# Space-Time Symmetry Restrictions on Transport Coefficients. III. Thermogalvanomagnetic Coefficients*

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Further development is given of the application to thermogalvanomagnetic coefficients of basic equations determining space-time symmetry restrictions. Material omitted from tables published by the author is supplied. Also, the thermogalvanomagnetic coefficients are expanded in powers of the components of the magnetic field, and the symmetry restrictions imposed on the expansion coefficients are discussed. The method is apparently also applicable to other transport coefficients and for other fields.

## 1. INTRODUCTION

THE effect of spatial and time-inversion symmetry on properties of magnetic systems has been much discussed since the early 1950's.[1] Recently, the distinction between symmetry restrictions on equilibrium properties and those on transport properties has been pointed out[2–4] and discussed in some detail.[3,4]

Here a further development is given of the application to thermogalvanomagnetic (TGM) coefficients of basic equations, derived in I, determining space-time symmetry restrictions. In Sec. 2 ideas presented in Secs. 3 B and 3 C of I are further developed for cases in which a magnetic field is present ($\mathbf{H}\neq 0$). In particular, it is pointed out that certain symmetry groups were omitted from some of the tables of I. The required modifications are detailed. In Sec. 3, the TGM coefficients $\tau(\mathbf{H})_{\mu\nu}$ are expanded in powers of the components of the magnetic field and the symmetry restrictions imposed on the expansion coefficients are discussed.

In I, a derivation was given of basic equations [(2.17) and (2.28) of I] which determine the restrictions on field-dependent transport coefficients arising from symmetry operations involving time inversion as well as spatial transformations. The derivation started from microscopic expressions for the transport coefficients in terms of thermal averages of products of quantum-mechanical operators. These equations reduce to equations of simpler form [(3.6) and (3.7) of I] when specialized to apply to the case of TGM coefficients.

The full (magnetic) space group symmetry of a crystal is not required for determining the symmetry restrictions on the TGM coefficients. It suffices to use the Laue group $\mathcal{K}^L(0)$ of the crystal obtained from the crystal point group by replacing the rotational part of any improper symmetry element by its proper counterpart (space inversion is everywhere replaced by the identity). The 32 crystal Laue groups are listed in Table II of I, and for each of these the symmetry-restricted matrices of thermoelectric coefficients (TGM coefficients with the magnetic field $\mathbf{H}=0$) can be found in Tables IV–VI of I.

## 2. TGM COEFFICIENTS $\tau(\mathbf{H})_{\mu\nu}$: FURTHER DISCUSSION

We want here to elucidate the symmetry restrictions on the TGM coefficients $\tau(\mathbf{H})_{\mu\nu}$ when a uniform magnetic field is present ($\mathbf{H}\neq 0$). When $\mathbf{H}\neq 0$, the symmetry restrictions are determined jointly by the crystal Laue group $\mathcal{K}^L(0)$ and the magnetic field direction (given by $\hat{H}=\mathbf{H}/H$), and were classified in I according to certain symmetry groups determined by $\mathcal{K}^L(0)$ and $\hat{H}$. These groups include the following: $\mathcal{G}^L(\mathbf{H})$—the subgroup of $\mathcal{K}^L(0)$ which leaves $\mathbf{H}$ invariant; $\mathcal{K}^L(\mathbf{H})$—the subgroup of $\mathcal{K}^L(0)$, elements of which leave $\mathbf{H}$ invariant or reverse its direction; $\mathcal{G}_L{}^L(\mathbf{H})$—the subgroup of $\mathcal{G}^L(\mathbf{H})$ not involving time inversion; and $\mathcal{K}_L{}^L(\mathbf{H})$—the subgroup of $\mathcal{K}^L(\mathbf{H})$ not involving time inversion. If $\mathcal{K}^L(0)$ is the three-dimensional pure rotation group together with time inversion, then $\mathcal{K}^L(\mathbf{H})=\infty 21'$ and $\mathcal{G}^L(\mathbf{H})=\infty 2'$; consequently, for crystals, $\mathcal{K}^L(\mathbf{H})$ is a subgroup of $\infty 21'$ and $\mathcal{G}^L(\mathbf{H})$ is a subgroup of $\infty 2'$. The classification in I was given in terms of case and category according to Table I of I, the five mutually exclusive cases corresponding to different values of the set of three indices: the index of $\mathcal{G}^L(\mathbf{H})$ in $\mathcal{K}^L(\mathbf{H})$, the index of $\mathcal{G}_L{}^L(\mathbf{H})$ in $\mathcal{G}^L(\mathbf{H})$, and the index of $\mathcal{K}_L{}^L(\mathbf{H})$ in $\mathcal{K}^L(\mathbf{H})$. Each of the five possible cases determines the category (a), (b), or (c).

To elucidate the types of symmetry restrictions on the TGM coefficients for $\mathbf{H}\neq 0$ the discussion of I is here extended by listing (in Table I), for each $\mathcal{K}^L(0)$, representative directions for the different possible types of symmetry-inequivalent directions of $\mathbf{H}$. For each $[\mathcal{K}^L(0),\hat{H}]$ pair in Table I, the groups $\mathcal{K}^L(\mathbf{H})$, $\mathcal{G}^L(\mathbf{H})$, and $\mathcal{K}_L{}^L(\mathbf{H})$, as well as the case and category, are specified. Table I provides an overview of the possible symmetries of TGM coefficients and serves as an aid in applying the tables of symmetry-restricted matrices in I. This table is, however, not restricted in application to TGM coefficients; it applies whenever the symmetry restrictions are determined by the zero-field Laue groups $\mathcal{K}^L(0)$ together with the direction of $\mathbf{H}$.

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[1] See Ref. 4 for earlier references and a brief history.
[2] S. Shtrikman and H. Thomas, Solid State Commun. 3, 147 (1965); 3, No. 9, p. *civ* (E) (1965).
[3] W. H. Kleiner, Phys. Rev. 142, 318 (1966). Referred to as I.
[4] W. H. Kleiner, Phys. Rev. 153, 726 (1967).

TABLE I. Laue groups $\mathcal{H}^L(\mathbf{H})$, $\mathcal{G}^L(\mathbf{H})$, and $\mathcal{H}_L{}^L(\mathbf{H})$ and the case and category of $\mathcal{H}^L(\mathbf{H})$ for the characteristic symmetry directions of $\mathbf{H}$ for each of the crystal Laue groups $\mathcal{H}^L(0)$. The groups $\mathcal{H}^L(0)$ are listed in the same order as in Table II of Ref. 3. The directions $\hat{H}$ of $\mathbf{H}$ are listed in decreasing order of the symmetry axes, first parallel to the axes, then perpendicular. An indicated range of symmetry directions of $\mathbf{H}$ is to be interpreted as excluding symmetry directions listed previously for the same $\mathcal{H}^L(0)$. For $\mathbf{H}$ in a direction of no special symmetry, the entry is given by that for the $\mathcal{H}^L(0)$ of lowest symmetry in the same category. The subscript on the symbol $2_\perp'$ indicates that the axis is perpendicular to $\mathbf{H}$. The $\mathcal{H}_L{}^L(\mathbf{H})$ are listed only for $\mathcal{H}^L(0)$ in category (c), since for $\mathcal{H}^L(0)$ in category (b), $\mathcal{H}_L{}^L(\mathbf{H})=\mathcal{H}^L(\mathbf{H})$ and for $\mathcal{H}^L(0)$ in category (a), $\mathcal{H}^L(\mathbf{H})=\mathcal{H}_L{}^L(\mathbf{H})1'$.

| $\mathcal{H}^L(0)$ | $\hat{H}$ | $\mathcal{H}^L(\mathbf{H})$ | $\mathcal{G}^L(\mathbf{H})$ | $\mathcal{H}_L{}^L(\mathbf{H})$ | Case | Category |
|---|---|---|---|---|---|---|
| 1 | ... | 1 | 1 | | i | b |
| 2 | ∥2 | 2 | 2 | | i | b |
| | ⊥2 | 2 | 1 | | iii | b |
| 222 | ∥2 | 222 | 2 | | iii | b |
| | ⊥2 | 2 | 1 | | iii | b |
| 4 | ∥4 | 4 | 4 | | i | b |
| | ⊥4 | 2 | 1 | | iii | b |
| 422 | ∥4 | 422 | 4 | | iii | b |
| | ∥2 | 222 | 2 | | iii | b |
| | ⊥4 | 2 | 1 | | iii | b |
| | ⊥2 | 2 | 1 | | iii | b |
| 3 | ∥3 | 3 | 3 | | i | b |
| 32 | ∥3 | 32 | 3 | | iii | b |
| | ∥2 | 2 | 2 | | i | b |
| | ⊥2 | 2 | 1 | | iii | b |
| 6 | ∥6 | 6 | 6 | | i | b |
| | ⊥6 | 2 | 1 | | iii | b |
| 622 | ∥6 | 622 | 6 | | iii | b |
| | ∥2 | 222 | 2 | | iii | b |
| | ⊥6 | 2 | 1 | | iii | b |
| | ⊥2 | 2 | 1 | | iii | b |
| 23 | ∥3 | 3 | 3 | | i | b |
| | ∥2 | 222 | 2 | | iii | b |
| | ⊥2 | 2 | 1 | | iii | b |
| 432 | ∥4 | 422 | 4 | | iii | b |
| | ∥3 | 32 | 3 | | iii | b |
| | ∥2 | 222 | 2 | | iii | b |
| | ⊥4 | 2 | 1 | | iii | b |
| | ⊥2 | 2 | 1 | | iii | b |
| 1′ | ... | 1′ | 1 | | iv | a |
| 21′ | ∥2 | 21′ | 2 | | iv | a |
| | ⊥2 | 21′ | 2′ | | v | a |
| 2221′ | ∥2 | 2221′ | 2′2′2 | | v | a |
| | ⊥2 | 21′ | 2′ | | v | a |
| 41′ | ⊥4 | 21′ | 2′ | | v | a |
| | ⊥4 | 21 | 2 | | v | a |
| 4221′ | ∥4 | 4221′ | 42′2′ | | v | a |
| | ∥2 | 2221′ | 22′2′ | | v | a |
| | ⊥4 | 21′ | 2′ | | v | a |
| | ⊥2 | 21′ | 2′ | | v | a |
| 3′ | ∥3 | 3′ | 3 | | iv | a |
| 3′2 | ∥3 | 3′2 | 32′ | | v | a |
| | ∥2 | 21′ | 2 | | iv | a |
| | ⊥2 | 21′ | 2′ | | v | a |
| 61′ | ∥6 | 61′ | 6 | | iv | a |
| | ⊥6 | 21′ | 2′ | | v | a |
| 6221′ | ∥6 | 6221′ | 62′2′ | | v | a |
| | ∥2 | 2221′ | 22′2′ | | v | a |
| | ⊥6 | 21′ | 2′ | | v | a |
| | ⊥2 | 21′ | 2′ | | v | a |
| 23′ | ∥3 | 3′ | 3 | | iv | a |
| | ∥2 | 2221′ | 2′2′2 | | v | a |
| | ⊥2 | 21′ | 2′ | | v | a |
| 43′2 | ∥4 | 4221′ | 42′2′ | | v | a |
| | ∥3 | 3′2 | 32′ | | v | a |
| | ∥2 | 2221′ | 22′2′ | | v | a |
| | ⊥4 | 21′ | 2′ | | v | a |
| | ⊥2 | 21′ | 2′ | | v | a |
| 2′ | ∥2′ | 2′ | 1 | 1 | iv | a |
| | ⊥2′ | 2′ | 2′ | 1 | ii | c |
| | ... | 1 | 1 | 1 | i | b |
| 2′2′2 | ∥2 | 2′2′2 | 2′2′2 | 2 | ii | c |
| | ∥2′ | 2′2′2 | $2_\perp'$ | 2 | v | a |
| | ⊥2 | 2 | 1 | 2 | iii | b |
| | ⊥2′ | 2′ | 2′ | 1 | ii | c |
| 4′ | ∥4′ | 4′ | 2 | 2 | iv | a |
| | ⊥4′ | 2 | 1 | 2 | iii | b |
| 4′22′ | ∥4′ | 4′22′ | 2′2′2 | 222 | v | a |
| | ∥2 | 222 | 2 | 222 | iii | b |
| | ∥2′ | 2′2′2 | $2_\perp'$ | 2 | v | a |
| | ⊥4′ | 2 | 1 | 2 | iii | b |
| | ⊥2 | 2 | 1 | 2 | iii | b |
| | ⊥2′ | 2′ | 2′ | 1 | ii | c |
| 42′2′ | ∥4 | 42′2′ | 42′2′ | 4 | ii | c |
| | ∥2′ | 2′2′2 | $2_\perp'$ | 2 | v | a |
| | ⊥4 | 2 | 1 | 2 | iii | b |
| | ⊥2′ | 2′ | 2′ | 1 | ii | c |
| 32′ | ∥3 | 32′ | 32′ | 3 | ii | c |
| | ∥2′ | 2′ | 1 | 1 | iv | a |
| | ⊥2′ | 2′ | 2′ | 1 | ii | c |
| 6′ | ∥6′ | 6′ | 3 | 3 | iv | a |
| | ⊥6′ | 2′ | 2′ | 1 | ii | c |
| 6′22′ | ∥6′ | 6′22′ | 32′ | 32 | v | a |
| | ∥2 | 22′2′ | 22′2′ | 2 | ii | c |
| | ∥2′ | 22′2′ | $2_\perp'$ | 2 | v | a |
| | ⊥6′ | 2′ | 2′ | 1 | ii | c |
| | ⊥2 | 2 | 1 | 2 | iii | b |
| | ⊥2′ | 2′ | 2′ | 1 | ii | c |
| 62′2′ | ∥6 | 62′2′ | 62′2′ | 6 | ii | c |
| | ∥2′ | 2′2′2 | $2_\perp'$ | 2 | v | a |
| | ⊥6 | 2 | 1 | 2 | iii | b |
| | ⊥2′ | 2′ | 2′ | 1 | ii | c |
| 4′32′ | ∥4′ | 4′22′ | 2′2′2 | 222 | v | a |
| | ∥3 | 32′ | 32′ | 3 | ii | c |
| | ∥2′ | 2′2′2 | $2_\perp'$ | 2 | v | a |
| | ⊥4′ | 2 | 1 | 2 | iii | b |
| | ⊥2′ | 2′ | 2′ | 1 | ii | c |

Several facts are evident from Table I. For given $\mathcal{H}^L(0)$, there are generally several distinct groups $\mathcal{H}^L(\mathbf{H})$ depending on the direction of $\mathbf{H}$. Also, different combinations $[\mathcal{H}^L(0),\hat{H}]$ can lead to the same $\mathcal{H}^L(\mathbf{H})$. In particular, it is possible for a given Laue group to occur as a group $\mathcal{H}^L(\mathbf{H})$ in different categories; for example,

$\mathcal{K}^L(\mathbf{H})=2'$ has category-case (a)-(iv) when $\mathbf{H}$ is parallel to the two-fold axis and $\mathcal{K}^L(\mathbf{H})=2'$ has category-case (c)-(ii) when $\mathbf{H}$ is perpendicular to the two-fold axis. Category-(a) groups $\mathcal{K}^L(0)$ have only category-(a) subgroups $\mathcal{K}^L(\mathbf{H})$, and category-(b) groups $\mathcal{K}^L(0)$ have only category-(b) subgroups $\mathcal{K}^L(\mathbf{H})$. However, a category-(c) group $\mathcal{K}^L(0)$ may in general have subgroups $\mathcal{K}^L(\mathbf{H})$ of category (a), (b), and/or (c).

The groups $\mathcal{K}^L(\mathbf{H})$ which are in category (a) and are subgroups of a group $\mathcal{K}^L(0)$ in category (c) were overlooked in the discussion before (3.16) of I and were hence omitted from the tables of I. The omitted groups $\mathcal{K}^L(\mathbf{H})$ are $2'$, $4'$, and $6'$ of category-case (a)-(iv) and $2'2'2$, $4'22'$, and $6'22'$ of category-case (a)-(v). Symmetry-restricted matrices of TGM coefficients for $2'$, $4'$, and $6'$ should have been included in Table VIII of I; similarly, matrices for $2'2'2$, $4'22'$, and $6'22'$ should have been included in Table IX. These groups should also have been listed correspondingly in Table III of I. These omissions are remedied by supplementary tables: Tables II–IV of the present paper, corresponding to Tables III, VIII, and IX of I, respectively.

TABLE II. Supplement to Table III of Ref. 3, which classifies Laue groups. The entries of this table are to replace the corresponding entries of that table. $\theta=1'$.

| Category | Case | Table | Groups |
|---|---|---|---|
| $H\neq 0$ (a) | (iv) | VIII | $\mathcal{K}^L=\mathcal{G}_L{}^L+\mathcal{G}_L{}^L b^L$,<br>$b^L=\theta$: $1', 21', 3', 41', 61'$; $\infty 1'$<br>$b^L\neq\theta$: $2', 4', 6'$; $\infty'$ |
| (a) | (v) | IX | $\mathcal{K}^L=\mathcal{K}_L{}^L+\mathcal{K}_L{}^L a^L=\mathcal{G}^L+\mathcal{G}^L b^L$, $\mathcal{G}^L\neq\mathcal{G}_L{}^L$<br>$a^L=\theta$: $21', 2221', 3'2, 4221', 6221'$; $\infty 21'$<br>$a^L\neq\theta$: $2'2'2, 4'22', 6'22'$; $(2n)'22'$ |

### 3. EXPANSION IN POWERS OF $H_\mu$

It is often useful to expand a field-dependent transport coefficient in powers of the components of the field, particularly when small values of the field are involved. It is then important to know the space-time symmetry restrictions on the coefficients in the expansion. We indicate here how these restrictions can be obtained in a simple way from the basic equations (mentioned in the Introduction and derived in I) which determine space-time symmetry restrictions on field-dependent transport coefficients. Although most of the discussion is for the case of TGM coefficients, the method is apparently applicable also to other transport coefficients and for other fields.

The procedure is simply to substitute the expansion for the transport coefficient

$$\tau_{B_\mu A_\nu}(\mathbf{H})=\sum_{k=0}\sum_{\alpha_1\alpha_2\cdots\alpha_k}\tau_{B_\mu A_\nu\alpha_1\alpha_2\cdots\alpha_k}H_{\alpha_1}H_{\alpha_2}\cdots H_{\alpha_k} \quad (1)$$

on both sides of Eqs. (2.17) and (2.28) of I, and to equate like powers of the components of the field for the

TABLE III. Symmetry-restricted matrices of TGM coefficients for $H\neq 0$, (a)-(iv): supplement to Table VIII of Ref. 3. $\mathbf{H}$ is parallel to the $(2n)'$ axis, $n=1, 2, \cdots$.

| $\mathcal{K}^L(\mathbf{H})$ | $\boldsymbol{\tau}'^e(\mathbf{H})$ | $\boldsymbol{\tau}'^0(\mathbf{H})$ | $\boldsymbol{\sigma}^e(\mathbf{H})$ | $\boldsymbol{\sigma}^0(\mathbf{H})$ |
|---|---|---|---|---|
| $2'$ | $\begin{pmatrix}\tau_{xx} & \tau_{yx} & -\tau_{zx}\\ \tau_{xy} & \tau_{yy} & -\tau_{zy}\\ -\tau_{xz} & -\tau_{yz} & \tau_{zz}\end{pmatrix}$ | $\begin{pmatrix}-\tau_{xx} & -\tau_{yx} & \tau_{zx}\\ -\tau_{xy} & -\tau_{yy} & \tau_{zy}\\ \tau_{xz} & \tau_{yz} & -\tau_{zz}\end{pmatrix}$ | $\begin{pmatrix}\sigma_{xx} & \sigma_{xy} & \sigma_{xz}\\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz}\\ -\sigma_{xz} & -\sigma_{yz} & \sigma_{zz}\end{pmatrix}$ | $\begin{pmatrix}0 & \sigma_{xy} & \sigma_{xz}\\ -\sigma_{xy} & 0 & \sigma_{yz}\\ \sigma_{xz} & \sigma_{yz} & 0\end{pmatrix}$ |
| $4'$ | $\begin{pmatrix}\tau_{yy} & -\tau_{xy} & 0\\ -\tau_{yx} & \tau_{xx} & 0\\ 0 & 0 & \tau_{zz}\end{pmatrix}$ | $\begin{pmatrix}-\tau_{yy} & \tau_{xy} & 0\\ \tau_{yx} & -\tau_{xx} & 0\\ 0 & 0 & -\tau_{zz}\end{pmatrix}$ | $\begin{pmatrix}\sigma_{xx} & 0 & 0\\ 0 & \sigma_{xx} & 0\\ 0 & 0 & \sigma_{zz}\end{pmatrix}$ | $\begin{pmatrix}\sigma_{xx} & \sigma_{xy} & 0\\ \sigma_{yx} & -\sigma_{xx} & 0\\ 0 & 0 & 0\end{pmatrix}$ |
| $(2n')$<br>$n=3, 4, \cdots$ | $\begin{pmatrix}\tau_{xx} & -\tau_{xy} & 0\\ \tau_{xy} & \tau_{xx} & 0\\ 0 & 0 & \tau_{zz}\end{pmatrix}$ | $\begin{pmatrix}-\tau_{xx} & \tau_{xy} & 0\\ -\tau_{xy} & -\tau_{xx} & 0\\ 0 & 0 & -\tau_{zz}\end{pmatrix}$ | $\begin{pmatrix}\sigma_{xx} & 0 & 0\\ 0 & \sigma_{xx} & 0\\ 0 & 0 & \sigma_{zz}\end{pmatrix}$ | $\begin{pmatrix}0 & \sigma_{xy} & 0\\ -\sigma_{xy} & 0 & 0\\ 0 & 0 & 0\end{pmatrix}$ |

TABLE IV. Symmetry-restricted matrices of TGM coefficients for $H\neq 0$, (a)-(v): supplement to Table IX of Ref. 3. $\mathbf{H}$ is parallel to the $(2n)'$ axis, $n=1, 2, \cdots$.

| $\mathcal{K}^L(\mathbf{H})$ | $\boldsymbol{\tau}'^e(\mathbf{H})$ | $\boldsymbol{\tau}'^0(\mathbf{H})$ | $\boldsymbol{\sigma}^e(\mathbf{H})$ | $\boldsymbol{\sigma}^0(\mathbf{H})$ |
|---|---|---|---|---|
| $2'2'2$<br>$(H\Vert 2_x')$ | $\begin{pmatrix}\tau_{xx} & -\tau_{yx} & 0\\ -\tau_{xy} & \tau_{yy} & 0\\ 0 & 0 & \tau_{zz}\end{pmatrix}$ | $\begin{pmatrix}0 & 0 & \tau_{zx}\\ 0 & 0 & -\tau_{zy}\\ \tau_{xz} & -\tau_{yz} & 0\end{pmatrix}$ | $\begin{pmatrix}\sigma_{xx} & \sigma_{xy} & 0\\ -\sigma_{xy} & \sigma_{yy} & 0\\ 0 & 0 & \sigma_{zz}\end{pmatrix}$ | $\begin{pmatrix}0 & 0 & \sigma_{xz}\\ 0 & 0 & \sigma_{yz}\\ 0 & 0 & \sigma_{yz}\end{pmatrix}$ |
| $4'22'$ | $\begin{pmatrix}\tau_{yy} & 0 & 0\\ 0 & \tau_{xx} & 0\\ 0 & 0 & \tau_{zz}\end{pmatrix}$ | $\begin{pmatrix}0 & \tau_{xy} & 0\\ \tau_{yx} & 0 & 0\\ 0 & 0 & 0\end{pmatrix}$ | $\begin{pmatrix}\sigma_{xx} & 0 & 0\\ 0 & \sigma_{xx} & 0\\ 0 & 0 & \sigma_{zz}\end{pmatrix}$ | $\begin{pmatrix}0 & \sigma_{xy} & 0\\ \sigma_{yx} & 0 & 0\\ 0 & 0 & 0\end{pmatrix}$ |
| $(2n)'22'$<br>$n=3, 4, \cdots$ | $\begin{pmatrix}\tau_{xx} & 0 & 0\\ 0 & \tau_{xx} & 0\\ 0 & 0 & \tau_{zz}\end{pmatrix}$ | $\begin{pmatrix}0 & \tau_{xy} & 0\\ -\tau_{xy} & 0 & 0\\ 0 & 0 & 0\end{pmatrix}$ | $\begin{pmatrix}\sigma_{xx} & 0 & 0\\ 0 & \sigma_{xx} & 0\\ 0 & 0 & \sigma_{zz}\end{pmatrix}$ | $\begin{pmatrix}0 & \sigma_{xy} & 0\\ -\sigma_{xy} & 0 & 0\\ 0 & 0 & 0\end{pmatrix}$ |

operators of a set generating the group $\mathcal{K}(0)$. The notation used here is defined in I. $\mathcal{K}(0)$ is the group of quantum-mechanical operators corresponding to space-time symmetry transformations with the property that an element of $\mathcal{K}(0)$ leaves the zero-field Hamiltonian for the system invariant. Note that the expansion and hence the expansion coefficients are symmetric in the indices $\alpha_1, \alpha_2, \cdots, \alpha_k$.

For TGM coefficients, Eqs. (2.17) and (2.28) [or (3.6) and (3.7)] of I reduce to the linear homogeneous equations

$$\tau_{B_\mu A_\nu \alpha_1\alpha_2\cdots\alpha_k} = \sum_{\kappa\lambda\beta_1\beta_2\cdots\beta_k} R_{\mu\kappa}R_{\nu\lambda}R_{\alpha_1\beta_1}R_{\alpha_2\beta_2}\cdots R_{\alpha_k\beta_k} \times \tau_{B_\kappa A_\lambda \beta_1\beta_2\cdots\beta_k} \quad (2)$$

and

$$\tau_{B_\mu A_\nu \alpha_1\alpha_2\cdots\alpha_k} = (-)^k \sum_{\kappa\lambda\beta_1\beta_2\cdots\beta_k} R_{\mu\kappa}R_{\nu\lambda}R_{\alpha_1\beta_1}R_{\alpha_2\beta_2}\cdots R_{\alpha_k\beta_k} \times \tau_{A_\lambda B_\kappa \beta_1\beta_2\cdots\beta_k} \quad (3a)$$

relating the expansion coefficients. The indices of $\tau$, $H$, and $R$ correspond to rectangular components. The matrix $R = D^{-1} = \tilde{D}$ is a $3\times3$ real orthogonal matrix with $D$ representing the proper rotation part of a quantum-mechanical operator, Eq. (2) applying if the quantum-mechanical operator does not involve time inversion, and Eq. (3a) applying if it does. As mentioned in the Introduction, for TGM coefficients the same restrictions result from using the Laue groups $\mathcal{K}^L(0)$ of $\mathcal{K}(0)$ as result from using $\mathcal{K}(0)$ itself.

The set of equations (2) determines the more spatial symmetry restrictions on the expansion coefficients $\tau_{B_\mu A_\nu \alpha_1\alpha_2\cdots\alpha_k}$. Equations of this type are well known, are usually derived using properties of tensor transformations, and solving them leads to relations among the coefficients of a type often tabulated.[5–8]

The similar set of equations (3a) is new. It determines the symmetry restrictions on $\tau_{B_\mu A_\nu \alpha_1\alpha_2\cdots\alpha_k}$ arising from symmetry operations involving time inversion. For equilibrium properties, the symmetry restrictions involving time inversion are, in general, different from those for transport properties. For an equilibrium property with the same tensor character as the TGM coefficients,[9] the space-time symmetry restrictions are determined by (2) and

$$\tau_{B_\mu A_\nu \alpha_1\alpha_2\cdots\alpha_k} = (-)^k \sum_{\kappa\lambda\beta_1\beta_2\cdots\beta_k} R_{\mu\kappa}R_{\nu\lambda}R_{\alpha_1\beta_1}R_{\alpha_2\beta_2}\cdots R_{\alpha_k\beta_k} \times \tau_{B_\kappa A_\lambda \beta_1\beta_2\cdots\beta_k}, \quad (3b)$$

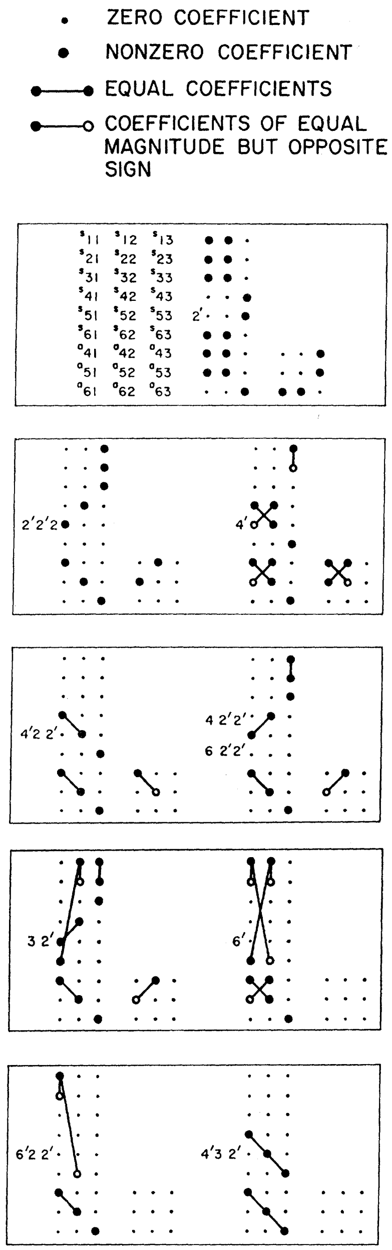


FIG. 1. Symmetry-restricted matrices of conductivity coefficients $\sigma_{\mu\nu\alpha}$ and corresponding equilibrium property coefficients. The matrices are given in the form shown at the upper left for each of the ten Laue groups $\mathcal{K}^L(0)$ of category (c) (Ref. 3). The first matrix gives $\sigma_{\mu\nu\alpha}$. The second matrix gives the corresponding equilibrium property; only the antisymmetric part is given, since the symmetric part is the same as for $\sigma_{\mu\nu\alpha}$. The choice of axes is as shown in Table V of Ref. 10: The principal axis is along $z$ (or $Ox_3$). If there exists, in addition, a two-fold axis ($2$, $\bar{2}=m$, $2'$, $\bar{2}'=m'$) perpendicular to the principal axis, it is taken along $Ox_1$; if more than one, the first in the list $2$, $m$, $2'$, $m'$ is taken along $Ox_1$. This choice of axes is also as given on p. 282 of Ref. 7, except that there the principal axis is taken along $Ox_2$ for monoclinic point groups. The numbers designate the components of $\sigma_{\mu\nu\alpha}$ (or the corresponding equilibrium property). The first of the two indices is an abbreviation for the index pair $\mu\nu$ according to

| $j$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|---|---|
| $\mu\nu$ | 11 | 22 | 33 | 23 | 31 | 12 | 32 | 13 | 21. |

The second index denotes $\alpha$. The superscripts $s$ and $a$ denote the symmetric and antisymmetric parts according to Eqs. (4). The notation used for the components is that of Ref. 7, p. 123.

[5] H. Jagodzinski, in *Encyclopedia of Physics*, edited by S. Flügge (Springer-Verlag, Berlin, 1955), Vol. 7/1, p. 1.

[6] C. S. Smith, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1958), Vol. 6, p. 175.

[7] J. F. Nye, *Physical Properties of Crystals* (Oxford University Press, London, 1960).

[8] S. Bhagavantam, *Crystal Symmetry and Physical Properties* (Academic Press Inc., New York, 1966).

[9] An example of such an equilibrium property, aside from its being symmetric in its two tensor indices, is isothermal magnetic susceptibility.

which differs from (3a) only in that $\tau_{A_\lambda B_\kappa \beta_1 \beta_2 \cdots \beta_k}$ on the right-hand side of (3a) is replaced by $\tau_{B_\kappa A_\lambda \beta_1 \beta_2 \cdots \beta_k}$; $\tau_{B_\mu A_\nu}$ here denotes the equilibrium property. Space-time symmetry-restricted matrices based on equations of this type have been tabulated by Le Corre[10] and by Birss.[11,12]

Equations (2), (3a), and (3b) hold also if $\tau$ is replaced by ${}^s\tau$ or ${}^a\tau$, where $s$ and $a$ denote the components symmetric and antisymmetric with respect to $B_\mu$ and $A_\nu$:

$$ {}^s\tau_{B_\mu A_\nu}(\mathbf{H}) \equiv \tfrac{1}{2}[\tau_{B_\mu A_\nu}(\mathbf{H}) + \tau_{A_\nu B_\mu}(\mathbf{H})], \quad (4a) $$

$$ {}^a\tau_{B_\mu A_\nu}(\mathbf{H}) \equiv \tfrac{1}{2}[\tau_{B_\mu A_\nu}(\mathbf{H}) - \tau_{A_\nu B_\mu}(\mathbf{H})]. \quad (4b) $$

Moreover, (3a) and (3b) reduces to the same equations for ${}^s\tau$, since ${}^s\tau_{B_\mu A_\nu \cdots} = {}^s\tau_{A_\nu B_\mu \cdots}$.

For $\mathcal{K}^L(0)$ in category (b), Eq. (3a) provides no restrictions. The symmetry restrictions are determined entirely by spatial symmetry and are the same for equilibrium and transport properties.

For $\mathcal{K}^L(0)$ in category (a), the spatial symmetry restrictions are augmented by Eq. (3a), which requires that

$$ \tau_{B_\mu A_\nu \alpha_1 \alpha_2 \cdots \alpha_k} = (-)^k \tau_{A_\nu B_\mu \alpha_1 \alpha_2 \cdots \alpha_k}, \quad (5) $$

representing restrictions imposed by the ordinary Onsager relations $\tau_{B_\mu A_\nu}(\mathbf{H}) = \tau_{A_\nu B_\mu}(-\mathbf{H})$; thus,

$$ {}^s\tau_{B_\mu A_\nu \alpha_1 \alpha_2 \cdots \alpha_k} = 0, \quad \text{for } k \text{ odd} \quad (6a) $$

$$ {}^a\tau_{B_\mu A_\nu \alpha_1 \alpha_2 \cdots \alpha_k} = 0, \quad \text{for } k \text{ even}. \quad (6b) $$

For equilibrium properties, on the other hand, (3b) gives

$$ \tau_{B_\mu A_\nu \alpha_1 \alpha_2 \cdots \alpha_k} = 0, \quad \text{for } k \text{ odd}. \quad (7) $$

For $\mathcal{K}^L(0)$ in category (c), Eq. (3a) leads to new restrictions. For $k=0$, these are given in Table VI of I for each of the ten crystallographic Laue groups in this category. For $k=1$, they are given[13,14] here in Fig. 1 for the electrical conductivity $\boldsymbol{\sigma}(\mathbf{H})$; the corresponding symmetry-restricted matrices for an equilibrium property with the same tensor character can be read directly from the table of piezomagnetic coefficients given in Ref. 10, Table V, by taking the transpose; these symmetry-restricted matrices are also given here in Fig. 1. The transport and equilibrium symmetry-restricted matrices for $k=1$ are the same for the symmetric part [since Eqs. (3a) and (3b) are equivalent for ${}^s\tau$], but are seen to be different in every case for the antisymmetric part. In every case, the restrictions on the antisymmetric part of the equilibrium matrix are more stringent in that the equilibrium matrix contains fewer independent components than the transport matrix.

From these results, we can conclude, in particular, that ${}^a\sigma_{\mu\nu}$ has the same symmetry as the spontaneous magnetization (see Ref. 10, Table IV) and that, apart from a transposition of the coefficient matrix, ${}^s\sigma_{\mu\nu\alpha} = {}^s\hat{\sigma}_{j\alpha}$ has the same symmetry as the matrix for the piezomagnetic effect (see p. 343 of Ref. 11, or p. 141 of Ref. 12). The same two conclusions were drawn (albeit for the resistivity rather than the conductivity) by Shtrikman and Thomas[2] using a different approach.

The set of equations (2) and (3) for all $k$ contains, in general, more information that the symmetry-restricted $\mathbf{H}$-dependent matrices tabulated in I. The reason is that the equations determining the symmetry-restricted matrices of I use only the subgroups $\mathcal{K}(\mathbf{H})$ of $\mathcal{K}(0)$ rather than $\mathcal{K}(0)$ itself; the restrictions corresponding to elements of $\mathcal{K}(0)$ not in $\mathcal{K}(\mathbf{H})$ are not taken into account in these symmetry-restricted matrices.


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