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On cross-correlation between thermal gradients and electric fields

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ABSTRACT

An important phenomenon in the field of thermoelectric conversion in certain materials is the *Seebeck* effect, which is characterized by an electrical field, $\boldsymbol{E}$ being produced by a temperature gradient, $\boldsymbol{E} = S\nabla\theta$, where S is known as the (isotropic) Seebeck number. The objective of this note is to develop bounds on the effective thermoelectric Seebeck property for heterogeneous mixtures of materials. Specifically, we develop bounds on $\langle \boldsymbol{E}\rangle_\Omega = S^*\langle\nabla\theta\rangle_\Omega$, where S^* is the effective Seebeck number for the mixture, where the averaging operator is defined as $\langle\cdot\rangle_\Omega \stackrel{\text{def}}{=} \frac{1}{|\Omega|}\int_\Omega(\cdot)\,d\Omega$ over a statistically representative volume element with domain Ω, using only the pointwise cross-correlation properties of the material and the average thermal fields. .

1. Introduction and objective

A cross-correlation phenomenon that has recently become of high interest is thermoelectricity, which deals with the conversion of thermal energy into electrical energy, and vice versa.[1] Unlike Joule-heating, the effects can be reversible. Essentially, one can generate current from a temperature difference. One important phenomena in this area is the *Seebeck Effect*, which is characterized by an electrical field, $\boldsymbol{E}$ being produced by a temperature gradient

$$\boldsymbol{E} = S\nabla\theta, \tag{1.1}$$

where S is known as the (isotropic) Seebeck number and where the thermal heat flux is related to the temperature gradient, for example, by $\boldsymbol{q} = \mathbb{K}\nabla\theta$, where $\mathbb{K}$ is the thermal conductivity. The objective in this note is to derive bounds for the effective Seebeck number for a heterogeneous materials, such as particulate-doped mixtures of materials (Fig. 1).

$$\langle \boldsymbol{E}\rangle_\Omega = S^*\langle\nabla\theta\rangle_\Omega, \tag{1.2}$$

where S^* is the effective Seebeck number for the mixture, where the averaging operator is defined as $\langle\cdot\rangle_\Omega \text{def} = \frac{1}{|\Omega|}\int_\Omega(\cdot)\,d\Omega$ over a statistically representative volume element with domain Ω, with only knowledge of the pointwise relations and the $\mathbb{K}^*$ is the effective thermal conductivity, relating the volume averaged thermal heat flux $\langle\boldsymbol{q}\rangle_\Omega$ to the temperature gradient $\langle\nabla\theta\rangle_\Omega$, $\langle\boldsymbol{q}\rangle_\Omega = -\mathbb{K}^*\langle\nabla\theta\rangle_\Omega$. As a model problem, we will consider a two-phase heterogeneous material. The analysis will proceed by developing phase field concentration functions for the thermal gradient in each component in the heterogeneous material and then using the concentration functions to develop estimates for the overall Seebeck number.

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[1] In particular, this interest is driven by thermal scavaging applications.

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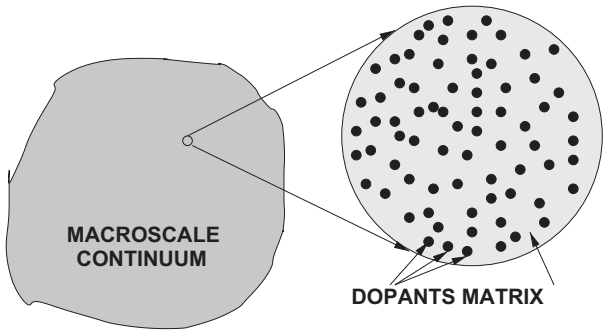

Fig. 1. A material doped with second phase particles.

Remark 1. Cross-correlations can be rather involved, for example in elastic applications, and we refer the reader to the extensive works of Kachanov, Sevostianov, and Shafiro (2001) and Sevostianov and Kachanov (2001, 2002, 2003, 2008a, 2008b, 2009a, 2009b) for cross-correlation property analysis connecting elastic and conductive properties. We note that in those works, the cross-correlated properties are not based on point-wise cross-correlations.

2. Phase-wise field decompositions

In this paper, as a model problem, we will consider a statistically representative volume element (RVE of volume $|\Omega|$) of a two-phase medium, as depicted in Fig. 1. The microscale properties are characterized by a spatially variable thermal conductivity $\mathbb{K}(\boldsymbol{x})$, electrical conductivity $\boldsymbol{\sigma}(\boldsymbol{x})$ and Seebeck $S(\boldsymbol{x})$ number. For example, for such a sample, one can decompose the thermal field carried by each phase in the material as follows

$$\langle \nabla\theta\rangle_{\Omega} = \frac{1}{|\Omega|}\left(\int_{\Omega_1} \nabla\theta\, d\Omega + \int_{\Omega_2} \nabla\theta\, d\Omega\right) = v_1\langle\nabla\theta\rangle_{\Omega_1} + v_2\langle\nabla\theta\rangle_{\Omega_2} \tag{2.1}$$

and for the electrical field

$$\langle \boldsymbol{E}\rangle_{\Omega} = \frac{1}{|\Omega|}\left(\int_{\Omega_1} \boldsymbol{E}\, d\Omega + \int_{\Omega_2} \boldsymbol{E}\, d\Omega\right) = v_1\langle\boldsymbol{E}\rangle_{\Omega_1} + v_2\langle\boldsymbol{E}\rangle_{\Omega_2}, \tag{2.2}$$

where Ω_1 is the domain of phase one and Ω_2 is the domain of phase two. v_1 and v_2 are the volume fractions of phases one and two respectively ($v_1 + v_2 = 1$). We denote $v_1\langle\nabla\theta\rangle_{\Omega_1}$ and $v_2\langle\nabla\theta\rangle_{\Omega_2}$ as the "thermal load shares", since[2]

$$v_1\langle\nabla\theta\rangle_{\Omega_1} + v_2\langle\nabla\theta\rangle_{\Omega_2} = \langle\nabla\theta\rangle_{\Omega}. \tag{2.3}$$

A key to obtaining the effective Seebeck number is to determine the load-shares as functions of known (a priori) quantities

$$\langle\nabla\theta\rangle_{\Omega_1} = \mathcal{F}_1(v_1, \mathbb{K}_1, \mathbb{K}_2, \langle\nabla\theta\rangle_{\Omega}) \tag{2.4}$$

and

$$\langle\nabla\theta\rangle_{\Omega_2} = \mathcal{F}_2(v_1, \mathbb{K}_1, \mathbb{K}_2, \langle\nabla\theta\rangle_{\Omega}), \tag{2.5}$$

where $\mathbb{K}_1$ and $\mathbb{K}_2$ are the conductivities of phase one and phase two respectively.

3. Concentration functions and load shares

A useful quantity that arises in the analysis of heterogeneous materials is the effective conductivity, $\mathbb{K}^*$, defined via[3]

$$\langle\mathbf{q}\rangle_{\Omega} = -\mathbb{K}^*\cdot\langle\nabla\theta\rangle_{\Omega}, \tag{3.1}$$

which is the macroscopic "property". Decomposing the righthand side yields

[2] For solids with cracks and non-spherical pores, such as thin platelets, the volume fraction is an inadequate microstructural parameter. For an indepth analysis of the proper microstructural parameters, we refer the reader to Kachanov (1999).

[3] Implicitly, we assume that (a) the contact between the phases is perfect and (b) the ergodicity hypothesis is satisfied (see Kröner (1972) or Torquato (2002)).