

## **EXTENDED IRREVERSIBLE THERMODYNAMICS AND NON-EQUILIBRIUM TEMPERATURE**

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**ABSTRACT.** We briefly review the concept of non-equilibrium temperature from the perspectives of extended irreversible thermodynamics, fluctuation theory, and statistical mechanics. The relations between different proposals are explicitly examined in two especially simple systems: an ideal gas in steady shear flow and a forced harmonic oscillator in a thermal bath. We examine with special detail temperatures related to the average molecular kinetic energy along different spatial directions, to the average configurational energy, to the derivative of the entropy with respect to internal energy, to fluctuation-dissipation relation and discuss their measurement.

### **1. Introduction**

One of the essential differences between equilibrium states and non-equilibrium steady states is that in the latter the system is crossed by a flux -of energy, matter, electric current or so on. Thus, it is logical to ask which will be 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. In the local equilibrium hypothesis [1], it is assumed that the fluxes have not an essential influence on the thermodynamics of the system: the thermodynamic potentials and, consequently, the equations of state of the system, keep their usual equilibrium form but at a local level, namely, for sufficiently small volume elements. In contrast, extended irreversible thermodynamics [2]-[4] incorporates the fluxes among the essential variables of the system. In fact, fluxes are of interest not only in thermodynamics but they are true protagonists of our time: migration fluxes, information fluxes, commercial fluxes, economic fluxes. The strength of the fluxes is changing our societies, mixing them, accelerating them, fostering progress in some fields and menacing some aspects of small cultures. Our society, then, is submitted to higher and higher fluxes of people, of information, of goods, and this certainly has important effects. The aim of EIT is to explore this question in the specialized domain of some physical systems.

In equilibrium, temperature may be defined by starting from several bases: Carnot's theorem, Gibbs equation, the expression for the entropy flux, expressions based on second moments of fluctuations, Einstein's relation, fluctuation-dissipation theorems, average molecular kinetic energy, average molecular potential energy, canonical form of the distribution function, Lagrange multiplier conjugated to the energy in maximum entropy formalisms. When applied to a system whatsoever in equilibrium, all these definitions lead

to a same result. However, out of equilibrium they lead to different results [5]-[7]. This is not surprising, because out of equilibrium there is not energy equipartition, and therefore different definitions -and consequently different measurements- implying different degrees of freedom will lead to different results.

There arise, then, several conceptual and practical problems. For example, how to define temperature?, which of these definitions -if any provides the best- is most realistic, most informative expression for temperature?, which information provide on the system the different measurements of temperature?, can these different temperatures be related to each other in relatively simple terms, i.e. through a small number of macroscopic parameters? In summary: is it still meaningful to use the concept of temperature beyond local equilibrium? We will focus our attention on non-equilibrium steady states, in order to avoid the additional difficulties arising from possible fast variations of the state of the system.

This problem is receiving an increasing interest: molecular dynamics simulations, for instance, explore situations very far from local equilibrium; the study of glasses, granular materials or nuclear collisions are practical situations where these problems arise in an acute way. Notwithstanding the wide and basic interest of this topic, the several groups of researchers working on different problems are using different definitions of effective non-equilibrium temperatures, which are especially fitted to their respective problems, but there is a lack of contact -and even some incongruences or incompatibilities- between the several perspectives. For instance, the groups working on macroscopic non-equilibrium thermodynamics and those starting from microscopic perspectives widely ignore the work carried out by each other; the groups working on different kinds of systems pay little attention to the research on other kinds of systems, and so on. We have tried to foster the contact through a wide review on these topics [5].

Here, we will formulate the problem in the framework of extended irreversible thermodynamics and will pay a special attention to two very simple systems: a dilute monatomic gas submitted to a plane Couette flow with shear viscous pressure  $P_{xy}^v$  and a forced harmonic oscillator in a thermal bath. In contrast with much more complex systems, as glasses and granular media, these two extremely simple situations allow a fruitful and illustrative discussion and an understanding of the problem for researchers not specialized in this field.

## 2. Extended irreversible thermodynamics

In extended thermodynamics, the fluxes are considered as independent variables. The most well known motivation arises in the analysis of fast phenomena, where the rate of variation of the properties of the system is faster than the time scale characterising the relaxation of the fluxes towards their respective local-equilibrium value. A detailed reasoning, repeated many times in the literature [2]-[4], [8] leads to the conclusion that for simple relaxational extensions of the Fourier law for the heat flux and the Newton-Stokes law for viscous pressure the entropy takes the form

$$(1) \quad s_{\text{EIT}}(u, v, \vec{q}) = s_{\text{leq}}(u, v) - \frac{1}{2} \frac{\tau_1 v}{\lambda T^2} \vec{q} \cdot \vec{q},$$

and

$$(2) \quad s_{\text{EIT}}(u, v, \mathbf{P}^v) = s_{\text{leq}}(u, v) - \frac{1}{4} \frac{\tau_2 v}{\eta T} \mathbf{P}^v : \mathbf{P}^v,$$

with  $u$  the internal energy,  $v$  the volume,  $s_{\text{leq}}$  the local-equilibrium entropy, all these quantities per unit mass,  $\vec{q}$  the heat flux,  $\mathbf{P}^v$  the viscous pressure tensor,  $\lambda$  the thermal conductivity,  $\eta$  the shear viscosity and  $\tau_1$  and  $\tau_2$  the relaxation times of the heat flux and the viscous pressure, respectively. Thus, extended thermodynamics is, in some sense, a thermodynamics of fluxes, besides a thermodynamics of classical variables. This expression is of interest not only for fast varying states, but also in non-equilibrium steady states. Indeed, assume a system submitted to a heat flow. The characteristic residence time of the energy in the system, i.e. the average time a parcel of energy supplied to the system will stay in it before leaving it, is of the order of  $U/Aq$ ,  $U$  being the internal energy of the system and  $Aq$  the total heat supplied to the system (and leaving the system) per unit time. Then, if the heat flux is high enough, the energy residence time will be of the order, or even shorter, than the relaxation time, in such a way that the energy entering into the system will not have time enough to distribute itself among the several degrees of freedom of the system before leaving the system. Then, the relaxation time is important not only for fast-varying states but also for steady states.

Since the entropy is modified by the fluxes, the corresponding equations of state obtained by differentiation of it will also be changed. Thus, EIT provides a framework to explore non-equilibrium modifications to the temperature, the pressure or the chemical potentials. This does not mean that one assumes that the simple expressions (1) and (2) are able to give all the quantitative details of these complex matters, but at least they provide a framework where this topic may be discussed semiquantitatively, in contrast with the local-equilibrium theory, where these matters do not arise at all.

In particular, the non-equilibrium temperature arising from (1) and (2) is

$$(3) \quad \theta^{-1}(u, v, \vec{q}) \equiv \left( \frac{\partial s}{\partial u} \right)_{v, \vec{q}} = T^{-1}(u, v) - \frac{\partial \alpha_1(u, v)}{\partial u} \vec{q} \cdot \vec{q},$$

$$(4) \quad \theta^{-1}(u, v, \mathbf{P}^v) \equiv \left( \frac{\partial s}{\partial u} \right)_{v, \mathbf{P}^v} = T^{-1}(u, v) - \frac{\partial \alpha_2(u, v)}{\partial u} \mathbf{P}^v : \mathbf{P}^v,$$

with  $\alpha_1 \equiv (\tau_1 v / 2 \lambda T^2)$  and  $\alpha_2 \equiv (\tau_2 v / 4 \eta T)$ . The problem, now, is to understand in physical terms the meaning of the non-equilibrium contributions.

For instance, one of the intuitive difficulties in considering non-equilibrium temperature is that temperature is associated with equilibrium between the thermometer and the system. Therefore, talking about a non-equilibrium temperature seems at first sight a contradiction. In the Gedanken (thought) experiment proposed in Fig. 1, this apparent contradiction is overcome [9]-[10]. Indeed, on the one side we take into consideration the heat flux  $q_{rs}$  between the thermometer and the system; on the other side, the heat flux  $q_s$  inside the system itself. Measuring non-equilibrium temperature means that the heat flux  $q_{rs}$  between the system and the thermometer vanishes, but that the heat flux in the system is different from zero. However, at the present stage of the presentation, (3) and (4) are only a formal definition. To relate it with measurement, we examine the operational meaning of

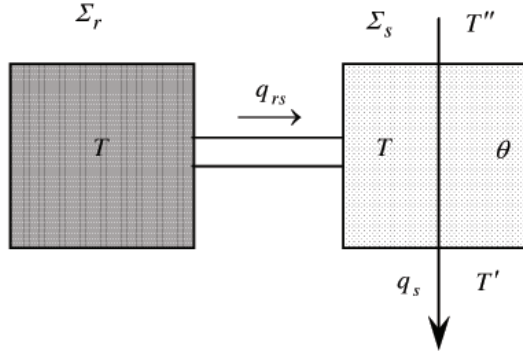


FIGURE 1. Gedanken experiment to analyze the physical meaning of non-equilibrium temperature of a system submitted to a heat flux (see the text for detailed explanation).

temperature by means of the Gedanken experiment of Fig. 1. We connect both systems by means of a good thermal conductor. One of them ( $\Sigma_r$ ) is at equilibrium whereas the other ( $\Sigma_s$ ) is in a non-equilibrium steady state characterized by a heat flux  $q_s$  perpendicular to the connection between both systems (Fig. 1), and which describes the heat exchange between  $\Sigma_s$  and other reservoirs not indicated in the figure. When the flux  $q_{rs}$  between both systems is zero, we will say, according to zeroth law, that both systems have the same temperature, at the points corresponding to the ends of the connecting bar. Note, however, that this statement does not clarify by itself whether the thermometer (the equilibrium system  $\Sigma_r$ ) indicates the local-equilibrium temperature or another temperature. To clarify this point, the second law is needed.

Indeed, the second law is able to relate the heat flux  $q_{rs}$  to the temperature gradient. In our analysis, there are at least two possibilities: one of them is that  $q_{rs}$  is proportional to  $\nabla T$  and the other one is that it is proportional to  $\nabla \theta$ , with  $\theta$  defined in (3). If  $q_{rs}$  is proportional to  $\nabla T$ , the thermometer will indicate the local-equilibrium temperature, because both systems must share the same value of  $T$  in order that the heat flux  $q_{rs}$  vanishes. If, in contrast,  $q_{rs}$  is proportional to  $\nabla \theta$ , the thermometer will indicate the non-equilibrium temperature defined by (3). According to EIT, the second law favors the second possibility over the first one, under conditions that will be examined there in detail.

To be more concrete, consider the situation in which both systems have the same local-equilibrium temperature  $T$  at both ends of the conducting bar (i.e. both systems have the same average kinetic energy per particle). However, one of them (system  $\Sigma_s$ ) is out of equilibrium. If the heat flux  $q_{rs}$  is proportional to the difference of the local-equilibrium temperature of both systems, it will be zero in this case. If, in contrast, it is proportional to the difference of the values of non-equilibrium temperature  $\theta$ , then one should have a nonvanishing heat flux  $q_{rs}$  despite the fact that the local-equilibrium temperature is the same in both systems.

Indeed, application of maximum-entropy analysis to an ideal monatomic gas submitted to a heat flux shows that the average kinetic energy along the direction of the flux is different that along the directions orthogonal to the heat flux. In particular, if  $q$  is directed along the  $y$  direction, it was found that [5, 11]

$$(5) \quad \left\langle \frac{1}{2} m v_x v_x \right\rangle = \left\langle \frac{1}{2} m v_z v_z \right\rangle = \frac{1}{2} k_B \theta < \frac{1}{2} k_B T,$$

$$(6) \quad \left\langle \frac{1}{2} m v_y v_y \right\rangle = \frac{1}{2} k_B (3T - 2\theta) > \frac{1}{2} k_B T.$$

In these expressions,  $k_B$  is the Boltzmann constant and  $T$  the local equilibrium temperature, defined as usual in terms of the average molecular translational kinetic energy as

$$(7) \quad \left\langle \frac{1}{2} m c^2 \right\rangle = \frac{3}{2} k_B T.$$

This consequence could be checked, for instance, by exciting a small region of a rarefied gas with two crossed laser beams and analyzing the Doppler broadening of emission lines from the excited region along the direction of the heat flux and perpendicularly to it. In this analysis, the temperature  $\theta$  obtained from the derivative of the entropy is related to the average kinetic energy in the directions perpendicular to the heat flux. The quantitative results are slightly different if, instead of maximum entropy approach, kinetic theory is used [12]-[13].

In the next section we will show a simple situation involving forced harmonic oscillators in a thermal bath which also shows that the temperature involved in heat exchange is different from the local-equilibrium temperature.

### 3. Forced oscillator in a thermal bath

In this section we deal with another very simple physical system, a one-dimensional harmonic oscillator, in which position contributes to the potential energy and velocity to the kinetic energy, thus leading in a natural way to ask for a kinetic and a configurational temperature. Though in equilibrium they coincide, out of equilibrium -for instance, in the presence of an external forcing giving energy to the oscillator- they become different from each other [14], thus adding a new question as which of these two temperatures is actually measured by a thermometer i.e. about the operational temperature being measured.

The simplest thermodynamic or statistical analysis of such systems assumes an ensemble of identical oscillators in a heat bath at a given temperature  $T$ . To analyze non-equilibrium effects, we introduce an external force acting on the oscillators, and consider that the system is described by

$$(8) \quad \ddot{x} + \gamma \dot{x} + kx = A \sin \omega t + \xi,$$

where the mass  $m$  of the oscillator is taken as unity,  $\gamma$  is the friction coefficient and  $k$  the elastic constant of the harmonic oscillator. The term  $A \sin \omega t$  corresponds to the external periodic forcing, and  $\xi$  is the stochastic noise describing the thermal bath, which has zero average and satisfies  $\langle \xi(t) \xi(t') \rangle = 2\gamma k_B T \delta(t - t')$ , where  $T$  is the absolute temperature of the bath defined by the noise.

In the absence of the external forcing, the probability distribution function of finding the system in a given position or momentum is Gaussian. The external force is giving an input power  $\dot{W}_{\text{ext}} = F\dot{x} = \dot{x}A \sin \omega t$  to the oscillator, which influences the average energy in the different degrees of freedom. In particular, Hatano [15] chose a situation in which the forcing period is longer than the momentum relaxation time and shorter than the position relaxation time, and found that the corresponding distribution functions for position and momentum are Gaussian and may be described in terms of kinetic and configurational temperatures given by

$$(9) \quad T_{\text{con}} = \frac{2}{k_{\text{B}}} \left\langle \frac{1}{2} k x^2 \right\rangle = T + \frac{k}{\gamma \omega^2} \dot{W},$$

$$(10) \quad T_{\text{kin}} = \frac{2}{k_{\text{B}}} \left\langle \frac{1}{2} k \dot{x}^2 \right\rangle = T + \frac{1}{\gamma} \dot{W}.$$

It is seen that both kinetic and configurational temperatures increase with respect to the temperature of the heat bath. The relative increase depends on the values of  $k$ ,  $\gamma$  and the frequency  $\omega$  of the external signal. When  $\omega$  is higher than  $\sqrt{k}$  the configurational temperature is lower than the kinetic one, and viceversa, and at resonance ( $k = \omega^2$ ) both temperatures are equal, but different from that of the bath. In the studies of heat transfer along one-dimensional lattices may be relevant to understand which is the relative contribution of kinetic and configurational temperatures in heat transport.

From a macroscopic point of view, there arises the problem of how these different microscopic temperatures are connected to macroscopic operational measurements. Since the different degrees of freedom may have different temperatures, the operational temperature will in general depend on the kind of connection between the thermometer and the system. To examine a situation which bears some similarities with the proposal in Fig. 1, it was considered [14] two coupled oscillators in contact with their respective heat baths, whose temperature may be controlled independently of each other, and connected through a spring. We will assume that one of them is forced to stay away from equilibrium (the system) while the other is unforced to remain in equilibrium (the thermometer). They are connected through a weak interaction potential  $V$ . The schematic picture of our situation is shown in Fig. 2.

The equations describing the dynamics of the system are

$$(11) \quad \ddot{x} + \gamma_1 \dot{x} + kx + \varepsilon \frac{\partial V(x-y)}{\partial x} = A \sin \omega t + \xi_1(t),$$

$$(12) \quad \alpha \ddot{y} + \gamma_1 \dot{y} + \varepsilon \frac{\partial V(x-y)}{\partial y} = \xi_2(t),$$

where  $k$  is the elastic constant of the spring connecting the oscillator to a wall,  $\varepsilon$  the elastic constant of the spring connecting both oscillators, and  $\alpha$  the mass of the oscillator in the thermometer, which may be different from the mass of the particles in the system. As in (8),  $\xi_1(t)$  and  $\xi_2(t)$  are again assumed to be Gaussian white noise describing the baths but

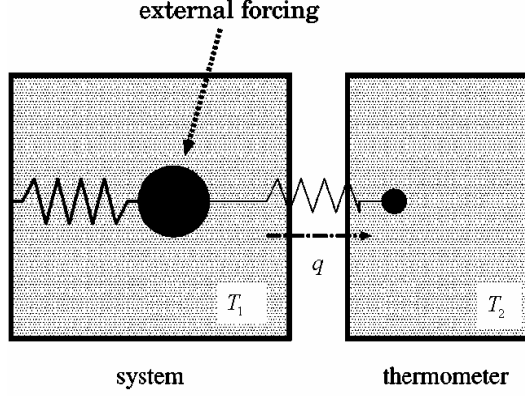


FIGURE 2. Schematic setting for an operational temperature between a forced harmonic oscillator and an equilibrium thermal bath.

characterized by different temperatures  $T_i$ , i.e.,

$$(13) \quad \langle \xi_i(t) \rangle = 0, \quad \langle \xi_i(t) \xi_j(t') \rangle = 2\gamma_i k_B \beta_i^{-1} \delta_{ij} \delta(t - t'),$$

with  $\delta_{ij}$  is Kronecker's delta. Sekimoto [16] studied in detail this system in absence of inertia and external forcing.

We may test two kind of interaction terms: the harmonic and bistable potentials

$$(14) \quad V(r) = \begin{cases} \frac{1}{2}r^2 \\ -\frac{1}{2}r^2 + \frac{1}{4}r^4 \end{cases}$$

The heat flux from the forced system to the thermometer is evaluated as

$$(15) \quad q = \varepsilon \frac{\partial V(x - y)}{\partial y} \dot{y}.$$

When both oscillators are unforced ( $A = 0$ ), the heat flux between them is proportional to the difference of the temperatures of the corresponding heat baths. When one of them is forced ( $A \neq 0$ ), it plays the role of the non-equilibrium system in Fig. 1 whereas the unforced oscillator plays the role of the thermometer, and the connecting spring simulates the thermal contact between them. The thermometer will indicate for the non-equilibrium system the temperature corresponding to a vanishing flux between the system and the thermometer. When the kinetic temperature is higher than the configurational one, it turns out [14] that the value of  $T'$  of the thermometer for which the heat flux vanishes is almost equal to the temperature of the heat bath  $T$  of the non-equilibrium system. In contrast, when configurational temperature is higher than the kinetic one, the temperature for which the heat flow vanishes is intermediate between the configurational and the kinetic ones.

It would be interesting to study how the operational temperature depends on the elastic constant of the connecting spring or the mass of the particles in the thermometer. Indeed, it is possible that different values will make the thermometer more sensitive to one degree of freedom or the other. This would mean that in non-equilibrium situations one must pay

much attention to the interaction between the thermometer and the system. In this case, the zero principle should be formulated only in a very restrictive form, by specifying the conditions of interaction between the systems.

#### 4. Dilute monatomic gas submitted to a shear viscous pressure

Dilute monatomic gases submitted to a plane Couette flow with shear viscous pressure  $P_{xy}^v$ , have become a paradigmatic situation in current thermodynamics of flowing fluids [3, 17], kinetic theory [18], non-equilibrium molecular dynamics [19]-[21] and fluctuation-dissipation theorem [22, 23]. In order to stress that different definitions of temperature lead to different values, but that these values may be related to each other if a sufficiently detailed knowledge of the system is available, we compute several temperatures and compare them.

The one-particle velocity distribution function for an ideal gas maximizing the entropy under the constraints on the average values of the internal energy  $U$  and the viscous pressure tensor  $\mathbf{P}^v$  has the form [3],[24]-[26]

$$(16) \quad f(\vec{r}, \vec{c}) = z^{-1} \exp\left[-\frac{1}{2}\mathbf{M} : m\vec{c}\vec{c}^\dagger\right],$$

with  $z$  the partition function,  $m$  the mass of the particles,  $\vec{c}$  their peculiar velocity, and  $\mathbf{M}$  the matrix of the Lagrange multipliers conjugated to  $U$  and  $\mathbf{P}^v$ , and the colon stands for a double scalar product. In plane Couette flow,  $\mathbf{M}$  is given by

$$(17) \quad \mathbf{M} = \begin{pmatrix} \beta & \lambda_{xy} & 0 \\ \lambda_{xy} & \beta & 0 \\ 0 & 0 & \beta \end{pmatrix},$$

where  $\beta$  and  $\lambda_{xy}$  are the Lagrange multipliers respectively conjugated to  $U$  and  $\mathbf{P}^v$ . A more general expression incorporating non-equilibrium normal pressures may be found in [25].

First of all, we compute the kinetic temperatures associated to the three spatial directions ( $x$ , along the flow,  $y$ , along the velocity gradient, and  $z$ , perpendicular to the previous two directions) of a flowing ideal gas. It follows from (16) and (17) that

$$(18) \quad \left\langle \frac{1}{2}mc_x^2 \right\rangle = \left\langle \frac{1}{2}mc_y^2 \right\rangle = \frac{1}{2} \frac{\beta}{\beta^2 - \lambda_{xy}^2} \equiv \frac{1}{2}k_B T_x > \frac{1}{2}k_B T,$$

and

$$(19) \quad \left\langle \frac{1}{2}mc_z^2 \right\rangle \equiv \frac{1}{2}k_B T_z < \frac{1}{2}k_B T.$$

Notice that, as in (7), equipartition of energy in the three spatial directions is broken. The average kinetic energy along  $z$  direction, perpendicular to the velocity and the velocity gradient, is less than in the other two directions (this is also found in non-equilibrium molecular dynamics for simple fluids with interacting molecules although in that case the temperature along the  $x$  and the  $y$  axis are not exactly equal [20]). Furthermore, it is seen that the kinetic temperature  $T_z$  coincides with the non-equilibrium thermodynamic temperature  $T_{\text{neq}}$ , similarly to the situation when a heat flux is present in the system (Fig.1),



in which the non-equilibrium temperature, denoted by  $\theta$  in 5, agrees with the kinetic temperature in the direction perpendicular to the heat flux [11]. It may be seen, after explicit calculation of the Lagrange multipliers [27], that  $T_z$  is reduced for increasing values of viscous pressure, whereas  $T_x$  and  $T_y$  increase with viscous pressure as it is shown in Fig. 3. The value of the temperature will depend, then, on the relative direction between the surface of the thermometer, the macroscopic velocity and its gradient.

Another way to define temperature is to start from the entropy, as in Section 2. From the thermodynamic point of view, this is the most fundamental definition of temperature. However, out of equilibrium, the entropy is usually not known, or it cannot be univocally defined. We refer to the non-equilibrium thermodynamic temperature  $T_{\text{neq}}$  stemming from the derivative of a non-equilibrium entropy [3, 25, 26]. The differential of the entropy for the plane Couette flow under consideration, characterized by  $U$  and  $P_{xy}^v$ , may be written as [2, 3, 24],

$$(20) \quad dS = k_B \beta dU + k_B \lambda_{xy} d(V P_{xy}^v),$$

where the entropy  $S$  is obtained from the distribution function (1) as  $S = -k_B \int f \ln f d\vec{c}$ . This leads for the non-equilibrium thermodynamic temperature [3, 24]

$$(21) \quad T_{\text{neq}} = \frac{1}{k_B \beta} = \left( \frac{\partial U}{\partial S} \right)_{V, P_{xy}^v} = \frac{3 [R^2 + (1 - Y)]}{1 - Y} T,$$

where  $R$  and  $Y$  stand for  $R \equiv V P_{xy}^v / U$  and  $Y = (1 + 3R^2)^{1/2}$ . The factor  $R$ , expressing the departure from equilibrium, is restricted to the interval  $0 \leq R \leq 1$ , as it is shown in detail in [24, 25]. In equilibrium, i.e. when  $R \rightarrow 0$ , it is found that  $T_{\text{neq}} \rightarrow T$ , whereas it decreases for increasing  $R$  and it tends to 0 when  $R \rightarrow 1$ . The physical interpretation of this fact is that in this regime the molecular energy is highly organized, and the disordered part of the energy contributing to the entropy is very small. Both  $T_z$  and  $T_{\text{neq}}$  decrease for increasing values of the viscous pressure.

Still another effective non-equilibrium temperature  $T_{\text{eff}}$  may be defined from the fluctuation-dissipation theorem [6, 22, 23, 28] relating response function and correlation function. In the situation we are studying, this temperature is defined as

$$(22) \quad \frac{\eta}{\tau_2} = \frac{1}{k_B T_{\text{eff}}} \langle \delta P_{xy}^v(0) \delta P_{xy}^v(0) \rangle,$$

where  $\eta$  is the dynamical shear viscosity,  $\tau_2$  the relaxation time of the viscous pressure and the angular brackets denote the equilibrium average. In equilibrium,  $T_{\text{eff}} = T$  and (22) becomes the Green-Kubo relation between shear viscosity and viscous pressure fluctuations when the decay of the latter is exponential with relaxation time  $\tau$  [2]. In the situation we are considering, we found [29]

$$(23) \quad T_{\text{eff}} = \frac{3}{2} \frac{\left\{ R^2 + [R^2 / (Y - 1)]^2 \right\} \left[ R^2 + \frac{2}{3} (Y - 1) \right]}{R^2 (Y - 1 - R^2)} T.$$

It is seen that  $T_{\text{eff}} \geq T \geq T_{\text{neq}}$  and that both  $T_{\text{eff}}$  and  $T_{\text{neq}}$  tend to the local-equilibrium temperature when the viscous pressure tends to zero but their asymptotic limit far from equilibrium is very different, as  $T_{\text{neq}} \rightarrow 0$  and  $T_{\text{eff}} \rightarrow \infty$ . Note that the several temperatures we have used are related by means of a small number of variables, namely, they may

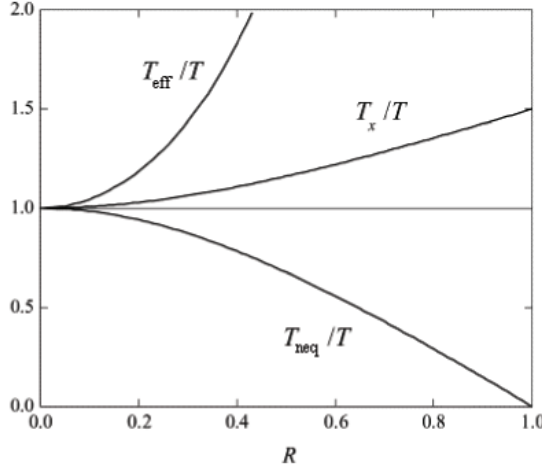


FIGURE 3. Several temperatures at a given value of  $U$  as a function of  $R = VP_{xy}^v/U$ . The temperatures shown here are: local equilibrium temperature  $T$ , thermodynamic non-equilibrium temperature  $T_{\text{neq}}$  (equal to the kinetic temperature along the  $x$  axis), the kinetic temperatures in the  $x$  and  $y$  directions ( $T_x = T_y$ ), and the fluctuation-dissipation effective temperature  $T_{\text{eff}}$ .

be expressed, all of them, in terms of the internal energy, the number of particles, and the viscous pressure.

Baranyai [20] studied, instead of an ideal gas, fluid systems composed of spherical particles interacting through a soft potential, and used non-equilibrium molecular dynamics to analyze their behavior in shear flow. He studied kinetic and configurational temperatures at different values of the shear rate and found both temperatures to be anisotropic. Furthermore, he proposed an operational temperature by simulating a physical thermometer in contact with the fluid and found that the operational temperature is closer to the configurational one than to the kinetic one. He found that the operational temperature depends on the mass of the particles composing the thermometer, in such a way that one must be careful in considering not only the properties of the system, but too of the thermometer and of its interaction with the system. In shear flow, he found that the operational temperature is closer to the temperature along the axis of the velocity gradient. In contrast, the configurational and kinetic temperatures along the direction of the flow are much lower than the operational temperature.

## 5. Concluding remarks

The topic of non-equilibrium temperature is playing a central role in recent theories of non-equilibrium thermodynamics, information theory, kinetic theory, non-equilibrium molecular dynamics, granular fluids, supercooled liquids under shear, radiative systems or

nanoscale heat transport (see [5, 6] for wide bibliographies). Thus, it deserves a detailed understanding from practical as well as fundamental grounds.

Here, we have seen that the different temperatures may be related amongst themselves, in such a way that the knowledge of one of them allows us to obtain the values of the other. They do not coincide because the different temperatures are related to different aspects of the system. Out of equilibrium there is no equipartition, in general, in such a way that different definitions of temperature, emphasizing on different aspects of the system, are expected to have different values.

As in extended irreversible thermodynamics, temperature is found to depend not only on the energy but also on the energy flux, i.e. the power input of the forcing to the oscillator, or the viscous pressure. In particular, a Gedanken experiment was proposed in order to clarify the meaning of non-equilibrium temperature from an operational point of view [8]. It is not yet clear how such operational temperature is related to the kinetic and configurational temperatures; probably, the contribution of both temperatures to the operational one will depend on the kind of thermometer being used. Analogous situations are found in some experimental systems, as for instance laser-induced plasmas in semiconductors under the presence of an electric current through them [30].

In summary, temperature is a concept which still has many open problems in non-equilibrium. For instance, in the situation studied here, the fact that the distribution functions of positions and momenta were Gaussian has made especially easy to define the temperature of the several degrees of freedom, but additional conceptual problems would appear if the distribution functions markedly differ from Gaussian one.

If such a wide diversity of temperatures arises out of equilibrium, is it legitimate to give a fundamental priority to one of them? May we still talk about temperature? In our opinion [5], one of the aims of non-equilibrium thermodynamics beyond local equilibrium is to relate the different temperatures in terms of the average energy and also of the fluxes acting on the system. In this case, one would need not only the global fluxes but also how these fluxes are distributed among the different degrees of freedom. The two situations briefly presented here have the interest of illustrating this point with simplicity.

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