Thermodynamics’ first law: what information theory tells us

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INTRODUCTION

Jaynes’ pioneering 1957 papers in The Physical Review 1 constitute a new theoretical foundation for the development of statistical mechanics providing us with a solid alternative on the basis of information theory (IT) 2. One of the main ingredients in Jaynes’ treatment was an intense use of the principle of parsimony (PP) 3. Our purpose here is to present an original derivation of thermodynamics’ first law from an IT viewpoint and, at the same time, provide a pedagogical example illustrating the principle of parsimony that explicitly invokes Jaynes’ discovery (of more than forty years ago) 1, 2, that no reference to equilibrium needs to be made in order to deal completely and successfully with all of thermodynamics. To some physicists, even theoreticians, the idea sounds revolutionary even today!

The PP, or Ockham’s razor, is a basic methodological principle that governs scientific endeavor 4. It dictates simplicity in theory construction, as for instance, in the number of axioms, or of parameters, involved in a theoretical construct.

As stated above, we will here apply this principle with regards to the usual IT-treatment of the first law of the thermodynamics 2. Appeal to Ockham’s razor will yield a simpler derivation than the usual textbook one.

3. The phase space probability distribution depends only on the system’s Hamiltonian.

4. This dependence is of exponential form.

Jaynes reformulated statistical mechanics in 1957 1 by recourse to information theory concepts 2, with quantum mechanics now providing the background. Instead of a distribution function in phase space we now use a density operator $\hat{\rho}$ to describe our system. $\hat{\rho}$ is obtained via the so called MaxEnt principle, namely, the constrained (Lagrange) maximization of Shannons’s logarithmic information measure $S$, regarded as a measure of ignorance 3, with

$$S = -k_B \text{Tr} \hat{\rho} \ln \hat{\rho},$$  \hspace{1cm} (1)$$

where $k_B$ is the Boltzmann constant, to be set equal to unity from now on. Jaynes’ basic axiom or postulate reads: the density operator that describes our system is that provided by the MaxEnt principle. One might argue that this postulate explicitly assumes Shannon’s entropy logarithmic form, but such an statement can be refuted by pointing out that other forms have been used in the literature to this effect with great success 3, 7, 8. A second axiom that one needs, however, is that $\hat{\rho}$ depends explicitly only on expectation values and implicitly on some Hamiltonian.

Most interestingly, no reference to either i) equal a priori probabilities or ii) equilibrium, needs to be made. On IT grounds, equilibrium refers to the state of knowledge of the observer, it is not an intrinsic property of the system. Information theory is essentially concerned with epistemology: equilibrium means that one’s knowledge is restricted to constants of the motion, so that one can forget about dynamics 2. The equilibrium notion plays no part whatsoever in our considerations.

On Ockham’s razor grounds, one might argue that Jaynes’ number of postulates is smaller that Gibbs’. In particular, since no mention of “equilibrium” is made, the associated theory has, at least potentially, a wider

JAYNES’ APPROACH AND OCKHAM’S RAZOR

The orthodox formulation of statistical mechanics is due to Gibbs 3, working on a classical mechanics substratum. It is based upon the following set of axioms 3:

1. Ensemble postulate: the system at equilibrium can be represented by an appropriately designed ensemble.

2. Equal a priori probabilities for cells in phase space.
outreach than that of Gibbs’\textsuperscript{2}. It is perhaps necessary to point out, at this point, that an entirely different information theory approach to non-equilibrium thermodynamics, based upon Fisher’s measure (a kind of “Fisher-MaxEnt”), has recently been advanced that exhibits definite advantages over both Gibbs’ and (the original) Jaynes’ treatments\textsuperscript{3,10,11}.

Returning to Jaynes’ approach, assume that we deal with a system with Hamiltonian $\hat{H}$. The system is characterized by the set of operators $\{\hat{O}_i\}$ ($i = 1,\ldots,M$, with $\hat{O}_i \equiv \hat{H}$) in the sense that one is supposed to know the expectation values of these operators. In other words

$$
\langle \hat{O}_i \rangle = a_i, \ (i = 1,\ldots,M)
$$

$$
Tr[\hat{\rho}] = 1,
$$

(2)

constitutes our a priori information concerning the system. We wish to find the appropriate, most unbiased $\hat{\rho}$ that reproduces this amount of information and otherwise maximizes our ignorance. The truth, all the truth, nothing but the truth\textsuperscript{3}. Using any other $\hat{\rho}$ is tantamount to inventing information that we actually do not possess. Extremizing then subject to the constraints\textsuperscript{2} leads to a density operator of the form\textsuperscript{2}

$$
\hat{\rho} = e^{-\sum_i \lambda_i \hat{O}_i} Z,
$$

(3)

where the $\{\lambda_i\}$ is a set of Lagrange multipliers ($\lambda_1 = \beta$ is the inverse temperature) that arise during the Lagrange formalism. The $\{\lambda_i\}$ are associated with the above expectation values that represent our foreknowledge\textsuperscript{3}. The normalization factor in Eq.\textsuperscript{3}

$$
Z = Tr[e^{-\sum_i \lambda_i \hat{O}_i}]
$$

(4)

is the partition function\textsuperscript{3}. The formalism allows for arbitrary variations in the expectation values to be carried out. Let us insist: thermodynamics has been derived more than 40 years ago from the IT formalism. If one relies on IT, it is clear that, epistemologically, no additional thermodynamic notions are to be presupposed in advance. Notice that predictions derived from the IT-formalism amply exceed the scope of themes that conventional thermodynamics is able to deal with\textsuperscript{1,2}. In order to obtain the first law, the usual text-book approach\textsuperscript{3} analyzes the variation of the internal energy $U$, which is regarded as a functional of both i) the density operator and ii) the Hamiltonian.

**OUR PRESENT GOAL**

We will show in this work that it is possible to perform a different treatment that considers the internal energy as a functional of solely the density operator. According to Ockham’s razor, this way of handling the first law is to be preferred to the traditional one, since now one can dispense with, in order to describe the thermodynamic work $W$, the two following theoretical assumptions (or needs) of the traditional approach\textsuperscript{3}:

**Assumptions that will be no longer needed**

- reference to “equilibrium”
- explicit dependence of the Hamiltonian on some “external” parameters $\chi$,
- recourse to the adiabatic theorem (AT)\textsuperscript{3}.

We can summarize the AT’s contents as follows\textsuperscript{3}: let us regard the Hamiltonian as depending on a parameter $\chi$ that evolves in time from an initial value $\chi_1$ to a final value $\chi_2$, during a time-interval $\tau$, in the fashion

$$
\chi(t) = \chi_1 + \frac{t}{\tau} (\chi_2 - \chi_1); \ (\chi(0) = \chi_1, \ \chi(\tau) = \chi_2).
$$

(5)

In the limit of an exceedingly slow, physically unrealizable $\chi$-change (i.e., for $\tau \rightarrow \infty$), the time evolution that $\hat{H}(\chi(t))$ generates during the temporal interval $[0, \tau]$ is such that, if the system is represented at $t = 0$ by an eigenstate of $\hat{H}(\chi_1)$, it will be found in an eigenstate of $\hat{H}(\chi_2)$ at $t = \tau$. Indeed, at any time $t$ in $[0, \tau]$ it will be encountered in an eigenstate of $\hat{H}(\chi(t))$.

**A RELATION FOR $dU$**

The possibility of eliminating recourse to the AT should be a relief to many who consider it a somewhat suspect subterfuge: to our knowledge there has been no direct, assumption free experimental confirmation of the claim that the final state of a system is really independent of its path from the initial state when work is performed\textsuperscript{12}. It goes without saying that the consequences of the first law are so well established that its validity is beyond any reasonable doubt\textsuperscript{12}. Nevertheless, in the light of this situation a new proof of the first law, specially one that avoids the awkward AT, should be of great interest.

We now proceed to derive a relationship for $dU$. For this we need to deal with the internal energy $U$, that is, with a special case ($i = 1$) of

$$
U = \langle \hat{O}_1 \rangle \equiv \langle \hat{H} \rangle = Tr[\hat{\rho} \hat{H}],
$$

(6)

and consider variations $\delta \hat{\rho}$ of the density operator, whose normalization entails

$$
Tr[\delta \hat{\rho}] = \delta Tr[\hat{\rho}] = \delta 1 = 0
$$
\[ Tr[\delta \rho \ln \rho] = \delta Tr[\rho \ln \rho]. \quad (7) \]

We also have, of course,
\[ Tr[\delta \rho \hat{O}] = \delta \langle \hat{O} \rangle. \quad (8) \]

Thus, we confront finding (Cf. (5))
\[ dU \equiv \delta \langle \hat{O}_{i=1} \rangle = Tr[\delta \rho \hat{H}]. \quad (9) \]

Appropriate manipulation of Eq. (3) allows one now to write \( \hat{H} \) in the fashion
\[ \ln \rho + \ln Z = - \left[ \beta \hat{H} + \sum_{i>1} \lambda_i \hat{O}_i \right], \quad (10) \]

and thus
\[ \hat{H} = -\frac{1}{\beta} \left( \ln \rho + \ln Z + \sum_{i>1} \lambda_i \hat{O}_i \right); \]
\[ \hat{O}_k = -\frac{1}{\lambda_k} \left( \ln \rho + \ln Z + \sum_{i \neq k} \lambda_i \hat{O}_i \right), \quad (11) \]

so that, replacing \( \hat{H} \) into Eq. (11), and minding also (6), yields
\[ dU = -\frac{1}{\beta} \delta \{ Tr[\rho \ln \rho] \} - \sum_{i>1} \frac{\lambda_i}{\beta} \delta \langle \hat{O}_i \rangle. \quad (12) \]

The first term in Eq. (12) is now to be recast in terms of the entropy of the system, as given by Eq. (14), which leads one to
\[ dU = T dS - \sum_{i>1} T \lambda_i \delta \langle \hat{O}_i \rangle, \quad (13) \]

where \( T = 1/\beta \) is the temperature of the system. More generally, one also has
\[ \delta \langle \hat{O}_k \rangle = \frac{dS}{\lambda_k} - \sum_{i \neq k} \frac{\lambda_i}{\lambda_k} \delta \langle \hat{O}_i \rangle. \quad (14) \]

We make now the identification
\[ \text{for heat (Q) change: } d'Q = TdS, \quad (15) \]

and we arrive at the promised relationship for \( dU \)
\[ dU = d'Q + dX, \quad (16) \]

with \( X = -T \sum_{i>1} \lambda_i \delta \langle \hat{O}_i \rangle. \)

**WHAT IS X?**

The derivation of (16) is straightforward. We are left with the interpretation of \( X \). Let us delve a little longer on the meaning of (16). We have assumed that our a priori information has slightly changed:
\[ \text{From } \langle \hat{O}_i \rangle = a_i \text{ to } \langle \hat{O}_i \rangle + \delta \langle \hat{O}_i \rangle = a_i + \delta a_i; \quad (i = 1, \ldots, M). \quad (17) \]

Necessarily then, the MaxEnt methodology yields a new density operator \( \rho + \delta \rho \), which, of course, entails in turn a change in the Lagrange multipliers
\[ \text{From } \lambda_i \text{ to } \lambda_i + \delta \lambda_i; \quad (i = 1, \ldots, M). \quad (18) \]

The essential IT-content of the first law (Cf. Eq. (16)) is that i) the \( \delta \langle \hat{O}_i \rangle \) are not independent quantities (Cf. Eq. (14)) and ii) they can be expressed solely in terms of the \( \lambda_i \). Of course, if one wishes to predict the value of \( \langle \hat{A} \rangle \), an operator not included in the set \( \{ \hat{O}_i \} \), one would need the \( \delta \lambda_i \).

If we call the differential of work \( (dW) \), effected at temperature \( T \),
\[ dW = -\sum_{i>1} T \lambda_i \delta \langle \hat{O}_i \rangle, \quad (19) \]

we obviously obtain, without further ado, the first law of thermodynamics in the fashion (16), where heat \( (dQ) \) and work \( (dW) \) terms acquire their traditional aspect. If we did not accept, for whatever the reason, the interpretation (19), we could not avoid the conclusion that the difference \( dU - dQ \) has two forms: one of them follows from (19) and *always* holds. In some particular instances, we would, in addition, have the conventional first law. On Ockham grounds, the first alternative, namely, Eq. (16), is clearly preferable. Consider the simple classical example posed by a probability distribution \( f(\tau) \) in phase-space (volume element \( d\tau \)), with two constraints:
\[ f(\tau) = Z^{-1} \exp ( -[\beta H(\tau) + p \beta \phi(\tau)] ) \]
\[ \int d\tau f(\tau) H(\tau) = U; \quad \int d\tau f(\tau) \phi(\tau) = V \quad (V = Volume; \quad p \equiv pressure), \quad (20) \]

where application of Eq. (16) immediately yields
\[ dU = TdS - p \ dv. \quad (21) \]

**DISCUSSION AND CONCLUSIONS**

We have shown that, within Jaynes’ information theory context, one may derive thermodynamics’ first law without appeal to the adiabatic theorem (5) or to a explicit
dependence of the pertinent Hamiltonian on hypothetical external parameters. This agrees with both Ockham’s razor and the Jaynes’ philosophy. Thus we avoid the slightly paradoxical contradiction between simultaneously stating

- on the one hand, that  \( \hat{\rho} \) contains all the available information concerning the system, and,
- on the other one, needing to add, to the theoretical description, putative infinitely slowly varying external parameters to obtain the first law.

There is no need to invoke the adiabatic theorem because, interestingly enough, the formalism itself demands that the process be undertaken at a constant temperature \( T \) (Cf. Eqs. (15)-(19)) that arises automatically in the constrained Lagrange extremization.

For a system characterized by the set of operators \( \{ \hat{O}_i \} \ (i = 1, \ldots, M); \hat{O}_1 \equiv \hat{H} \), in the sense that we know a priori the pertinent expectation values \( \{ \langle \hat{O}_i \rangle \}; \ (i = 2, \ldots, M) \). These constituted part of our prior knowledge. If a posteriori we encounter changes, this entails that work has been performed, on or by the system.

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