Reply to "Comments on 'Possible experiment to check the reality of a nonequilibrium temperature'"

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A simple mechanistic interpretation of our proposed experiment is presented, which allows us to clarify the points raised by the preceding Comments by Hoover, Holian, and Posch [Phys. Rev. E **48**, 3191 (1993)] and Henjes [Phys. Rev. E **48**, 3194 (1993)].

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The two previous Comments [1,2] raise interesting points about our proposed experiment [3] on a nonequilibrium absolute temperature. The Comment by Henjes [1] outlines the problem of a possible ambiguity in the interpretation of our proposed experiment [3], according to whether one uses $\nabla\Theta$ or ∇T to describe the heat flux q_y in the nonequilibrium system, thus leading to no conclusion about whether T or Θ is measured in a real experiment. Here, Θ is a generalized absolute temperature obtained by differentiation of the nonequilibrium entropy in the presence of a heat flux [4,5] and T is the usual local-equilibrium absolute temperature. On the other hand, the Comment by Hoover, Holian, and Posch [2] emphasizes the utility of the ideal-gas temperature scale and raises the question of the compatibility of the nonequilibrium temperature with the ideal-gas temperature or local-equilibrium temperature.

To clarify these questions, we propose a mechanistic interpretation of our suggested experiment, based on the kinetic theory of gases. This experiment allows us to avoid the ambiguity pointed out by Henjes [1] and, on the other side, in response to the Comment by Hoover, Holian and Posch [2], it stresses the fact that in this situation an ideal-gas thermometer would read the generalized temperature rather than the local temperature. Indeed, this mechanistic interpretation may provide the basis for a computer simulation, which allows us to specify the local-equilibrium absolute temperature T, related in the usual way to the mean kinetic energy of the particles.

For instance, we imagine that both systems at the ends of the connecting bar of Fig. 1 consist of an ideal monatomic gas, and we study the power delivered to each end of the bar by molecular collisions. It is easy to show, in a qualitative way, that if both ends of the bar are at the same local-equilibrium temperature, but the system on the right is in a nonequilibrium steady state under a heat flux q_y, the end corresponding to the nonequilibrium system is receiving less power than the end at equilibrium, so that heat will flow from the latter system to the former one, according to the macroscopic reasoning in our paper.

We will consider the kinetic energy arriving at the wall corresponding to collisions of particles whose trajectory makes an angle $\pm\alpha$ with the normal to the surface of the bar. A fraction of this energy will be delivered to the bar if it is heat conducting. The energy per unit time and unit area (the energy flux) arriving at the wall will be proportional to

$$J_u(\alpha)\approx a(\alpha)[n_+T_+\sqrt{T_+}+n_-T_-\sqrt{T_-}]\,, \tag{1}$$

where $a(\alpha)$ is a function of the collision angle α and subscripts + and − stand for labeling the upper and lower regions shown in Fig. 1. Indeed, $n\sqrt{T}$ is proportional to the flux of particles arriving at the wall [(density)×(speed)] whereas T is proportional to the mean energy carried per particle. Thus, $nT\sqrt{T}$ is the flux of energy carried by the particles colliding with the wall, expressed in k units.

In the equilibrium system, n and T do not depend on the position, so that $n_+=n_-=n$ and $T_+=T_-=T$. In the nonequilibrium system, $n(y)$ and $T(y)$ depend on the position y; however, the absence of convection imposes $n(y)T(y)=\text{const}$ (constant pressure condition); from here it follows that $n_+T_+=n_-T_-$. We will write $T_+=T+\delta T$, $T_-=T-\delta T$, with $\delta T\approx l\nabla T\sin\alpha$ (particles coming from distances longer than l will not arrive at the wall due to collisions). Then, the energy arriving at the wall per unit time and unit area, i.e., the energy flux, will be, in the equilibrium system,

$$J_u^{\text{eq}}(\alpha)\approx 2a(\alpha)nT\sqrt{T}\,, \tag{2}$$

whereas in the nonequilibrium system it will be

$$J_u^{\text{neq}}(\alpha)\approx a(\alpha)nT\sqrt{T}\,\{[1+(\delta T/T)]^{1/2}+[1-(\delta T/T)]^{1/2}\}\,, \tag{3}$$

which, up to the second order in δT, is

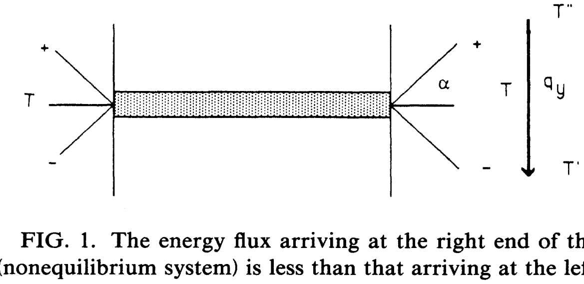

FIG. 1. The energy flux arriving at the right end of the bar (nonequilibrium system) is less than that arriving at the left end of the bar (equilibrium system). Thus it follows that energy should flow from the left to the right.

$$J_u^{\mathrm{neq}}(\alpha)\approx 2a(\alpha)nT\sqrt{T}\,\{1-(1/8)(\delta T/T)^2\}<J_u^{\mathrm{eq}}(\alpha)\ . \tag{4}$$

Integration over all angles α from 0 to $\pi/2$ indicates that the energy flux arriving at the end of the bar in the system at equilibrium is higher than the energy arriving at the end in the nonequilibrium system, in spite of the fact that both systems are at the same local-equilibrium temperature (both systems have the same mean molecular energy). Thus, a heat flux q_x proportional to $(l\nabla \ln T)^2$ will appear in the situation of Fig. 1, according to our predictions.

This experiment does not present the ambiguity mentioned by Henjes [1] because both T and q_y may be unequivocally controlled in a computer simulation. On the other hand, the system on the left (equilibrium system) may be considered as an ideal-gas thermometer: this thermometer will read the nonequilibrium temperature Θ, because only when the T of the thermometer is equal to the Θ of the nonequilibrium system in contact with it will the heat exchange between the thermometer and the system vanish. Note that in comparison with the thermometer assumed by Hoover, Holian, and Posch [2], our thermometer does not involve any material exchange between it and the system

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