

Temperature of a closed system at equilibrium: the total energy is a "sufficient statistic"

◆ **Abstract.** An unexpected formal identity is revealed between the technical notion of statistical sufficiency and a property of thermal equilibrium that has been observed by L. Szilard and G.N. Lewis. Promoting this formal identity into a postulate yields a new and *purely phenomenological* axiomatic approach to thermodynamics. It is based on the theory of the estimation of parameters just as the axioms of quantum mechanics are based on the analysis of the process of observation. ◆

1. The ill-defined term "statistics;" difference between probability theory and estimation of parameters

To account for our incomplete knowledge of the state of a macroscopically observed system, Gibbs proposed two representative statistical "ensembles:" the *canonical* ensemble of known temperature and random energy, and the *micro-canonical* ensemble of known energy. But Khinchin 1949, having examined concepts that Gibbs used, including laws as fundamental as " $S = \log W$," found that many could not be made rigorous and concluded that they should be avoided. His suggestion would, however, destroy the very useful complementarity between the two Gibbs ensembles.

This paper proposes to show that, in fact, sufficiently general mathematics makes a rigorous formulation possible. Indeed, Khinchin limits himself to *probability theory*. This has been the appropriate tool for the goal of deducing macroscopic properties from microscopic statistical hypotheses. But the step from microcanonical to canonical, including the definition of a temperature for an isolated system, demands a different

kind of mathematics. It will be shown that theory of the estimation of parameters, which is a proper part of statistics, is particularly appropriate for the study of the foundations of thermodynamics.

It is understood that this increase in precision of the foundations of the theory does not affect the predictions relative to large systems. But it may have practical consequences for small systems.

2. A property of the Gibbs canonical distribution of energy

Let us begin by showing how the Gibbs distribution $p(u) = \Omega(u)^{-1} e^{-\beta u}$, is related to a properly statistical axiom. We will start by describing the converse, due to Szilard 1925, Darmais 1936, Koopman 1936 and Pitman 1931, of a classical and banal theorem of thermo-statistical mechanics:

Theorem. Put in contact two systems that have previously been in contact with the same heat reservoir. Consider the distribution $p'(u_1)$ of the energy U_1 of one of the systems. This distribution is independent of the initial temperature of the heat reservoir, and uniquely conditioned by the total energy u .

Proof: It follows from $\Omega(u) = \Omega_1(u_1) \Omega_2(u_2)$ that

$$p'(u_1) = \frac{p_1(u_1)p_2(u_2)}{p(u)} = \frac{\Omega_1(u_1)^{-1} e^{-\beta u_1} \Omega_2(u_2)^{-1} e^{-\beta u_2}}{\Omega(u)^{-1} e^{-\beta u}} = \frac{\Omega_1(u_1) \Omega_2(u_2)}{\Omega(u)}.$$

3. Derivation of the canonical distribution from the microcanonical

The usual method to introduce the Gibbs canonical distribution derives the same expression for $p'(u_1)$ from a microcanonical hypothesis. A system of energy u can be found in $\Omega(u)$ different "states" and all configurations of this system are assumed to have equal probabilities. This hypothesis follows from the ergodic property (taken as a theorem or a hypothesis). But it implies the introduction of randomness, which is basically not justified in a dynamic theory. In fact, if the system of energy u_1 is very small compared to its complement of energy use, the formula for $p'(u_1)$ becomes

$$p'(u_1) = \Omega_1(u_1)^{-1} e^{-\beta' u_1}, \quad \text{with} \quad \beta' = -\frac{\log \Omega(u)}{u}.$$

This is again the Gibbs distribution, but with a factor β' differing from the initial β .

4. The work of Szilard and Lewis

Szilard 1925 (and, in less complete detail, Lewis 1931) has shown that the method used in Section 3 has a very important and unjustly neglected variant, one that involves the converse of the theorem in Section 2. The objective is to base statistical thermodynamics on phenomenological principles taking ergodicity to be out of reach of observation, because it is related to “states” that are inobservable by definition.

Szilard starts with two axioms: (a′) the axiom that the energy of a canonical system is intrinsically random (refer to quantum theory, von Neumann 1932), and (b′) a conclusion of the theorem of section 2, which is expected to hold only after a long enough time: the axiom that the “nature” of thermal equilibrium is such that any property observed long after the system has been isolated independent of the way it has initially been prepared (example: by contact with a thermostat, or by putting together two parts that were initially in contact with different thermostats); in particular, $p'(u_1)$ can not be conditioned by u . Szilard shows:

Converse theorem. Only the Gibbs distribution satisfies (b′).

5. Role of statistical sufficiency in thermodynamics

More direct than (a) and (b), the postulates (a′) and (b′) are not subject to limitations imposed on a macroscopic physicist, therefore they are not yet “phenomenological”, in the meaning usually applied to the laws of Carnot, Clausius, etc. They may, however, be made phenomenological by a translation that is immediate (but not at all evident, as it seems).

In fact, Szilard's *criterion* (b′), implies that $p'(u_1)$ cannot be conditioned by any quantity other than u , hence is precisely identical to the most general definition of “statistical sufficiency.” It asserts the measured u is a sufficient statistic for the estimation of θ . Hence, the concept of sufficiency is related to the “indirect measurements” of the θ of a thermostat Th., as given by the examination of “samples” of a system that has been in contact with Th. Sufficiency expresses the macroscopic character of the temperature $1/\theta$: for the estimation of θ , it is neither necessary to measure independently the energies of all the parts of the system, nor to know the empirical distribution of the energy among the parts. Whatever the criterion for “good estimation” may be, the estimate based on the whole is as good as an estimate based on the knowledge of all the parts. The process will never be perfect, because to estimate a parameter means to guess its value, which can be done in a “reasonable” way, but never in a logically necessary fashion.

