partial u_n}{\partial k_\alpha} \left| \frac{\partial u_n}{\partial k_\beta} \right| \right\rangle, \tag{14}
\]
where $\rho_n = \rho(\varepsilon_{n,k})$, and the thermal coefficients $L^B (= S^B + M^B)$ are obtained as

\[
(L^B)^{\alpha\beta}_{11} = - \frac{1}{hV} \sum_{n,k} \rho_n \Omega_n^z(k),
\]

\[
(L^B)^{\alpha\beta}_{12} = - \frac{1}{hV} \sum_{n,k} (\mu \rho_n + k_BT c_1(\rho_n)) \Omega_n^z(k),
\]

\[
(L^B)^{\alpha\beta}_{22} = - \frac{1}{hV} \sum_{n,k} (\mu^2 \rho_n + 2\mu k_BT c_1(\rho_n) + (k_BT)^2 c_2(\rho_n)) \Omega_n^z(k),
\]

where $\Omega_n^z(k)$ is the Berry curvature in momentum space: $\Omega_n^z(k) = i \left[ \frac{\partial u_n}{\partial k} \times \frac{\partial u_n}{\partial k} \right]_z$. Thus we can derive the thermal Hall conductivity $\kappa^{xy} = \left( (L^B)^{xy}_{22} - 2\mu (L^B)^{xy}_{12} + \mu^2 (L^B)^{xy}_{11} \right)/T$ from equation (15)-(17), and obtain

\[
\kappa^{xy} = \frac{2k_B^2 T}{hV} \sum_{n,k} c_2(\rho_n) \text{Im} \left( \frac{\partial u_n}{\partial k_x} \frac{\partial u_n}{\partial k_y} \right) = - \frac{k_B^2 T}{hV} \sum_{n,k} c_2(\rho_n) \Omega_{n,z}(k).
\]

As we can see from these equations (15)-(18), the thermal transport coefficients are expressed by the Berry curvature. Therefore, the thermal Hall effect of magnon is totally due to the magnon band structure because $\Omega_n^z(k)$ depends only on the magnon band structure. Compared with the previous work [5, 6], which includes only the $(S^B)^{\alpha\beta}_{ij}$, our results include both $(S^B)^{\alpha\beta}_{ij}$ and $(M^B)^{\alpha\beta}_{ij}$.

4. Conclusion

We calculated the thermal transport coefficients in the magnon system, as an example of the boson system, by using the linear response theory in analogy with the electron system. We expressed these coefficients in terms of the Bloch wave function, and found that these coefficients and the corresponding thermal Hall conductivity are described by the Berry curvature in momentum space. Consequently, we conclude that the thermal Hall effect of the magnon in the clean limit is purely due to the magnon band structure.

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