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REMARKS ON THE ENTROPY IN QUANTUM MACROPHYSICS

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The ordinary formalism of quantum theory may be described in hurried outline as follows. To every physical system there corresponds a Hilbert space $\mathfrak{H}$. All elements ψ belonging to the unit sphere of $\mathfrak{H}$ are called *microstates* of the physical system. Further, to every physical quantity or observable there corresponds a self-adjoint (not necessarily bounded) linear operator on $\mathfrak{H}$. Let A be an operator corresponding to an observable and let

$$A = \int_{-\infty}^{\infty} \lambda \, \Pi_A(d\lambda)$$

be its spectral decomposition (see [5], p. 318, [6], p. 180). It should be noted that the projector-valued spectral measure Π_A defined on Borel subsets of the real line is uniquely determined. The fundamental statistical law of quantum theory states that the formula $p_A^\psi(\mathscr{E}) = \big(\Pi_A(\mathscr{E})\psi, \psi\big)$ gives the probability that a measurement at a microstate ψ of the observable corresponding to the operator A will lie in the set $\mathscr{E}$. The mean value of the observable A at a microstate ψ, i. e. the intergal $\int_{-\infty}^{\infty} \lambda P_A^\psi(d\lambda)$, will be denoted by $m_A(\psi)$, provided that it exists. Further, the entropy $s_A(\psi)$ of A at the microstate ψ is defined by the formula

$$s_A(\psi) = \sup \Big(- \sum_{k=1}^{n} p_A^\psi(\mathscr{E}_k) \log p_A^\psi(\mathscr{E}_k) \Big),$$

where the supremum is extended over all finite decompositions of the real line into Borel sets $\mathscr{E}_1, \mathscr{E}_2, \ldots, \mathscr{E}_n$.

We shall now quote some basic notions of macrophysics introduced in [2]. Two microstates φ and ψ are said to be *equivalent* with respect to the observable A, in symbols $\varphi \underset{A}{\sim} \psi$, if $m_A(\varphi) = m_A(\psi)$. The relation $\underset{A}{\sim}$ divides the set of all microstates in which A has finite mean value into disjoint classes. These classes will be called *macrostates* with respect to A

or shortly macrostates and denoted by capital Greek letters $\Phi, \Psi, \ldots$ The macrostate containing a microstate φ will be also denoted by $[\varphi]$. The *mean value* $M_A(\Phi)$ of the obsevable A at the macrostate Φ is defined as the common value $m_A(\varphi)$ for all microstates φ belonging to Φ. In order to define the *entropy* $S_A(\Phi)$ of A at the macrostate φ we apply the principle of maximum uncertainty formulated by Jaynes [3]. This principle may be regarded as a precise and mathematically correct replacement of the ambiguous Laplace principle of insufficient reason. According to Jaynes principle we define $S_A(\Phi)$ as the maximal uncertainty concerning A when the mean value $M_A(\Phi)$ is known. More precisely, we put $S_A(\Phi) = \sup\{s_A(\varphi):\varphi\in\Phi\}$. It was proved in [2] that the entropy $S_A(\Phi)$ is finite at every macrostate Φ if and only if the spectrum of A is discrete and if there exists a real constant c such that

$$\sum_{k=1}^{\infty}\exp(c\lambda_k) < \infty,$$

where $\lambda_1, \lambda_2, \ldots$ are proper values of the operator A. Each operator A satisfying the last condition is called *thermodynamically regular*. The class of thermodynamically regular operators is the largest class of operators for which the generalized thermodynamics can be developed (see [2]). In what follows we shall consider only thermodynamically regular operators.

The evaluation of the physical system in time brings about a systematic and continuous change of microstates. This change is determined by the equation

$$\psi(t) = \exp\left(-\frac{it}{\hbar}H\right)\psi \quad (t \geqslant 0),$$

which may be written in differential form as the Schrödinger equation of the motion

$$i\hbar\frac{\partial\psi(t)}{\partial t} = H\psi(t)$$

with the initial condition $\psi(0) = \psi$ (see [1], p. 110, [4], p. 108). Here H is the Hamiltonian operator, i. e. the total energy operator for the system in question and $\hbar$ is an abbreviation for Planck's constant divided by 2π. In what follows we assume that the Hamiltonian does not depend on the time t.

The entropy in evolving physical systems was discussed in [7] and [8]. Since, in general, macrostates with respect to operators non-commuting with the Hamiltonian branch out during the motion of the system, it was necessary to introduce a new concept of *entropy at an instant* t for a macrostate Φ, in symbols $S^t_A(\Phi)$. According to Jaynes principle, $S^t_A(\Phi)$ is defined to be the maximal uncertainty at time t concerning A when the initial mean value $M_A(\Phi)$ is known. More precisely, we put

$$S^t_A(\Phi) = \sup\{S_A([\varphi(t)]) : \varphi(0) \in \Phi\}.$$

In [8] (see also [7]) the principle of increase of entropy for spin operators, i. e. the inequality

$$S^t_A(\Phi) \geqslant S_A(\Phi) \qquad (t \geqslant 0)$$

was established. Moreover, for arbitrary operators A a limiting principle of increase of entropy was proved.

We have seen that the definition of fundamental quantities of macrophysics $S_A(\Phi)$ and $S^t_A(\Phi)$ is based on Jaynes principle of maximum uncertainty. It is natural to ask whether the Jaynes principle can be replaced by a less pessimistic statistical principle which also would imply the law of increase of entropy. A possible way is to regard the uncertainty of a macrostate as an average of uncertainties of its microstates. Thus the question can be formulated as follows. Consider a thermodynamically regular operator A. One wants to associate with every macrostate Φ with respect to A a probability measure P_Φ defined on Borel subsets of Φ such that for average entropies

$$\overline{S}_A(\Phi) = \int_\Phi s_A(\varphi) P_\Phi(d\varphi) \tag{1}$$

and

$$\overline{S}^t_A(\Phi) = \int_\Phi s_A(\varphi(t)) P_\Phi(d\varphi) \tag{2}$$

the law of increase of entropy is valid, i. e.

$$\overline{S}^t_A(\Phi) \geqslant \overline{S}_A(\Phi) \qquad (t \geqslant 0)$$

for every motion of the physical system in question. We note that the definition of average entropy at an instant t for a macrostate Φ admits another reasonable version. Namely,

$$\tilde{S}^t_A(\Phi) = \int_\Phi \overline{S}_A([\varphi(t)]) P_\Phi(d\varphi). \tag{3}$$

Of course, this definition requires some obvious measurability conditions for $\overline{S}_A([\varphi(t)])$ regarded as a function of microstates φ. The corresponding principle of increase of entropy can be written in the form

$$\tilde{S}^t_A(\Phi) \geqslant \overline{S}_A(\Phi) \qquad (t \geqslant 0).$$

The aim of the present note is to prove that, unfortunately, for some simple physical quantities A probability measures P_Φ described above do not exist. This result shows that the theory of macrophysics based on the Jaynes principle cannot be seriously modified without having spoilt the law of increase of entropy.

Consider non-relativistic spin component operators $\sigma_x, \sigma_y, \sigma_z$ for a single fermion with the spin $\frac{1}{2}$ (e. g. electron, proton, neutron) fixed in the configuration space, i. e. whose behaviour can be described by spin variables only. In this case the Hilbert space $\mathfrak{H}_0$ is two-dimensional and the operators σ_x, σ_y and σ_z can be represented by Pauli's matrices

$$\sigma_x = \tfrac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \tfrac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \tfrac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{4}$$

referring to a basis consisting of proper vectors of σ_z (see [1], p. 149).

LEMMA. *Let $\xi \in \mathfrak{H}_0$. If for every $t \geqslant 0$ the equations*

$$(\sigma_z e^{-it\sigma_x}\xi, e^{-it\sigma_x}\xi) = (\sigma_z e^{-it\sigma_y}\xi, e^{-it\sigma_y}\xi) = 0 \tag{5}$$

hold, then $\xi = 0$.

Proof. From (4) we get the well-known relations:

$$\sigma_x\sigma_y = -\sigma_y\sigma_x = \tfrac{1}{2}i\sigma_z, \tag{6}$$

$$\sigma_y\sigma_z = -\sigma_z\sigma_y = \tfrac{1}{2}i\sigma_x, \tag{7}$$

$$\sigma_z\sigma_x = -\sigma_x\sigma_z = \tfrac{1}{2}i\sigma_y, \tag{8}$$

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \tfrac{1}{4}I, \tag{9}$$

where I is the unit operator in H_0. Further, by the last equation, we have

$$e^{-it\sigma_x} = \cos\tfrac{1}{2}t\cdot I - 2i\sin\tfrac{1}{2}t\cdot\sigma_x,$$

$$e^{-it\sigma_y} = \cos\tfrac{1}{2}t\cdot I - 2i\sin\tfrac{1}{2}t\cdot\sigma_y.$$

Hence and from (6), (7) and (8), by a simple computation, we obtain the equations

$$(\sigma_z e^{-it\sigma_x}\xi, e^{-it\sigma_x}\xi) = \cos t\cdot(\sigma_z\xi, \xi) + \sin t\cdot(\sigma_y\xi, \xi),$$

$$(\sigma_z e^{-it\sigma_y}\xi, e^{-it\sigma_y}\xi) = \cos t\cdot(\sigma_z\xi, \xi) - \sin t\cdot(\sigma_x\xi, \xi)$$

which, by virtue of (5), imply

$$(\sigma_x\xi, \xi) = (\sigma_y\xi, \xi) = (\sigma_z\xi, \xi) = 0.$$

Hence, by (6),

$$(\sigma_x\xi, \sigma_y\xi) = (\sigma_y\sigma_x\xi, \xi) = -\tfrac{1}{2}i(\sigma_z\xi, \xi) = 0$$

and, similarly, in view of (7) and (8),

$$(\sigma_y\xi, \sigma_z\xi) = (\sigma_x\xi, \sigma_z\xi) = 0.$$

Thus, the vectors $\sigma_x \xi$, $\sigma_y \xi$ and $\sigma_z \xi$ are mutually orthogonal. Since the space $\mathfrak{H}_0$ is two-dimensional and, by (9),

$$(\sigma_x \xi, \sigma_x \xi) = (\sigma_y \xi, \sigma_y \xi) = (\sigma_z \xi, \sigma_z \xi) = \tfrac{1}{4}(\xi, \xi),$$

we infer that $(\xi, \xi) = 0$, which completes the proof.

Now we shall prove the following statement:

There exists no family P_Φ of probability measures on macrostates Φ with respect to the observable σ_z for a spatially fixed fermion such that at least one of the inequalities

$$\overline{S}^t_{\sigma_z}(\Phi) \geqslant \overline{S}_{\sigma_z}(\Phi) \quad (t \geqslant 0), \tag{10}$$

$$\tilde{S}^t_{\sigma_z}(\Phi) \geqslant \overline{S}_{\sigma_z}(\Phi) \quad (t \geqslant 0) \tag{11}$$

holds for every motion.

Indeed, suppose the contrary. Let P_Φ be a family of probability measures on macrostates Φ such that one of inequalities (10), (11) holds for every motion of the system. Let ψ_+ and ψ_- be proper vectors of σ_z corresponding to proper values $\frac{1}{2}$ and $-\frac{1}{2}$ respectively. Each microstate $\psi \in \mathfrak{H}_0$ can be written in the form $\psi = a_+ \psi_+ + a_- \psi_-$, where a_+ and a_- are complex numbers satisfying the condition $|a_-|^2 + |a_+|^2 = 1$. Hence it follows that

$$m_{\sigma_z}(\psi) = \tfrac{1}{2}|a_+|^2 - \tfrac{1}{2}|a_-|^2,$$
$$s_{\sigma_z}(\psi) = -|a_+|^2 \log|a_+|^2 - |a_-|^2 \log|a_-|^2.$$

Thus the equations $m_{\sigma_z}(\psi) = 0$ and $s_{\sigma_z}(\psi) = \log 2$ are equivalent. Since $\log 2$ is the maximum of the entropy $s_{\sigma_z}(\psi)$ for all microstates $\psi \in \mathfrak{H}_0$, for any macrostate Φ the equation

$$\overline{S}_{\sigma_z}(\Phi) = \int_\Phi s_{\sigma_z}(\psi) P_\Phi(d\psi) = \log 2$$

implies the formula $s_{\sigma_z}(\psi) = \log 2$ P_Φ-almost everywhere. Thus

$$M_{\sigma_z}(\Phi) = 0 \text{ if and only if } S_{\sigma_z}(\Phi) = \log 2. \tag{12}$$

Let Φ_0 be the macrostate with $M_{\sigma_z}(\Phi_0) = 0$. By (12), taking into account hypothesis (10) and (11) and the inequalities $\overline{S}^t_{\sigma_z}(\Phi) \leqslant \log 2$, $\tilde{S}^t_{\sigma_z}(\Phi) \leqslant \log 2$, we conclude that at least one of the equations

$$\overline{S}^t_{\sigma_z}(\Phi_0) = \log 2 \quad (t \geqslant 0), \tag{13}$$

$$\tilde{S}^t_{\sigma_z}(\Phi_0) = \log 2 \quad (t \geqslant 0) \tag{14}$$

holds for every motion of the considered fermion. Hence, by (2) and (3), we obtain, for every instant t, the equation $s_{\sigma_z}(\varphi(t)) = \log 2$ P_Φ-almost everywhere in the case (13) and $\overline{S}_{\sigma_z}([\varphi(t)]) = \log 2$ P_{Φ_0}-almost everywhere in the case (14). Now, by (12), in both cases we get the equation $m_{\sigma_z}(\varphi(t)) = 0$ P_{Φ_0}-almost everywhere. Applying an argument of Fubini's type and taking into account the continuity of $m_{\sigma_z}(\varphi(t))$ with respect to t, we obtain for every motion the equation

$$(15) \qquad m_{\sigma_z}(\varphi(t)) = 0 \quad \text{for} \quad P_{\Phi_0}\text{-almost all } \varphi \in \Phi_0 \text{ and all } t \geqslant 0.$$

Now consider the evolution of the particle in question in an external uniform magnetic field. For uniform fields directed along the x-axis and y-axis the corresponding Hamiltonians H_x and H_y are multiples of σ_x and σ_y respectively. For simplicity of our considerations we may assume that $H_x = \hbar\sigma_x$ and $H_y = \hbar\sigma_y$. Consequently, in the first case the evolution of a microstate φ is given by the equation $\varphi(t) = e^{-it\sigma_x}\varphi$ and in the second case by the equation $\varphi(t) = e^{-it\sigma_y}\varphi$. By formula (15), valid for every motion, there exists a microstate $\varphi_0 \in \Phi_0$ such that

$$m_{\sigma_z}(e^{-it\sigma_x}\varphi_0) = m_{\sigma_z}(e^{-it\sigma_y}\varphi_0) = 0$$

for all $z \geqslant 0$. Since

$$m_{\sigma_z}(e^{-it\sigma_x}\varphi_0) = (\sigma_z e^{-it\sigma_x}\varphi_0, e^{-it\sigma_x}\varphi_0)$$

and

$$m_{\sigma_z}(e^{-it\sigma_y}\varphi_0) = (\sigma_z e^{-it\sigma_y}\varphi_0, e^{-it\sigma_y}\varphi_0),$$

we have, by Lemma, $\varphi_0 = 0$. But this contradicts the equation $(\varphi_0, \varphi_0) = 1$. Our statement is thus proved.

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