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FINITE SPEED HEAT PROPAGATION AS A CONSEQUENCE OF MICROSTRUCTURAL EVENTS

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ABSTRACT

The standard Fourier's proposal to consider the heat flux q proportional to the gradient of the phenomenological temperature leads to a well-known paradox: the instantaneous propagation of temperature disturbances in a rigid conductor. Several analyses aimed so far to overcome such a physical inconsistency. The pertinent literature is wide. A book by B. Straugham [12] reviews largely the matter. Proposals go from ad hoc modifications of the Fourier's law to a viewpoint resting on moment expansion of the velocity distribution of particles, as it is the case of I. Müller and T. Ruggeri extended thermodynamics [10]. As regards modifications of Fourier's law, Maxwell-Cattaneo's approach (see [1], [7]) is the most popular (also called Maxwell-Cattaneo-Vernotte [14]), often reinterpreted by specifying differently what I. Müller pointed out (see [8], [9]): the heat flux is given by

$$\mathsf{q} = -k\nabla\vartheta + \mathsf{h}, \tag{1}$$

where k is a material positive constant in the case of isotropic heat propagation, ϑ the value of a differentiable scalar field $(x,t) \longmapsto \vartheta := \tilde{\vartheta}(x,t)$ describing pointwise and in time what we consider as a phenomenological temperaure, h is an *extra* flux to be assigned on the basis of phenomenological information, in a form able to adjust temperature time evolution, assuring it finite speed propagation. More precisely, in its primary formulation, Maxwell-Cattaneo's modification of Fourier's law reads

$$\tau\dot{\mathsf{q}} + \mathsf{q} = -k\nabla\vartheta, \tag{2}$$

where the constant τ is interpreted as a relaxation time and the additional flux $\tau\dot{\mathsf{q}}$ as a sort of *thermal inertia* [2], not otherwise specified unless stating that it is a term avoiding the infinite speed propagation of temperature variations. Modifications of equation (2) rest often on the need of regularization for analytical and/or computational purposes. We can list, for example, incremental (or differential) constitutive laws like

$$\tau\dot{\mathsf{q}} + \mathsf{q} = -k\nabla\vartheta + a_1\nabla\mathrm{div}\vartheta + a_2\Delta\mathsf{q}, \tag{3}$$

$$\tau\dot{\mathsf{q}} + \mathsf{q} = -k\nabla\vartheta + a_3\nabla\dot{\vartheta}, \tag{4}$$

$$\tau\dot{\mathsf{q}} = -k\nabla\vartheta + a_2\Delta\mathsf{q} \tag{5}$$

(see [4] and [13] for detailed analyses of these expressions).

Notwithstanding the effectiveness of various proposals, starting from Maxwell-Cattaneo's one, in overcoming Fourier's paradox a question remaining not completely specified is the physical nature of additional terms summarized by h, precisely their link with the structure of the matter in hands. In other words, in question is, more generally, the nature of heat's description in continuum models, besides the definition of temperature.

The question deals with choices we do in constructing models of the world we perceive. In this sense it has also a philosophical character. When we start describing the mechanics of a body, in fact, with our modeling choices–the first one is the representation of body's morphology–we decide a level of accurateness: we include a number of details in what we call mechanics, even concerning dissipative structures, and put the rest in what we call heat. Although such a remark is vague in this stage, it is what suggests this work.

When we consider a rigid conductor as a portion of space, which is the domain of a scalar field that we call *temperature*, satisfying in its evolution the first law of thermodynamics, a question is what kind of structure we attribute to such a law, i.e. whether we neglect, at least at the level of the geometric description, that the matter constituting a body has an internal articulate structure, which may undergo irreversible changes.

My idea is that just these microscopic changes are those mechanisms determining a finite speed propagation of heat, independently of the type of microstructure–in this sense the mechanism is universal–provided that such mutations are sensitive to temperature variations, considered in a macroscopic phenomenological way.

In what follows, I try to formalize this point of view. Mine is just a first tentative, which requires further refinements; however, it may be a way of starting a discussion. With $\mathcal{B}$ we indicate the fit region occupied by a rigid conductor in the three-dimensional point space $\mathcal{E}^3$, considered endowed with Euclidean structure. The body is rigid in the sense that the sole admissible deformations are isometric and orientation-preserving. The circumstance does not exclude the possibility of microscopic changes in the matter, i.e. events occurring at a spatial scale lower than the one of (average) naked-eye observation. Such changes are alterations of the low-scale geometry in the arrangements of atoms and molecules. We may describe in time and space those microstructural geometric features that we consider essential by a field

$$(x,t) \longmapsto \nu := \tilde{\nu}(x,t) \in \mathcal{M}, \tag{6}$$

which takes values in a finite-dimensional differentiable manifold $\mathcal{M}$ left abstract just to include a wide range of descriptive possibilities and to furnish result independent of a specific microstructural shapes, so universal results in this sense, as I have already remarked. I assume minimal geometric structures over $\mathcal{M}$, although some analytical questions (see [5], [3]) may suggest to consider it Riemannian and complete.

I do not consider macroscopic changes of places, so that I do not distinguish between $\mathcal{E}^3$ and an isomorphic copy of it, where we commonly embed (or better detect) what we consider deformed shapes with respect to $\mathcal{B}$. In this way, to me an *observer* is just a pair made of a coordinate atlas over $\mathcal{E}^3$ and another one over $\mathcal{M}$. This is in agreement with a definition I have already proposed in other papers (see, e.g., [6]): an observer is a collection of frames of reference on *all* geometric environments necessary to describe its morphology and its motion. Here motion is intended in generalized sense and includes the time-variation of the microstructure descriptor field $\tilde{\nu}$.

When we translate a frame of reference in the ambient space, our perception of the microstructure remains unaltered–this is a key point–while rotations in space may alter it. Imagine, for example, that ν is a vector–say the polarization at a point. When we rotate the frame of reference in space, our representation of that vector is also rotated. In general, we can say that if $\dot{\nu}$ is the time rate of ν as perceived by an observed O and $\dot{\nu}^*$ the pull-back into O of the analogous rate perceived by another observer translating with velocity c and rotating by speed q with respect to O, we get (see also [6])

$$\dot{\nu}^* = \dot{\nu} + \mathcal{A}(\nu)q. \tag{7}$$

If the special orthogonal group $SO(3)$ may act on $\mathcal{M}$, the linear operator $\mathcal{A}(\nu)$ is the infinitesimal generator of its action. Otherwise, it is a general linear operator $\mathcal{A}(\nu) \in \mathrm{Hom}(\mathbf{R}^3, T_\nu\mathcal{M})$ with formal adjoint $\mathcal{A}^*(\nu) \in \mathrm{Hom}(T^*_\nu\mathcal{M}, \mathbf{R}^{3*})$, where $T^*_\nu\mathcal{M}$ is the cotangent space of $\mathcal{M}$ at ν and $\mathbf{R}^{3*}$ is the dual of $\mathbf{R}^3$. Its specification, once a manifold $\mathcal{M}$ has been selected for a specific material class, characterizes a change in observer.

We consider a metric g in space and distinguish from now on between contravariant and covariant components of tensor entities. Specifically, we write Da for the derivative of a differentiable field $x \longmapsto a := \tilde{a}(x)$. It differs from the gradient ∇a by the action of the metric, namely $\nabla a = (Da)g^{-1}$. Consequently, we shall write the Fourier law as $\mathsf{q} = -kD\vartheta$, considering in this way the heat flux as a covector rather than a vector. Such a choice is natural in this setting, as it will appear (I hope) from the following developments. Finally, as a matter of notation we recall that we use the dot to indicate duality pairing.

We call *part* any subset b of $\mathcal{B}$ with non-vanishing volume and the same regularity of $\mathcal{B}$. We define the actions over a generic part through the power they perform in a certain class of chances in body's morphology and placement. Here, I exclude macroscopic motion of the body and any external action performing power in a (even virtual) change of placement. I consider just actions associated with microstructural changes and divide them into bulk and contact families, by following a common practice in continuum mechanics. Consequently, I define just the external power $\mathcal{P}_\mathsf{b}(\dot{\nu})$ performed by these actions in the rate $\dot{\nu}$:

$$\mathcal{P}_\mathsf{b}(\dot{\nu}) := \int_\mathsf{b} \beta^\dagger \cdot \dot{\nu}\, d\mu(x) + \int_{\partial\mathsf{b}} \tau \cdot \dot{\nu}\, d\mathcal{H}^2, \tag{8}$$

where $d\mathcal{H}^2$ is the surface measure along $\partial\mathsf{b}$ and $d\mu(x)$ the volume measure in $\mathcal{B}$; $\beta^\ddagger$ represents possible external bulk actions on the microstructure, while τ the contact ones. By mimicking Cauchy's assumption about the structure of standard (deformational) contact actions, we assume that τ depends on the place and the normal n to the boundary, besides time left unexpressed for the sake of simplicity, so that we assume $\tau = \tilde{\tau}(x,n)$.

An **invariance axiom** has here basic character: We impose that

$$\mathcal{P}_\mathsf{b}(\dot{\nu}) = \mathcal{P}_\mathsf{b}(\dot{\nu}^*) \tag{9}$$

for any choice of the part considered and q.

The invariance axiom implies the following assertions:

1) If the fields $x \longmapsto \mathcal{A}^*\beta^\dagger$ and $x \longmapsto \mathcal{A}^*\tau$ are integrable, the following *integral balance* holds true:

$$\int_\mathsf{b} \mathcal{A}^*\beta^\dagger\, d\mu(x) + \int_{\partial\mathsf{b}} \mathcal{A}^*\tau\, d\mathcal{H}^2 = 0. \tag{10}$$

2) If $x \longmapsto |\mathcal{A}^*\beta^\dagger|$ is bounded over $\mathcal{B}$ and $\tilde{\tau}(\cdot,n)$ is continuous for any n, the following *nonstandard action-reaction principle* holds:

$$\mathcal{A}^*(\tilde{\tau}(x,n) - \tilde{\tau}(x,-n)) = 0. \tag{11}$$

3) In the assumptions of item (2), there exists a second-rank tensor $S := \tilde{S}(x,t) \in \mathrm{Hom}(T^*_x\mathcal{B}, T^*_{\tilde{\nu}(x,t)}\mathcal{M})$ such that

$$\tilde{\tau}(x,n,t) = S(x,t)n(x,t). \tag{12}$$

4) If the field $x \longmapsto S(x)$ is $C^1(\mathcal{B}) \cap C(\partial\mathcal{B})$, there exist a field $(x,t) \longmapsto z(x,t) \in T^*_{\tilde{\nu}(x,t)}\mathcal{M}$ such that, with $\rceil$ Ricci's alternating symbol,

$$\beta^\dagger - z + \mathrm{Div}S = 0, \tag{13}$$

$$\mathsf{e}(\mathcal{A}^*z + (D\mathcal{A}^*S)) = 0. \tag{14}$$

5) Under the validity of the previous item, the following identity holds true:

$$\mathcal{P}_\mathsf{b}(\dot{\nu}) = \int_\mathsf{b} (z \cdot \dot{\nu} + S \cdot D\dot{\nu}) := \mathcal{P}^{inn}_\mathsf{b}(\dot{\nu}). \tag{15}$$

Previous items are a special case of a theorem in [6]. To exploit them in thermodynamical setting, we recall once again the **temperature** field $(x,t) \longmapsto \vartheta := \tilde{\vartheta}(x,t)$, considered here–I repeat–as *a phenomenological quantity defined by the rules it satisfies*, and the **first law of thermodynamics**, expressed by

$$\frac{d}{dt}\int_\mathsf{b} e\, dx = \mathcal{P}_\mathsf{b}(\dot{\nu}) + \int_\mathsf{b} r\, dx - \int_{\partial\mathsf{b}} \mathsf{q}\, d\mathcal{H}^2 \tag{16}$$

for any part b considered. In the previous balance $r \in \mathbf{R}$ and $\mathsf{q} \in \mathbf{R}^{3*}$ are heat source and flux, respectively. Notice that we consider the heat flux as a covector. By exploiting item (5) above, we can rewrite the first principle as

$$\frac{d}{dt}\int_\mathsf{b} e\, dx = \mathcal{P}^{inn}_\mathsf{b}(\dot{\nu}) + \int_\mathsf{b} r\, dx - \int_{\partial\mathsf{b}} \mathsf{q}\, d\mathcal{H}^2. \tag{17}$$

Further specific assumptions characterize the analysis presented here.

Assumption 1: $\beta^\dagger = 0$. It means that we exclude both microstructural inertia relative to the macroscopic motion and direct external bulk actions on the microstructure.

The assumption implies

$$\mathcal{P}^{inn}_{\mathsf{b}}(\dot{\nu}) = \int_{\mathsf{b}} \operatorname{div}(S^* \dot{\nu})\, d\mu(x) \tag{18}$$

and we indicate by $-\mathsf{p}$ the flux $S^*\dot{\nu}$. Consequently, since b does not depend on time, its arbitrariness implies the local energy balance

$$\dot{e} = r - \operatorname{div}(\mathsf{q} + \mathsf{p}). \tag{19}$$

In this way, we find an additional heat flow clearly due to microstructural changes, independently of the type of microstructure.

Assumption 2: We presume that the microstructural actions (i.e. self-action z and microstress S) do not have energetic component and display just dissipative nature (see [6] for further remarks on such a decomposition). Moreover, we presume that p is a differentiable function

$$\mathsf{p} = \tilde{\mathsf{p}}(\vartheta, \nu, \dot{\nu}, N, \dot{N}), \tag{20}$$

with $N := D\nu$. Such an assumption is also compatible the structure of the internal energy density e assumed in the next hypothesis.

Assumption 3: $e = \tilde{e}(\vartheta)$, with $\tilde{e}$ a differentiable function of its argument.

Assumption 4: Fourier's law holds true: $\mathsf{q} = -kD\vartheta$, with k a positive constant (i.e. we consider isotropic conduction properties in the material for the sake of simplicity).

Assumption 5: We introduce a constraint prescribing that it is just temperature variations alter the material microstructure, i.e. we assume the existence of a differentiable function $\lambda(x, \vartheta)$ such that

$$\dot{\nu} = \lambda(x, \vartheta)\dot{\vartheta}, \tag{21}$$

with $\lambda \in T_{\tilde{\nu}(x)}\mathcal{M}$.

By exploiting previous assumptions and computing the derivatives in the local form of the energy balance (19), we get

$$\zeta \cdot \nabla\dot{\vartheta} - k\Delta\vartheta + (c + \delta)\dot{\vartheta} + \xi \cdot \nabla\vartheta + (\gamma - r) + \frac{\partial \mathsf{p}}{\partial N} \cdot \nabla N + \frac{\partial \mathsf{p}}{\partial \dot{N}} \cdot \nabla \dot{N} = 0, \tag{22}$$

where $\zeta := \frac{\partial \mathsf{p}}{\partial \dot{\nu}}\lambda \in \mathbf{R}^{3*}$, $c := \frac{\partial e}{\partial \vartheta} \in \mathbf{R}$, $\delta := \frac{\partial \mathsf{p}}{\partial \dot{\nu}} \cdot D\lambda \in \mathbf{R}$, $\xi := \frac{\partial \mathsf{p}}{\partial \vartheta} \in \mathbf{R}^{3*}$, $\gamma := \frac{\partial \mathsf{p}}{\partial \nu} \cdot D\nu \in \mathbf{R}$.

Let us consider a simplified version of the previous equation given by

$$\zeta \cdot \nabla\dot{\vartheta} - k\Delta\vartheta + (c + \delta)\dot{\vartheta} + \xi \cdot \nabla\vartheta + (\gamma - r) = 0. \tag{23}$$

It correspond to the case in which the inner power is given by the sole self-action z, i.e. when $\dot{N} = 0$, a condition under which we can presume that the dissipative microstress vanishes (see [6] for further remarks about). In this case, rather idealized indeed, the pertinent characteristic matrix has eigenvalues $-k$ with multiplicity 2, and $\frac{-k \pm \sqrt{k^2 + 4|\zeta|^2}}{2}$. Since $\sqrt{k^2 + 4|\zeta|^2} > k$ for any $\zeta \neq 0$, the matrix signature is $(1, 3, 0)$, i.e. the evolution equation (23) is hyperbolic with consequent finite-speed propagation of temperature disturbances. When $\zeta = 0$, i.e. when even the dissipative self-action vanishes with consequent absence of microstructural effects, the evolution equation (23) would re-attain parabolic nature with consequent re-appearance of Fourier's paradox.

The analysis presented so far connects the finite speed propagation that we record in the phenomenological world to the occurrence of microscopic events within the material. Alternative approaches not accounting for a direct description of the material microstructures are possible and available. Evaluation on whether points of view or specific assumption have cogent physical significance, or else they are essentially analytical tricks useful to eliminate Fourier's paradox, may allow one to prefer a given approach to another.

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