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ON THE EXACT IDENTITY BETWEEN THERMODYNAMIC AND INFORMATIC ENTROPIES IN A UNITARY MODEL OF FRICTION

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We consider an elementary collision model of a molecular reservoir upon which an external field is applied and the work is dissipated into heat. To realize macroscopic irreversibility at the microscopic level, we introduce a "graceful" irreversible map which randomly mixes the identities of the molecules. This map is expected to generate informatic entropy exactly equal to the independently calculable irreversible thermodynamic entropy.

Keywords: Microscopic irreversibility; thermodynamic irreversibility; entropy production; information loss; relative entropy; quantum entropy; Gibbs paradox.

1. Introduction

The thermodynamic entropy S_R^{thermo} of a given equilibrium reservoir is equal to the informatic (Shannon–von Neumann) entropy

$$S[\rho_R] \equiv -\text{tr}(\rho_R \log \rho_R). \tag{1}$$

The ρ_R is the corresponding Gibbs canonical state of the reservoir, taken in the infinite volume (thermodynamic) limit. If we switch on a certain external macroscopic field to perform work on the reservoir then the state $\rho_R(t)$ starts to evolve reversibly while, from the thermodynamic viewpoint, part of the work will be dissipated into heat in the reservoir. There is a common expectation that the irreversible thermodynamic entropy production also equals the change of the informatic entropy of the reservoir:

$$\Delta_{\text{irr}} S_R^{\text{thermo}} = S[\rho_R(t + \Delta t)] - S[\rho_R(t)]. \tag{2}$$

As is well-known, this equation does not hold because $\rho_R(t)$ evolves unitarily and the right-hand side is always zero. This is the notorious conflict between the reversibility of the reservoir's microscopic dynamics and the macroscopically observed irreversible dissipation. In our case, this dissipation is "friction" against the external field. Various resolutions of this contradiction between the microscopic and macroscopic theories are possible. None of them are general and none of them are able to prove the exact identity of the thermodynamic and informatic entropy productions. Obviously, any resolution must *impose some deliberate irreversibility* on the unitary dynamics. For a systematic study, we formalize this irreversibility as a completely positive map $\mathcal{M}$ applied to the reservoir state repeatedly. Then, we expect that

$$\Delta_{\mathrm{irr}}S_R^{\mathrm{thermo}} = S[\mathcal{M}\rho_R(t + \Delta t)] - S[\rho_R(t)] \tag{3}$$

holds exactly for microscopically short intervals Δt. The map $\mathcal{M}$ we are looking for must be *graceful*. It should not alter the macroscopic reaction (e.g. the friction force) of the reservoir on the field. Moreover, it should be such that it conserves the free dynamics of the reservoir:

$$\mathcal{M}[H_R, \rho_R(t + \Delta t)] = [H_R, \mathcal{M}\rho_R(t + \Delta t)], \tag{4}$$

where H_R is the reservoir's Hamiltonian.

In our work, we construct an elementary reservoir model composed of distinguishable molecules and postulate a discrete reversible (unitary) collision dynamics for its interaction with the external field. In this model, the thermodynamic entropy production $\Delta_{\mathrm{irr}}S^{\mathrm{thermo}}$ is exactly calculable. Then, a natural projection $\mathcal{M}$ is found that expected to increase the information entropy of the reservoir by $\Delta_{\mathrm{irr}}S^{\mathrm{thermo}}$ exactly. The map $\mathcal{M}$ symmetrizes the state ρ_R for all distinguishable molecules, i.e. it mixes the ones which collided with the external field among all molecules throughout the reservoir. The identity (3) relies upon a novel conjecture concerning the increase of the informatic entropy under the projection $\mathcal{M}$. We have heuristically proved the theorem for the classical case.

2. The Reservoir, Collisions

Assume a single molecule with a Hamiltonian H in the Gibbs-equilibrium state ρ at inverse temperature β:

$$\rho = \frac{1}{Z(\beta)}e^{-\beta H}. \tag{5}$$

Let the molecule interact with a certain external field and let us describe the interaction by the following "collision":

$$\rho \to U\rho U^\dagger \equiv \sigma, \qquad [U, H] \neq 0, \tag{6}$$

where U is unitary. Suppose our reservoir is formed by the ideal gas of n such *distinguishable* molecules in equilibrium:

$$\rho_R = \rho \otimes \rho \otimes \cdots \rho \equiv \rho^{\otimes n}, \tag{7}$$

with the Hamiltonian

$$H_R = H \otimes I^{\otimes(n-1)} + I \otimes H \otimes I^{\otimes(n-2)} + I^{\otimes(n-1)} \otimes H, \tag{8}$$

and its thermodynamic limit is $n \to \infty$. Let us assume that the molecules will reversibly collide with the field in succession, see Eq. (6). Without restricting the generality, we can assume that the first molecule collides first, the second collides second, and so on:

$$\rho^{\otimes n} \to \sigma \otimes \rho^{\otimes(n-1)} \to \sigma \otimes \sigma \otimes \rho^{\otimes(n-2)} \to \cdots . \tag{9}$$

Since $S[\sigma] = S[\rho]$, the informatic entropy of the reservoir has not changed at all in the above reversible collisions:

$$S[\rho^{\otimes n}] = S[\sigma \otimes \rho^{\otimes(n-1)}] = S[\sigma \otimes \sigma \otimes \rho^{\otimes(n-2)}] = \cdots = nS[\rho] = nS[\sigma]. \tag{10}$$

For simplicity, we consider the first collision and implement our idea for it. If we calculate the mean energy transfer from the field to the molecule, we obtain

$$\Delta E \equiv \mathrm{tr}(\sigma H) - \mathrm{tr}(\rho H) = \frac{\mathrm{tr}(\sigma \log \sigma) - \mathrm{tr}(\sigma \log \rho)}{\beta} > 0. \tag{11}$$

The proof is straightforward if we express $\log \rho = -\beta H - \log Z$ from (5), substitute it, and observe that $\mathrm{tr}(\rho \log \rho) = \mathrm{tr}(\sigma \log \sigma)$. The right-hand side above is proportional to the informatic relative entropy $S[\sigma|\rho]$ of the post- and pre-collision states, which is always positive. In a reversible process, a Gibbs-state will always *absorb* energy from the field. If the molecule is part of a reservoir and the field interacts with many molecules in succession then, thermodynamically, we expect that the above mean energy is dissipated to the reservoir. Therefore, the average thermodynamic entropy production per collision is, on thermodynamic grounds:

$$\Delta_{\mathrm{irr}} S^{\mathrm{thermo}} = \beta \Delta E = S[\sigma|\rho]. \tag{12}$$

We see that $\Delta_{\mathrm{irr}} S^{\mathrm{thermo}}$ is always positive since $S[\sigma|\rho]$ is always positive if $\sigma \neq \rho$. We emphasize that the above identity is part of common knowledge and is different from our target identity. The relative entropy which is microscopic plays an auxiliary role in the calculations. We are looking for the informatic entropy production whose value shall coincide with the relative entropy. Our target identity is

$$\Delta_{\mathrm{irr}} S^{\mathrm{thermo}} = \Delta S_R , \tag{13}$$

where ΔS_R is the *increase* of the informatic entropy between the post- and pre-collision states of the *whole reservoir*. We already noticed that ΔS_R would remain zero after the first unitary collision. The point is that we have to define a new post-collision state of the reservoir, which differs from $\sigma \otimes \rho^{\otimes(n-1)}$.

3. The Graceful Irreversible Map

Now we have to *postulate* a (completely) positive map $\mathcal{M}$ which is irreversible and *graceful*:

$$\sigma \otimes \rho^{\otimes(n-1)} \rightarrow \mathcal{M}\left(\sigma \otimes \rho^{\otimes(n-1)}\right). \tag{14}$$

The map should correlate the molecules. Single-molecule maps can increase the informatic entropy but they would not produce the requested value $S[\sigma|\rho]$. We need a map which only smears out information whose loss is heuristically justifiable in a molecular reservoir. Let the map $\mathcal{M}$ be the total randomization over the identity of the n molecules. In our case:

$$\mathcal{M}\left(\sigma \otimes \rho^{\otimes(n-1)}\right) = \frac{\sigma \otimes \rho^{\otimes(n-1)} + \rho \otimes \sigma \otimes \rho^{\otimes(n-2)} + \cdots + \rho^{\otimes(n-1)} \otimes \sigma}{n}. \tag{15}$$

It is clear that this post-collision map is irreversible and increases the informatic entropy of the reservoir. Moreover, it is consistent with Eq. (4) in conserving the energy.

In the appendix, we are going to illustrate for the classical case that the informatic entropy increases by the relative entropy of the post- and pre-collision states. According to this novel mathematical conjecture:

$$\Delta S_R \equiv \lim_{n=\infty}\left(S[\mathcal{M}(\sigma \otimes \rho^{\otimes(n-1)})] - S[\sigma \otimes \rho^{\otimes(n-1)}]\right) = S[\sigma|\rho]. \tag{16}$$

This would confirm the central physical identity (3). This says that our model yields exact identity between the independently defined thermodynamic and informatic entropies. The key element of the model is a graceful irreversible map postulated after each reversible interaction of the field with a molecule.

4. Discussion

Realistic microscopic models of dissipation are not calculable exactly. Note that both the irreversible thermodynamic $\Delta_{\mathrm{irr}}S^{\mathrm{thermo}}$ and the informatic ΔS_R entropies should be calculable independently and exactly. Our model is less realistic while it allows exact calculation and confirmation of $\Delta_{\mathrm{irr}}S^{\mathrm{thermo}} = \Delta S_R$. Our elementary model can be improved or varied in certain ways. For instance, the map $\mathcal{M}$ does not need to be repeated after each collision, it may be applied after several collisions — the main result remains. The collision dynamics is, however, essential. If we resolved it into a smooth Hamiltonian evolution the model would become fundamentally sensitive to the repetition frequency of the irreversible map $\mathcal{M}$.

In the spirit of the present work, a particular version of the model already appeared in Ref. 2 as the model of classical mechanical friction. The relationship of the map $\mathcal{M}$ to the Gibbs principle of molecular undistinguishability has been discussed although not fully persued. This is probably a deeper issue and a subject of future research.

Analysis of friction phenomena in a reduced single molecule description can be based on a two step cyclic process.[5] The first is identical to Eq. (6). The second step is an irreversible map generated by the phenomenological Lindblad operator which restores the system to its initial state. The cyclic requirement means that all entropy has to be generated in the reservoir. Unlike the present model, in the Lindblad formulation there is no explicit description of the graceful map that generates the desired entropy production.

5. Asher

Asher strived for internal consistency between independent but related branches of physics. This outlook is reflected in his book,[1] where he has linked numerous thermodynamical aspects to quantum theory and *vice versa*.

Following von Neumann, Asher proves that the equilibrium quantum informatic entropy is genuine thermodynamic entropy (p. 270). One can read the derivation of a version of our Eq. (11) [see p. 269, Eq. (9.24)]. One also learns the heuristic derivation of the Shannon informatic entropy (p. 260), we exploited in the appendix. Asher invoked thermodynamical argument particularly in a debate on hypothetic nonlinear Schrödinger equations (p. 278; see also Refs. 3 and 4). The power of thermodynamic arguments may show itself in our present work: the novel mixing entropy conjecture (appendix) for quantum entropies has so far not been proven but it is strongly supported by the physical wisdom that the thermodynamic and informatic entropy productions should coincide.

Acknowledgment

Appendix A. Conjecture on Entropy of Mixing

We consider $n + 1$ uncorrelated identical systems, where n systems have the same state ρ and a single system has a certain different state σ, and where both ρ and σ can be given arbitrarily. Consider the following uncorrelated composite state:

$$\sigma \otimes \rho^{\otimes n}. \tag{17}$$

Then, we assume that the single different system "loses" its identity among the other components, i.e. it becomes totally mixed with them. Let the resulting state be

$$R = \frac{\sigma \otimes \rho^{\otimes n} + \rho \otimes \sigma \otimes \rho^{\otimes(n-1)} + \cdots + \rho^{\otimes n} \otimes \sigma}{n + 1}. \tag{18}$$

We define the entropy of mixing:

$$S^{\mathrm{mix}}[\sigma|\rho; n] = S[R] - nS[\rho] - S[\sigma]. \tag{19}$$

We conjecture that in the limit $n \to \infty$ the entropy of mixing is identical to the relative entropy of σ with respect to ρ:

$$S^{\mathrm{mix}}[\sigma|\rho;\infty] = -\mathrm{tr}(\sigma \log \rho) - S[\sigma] \equiv S[\sigma|\rho]. \tag{20}$$

The proof of the general quantum case is missing. We present a heuristic proof for the classical case $[\sigma, \rho] = 0$.

Heuristic proof — Classical case. We can directly estimate the increase of Shannon entropy caused by mixing. Let us consider a discrete d-state system and its diagonal density matrices with elements $\rho_{ab} = \rho_a \delta_{ab}$ and $\sigma_{ab} = \sigma_a \delta_{ab}$, where $a, b = 1, 2, \ldots, d$. If n is large, we can ignore all but the statistically relevant terms in $\hat{\rho}^{\otimes n}$. Look at the components

$$\rho_{a_1} \rho_{a_2} \cdots \rho_{a_n}, \tag{21}$$

and consider the string

$$a_1 a_2 a_3 \cdots a_n \tag{22}$$

of labels. In the statistically relevant terms, the multiplicity of a given index a must approximately be $n\rho_a$ for each $a = 1, 2, \ldots, d$. Therefore, each relevant term has the same weight and the total number of relevant terms can be estimated combinatorically as

$$\frac{n!}{(n\rho_1)!(n\rho_2)! \cdots (n\rho_d)!} \sim 2^{nS[\rho]}, \tag{23}$$

which is the number of all different orderings within the string (22). Now, take the single state described by σ_a, insert the latter into the string at random and try to calculate the expected increase of the number of relevant configurations. Assume temporarily that $\sigma_a = \delta_{a1}$. Then, the above number of combinations acquires a factor

$$\frac{n+1}{n\rho_1 + 1} \sim \frac{1}{\rho_1}. \tag{24}$$

Equation (24) means that the entropy increases by $-\log \rho_1$. Generalizing this result, we can estimate the average increase of the entropy for any distribution σ_a:

$$-\sum_a \sigma_a \log \rho_a - S[\sigma] = S[\sigma|\rho], \tag{25}$$

which is the classical special case of our conjecture (20).

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