

On the Entropy Flow between Parts of Multi-component Systems, Partial Entropies and the Implications for Observations

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The concept of the time dependent *instantaneously occupied phase space volume* is applied to multi-component systems. It allows for the investigation of entropy flows between the components of the system and the evaluation of partial entropies assigned to the subsystems. We give numerical examples by means of molecular dynamics simulations of a 100-particle gas. Using a symplectic exactly reversible algorithm, a consistent and reliable evaluation of energy and entropy exchanges as well as the intake of work is achieved. The entropy flow which is related to an information flow is linked to an observational situation. This yields a further indication for the necessity of an intrinsic observer for a better understanding of the physical world. In addition, it indicates the Gödelian structure of cognition in a most serious way because only “first-principle” assumptions are made. Thereby, the paradoxical situation which is created by Jaynes’ concept of an “anthropomorphic entropy” can be resolved by putting the anthropomorphic contents of thermodynamics down to an ontological basis. This is a straightforward extension of Szilard’s and Brillouin’s information theoretical treatment of cognition.

Key words: Information Flow; Intrinsic Observer; Phase Space Volume; Molecular Dynamics; Entropy Flow.

1. Introduction

In order to become aware of and to gain knowledge on an object one has to interact with it [1 - 3]. An interaction in turn has mutual impact on both the measuring subject and the measured object. Subject and object exchange momenta and energy and possibly mass [2]. Eventually, they may change internal entropic states. In this paper we investigate the entropic flow between the parts of multi-component systems using the entropy formula recently derived by Diebner and Rössler [4, 5] in the molecular dynamics context.

If one of the subsystems has self-organizing properties in a sophisticated way that it can be called “observer” there is no obvious reason to treat it differently from other physical subsystems. We show by means of molecular dynamics simulations (MDS) that the entropy flow quantitatively depends on the thermodynamic states the subsystems had before interacting with each other. For an observer this means that his gain of knowledge depends not only on the states of the external world but also on his own state.

Let us briefly recapitulate some thermodynamics as far as it concerns here. Assume a gas which consists

of N identical particles within a volume V . Configurations and momenta define the entropy. Boltzmann’s entropy

$$\begin{aligned} S_B[\gamma_B(t)] &= -k \int_{\Gamma_B} \rho(\gamma_B(t)) \ln \rho(\gamma_B(t)) d\gamma_B \\ &= -k \langle \ln \rho \rangle_{\Gamma_B}, \end{aligned} \quad (1)$$

where the integral is taken over the 6-dimensional 1-particle phase space, Γ_B , with ρ being the distribution of the particles’ states, γ_B , uses the micro-canonical ensemble to be interpreted when only macrostates are measured [6]. In MDS, micro-canonical ensembles play a superior role at least with respect to the computation of the entropy which is calculated from the explicitly known micro states. A frequently calculated entropic measure in this context is Boltzmann’s H -function,

$$H[v(t)] = k \int_{\Gamma_v} \rho(v(t)) \ln \rho(v(t)) dv, \quad (2)$$

whereby the integral is taken over the 3-dimensional velocity part, Γ_v , of the 6-dimensional 1-particle

phase space, Γ_B , where $\rho(v)$ is the distribution of the velocities [7].

The advantage of Boltzmann's entropy is its explicit time dependency. It can be calculated at each time instant because the cloud of N state points forms a distribution in the limit $N \rightarrow \infty$ which can be approximated by means of binning, for example. Not so in the case of Gibbs' entropy,

$$S_G = -k \langle \ln \rho \rangle_{\Gamma_G}, \quad (3)$$

where the integral is taken over the total $6N$ -dimensional phase space, Γ_G , and ρ being the distribution of the $6N$ -dimensional states γ_G of the system. A time dependent calculation of this entropy seems not to be available because a state at a time instant marks a point in the phase space and only the trajectory defines a density in the continuum limit. This entropy is inexpedient for MDS especially in the case of non-equilibrium systems, i. e., in the case of transient behavior. In such a transient case it is obviously contradictory to estimate a density by means of computing a long trajectory. The latter strategy will work only in the case of equilibrium. Even, or perhaps just analytically, a consistent non-equilibrium thermodynamics is one of the toughest challenges of physics.

Moreover, the interpretation of Gibbs' entropy formula seems to be an anthropomorphic one as stressed by Jaynes [8], since it depends on our knowledge of a system which entropy this system has. In fact, the full phase space density ρ in the Liouville equation,

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \dot{q} \frac{\partial \rho}{\partial q} + \dot{p} \frac{\partial \rho}{\partial p}, \quad (4)$$

is usually interpreted as an uncertainty resulting from our restricted knowledge [9]. This uncertainty may eventually increase with time and, thus, has implications on the accuracy of predictions. As Jaynes mentioned, if we had perfect knowledge on a system, the entropy of that system would vanish. The density ρ in (4) converges to a δ -distribution in that limit, describing a precise trajectory in the time course. However, that the N -particle system then should have zero entropy seems to be absurd.

Not surprising, the Gibbs entropy can be derived by applying Shannon's theory of communication [10] to thermodynamical systems [11, 8]. From the so-called *Landauer limit* $\ln(2)kT$ [12] – the dissipated energy after the erasure of 1 bit of information – it is clear

that for preparing an information processing device in an exactly known initial state a huge amount of energy is necessary. The CPU then has zero entropy, but this intake of “neg-entropy” has to be taken from the surrounding. If an observing subject and the observed object were the only systems, i. e., if there were no additional surrounding, it is clear from the above argument that gaining full knowledge on the exact state of the object necessitates such a strong subject-object interaction that the object may be totally destroyed like a photon when being observed. Thus, Jaynes' at first absurdly sounding “anthropomorphism” indeed seems not to be too far from Boltzmann's concept of treating entropy as a function of the actual states of the systems. The absurdity stems from the fact that the observer's physical state and his impact on the object has so far been neglected. Brillouin's insight “Maxwell's demon cannot operate” [2] can thus be strengthened: Maxwell's demon does not even exist in relational terms; it is a metaphysical concept. Laplace's demon, the predecessor of Maxwell's demon, can be viewed as a metaphor which illustrates the concept of determinism and has no relational counterpart. Maxwell's demon is an attempt to apply a non-relational concept to the relational aspects of the world. A demon realized by relational means, i. e., by means of an interaction between the demon and the observed object is no longer a demon but rather an intrinsic observer with an impact on the object.

Although Jaynes' concept according to the above argumentation may be undisputable, in the MDS context, however, the Gibbs entropy is unworkable. For other objections against Gibbs entropy like non-ergodicity of real systems, for example, please confer [13]. In order to investigate the dynamics of a subject-object interaction one has to search for an adequate deterministic time-dependent entropy as a function of given microstates. Boltzmann's entropy in the form of (1) is a candidate. However, it uses distributions in the 1-particle phase space only and, thus, is of local character in the sense that configurations only with respect to the next neighbors are taken into account. However, it has been shown in [4, 5] that a correlation-like time-dependent entropy formula can be derived using the concept of *instantaneously occupied phase space volume* in the full phase space. The full arrangement of the particles is taken into account with that entropy. For a 3-dimensional N -particle gas this entropy reads

$$S_{\text{DR}} [r(t)] = k \left\{ \ln(N) + \frac{1}{N(N-1)} \left[\sum_{i=1}^N \sum_{\substack{j=1 \\ j \neq i}}^N \ln \left(\frac{1}{6} \pi^3 \gamma_{ij}^6(t) \right) \right] \right\}. \quad (5)$$

Thereby, γ_{ij} is the normalized distance of particles i and j in the 6-dimensional 1-particle phase space. For the normalization a maximum distance in the configuration space, given by the collateral extension of the gas, and the maximum momentum, given by $p_{\text{max}} = \sqrt{2E}$ with total energy E , is used. S_{DR} indeed is a compromise between the Boltzmann entropy of (1) and the Gibbs entropy of (3). We are now able to investigate the dynamical entropic behavior of multi-component systems.

2. Entropy of a Two-Component System

Assume given an N -particle gas within volume V . The N identical point-shaped particles interact with each other through a repelling potential, the concrete form of which is not important for the effect to be shown. We choose a repelling Coulomb-potential to amplify the effect artificially, though being unrealistic for a molecular gas. It rather mimics a free electron gas.

According to an argument given by Hoover [14], which is in line with the concept of occupied phase space [4, 5], “a kind of free volume made of holes distributed through the system gives a direct measure of the instantaneous work required to insert another particle”:

$$\mu = \left(\frac{\partial A}{\partial N} \right)_{V,T}. \quad (6)$$

Here we stick with the micro-canonical formulation and calculate a slightly different entity, namely the work carried out with respect to a conserved total energy. Therefore, a second system composed of M particles of the same species is moved from a large distance (ideally from infinity) to the vicinity of the first system until they are side by side. In the case of $N = M = 1$ this is nothing else than the usual derivation of the electro-static potential between two electrons. However, if $N > 1$ and/or $M > 1$, than the subsystems have internal degrees of freedom. The resulting additional internal dynamics are usually not treated within electro-static derivations. Instead, only the total charge of a metallic sphere, for example, is

taken into account. However, with respect to the entropic behavior these internal dynamics become important.

We now describe a first simulation example realized by a 100-particle MDS. Hereby, $N = 99$ particles are confined within the unit cube $[0, 1] \times [0, 1] \times [0, 1]$. One particle (i.e. $M = 1$), arbitrarily labeled with $n = 1$, is separated from that subsystem and initially located at $q_1 = (5.0, 0.5, 0.5)^T$. The 99 particles of the first subsystem are initially equi-distributed at rest within the left half of the cube. The Hamiltonian of that system reads

$$H = T(\{\mathbf{p}^n\}) + V(\{\mathbf{q}^n\}) \quad (7)$$

$$= \sum_{n=1}^{\hat{N}} \frac{\mathbf{p}^n \cdot \mathbf{p}^n}{2} + \sum_{i=1}^{\hat{N}} \sum_{j>i}^{\hat{N}} \frac{\epsilon}{r^{i,j}} + \text{wall potential}.$$

Hereby, $\hat{N} = N + M$ and $r^{i,j}$ is the distance of particles i and j . Here and in the following, superscripts are used for particle labels whereas subscripts are reserved for the spatial components. The masses of the particles have been set to unity and ϵ is set equal to 10^{-2} throughout the paper. The wall potential, acting only on the 99 particles of the first system, is regarded as infinite, which leads to fully elastic reflections. The latter can easily be implemented using the symplectic two-step integrator recently derived from a variational principle [15] applied in discretized space and time. The discretization of space-time with spacing parameters Δq and Δt , respectively,

$$t = t_0 + k\Delta t; \quad q_j^n = q_{j,0}^n + x_j^n \Delta q; \quad k, x_j^n \in \mathbb{Z}, \quad (8)$$

leads to an integer representation of the positions and the time given by x_j^n and k , respectively. The arbitrary origin, q_0 , of the frame is chosen to be zero in the following. The superscript $n \in \{1, \dots, \hat{N}\}$ labels the particle and the subscript $j \in \{1, 2, 3\}$ is the spatial component, respectively. The application of the principle of least action to the discrete space-time eventually yields a symplectic integrator that ensures an exactly reversible dynamics. This algorithm reads

$$x_j^n(k+1) = 2x_j^n(k) - x_j^n(k-1) - \text{ROUND} \left\{ \frac{(\Delta t)^2}{2(\Delta q)^2} \tilde{V} \right\};$$

$$\tilde{V} = V[x_1^1(k)\Delta q, \dots, (x_j^n(k)+1)\Delta q, \dots, x_3^N(k)\Delta q]$$

$$- V[x_1^1(k)\Delta q, \dots, (x_j^n(k)-1)\Delta q, \dots, x_3^N(k)\Delta q];$$

$$n = 1, \dots, \hat{N}; \quad j = 1, 2, 3. \quad (9)$$

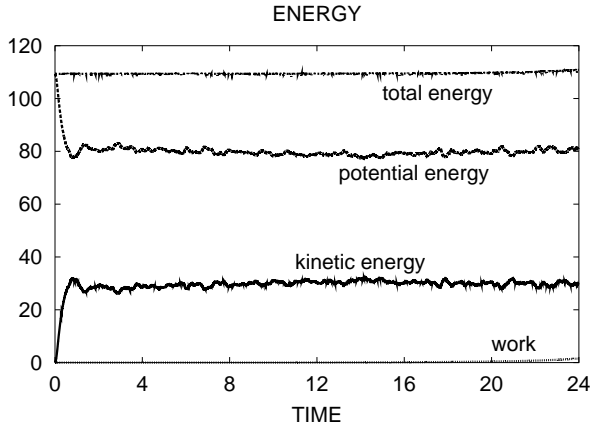


Fig. 1. Time series of the energy contributions in a 100-particle MDS. Before $t = 10$, a single far outlying particle is fixed at its initial position and then moved towards the gas. The lowermost graph shows the concomitant intake of work. Note, that the total energy (uppermost graph) increases by the same amount. The early transient behavior in potential and kinetic energy is due to a relaxation process. Cf. text for details.

The ROUND-function represents the closest integer of its argument. The discretization constants are chosen to be $L = \frac{1}{\Delta q} = 2^{35}$ and $\Delta t = 10^{-4}$, respectively, throughout all simulations described in this paper. The momenta of the particles are given by

$$p_j^n(k) = \frac{(x_j^n(k) - x_j^n(k-1))\Delta q}{\Delta t}; \quad (10)$$

$$n = 1, \dots, \hat{N}; \quad j = 1, 2, 3.$$

The reflection rule at the walls reads

$$\tilde{x}_j^n(k+1) = \text{r.h.s. of (9)}, \quad (11)$$

$$x_j^n(k+1) = \begin{cases} \tilde{x}_j^n(k+1), & \text{if } 0 < \tilde{x}_j^n(k+1) < L; \\ x_j^n(k) & \text{otherwise,} \end{cases}$$

$$x_j^n(k) = \begin{cases} x_j^n(k), & \text{if } 0 < \tilde{x}_j^n(k+1) < L; \\ \tilde{x}_j^n(k+1) & \text{otherwise,} \end{cases}$$

$$j = 1, 2, 3; \quad n = 2, \dots, \hat{N}.$$

Hereby, \tilde{x}_j^n is an intermediate algorithmic step which is retained if it lies within the cube, otherwise the reflection is carried out. (Note, the reflection does not apply to particle $n = 1$ in our example.)

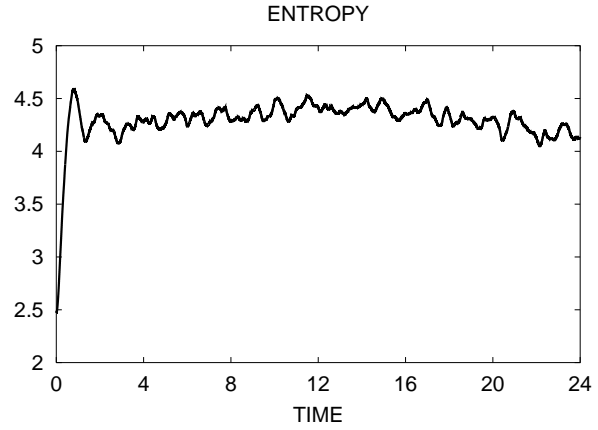


Fig. 2. Entropy of the 100-particle MDS as in Figure 1. There is a strong early increase of entropy due to the expansion of the gas. From $t = 10$ on, the entropy decreases due to an intake of work. Cf. text for details.

The algorithm of (9), together with the reflection rule of (11) allows for a consistent statistical mechanical analysis of the systems given by the Hamiltonian of (7). The integration of the 100-particle-system is carried out in two steps. First, the separated particle labeled $n = 1$ is fixed at its initial position up to $t = 10$. During that period a relaxation process of the gas takes place by expanding into the whole volume. This relaxation process reveals in the transiency of the energy as well as the entropy of the gas. The corresponding graphs are depicted in Figs. 1 and 2. The entropy calculated according (5) increases by about two units. From $t = 10$ on, the initially separated particle, labeled $n = 1$, is moved towards the cube which confines the gas. The velocity of that particle is 0.291, which is close to the mean velocity of a particle of the gas. Thereby work is carried out which changes the internal energy of the gas. This work is shown in Fig. 1 to be compared with the other graphs and replotted in Fig. 3 (smooth graph) using a magnified scale to see the details. In addition to this electro-static treatment of energy, the concomitant entropy change has been evaluated which can be seen in Figure 2. The entropy slowly decreases after $t = 10$.

It goes without saying that the internal energy can no longer be conserved. However, the energy change is exactly balanced by the work intake – even in our discrete simulated mini-universe, which is why we mention it. This is the merit of the exactly reversible algorithm used. Note that Orban and Bellemans in 1967 [16] recognized a numerical dissipation which

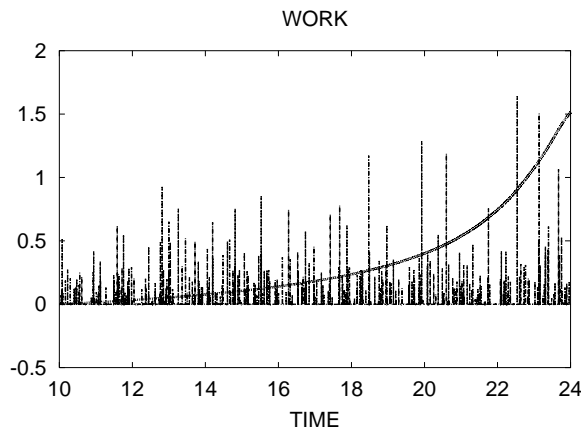


Fig. 3. Work intake (smooth graph) of the same system as in Figs. 1 and 2 during the relevant episode from $t = 10$ on, together with the fluctuations (spiking graph) of the total energy minus the work.

is superimposed to an originally conservative system frustrating a reliable entropic analysis. Only recently it has been shown, that such a purely numeric dissipation can be avoided [17, 15, 18]. Indeed, the difference of the momentary energy minus the initial energy minus the work has no drift and shows only minor fluctuations about zero, which can be seen in Fig. 3 (spiking graph). These fluctuations are of purely numerical origin and do neither destroy the exact symplecticity nor a consistent entropy analysis. For an elaborate discussion please confer to [15, 18].

3. Partial Entropies of Subsystems

The structure of the correlation-like entropy of (5) allows for the evaluation of “partial entropies” of subsystems. Let $A \subseteq \{1, 2, \dots, N\}$ be a subset of indices (particle labels) the corresponding particles of which define a subsystem. We interchangeably use A for the denotation of the subsystem and the corresponding set of indices. If one restricts the first summation of (5) to subset A, this defines a partial entropy related to subsystem A. In the above described simulation of a 100-particle system, we called particle $n = 1$ a first subsystem, henceforth denoted A, and the remaining particles a second one, henceforth denoted B. Thus, the corresponding partial entropies can be evaluated by restricting the first summation to the index $i = 1$ and to the set of indices $\{2, 3, \dots, \hat{N}\}$, respectively.

A further entropy related to the 99-particle system can be evaluated by using the states of that very system

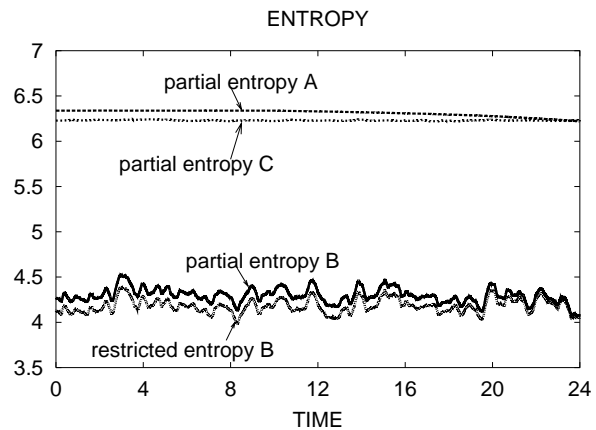


Fig. 4. Entropy by time of a 100-particle gas as in Fig. 1, however without the expansion process in the beginning. The labels are consistent with the notation used in the text, where a full discussion is given.

exclusively, i. e., by neglecting the interaction with the 1-particle system. In this case, both summations in (5) are restricted to the corresponding indices and, additionally, the total number of particles is reduced accordingly. We call this entity “restricted entropy” of subsystem B.

Finally, we allocate C to the 1-particle subsystem given by the particle with label $n = 100$. This is an arbitrary choice since there is no obvious characteristic which would allow to distinguish particle $n = 100$ from the other particles $n = 2, \dots, 99$ that belong to B. The definition of subsystem C is for the sake of a comparison with subsystem A with respect to their entropic behavior.

Figure 4 shows the results of an MDS which has been performed in the same way as in the previous section with the exception that an already relaxed initial state for the 99-particle subsystem has been used, namely the final state of the previously performed simulation. Again, from $t = 10$ on, particle $n = 1$ is moved constantly towards the 99-particle subsystem, whereas before $t = 10$ it has been fixed at its initial position. The labeling of the graphs in Fig. 4 is consistent with the above introduced notation. “Partial entropy C” is almost constant over the whole time range whereas “partial entropy A” decreases after $t = 10$. This can intuitively be understood quite easily because the (relative) movement of subsystem B towards A has a non-negligible impact on A. The partial entropy of C, in contrast, is mainly determined by the contributions of the particles of sub-

system B which have an almost constant relative configuration.

A comparison of the graphs “partial entropy B” and “restricted entropy B” shows that an initially given difference approximately vanishes in the time course after $t = 10$. The slight remaining difference is mainly due to the different total numbers of particles that determine the constant contributions to the entropies. It follows that a restriction to subsystem B from the very beginning would not have allowed for a reliable evaluation of the entropy transfer between the systems. With respect to observational situations it is to assume, that exactly this difference has so far not been taken into account. One can easily accept that such a disregard has a vanishing influence in most technical applications. However, in small (micro- and mesoscopic) systems the entropic impact of an observation may become important, which is evident from the simulation examples given.

4. Conclusions

The concept of an entropy flow between subsystems has been introduced, and MDS examples have been given. This concept allows for the evaluation of a time-dependent entropy exchange between subsystems that interact with each other. We further argued that a relational treatment of an observation process is qualitatively of the same kind, i. e., an interaction between the parts of a multicomponent system. This leads to the concept of an intrinsic observer which is indeed not a new concept [19 - 21]. However, through the comparison of an observer with Maxwell’s demon some paradoxical phenomena can be clarified. A demon is a metaphor for the fruitful concept of determinism and is clearly distinct from an observer which is an (intrinsic) subsystem of a multi-component system. This insight suggests that via an endophysical approach (as it is called by Rössler [20]) a deeper

understanding of physics may be possible and that at the same time a Gödel-like antinomy [22] becomes evident. It is sometimes argued that cognition has self-referential character and that we therefore cannot fully understand the world [23]. However, we here gave more than a plausible hand-waving argument and it seems that the limitation of our knowledge has a much less profound origin than is suggested by brain theoretical considerations. We did not use any anthropomorphic entities or concepts – we only used fundamental physical concepts which are of much more evidence.

The introduced concept encourages experiments that allow for a more detailed quantitative investigation of the observer’s impact on objects even with “real” observers. The latter can be coupled in a controlled way to virtual environments via adequate haptic interfaces by using, for instance, the “flotor” developed by Ralph Hollis et al. [24 - 26]. Such experiments are in preparation and partially already in progress.

To conclude, the introduced entropy flow enables investigations of time-dependent thermodynamical processes in a quantitative way. Moreover, apparent anthropomorphic contents of communication theory can be put down to an ontological basis by introducing “intrinsic observers”. If one accepts that the human knowledge is uniquely related to the entity “information” and thus to “entropy” a consistent thermodynamics follows and the evidence for the Gödelian structure gets the character of a proof. An observational entropic impact on an object becomes important in small systems especially in quantum mechanical systems.

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