# Thermodynamic definition of mean temperature

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The notion of mean temperature is crucial for a number of fields, including climate science, fluid dynamics, and biophysics. However, so far its correct thermodynamic foundation is lacking or even believed to be impossible. A physically correct definition should not be based on mathematical notions of the means (e.g., the mean geometric or mean arithmetic), because they are not unique, and they ignore the fact that temperature is an ordinal level variable. We offer a thermodynamic definition of the mean temperature that is based upon the following two assumptions. First, the correct definition should necessarily involve equilibration processes in the initially nonequilibrium system. Among such processes, reversible equilibration and fully irreversible equilibration are the two extreme cases. Second, within the thermodynamic approach we assume that the mean temperature is determined mostly by energy and entropy. Together with the dimensional analysis, the two assumptions lead to a definition of the mean temperature for ideal and (van der Waals) nonideal gases with temperature-independent heat capacities and concentration of gases. Our method works for any nonequilibrium initial state, not only two-temperature states.

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## I. INTRODUCTION

Many nonequilibrium situations are described by mean temperature in a quasiequilibrium manner. Climate is defined with respect to a mean temperature, while climate change discussions are largely based on global mean temperatures of Earth's surface [1–6]. These mean temperatures come from mathematical averaging of experimental results obtained via different instrument readings. Mean temperature and deviations from it are widely used in turbulence [7–9], granular gases [10], cellular biophysics [11], material science (including radiative heat transfer) [12], etc. Particularly, temperature is considered as a function of mechanical variables, namely, energy and volume (the form of this function is taken from macroscopic thermodynamics), and mean temperature and variance are calculated as for ordinary random variables [11,13].

Despite this widespread usage, the notion of mean temperature so far lacks physical foundations [6]. There are several interrelated reasons for that.

(i) Mathematical definitions of the mean are not unique (mean arithmetic, geometric or harmonic?), though in one way or another they are employed for defining the mean temperature.

(ii) The mean arithmetic is selected for additive quantities, e.g., length, volume, and energy.<sup>1</sup> Here defining the mean

amounts to taking the two systems with different (say) volumes together, calculating the total volume, and dividing over the number of systems [14]. But temperature is not an additive quantity.

(iii) Temperature is defined with respect to a conventionally chosen thermometer [13–16]. The readings  $t_1$  and  $t_2$  of two thermometers 1 and 2 relate to each other via a monotonous transformation  $t_1 = f(t_2)$  [13–16]. Hence the notions of larger and smaller are well defined for temperature, but mathematical means are not covariant with respect to f(x), in contrast to physical quantities (energy, entropy, pressure, etc.) that are invariant. Using the language of statistics, temperature belongs to ordinal-level variables [17–21]. One particular example of f(x) is an affine transformation f(x) = ax + b, where a and b are constants. Three basic scales—Celsius, Fahrenheit, and Kelvin|relate to each other via affine transformations:

$$T_{\rm C} = \frac{5}{9}(T_{\rm F} - 32), \quad T_{\rm C} = T_{\rm K} - 273.15,$$
 (1)

where the coefficients here are conventional (e.g., due to historic accidents).

The arithmetic mean (but not other means) is covariant with respect to an affine transformations but is not covariant with respect to more general monotonous transformations, e.g., to f(x) = 1/x. Indeed, frequently the inverse temperature  $\beta = 1/T$  provides a better physical description than *T* itself, e.g., because it provides a better of account nonequilibrium physics [13,22,23]. Spin physics employs  $\beta$  instead of *T*, also because in that field  $\beta$  passing through zero is usual, unlike

<sup>&</sup>lt;sup>1</sup>For energy this holds to a limited extent due to interaction energy.

"dramatic" changes implied by  $T = 1/\beta$  passing through the infinity [22]. Also, the usage of  $\beta$  (instead of T) makes the third law intuitive, since this law now tells about the impossibility to reach  $\beta = \infty$  [13]. Given these advantages of  $\beta$  with respect to T, one can try to define the mean temperature via the mean arithmetic of  $\beta$ , which amounts to mean harmonic in terms of T. This illustrates the above point (i).

(iv) Temperature is defined only in equilibrium [13]. This means that for defining a mean temperature in a nonequilibrium state we should invoke physically meaning-ful equilibration processes that correspond to the operational notion of putting the systems together [14]. Such processes depend on how precisely (i.e., under which external conditions) the equilibration was achieved.<sup>2</sup>

We propose a thermodynamic definition of the mean temperature that solves the above issues. We start by setting upper and lower bounds to the mean temperature. These bounds describe two extremes of equilibration processes: one that is reversible and thermally-isolated, releasing work, and one that is completely irreversible and energy-isolated, increasing entropy by dissipating the available work. Respective temperatures  $\hat{T}$  and  $\bar{T}$  refer to entropy-conserving and energy-conserving processes. We suggest, and then prove from the definition, that  $\hat{T}$  and  $\tilde{T}$  ( $\hat{T} < \tilde{T}$ ) are lower and upper bounds of the mean temperature  $\overline{T}$ . Next, we assume that within the thermodynamic description, the mean temperature  $\overline{T}$  is defined only via entropies and energies of the initial (nonequilibrium) state and possible final equilibrium state. This assumption, along with a dimensional analysis and the maximum ignorance principle, suffices to define the mean temperature  $\overline{T}$ . It holds that  $\hat{T} \leq \overline{T} \leq \widetilde{T}$ , depending both on the initial nonequilibrium state of the considered system and also on the very substance it refers to, e.g., the mean temperature for two pieces of iron having temperatures  $T_1$ and  $T_2$  will be different from two pieces of wood having the same temperatures  $T_1$  and  $T_2$ . However, for a class of systems relevant for atmospheric physics-ideal and van der Waals nonideal gases with a temperature-independent heat capacity (cf. Appendix A)— $\overline{T}$  holds a general expression that (aside from the initial temperatures) depends only on heat capacities and concentrations of gases.

It turns out that  $\tilde{T}$  formally coincides with the temperature estimator from energy measurements, as deduced from the maximum-likelihood method; see Appendix C. Reference [24] developed this approach to temperature estimation from energy measurements, and it is the standard approach for temperature fluctuations; see [25,26] for reviews. According to that approach, the temperature estimator also maintains covariance for monotonous transformations.

The rest of this paper is organized as follows. The next section discusses the general setup of our problem. Section III defines the mean temperature. Section III C indicates its generalizations. Section III D compares our definition with several notions of effective temperature and nonequilibrium temperature proposed in the literature. Section IV applies our

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definition to the ideal gas model. The application to nonideal gases is given in Appendix A. We summarize in the last section with a discussion of the physical meaning of our approach and its limitations.

## **II. SETUP**

Consider *M* equilibrium systems  $A_k$ , k = 1, ..., M. Each system has absolute temperature  $T_k$ , number of particles  $N_k$ , volume  $V_k$ , internal energies  $U_k(T_k, V_k, N_k)$ , and entropy  $S_k(T_k, V_k, N_k)$ . For simplicity we shall work with M = 2, but the extension of our results to M > 2 is straightforward and amounts to replacing  $U_1 + U_2$  by  $\sum_{k=1}^{M} U_k$  and  $S_1 + S_2$  by  $\sum_{k=1}^{M} S_k$ . We will explain how our results apply to more general initial states of  $A_k$  in Sec. III C.

We shall work with the absolute temperature scale (in energy units, i.e., with  $k_{\rm B} = 1$ ), but at several places we emphasize the covariance of our conclusions with respect to monotonous transformations of temperature.

We assume that  $A_1 + A_2$  is a thermally isolated system. We allow  $A_1 + A_2$  to equilibrate and reach some joint temperature which can be then related to the mean temperature. The equilibration process depends on the external conditions [13]; e.g., it depends on whether and to which extent we allow for work extraction from  $A_1 + A_2$ . We consider only processes that proceed via thermal contacts, i.e., they are realized at fixed values of the volumes  $(V_1, V_2)$  and the particle numbers  $(N_1, N_2)$ . The reason for this is discussed in Appendix B. Hence we omit the arguments  $(V_1, N_1)$  and  $(V_2, N_2)$  for energy and entropy.

#### A. Reversible equilibration

 $A_1$  and  $A_2$  couple through a working body B, which sequentially interacts with  $A_1$  and  $A_2$  via weak thermal contacts. Between interactions B delivers work to the external source [13]. The thermodynamic state of B changes cyclically. Hence the overall entropy change is given by the change of the entropies of  $A_1$  and  $A_2$ . The process is reversible, and the overall entropy stays constant:

$$S_1(T_1) + S_2(T_2) = S_1(\hat{T}) + S_2(\hat{T}),$$
 (2)

where  $\hat{T}$  is the final temperature, which is the same for  $A_1$  and  $A_2$ . Since  $A_1 + A_2$  is thermally isolated due to (2), the overall energy deficit is the extracted work:

$$U_1(T_1) + U_2(T_2) - U_1(\hat{T}) - U_2(\hat{T}) \ge 0.$$
(3)

Figure 1 illustrates the situation of Eqs. (2) and (3) on the energy-entropy diagram. It is seen that possible nonequilibrium states  $(U_{in}, S_{in})$  are bound (from left) by an an increasing and concave equilibrium energy-entropy curve. The reason for concavity is noted in the caption of Fig. 1. For our situation,  $U_{in} = U_1(T_1) + U_2(T_2)$  and  $S_{in} = S_1(T_1) + S_2(T_2)$ . Note from Fig. 1 that Eq. (3) is the maximal work that can be extracted under the restriction of the second law and fixed  $(V_1, N_1)$  and  $(V_2, N_2)$ :

$$U_1(\hat{T}) + U_2(\hat{T}) = \min_{\hat{T}_1, \hat{T}_2} [U_1(\hat{T}_1) + U_2(\hat{T}_2)|], \qquad (4)$$

where the minimization is conditioned by  $S_1(T_1) + S_2(T_2) \leq S_1(\hat{T}_1) + S_2(\hat{T}_2)$ . This conditioning is indicated in Eq. (4) by |.

<sup>&</sup>lt;sup>2</sup>There are attempts to define temperature also *directly* in nonequilibrium states; see Sec. III D for a discussion.

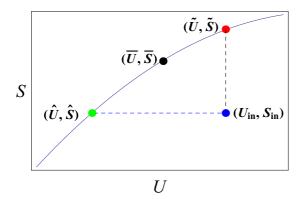


FIG. 1. A schematic representation of the entropy-energy diagram. The blue concave curve shows S(U): the equilibrium entropy S as a function of equilibrium energy U for a fixed volume and particle number. This curve is growing, S'(U) > 0, since the temperature is positive. The curve is concave, S''(U) < 0, because the heat capacity (at a fixed volume and particle number) is positive due to thermodynamic stability [13]. Now  $(U_{in}, S_{in})$ , denoted by the blue point, indicates the initial nonequilibrium state; e.g., this can be a two-temperature state for two systems  $A_1 + A_2$ . This state can equilibrate via at least two processes: the irreversible scenario refers to a constant energy and monotonically increasing entropy; see the black-dashed (vertical) line. Equilibrium values are denoted as  $(\tilde{U}, \tilde{S})$  (red point) and refer to temperature  $\tilde{T}$ ; cf. (7). In the reversible process, the entropy remains constant while the energy decreases until it reaches the equilibrium point  $(\hat{U}, \hat{S})$  at temperature  $\hat{T}$  [cf. (4)]; see the blue-dashed (horizontal) line reaching the green point. The mean temperature  $\bar{T}$  refers to an equilibrium state  $(\bar{U}, \bar{S})$  located in between:  $\hat{T} < \bar{T} < \tilde{T}$ ; see Eq. (13).

Indeed, if we allow more general processes, where the final entropy is larger than  $S_{in} = S_1(T_1) + S_2(T_2)$ , then the final energy is also larger than  $U_1(\hat{T}) + U_2(\hat{T})$  due to the fact that the equilibrium energy-entropy curve S(E) is increasing; see Fig. 1.

It is natural for relaxation to be accompanied by work extraction. Within atmospheric thermodynamics, work extraction means increasing the hydrodynamic kinetic energy due to internal energy and refers to the emergence of a macroscopic motion (wind, storm, or circulation) in a nonequilibrium state [27,28]; see [29,30] for reviews. Carefully accounting for this energy balance requires fluid dynamic consideration; see, e.g., [31]. Reference [32] studied the maximal extracted work and the maximal entropy increase as features of a nonequilibrium atmosphere; see [30] for a review.

## B. Fully irreversible equilibration

The second pertinent scenario of equilibration looks at another extreme. Now  $A_1$  and  $A_2$  are isolated from the rest of the world and are subject to the fully irreversible equilibration via thermal contacts; i.e., again  $(V_1, N_1)$  for  $A_1$  and  $(V_2, N_2)$ for  $A_2$  stay fixed. Now the total energy is conserved,

$$U_1(T_1) + U_2(T_2) = U_1(\widetilde{T}) + U_2(\widetilde{T}),$$
(5)

defining the final temperature  $\tilde{T}$ . The entropy increase is clearly positive:

$$S_1(\tilde{T}) + S_2(\tilde{T}) - S_1(T_1) - S_2(T_2) > 0.$$
(6)

As seen from Fig. 1, Eq. (6) is the maximal entropy increase for the conserving energy plus fixed  $(V_1, N_1)$  and  $(V_2, N_2)$ :

$$S_1(\widetilde{T}) + S_2(\widetilde{T}) = \max_{\widetilde{T}_1, \widetilde{T}_2} [S_1(\widetilde{T}_1) + S_2(\widetilde{T}_2)], \qquad (7)$$

where the maximization is conditioned by  $U_1(T_1) + U_2(T_2) = U_1(\tilde{T}_1) + U_2(\tilde{T}_2)$ . We note that the structure of (5) is formally similar to the temperature estimator developed in Ref. [24]. This connection is explained in Appendix C.

# **III. MEAN TEMPERATURE**

# A. Upper and lower bounds for the mean temperature

As we confirm below, the temperatures  $\hat{T}$  and  $\tilde{T}$  hold,

$$\min[T_1, T_2] \leqslant \hat{T} \leqslant \tilde{T} \leqslant \max[T_1, T_2], \tag{8}$$

which naturally implies that all other temperatures found via partially irreversible processes will be located between  $\hat{T}$  and  $\tilde{T}$ ; see Fig. 1.

Below we show that the mean temperature  $\overline{T}$  also locates between  $\hat{T}$  and  $\widetilde{T}$ :

$$\hat{T} \leqslant \bar{T} \leqslant \tilde{T}.$$
(9)

The rationale for (9) is that once the temperature relates to the heat content, we should decide what to do with the available work. Two extreme options are to dissipate it completely  $(\tilde{T})$  or to extract it fully  $(\hat{T})$ . We cannot add any external work, since this will potentially change the heat content. Moreover, if we start adding work to the overall system  $A_1 + A_2$ , the final temperature can be made arbitrarily large.

Note that all thermalization processes with the final temperature  $\bar{T}$  holding (9) are consistent with the statement of the second law: entropy of a thermally isolated system does not decrease. In that sense the second law alone is not able to fix the final temperature, which is not surprising.<sup>3</sup>

We emphasize that  $\hat{T}$  and  $\tilde{T}$  are covariant with respect to monotonous transformations of the absolute temperature. This follows from the very definitions (2) and (5). Put differently,  $\hat{T}$  and  $\tilde{T}$  are covariant with respect to employing any other reasonable thermometer instead of the thermometer that leads to the absolute temperature.

# **B.** Definition of mean temperature

We assume that the mean temperature  $\bar{T}$  is an equilibrium temperature holding (9), and it is determined via energy and entropy only [by analogy to Eqs. (4) and (7)]. The physical basis of this assumption is the known thermodynamic fact that the state of an equilibrium system with a fixed number of particles is determined by two variables that can be taken entropy and energy<sup>4</sup> [13]. Now we need a concrete mathematical form of the physical assumption, e.g., we postulate that the mean temperature  $\bar{T}$  is found through a four-variable function of the

<sup>&</sup>lt;sup>3</sup>A similar situation, where the second law alone is not capable to determine the final equilibrium state, is realized for the adiabatic piston problem [33].

<sup>&</sup>lt;sup>4</sup>There are exclusions from this thermodynamic rule, e.g., for magnets in external fields, but we do not focus on them here.

initial and final energy and entropy:

$$\bar{T} = \operatorname{argmax}_{T} F[U_{1}(T) + U_{2}(T), S_{1}(T) + S_{2}(T), S_{1}(T_{1}) + S_{2}(T_{2}), U_{1}(T_{1}) + U_{2}(T_{2})].$$
(10)

 $\overline{T}$  in (10) should be invariant with respect to changing dimensions of the entropy and energy, as well as adding to these quantities arbitrary constants *b* and *d* [13]:

$$S \to aS + b$$
,  $U \to cU + d$ ,  $a > 0$ ,  $c > 0$ , (11)

where the constants a and c come from changing the dimensions. In addition, (10) should hold (9). Indeed, the invariance with respect to changing the dimensions is a natural condition to demand, while the invariance with respect adding arbitrary constants reflects the freedom energy and entropy have in thermodynamics.<sup>5</sup>

The only expression that holds all the above conditions and is invariant with respect to (11) reads [34–36]

$$\bar{T}(\alpha_1, \alpha_2) = \operatorname{argmax}_T \{ [U_1(T_1) + U_2(T_2) - U_1(T) - U_2(T)]^{\alpha_1} [S_1(T) + S_2(T) - S_1(T_1) - S_2(T_2)]^{\alpha_2} \},$$
(12)

where  $\alpha_1 \ge 0$  and  $\alpha_2 \ge 0$  are weights. All other possibilities are equivalent to (12) in one way or another.

Note that for  $\alpha_1 \to 0$  and  $\alpha_2 \to 0$  we revert to (resp.) Eqs. (7) and (4). It should also be clear that  $\hat{T} \leq \bar{T}(\alpha_1, \alpha_2) \leq \tilde{T}$ ; cf. (9).

How do we choose  $\alpha_1$  and  $\alpha_2$ ? First note that instead of the function to be maximized in (12) we can maximize its logarithm, which makes clear that only the ratio  $\alpha_1/\alpha_2$  is important for  $\overline{T}(\alpha_1, \alpha_2)$ . In other words, we can assume  $\alpha_1 + \alpha_2 = 1$ . Once we do not know these weights, the ignorance (or the most unbiased, or the maximum entropy) interpretation forces us to choose  $\alpha_1 = \alpha_2 = 1/2$ . Thus we end up from (12) to the final definition of the mean temperature:

$$\bar{T} = \bar{T}(1/2, 1/2).$$
 (13)

It is important to emphasize that maximum ignorance is not a physical principle, so choosing  $\alpha_1 = \alpha_2 = 1/2$  is a plausible assumption.<sup>6</sup>

Equation (13) achieves a balance between no work extraction (complete irreversibility) and the complete reversibility: now some work is still extracted, but the entropy does increase. The unique argmax of (13) automatically appears in the interval  $[\hat{T}, \tilde{T}]$ . In contrast to a naive definition  $(\tilde{T} + \hat{T})/2, \bar{T}$  in (13) is invariant with respect to monotonic changes of temperature (i.e., going from one reasonable thermometer to another), since it is defined via optimization of thermodynamic variables.

The freedom of at least one weight factor is present in any definition of the mean, e.g., the mean arithmetic of two lengths  $L_1$  and  $L_2$  is generally defined as  $\overline{L} = \alpha_1 L_1 + \alpha_2 L_2$ , with non-negative  $\alpha_1$  and  $\alpha_2$  holding  $\alpha_1 + \alpha_2 = 1$ . In that situation the weights  $\alpha_1$  and  $\alpha_2$  refer to relative importance of  $L_1$  and  $L_2$ . In our situation the weights refer to the relative importance of energy decrease versus entropy decrease during equilibration.

Finally, note an obvious interpretation of  $\overline{T}$ . If the composite system  $A_1 + A_2$  is coupled to an external thermal bath  $B^*$  at temperature  $T^*$ , and if this coupling is sufficiently weak for the energy transfer to  $B^*$  to be much slower than the equilibration time of  $A_1 + A_2$ , then  $B^*$  will deliver heat for  $T^* > \overline{T}$  and will get heat for  $T^* < \overline{T}$ . If only upper  $\widetilde{T}$  and lower  $\overline{T}$  bounds are employed (and not the value of  $\overline{T}$ ), then a weaker statement is found:  $B^*$  will deliver heat for  $T^* > \widetilde{T}$  and will get heat for  $T^* < \widehat{T}$ .

#### C. Generalizations

To extend the physical meaning of Eqs. (13) and (12), note that  $\overline{T}$  from (13) is the temperature that corresponds to values  $(\overline{U}, \overline{S})$  found via

$$(\overline{U}, \overline{S}) = \operatorname{argmax}_{S,U}[(S - S_{\text{in}})(U_{\text{in}} - U)], \qquad (14)$$

where the maximization is carried out over all allowed physical (also nonequilibrium) values of *S* and *U*. For consistency with (13) we have  $S_{in} = S_1(T_1) + S_2(T_2)$ , and  $U_{in} = U_1(T_1) + U_2(T_2)$ , but (14) applies to any nonequilibrium initial state ( $S_{in}, U_{in}$ ); e.g., several initially noninteracting equilibrium systems at different temperatures.

To understand Eq. (14), recall from Fig. 1 that those physical values of energy and entropy are bound into a convex domain by the equilibrium curve S(U). The maximization in (14) is reached in that curve; otherwise, one can always increase S or decrease U so as to reach this curve. We also naturally have  $\hat{S} \leq \bar{S} \leq \tilde{S}$  and  $\hat{U} \leq \bar{U} \leq \tilde{U}$ ; see (14) and Fig. 1. The maximum in (14) [i.e., also in (13)] is unique; see Appendix D. Equation (14) can be applied without demanding that  $(\bar{U}, \bar{S})$  are in equilibrium, and without requiring the bounds (9). These features come out automatically from (14), which can be generalized to cases where there are additional (dynamic) restrictions towards attaining the equilibrium curve. In this context, note that the S(U) curve in Fig. 1 needs to be concave and continuous for our analysis to apply; it need not be smooth. Thus the above formalism also treats equilibrium phase transitions.

# D. Effective temperature and nonequilibrium temperature versus mean temperature

There are nonequilibrium systems where different degrees of freedom can acquire different temperatures during relaxation to equilibrium, or in nonequilibrium steady states [40,41]. These degrees of freedom are effectively in equilibrium, and hence the temperature for them is well defined.

<sup>&</sup>lt;sup>5</sup>Note that within the reasoning of (11), the dimension of temperature is kept fixed, even though the dimensions of *S* and *U* are changing. This implies the usage of a nonminimal dimension system which is frequently applied in dimensional analysis, especially with respect to temperature *T* that is given an independent dimension [37,38]. The equilibrium relation between *S*, *U*, and *T* is now given via the conversion factor *k*:  $\frac{\partial U}{\partial S}|_V = kT$ , where *k* (related to Boltzmann's constant  $k_B$ ) compensates the dimension mismatch. Recall that several pertinent results in fluid dynamic dimensional analysis can be found only via nonminimal dimension systems with an independent dimension of temperature [37,38].

<sup>&</sup>lt;sup>6</sup>The maximum ignorance principle belongs to probabilistic inference. Its applicability to physics does involve assumptions, although such applications work in physics fairly well [39].

Clearly, effective temperatures in such systems are not directly helpful for defining or interpreting the mean temperature. A similar situation takes place in glassy materials, where different processes (instead of different degrees of freedom) are described by different (effective) temperatures [42].

The related notion of nonequilibrium temperature (having no unique definition) can be more helpful for interpreting the mean temperature, though strictly speaking this goes against our premise (iv) [cf. Sec. I] that the temperature is to be defined only in equilibrium. Various proposals for nonequilibrium temperature are reviewed in [43,44]. We shall comment on those that are relevant for our definition of mean temperature. Reference [45] found interesting applications of the temperature  $\hat{T}$  [see (4) and (16) below] to heat-conduction physics. The proposal for a nonequilibrium temperature made in [46] applies only to finite-level quantum systems, and for two identical quantum systems at different temperatures it reduces to the harmonic mean temperature; cf. our discussion in Sec. I. Reference [47] introduces (again for finite-level quantum systems) two nonequilibrium temperatures. They govern the interaction with an external thermal bath, and in that sense they are similar to the temperatures  $\hat{T}$  and  $\hat{T}$ ; see the discussion at the end of Sec. III A. Reference [48] proposes a quantum observable for temperatures, although the form of this observable turns out to be system dependent, in contrast to more generic quantum observables, e.g., coordinate or momentum.

## **IV. IDEAL GASES**

The simplest case for illustrating the above definition of  $\overline{T}$  is that of M ideas gases. Each gas k (k = 1, ..., M) has volume  $V_k$ , number of particles  $N_k$ , internal energy  $U_k$ , entropy  $S_k$ , constant (i.e., temperature independent) fixed-volume heat capacity  $c_k$ , and temperature  $T_k$  [13]:

$$S_k = N_k \ln \frac{V_k}{N_k} + N_k c_k \ln T_k, \quad U_k = N_k c_k T_k,$$
 (15)

where in  $S_k$  and in  $U_k$  we omitted certain inessential constants. Now  $\hat{T}$  and  $\tilde{T}$  read from (4), (7)

$$\hat{T} = \prod_{l=1}^{M} T_l^{n_l c_l/\bar{c}}, \quad \widetilde{T} = \sum_{l=1}^{M} \frac{n_l c_l}{\bar{c}} T_l, \quad (16)$$

$$\bar{c} = \sum_{l=1}^{M} n_l c_l, \quad n_l = \frac{N_l}{N}, \quad N = \sum_{l=1}^{M} N_l, \quad (17)$$

where  $\bar{c}$  is the mean heat capacity and  $n_l$  are concentrations. Hence  $\hat{T}$  ( $\tilde{T}$ ) in (16) reduces to a weighted geometric (arithmetic) average with weights  $n_k c_k/\bar{c}$ . The arithmetic and geometric means in (16) are valid only for ideal (and van der Waals nonideal) gases having temperature-independent heat capacities, i.e., they do not hold generally. This implication of our analysis challenges the uncritical use of the mean arithmetic formula to estimate the mean temperature of gases; e.g., granular gases [10].

Now the extension of (13) to M > 2 is represented as  $\max_T[(\tilde{T} - T)\ln(T/\hat{T})]$ . The maximization of this expression is carried out by differentiating

$$\bar{T} = \tilde{T} / W[e \,\tilde{T} / \hat{T}], \tag{18}$$

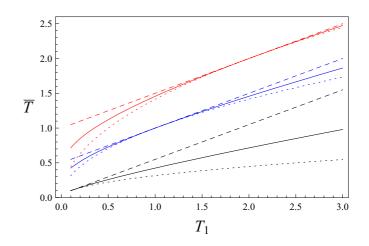


FIG. 2. The mean temperature  $\overline{T}$  for a two-temperature system vs temperature  $T_1$  of one of the systems; see (20). From top to bottom (red, blue, black curves):  $T_2 = 2$ , 1, 0.1. For each curve its dashed (dotted) counterpart of the same color denotes the arithmetic mean  $\widetilde{T} = (T_1 + T_2)/2$  (geometric mean  $\widehat{T} = \sqrt{T_1T_2}$ ) calculated at the same value of  $T_2$ . It is seen that  $\widetilde{T} \ge \overline{T} \ge \widehat{T}$ .

where  $\hat{T}$  and  $\tilde{T}$  are given by (16), and where W[z] is the Lambert special function that solves the equation [49]

$$W[z] e^{W[z]} = z.$$
 (19)

It has various applications in physics [49] and is tabulated with major computational platforms, e.g., PYTHONand MATHE-MATICA (as ProductLog[z]). In the simplest case of equal heat capacities,  $c_1 = ... = c_M$ , we find from (18) for M = 2 (with obvious generalization to M > 2)

$$\bar{T} = \frac{T_1 + T_2}{2W[e(T_1 + T_2)/(2\sqrt{T_1T_2})]}.$$
(20)

Figure 2 shows the behavior of (20) along with  $\hat{T}$  and  $\tilde{T}$ .

The same formulas (16)–(20) apply also to the case, where each system k (k = 1, ...M) at temperature  $T_k$  is not a single ideal gas but a mixture of ideal gases. Then the only change in (16)–(20) is that  $c_k$  (k = 1, ...M) is the average (temperatureindependent) heat capacity of the mixture. This case refers to the mean temperature of two stations that measured temperatures  $T_1$  and  $T_2$  (resp.) for air with different compositions of the main atmospheric gases: nitrogen, oxygen, and argon. This difference translates into different values of  $c_1$  and  $c_2$ , and then (16)–(20) apply. Importantly, the same (16)–(20) apply for van der Waals nonideal gases; see Appendix A.

Equations (16)–(20) do not apply if the heat capacity c depends on temperature. Here we should proceed directly from (13). This temperature dependence is small for air: c changes by 0.4% for temperature T varying between 300 and 350 K. Thus Eqs. (16)–(20) directly apply to calculating the mean temperature of air.

#### V. SUMMARY

Multiple problems arise when mean temperature is used to explain inhomogeneous temperature situations; see (i)–(iv) in the Introduction. These problems will likely become more serious, once temperature methods go deeper into microscales [47,50,51]. We proposed a solution to these problems based on thermodynamics. The mean temperature results from putting the systems together and hence allowing for a joint equilibration. Here we employ the operational way of defining thermodynamic quantities that goes back to Bridgman [14]. The definition allows for work extraction from the overall system  $A_1 + A_2$ . In particular, this feature is needed for applications in climate science, since there work extraction refers, e.g., to wind formation; see the discussion that follows Eq. (4). The work extraction is achieved via external fields, and the work is a response to such fields. Our setup also describes the direction of the heat flow; cf. the discussion at the end of Sec. III B.

Our definition of the mean temperature does not take into account dynamical factors, e.g., those given by hydrodynamics or kinetic theory. This is both weakness and strength, also because our results are independent on dynamical details, and they are potentially applicable to systems outside of the traditional thermodynamical realm; see, e.g., [44,52–54]. Our method works for any nonequilibrium initial state, not only two-temperature states.

We note that our method of placing upper and lower bounds on the mean temperature, and then determining the latter from more fine-grained reasoning, will be useful also in more specific, dynamic situations, also because those situations do assume fixed reference states [29]. We think that at least some of dynamical factors can be added as constraints in our method. A similar situation is realized in dynamic applications of the maximum entropy principle [39]. In fact, our approach can be regarded as a generalized maximum entropy method.

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### APPENDIX A: VAN DER WAALS NONIDEAL GAS

For the van der Waals nonideal gas model entropy and energy read, respectively [13] [cf. (15)]:

$$S_k = c_k N_k \ln T_k + N_k \ln \left[ \frac{V_k - N_k b_k}{N_k} \right], \tag{A1}$$

$$U_k = c_k N_k T_k - \frac{N_k^2 a_k}{V_k}, \quad k = 1, ..., M,$$
 (A2)

where  $c_k$  is the constant-volume heat capacity—which are again assumed to be constants|while  $a_k$  and  $b_k$  are van der Waals parameters. Recall that  $a_k > 0$  enters only into the energy, i.e., it characterizes the interparticle interaction, while  $b_k > 0$  enters only the entropy, as it stands for the excluded volume. It should be clear from (A1) that  $\frac{N_k b_k}{V_k}$  holds  $0 < 1 - \frac{N_k b_k}{V_k}$ . An upper bound on  $1 - \frac{N_k b_k}{V_k}$  comes from the thermodynamic stability condition  $\frac{\partial P}{\partial V}|_T < 0$  [13]. Hence two bounds together can be written as

$$0 < 1 - \frac{N_k b_k}{V_k} < \sqrt{\frac{T_k}{2a_k \frac{N_k}{V_k}}}.$$
 (A3)

Given these restrictions on the van der Waals parameters, we find back from Eqs. (13) and (12) the same formulas (16)–(20). In particular, they apply for defining averages between metastable states described by the van der Waals equation.

## APPENDIX B: MORE GENERAL EQUILIBRATION PROCESSES

In the main text we restricted ourselves with reversible and fully irreversible processes that proceed via thermal contacts, i.e., they are realized at fixed values of the volumes  $(V_1, V_2)$ and the particle numbers  $(N_1, N_2)$ . In particular, we did not involve pressure differences into the work extraction, because even when the equilibrium systems  $A_1$  and  $A_2$  have initially the same temperature T, their final temperature (after work has been extracted from pressure differences as well) will be lower than T, as we show below. This would obviously contradict our intention of defining the mean temperature, since, e.g., condition (8) will not hold anymore. Similar issues arise when  $A_1$  and  $A_2$  are composed of different (distinguishable) particles and we allow the mixing of gases during the work extraction. Then the final temperature will be lower than Tdue to the Gibbs mixing term, even when initial pressures and temperatures are equal; see below.

This issue is not restricted to the reversible mode of operation only. For example, during an irreversible mixing of two *nonideal* gases  $A_1$  and  $A_2$  having initially the same temperature T, their final temperature will be lower than T if the irreversible process is extended to include pressure differences; see below.

Thus the definition of a mean temperature in a nonequilibrium system requires equilibration processes that proceed mostly thorough thermal conductivity. Sections B 1 and B 2 show that there are reversible and irreversible processes that are not restricted to thermal contacts and that are not suitable for determining the mean temperature for a number of interesting reasons.

#### 1. Ideal gases

Let us return to the situation of M gases (k = 1, ..., M) discussed in Sec. IV. We do not anymore assume that these gases are ideal.

Recall Eq. (15) for entropy and energy of k = 2 ideal gases at (initial) temperatures  $T_k$ . The two gases together form a thermally isolated system. The total volume  $V_1 + V_2$  and the total number of particles  $N_1 + N_2$  are conserved.

First we assume that  $c_1 \neq c_2$ , i.e., the gases are different. Let it be that now they mix together and equilibrate via an entropy-conserving process. Hence only  $V_1 + V_2$  and  $N_1 + N_2$ are conserved but not  $V_1$  and  $N_1$  separately. In the final equilibrated state each gas occupies volume  $V = V_1 + V_2$  and they both have the same temperature  $\hat{T}$ . Hence the condition that the final entropy equals initial entropy reads from (15)

$$\sum_{k=1}^{2} N_k \left( \ln \frac{V}{N_k} + c_k \ln \hat{T} \right) = \sum_{k=1}^{2} N_k \left( \ln \frac{V_k}{N_k} + c_k \ln T_k \right).$$
(B1)

Now (B1) leads to

$$\hat{T} = e^{-\frac{1}{\bar{c}}\sum_{l=1}^{2}n_l \ln \frac{1}{v_l}} \prod_{l=1}^{2} T_l^{n_l c_l/\bar{c}},$$
(B2)

$$n_k = \frac{N_k}{\sum_{l=1}^2 N_l}, \quad v_k = \frac{V_k}{\sum_{l=1}^2 V_l}, \quad \bar{c} = \sum_{l=1}^2 n_l c_l,$$
 (B3)

where  $\sum_{l=1}^{2} n_l \ln \frac{1}{v_l} \ge 0$  is the Gibbs mixing term. We now have the following for  $T_1 = T_2$ :

$$\hat{T} = e^{-\frac{1}{c}\sum_{l=1}^{2} n_l \ln \frac{1}{v_l}} < T_1 = T_2,$$
(B4)

i.e., this equilibration scheme is not suitable for the definition of a mean temperature.

Now assume that the gases are identical, hence  $c_1 = c_2 = c$ . The final equilibrated gas should be treated as a single entity with number of particles  $N = N_1 + N_2$ , temperature  $\hat{T}_{id}$ , and volume  $V = V_1 + V_2$ . The constant entropy condition reads instead of (B2)

$$N\ln\frac{V}{N} + c\ln\hat{T}_{\rm id} = \sum_{k=1}^{2} N_k \left(\ln\frac{V_k}{N_k} + c\ln T_k\right), \quad (B5)$$

which implies [cf. (B3)]

$$\hat{T}_{id} = e^{-\frac{1}{c}\sum_{l=1}^{2} n_l \ln \frac{n_l}{v_l}} \prod_{l=1}^{2} T_l^{n_l}.$$
 (B6)

Recall from the fact that  $\sum_{l=1}^{2} n_l \ln \frac{n_l}{n_l}$  is a relative entropy,

$$\sum_{l=1}^{2} n_l \ln \frac{1}{v_l} \ge \sum_{l=1}^{2} n_l \ln \frac{n_l}{v_l} \ge 0, \tag{B7}$$

and  $\sum_{l=1}^{2} n_l \ln \frac{n_l}{v_l} = 0$  only when  $n_l = v_l$  (l = 1, 2). It is seen again that even when  $T_1 = T_2$  in (B6) we still have that  $\hat{T}_{id} < T_1 = T_2$ . Noting the equation of state  $P_k V_k = N_k T_k$  (where  $P_k$  is pressure and k = 1, 2) for initial gases, we see that for  $T_1 = T_2$ we can have  $\sum_{l=1}^{2} n_l \ln \frac{n_l}{v_l} > 0$  only when  $P_1 \neq P_2$ . Hence the inequality of pressures in the initial state makes  $\hat{T}_{id} < T_1 = T_2$ . Thus, due to  $\hat{T}_{id} < T_1 = T_2$  and  $\hat{T} < T_1 = T_2$ , the processes described by Eqs. (B2) and (B5) are not suitable for defining a lower bound on the mean temperature.

#### 2. Nonideal gases

The above analysis will be repeated for nonideal gases, since there are novel points in this case. Recall from (A1) the van der Waals nonideal gas model. For simplicity we take  $c_k = c > 0$  (temperature-independent constant),  $a_k = a > 0$ ,  $b_k = b > 0$ , and k = 1, 2. Let us assume that the two gases

mix in a completely irreversible way and reach temperature  $\tilde{T}$  (or  $\tilde{T}_{id}$ ) that is determined from the energy conservation:

$$\widetilde{T} = \sum_{k=1}^{2} n_k T_k - \frac{aN}{cV} \sum_{k=1}^{2} n_k \left(\frac{n_k}{v_k} - 1\right),$$
(B8)

$$\widetilde{T}_{id} = \sum_{k=1}^{2} n_k T_k - \frac{aN}{cV} \sum_{k=1}^{2} n_k^2 \left(\frac{1}{v_k} - 1\right),$$
(B9)

where  $n_k$  and  $v_k$  are defined by (B3). Equation (B8) refers to the distinguishable situation (nonidentical gases), where in the final state we still have two gases with particle numbers  $N_1$  and  $N_2$  occupying volume  $V = V_1 + V_2$ . Equation (B9) refers to identical gases, where the final state is a single gas at volume  $V = V_1 + V_2$ , particle number  $N = N_1 + N_2$ , and temperature  $\tilde{T}_{id}$ . We emphasize that for nonideal gases also the irreversible mixing temperature starts to feel whether the particles are identical. This is because we assumed that for the distinguishable situation particles from gas 1 do not interact with particles from gas 2, not only in the initial state but also in the final state. For the distinguishable situation this assumption is clearly incorrect: in the final state all particles interact with each other. This difference is reflected in (B8) and (B9).

Note from Eqs. (B8), (B9) that

$$\widetilde{T} < \sum_{k=1}^{2} n_k T_k, \quad \widetilde{T}_{id} < \sum_{k=1}^{2} n_k T_k.$$
 (B10)

The second relation in (B10) is obvious from  $v_k < 1$ . The first relation follows from (B7) upon noting there  $\ln \frac{n_l}{v_l} \leq \frac{n_l}{v_l} - 1$ . Equation (B10) confirms that  $T_1 = T_2 > \widetilde{T}$  and  $T_1 = T_2 > \widetilde{T}_{id}$ , i.e., this irreversible process is not suitable for defining an upper bound on the mean temperature.

# APPENDIX C: A RELATION BETWEEN $\tilde{T}$ AND THE TEMPERATURE ESTIMATOR

The structure of (5) is formally similar to the temperature estimator developed in Ref. [24]; in this context see also [25] and [26] for a recent review. Here the unknown temperature *T* of an equilibrium Gibbsian system is estimated from an identical, independently distributed sample  $E_1, ..., E_N$ of energy values. Thus, each  $E_k$  (k = 1, ..., N) is generated from the Gibbs probability density  $P(E) = e^{-\beta E}/Z(\beta)$ , where  $\beta = 1/T$  is the inverse temperature, which is regarded to be an unknown parameter. Now the maximum-likelihood method finds the temperature estimator  $\beta^{\circ}(E_1, ..., E_N)$  from maximizing over  $\beta$  the likelihood function  $P(E_1)...P(E_N)$ . It should be clear from the form of the Gibbs distribution that the maximizator  $\beta^{\circ}(E_1, ..., E_N)$  is unique. Then the very maximum-likelihood method implies that it is covariant with respect to bijective transformations of  $\beta$ . It is found from

$$\frac{1}{\mathcal{N}}\sum_{k=1}^{\mathcal{N}} E_k = U(\beta^\circ), \quad U(\beta) = \frac{1}{Z(\beta)}\sum_E Ee^{-\beta E}, \quad (C1)$$

where  $U(\beta)$  is the mean energy of the system. The analogy between (C1) (for  $\mathcal{N} = 2$ ) and (5) is now obvious. Though suggestive, this analogy is formal, because  $E_k$  in (C1) refers to different energy measurement results of a system with the same (unknown) temperature, while in (5) we have different mean energies due to different temperatures.

## **APPENDIX D: THE MAXIMUM IN (14) IS UNIQUE**

Let us show that the maximum in (14) [hence also in (13)] is unique. The mathematical structure of this argument is taken from [35]; cf. also [36]. Indeed, if the maximum is reached at two different points  $(U_1, S_1)$  and  $(U_2, S_2)$  such that

$$(S_1 - S_{in})(U_{in} - U_1) = (S_2 - S_{in})(U_{in} - U_2),$$
 (D1)

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then  $\frac{1}{2}(U_1 + U_2, S_1 + S_2)$  is also in the maximization domain of (14), because that domain is a convex set. This fact follows from the concavity of the S(U) curve in Fig. 1. Now

$$\frac{1}{4}(S_1 - S_{in} + S_2 - S_{in})(U_{in} - U_1 + U_{in} - U_2)$$
  
>  $(S_1 - S_{in})(U_{in} - U_1) = (S_2 - S_{in})(U_{in} - U_2)$  (D2)

contradicts the assumption that  $(S_1 - S_{in})(U_{in} - U_1) = (S_2 - S_{in})(U_{in} - U_2)$  provides the maximum. Hence, the maximum in (14) is unique:  $(U_1, S_1) = (U_2, S_2)$ .

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