On the non-singularity of the thermal conductivity tensor and its consequences

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Abstract

In this paper, the symmetric character of the thermal conductivity tensor for linear anisotropic material is established as the result of arguments from tensor analysis for Duhamel's generalization of Fourier's heat conduction. The non-singular nature of the conductivity tensor plays the fundamental role in establishing this symmetry, as well as its positive (or negative) definiteness. Significantly, the second law of thermodynamics does not contribute here in establishing these characteristics, but does ultimately decide that the conductivity tensor is indeed positive definite.

1. Introduction

The conductivity tensor characterizes the general linear heat conduction relation between temperature gradients and heat flux in heterogeneous anisotropic material. By using non-equilibrium statistical mechanics, Onsager [1] has shown that the conductivity tensor is symmetric. Since classical continuum thermodynamics did not provide any direct reasoning for this property for a long time, there had been the general belief that the symmetry condition can only be derived based on additional physical assumptions. For instance, Day and Gurtin [2] have introduced the requirement that the thermal work functional has a weak relative minimum at equilibrium.

Recently, Hadjesfandiari [3] has established the symmetric character of the conductivity tensor by using arguments from tensor analysis and linear algebra regarding the generalization of Fourier's heat conduction law. Interestingly, the fundamental ground in this establishment is the non-singularity of the conductivity tensor. The method of proof is based on the consistency of the system of linear equations representing the heat conduction law in different coordinate systems. This proof clearly demonstrates that classical continuum thermodynamics can provide the mathematical reason for the symmetric character of the conductivity tensor, which is a necessary condition for having consistent tensorial relations in classical heat conduction theory. As a result, one might speculate that there are other ways to establish this character, although the fundamental step still remains the non-singularity of the conductivity tensor.

Here we establish the symmetric character of the conductivity tensor by focusing on the conductivity tensor itself, without using the linear heat conduction equation. As mentioned, the fundamental ground in this establishment is also the non-singularity of the conductivity tensor. The method of proof is based on the fact that the conductivity tensor cannot be skew-symmetric. Significantly, this proof shows the subtle character of tensors in three-dimensional space, which has not been recognized previously. Interestingly, the form of this proof also shows that the conductivity tensor is either positive or negative definite. It should be emphasized that the second law of thermodynamics and Clausius-Duhem inequality do not have any role here in establishing the symmetry character of the conductivity tensor. They only establish that the conductivity tensor is positive, rather than negative, definite.

The paper is organized as follows. In Section 2, we provide an overview of the classical heat conduction relations for linear anisotropic material. After that in Section 3, the symmetric character of the conductivity tensor is established by using the arguments from tensor analysis. Finally, Section 4 contains a summary and some general conclusions. Appendix A presents properties of the eigenvalue problem for second order tensors.

2. Linear heat conduction theory

Consider the three dimensional orthogonal coordinate system $x_1x_2x_3$ as the reference frame. For linear anisotropic material, Duhamel's generalization of Fourier's heat conduction law [4] is

$$q_i = -k_{ij} T_{,j} . \qquad (1)$$

Here the tensor k_{ij} is the material thermal conductivity tensor, which relates the heat flux vector q_i to the gradient of the temperature field T. The minus sign in (1) assures that the heat flow occurs from a higher to a lower temperature when the material is isotropic with positive conductivity in Fourier's original law. From a physical standpoint, we postulate that there is a one to one relationship between the temperature gradient $T_{,i}$ and the heat flux q_i in (1). This condition requires that the conductivity tensor be non-singular, as will be demonstrated in detail in the next section.

In terms of components, the second order conductivity tensor $\mathbf{k}$ in the coordinate system $x_1 x_2 x_3$ can be written as

$$\left[k_{ij}\right] = \begin{bmatrix} k_{11} & k_{12} & k_{13} \\ k_{21} & k_{22} & k_{23} \\ k_{31} & k_{32} & k_{33} \end{bmatrix}. \qquad (2)$$

Since we have not established the symmetry character of k_{ij}, the nine components of k_{ij} are independent of each other at this stage. Therefore, the conductivity tensor k_{ij} is specified by nine independent components in the general case. As a result, the conductivity tensor can be represented by points of an abstract nine-dimensional space. However, as will be seen, there are some restrictions on the conductivity tensor, which confines the domain of the conductivity tensor in this abstract space.

By decomposing the thermal conductivity tensor k_{ij} into symmetric $k_{(ij)}$ and skew-symmetric $k_{[ij]}$ parts, we have

$$k_{ij} = k_{(ij)} + k_{[ij]} , \qquad (3)$$

where

$$k_{(ij)} = \frac{1}{2}\left(k_{ij} + k_{ji}\right) = k_{(ji)} , \qquad (4)$$

$$k_{[ij]} = \frac{1}{2}\left(k_{ij} - k_{ji}\right) = -k_{[ji]}. \tag{5}$$

Notice that here we have introduced parentheses surrounding a pair of indices to denote the symmetric part of a second order tensor, whereas square brackets are associated with the skew-symmetric part. Since the general conductivity tensor k_{ij} is specified by nine independent components, the tensors $k_{(ij)}$ and $k_{[ij]}$ are specified by six and three independent components, respectively. In the following section, we prove that $k_{[ij]}$ vanishes based exclusively on tensor analysis.

3. Symmetric character of the conductivity tensor

Now we establish that the conductivity tensor k_{ij} cannot be singular. Appendix A demonstrates that singular tensors have at least one zero eigenvalue. Therefore, if we assume that the conductivity tensor is singular, at least one of its eigenvalues vanishes. Let us arbitrarily choose the third eigenvalue to be one of these eigenvalues, that is, $\lambda_3 = 0$, where its corresponding real eigenvector is $\mathbf{v}^{(3)}$. For a non-zero temperature gradient $T_{,i}$ in the direction of $\mathbf{v}^{(3)}$, where

$$T_{,i} = \vartheta v_i^{(3)}, \tag{6}$$

with ϑ as an arbitrary non-zero constant, there would be no heat flux; that is

$$q_i = -k_{ij}T_{,j} = -\vartheta k_{ij} v_i^{(3)} = 0. \tag{7}$$

However, this physically contradicts the fact that there is a one to one relationship between the temperature gradient $T_{,i}$ and the heat flux q_i in (1). Therefore, this contradiction requires that the conductivity tensor k_{ij} be non-singular, that is

$$\det(\mathbf{k}) = \det\left[k_{ij}\right] \neq 0. \tag{8}$$

This shows that the conductivity tensor is invertible.

Interestingly, we notice that $\det(\mathbf{k}) = 0$ specifies an eight-dimensional hyper-surface in the abstract nine-dimensional space of the conductivity tensor. This hyper-surface divides the nine-dimensional space into two exclusive subspaces. Since the domain of the conductivity tensor is continuous in the abstract nine-dimensional space, the constraint (8) requires that this domain be in only one of these two subspaces. The more fundamental meaning of this restriction will be elucidated shortly.

In Appendix A, we demonstrate the well-known fact that all three-dimensional skew-symmetric tensors are singular. As a result, the non-singular conductivity tensor k_{ij} cannot be skew-symmetric. For now, we concentrate on this important character and ignore the general non-singularity character of the conductivity tensor k_{ij}.

For further investigation, we consider the decomposition

$$k_{ij} = k_{(ij)} + k_{[ij]} . \tag{9}$$

Let us assume the skew-symmetric tensor $k_{[ij]}$ part is non-zero. Since, the conductivity tensor cannot become skew-symmetric, the symmetric part $k_{(ij)}$ is also non-zero. However, the symmetric part $k_{(ij)}$ can become as arbitrarily small as we wish. This means that the tensor k_{ij} can approach to the non-zero limit value $k_{[ij]}$ in many arbitrary ways, but it cannot become equal to $k_{[ij]}$. Mathematically, this states that the conductivity tensor is not defined at $k_{[ij]}$, although it is defined in its neighborhood. However, we notice that this restriction is in contradiction with the continuity of the domain of definition of the conductivity tensor. Therefore, this contradiction requires that the skew-symmetric part $k_{[ij]}$ vanish, that is

$$k_{[ij]} = 0 , \quad k_{ij} = k_{(ij)} . \tag{10}$$

This result states that the conductivity tensor is symmetric, that is

$$k_{ij} = k_{ji} . \tag{11}$$

Therefore, the general conductivity tensor is specified by six independent components.

For more clarification, we demonstrate the above reasoning by using the symbolic three-dimensional coordinate system in Fig. 1, where the horizontal plane including two coordinate axis represents the six-dimensional space of $k_{(ij)}$, and the vertical axis represents the three-dimensional space of $k_{[ij]}$. Notice that the origin corresponds to the zero of $k_{(ij)}$ and $k_{[ij]}$. Since the conductivity tensor k_{ij} cannot be skew-symmetric, it cannot be on the vertical line, although it can be at any point around it. Therefore, the vertical line is the location of impossible values for the conductivity tensor. However, this is inconsistent with the continuity of the conductivity tensor in its domain. As a result, this contradiction requires that points representing the consistent conductivity tensor must lie in the horizontal plane that passes continuously through the point $k_{[ij]} = 0$. Only in this plane is the conductivity tensor continuous. Since the skew-symmetric part is zero everywhere in this plane, the thermal conductivity tensor must be symmetric.

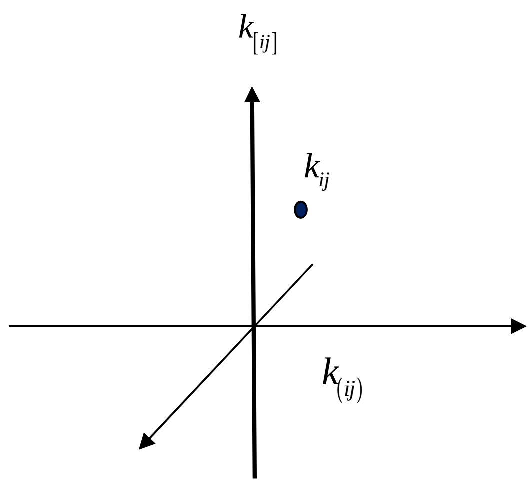

Fig. 1 Symbolic representation of abstract nine-dimensional conductivity space

Now we notice that the eigenvalues of the symmetric conductivity tensor k_{ij} are all real and their corresponding real eigenvectors are mutually orthogonal for distinct eigenvalues or can be taken mutually orthogonal for repeated eigenvalues. Consequently, we can generally diagonalize the conductivity tensor by choosing the new coordinate system $x_1'x_2'x_3'$, such that the coordinate axes x_1', x_2' and x_3' are along the orthogonal eigenvectors $\mathbf{v}^{(1)}$, $\mathbf{v}^{(2)}$ and $\mathbf{v}^{(3)}$. As a result, the representation of the conductivity tensor in this new coordinate system becomes

$$\left[k'_{ij}\right] = \begin{bmatrix} k'_{11} & 0 & 0 \\ 0 & k'_{22} & 0 \\ 0 & 0 & k'_{33} \end{bmatrix}, \tag{12}$$

where we have

$$\lambda_1 = k'_{11}, \quad \lambda_2 = k'_{22}, \quad \lambda_3 = k'_{33}. \tag{13}$$

On the other hand, the non-singularity of the conductivity tensor also imposes more restrictions on this symmetric tensor. In particular, if there is no restriction on the signs of eigenvalues λ_1, λ_2 and λ_3, then they can also become zero. However, this result is in contradiction to the non-singularity of the conductivity tensor. Therefore, the strictly non-singular conductivity tensor is symmetric and is either positive or negative definite. Interestingly, we notice that this shows that the hyper-surface $\det(\mathbf{k}) = 0$ divides the abstract space of the symmetric conductivity tensor space into positive and negative definite conductivity tensor subspaces. Notice that to this stage, there has been no reference to the second law of thermodynamics.

The combination of the first and second law of thermodynamics [5] results in the Clausius-Duhem inequality

$$q_i T_{,i} \le 0. \tag{14}$$

This inequality shows that the heat flux vector cannot have any positive component in the direction of temperature gradient. By using the relation (1) for heat flux, we can write the Clausius-Duhem inequality (14) as

$$k_{ij} T_{,i} T_{,j} \ge 0. \tag{15}$$

Since the conductivity tensor is a non-singular symmetric tensor, the Clausius-Duhem inequality in the form of (15) shows that this tensor is positive definite. This means that all of the eigenvalues (13) are positive.

As mentioned before, the second law of thermodynamics and Clausius-Duhem inequality do not have any role here in establishing the symmetric character of the conductivity tensor. The proof has been solely based on the tensorial character of quantities in Duhamel's generalization of

Fourier's heat conduction law (1). The Clausius-Duhem inequality (14) imposes only the positive definite restriction on the symmetric conductivity tensor k_{ij}.

4. Conclusions

By using arguments from tensor analysis, we have established the symmetric character of the conductivity tensor for linear anisotropic material. Interestingly, the non-singular character of the conductivity tensor is fundamental in establishing this statement. The proof here shows that classical continuum thermodynamics can provide the mathematical reason for the symmetric character of the conductivity tensor. Remarkably, this method of proof also shows that the conductivity tensor is either positive or negative definite. However, the Clausius-Duhem inequality requires this tensor to be positive definite.

The method of proof used here shows the subtle character of tensors and their interrelationships in three-dimensional space, which has not been fully exploited in studying physical phenomena from this mathematical view. By using the character of tensors, we may find important results, which could not have been imagined previously in classical physics. As shown in this paper, the tensorial proof refutes the general belief that the symmetry condition for the conductivity tensor can be derived only based on additional physical assumptions, such as the requirement that the thermal work functional have a weak relative minimum at equilibrium.

It should be emphasized that the singularity of all three-dimensional skew-symmetric tensors has played a vital role in establishing the symmetric character of the conductivity tensor. However, we should remember that skew-symmetric tensors are only singular in odd dimensional spaces, such as the three-dimensional physical space considered here. Skew-symmetric tensors in even dimensional spaces are not necessarily singular. This means that if our physical space had been even dimensional, e.g., two-dimensional, the conductivity tensor would not have been symmetric, unless other physical arguments were imposed.

As one might expect, the symmetric character of the resistivity tensor in Ohm's law for electric conduction and the diffusion coefficient tensor for Fick's law in mass transfer and other diffusive systems can be established using analogous methods.

Appendix A. Eigenvalue problem for second order tensors

Consider the general second order tensor $\mathbf{C}$ in three-dimensional space. The eigenvalue problem for this tensor is defined as

$$C_{ij}v_j = \lambda v_i , \tag{A1}$$

where the parameter λ is the eigenvalue or principal value and the vector $\mathbf{v}$ is the eigenvector or principal direction. The eigenvalue problem (A1) can be written as

$$\left(C_{ij} - \lambda\delta_{ij}\right)v_j = 0 . \tag{A2}$$

The condition for (A2) to possess a non-trivial solution for v_i is

$$\det\left(C_{ij} - \lambda\delta_{ij}\right) = 0 , \tag{A3}$$

which in terms of elements can be written as

$$\det\begin{bmatrix} C_{11}-\lambda & C_{12} & C_{13} \\ C_{21} & C_{22}-\lambda & C_{23} \\ C_{31} & C_{32} & C_{33}-\lambda \end{bmatrix} = 0 . \tag{A4}$$

This gives the cubic characteristic equation for λ as

$$\lambda^3 - I_1\lambda^2 + I_2\lambda - I_3 = 0 , \tag{A5}$$

where the real coefficients I_1, I_2 and I_3 are the invariants of the tensor $\mathbf{C}$ expressed as

$$I_1 = \mathrm{trace}\left(\mathbf{C}\right) = C_{ii} , \tag{A6}$$

$$I_2 = \frac{1}{2}\left[\left(\mathrm{trace}\ \mathbf{C}\right)^2 - \mathrm{trace}\ \left(\mathbf{C}^2\right)\right] = \frac{1}{2}\left[\left(C_{ii}\right)^2 - C_{ij}C_{ji}\right], \tag{A7}$$

$$I_3 = \det\left(\mathbf{C}\right) = \frac{1}{6}\varepsilon_{ijk}\varepsilon_{pqr}C_{ip}C_{jq}C_{kr} . \tag{A8}$$

The symbol ε_{ijk} in (A8) is the alternating or Levi-Civita symbol.

It should be noticed that since the vector $\mathbf{v}$ is normalized, we have

$$v_i\bar{v}_i = 1 , \tag{A9}$$

where $\bar{v}_i$ is the complex conjugate of v_i .

Let us call the eigenvalues λ_1, λ_2 and λ_3. The cubic equation (A5) with real coefficients has at least one real root. Therefore, in any case, one eigenvalue and its corresponding eigenvector are real, which we denote as the third eigensolution λ_3 and $\mathbf{v}^{(3)}$. We notice that the other two eigenvalues λ_1 and λ_2, and their corresponding eigenvectors $\mathbf{v}^{(1)}$ and $\mathbf{v}^{(2)}$ are either real or complex conjugate of each other. However, for the real eigenvalue λ_3 with the corresponding real normalized eigenvector $\mathbf{v}^{(3)}$, we have

$$v_i^{(3)} v_i^{(3)} = 1 . \quad \text{(A10)}$$

Interestingly, we notice that the invariants of the tensor $\mathbf{C}$ can be expressed in terms of eigenvalues, where

$$I_1 = \lambda_1 + \lambda_2 + \lambda_3 , \quad \text{(A11)}$$

$$I_2 = \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1 , \quad \text{(A12)}$$

$$I_3 = \lambda_1\lambda_2\lambda_3 . \quad \text{(A13)}$$

If a tensor is singular, the relation (A13) shows that at least one of the eigenvalues vanishes.

A second order tensor $\mathbf{P}$ is symmetric, if

$$\mathbf{P}^t = \mathbf{P} , \qquad P_{ji} = P_{ij} . \quad \text{(A14)}$$

It is seen that a general symmetric second order tensor in three-dimensional space is specified by six independent values. The eigenvalues of the symmetric tensor P_{ij} are all real and their corresponding real eigenvectors are mutually orthogonal for distinct eigenvalues or can be taken mutually orthogonal for repeated eigenvalues. This means there is a primed orthogonal coordinate system $x_1' x_2' x_3'$, where the representation of P_{ij}' is diagonal, that is

$$\left[P_{ij}' \right] = \begin{bmatrix} P_{11}' & 0 & 0 \\ 0 & P_{22}' & 0 \\ 0 & 0 & P_{33}' \end{bmatrix} . \quad \text{(A15)}$$

A second order tensor $\mathbf{Q}$ is skew-symmetric, if

$$\mathbf{Q}^t = -\mathbf{Q}\,, \qquad Q_{ji} = -Q_{ij}\,. \tag{A16}$$

As a result, a general skew-symmetric tensor in three-dimensional space is specified by three independent values. For the determinant of this tensor, we have

$$\det(\mathbf{Q}) = \det(-\mathbf{Q})\,. \tag{A17}$$

Since the tensor $\mathbf{Q}$ is three-dimensional, we have

$$\begin{aligned}\det(-\mathbf{Q}) &= (-1)^3 \det(\mathbf{Q}) \\ &= -\det(\mathbf{Q})\end{aligned}\,. \tag{A18}$$

Therefore, (A17) becomes

$$\det(\mathbf{Q}) = -\det(\mathbf{Q})\,. \tag{A19}$$

This shows that the determinant of the tensor $\mathbf{Q}$ vanishes; that is

$$\det(\mathbf{Q}) = 0\,. \tag{A20}$$

This in turn shows that one of the eigenvalues of the skew-symmetric tensor Q_{ij} is zero. Therefore, all three-dimensional skew-symmetric tensors are singular and have one zero eigenvalue. Interestingly, the other two eigenvalues of any skew-symmetric tensor Q_{ij} form a purely imaginary conjugate pair.

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