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# Two Uniqueness Problems Connected with Lewis' Principle. (**)

## 1. - Introduction.

LEWIS has proposed [1] a simple principle that enables to obtain the fundamental formulas of Statistical Mechanics. This principle generalizes JAYNES' method of maximum uncertainty [2] to time dependent situations and at the same time, widens the scope of its applications. Moreover it answers perfectly to GRAD's interpretation [3] of the appearance of several expressions for the entropy. The application of LEWIS' principle depends on the existence and the uniqueness of the solutions of a certain class of variational problems. Both these properties are postulated by LEWIS; here we intend to show that, in two cases of particular physical interest, they can be established in a rigorous manner. Since the principle has not been the object of much attention, we think it useful to recall its premises and its statement.

Let a conservative system with $s$ degrees of freedom be described by the Hamiltonian $H(z)$, where $z$ represents the set of generalized coordinates and conjugated momenta: $z=(q_1, q_2, \ldots, q_s, p_1, p_2, \ldots, p_s)$. The Hamiltonian is assumed to be bounded below by a constant (this assumption is not restrictive, since it is satisfied by practically every physical system); as is usual, the constant is assumed to be equal to zero.

In a somewhat imprecise language, a state function is a function that describes the state of a given system. Examples of state functions are pro-

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vided by the probability density $w(t, z)$ in the phase space $\Gamma$ of the system, or by the « $n$-particle functions » defined by

$$f_n(t, z_1, z_2, \ldots, z_n) = \int w(t, z_1, \ldots, z_s)\, dz_{n+1}\, dz_{n+2} \ldots dz_s \qquad (1 \leqslant n \leqslant s)\,.$$

For a given state function $u$, a complete description of the system consists of an equation of motion:

$$\frac{\partial u}{\partial t} = Mu$$

and of an entropy functional:

$$S = S[u]\,. \tag{1}$$

The operator $M$ is not linear in general; the functional $S$ is real-valued. The « original » (in a sense which will be made clear by the statement of the principle) state function is $w(t, z)$; the complete description of the system is then given by the Liouville's equation and by the following entropy functional:

$$S[w] = -k \int_\Gamma w(t, z) \lg w(t, z)\, dz \tag{2}$$

where $k$ is the BOLTZMANN constant. LEWIS' principle states what follows

« Given a complete description of the system in terms of the state function $u$, let

$$f = Lu \tag{3}$$

be a new state function, $L$ being a linear, in general not invertible, operator. Let $u[f]$ be the unique state function that maximizes the functional (1) subject to (3) and, possibly, other conditions such as normalization or symmetry. The equation of motion for $f$ is then given by:

$$\frac{\partial f}{\partial t} = LMu[f] \tag{4}$$

while the new entropy functional is:

$$S_1[f] = S[u[f]]\,. \tag{5}$$

The equations (4) and (5) represent the new complete description of the system in terms of $f$ ».

The principle contains the unproven assertion that a unique function $u[f]$ exists that maximizes the entropy functional (1).

## 2. - The case of the canonical ensemble.

When the new description is given in terms of the scalar:

$$U(t) = \int_\Gamma H(z) w(t, z)\, dz \tag{6}$$

the function that maximizes (2) subject to the condition (6) and the normalization condition:

$$\int_\Gamma w(t, z)\, dz = 1 \qquad \forall t \in R$$

is (see [**1**], p. 1458):

$$w[U] = Z^{-1} \exp[-\beta H(z)] \tag{7}$$

where $Z$ is the partition function:

$$Z(\beta) = \int_\Gamma \exp[-\beta H(z)]\, dz\,.$$

It is important to remark that, since the system is conservative, the scalar $U(t)$ of equation (6) is actually a constant. The equation of motion for $U$ is in fact (see [**1**], eq. (9.5)):

$$\frac{dU}{dt} = 0$$

which implies $U =$ constant. As a consequence, $w[U]$ is also independent of time, as was already obvious from (7).

We shall now prove the uniqueness of the solution (7). This is equivalent to proving that a unique real number $\beta^*$ exists that satisfies (6), that is that the following equation in the unknown $\beta$:

$$\int_\Gamma H \exp(-\beta H)\, dz \Big/ \int_\Gamma \exp(-\beta H)\, dz = U \tag{8}$$

has a unique solution $\beta^*$.

Because of the assumption on $H$, we have $U \geqslant 0$; we can discard the case $U = 0$, which has little physical interest (Hamiltonian identically equal to zero), and assume $U > 0$. By making use of the partition function, equation (8) may be written as follows:

$$-Z'(\beta)/Z(\beta) = U . \tag{9}$$

But a result of KHINCHIN ([4], p. 77), under assumptions identical with ours, shows that the equation (9) has a unique solution for $U > 0$. The uniqueness of (7) is thus established.

## 3. - The case of Vlasov equation.

The function $w^*(t, z_1, \ldots, z_s)$ that maximizes (2) under the conditions:

(i) $f_1(t, z_1) = \int w(t, z_1, \ldots, z_s)\, dz_2 \ldots dz_s$;

(ii) $\int_\Gamma w(t, z)\, dz = 1 \quad \forall t \in R$;

(iii) $w$ is symmetric in $z_1, z_2, \ldots, z_s$,

is (see [1], eq. (4.7)):

$$w^*(z_1, \ldots, z_s) = \prod_{i=1}^{s} f_1(z_i) . \tag{10}$$

The dependence on time is understood, although it is not explicitly noted. The function $f_1$ of condition (i) is the new state function. We show here that (10) is the unique function that maximizes (2) subject to the conditions (i), (ii) and (iii).

Let, ab absurdo, $\boldsymbol{w}$ be a function that satisfies (i), (ii) and (iii), and such that

$$S[\boldsymbol{w}] \geqslant S[w^*]$$

or, explicitly:

$$-k\int_\Gamma \boldsymbol{w} \lg \boldsymbol{w}\, dz \geqslant -k\int_\Gamma w^* \lg w^*\, dz . \tag{11}$$

According to (5), the entropy functional provided by the principle is given by:

$$S_1[f_1] = -k\int_\Gamma w^* \lg w^* \,\mathrm{d}z = -k\int \{\prod_{i=1}^{s} f_1(z_i)\} \lg \{\prod_{j=1}^{s} f_1(z_j)\}\,\mathrm{d}z =$$

$$= -k\int \{\prod_{i=1}^{s} f_1(z_i)\} \sum_{j=1}^{s} \lg f_1(z_j)\,\mathrm{d}z_1\,\mathrm{d}z_2 \ldots \mathrm{d}z_s =$$

$$= -k\sum_{j=1}^{s} \int \prod_{\substack{i=1\\ i\neq j}}^{s} \{f_1(z_i)\,\mathrm{d}z_i\} \int f_1(z_j) \lg f_1(z_j)\,\mathrm{d}z_j =$$

$$= -k\sum_{j=1}^{s} \int f_1(z_j) \lg f_1(z_j)\,\mathrm{d}z_j =$$

$$= -ks \int_\gamma f_1(z_1) \lg f_1(z_1)\,\mathrm{d}z_1\,.$$

In the last integral, the integration is to be performed on the configuration space $\gamma$ of the first particle. If we substitute the last result into (11), we obtain:

$$-k\int_\Gamma \boldsymbol{w} \lg \boldsymbol{w}\,\mathrm{d}z \geqslant -ks\int_\gamma f_1(z_1) \lg f_1(z_1)\,\mathrm{d}z_1\,. \tag{12}$$

This latter inequality proves the assumption (11) wrong. In fact,

$$H_G = \int_\Gamma \boldsymbol{w} \lg \boldsymbol{w}\,\mathrm{d}z$$

is GIBBS' $H$ function, whilst

$$H_B = \int_\gamma f_1(z_1) \lg f_1(z_1)\,\mathrm{d}z_1$$

is BOLTZMANN's $H$ function. On the other hand, it is well known (see for example: [**3**], p. 336, or [**5**], p. 393) that $H_G$ and $H_B$ satisfy the following inequality:

$$H_G \geqslant sH_B \tag{13}$$

namely (12) in which the sign has been reversed. The inequality (11) must therefore be written in the form:

$$-k\int_\Gamma \boldsymbol{w} \lg \boldsymbol{w}\,\mathrm{d}z \leqslant -k\int_\Gamma w^* \lg w^*\,\mathrm{d}z = -ks\int_\gamma f_1(z_1) \lg f_1(z_1)\,\mathrm{d}z_1\,. \tag{14}$$

The last relationship holds for any $\boldsymbol{w}$ that satisfies the three conditions (i), (ii) and (iii). The inequality (13) is a direct consequence of the relationship: $\lg x \leqslant x - 1$ (see [**3**] or [**5**]), in which the equality is possible if and only if $x = 1$. The equality in (14) is therefore possible if and only if $\boldsymbol{w} = w^*$.

The equation of motion for the state function $f_1$ turns out to be VLASOV equation. The importance of this case is enhanced by the fact, that, after adding a few simplifying assumptions, LEWIS was able to deduce BOLTZMANN equation.

As a last remark, we shall point out that the problem of establishing the existence and the uniqueness of the function that maximizes the functional (2) subject to general conditions, rather than to the particular ones that we have considered in the present work, is still open.

## References

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## Summary

*Lewis' principle postulates the existence and the uniqueness of the solutions of a class of variational problems. The validity of these assumptions is however not investigated. We prove here the uniqueness of the probability density that maximizes the functional* $-k\int_\Gamma w(t, z) \lg w(t, z)\, dz$ *in two cases of physical interest,the uniqueness having been proved for the two cases by Lewis.*

## Sommario

*Il principio di Lewis postula l'esistenza e l'unicità delle soluzioni di una classe di problemi variazionali. Non vi si esamina tuttavia la fondatezza di tali ipotesi. Si dimostra qui l'unicità della densità di probabilità che massimizza il funzionale* $-k\int_\Gamma w(t, z) \lg w(t, z)\, dz$ *in due casi di particolare interesse per la fisica; l'esistenza era già stata provata da Lewis.*

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