Note on geometrical description of weak-field Hall conductivity in metals

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Abstract

The geometrical formulae due to Tsuji (for 3D cubic metals) and Ong (for 2D metals) for the weak-field Hall conductivity are reviewed. Especially the Tsuji formula is discussed in Haldane's perspective.

1 Introduction

In this note we review the geometrical formulae [1, 2] for the weak-field Hall conductivity in metals.

In 2D the Ong [2] formula for the Hall conductivity is expressed only by the mean free path. In 3D the Tsuji [1] formula is expressed not only by the mean free path but also the curvature of the Fermi surface.

These formulae are geometrical interpretations of the Boltzmann conductivity and well understood in Haldane's perspective [3].

2 Boltzmann conductivity

The weak-field DC Hall conductivity σ^{xy} per spin is given by

$$\sigma^{xy} = e^3 B \sum_{\boldsymbol{k}} l^x \left(v^x \frac{\partial}{\partial k_y} - v^y \frac{\partial}{\partial k_x} \right) l^y \left(-\frac{\partial f}{\partial \varepsilon} \right), \tag{1}$$

using the solution of the linearized Boltzmann equation. Here the magnetic field is chosen as $\boldsymbol{B} = (0, 0, B)$ for simplicity. The mean free path vector $\boldsymbol{l} =$

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(l^x, l^y, l^z) is given as $\boldsymbol{l} = \tau \boldsymbol{v}$ where $\boldsymbol{v} = (v^x, v^y, v^z)$ is the velocity of the quasi-particle and τ is its renormalized transport life-time. $\partial f/\partial \varepsilon$ is the derivative of the Fermi distribution function f with respect to the quasi-particle energy ε. Although we have suppressed the argument of $\boldsymbol{v}$, τ and ε, they are the functions of the position $\boldsymbol{k} = (k^x, k^y, k^z)$ in $\boldsymbol{k}$-space. The component of the quasi-particle velocity v^α $(\alpha = x, y, z)$ is given as $v^\alpha = \partial\varepsilon/\partial k^\alpha \equiv \varepsilon_\alpha$.

Eq. (1) is valid when x- and y- directions are equivalent. For general case we should employ $\hat{\sigma}^{xy} \equiv (\sigma^{xy} - \sigma^{yx})/2$. Consequently we obtain[1]

$$\hat{\sigma}^{xy} = \frac{1}{2} e^3 B \sum_{\boldsymbol{k}} (v^x,\ v^y) \begin{pmatrix} M^{-1}_{yy} & -M^{-1}_{xy} \\ M^{-1}_{xy} & -M^{-1}_{xx} \end{pmatrix} \begin{pmatrix} v^x \\ v^y \end{pmatrix} \tau^2 \left(-\frac{\partial f}{\partial \varepsilon} \right), \tag{2}$$

where

$$M^{-1}_{\alpha\beta} \equiv \frac{\partial^2 \varepsilon}{\partial k^\alpha \partial k^\beta} \tag{3}$$

is the effective mass tensor.

It is remarkable that the derivatives of τ cancel out[2] through the anti-symmetrization $(\sigma^{xy} - \sigma^{yx})$.

Eq. (2) is the general result for the Hall conductivity so that you have only to estimate it numerically if you are not interested in its geometrical interpretation.

3 Fermi surface contribution

In the case of Fermi degeneracy we can estimate $-\partial f/\partial\varepsilon$ by the delta function:

$$\int \mathrm{d}\boldsymbol{k} \left(-\frac{\partial f}{\partial \varepsilon} \right) = \int \frac{\mathrm{d}S}{|\boldsymbol{v}|}, \tag{4}$$

where $\boldsymbol{v} = \partial\varepsilon/\partial\boldsymbol{k}$ and the integral in the right-hand-side is over the Fermi surface. Thus the Fermi surface contribution becomes

$$\hat{\sigma}^{xy} = \frac{1}{2} e^3 B \int \frac{\mathrm{d}S}{(2\pi)^3} (v^x,\ v^y) \begin{pmatrix} M^{-1}_{yy} & -M^{-1}_{xy} \\ M^{-1}_{xy} & -M^{-1}_{xx} \end{pmatrix} \begin{pmatrix} v^x \\ v^y \end{pmatrix} \frac{\tau^2}{|\boldsymbol{v}|}. \tag{5}$$

Throughout this note we only consider the contribution from a single sheet[3] of the Fermi surface.

[1] See [4] for $\hat{\sigma}^{xy}$. See, for example, [5]-(2.56) for σ^{xy}.

[2] Thus the expression for the Hall conductivity σ_{H} which contains the derivatives of τ, for example [5]-(2.53), is a bad expression.

[3] In the case of multi-sheets we should sum the contributions from all the sheets [3].

4 Haldane's perspective

The above expressions are derived using the factor $(\boldsymbol{v} \times \partial/\partial \boldsymbol{k}) \cdot \boldsymbol{B}$. If we switch the expression from $(\boldsymbol{v} \times \partial/\partial \boldsymbol{k}) \cdot \boldsymbol{B}$ to its equivalence $(\boldsymbol{B} \times \boldsymbol{v}) \cdot \partial/\partial \boldsymbol{k}$, we obtain the last equation in p.2-[3]:

$$\sigma^{xy} = e^3 \int \frac{\mathrm{d}S}{(2\pi)^3} l^x \left[(\boldsymbol{B} \times \boldsymbol{n}) \cdot \frac{\partial}{\partial \boldsymbol{k}} \right]_z l^y, \tag{6}$$

for the case of Fermi degeneracy. The unit normal vector is introduced as $\boldsymbol{n} = \boldsymbol{v}/|\boldsymbol{v}| = (n^x, n^y, n^z)$. The anti-symmetrization of Eq. (6) becomes Eq. (5).

Haldane introduced the symmetric tensor $\gamma_{\mu\nu}$ as[4]

$$\hat{\sigma}^{\alpha\beta} \equiv e^3 \epsilon^{\alpha\beta\mu} \gamma_{\mu\nu} B^\nu. \tag{8}$$

In our restricted case[5] Eq. (5) is written as $\hat{\sigma}^{xy} = e^3 \epsilon^{xyz} \gamma_{zz} B^z$ with[6]

$$\gamma_{zz} = \frac{1}{2} \int \frac{\mathrm{d}S}{(2\pi)^3} (v^x,\, v^y) \begin{pmatrix} M_{yy}^{-1} & -M_{xy}^{-1} \\ -M_{xy}^{-1} & M_{xx}^{-1} \end{pmatrix} \begin{pmatrix} v^x \\ v^y \end{pmatrix} \frac{\tau^2}{|\boldsymbol{v}|}. \tag{9}$$

This 2×2 representation can be related to the 3×3 representation

$$\begin{pmatrix} \kappa^{xx} & \kappa^{yx} & \kappa^{zx} \\ \kappa^{xy} & \kappa^{yy} & \kappa^{zy} \\ \kappa^{xz} & \kappa^{yz} & \kappa^{zz} \end{pmatrix}, \tag{10}$$

as discussed in the next section. See the Appendix C for the relation to the usual 2×2 representation[7]. The 3×3 matrix can be diagonalized as

$$\begin{pmatrix} \kappa_1 & 0 & 0 \\ 0 & \kappa_2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{11}$$

[4] We use Einstein's convention:

$$\epsilon^{\alpha\beta\mu} \gamma_{\mu\nu} B^\nu = \sum_\mu \sum_\nu \epsilon^{\alpha\beta\mu} \gamma_{\mu\nu} B^\nu. \tag{7}$$

[5] We measure the current in x-direction under the electric field in y-direction and the magnetic field in z-direction.

[6] In [3]

$$\gamma_{zz} = \frac{1}{2} \int \frac{\mathrm{d}S}{(2\pi)^3} (v^x,\, v^y) \begin{pmatrix} \kappa^{yy} & -\kappa^{yx} \\ -\kappa^{xy} & \kappa^{xx} \end{pmatrix} \begin{pmatrix} v^x \\ v^y \end{pmatrix},$$

since the integrand of $\gamma_{\alpha\beta}$ is given by $\epsilon_{\alpha\mu\delta}\epsilon_{\beta\nu\sigma} n^\mu n^\nu \kappa^{\delta\sigma} l^2$ and thus $\epsilon_{z\mu\delta}\epsilon_{z\nu\sigma} n^\mu n^\nu \kappa^{\delta\sigma} l^2 = (n^x n^x \kappa^{yy} - n^x n^y \kappa^{yx} - n^y n^x \kappa^{xy} + n^y n^y \kappa^{xx}) l^2$. This expression does not coincide with our Eq. (9), since ours needs only $(\partial v^x/\partial k^y)/|\boldsymbol{v}|$, for example, but Haldane's needs $\partial(v^x/|\boldsymbol{v}|)/\partial k^y$. In other words γ_{zz} should be compared with $\kappa^{\delta\sigma}$ but not with $n^\mu n^\nu \kappa^{\delta\sigma}$.

[7] The usual discussions of the 2×2 representation are summarized in the Appendices A and B.

as stated in the below Eq. (5) of [3]. The pair of the eigenvalues (κ_1 and κ_2) is the basis of the geometrical interpretation: $G = \kappa_1\kappa_2$ and $2H = \kappa_1 + \kappa_2$ where G is the Gaussian curvature and H is the mean curvature.

Especially the trace $2H$, which is independent of the choice of the local coordinate, is the target in the next section.

5 Tsuji formula in 3D

Our master equation (9) should be viewed as

$$\gamma_{zz} = \int \frac{\mathrm{d}S}{(2\pi)^3} h_{zz}\tau^2, \tag{12}$$

since h_{zz} is determined solely by the derivative of ε:

$$h_{zz} = \frac{1}{2|\boldsymbol{v}|}\left(\varepsilon_x\varepsilon_x\varepsilon_{yy} + \varepsilon_y\varepsilon_y\varepsilon_{xx} - \varepsilon_x\varepsilon_y\varepsilon_{yx} - \varepsilon_y\varepsilon_x\varepsilon_{xy}\right), \tag{13}$$

with $\varepsilon_\alpha \equiv v^\alpha$ and $\varepsilon_{\alpha\beta} \equiv M^{-1}_{\alpha\beta}$. This h_{zz} reflects the Fermi surface geometry but τ has no geometrical meaning. We should discuss the geometrical property by the symmetric tensor γ_{zz}.

On the other hand, the trace $2H$ of the 3×3 representation (10) becomes[8]

$$\begin{aligned} 2H \;=\; & \frac{1}{|\boldsymbol{v}|^3}\cdot\Big[\varepsilon_x\varepsilon_x(\varepsilon_{yy}+\varepsilon_{zz}) + \varepsilon_y\varepsilon_y(\varepsilon_{zz}+\varepsilon_{xx}) + \varepsilon_z\varepsilon_z(\varepsilon_{xx}+\varepsilon_{yy}) \\ & - \varepsilon_x(\varepsilon_y\varepsilon_{yx}+\varepsilon_z\varepsilon_{zx}) - \varepsilon_y(\varepsilon_x\varepsilon_{xy}+\varepsilon_z\varepsilon_{zy}) - \varepsilon_z(\varepsilon_x\varepsilon_{xz}+\varepsilon_y\varepsilon_{yz})\Big]. \end{aligned} \tag{14}$$

The mean curvature is given by this expression (14) for any shape of the Fermi surface.

By comparing (13) and (14) we see that h_{zz} is a piece of H. By summing three pieces we can construct H: $H = (h_{zz} + h_{xx} + h_{yy})/|\boldsymbol{v}|^2$ where

$$h_{xx} = \frac{1}{2|\boldsymbol{v}|}\left(\varepsilon_y\varepsilon_y\varepsilon_{zz} + \varepsilon_z\varepsilon_z\varepsilon_{yy} - \varepsilon_y\varepsilon_z\varepsilon_{zy} - \varepsilon_z\varepsilon_y\varepsilon_{yz}\right), \tag{15}$$

and

$$h_{yy} = \frac{1}{2|\boldsymbol{v}|}\left(\varepsilon_z\varepsilon_z\varepsilon_{xx} + \varepsilon_x\varepsilon_x\varepsilon_{zz} - \varepsilon_z\varepsilon_x\varepsilon_{xz} - \varepsilon_x\varepsilon_z\varepsilon_{zx}\right). \tag{16}$$

h_{zz} is obtained from the measurement: $\hat{\sigma}^{xy} = e^3\epsilon^{xyz}\gamma_{zz}B^z$. In the same manner h_{xx} and h_{yy} are obtained from the measurements: $\hat{\sigma}^{yz} = e^3\epsilon^{yzx}\gamma_{xx}B^x$

[8]Here $2H = \kappa^{xx} + \kappa^{yy} + \kappa^{zz}$. See Eq. (41) in the Appendix C for κ^{zz}. κ^{xx} and κ^{yy} are obtained in the same way.

and $\hat{\sigma}^{zx} = e^3 \epsilon^{zxy} \gamma_{yy} B^y$, respectively. By summing three experimental results with different configurations we obtain

$$\gamma_{zz} + \gamma_{xx} + \gamma_{yy} = \int \frac{\mathrm{d}S}{(2\pi)^3} H l^2, \tag{17}$$

with $l^2 = |\boldsymbol{l}|^2 = |\boldsymbol{v}|^2 \tau^2$.

In the case of cubic symmetry we obtain the Tsuji formula[9]

$$\gamma_{zz} = \gamma_{xx} = \gamma_{yy} = \int \frac{\mathrm{d}S}{(2\pi)^3} \frac{H}{3} l^2. \tag{18}$$

This form (18) is given in Eq. (4) of [3].

6 Ong formula in 2D

Although Haldane [3] discusses the relation between 2D and 3D formulae, we shall discuss the 2D case as a separate issue.

For simplicity, we put $\boldsymbol{B} = (0, 0, B)$ as in the previous section and set the 2D system in xy-plane. The 2D version of (6), Eq. (2) in [2], is given as

$$\sigma^{xy} = e^3 \int \frac{\mathrm{d}k_t}{(2\pi)^2} l^x \left[(\boldsymbol{B} \times \boldsymbol{n}) \cdot \frac{\partial}{\partial \boldsymbol{k}} \right]_z l^y, \tag{19}$$

where $\mathrm{d}k_t$ is the length along the Fermi line. Since $\boldsymbol{B} \times \boldsymbol{n} = B\boldsymbol{t}$ and $\boldsymbol{t} \cdot (\partial/\partial \boldsymbol{k}) = \partial/\partial k_t$, $(\boldsymbol{B} \times \boldsymbol{n}) \cdot (\partial/\partial \boldsymbol{k}) = B\partial/\partial k_t$ where $\boldsymbol{t}$ is the unit tangent vector along the Fermi line, Eq. (19) is written as

$$\sigma^{xy} = \frac{e^3 B}{(2\pi)^2} \int l^x \mathrm{d}l^y, \tag{20}$$

where $\mathrm{d}l^y = (\partial l^y/\partial k_t)\mathrm{d}k_t$. After the anti-symmetrization we obtain the Ong formula

$$\hat{\sigma}^{xy} = \frac{e^3 B}{(2\pi)^2} \int \frac{1}{2} \Big[l^x \mathrm{d}l^y - l^y \mathrm{d}l^x \Big] = \frac{e^3 B}{(2\pi)^2} \int \frac{1}{2} \Big[\boldsymbol{l} \times \mathrm{d}\boldsymbol{l} \Big]_z. \tag{21}$$

This form (21) is given in Eq. (3) of [2]. Moreover, Ong [2] discussed the "Stokes" area in $\boldsymbol{l}$-space.

[9] The derivation of the Tsuji formula is shown in the Appendix A of [5].

A Curvature in differential forms

In this appendix we review the minimum fundamentals[10] of a smooth surface Σ in 3D Euclidean space.

Let us choose a point $\boldsymbol{x}$ on the surface Σ and consider the vector $\boldsymbol{n}$ normal to Σ at $\boldsymbol{x}$. Then we move to another point $\boldsymbol{x}'$ on Σ and consider the normal vector $\boldsymbol{n}'$ there. Both $\boldsymbol{n}$ and $\boldsymbol{n}'$ are unit vectors. We assume that the movement is infinitesimally small so that both $\mathrm{d}\boldsymbol{x} \equiv \boldsymbol{x}' - \boldsymbol{x}$ and $\mathrm{d}\boldsymbol{n} \equiv \boldsymbol{n}' - \boldsymbol{n}$ are in the tangent plane[11] at the point $\boldsymbol{x}$.

The vectors in the tangent plane are expanded as $\mathrm{d}\boldsymbol{x} = \sigma_1 \boldsymbol{e}_1 + \sigma_2 \boldsymbol{e}_2$ and $\mathrm{d}\boldsymbol{n} = \omega_1 \boldsymbol{e}_1 + \omega_2 \boldsymbol{e}_2$ where $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ are the basis vectors of the tangent plane. Here σ_1, σ_2, ω_1 and ω_2 are 1-forms. The 2-form $\sigma_1\sigma_2$ represents the element of area of Σ. The 2-form $\omega_1\omega_2$ represents the element of area of the unit sphere. The Gaussian curvature K is introduced as the magnification factor between two areas: $\omega_1\omega_2 = K\sigma_1\sigma_2$.

Two sets of 1-forms are related by a symmetric matrix ($c = b$) as

$$\begin{pmatrix} \omega_1 \\ \omega_2 \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix}. \tag{22}$$

The determinant of this matrix is the Gaussian curvature: $K = ad - bc$. The trace is related to the mean curvature H: $2H = a + d$. If this 2×2 matrix is diagonalized as

$$\begin{pmatrix} \kappa_1 & 0 \\ 0 & \kappa_2 \end{pmatrix}, \tag{23}$$

$K = \kappa_1\kappa_2$ and $2H = \kappa_1 + \kappa_2$. Here the eigenvalues, κ_1 and κ_2, are principal curvatures.

B Components of 2×2 representation

In this appendix we calculate the components of the 2×2 matrix[12] in the Appendix A explicitly.

We give the point on the surface Σ as $\boldsymbol{x} = (x^1, x^2, u)$ with $u = u(x^1, x^2)$. Accordingly $\mathrm{d}\boldsymbol{x} = (\mathrm{d}x^1, \mathrm{d}x^2, \mathrm{d}u)$ where $\mathrm{d}u = p_1\mathrm{d}x^1 + p_2\mathrm{d}x^2$ with $p_i \equiv \partial u/\partial x^i$ ($i = 1, 2$). Introducing the vectors $\boldsymbol{t}_1 = (1, 0, p_1)$ and $\boldsymbol{t}_2 = (0, 1, p_2)$ the small tangent vector is written as $\mathrm{d}\boldsymbol{x} = \boldsymbol{t}_1\mathrm{d}x^1 + \boldsymbol{t}_2\mathrm{d}x^2$. The unit normal[13] vector is given by $\boldsymbol{n} = \boldsymbol{w}/|\boldsymbol{w}|$ with $\boldsymbol{w} = (-p_1, -p_2, 1)$.

[10] See, for example, §4.5 of [6].

[11] The normalization $\boldsymbol{n} \cdot \boldsymbol{n} = 1$ leads to $\mathrm{d}\boldsymbol{n} \cdot \boldsymbol{n} = 0$.

[12] See, for example, §8.2 of [6].

[13] It is apparent that $\boldsymbol{w} \cdot \boldsymbol{t}_1 = 0$ and $\boldsymbol{w} \cdot \boldsymbol{t}_2 = 0$.

Let us consider the map $\hat{A}$: $\mathrm{d}\boldsymbol{x} \to \mathrm{d}\boldsymbol{n}$ and introduce the 2×2 representation by

$$(\mathrm{d}\boldsymbol{n} \cdot \boldsymbol{t}_i) = \sum_{j=1}^{2} a_{ij} (\mathrm{d}\boldsymbol{x} \cdot \boldsymbol{t}_j), \tag{24}$$

where the inner product is defined as

$$\boldsymbol{x} \cdot \boldsymbol{t} = (x, y, z) \cdot (t, u, v)^{\mathrm{t}} = (x, y, z) \cdot \begin{pmatrix} t \\ u \\ v \end{pmatrix} = xt + yu + zv. \tag{25}$$

Since $\mathrm{d}\boldsymbol{n} \cdot \boldsymbol{t}_i = -(1/|\boldsymbol{w}|) \sum_j r_{ij} \mathrm{d}x^j$ and $\mathrm{d}\boldsymbol{x} \cdot \boldsymbol{t}_j = \sum_k (\delta_{jk} + p_j p_k) \mathrm{d}x^k$ with $r_{ij} = \partial^2 u / \partial x^i \partial x^j$, a_{ij} satisfies

$$\sum_{j=1}^{2} a_{ij} \left(\delta_{jk} + p_j p_k\right) = -\frac{1}{|\boldsymbol{w}|} r_{ik}. \tag{26}$$

In terms of Monge's notation ($p = \partial u/\partial x$, $q = \partial u/\partial y$, $r = \partial^2 u/\partial x^2$, $s = \partial^2 u/\partial x \partial y$, $t = \partial^2 u/\partial y^2$ with $x^1 = x$ and $x^2 = y$) Eq. (26) is written as

$$\hat{A} \begin{pmatrix} 1 + p^2 & pq \\ pq & 1 + q^2 \end{pmatrix} = -\frac{1}{|\boldsymbol{w}|} \begin{pmatrix} r & s \\ s & t \end{pmatrix}. \tag{27}$$

Thus

$$\hat{A} = \frac{1}{|\boldsymbol{w}|^3} \begin{pmatrix} pqs - (1 + q^2) r & pqr - (1 + p^2) s \\ pqt - (1 + q^2) s & pqs - (1 + p^2) t \end{pmatrix}. \tag{28}$$

The trace is readily obtained as

$$2H = \mathrm{trace}\left(\hat{A}\right) = \frac{1}{|\boldsymbol{w}|^3} \Big[2pqs - (1 + p^2) t - (1 + q^2) r \Big]. \tag{29}$$

After some calculations the determinant is obtained as

$$G = \det\left(\hat{A}\right) = \frac{1}{|\boldsymbol{w}|^4} \Big[rt - s^2 \Big]. \tag{30}$$

The components a_{ij} are also[14] obtained by the derivative of the unit normal vector $\boldsymbol{n} = (n^x, n^y, n^z)$ where $\boldsymbol{n} = \boldsymbol{w}/w$ with $\boldsymbol{w} = (-p, -q, 1)$ and $w^2 \equiv p^2 + q^2 + 1$. Here we put $p_x \equiv r$, $q_y \equiv t$ and $s \equiv p_y = q_x$ for the convenience of the calculation. The results[15] are

$$a_{11} = \frac{\partial n^x}{\partial x} = -\frac{1}{w} p_x + \frac{p}{w^3} (p p_x + q q_x) = \frac{1}{w^3} \Big[pqs - (1 + q^2) r \Big], \tag{31}$$

[14] If we set the view point at $(0, 0, \infty)$, the identification, $a_{11} = \partial n^x / \partial x$, $a_{21} = \partial n^x / \partial y$, $a_{12} = \partial n^y / \partial x$ and $a_{22} = \partial n^y / \partial y$, is naturally understood.

[15] Here we should take care that $\mathrm{d}\boldsymbol{n} = \mathrm{d}\boldsymbol{x} \hat{A}$.

$$a_{21} = \frac{\partial n^x}{\partial y} = -\frac{1}{w}p_y + \frac{p}{w^3}(pp_y + qq_y) = \frac{1}{w^3}\Big[pqt - (1+q^2)s\Big], \tag{32}$$

$$a_{12} = \frac{\partial n^y}{\partial x} = -\frac{1}{w}q_x + \frac{q}{w^3}(pp_x + qq_x) = \frac{1}{w^3}\Big[pqr - (1+p^2)s\Big], \tag{33}$$

$$a_{22} = \frac{\partial n^y}{\partial y} = -\frac{1}{w}q_y + \frac{q}{w^3}(pp_y + qq_y) = \frac{1}{w^3}\Big[pqs - (1+p^2)t\Big]. \tag{34}$$

C 3×3 representation

Here we move from $\boldsymbol{x}$-space to $\boldsymbol{k}$-space. In the Appendix B we have assumed that the z-component is given by the function $u(x, y)$ explicitly. In the following we assume that the point $\boldsymbol{k} = (k^x, k^y, k^z)$ on the Fermi surface is given by $\varepsilon(\boldsymbol{k}) = 0$ implicitly.

The 2×2 matrix introduced in the Appendix B is written as

$$\begin{pmatrix} \kappa^{xx} & \kappa^{yx} \\ \kappa^{xy} & \kappa^{yy} \end{pmatrix}, \tag{35}$$

which is a part of the 3×3 matrix

$$\begin{pmatrix} \kappa^{xx} & \kappa^{yx} & \kappa^{zx} \\ \kappa^{xy} & \kappa^{yy} & \kappa^{zy} \\ \kappa^{xz} & \kappa^{yz} & \kappa^{zz} \end{pmatrix}, \tag{36}$$

where

$$\kappa^{ab} \equiv \frac{\partial n^a}{\partial k^b}, \tag{37}$$

with $a, b = x, y, z$.

If the 2×2 matrix is diagonalized as

$$\begin{pmatrix} \kappa_1 & 0 \\ 0 & \kappa_2 \end{pmatrix}, \tag{38}$$

then the 3×3 matrix is diagonalized as

$$\begin{pmatrix} \kappa_1 & 0 & 0 \\ 0 & \kappa_2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{39}$$

since both $\mathrm{d}\boldsymbol{n}$ and $\mathrm{d}\boldsymbol{x}$ are in the tangent plane so that the normal vector becomes the eigenvector of the 3×3 matrix with zero eigenvalue. Consequently the trace of the 3×3 matrix is equal to the trace of 2×2 matrix.

The components κ^{ab} are expressed in terms of the derivative of the quasi-particle energy ε. For example,

$$\kappa^{zz} = \frac{\partial n^z}{\partial k^z} = \frac{\partial}{\partial k^z} \frac{\varepsilon_z}{(\varepsilon_x^2 + \varepsilon_y^2 + \varepsilon_z^2)^{1/2}} = \frac{\varepsilon_{zz}}{|\boldsymbol{v}|} - \frac{\varepsilon_z}{|\boldsymbol{v}|^3}(\varepsilon_x \varepsilon_{xz} + \varepsilon_y \varepsilon_{yz} + \varepsilon_z \varepsilon_{zz}), \quad (40)$$

where $|\boldsymbol{v}|^2 = \varepsilon_x^2 + \varepsilon_y^2 + \varepsilon_z^2$. In Eq. (40) the term $\varepsilon_z \varepsilon_z \varepsilon_{zz}$, which is not expected for the off-diagonal conductivity, disappers by the subtraction so that we obtain

$$\kappa^{zz} = \frac{1}{|\boldsymbol{v}|^3} \Big[(\varepsilon_x \varepsilon_x + \varepsilon_y \varepsilon_y) \varepsilon_{zz} - \varepsilon_z (\varepsilon_x \varepsilon_{xz} + \varepsilon_y \varepsilon_{yz}) \Big]. \quad (41)$$

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