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THEORETICAL PHYSICS

On the Quantum Informational Thermodynamics

by

A. KOSSAKOWSKI

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The information-theoretical approach to thermodynamics (informational thermodynamics for short) has been developed by Ingarden and Urbanik [1]—[11] (cf. also Jaynes [12]—[14]). In the present paper their ideas are generalized and further developed.

We shall first restrict our discussion to the case of a finite-dimensional Hilbert space. The condition under which the extension to the case of an infinite-dimensional Hilbert space is possible will be presented at the end of the present paper.

Let $\mathcal{H}$ be a finite-dimensional Hilbert space corresponding to a physical system and let $N = \dim \mathcal{H}$, Denote by P the set of all density operators on $\mathcal{H}$. Each element $\varrho \in P$ will be called a *microstate*. To every observable there corresponds a self-adjoint linear operator on $\mathcal{H}$. The mean value of the observable A at a microstate ϱ, i.e., $\mathrm{Tr}(A\varrho)$, will be denoted by $m_A(\varrho)$. Let H be the Hamiltonian of the system in question. In the Schrödinger picture the time evolution of the microstate $\varrho(t)$ is described by the von Neumann equation

$$i\hbar \frac{d}{dt} \varrho(t) = [H, \varrho(t)]. \tag{1}$$

When the microstate $\varrho(0)$ is known at the time $t = 0$ we can calculate from (1) $\varrho(t)$ $(t \geqslant 0)$ and, in consequence, find the time evolution of mean values for all observables.

The entropy, $s(\varrho)$, of a microstate ϱ is given by the von Neumann formula, i.e., $s(\varrho) = -\mathrm{Tr}(\varrho \ln \varrho)$. It was shown in [15] that $s(\varrho)$ is the only (up to an additive constant) measure of information contained in ϱ, compatible with the axiomatic definition [16], which is invariant under all unitary transformations in $\mathcal{H}$. In particular, $s(\varrho(t)) = s(\varrho(0))$ for all $\varrho(0) \in P$ and $t \geqslant 0$.

Suppose that we have determined (measured) the mean values of observables $A_1, \ldots, A_p$ $(p \leqslant N^2 - 1)$ at the time $t = 0$. The problem is to assign for every observable X and for every $t \geqslant 0$ the estimated value of X at the time $t \geqslant 0$ in a consistent way with the quantum-mechanical description. The proposed solution of this problem is based on the information-theoretical approach.

Let $A^{(p)} = (A_1, \ldots, A_p)$ (A for short) be a set of p observables such that operators $I, A_1, \ldots, A_p$ are linearly independent and $p \leqslant N^2 - 1$, $N = \dim \mathcal{H}$, I is the identity operator. Two microstates ϱ' and ϱ'' are said to be *equivalent* with respect to A, in symbols $\varrho' \underset{A}{\sim} \varrho''$, if $m_{A_i}(\varrho') = m_{A_i}(\varrho'')$ for $i = 1, \ldots, p$. The relation $\underset{A}{\sim}$ divides the set P of all microstates into disjoint classes. These classes will be called *A-macrostates* and will be denoted by capital Greek letters $\Phi_A, \Psi_A, \ldots$, The A-macrostate containing a microstate ϱ will also be denoted by $[\varrho]_A$. The value, $M_{A_i}(\Phi_A)$, of the observable A_i $(i = 1, \ldots, p)$ at a macrostate Φ_A is defined as the common value of $m_{A_i}(\varrho)$ $(i = 1, \ldots, p)$ for all $\varrho \in \Phi_A$.

In order to define the entropy of the macrostate we apply the principle of maximum uncertainty formulated by Jaynes, Ingarden and Urbanik. According to this principle, we define the *entropy*, $S(\Phi_A)$, of the macrostate Φ_A as the maximum uncertainty concerning microstate ϱ when the macrostate Φ_A is known. More precisely,

$$S(\Phi_A) = \sup\{s(\varrho) : \varrho \in \Phi_A\}. \tag{2}$$

Wichmann [17] has proved the following

THEOREM 1. *Let Φ_A be a macrostate. Then there exists a unique microstate $\varrho^* \in \Phi_A$ such that*

$$S(\Phi_A) = s(\varrho^*), \tag{3}$$

where

$$\varrho^* = \varrho^*(a_1, \ldots, a_p) = \left[\mathrm{Tr}\exp\left(-\sum_{i=1}^{p} a_i A_i\right)\right]^{-1} \exp\left(-\sum_{i=1}^{p} a_i A_i\right), \tag{4}$$

and the equations

$$M_{A_i}(\Phi_A) = \mathrm{Tr}(A_i \varrho^*(a_1, \ldots, a_p)) \quad (i = 1, \ldots, p) \tag{5}$$

have the unique solution in $a_1, \ldots, a_p$.

The microstate ϱ^* will be called the *representative microstate* for the macrostate Φ_A.

Let Ω be a closed convex set of microstates and let X be an observable. The relation $\underset{X}{\sim}$ divides the set Ω into disjoint classes. These classes will be called *Ω-relative X-macrostates* and will be denoted by $\Phi_X(\Omega)$, $\Psi_X(\Omega), \ldots$.

Let Φ_A be a macrostate known at time $t = 0$, and let us denote by Ω_t the closed convex set of microstates at the time $t \geqslant 0$ which have belonged to Φ_A at the time $t = 0$, i.e., $\Omega_t = \{\varrho(t) : \varrho(0) \in \Phi_A\}$. Consider the family

$$F_X^t(\Phi_A) = \{[\varrho(t)]_X \cap \Omega_t : \varrho(0) \in \Phi_A\} \tag{6}$$

of all Ω_t-relative X-macrostates which can be composed of the microstates belonging to Φ_A at time $t = 0$. All elements of $F_X^t(\Phi_A)$ are indistinguishable by the measurement of the mean values of observables $A_1, \ldots, A_p$. In order to decide which element of the family $F_X^t(\Phi_A)$ has to be chosen, the principle of maximum uncertainty will be applied. Namely, the *Ω_t-relative X-macrostate at the time* $t \geqslant 0$, $\Phi_X^t(\Omega_t)$, is defined as the maximally uncertain Ω_t-relative X-macrostate from the family $F_A^t(\Phi_A)$. More precisely,

$$\Phi_X^t(\Omega_t) : S\left(\Phi_X^t(\Omega_t)\right) = \sup\left\{S\left(\Psi_X(\Omega_t)\right) : \Psi_X(\Omega_t) \in F_X^t(\Phi_A)\right\}. \tag{7}$$

Moreover, the *estimated value at time* $t \geqslant 0$, $M_X^t(\Phi_A)$, of an observable X is defined by the equality

$$M_X^t(\Phi_A) = M_X\left(\Phi_X^t(\Omega_t)\right). \tag{8}$$

By the convexity of $F_X^t(\Phi_A)$ and by Theorem 1 it follows that the macrostate $\Phi_X^t(\Omega_t)$, and in consequence $M_X^t(\Phi_A)$, is uniquely determined.

The X-macrostate containing the macrostate $\Phi_X^t(\Omega_t)$ will be denoted by Φ_X^t (it is assumed that the initial macrostate Φ_A is fixed).

The presented description in terms of macrostates is called the *quantum informational thermodynamics.*

THEOREM 2. *Let Φ_A be a macrostate known at the time $t = 0$, and let X be an observable. Then the relations*

$$\Phi_X^t(\Omega_t) = [\varrho^*(t)]_X \cap \Omega_t, \tag{9}$$

and

$$M_X^t(\Phi_A) = \mathrm{Tr}\left(X \varrho^*(t)\right) \tag{10}$$

hold. The microstate $\varrho^*(t)$ is determined by means of the von Neumann equation

$$i\hbar \frac{d}{dt} \varrho^*(t) = [\varrho^*(t), H] \tag{11}$$

with the initial condition $\varrho^*(0) = \varrho^*$, where ϱ^* is the representative microstate for Φ_A.

THEOREM 3. *Let Φ_A be a macrostate known at the time $t = 0$. Then the following inequality*

$$S(\Phi_A^t) \geqslant S(\Phi_A) \tag{12}$$

holds, where $\Phi_A^t = [\varrho^*(t)]_A$.

This Theorem may be interpreted as an analogue to the Boltzmann's H-Theorem in the case of macrostates.

A macrostate Φ_A is said to be *invariant* under the motion if for every $t \geqslant 0$ the microstate $\varrho(t)$ belongs to Φ_A, whenever the initial microstate $\varrho(0)$ has belonged to Φ_A.

THEOREM 4. *All A-macrostates are invariant under the motion iff every operator A_i $(i = 1, ..., p)$ commutes with the Hamiltonian of the system in question.*

Every macrostate invariant under the motion will be called the *equilibrium macrostate*. The equilibrium quantum thermodynamics may be characterized as the theory of equilibrium macrostates.

Let us consider a set $X^{(r)} = (X_1, \ldots, X_r)$, which will be denoted by X for short, of observables such that operators $I, X_1, \ldots, X_r$ are linearly independent and $r \leqslant N^2 - 1$. The value $M^t_{X_i}(\Phi_A)$ will be denoted by $M_{X_i}(t)$ $(i = 1, \ldots, r)$. For every time $t \geqslant 0$ there exists the representative microstate $\tilde{\varrho}_t$ for the macrostate $[\varrho^*(t)]_X$. By Theorem 1 $\tilde{\varrho}_t$ has the form

$$\tilde{\varrho}_t = \left[\operatorname{Tr} \exp\left(-\sum_{i=1}^{r} b_i(t) X_i\right)\right]^{-1} \exp\left(-\sum_{i=1}^{r} b_i(t) X_i\right), \tag{13}$$

where $b_i(t)$ $(i = 1, \ldots, r)$ can be uniquely expressed in terms of $M_{M_i}(t)$ $(i = 1, \ldots, r)$ from the equations

$$M_{X_i}(t) = \operatorname{Tr}(X_i \tilde{\varrho}_t) \quad (i = 1, \ldots, r). \tag{14}$$

Taking into account (10) and (11) the equations of motion for $M_{X_i}(\mathrm{t})$ $(i = 1, \ldots, r)$ can be written as follows

$$i\hbar \frac{d}{dt} M_{X_i}(t) + \operatorname{Tr}\left(\tilde{\varrho}_t [H, X_i]\right) = \operatorname{Tr}\left(\left(\varrho^*(t) - \tilde{\varrho}_t\right)[X_i, H]\right) \tag{15}$$

$$(i = 1, \ldots, r)$$

with the initial conditions

$$M_{X_i}(0) = \operatorname{Tr}\left(X_i \varrho^*(0)\right) \quad (i = 1, \ldots, r), \tag{16}$$

where $\varrho^*(t)$ $(t \geqslant 0)$ is determined by (11).

It may be observed that the left-hand side of (15) is expressible only in terms of $M_{X_i}(t)$ $(i = 1, \ldots, r)$, since $\tilde{\varrho}_t$ is a function of $M_{X_i}(t)$ $(i = 1, \ldots, r)$ by (13) and (14).

THEOREM 5. *Let $M_{X_i}(t)$ $(i = 1, \ldots, r)$ be the solution of the equations*

$$i\hbar \frac{d}{dt} M_{X_i}(t) + \operatorname{Tr}\left(\tilde{\varrho}_t [H, X_i]\right) = 0 \quad (i = 1, \ldots, r) \tag{17}$$

with the initial conditions $M_{X_i}(0) = \operatorname{Tr}(X_i \varrho^*)$ $(i = 1, \ldots, r)$, and let $\Psi_X(t)$ be the X-macrostate corresponding to the values $M_{X_i}(t)$ $(i = 1, \ldots, r)$. Then for every $t \geqslant 0$ the equality

$$S(\Psi_X(t)) = S(\Psi_X(0)) \tag{18}$$

holds.

With regard to the equality (18), the time evolution described by (17) may be called the *iso-entropic motion* with respect to observables $X_1, \ldots, X_r$. Moreover, the right-hand side terms in (15) may be interpreted as the *collision* terms for observables $X_1, \ldots, X_r$.

Until now we have considered the case of a finite-dimensional Hilbert space. In this case the entropy of any macrostate is finite. In the case of an infinite-dimensional Hilbert space, entropy (2) may, or may not, be finite. In this case the formalism presented above has to be subjected to some restrictions imposed on admissible sets of observables in order to make the entropy (2) finite.

Let $\mathcal{H}$ be o separable Hilbert space, and let $A_1, \ldots, A_p$ be a set of observables such that operators $I, A_1, \ldots, A_p$ are linearly independent. The set $A_1, \ldots, A_p$ of observables is called a *thermodynamically regular set* (regular for short) if there exists a sequence $c_1, \ldots, c_p$ of p real numbers such that

$$\mathrm{Tr}\,(c_1 A_1 + \ldots + c_p A_p) < \infty. \tag{19}$$

The notion of regularity given here is a generalization of that introduced in [1] for one observable. We observe that informational thermodynamics in the case of an infinite-dimensional Hilbert space can be formulated only for regular operators.

The classical informational thermodynamics can be formulated exactly in the same manner as the quantum one in the case of an infinite-dimensional Hilbert space. The following changes are necessary. Let Γ be the phase space corresponding to a physical system, and let $d\Gamma$ be the Liouville measure on Γ. A microstate $\varrho(q, p)$ is the Radon—Nikodym derivative of a probabilistic measure on Γ with respect to the Liouville measure. An observable $A = A(q, p)$ is a real measurable function on Γ. Finally, the commutator has to be changed into $i\hbar\{\cdot, \cdot\}$ ($\{\cdot, \cdot\}$ denotes the Poisson bracket) and $\mathrm{Tr}\, A$ has to be replaced by $\int_\Gamma A(q, p)\, d\Gamma$.

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DEPARTMENT OF THERMODYNAMICS AND THEORY OF RADIATION, UNIVERSITY, TORUŃ
(KATEDRA TERMODYNAMIKI I TEORII PROMIENIOWANIA, UNIWERSYTET, TORUŃ)

REFERENCES

[1] R. S. Ingarden and K. Urbanik, Acta Phys. Polon., **21** (1962), 281.

[2] R. S. Inagrden, Bull. Acad. Polon. Sci., Sér. sci. math., astronom. et phys., **11** (1963), 209—212.

[3] — , *Physics and Technics of Low Temperatures*, Proc. 3rd Reg. Conference held in Prague, 1963.

[4] K. Urbanik, Bull. Acad. Polon. Sci., Sér. sci. math., astronom. et phys., **10** (1962), 349—352.

[5] — , *Statistical Decision Functions and Random Processes*, Transactions of the 3rd Prague Conference on Information Theory, 1963, p. 743—764.

[6] — , Forschritte der Physik, **12** (1964), 567.

[7] — , ibid., **13** (1965), 755.

[8] K. Urbanik, Colloquium Math., **12** (1964), 271.

[9] R. S. Inagrden, Bull. Acad. Polon. Sci., Sér. sci. math., astronom. et phys., **13** (1965), 69—72.

[10] — , Acta Phys. Polon., **27** (1965), 179.

[11] R. S. Inagrden and A. Kossakowski, ibid., **28** (1965), 499.

[12] E. T. Jaynes, Phys. Rev., **106** (1957), 620.

[13] — , ibid., **108** (1957), 171.

[14] — , Brandais Summer Institute, 1962, Vol. 3, Statistical Physics, N. Y., Benjamin, 1963.

[15] R. S. Inagrden and A. Kossakowski, Bull. Acad. Polon. Sci., Sér. sci. math., astronom. et phys., **16** (1968), 61—65.

[16] A. Kossakowski, ibid., **17** (1969), 77.

[17] E. H. Wichmann, J. Math. Phys., **4** (1963), 884.