Weak Convergence of States in Quantum Statistical Mechanics

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This paper considers the convergence (in the sense defined later on) of the initial state of a quantum system to the microcanonical distribution. The results are related to paper [1] by von Neumann at some points, but the setting of the problem considered by von Neumann differs essentially from that considered in this paper (which contains, in particular, quantum versions of some results of [2, Chapter 2]).

In addition to the definition of the entropy of a quantum system as the information entropy of its density operator [3] (see also [4] and this paper), which has become classical, von Neumann considered another definition of quantum mechanical entropy (due to Wigner, as von Neumann mentions in [1]), which is, in fact, a quantum version of the definition of coarse entropy [7]. Moreover, von Neumann proved that the time-mean of Wigner entropy increases (see [1, 3, 4]). A discussion of this von Neumann’s result and some critical comments on his interpretation can be found in [11] and the references therein. On the other hand, it is well known that von Neumann information entropy, like Gibbs entropy in the classical case [10], is an integral of motion (see, e.g., [9]); thus, it by no means always coincides with the increasing thermodynamic entropy of a nonequilibrium state (we assume that the information entropies of the canonical and the microcanonical state coincide with the thermodynamic entropy of the equilibrium state).

Wigner entropy is defined as the information entropy of some (fictitious) state of the quantum system under consideration in which all observables that are referred to as macroscopic in [1] have the same means as in the real state of the quantum system (a similar definition of entropy was given in the footnote of D.V. Zubarev on pp. 178–179 in book [8]; applications of information entropy in quantum mechanics are discussed in books [5, 6]). Wigner entropy is a special case of $F$-entropy introduced by these authors in [4] ($F$ is the set of observables); the $F$-entropy of a state $\nu$ of a quantum system is defined as the least upper bound of the information entropies of all those states in which observables from the set $F$ have the same means as in the state under consideration. If this upper bound is finite, then it is attained in some state $Q_F(\nu)$, which is similar to the microcanonical state; it is natural to call this state the quasi-microcanonical state generated by the set $F$ and the state $\nu$. If the set $F$ contains only one element, namely, a projector onto the subspace of the Hilbert space of the quantum system under consideration generated by the eigenvectors of the Hamiltonian contained in the interval $[E - \varepsilon, E + \varepsilon]$, then, for any state $\nu$, $Q_F(\nu)$ is the microcanonical state in the traditional sense (corresponding to the given interval).\footnote{In [1], von Neumann uses the term “microcanonical” for the quasi-microcanonical state $Q_F(\nu)$ generated by the set $F$ of all macroscopic observables commuting with the Hamiltonian.}

In this paper, we show that if $\nu(t)$ is a state of the system at an arbitrary moment $t \geq 0$, then, for an appropriate initial state $\nu(0)$, the difference between the states $\nu(t)$ and $Q_F(\nu(t))$ tends to zero with increasing time in the weak topology of the state space determined by the set of observables described in this paper. Since the evolution of a quantum system is determined by equations invariant with respect to reversing time, it follows that this difference tends to zero in the same topology as $t \to -\infty$ too (here and in what follows, all limits are in the sense of Cesàro). In particular, in the same topology, the state $\nu(t)$ (and, therefore, $Q_F(\nu(t))$) tends to the microcanonical state as $t \to \pm\infty$;\footnote{We do not consider the rate of convergence to the limit. Nevertheless, it seems to be likely that, with increasing the set $F$, the rate of convergence of the difference between the states $\nu(t)$ and $Q_F(\nu(t))$ to zero increases as well. Note also that if, for $t_2 \geq t_1 \geq 0$, the symbol $A_1^{t_2}$ denotes the evolution of the operator mapping the state of the system at the moment $t_1$ into the state of the system at the moment $t_2$, then, generally, $A_0^{t_1}(Q_F(\nu(0))) \neq Q_F(\nu(t)) = Q_F(A_0^{t_1}(\nu(0)))$.} this assertion

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can be regarded as a weak version of the ergodic theorem.\textsuperscript{3}

We also consider two interpretations of a quantum system as an infinite-dimensional Hamiltonian system. In one of them, the phase space is the Hilbert space of the quantum system endowed with the symplectic structure generated by its complex structure; in the other, this is the corresponding projective Hilbert space. In both cases, it turns out that both with increasing and decreasing time, the difference between the classical states assigned to the quantum states considered above tends to zero in the weak topology on the set of classical states (i.e., measures on the phase space) determined by certain quadratic forms. Of course, in neither case, the difference between the information entropies of the states to be compared can tend to zero, because the information entropies of both the state $S$ and its classical image are integrals of motion.

1. PRELIMINARIES

We use the terminology of [4]. Below, we recall some definitions from [4]. If $\mu$ and $\nu$ are (countably additive nonnegative) measures on a measurable space $(\Omega, \mathcal{B})$ and $\nu(\Omega) = 1$ (i.e., $\nu$ is a probability measure) and $\nu$ is absolutely continuous with respect to $\mu$, then the information entropy of the measure $\nu$ with respect to $\mu$ is the number $S(\nu, \mu)$ defined by

$$S(\nu, \mu) = -\int_{\Omega} \frac{d\nu}{d\mu} \ln \frac{d\nu}{d\mu} \, d\mu.$$ 

If the measure $\nu$ is concentrated on a countable subset $\mathcal{C}$ of the set $\Omega$ and $\mu$ is a counting measure on $\mathcal{C}$, then the information entropy $S(\nu)$ of $\nu$ is the information entropy of the measure $\nu$ with respect to $\mu$; i.e., $S(\nu) = S(\nu, \mu)$.

A state of a quantum system can be determined by any probability Borel measure $\nu$ on the complex separable Hilbert space of the system\textsuperscript{4} admitting a covariance operator coinciding with the von Neumann density operator.\textsuperscript{5} A bounded quantum observable is identified with a bounded self-adjoint operator on the Hilbert space. Moreover, it is assumed that if $\nu$ is a probability Borel measure determining a state $r$ of the quantum system and $A$ is a bounded quantum observable, then $\int (Ax, x)\nu(dx)$ is the mean value of the results of measurements of the observable $A$ performed on copies of the quantum system, each in the state $r$. Thus,

$$\int (Ax, x)\nu(dx) = \text{tr} AT,$$

where $T$ is the correlation operator of the measure $\nu$, i.e., the von Neumann density operator $(T = \int (x \otimes x)\nu(dx))$. This assumption includes von Neumann’s postulate about a relation of observables and states to experimental results.

The state of a classical Hamiltonian system is identified with a probability Borel measure on its phase space. A bounded classical observable is identified with a measurable bounded function on the phase space of the system. If $\nu$ and $f$ are a state and an observable of a Hamiltonian system, then $\int f(x)\nu(dx)$ is the mean value of the results of measurements of the observable $f$ performed on copies of the Hamiltonian system, each in the state $\nu$.

We denote the set of all states of the classical or quantum system under consideration by $\mathcal{R}$. For each state $r \in \mathcal{R}$, the symbol $S(r)$ denotes its information entropy (which is defined below).

If a state $r$ of a classical system is determined by a measure concentrated on a countable subset of the phase space, then the information entropy of the state $r$ is defined to be the information entropy of this measure.

For a quantum system, among all probability measures on the Hilbert space determining a state $r$ is a measure $\rho_r$ whose support is the set $\{e_n\}$ of normalized eigenvectors of the density operator $T$ corresponding to the state $r$. The information entropy $S(r)$ of this state is, by definition, the information entropy of the measure $\rho_r$; thus,

$$S(r) = -\text{tr} T \ln T = -\sum \rho_r(e_n) \ln \rho_r(e_n).$$

The information entropy of any other measure with countable support determining the same quantum state is at most $S(r)$. If the Hilbert space of the quantum system is finite-dimensional, then information entropy can also be defined for any probability measure $\nu$ absolutely continuous with respect to the measure $\mu$ on the Hilbert space that is determined by inner product in this space as the information entropy with respect to $\mu$. If the measure $\nu$ determines a state of the quantum system, then its information entropy is smaller than that of such a measure. Thus, in studying the entropy properties of such quantum systems, it is unnatural to specify states by measures absolutely continuous with respect to the measure $\mu$, in particular, by Gaussian measures.

\textsuperscript{3} Of course, the difference between the information entropies of the states $\nu(t)$ and $Q_r \nu(t)$ must not tend to zero, because the information entropy of the state $\nu(t)$ does not depend on time, while the information entropy of the state $Q_r \nu(t)$ (it is this entropy that we call the $F$-entropy of the state $\nu(t)$) increases. On the other hand, it is the fact that the state $\nu(t)$ and $Q_r \nu(t)$ are asymptotically (as $t \to \pm \infty$) indistinguishable (in the weak topology) that renders the definition of $F$-entropy suggested in [4] natural.

\textsuperscript{4} This is the phase space of the infinite-dimensional classical Hamiltonian system associated with the quantum system under consideration in the first interpretation.

\textsuperscript{5} There is precisely one Gaussian measure with zero mean among such measures.
2. DEFINITION OF QUASIMICROCANONICAL STATES

For each state \( \nu \) of a quantum system and every set \( F \) of its bounded observables, we use \( R_t(F, \nu) \) to denote the subset of \( \mathcal{H} \) determined by the relation \( \rho \in R_t(F, \nu) \Leftrightarrow \forall f \in F(f, \nu) = (f, \rho) \); the symbol \( R(F, \nu) \) denotes the subset of \( R_t(F, \nu) \) consisting of the eigenvectors determined of density operators whose ranges are subspaces of the linear hull \( H_1 \) of the set of eigenvectors of the Hamiltonian operator corresponding to the eigenvalues contained in the interval \( [E - \varepsilon, E + \varepsilon] \), where \( \varepsilon > 0 \) and \( E > 0 \); in what follows, we assume \( \varepsilon \) and \( E \) to be fixed.

For each subset \( F \) of the set of all bounded observables of a quantum or a classical system, the \( F \)-entropy of a state \( \nu \in \mathcal{H} \) of this system [4] is the number \( S_F(\nu) \) defined by \( S_F(\nu) = \sup \{ S(r): r \in R(F, \nu) \} \). If \( S_F(\nu) < \infty \), then there exists a unique state \( r \in R(F, \nu) \) for which the upper bound is attained; this state is denoted by \( Q_F(\nu) \). Thus, \( S_F(\nu) = S(Q_F(\nu)) \).

**Definition 1.** Suppose that \( S_F(\nu) < \infty \). Then, the quasimicrocanonical state generated by the set \( F \) and the state \( \nu \) is defined as the state \( Q_F(\nu) \in R(F, \nu) \).

**Remark 1.** If \( F \) contains only one element, which is the orthogonal projector \( P_K \) onto some vector subspace \( K \) of the space \( H_1 \), and the state \( \nu \) is determined by a density operator whose image is contained in the image of the projector \( P_K \), then \( Q_F(\nu) = P_K \).

**Remark 2.** Using the technique of rigged Hilbert spaces, we can give a definition of a quasimicrocanonical state not assuming that \( S_F(\nu) < \infty \). However, such a state cannot belong to the initial Hilbert space.

3. CLASSICAL MODELS

By a dequantization we mean a mapping that takes quantum systems to classical systems (we do not formalize this notion here). In this section, we describe two dequantizations. Although they are known fairly well, a number of their properties has not been mentioned explicitly. In particular, like the quantization operation, these dequantizations may not commute with some transformations (as in the quantum case, it is natural to refer to such phenomena as anomalies).

A symplectic locally convex space (LCS) is a pair \((E, I)\), where \( E \) is a real LCS and \( I \) is linear mapping (determining the symplectic structure) from the dual space \( E^* \) of \( E \) endowed with a suitable locally convex topology to \( E \) such that \( I^* = -I \). A Hamiltonian system (with a linear phase space) is a triple \((E, I, \mathcal{H})\), where \((E, I)\) is a symplectic LCS and \( \mathcal{H} \) is a number function on \( E \), which is called the Hamiltonian function. The equation \( f'(t) = I(\mathcal{H}(f(t))) \) with respect to \( f: \mathbb{R} \to E \) is called the Hamilton equation for the Hamiltonian system \((E, I, \mathcal{H})\).

Suppose that \( H \) is the complex Hilbert space of a quantum system, \( \mathcal{H} \) is its Hamiltonian, \( H_R \) is the realification of the Hilbert space \( H \), and a mapping \( I_H: H_R \to H \) is defined by \( h \mapsto ih \), where \( i = \sqrt{-1} \). Then, the pair \((H_R, I_H)\) is a symplectic LCS.

Suppose also that \( b_A(x) = \frac{1}{2} (\mathcal{H}x, x) \) for \( x \in H \). Then, the triple \((H_R, I_H, b_A)\) is a Hamiltonian system, and its Hamilton equation coincides with the Schrödinger equation for the initial quantum system. The probability measure \( \nu \) on \( H \), which determines a state of the quantum system, determines also a state of the infinite-dimensional classical Hamiltonian system \((H_R, I_H, b_A)\), if each quantum observable \( A \) is assigned the classical observable \( b_A \) defined by \( b_A(x) = (Ax, x) \), then, according to the above considerations, the means of the results of measurements of the quantum observable and the corresponding classical observable are the same. This passage from a quantum system to a classical one is one of the dequantization operations mentioned above. To describe the second dequantization, we pass from the Hilbert phase space of the Hamiltonian system obtained as the result of the dequantization described above to the corresponding projective Hilbert space.

We emphasize that the probability distributions of the results of measurements of quantum and classical observables corresponding to each other under both dequantizations may be quite different. Yet another anomaly of these dequantizations is that, at the quantum level, the passage to composite systems is realized by using the tensor multiplication of the corresponding spaces, while at the classical level, it is realized by using Cartesian multiplication. This anomaly means that it is impossible to interpret elements of the phase spaces of the Hamiltonian systems obtained by such dequantizations as hidden parameters determining results of experiments on quantum systems.

4. MAIN RESULTS

In what follows, we assume that the Hamiltonian operator has a purely discrete simple spectrum; \( F, F_1, \) and \( F_2 \) are finite sets if observables; \( \mathcal{E} = \{e_n\} \) is an orthonormal basis of the space \( H_1 \), consisting of eigenvectors of the Hamiltonian \( \mathcal{H} \); and \( \eta_0 \) is a uniform measure on \( \mathcal{H} \). By \( \mathcal{A} \) we denote the subset of \( \mathcal{A} \) defined as follows: \( A \in \mathcal{A} \) if and only if \( A = \sum a_n e_n \), where \( |a_n| = |a_{nk}| \) for all \( n, k \in \mathbb{N} \); by \( \nu_{\mathcal{A}} \) we denote the set of states of the quantum system determined by measures concentrated on the set \( \mathcal{A} \). Let \( \mathcal{P} \) be a set of pairwise orthogonal subspaces of \( H_1 \) such that the linear hull of the union of these subspaces coincides with \( H_1 \); by \( F_1 \) we denote the vector space of finite linear combinations of orthogonal projectors onto subspaces from \( \mathcal{P} \), and \( F \) is the subspace of \( F_1 \) consisting of all operators commuting.
with the Hamiltonian. Let \( \tau \) be the weak topological on the state space of the quantum system determined by elements of \( F_j \) (of course, this topology may be non-Hausdorff), and let \( \tau \) be the topology on the state space of the Hamiltonian system \( (H, L, b, \nu) \) determined by the set of functions \( \{ b \}; A \in F_j \} \) (it is non-Hausdorff).

**Theorem 1.** If a function \( \nu: [0, \infty) \to \mathbb{R} \) describes the evolution of the quantum system with Hamiltonian \( H \), and its initial state \( \nu(0) \in \mathcal{V}_d \), then

\[
\frac{1}{t} \int_0^t \nu(t) \to P_H, \quad \text{as } t \to \pm \infty \text{ in the topology } \tau_q.
\]

The proof of this theorem is similar to that of the main result of \([4]\). Suppose that \( \nu(0) = \sum_n a_n e_n \) where \( |a_n| = \frac{1}{\dim H_1} \) for all \( n \in \mathbb{N} \). Let \( F = \{ P_{T_1}, P_{T_2}, \ldots, P_{T_n} \} \), where the \( T_j \) with \( j = 1, 2, \ldots, n \) are pairwise orthogonal vector subspaces of \( H \) such that the linear hull of their union coincides with \( H \). For each \( k \in \{ 1, 2, \ldots, n \} \), by \( \{ e_j^k \} \) we denote an orthonormal basis in \( T_k \) and assume that \( e_j^k = \sum_{p} c_{jp}^k e_p \). For each \( t \geq 0 \), let \( \nu(t) = \sum_{p} a_{p} e^{i \epsilon_{p} t} e_{p} \) be a vector determining a pure state of the quantum system at the moment \( t \), where \( c_{p} \) are the eigenvalues of the Hamiltonian corresponding to the eigenvectors \( e_{p} \). Then, for all admissible \( k \) and \( j \), we have \( \nu(t), e_j^k = \sum_{p} a_{p} e^{i \epsilon_{p} t} c_{jp}^k \), where \( (\cdot, \cdot) \) denotes inner product in the Hilbert space \( H \) and the bar over the symbol \( c \) denotes complex conjugation. Therefore,

\[
\left\| P_{H_1} \right\|^2 = \frac{1}{\dim H_1} \sum_p \sum_j |c_{jp}^k|^2 + \sum_{j=1}^{n} a_{p} \bar{a}_{p} e^{i \epsilon_{p} t} c_{jp}^k \bar{c}_{jp}^k = \frac{\dim H_k}{\dim H_1} \sum_{j=1}^{n} a_{p} \bar{a}_{p} e^{i \epsilon_{p} t} c_{jp}^k \bar{c}_{jp}^k.
\]

This equality implies the assertion of the theorem.

**Theorem 2.** Under the assumptions of Theorem 1,

\[
\frac{1}{t} \int_0^t (Q_t(\nu(t)) - \nu(t)) \to 0
\]

as \( t \to \pm \infty \) in the topology \( \tau_q \).

This theorem is a strengthening of Theorem 1, and its proof is quite similar to that of Theorem 1.

**Remark 3.** Theorem 1 remains valid without the assumption \( \nu(0) \in \mathcal{V}_d \) provided that the sets \( F \) and \( F_j \) satisfy certain additional conditions; the proof uses considerations similar to those of \([1, 11]\).

Theorem 2 implies the following assertion.

**Theorem 3.** Suppose that the assumptions of Theorem 1 hold, \( \eta(t), \) where \( t \in (0, \infty) \), is a measure on \( H_k \) determining a state \( \nu(t) \), and \( \eta(t) \) is a measure on \( H_k \) determining the state \( Q_t(\nu(t)) \). Then,

\[
\frac{1}{t} \int_0^t (\eta(t) - \eta(t)) dt \to 0
\]

as \( t \to \pm \infty \) in the topology \( \tau_c \).

**Corollary 1.** Under the assumptions of Theorem 2,

\[
\frac{1}{t} \int_0^t \eta(t) \to \eta_0
\]

as \( t \to \pm \infty \) in the topology \( \tau_c \).

Theorem 3 has an analogue for the second dequantization.

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