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Rosenfeld-Prigogine complementarity of descriptions in the context of informational statistical thermodynamics

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Within the framework of informational statistical thermodynamics, we consider the case of a particular dissipative dynamical system, namely, a system of harmonic oscillators weakly interacting with a thermal bath. Informational entropy and informational-entropy production are obtained. In terms of them we derive the information gain in alternative pictures and a Rosenfeld-like complementarity principle between microdescription and macrodescription. This complementarity is related to a kind of measure of the incompleteness of both descriptions and to Prigogine's theory of irreversible processes. The fundamental role of the universal Boltzmann constant for the characterization of this complementarity is discussed. [S1063-651X(98)06501-5]

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I. INTRODUCTION

The connection and interplay of the microscopic and macroscopic levels of description in matter, that is, between mechanics and thermodynamics, have been the object of discussion since the emergence of thermodynamics, as an offshoot of the Industrial Revolution, in last century. In particular, Rosenfeld [1] has argued that in this case is at work a kind of logical relationship to which the name of *complementarity* may be applied. This was conjectured by Bohr [2], and is contained in a particular form in Prigogine's work [3]. In Rosenfeld's words, it should characterize the mutual exclusiveness of the two descriptions: conditions allowing for a complete microscopic mechanical description of a system exclude the possibility of applying to the system any of the typical thermodynamic concepts; and, conversely, the macroscopic description in terms of the latter requires conditions of observation under which the mechanical parameters scape our control.

We consider here the ideas of Rosenfeld and Prigogine in the framework of an emerging theory, namely, the so-called informational statistical thermodynamics (IST for short). It is applied to the study of a particular system consisting into an assembly of two subsystems of linear oscillators in mutual interaction (it constitutes an excellent model for the description of particular sets of collective elementary excitations in solids like, for example, polaritons, magnetoplasma waves, etc.).

IST (sometimes also called information-theoretic thermodynamics) was pioneered by Hobson [4], sometime after the publication of Jaynes's seminal papers [5] on the foundations of statistical mechanics on the basis of information theory (brief considerations and short historical notes on IST are given in Ref. [6], and additional topics in Ref. [7]). It may be noted that, as thermostatics (thermodynamics of equilibrium systems) has microscopic foundations provided by Gibbs' equilibrium statistical mechanics (and then is referred as Gibbs Thermostatics [8]), IST (a thermodynamics for irreversible processes) has its mechanical-statistical foundations in the statistical mechanics for nonequilibrium systems, in particular, the so-called nonequilibrium statistical operator method (NESOM for short, reviewed in Ref. [9]), with Zubarev and co-workers' construction [10,11] apparently being the most concise, elegant, practical, and physically sound approach [12,13].

In continuation, the method is applied to the particular model system mentioned above, which admits exact solutions, and for which particular thermodynamic aspects, in the context of IST, are obtained in order to used them to characterize Rosenfeld's arguments. We discuss this kind of complementarity principle, analyze its connection to the one due to Prigogine, and give the form of a principle of incompleteness of description. In Sec. IV we present a critical discussion and some concluding remarks.

II. MODEL AND ITS DESCRIPTION IN IST

Consider the system composed by two subsystems of harmonic oscillators, coupled through a particular interaction, as described by the Hamiltonian

$$\hat{H}(\hat{\mathbf{x}},\hat{\mathbf{p}};\hat{\mathbf{X}},\hat{\mathbf{P}})=\hat{H}_{01}(\hat{\mathbf{x}},\hat{\mathbf{p}})+\hat{H}_{02}(\hat{\mathbf{X}},\hat{\mathbf{P}})+\hat{H}'(\hat{\mathbf{x}},\hat{\mathbf{p}},\hat{\mathbf{X}},\hat{\mathbf{P}}), \quad (1)$$

where $\hat{\mathbf{x}}\equiv\hat{x}_1,\ldots,\hat{x}_N$ and $\hat{\mathbf{X}}\equiv\hat{X}_1,\ldots,\hat{X}_N$, are the generalized coordinates of the two types of N and N' oscillators, respectively, and $\hat{\mathbf{p}}$ and $\hat{\mathbf{P}}$ are the corresponding sets of linear momenta. In Eq. (1), H_{01} and H_{02} are the Hamiltonians of the free subsystems, namely,

$$\hat{H}_{01}=\sum_{j=1}^{N}\tfrac{1}{2}(\hat{p}_j^2+\omega_j^2\hat{x}_j^2), \quad (2a)$$

$$\hat{H}_{02}=\sum_{\mu=1}^{N'}\tfrac{1}{2}(\hat{P}_\mu^2+\Omega_\mu^2\hat{X}_\mu^2) \quad (2b)$$

and H' is the interaction energy, which is taken in the form of the bilinear interaction,

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$$H' = \sum_{j,\mu} \Gamma_{j\mu} \hat{x}_j \hat{X}_\mu, \quad j=1,...,N; \mu=1,...,N', \tag{2c}$$

where Γ stands for the coupling strength of the interaction.

Given the Hamiltonian of Eq. (1) we can proceed to build the informational mechanostatistical description of the system in NESOM, a description which may be considered to be encompassed within the scope of Jaynes's predictive statistical mechanics [14] (see Refs. [9–13]), and which, as noticed, provides the foundations of IST. We recall that the IST (or informational-statistical) entropy is given by

$$\overline{S(t)} = -\mathrm{Tr}\{\rho(t) \ln \overline{\rho(t,0)}\} \equiv -\mathrm{Tr}\{\rho(t)\mathcal{P}(t) \ln \rho(t)\}, \tag{3}$$

where $\overline{\rho(t,0)}$ is an auxiliary coarse-grained distribution, and $\rho(t)$ is the distribution that describes the macroscopic state of the system and its evolution in nonequilibrium conditions. The latter contains nonlinear, nonlocal in space, and memory effects, and it is an operator uniquely defined by the former and the system's Hamiltonian [9–13]. Moreover, $\mathcal{P}(t)$ is a time-dependent projection operator, which projects on the so-called informational subspace composed by the dynamical variables used for the description of the system [9,15].

The informational entropy of Eq. (3) increases in time, which is a consequence of the loss of information in the interpretation of the measurements performed on the system [9,15,16]. According to the method $\overline{\rho(t,0)}$ is a superoperator depending on a set of basic dynamical variables $\{\hat{P}_j\}$, with $j=1,...,n$, chosen to provide for the sought-after statistical description of the system [9–13], and also depending on an accompanying set of Lagrange multipliers $\{F_j(t) = k_B^{-1}\mathcal{F}_j(t)\}$, where k_B is a Boltzmann constant. It takes the form of an instantaneous generalized Gibbsian-like distribution given by [9–13]

$$\overline{\rho(t,0)} = \exp\left\{ -\phi(t) - \sum_{j=1}^{n} F_j(t)\hat{P}_j \right\}, \tag{4}$$

where ϕ, playing the role of the logarithm of a generalized nonequilibrium partition function, ensures its normalization. Moreover, the Lagrange multipliers (or intensive thermodynamic variables) satisfy that

$$\mathcal{F}_j(t) = k_B \delta\overline{S(t)}/\delta Q_j(t) \equiv \mathcal{F}_j\{Q_1(t),\ldots,Q_n(t)\}, \tag{5a}$$

where δ stands for functional differential, and they are determined by the constraints that

$$Q_j(t) = \mathrm{Tr}\{\hat{P}_j \rho(t)\} \equiv Q_j\{\mathcal{F}_j(t),\ldots,\mathcal{F}_n(t)\}. \tag{5b}$$

The set $\{Q_j(t)\}$ is composed by the macroscopic variables that describe the nonequilibrium thermodynamic state of the system, with their irreversible evolution governed by generalized nonlinear quantum transport equations of the type

$$\frac{d}{dt} Q_j(t) = \mathrm{Tr}\left\{ \frac{1}{i\hbar} [\hat{P}_j, H]\rho(t) \right\} \equiv \Phi_j\{Q_1(t),\ldots,Q_n(t);t\}, \tag{6}$$

where the explicit form of the nonlinear, nonlocal in space, and memory-dependent functionals Φ_j is given elsewhere [9–11,17,18]. Although the term after the first equal sign is dependent, through ρ, on the set $\{F_j\}$, Eq. (5a) allows us to close the equations in terms of variables Q_j.

Two other relevant results are that the informational-entropy production is given by [9–11,15],

$$\overline{\sigma(t)} = d\overline{S(t)}/dt = \sum_{j=1}^{n} F_j(t)[dQ_j(t)/dt], \tag{7}$$

and a particularly well-defined relationship between the root-mean-square deviations of the macrovariables and of the Lagrange multipliers is satisfied, namely,

$$[\Delta^2\mathcal{F}_j(t)]^{1/2}[\Delta^2 Q_j(t)]^{1/2} = k_B[G_{jj}(t)]^{1/2}, \tag{8}$$

where G is a quantity equal to the product of the diagonal element j of the correlation matrix and that of its inverse, and equal to 1 in the case of uncorrelated variables, as shown in Appendix A. Equation (8) resembles a kind of uncertainty principle in the way proposed by Rosenfeld [1], which is *valid for arbitrarily far-from-equilibrium conditions and at any time during the evolution of the dissipative macrostate of the system*. It ought to be noticed that the root-mean-square deviations $\Delta^2\mathcal{F}_j(t)$ are to be understood in the same sense as is done in equilibrium, what is described in Ref. [19]; on the other hand, the $\Delta^2 Q_j(t)$ represent the statistical fluctuations of the macrovariables.

Let us return to the specific case of the system of oscillators characterized by the Hamiltonian of Eq. (1). We consider two different statistical descriptions of it: First, we consider the description in terms of

$$\text{(I)} \quad \{\hat{H}_{01}, \hat{H}_{02}\}, \quad \{\beta_{1I}(t);\beta_{2I}(t)\}, \quad \{E_1(t);E_2(t)\}, \tag{9}$$

which consists of collective variables corresponding to the energies of each of the subsystems; that is, here we have a kind of canonical description of each one in nonequilibrium conditions, with the auxiliary (coarse-grained) statistical probability distribution given by [cf. Eq. (4)]

$$\overline{\rho_I}(t,0) = \exp\{-\phi_I(t) - \beta_{1I}(t)\hat{H}_{01} - \beta_{2I}(t)\hat{H}_{02}\}. \tag{10}$$

Let us consider the equations of evolution for the two basic variables, that is, the equations of the type of Eqs. (6) for $Q_1(t) \equiv E_1(t)$ and $Q_2(t) \equiv E_2(t)$ in this case. As already noted, the right-hand side of these equations is in fact a functional of the two Lagrange multipliers $\beta_{1I}(t)$ and $\beta_{2I}(t)$, on which $\rho(t)$ depends. But these Lagrange multipliers are related to the basic variables through Eqs. (5), which in this case, and in a classical-mechanical approach, are

$$E_1(t) = \mathrm{Tr}\{\hat{H}_{01}\rho(t)\} = N\beta_{1I}^{-1}(t), \tag{11a}$$

$$E_2(t) = \mathrm{Tr}\{\hat{H}_{02}\rho(t)\} = N'\beta_{2I}^{-1}(t). \tag{11b}$$

Therefore, the equations of evolution for the basic variables can be transformed into equations of evolution for the Lagrange parameters $\beta_{1I}(t)$ and $\beta_{2I}(t)$. This is done using the nonlinear transport theory that the method provides [9–11,17,18], but resorting to the so-called second order approximation in relaxation theory [17], that is, the one that keeps the interaction up to second order (binary collisions), restricted then to weak interactions. Moreover, we take the limit of N' going to infinity, that is, the second system of oscillators plays the role of an ideal reservoir at, say, temperature T_0. The resulting system of equations of evolution is solved to finally obtain (see Appendix B), after introducing the definitions $\beta_{1I}^{-1}(t)=k_B T_{1I}^*(t)$ and $\beta_{2I}^{-1}(t)=k_B T_{2I}^*(t)$, with both T^* playing the role of nonequilibrium temperature-like variables (usually referred to as quasitemperatures [20]), that

$$T_{1I}^*(t)=T_\infty+A_I e^{-t/\tau}, \quad T_{2I}^*(t)=T_\infty=T_0, \tag{12}$$

with the IST entropy production being

$$\overline{\sigma_I}(t)=N\tau^{-1}[T_{1I}^*(t)-T_{2I}^*(t)]^2/T_{1I}^*(t)T_{2I}^*(t), \tag{13}$$

where T_∞ (corresponding to the temperature when final thermal equilibrium is achieved; that is, for $t\to\infty$ the temperature of the system and reservoir coincide), and A_I are fixed by the initial conditions. In Eqs. (12), τ is a relaxation time given by

$$\frac{1}{\tau}=\frac{1}{N}\sum_j \quad \frac{1}{\tau_j}=\frac{1}{N}\sum_j \;(\pi/2)\sum_\mu \;(|\Gamma_{j\mu}|^2/\omega_j^2)\,\delta(\omega_j-Q_\mu). \tag{14}$$

The entropy production of Eq. (13) is positive, and becomes null when final equilibrium is achieved ($T_{1I}^*=T_{2I}^*=T_\infty=T_0$ for $t\to\infty$).

Consider now the description

$$\text{(II)}\quad \{\hat{H}_{10},\hat{\mathbf{x}},\hat{\mathbf{p}};\hat{H}_{20}\};\{\beta_{1II}(t),\boldsymbol{\varphi}_{II}(t),\boldsymbol{\gamma}_{II}(t);\beta_{2II}(t)\};$$
$$\{E_1(t),\overline{\mathbf{x}}(t),\overline{\mathbf{p}}(t);E_2(t)\}, \tag{15}$$

which is a mixed one, involving the microscopic individual coordinates and momenta of the oscillators in subsystem 1 and the collective variables energy [as in (I); cf. Eq. (9)]. Therefore, the coarse-grained auxiliary distribution in this case is [cf. Eq. (4)]

$$\overline{\rho}(t,0)=\exp\Big\{-\phi_{II}(t)-\beta_{1II}(t)\hat{H}_{10}-\beta_{2II}(t)\hat{H}_{20}$$
$$-\sum_{j=1}^{N}[\varphi_{jII}(t)\hat{x}_j+\gamma_{jII}(t)\hat{p}_j]\Big\}, \tag{16}$$

and, while $E_2(t)$ is again the one given in Eq. (11b), we now have that

$$E_1(t)=N\beta_{1II}^{-1}(t)+\tfrac{1}{2}\sum_{j=1}^{N}\beta_{1II}^2(t)[\gamma_{jII}^2(t)+\omega_j^2\varphi_{jII}^2(t)], \tag{17a}$$

$$\omega_j^2\overline{x_j}(t)=-\beta_{1II}^{-1}\varphi_{jII}(t), \tag{17b}$$

$$\overline{p_j}=-\beta_{1II}^{-1}(t)\gamma_{jII}(t). \tag{17c}$$

Proceeding as in the previous case (I) (see Appendix B), we derive and solve the equations of evolution to find that

$$T_{1II}^*(t)=T_\infty+A_{II}e^{-t/\tau}, \tag{18a}$$

$$T_{2II}^*(t)=T_\infty=T_0, \tag{18b}$$

$$\overline{x_j}(t)=(a_j/\omega_j)\exp(-t/2\tau_j)\sin(\omega_j t+\theta_j), \tag{18c}$$

$$\overline{p_j}(t)=-\overline{x(t)}/2\tau_j+a_j\,\exp(-t/2\tau_j)\cos(\omega_j t+\theta_j), \tag{18d}$$

$$\hat{\sigma}_{II}(t)=N\tau^{-1}\{[T_{1II}^*(t)-T_{2II}^*(t)]^2/T_{1II}^*(t)T_{2II}^*(t)\}$$
$$+[f(t)/k_B T_{2II}^*(t)], \tag{19}$$

where a_j and θ_j are determined by the initial conditions

$$f(t)=\sum_j [(\omega_j^2/\tau_j)\overline{x_j^2}(t)+\Lambda_j\overline{x_j}(t)\overline{p_j}(t)], \tag{20a}$$

τ_j is defined in Eq. (14), and

$$\Lambda_j=\sum_\mu (|\Gamma_{j\mu}|^2)(\Omega_\mu^2-\omega_j^2)^{-1}. \tag{20b}$$

We recall that subsystem 2 acts as an ideal reservoir at constant temperature $T_0=T_{2II}^*(0)=T_\infty$.

Next we compare both descriptions (I) and (II) [cf. Eqs. (10) and (16)] using, evidently, the same initial conditions in both cases. We fix the initial energies of both systems, which, using Eqs. (11) and (17), can be written in the form

$$\text{(I)}\qquad \Delta E=E_1(0)-Nk_BT_\infty=\delta q_{1I}, \tag{21a}$$

$$\delta q_{1I}=Nk_B[T_{1I}^*(0)-T_\infty]=Nk_BA_I, \tag{21b}$$

$$\text{(II)}\qquad \Delta E=E_1(0)-Nk_BT_\infty=\delta q_{1II}+\delta w_{1II}, \tag{21c}$$

$$\delta w_{1II}=\sum_j (a_j^2/2), \tag{21d}$$

$$\delta q_{1II}=Nk_B[T_{1II}^*(0)-T_\infty]=Nk_BA_{II}, \tag{21e}$$

we recall that the energy of the reservoir E_2 is fixed by its temperature, $T_0=T_\infty$, and for the sake of simplicity, without losing generality, we have chosen the initial conditions $\overline{x_j}(0)=0$ and $\overline{p_j}(0)=a_j$. Equations (21) provide the initial energy in excess of the values in final equilibrium, ΔE, which is composed of two terms: one, δq, which we call a "heatlike contribution," and the other, δw, dubbed a "worklike contribution."

We proceed to compare both descriptions for which purpose, first, we resort to a quantum description—more appropriate for a full analysis in what follows (see Appendix C)—and, second, we define what we call an *order parameter* given by

$$\Delta(t)=[\overline{S_1}(t)-\overline{S_{II}}(t)]/\overline{S_I}(t)=K(t)/\overline{S_I}(t), \tag{22}$$

where we have introduced

$$K(t)=-\mathrm{Tr}\{\overline{\rho_{II}}(t,0)[\ln\,\overline{\rho_I}(t,0)-\ln\,\overline{\rho_{II}}(t,0)]\}, \tag{23}$$

namely, an analog of Kullback's information measure [21], which is interpreted as a measure of the gain in information in the description using $\overline{\rho_{II}}$ in comparison with the one using $\overline{\rho_1}$. In Fig. 1 we show the evolution of Δ for the choice T_0

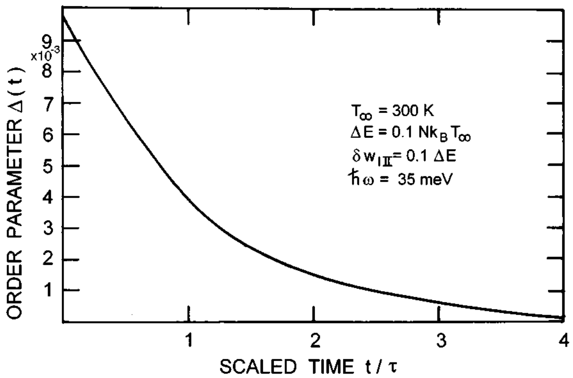

FIG. 1. Evolution in time of the order parameter of Eq. (22).

$=300$ K; $\Delta E = 0.1\, Nk_B T_0$, $\delta w_{1II} = 0.1\Delta E$, and all $\hbar\omega_j$ equal to 35 meV. The IST entropy in description (II) is smaller than in description (I), as expected, since the former carries more information, but they asymptotically coincide once final thermodynamic equilibrium is achieved, as it should. Further considerations on the informational entropy and its production are given in Refs. [9,15,16], and a geometrical-topological discussion of the method is due to Ref. [22].

III. ROSENFELD-PRIGOGINE COMPLEMENTARITY IN IST

Taking into account the results of Sec. II together with the relationship of Eq. (8), we explore the role of Boltzmann constant resorting to, at a given time (say the initial one $t = 0$), introducing in the expression for Δ of Eq. (22) a scaling ξ of the Boltzmann constant (writting ξk_B), with ξ varying from zero to infinity. The resulting ξ-dependent $\Delta(0|\xi)$ is shown in Fig. 2. It is verified that $0 \leqslant \Delta \leqslant 1$, with Δ going to one for ξ going to zero and Δ going to zero for ξ going to infinity, implying in maximum information gain and no information gain at all, respectively. For the numbers used (and we recall that δw_{1II} is 10% of the input of exciting energy ΔE, while δq_{1II} is 90% of ΔE), for $\xi = 1$, that is the real case in nature for $k_B = 8.617 \times 10^{-5}$ eV/K, the information gain is roughly 1% of S_I. Moreover, it follows that for

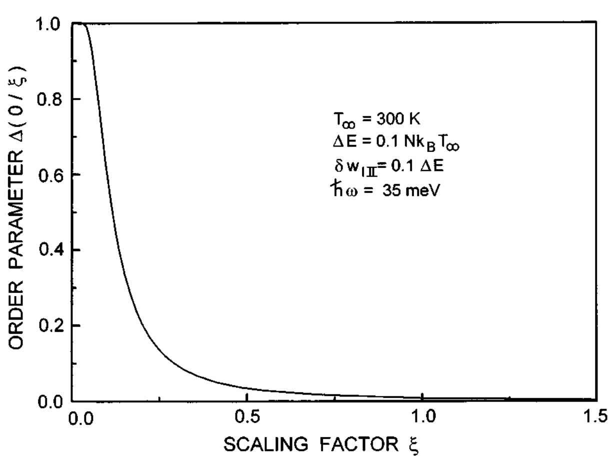

FIG. 2. Dependence of the order parameter of Eq. (22) for $t = 0$ on a scaled Boltzmann constant.

ξ small the heatlike contribution δq_{1II} goes to zero, while, the worklike contribution δw_{1II} acquires the maximum value ΔE, which can be interpreted as meaning that one can only pump mechanical work on the system, and that no heating is possible. For nonzero value of ξ both contributions are present, and for ξ of the order and larger than 0.5, we obtain that they very approximately maintain the distribution of 90% and 10% of the pumped energy ΔE, for δq_{1II} and δw_{1II} respectively.

We may summarize these results as implying that for a ''small Boltzmann constant'' a mechanical-like description predominates, while for the universal value of the Boltzmann constant, and also for ''larger values of it,'' both heatlike and worklike contributions can be pumped simultaneously on the system. Furthermore, in the former case, the informational entropy S_{II} tends to zero, in accord with the fact of having what can be considered as a purely mechanical description, and the informational-entropy production vanishes. Then we may say that in such a limiting situation (''null Boltzmann constant'') no statistical thermodynamics exists, quite in agreement with Jaynes's statements, in his already classical paper of 1965 [23] (see also Ref. [24]).

On the other hand, to make contact with Prigogine's approach, we introduce in IST the entropy operator

$$\mathcal{S}(t) = k_B \hat{\hat{S}}(t) = -k_B \mathcal{P}(t) \ln \rho(t) = -\mathcal{F}_0(t) - \sum_{j=1}^{n} \mathcal{F}_j(t) \hat{P}_j , \tag{24}$$

where $\mathcal{F}_0 = k_B \phi$ and $P(t)$ is the time-dependent projection operator present in Eq. (3) and defined elsewhere [9] (which projects at each time t over the subspace defined by the basic set of dynamical variables, the so-called informational subspace; see also Ref. [22]). The statistical average with $\rho(t)$ of this entropy operator is the IST entropy of Eq. (3). Furthermore, if we indicate by L the Liouville operator of the system, then it follows that

$$k_B \hat{\hat{\sigma}}(t) \equiv i\mathsf{L}\mathcal{S}(t) = \sum_j \mathcal{F}_j(t) i\mathsf{L} P_j , \tag{25}$$

which introduces the entropy production operator, $\hat{\hat{\sigma}}$ whose average is the IST entropy production of Eq. (7). The connection of the entropy operator of Eq. (24) and the one introduced in a general form by Prigogine is made through the identification $-k_B \mathcal{P}(t) \ln\rho(t) = M\rho(t)$, with operator M defined in Ref. [3]. Let us take the commutator of the Liouville operator and the entropy operator, and next the average value of it, to obtain that

$$\begin{aligned} \mathrm{Tr}\{[i\mathsf{L}, \hat{\mathcal{S}}(t)]\rho(t)\} &= \frac{1}{i\hbar} \mathrm{Tr}\{[\hat{\mathcal{S}}, \hat{H}] - \hat{\mathcal{S}}[\rho, \hat{H}]\} \\ &= \mathrm{Tr}\{\rho i\mathsf{L}\hat{\mathcal{S}}\} = k_B \overline{\sigma(t)}. \end{aligned} \tag{26}$$

According to Prigogine [3], the non-null commutator $[i\mathsf{L}, \hat{\mathcal{S}}]$ in this Eq. (26) leads to a *complementarity principle* that implies that either we consider eigenfunctions of the Liouville operator to determine the mechanical evolution of the system, or we consider eigenfunctions of the entropy operator [25], but they do not have common eigenfunctions.

IV. CONCLUDING REMARKS

We can say that the results presented above point to the plausibility that the incommensurability of the Liouville operator (mechanical level) and the entropy operator (thermodynamical level) implies a kind of uncertainty relation, or, more appropriately, a kind of *measure of incompleteness of descriptions*: A simultaneous determination of the informational content of the solutions of the equations of evolution of the macrostate and a detailed microscopic positioning (point in phase space or quantum state) is not possible. This fact is governed by the presence of the Boltzmann constant, as quantified in Eqs. (8) and (26) (see Fig. 2, where the role of k_B—scaled by the factor ξ—in characterizing this complementarity principle is evidenced).

It has been argued [26] that k_B introduces an influence on the microscopic level of the experiment at the macroscopic level. Heat and work are considered as intrinsic properties of matter, and heat flux as a movement of ''thermal charges'' under the action of a gradient of temperature. In this context k_B may then be—as reinforced by the results in this paper—considered as a ''quantum of thermal charge,'' namely, the minor amount of heat to be displaced by unit of temperature gradient. It would *represent the unit of measure of the uncertainty of the description of the mechanical state on the basis of the given reduced macroscopic characterization of the system*. This point has also been stressed by Tisza [8]. Hence it may be argued that, as Planck's constant defines the interaction between the quantum system and the measurement device as nondecomposable, Boltzmann's constant also defines the microscopic and macroscopic descriptions as nondecomposable [27]. In this case, we reiterate, there is at work a kind of logical relationship to which the name of *complementarity*—as an extension of Bohr's ideas—may be applied [1]: As shown (and we stress that this is in the realm of IST) it can be characterized by a kind of uncertainty relation [cf. Eq. (8)] and the interplay of two noncommutative operators [cf. Eq. (26)], and it becomes tempting, or, better, conjecturable, to consider the Boltzmann constant as playing the role of an elementary quantum of heat transfer, and being responsible for the necessary duality of descriptions.

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APPENDIX A: CORRELATION MATRIX AND AN UNCERTAINTYLIKE LAW

Given $\phi(t)$ and $\overline{S(t)}$ of Eqs. (3) and (4), their differential coefficients give $Q_j(t)$ and $F_j(t)$; that is [9–11],

$$Q_j(t) = -\delta\phi(t)/\delta F_j(t), \quad F_j(t) = \delta\overline{S(t)}/\delta Q_j(t), \tag{A1}$$

where δ stands for functional derivative [28]. Moreover, the second order functional derivatives allow us to introduce the fluctuations of the basic variables, also providing for a generalization of Maxwell's relations to nonequilibrium situations, namely,

$$\begin{aligned}\delta^2\phi(t)/\delta F_j(t)\,\delta F_k(t) &\equiv \mathsf{C}_{jk}(t)\\ &= -\delta Q_j(t)/\delta F_k(t) = -\delta Q_k(t)/\delta F_j(t)\\ &= \int d\Gamma\,\Delta\hat{P}_j(t)\Delta\hat{P}_k(t)\overline{\rho(t,0)},\end{aligned} \tag{A2}$$

where

$$\Delta\hat{P}_j(t) = \hat{P}_j - Tr\{\hat{P}_j\overline{\rho(t,0)}\} = \hat{P}_j - Q_j(t), \tag{A3}$$

and $\mathsf{C}_{jk}(t)$ is the matrix of correlations of the basic dynamical variables, which is symmetric, namely, $\mathsf{C}_{jk} = \mathsf{C}_{kj}$, and, as noted, is a generalization to the nonequilibrium situation (in the context of IST) of Maxwell's relations in thermostatics. Furthermore [9–11],

$$\delta^2\overline{S(t)}/\delta Q_j(t)\,\delta Q_k(t) = \delta F_j(t)/\delta Q_k(t) = \delta F_k(t)/\delta Q_j(t) \tag{A4}$$

and

$$\begin{aligned}\sum_{\ell} \frac{\delta^2\phi(t)}{\delta F_j(t)\,\delta F_\ell(t)}\frac{\delta^2\overline{S(t)}}{\delta Q_\ell(t)\,\delta Q_k(t)} &= -\sum_{\ell}\frac{\delta Q_j(t)}{\delta F_\ell(t)}\frac{\delta F_l(t)}{\delta Q_k(t)}\\ &= -\delta_{jk},\end{aligned} \tag{A5}$$

and then the second differential coefficients of the informational entropy are the elements of minus the inverse $\hat{\mathsf{C}}^{(-1)}$ of the matrix of correlations $\hat{\mathsf{C}}$. Let us next introduce the alternative definitions (thus introducing Boltzmann constant)

$$k_B\overline{S(t)} = \mathsf{S}(t), \quad \mathcal{F}_j(t) = k_B F_j(t) = \delta\mathsf{S}(t)/\delta Q_j(t). \tag{A5}$$

The fluctuation of the informational entropy is

$$\begin{aligned}\Delta^2\mathsf{S}(t) &= \sum_{j,k}\frac{\delta\mathsf{S}(t)}{\delta Q_j(t)}\frac{\delta\mathsf{S}(t)}{\delta Q_j(t)}C_{jk}(t)\\ &= \sum_{j,k}\mathsf{C}_{jk}(t)\mathcal{F}_j(t)\mathcal{F}_k(t),\end{aligned} \tag{A6}$$

and that of the intensive variables $\mathcal{F}$ are

$$\begin{aligned}\Delta^2\mathcal{F}_j(t) &= \sum_{k,l}\frac{\delta F_j(t)}{\delta Q_k(t)}\frac{\delta F_j(t)}{\delta Q_\ell(t)}\mathsf{C}_{k\ell}(t)\\ &= k_B^2\sum_{k,\ell}\mathsf{C}_{jk}^{(-1)}(t)\mathsf{C}_{jl}^{(-1)}(t)\mathsf{C}_{k\ell}(t) = k_B^2\mathsf{C}_{jj}^{(-1)}(t).\end{aligned} \tag{A7}$$

Therefore,

$$\Delta^2 Q_j(t)\Delta^2\mathcal{F}_j(t) = k_B^2 G_{jj}(t), \tag{A8}$$

$$G_{jj}(t) = \mathsf{C}_{jj}(t)\mathsf{C}_{jj}^{(-1)}(t). \tag{A9}$$

In the particular case when the basic variables are uncorrelated, viz. $\mathsf{C}_{jk}=0$ for $j \neq k$, as in the case of equilibrium, then

$$\Delta^2 Q_j(t)\Delta^2\mathcal{F}_j(t) = k_B^2 \tag{A10}$$

and

$$[\Delta^2 Q_j(t)]^{1/2}[\Delta^2\mathcal{F}_j(t)]^{1/2} = k_B. \tag{A11}$$

Equations (A8) and (A11) have a similarity with an uncertainty law, as is the case in quantum mechanics for the case of two noncommuting Hermitian operators.

APPENDIX B: EQUATIONS OF MOTION

1. First description [cf. Eq. (9)]

In the Markovian limit of the NESOM-based kinetic theory [9,17,18,29] we find that

$$\frac{d}{dt}E_1(t) = J_1^{(2)}(t), \quad \frac{d}{dt}E_2(t) = J_2^{(2)}(t), \tag{B1}$$

where the collision operator $J^{(2)}$ is given by

$$J_{1(2)}^{(2)}(t) = \int_{-\infty}^{0} dt' e^{\epsilon t'} \int d\Gamma_1 d\Gamma_2 \times \{H'(t')_0, \{H', H_{01}\}\}\overline{\rho_1}(\Gamma_1,\Gamma_2|t,0), \tag{B2}$$

where subindex zero indicates an evolution in time under H_0, and, we recall, ε is a positive infinitesimal that goes to zero after the calculation of the average has been performed; Γ_1 and Γ_2 are phase points in the phase space of each subsystem. After some lengthy but straightforward algebra, we find that

$$\begin{aligned} J_1^{(2)}(t) = \int_{-\infty}^{0} dt' e^{\varepsilon t'} \int d\Gamma_1 \int d\Gamma_2 \Bigg\{ & \sum_{j,\mu,\nu} \Gamma_{j\mu}\Gamma_{j\mu} \\ & \times [X_\mu X_j \cos(\omega_j t')\cos(\Omega_\mu t') \\ & + P_\mu X_\nu \Omega_\mu^{-1} \cos(\omega_j t')\sin(\Omega_\mu t')] \\ & - \sum_{j,k,\mu} \Gamma_{j\mu}\Gamma_{k\mu}\Omega_\mu^{-1}[p_j x_k \cos(\omega_k t')\sin(\Omega_\mu t') \\ & + p_j p_k \omega_k^{-1} \sin(\omega_k t')\sin(\Omega_j t')]\Bigg\} \overline{\rho_1}(\Gamma_1,\Gamma_2|t,0), \end{aligned} \tag{B3}$$

where x, p, X, and P are given at time $t'=0$. A similar equation follows for $J_2^{(2)}(t)$ which we omit for the sake of brevity. The average values that appear in Eq. (B3) are evaluated to obtain that

$$\langle p_j x_k|t\rangle = 0, \quad \langle p_j p_k|t\rangle = \delta_{jk}\beta_{I1}^{-1}(t), \tag{B4}$$

$$\langle P_\mu X_\nu|t\rangle = 0, \quad \langle X_\mu X_v|t\rangle = \delta_{\mu\nu}\Omega_\mu^{-2}\beta_{I2}^{-1}(t), \tag{B5}$$

and, introducing these results into Eq. (B1), we find that

$$\frac{d}{dt}E_1(t) = \frac{N}{\tau_1}[\beta_{I1}^{-1}(t) - \beta_{I2}^{-1}(t)], \tag{B6}$$

$$\frac{d}{dt}E_2(t) = -\frac{d}{dt}E_1(t), \tag{B7}$$

where

$$\frac{N}{\tau_1} = \frac{\pi}{2}\sum_{j,\mu}\frac{\Gamma_{j\mu}^2}{\omega_j^2}\delta(\omega_j - \Omega_\mu), \tag{B8}$$

and the final form of Eq. (B7) is a result of the conservation of energy in the global system. Moreover, taking into account Eqs. (11), we have a closed system of two equations for the two Lagrange parameters β_{I1} and β_{I2}.

2. Second description [cf. Eq. (15)]

The calculation runs quite similarly to the previous one, and we omit the details for the sake of brevity, only noticing that the average values of the basic variables in terms of the Lagrange multipliers are

$$E_1(t) = \frac{N}{\beta_{II1}(t)} + \sum_j \tfrac{1}{2}[\tilde{p}_j^{\,2}(t) + \omega_j^2\tilde{x}_j^{\,2}(t)], \tag{B9}$$

$$E_2(t) = \frac{N'}{\beta_{II2}(t)}, \tag{B10}$$

$$\tilde{x}_j(t) = -\sigma_{jII}(t)|\omega_j^2\beta_{II1}(t), \tag{B11}$$

$$\tilde{p}_j(t) = -\gamma_{jII}(t)|\beta_{II1}(t). \tag{B12}$$

APPENDIX C: QUANTUM-MECHANICAL APPROACH

In a quantal approach the two descriptions of Sec. II are, in terms of the dynamical quantities, in the first case [cf. Eq. (9)] of the Hamiltonian operators

$$\hat{H}_{01} = \sum_j \hbar\omega_j(a_j^\dagger a_j + \tfrac{1}{2}), \tag{C1}$$

$$\hat{H}_{02} = \sum_\mu \hbar\omega_\mu(b_\mu^\dagger b_\mu + \tfrac{1}{2}), \tag{C2}$$

where a ($a^\dagger$) and b ($b^\dagger$) are annihilation and creation operators in the corresponding states. In the second case [cf. Eq. (15)], besides the two Hamiltonians above, are incorporated the quantities a_j and $a_j^\dagger$, which, through appropriate linear combinations, produce the operators for coordinate and momentum of the oscillator in the second quantization representation. The auxiliary coarse-grained statistical operators are, in this case,

$$\overline{\rho_I}(t,0) = \exp\{-\phi_I(t) - \beta_{1I}(t)\hat{H}_{01} - \beta_{2I}(t)\hat{H}_{02}\}, \tag{C3}$$

$$\overline{\rho_{II}}(t,0)=\exp\Bigg\{-\phi_{II}(t)-\beta_{1II}(t)\hat{H}_{01}-\beta_{2II}(t)\hat{H}_{02}-\Bigg(\sum_j f_j(t)a_j+\text{H.c.}\Bigg)\Bigg\}, \qquad \text{(C4)}$$

where ϕ, β, and f are the corresponding Lagrange multipliers. The macrovariables are

$$E_1(t)=\text{Tr}\{\hat{H}_{01}\overline{\rho_I}(t,0)\},\quad E_2(t)=\text{Tr}\{\hat{H}_{02}\overline{\rho_1}(t,0)\} \qquad \text{(C5)}$$

in the first description, and

$$E_1(t)=\text{Tr}\{\hat{H}_{01}\overline{\rho_{II}}(t,0)\},\quad E_2(t)=\text{Tr}\{\hat{H}_{02}\overline{\rho_{II}}(t,0)\}, \qquad \text{(C6)}$$

in the second, together with

$$\langle a_j|t\rangle=\text{Tr}\{a_j\overline{\rho_{II}}(t,0)\},\quad \langle a_j|t\rangle^*=\text{Tr}\{a_j^\dagger\overline{\rho_{II}}(t,0)\}, \qquad \text{(C7)}$$

It ought to be noted that the statistical operator $\overline{\rho_{II}}(t,0)$ of Eq. (C4) can be expressed in terms of only the population operators for a new set of quantities, say $\widetilde{a}$, once the Glauber-like transformation

$$a_j=a_j+\langle a_j|t\rangle \qquad \text{(C8)}$$

is performed. The calculations are then greatly simplified, and it can be shown that

$$\widetilde{\nu}_j=\text{Tr}\{\widetilde{a}_j^\dagger\widetilde{a}_j\overline{\rho_2}(t,0)\}=[\exp(\beta_{1I}(t)\hbar\omega_j)-1]^{-1}+|\langle a_j|t\rangle|^2, \qquad \text{(C9)}$$

$$\langle a_j|t\rangle=-f_j(t)/\beta_{1II}(t)\hbar\omega_j\,. \qquad \text{(C10)}$$

Using the results listed above, after some algebra, the different statistical-thermodynamic functions can be calculated to obtain in the first description that

$$E_1/N=\tfrac{1}{2}\hbar\omega_0\coth(\tfrac{1}{2}\beta_{1I}\hbar\omega_0), \qquad \text{(C11)}$$

$$\phi_I/N=-\ln[2\sinh(\tfrac{1}{2}\beta_{1I}\hbar\omega_0)], \qquad \text{(C12)}$$

$$\begin{aligned}\overline{S_I}/N&=(\phi/N)+\beta_{1I}(E/N)\\&=-\ln[2\sinh(\tfrac{1}{2}\beta_{1II}\hbar\omega_0)]\\&\quad+\tfrac{1}{2}\beta_{1II}\hbar\omega_0\coth(\tfrac{1}{2}\beta_{1II}\hbar\omega_0).\end{aligned} \qquad \text{(C13)}$$

In the derivation of these equations, we have taken a unique frequency for all the oscillators, and the second system is taken as an ideal reservoir (see the main text). In the second description, we find that

$$E_1/N=\tfrac{1}{2}\hbar\omega_0\coth(\tfrac{1}{2}\beta_{1II}\hbar\omega_0)+\beta_{1II}^{-2}(\Lambda/k_B^2), \qquad \text{(C14)}$$

$$\phi_{II}/N=-\ln[2\sinh(\tfrac{1}{2}\beta_{1II}\hbar\omega_0)]-\beta_{1II}^{-1}(\Lambda/k_B^2), \qquad \text{(C15)}$$

$$\begin{aligned}\overline{S_{II}}/N&=-\ln[2\sinh(\tfrac{1}{2}\beta_{1II}\hbar\omega_0)]\\&\quad+\tfrac{1}{2}\beta_{1II}\hbar\omega_0\coth(\tfrac{1}{2}\beta_{1II}\hbar\omega_0),\end{aligned} \qquad \text{(C16)}$$

where $\Lambda=\Delta\omega/N$ and

$$\Delta\omega=k_B^2\sum_j|f_j|^2. \qquad \text{(C17)}$$

We use these results in the numerical calculations, proceeding in the same way as done in the classical approach.

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