

NON-EQUILIBRIUM TEMPERATURES IN SYSTEMS WITH INTERNAL VARIABLES

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ABSTRACT

We discuss different definitions of non-equilibrium temperature in systems with internal variables. In equilibrium states, all the different definitions of temperature (caloric, entropic, kinetic, vibrational, configurational, fluctuational, and so on) lead to the same value, but in non-equilibrium they lead to different values. Out of equilibrium, equipartition is not to be expected and therefore the "temperatures" of the different degrees of freedom will be different from each other. Here, we focus our attention on the caloric temperature, based on the internal energy corresponding to the internal variable, the entropic temperature, based on the entropy, and several thermometric or empirical temperatures, based on the zeroth law. We illustrate the difference and the connections between them in some simple systems with a heat flux (two-level and three-level systems, ideal gases), and we also consider a solid system with internal variables. These variables may be measured, but not controlled, and they appear in the Gibbs equation like the classical thermodynamic variables. As an example, we consider a crystal with dislocations submitted to an external flux of energy (like a wall of a fusion reactor bombarded by energetic particles).

INTRODUCTION

Temperature is a concept common to all thermodynamic approaches. However, the meaning and measurement of temperature in non-equilibrium steady states beyond the local-equilibrium approximation is one of the fundamental problems in advanced non-equilibrium thermodynamics. Thus, it is logical that different approaches may consider temperature from different perspectives. For instance, in rational thermodynamics, it is considered as a primitive quantity. In theories with internal variables, each variable could have in principle its own temperature. In extended thermodynamics, temperature is assumed to depend also on the fluxes. In statistical theories, temperature may be related to the form of the distribution functions. Thus, a comparative discussion of the several thermodynamic approaches requires as a preliminary condition to compare and clarify the role of temperature.

Wide surveys of this topic are in [1]-[5]. Out of equilibrium, energy equipartition is not expected and, therefore, different measurements of temperature, sensitive to different sets of degrees of freedom, will yield different values for the temperature. From the theoretical perspective as well, different definitions of temperature will also lead to different values of this quantity.

For instance, in a system composed of matter and radiation, a thermometer with purely reflecting walls will give the temperature of matter, as it will be insensitive to radiation. In contrast, a thermometer with perfectly black walls will yield a temperature related both to matter and radiation. In equilibrium, both thermometers will give the same temperature, but in a non-equilibrium steady state (for instance, with photons transmitting heat and colliding against the particles of a gas) these thermometers will give different temperatures.

Another situation with several -or many-temperatures arises

in mixtures of gases with internal degrees of freedom and at high temperatures, as in the entry of spaceships into a planetary atmosphere. In such a case, one may have different kinetic temperatures for different gases, and different electronic temperatures (related to the relative occupancy of electrons at the several energy levels), and different vibrational and rotational temperatures. All these temperatures may be experimentally obtained by means of spectrometric methods, by measuring the intensity of the spectral lines emitted by the gases.

As it was pointed out in [1], instead of trying to attribute to some of the mentioned temperatures a more relevant role than to others (this will be indeed the case, but for different kinds of temperatures depending on the problem being addressed to), one should try to obtain the relations between them when the conditions on the system (total energy, energy flux, and so on) are specified. In fact, the ensemble of these different temperatures yields a very rich information about the system: about their internal energy transfers and their internal energy contents for the several degrees of freedom.

Here, we will discuss in detail the thermometric, caloric and entropic temperatures for systems with internal variables, the first one related to the zeroth law, the second one being based on the internal energy of the variable, and the third one related to its entropy.

TEMPERATURE DEFINITIONS IN EQUILIBRIUM THERMODYNAMICS

In equilibrium thermodynamics there are several definitions of temperature: empirical (based on the zeroth law), caloric (based on the first law), and entropic (based on the second law). Here, we remind the reader these definitions.

Empirical definition:

Empirical (or thermometric) temperature is defined by the zeroth law, which states the transitive character of thermal equilibrium. In particular, it states that if a state A of a system is in equilibrium with state B of another system, and state B is in equilibrium with state C of a third system, states A and C are in mutual thermal equilibrium.

Entropic definition:

The most fundamental definition of temperature in equilibrium thermodynamics is that appearing in the Gibbs equation.

$$\frac{1}{T} \equiv \left(\frac{\partial S}{\partial U} \right)_{\text{all other extensive variables}}, \quad (1)$$

where the subscript "all other extensive variables" means that the derivative must be carried out keeping constant all the other extensive variables appearing in the entropy, as for instance the volume V , the number of particles N_i of the species i and so on.

Caloric definition:

Another definition of temperature - we will call it the caloric definition, because it uses the so-called caloric equation of state relating internal energy and temperature - is obtained from the internal energy of the different degrees of freedom. For instance

$$U = U(T, V, N_i). \quad (2)$$

Since U is defined by the first principle, this definition is related to this principle.

TEMPERATURE DEFINITIONS IN STEADY STATE NON-EQUILIBRIUM THERMODYNAMICS

Our aim is to explore in a few simple situations how the temperatures defined by (1) and (2) differ in non-equilibrium steady states. Non-equilibrium steady states are different than equilibrium states because in them the system is crossed by fluxes of energy, matter, electric current and so on. Thus, it is interesting to investigate the influence of such fluxes on the thermodynamics of the system. The presence of fluxes is related to inhomogeneities in the system: the presence of a gradient of temperature, concentration, electrical potential or barycentric velocity.

Illustration 1: caloric and entropic temperatures in two-level system with an energy flux

First, we present an example related to a statistical description [6]. We illustrate the mentioned concepts of temperature with a two-level system, with N_1 particles at level 1 (with energy E_1) and N_2 particles at level 2 (with energy E_2). For instance, this could refer to electrons in two electronic levels, or to spins under an external magnetic field, or some other situations. The total internal energy will be $U = N_1 E_1 + N_2 E_2$; from here, one may define a caloric temperature T as

$$k_B T \equiv \frac{N_1}{N} E_1 + \frac{N_2}{N} E_2, \quad (3)$$

with N the total number of particles $N = N_1 + N_2$, and k_B the Boltzmann constant. On the other side, in equilibrium situations following the canonical distribution function, the temperature

will be defined as

$$k_B T \equiv \frac{E_2 - E_1}{\ln(N_1/N_2)}. \quad (4)$$

Assume now that the system is submitted to an energy flow q (energy per unit time), in such a way that the relative proportion of particles in states 1 and 2 is modified (for instance, the higher energy level 2 becomes more populated than in equilibrium, and the lowest level, which is receiving the external energy, becomes less populated).

Assume that the dynamics of the populations N_1 and N_2 is given by

$$\frac{dN_1}{dt} = -\frac{dN_2}{dt} = -\alpha N_1 + \beta N_2 - \gamma q N_1, \quad (5)$$

where α and β are the transition rates from 1 to 2 and from 2 to 1 respectively, and γ is a coefficient related to efficiency of energy absorption by particles in the lower level 1 bringing them to the higher level 2. The steady state solution of (5) is

$$\frac{N_1}{N_2} = \frac{\beta}{\alpha + \gamma q}. \quad (6)$$

For $q = 0$, one has

$$\frac{N_1}{N_2} = \frac{\beta}{\alpha} = \exp \left[-\frac{E_1 - E_2}{k_B T} \right]. \quad (7)$$

This is the detailed-balance relation amongst the rates. By keeping the definitions (3) and (4) but related to the non-equilibrium populations, one gets the following expressions for the non-equilibrium caloric temperature

$$T_{\text{neq,cal}} = T \frac{\alpha + \beta}{\alpha + \beta + \gamma q} \frac{E_1 + (\alpha + \gamma q) \beta^{-1} E_2}{E_1 + \alpha \beta^{-1} E_2}. \quad (8)$$

The entropy is

$$S = -k \left[\frac{N_1}{N} \ln N_1/N + \frac{N_2}{N} \ln N_2/N \right], \quad (9)$$

which in presence of q takes the form

$$S = S_{\text{eq}} - k_B \frac{\gamma^2}{\beta^2} \left[\frac{N}{N_1} + \frac{N}{N_2} \right] q^2. \quad (10)$$

This leads to

$$\frac{1}{T_{\text{neq,ent}}} = \frac{1}{T_{\text{cal}}} + k_B \frac{\gamma^2}{\beta^2} \frac{1}{(E_1 - E_2)N} \left[\frac{N^2}{N_1^2} - \frac{N^2}{N_2^2} \right] q^2. \quad (11)$$

Finally, the non-equilibrium thermometric temperature from (4) and (6) will be

$$T_{\text{neq,th}} = T \frac{1}{1 - \frac{\ln[1+(\gamma/\alpha)q]}{E_2 - E_1} k_B T}. \quad (12)$$

It is seen that these temperatures are different from each other when $q \neq 0$. Here, T is the equilibrium temperature, which is equal to the temperature of a thermal bath in which these systems are in contact. Note that in the extreme situations that the higher-level population 2 becomes higher than the lower level population 1, namely, for q higher than $(\beta - \alpha)/\gamma$, the entropic temperature becomes negative, whereas the caloric temperature remains positive. Note that a thermometer in equilibrium in contact with the system will measure temperature (12), rather than temperature (8) or (11). From temperature (12) it would be possible measure γ . Spectrometric methods allow to measure temperature (12) through the intensity of spectral emission line corresponding to $2 \rightarrow 1$.

Illustration 2: thermometric temperature in three-level system with an energy flux

To discuss the problems related to zeroth law and thermometric temperature we consider a three-level system, with energies $E_1 < E_2 < E_3$, and assume, for the sake of simplicity, the simplest triangular scheme for its possible internal transitions, namely $1 \rightarrow 2 \rightarrow 3 \rightarrow 1$. More realistic schemes are possible, but here we want to stick to the simplest illustrations. The evolution of the atomic populations N_1, N_2 and N_3 will be given by

$$\begin{aligned} \frac{dN_1}{dt} &= -\alpha_1 N_1 + \beta N_3 - \gamma_1 q N_1, \\ \frac{dN_2}{dt} &= -\alpha_2 N_2 - \gamma_2 q N_2 + \alpha_1 N_1 + \gamma_1 q N_1, \\ \frac{dN_3}{dt} &= -\frac{dN_1}{dt} - \frac{dN_2}{dt}, \end{aligned} \quad (13)$$

where α_1, α_2 and β stand for the rate transitions coefficients; in particular, γ_1 and γ_2 stand for the part of the energy flux which interacts with particles in state 1 and in state 2. The steady state populations will be

$$\begin{aligned} \frac{N_1}{N_2} &= \frac{\alpha_2 + \gamma_2 q}{\alpha_1 + \gamma_1 q}, \\ \frac{N_1}{N_3} &= \frac{\beta}{\alpha_1 + \gamma_1 q}. \end{aligned} \quad (14)$$

The equilibrium temperature will be

$$k_B T = \frac{E_2 - E_1}{\ln(N_1/N_2)} = \frac{E_3 - E_1}{\ln(N_1/N_3)}. \quad (15)$$

The thermometric temperatures related to populations 1 and 2, as 1 and 3, will be the following non-equilibrium temperatures

$$T_{neq,12} = T \frac{1}{1 - \frac{\ln[(1+(\gamma_1/\alpha_1)q)/(1+(\gamma_2/\alpha_2)q)]}{E_2 - E_1}},$$

$$T_{neq,13} = T \frac{1}{1 - \frac{\ln[1+(\gamma_1/\beta_1)q]}{E_3 - E_1}}. \quad (16)$$

A thermometer in contact with levels 1 and 2 would measure T_{12} , and a thermometer in contact with 1 and 3 would measure T_{13} ; analogously, a thermometer in contact with 2 and 3 would measure a temperature T_{23} defined in analogy with (16)_a and (16)_b. Of course, in equilibrium all these temperatures would be the same. It is not clear, instead, what would measure a thermometer in contact with 1, 2 and 3. From expressions (16) it would be possible to obtain γ_1 and γ_2 . Note, therefore, that the zeroth-principle of equilibrium thermodynamics cannot be applied to non-equilibrium steady states.

Illustration 3: caloric and entropic temperatures in non-equilibrium ideal gas

Ideal gases are a system for conceptual discussion of thermodynamic concepts [7], [8]. In kinetic theory, the temperature of a gas is usually defined as the kinetic temperature, which is a form of caloric temperature, through the relation

$$\frac{3}{2} k_B T = \langle \frac{1}{2} m C^2 \rangle, \quad (17)$$

where m and C are the mass and the velocity intensity of a gas particle, respectively. This relation has nothing to do with the special form of the distribution function. In non-equilibrium states, the distribution function may be written as

$$f(\mathbf{r}, C, t) = f_{eq}(\mathbf{r}, C, t) [1 + \Phi], \quad (18)$$

with f_{eq} the equilibrium distribution function characterized by the local values of the thermodynamic parameters, and Φ a non-equilibrium contribution. Up to the second order in Φ , the "entropy" s obtained from the H -function has the form

$$s = s_{eq} - \frac{1}{2} k_B \int f_{eq} \Phi^2 dC, \quad (19)$$

with s the entropy per unit volume. It is seen that, in principle, s will be different from the local-equilibrium entropy s_{eq} . Then one may define the entropic temperature as

$$\frac{1}{T_{neq,ent}} = \frac{\partial s}{\partial u} = \frac{1}{T} - \frac{k_B}{2c} \frac{\partial}{\partial T} \int f_{eq} \Phi^2 dC. \quad (20)$$

In a system submitted to a heat flux, the entropy (19) has the form, up to the second order in the heat flux,

$$s = s_{eq} - \frac{\tau}{2\lambda T^2} \mathbf{q} \cdot \mathbf{q}, \quad (21)$$

where τ is the collision time and λ the thermal conductivity. In more explicit terms, taking into account that

$$\lambda = \frac{5}{2} k_B \frac{p}{m} \tau, \quad (22)$$

the general expression (21) combined with definition (20) yields

$$\frac{1}{T_{neq,ent}} = \frac{1}{T} + \frac{2}{5} \frac{nm}{p^3 T} \mathbf{q} \cdot \mathbf{q}. \quad (23)$$

This temperature would be merely formal unless a method of measurement of it may be specified. It has been shown that this non-equilibrium temperature corresponds to the kinetic temperature in the plane perpendicular to the heat flux. Thus, if the heat flux is in the z direction, one has

$$\left\langle \frac{1}{2} m C_x^2 \right\rangle = \left\langle \frac{1}{2} m C_y^2 \right\rangle = \frac{1}{2} k_B T_{neq,ent} < \frac{1}{2} k_B T$$

and

$$\left\langle \frac{1}{2} m C_x^2 \right\rangle = \frac{1}{2} k_B (3T_{neq,ent} - 2T) > \frac{1}{2} k_B T \quad (24)$$

in such a way that the usual definition of T given in (18) is satisfied. Thus, the concept of the entropic definition of temperature is not in contradiction with that of the kinetic definition.

NON-EQUILIBRIUM TEMPERATURES IN CONTINUUM THERMODYNAMICS

Here, we formulate the problem in the framework of continuum thermodynamics and we consider non-equilibrium steady states, different than equilibrium states because in them the system is crossed by fluxes of energy, matter, electric current or so on. In classical irreversible thermodynamics it is assumed the local equilibrium hypothesis, that states that the fluxes have not an essential influence on the thermodynamics of the system. It assumes that a continuous system out of equilibrium may be decomposed in many small subsystems, each of which behaves, from a thermodynamic point of view, as if it was in local equilibrium.

Non-equilibrium steady states are the natural generalization of equilibrium states: in them, the values of the variables do not depend on time but, in contrast to equilibrium states, a continuous flux of energy - or matter, or momentum, or charge - must be supplied and extracted from the system. We recall the well-known Fourier's transport equation for heat flow \mathbf{q}

$$\mathbf{q} = -\lambda \nabla T, \quad (25)$$

with λ the thermal conductivity.

Beyond local equilibrium, for an ideal monoatomic gas, the entropy takes the form (21), which writes as

$$s(u, \mathbf{q}) = s_{eq}(u) - \alpha(u) \mathbf{q} \cdot \mathbf{q}, \quad (26)$$

where s and u are the entropy and the internal energy, respectively, per unit volume and $\alpha = -\tau(2\lambda T^2)^{-1}$. Using definition (1) we have for the entropic temperature θ

$$\frac{1}{\theta} = \left(\frac{\partial s}{\partial u} \right)_{\mathbf{q}} = \frac{1}{T} - \left(\frac{\partial \alpha(u)}{\partial u} \right) \mathbf{q} \cdot \mathbf{q}, \quad (27)$$

with T the caloric temperature. In a steady state we can use $\mathbf{q} = -\lambda \nabla T$ and rewrite relation (27) in the form

$$s(u, \mathbf{q}) = s_{eq}(u) - \frac{\tau \lambda}{2T^2} \nabla T \cdot \nabla T. \quad (28)$$

Non-equilibrium temperatures in solid systems with internal variables

In this section we will discuss the caloric and entropic non-equilibrium temperatures in a crystal with dislocations, submitted to a given energy flux. We have in mind, for instance, the walls of a fusion nuclear reactor, which are submitted to an intense neutron flux supplied by the nuclear reaction or an electronic device with hot electrons. The neutron flux has two effects on the walls: a thermal effect (it heats them), and a mechanical effect (it produces dislocations in the walls). The second effect is unwanted, because it may reduce the mechanical resistance of the wall.

We assume that in the considered medium we have following fields [9]-[11]: *the elastic field* described by the total stress tensor t_{ij} and the small-strain tensor ϵ_{ij} , defined by $\epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$ (being u_i the components of the displacement vector), *the thermal field* described by the local temperature θ , and the heat flux q_i . However, we assume that the description of the evolution of the system requires the introduction of further dynamical variables in the thermodynamic state space like, for instance, an internal variable. But, whereas the classical variables may be measured and controlled, the internal variables cannot be controlled. In solid media they can describe internal defects like dislocation lines, point defects, porous channels, disclinations and so on. They appear in the Gibbs equation like the classical thermodynamical variables. The evolution of internal variables is described by rate equations, different from the constitutive relations, the transport equation of heat, the balance equations of mass, momentum, momentum of momentum and energy. The whole set of these equations describe the evolution of the system.

Thus, we introduce in the thermodynamic state space the internal variable a_{ij} and its flux V_{ijk} .

We assume that the *evolution equation* for the tensorial internal variable is the following

$$\frac{da_{ij}}{dt} + V_{ijk,k} = A_{ij}, \quad (29)$$

where a_{ij} is the dislocation core tensor, V_{ijk} is its flux and A_{ij} is a field source. The tensor a_{ij} , introduced by Maruszewski [12], describes the local structure of dislocations lines, which form a network of very thin lines disturbing the otherwise perfect periodicity of the crystal lattice. Since these very thin channels, in general, are not distributed isotropically, it is natural to describe them by a tensor, taking into account the local density of the dislocation channels along several directions

The tensor A_{ij} represents the source-like term describing the net effects of formation and annihilation of dislocation lines, which may be a function of temperature T , the strain tensor ϵ_{ij} , the energy flux \mathbf{q} , or the stress tensor t_{ij} . Equation (29) could be simplified, for instance, by assuming for the dislocation flux $V_{ijk} = -D \frac{\partial a_{ij}}{\partial x_k}$, with D being a diffusion coefficient for dislocations. On the other hand, the production term may be seen as the

combination of a dislocation-formation term and a dislocation-destruction term, namely, $A_{ij} = A_{ij}$ (formation) $-A_{ij}$ (destruction).

Then, we consider for the evolution equation for the internal variables the simple form

$$\frac{da_{ij}}{dt} - D\nabla^2 a_{ij} = A_{ij,eq} + \tilde{\alpha} q_i q_j. \quad (30)$$

Here, $A_{ij,eq}$ is the net formation tensor in the absence of an external energy flux ($\mathbf{q} = 0$), and we have added to it a tensor depending on the energy flux.

This form does not pretend to be especially realistic, but only to illustrate that thermal stresses related to $q_i q_j$ could influence the evolution of dislocation lines. More realistic than a simple energy flux, would be to consider, for instance, an energy flux due to the bombardment of the crystal with particles having relatively high energy, which could produce new defects or modify the structure of the dislocation lines.

Non-equilibrium entropic temperature

The entropic definition of absolute temperature is related to the Gibbs equation which, for the system we are considering, has the form

$$ds = \theta^{-1} dU + \theta^{-1} \sigma_{ij} d\varepsilon_{ij} - \theta^{-1} \pi_{ij} da_{ij} - \theta^{-1} \pi dq_i, \quad (31)$$

with π_{ij} the corresponding thermodynamic potential conjugate of the dislocation tensor a_{ij} and π the corresponding thermodynamic potential conjugate of the heat flux q_i . Here, u is the total internal energy of all the degrees of freedom, and we call θ the entropic (absolute) temperature to distinguish it from the T related to the caloric definition.

We have assumed that only the internal variable under consideration is modified by the presence of an external energy flow. Of course the classical variables, like U and ε_{ij} will also be modified by the flux, but here we refer to the modification of temperature for given values of the classical variables.

The thermodynamic absolute temperature is given by (1). In particular, for given values of the classical variable ε_{ij} and in steady states, the equilibrium temperature and the non-equilibrium temperature are defined by

$$\theta_{eq}^{-1} \equiv \left(\frac{\partial s}{\partial u} \right)_{\mathbf{q}=0}; \quad \theta_{neq}^{-1} \equiv \left(\frac{\partial s}{\partial u} \right)_{\mathbf{q} \neq 0}. \quad (32)$$

The quantity θ_{neq}^{-1} can be expanded around its equilibrium counterpart obtaining

$$\theta_{neq}^{-1} = \theta_{eq}^{-1} - \theta_{eq}^{-2} \frac{\partial \theta_{eq}}{\partial a_{ij}} \Delta a_{ij}, \quad (33)$$

where in steady states

$$\Delta a_{ij} = a_{ij}(\mathbf{q} \neq 0) - a_{ij}(\mathbf{q} = 0). \quad (34)$$

Then, in the first approximation, the non-equilibrium temperature θ_{neq} will be related to the equilibrium temperature corre-

sponding to a_{ij} ($\mathbf{q} = 0$) as

$$\theta_{neq} = \frac{\theta_{eq}}{1 - \theta_{eq}^{-1} \frac{\partial \theta_{eq}}{\partial a_{ij}} \Delta a_{ij}} \approx T \left(1 + T^{-1} \left(\frac{\partial T}{\partial a_{ij}} \right) \Delta a_{ij} \right) = T + \left(\frac{\partial T}{\partial a_{ij}} \right) \Delta a_{ij}, \quad (35)$$

where we have taken into account that in equilibrium (or local-equilibrium) all the definitions of temperature coincide, therefore $\theta_{eq} = T$, and we have used the approximation $(1 - x)^{-1} \approx 1 + x$, for $x \ll 1$.

Non-equilibrium caloric temperature

To define the caloric definition of temperature first we consider the caloric equation of state at the equilibrium of the system for given values of ε_{kl} and for vanishing values of the external flux \mathbf{q} : $U_{dis} = U(a_{ij}(T, \varepsilon_{kl}), T, \varepsilon_{kl})$, where we have taken in consideration that at equilibrium the internal variable depends on temperature and the stress tensor. Then, we define the caloric non-equilibrium temperature field T_{neq} related to a_{ij} in a steady state in the following way

$$U_{dis}(a_{ij}(T_{neq}, \varepsilon_{kl}, \mathbf{q} = 0), T_{neq}, \varepsilon_{kl}) \equiv U_{dis}(a_{ij}(T, \varepsilon_{kl}, \mathbf{q}), T, \varepsilon_{kl}). \quad (36)$$

Then, to define the caloric non-equilibrium temperature assume that the formal expression of the relation between internal energy and temperature keeps, out of equilibrium, the same form as in equilibrium ($U_{dis} = U(a_{ij}(T, \varepsilon_{kl}), T, \varepsilon_{kl})$), where $\mathbf{q} = 0$, and we equate it to the value of internal energy in non-equilibrium, where $\mathbf{q} \neq 0$. Thus, we define the temperature in non-equilibrium state as that temperature which, introduced in the caloric state equation would give for the internal energy the actual value corresponding to the non-equilibrium state. Namely, we will have

$$T_{neq} = T + \left(\frac{\partial T}{\partial U_{dis}} \right) \Delta U_{dis} = T + \left(\frac{1}{c_{dis}} \right) \Delta U_{dis}, \quad (37)$$

where $\left(\frac{\partial T}{\partial U_{dis}} \right) \Delta U_{dis}$ is the non-equilibrium contribution due to the presence of $\mathbf{q} \neq 0$, and c_{dis} is the specific heat associated to the changes of the internal energy of dislocation lines, per unit volume, namely $c_{vdis} = \frac{\partial U_{dis}}{\partial T}$. The specific heat plays thus an important role in the caloric definition of temperature.

Entropic flux in the definition of non-equilibrium temperature

In [1] it was seen that in the case of a crystal with dislocations, the entropy flux has the form

$$J_k^s = \theta^{-1} q_k - \pi_{ij} \theta^{-1} V_{ijk}. \quad (38)$$

Here, the variable π_{ij} is the conjugate to a_{ij} as introduced in (31). It has been proposed that a convenient definition of a non-equilibrium contribution could be based on this expression (38),

taking as the reciprocal of thermodynamic temperature the coefficient linking the heat flux \mathbf{q} with the entropy flux \mathbf{J}^S . Based on the idea of perfect interfaces between systems, in which both the heat flux and the entropy flux would be continuous, Muller gave the definition of the so-called "coldness", namely, of the reciprocal of absolute temperature.

Considering the entropy flux and the heat flux through an interface between two systems (let us say, a thermometer and a system) is convenient, because this reminds us the importance of the contact between the system and the thermometer in measuring temperature.

In this aspect, problematic questions arise. In first place, the existence of ideal interfaces is a nice theoretical concept, but in general the interfaces between different materials are not ideal, but exhibit the so-called "thermal boundary resistance", which implies a discontinuity of temperature through the surface, and a corresponding discontinuity of the entropy flux, due to entropy production across the wall, due to the fact that heat is flowing between two different temperatures.

FINAL COMMENTS

In this presentation we have emphasized that one of the aims of non-equilibrium thermodynamics should be to find the transformation laws relating several thermometric, entropic, caloric and other temperatures in systems submitted to given energy flux.

This program has been partially carried out in [1] for forced harmonic oscillators in a thermal bath, in which case kinetic and vibrational temperatures play a special role, and for ideal gases in Couette flow [13], for kinetic temperatures along the three spatial axes, thermodynamic absolute temperature, local-equilibrium temperature, and fluctuation dissipation temperature, or the relation among some non-equilibrium temperatures in heat transport along nanowires [14].

Here, we have tried to be more general, both by the use of simple illustrations of two-level, three-level systems and ideal gases, as by the statement of this problem in the context of a more difficult and demanding situation of solids systems with dislocations.

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