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О непрерывности энтропии

Показано, что для квантово-механической системы с конечной степенью свободы при учёте неограниченных наблюдаемых получаем физические топологии на системе состояний-наблюдаемых, относительно которой энтропия является непрерывной функцией.

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On the Continuity of the Entropy

In the paper it is shown for a quantum-mechanical system with finite degree of freedom that taking into account also unbounded observables one gets physical topologies on the state-observable system with respect to which the entropy becomes a continuous function.

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1. The Physical Topologies

For infinite dimensional density matrices $\varrho \geq 0$, tr $\varrho = 1$, the entropy $S(\varrho) = -\mathrm{tr}\,\varrho \ln \varrho$ is not always finite /10/. Moreover, $S(\varrho)$ is uncontinuous with respect to the metric $d(\varrho, \mu) = \|\varrho - \mu\|_1$, naturally given on the density matrices by the trace norm $\|\varrho\|_1 = \mathrm{tr}\,|\varrho|$. In this paper we shall show that taking into account also unbounded observables in the case of a quantum mechanical system with finite degree of freedom one will be let to a strong topology on the set of density matrices with respect to which the entropy is continuous.

Let us begin with a general definition of the physical topology. For that we assume that the states ϱ of the physical system are normed positive functionals on the $*$-algebra with the unity I, i.e. $\varrho(A^+A) \geq 0$ for $A \in \mathcal{A}$ and $\varrho(I) = 1$. We call $\mathcal{A}$ the observable algebra of the physical system. By $\mathfrak{Z}$ we denote the set of states and by $\mathfrak{S}$ the complex space of linear functionals on $\mathcal{A}$ generated by $\mathfrak{Z}$. Further we assume that the states separate the observables, i.e. for every $A \in \mathcal{A}$, $A \neq 0$, there exists a $\varrho \in \mathfrak{Z}$ with $\varrho(A) \neq 0$.

$(\mathfrak{S}, \mathcal{A})$ form a dual pair in the sense of the theory of linear spaces with respect to the bilinear form $(\varrho, A) = \varrho(A)$. We denote by $\beta^* = \beta(\mathfrak{S}, \mathcal{A})$ the strong topology in $\mathfrak{S}$ and by

$\beta = \beta(\mathcal{A}, \sigma)$ the strong topology in $\mathcal{A}$ (/8/, V.7).

β^* on σ is defined by the system of all seminorms

$$\beta^* : \qquad q_{\mathfrak{A}}(\varrho) = \sup_{A \in \mathfrak{A}} |\varrho(A)|,$$

where $\mathfrak{A}$ runs over all weakly bounded sets in $\mathcal{A}$. These are exactly the subsets $\mathfrak{A} \subset \mathcal{A}$ for which $q_{\mathfrak{A}}(\varrho)$ is finite for $\varrho \in \sigma$. Quite analogously one gets the seminorms defining the topology β.

We call β and β^* the (uniform) <u>physical topologies</u> of the state-observable system $(\mathcal{Z}, \mathcal{A})$. This notion is justified by the fact that a sequence ϱ_n of states converges to a state ϱ with respect to the physical topology β^* if and only if the expectation values $\varrho_n(A)$ converge to $\varrho(A)$ uniformly on every weakly bounded set $\mathfrak{A}$ of observables, i.e. $\sup_{A \in \mathfrak{A}} |\varrho_n(A) - \varrho(A)| \longrightarrow 0$. Quite analogous is the physical interpretation of the topology β on the observable algebra.

Let us now regard the case that $\mathcal{A} = \mathcal{L}^+(\mathcal{D})$ is the $*$-algebra of all (unbounded) operators A in a Hilbert space $\mathcal{H}$ so that A and its adjoint A^* are defined on the dense domain $\mathcal{D}$ and leave $\mathcal{D}$ invariant, i.e. $A\mathcal{D} \subset \mathcal{D}$, $A^*\mathcal{D} \subset \mathcal{D}$. Involution in $\mathcal{L}^+(\mathcal{D})$ is defined by $A \to A^+ = A^*|_{\mathcal{D}}$, the restriction of A^* to $\mathcal{D}$ /4/. $\langle\, ,\, \rangle$ denotes the scalar product in $\mathcal{H}$.

<u>Definition 1</u>

By $\sigma_1(\mathcal{D})$ we denote the set of all operators $\varrho \in \mathcal{L}^+(\mathcal{D})$ for which $A \varrho B$ is a nuclear operator in $\mathcal{H}$ for all $A, B \in \mathcal{L}^+(\mathcal{D})$. We call the $\varrho \in \sigma_1(\mathcal{D})$ <u>$\mathcal{D}$-nuclear operators</u> and if $\varrho \gg 0$ and $\operatorname{tr} \varrho = 1$, so we call ϱ <u>$\mathcal{D}$-density matrix</u>. The set of all $\mathcal{D}$-density matrices we denote by $\mathcal{Z}(\mathcal{D})$.

$(\sigma_1(\mathcal{D}), \mathcal{L}^+(\mathcal{D}))$ forms a dual pair with respect to the bilinear form $(\varrho, A) = \varrho(A) = \operatorname{tr} \varrho A$, $\varrho \in \sigma_1(\mathcal{D})$, $A \in \mathcal{L}^+(\mathcal{D})$.

If ϱ is a $\mathcal{D}$-density matrix, then $\varrho(A) = \operatorname{tr} \varrho A$ is a normal state on the $*$-algebra $\mathcal{L}^+(\mathcal{D})$. In what follows we restrict ourselves now to the special state-observable

sytem $(\mathcal{Z}(\mathcal{D}), \mathcal{L}^+(\mathcal{D}))$. Let us remark, that the physical topology β^* is automatically defined on $\sigma_1(\mathcal{D}) \supset \mathcal{Z}(\mathcal{D})$. A more general description of the so-called β-topologies on operator systems is given in /7/.

The special case $\mathcal{D} = \mathcal{H}$ is the up to now mostly regarded case in the algebraic approach to statistical physics. Then $\mathcal{L}^+(\mathcal{D}) = \mathcal{B}(\mathcal{H})$, the W^*-algebra of all bounded operators on $\mathcal{H}$ /4/, and $\sigma_1(\mathcal{D}) = \sigma_1$, the ideal of all nuclear operators on $\mathcal{H}$. Now the topology β is the usual uniform topology on $\mathcal{B}(\mathcal{H})$ defined by the operator norm $\| A \|$ and β^* on σ_1 is the topology defined by the trace-norm $\| \varrho \|_1 = \operatorname{tr} |\varrho|$ /9/. These both uniform topologies on the bounded operators and on the density matrices are the most applied topologies on observables and states.

2. The Continuity of the Entropy

In what follows we only regard domains $\mathcal{D} \subset \mathcal{H}$ of the form $\mathcal{D} = \bigcap_{n=0}^{\infty} \mathcal{D}(T^n)$ where $T \geqslant I$ is a selfadjoint operator in $\mathcal{H}$ with nuclear inverse T^{-1}. $\mathcal{D}(T^n)$ is the domain of definition of the operator T^n. $\mathcal{D}$ is then a domain of type I in the sense of /6/. The β^* topology on $\sigma_1(\mathcal{D})$ has some interesting properties.

<u>Theorem 1</u>

i) The topology β^* on $\sigma_1(\mathcal{D})$ is given by the denumerable system of norms

$$\| \varrho \|_k = \| T^k \varrho T^k \|, \qquad k=0,1,2,\dots$$

where $\| T^k \varrho T^k \|$ is the usual operator norm of the bounded operator $T^k \varrho T^k$, $\varrho \in \sigma_1(\mathcal{D})$.

ii) $\sigma_1(\mathcal{D})$ is a Frechet $*$-algebra with respect to the topology β^* and the norms $\| \cdot \|_k$ are multiplicative,

$$\| \mu \cdot \varrho \|_k \le \| \mu \|_k \| \varrho \|_k \qquad \varrho, \mu \in \sigma_1(\mathcal{D}), \; k=0,1,2,\dots$$

and symmetric, $\| \varrho^* \|_k = \| \varrho \|_k$.

The proof of this theorem and some other important properties of $\sigma_1(\mathcal{D})$ is given in the next section. Here we will discuss an interesting application of this theorem

<u>Theorem 2</u>

The entropy $S(\rho) = -\mathrm{tr}\,\rho \log \rho$ is a finite function on the set $\mathfrak{S}_{1+}(\mathcal{D})$ of positive $\mathcal{D}$-nuclear operators, $\rho \in \mathfrak{S}_1(\mathcal{D})$, $\rho \geqslant 0$, and $S(\rho)$ is continuous with respect to the physical topology β^* on $\mathfrak{S}_{1+}(\mathcal{D})$.

Before we prove this theorem we want to give a special, more physical formulation of that theorem. We can say, that for a quantum-mechanical system of finite degree of freedom generated by the Schrödinger operators $Q_n = x_n$, $P_n = \frac{1}{i}\frac{\partial}{\partial x_n}$, $n=1,\dots,3f$, the entropy is finite and continuous with respect to the uniform physical topology on the set $\mathcal{Z}$ of all density matrices ρ which have finite expectation values $\rho(Q_n) = \mathrm{tr}\,\rho\, Q_n$ and $\rho(P_n) = \mathrm{tr}\,\rho\, P_n$ for position and momentum operators. Namely, the natural domain $\mathcal{D}$ of definition for the operators Q_i, P_i is the Schwartz space $\mathcal{S} = \mathcal{S}(R^{3f})$ of rapidly decreasing functions $\phi(x)$ in $3f$ variables. As a dense subspace of $L_2(R^{3f})$ $\mathcal{S}$ is of the form $\mathcal{S} = \bigcap_{n=0}^{\infty} \mathcal{D}(T^n)$ where we can take for T the operator $T = (N+1)^2$, $N = \sum A_n^+ A_n$ the number operator, $A_n^+ = \frac{1}{\sqrt{2}}\left(x_n - \frac{\partial}{\partial x_n}\right)$, $A_n = \frac{1}{\sqrt{2}}\left(x_n + \frac{\partial}{\partial x_n}\right)$ (see /8/,V3). Then $Q_n, P_n \in \mathcal{L}^+(\mathcal{S})$ and the density matrices ρ with finite expectation values for the position and momentum operators Q_n, P_n are exactly the $\mathcal{S}$-density matrices $\rho \in \mathcal{Z}(\mathcal{S})$.

Let us now remark that the applications of Theorem 2 are not restricted to the Schwartz space $\mathcal{S}$. For many quantum mechanical systems (a.e. Harmonic oscillator, electron in central potential /1/) the operators are defined on a domain of type I (nuclear space) and Theorem 2 can be applied.

<u>Proof of Theorem 2:</u> To prove the continuity of the entropy $S(\rho)$ with respect to the physical topology β^* we show $S(\rho) \longrightarrow S(\rho')$ if $\|\rho - \rho'\|_2 \longrightarrow 0$, where $\|\rho\|_2 = \|T^2 \rho\, T^2\|$ is one of the norm of Theorem 1 defining β^*.

Let $\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3 \geqslant \dots$ be the eigenvalues of T and $\rho_1 \geqslant \rho_2 \geqslant \rho_3 \geqslant \dots$ the eigenvalues of $\rho \in \mathfrak{S}_{1+}(\mathcal{D})$ then from $\rho = T^{-2}(T^2\rho)$ we get the estimation (/2/ II, §2.1)

$$\rho_n \leq \lambda_n^{-2} \|T^2\rho\| \leq \lambda_n^{-2}\|\rho\|_2 .$$

$\|T^2\rho\| \leq \|\rho\|_2$ holds as a consequence of $T^2 \geqslant 1$. Let $\rho' \in \mathfrak{S}_{1+}(\mathcal{D})$ be fixed. First we can choose a natural number L so large that for $n > L$ $\lambda_n^{-2}\|\rho\|_2 < \frac{1}{e}$ for all ρ with $\|\rho - \rho'\|_2 \leq 1$. Since $-x\ln x$ is monotonically increasing for $0 < x < \frac{1}{e}$ we get for these ρ the following estimation

$$R_L(\rho) = \sum_{n>L} -\rho_n \ln \rho_n < \sum_{n>L} \frac{\|\rho\|_2}{\lambda_n^2}\left(2\ln\lambda_n - \ln\|\rho\|_2\right).$$

Let $\varepsilon > 0$. Since $\sum_n \frac{1}{\lambda_n} < \infty$, we can yet take L so large that $R_L(\rho) \leq \frac{\varepsilon}{3}$ for all ρ with $\|\rho - \rho'\|_2 \leq 1$.
From this we also see that $S(\rho)$ is finite.

Further we get the following estimation for the entropies

$$|S(\rho) - S(\rho')| \leq \left|\sum_{n=1}^{L}(\rho_n \ln \rho_n - \rho'_n \ln \rho'_n\right| + \tfrac{2}{3}\varepsilon .$$

Since $|\rho_n - \rho'_n| \leq \|\rho - \rho'\|_2$, $n=1,2,3,\dots$ we can now find a $0 < \delta < 1$ so that also the first part on the right-hand side of the estimation is less than $\frac{\varepsilon}{3}$ for $\|\rho - \rho'\|_2 < \delta$. For These ρ we have then $|S(\rho) - S(\rho')| < \varepsilon$. H

3. The Ideal of $\mathcal{D}$-Nuclear Operators

The main aim of this section is to prove Theorem 1. As a preparation of that we derive some important properties of $\mathcal{D}$-nuclear operators.

Let us recall that we regard only domains $\mathcal{D} \subset \mathcal{H}$ of the form described at the beginning of section 2. For any real s $-\infty < s < +\infty$ we define on $\mathcal{D}$ the norm $\|\phi\|_s = \|T^s\phi\|$ and denote by $\mathcal{H}_s$ the completion of $\mathcal{D}$ with respect to $\|\cdot\|_s$. Then $\{\mathcal{H}_s\}$ is a scale of Hilbert spaces with $\mathcal{D} = \mathcal{H}_\infty = \bigcap_{-\infty<s} \mathcal{H}_s$, $\mathcal{H}_0 = \mathcal{H}$.

<u>Lemma 1</u>

i) $\mathcal{D}$ is a nuclear Frechet space with respect to the topology t given by all norms $\|\cdot\|_s$, $-\infty < s < +\infty$.

ii) Any operator $A \in \mathcal{L}^+(\mathcal{D})$ is a continuous mapping of $\mathcal{D}[t]$ into itself and there exists an $r > 0$ depending on A so that $T^{-r}A$, AT^{-r} are bounded operators on $\mathcal{H}$.

<u>Proof:</u> i) $\mathcal{D}[t]$ is the projective limit of the Banach spaces $\mathcal{D}(T^n)$ with the norm $\|\phi\|_n = \|T^n\phi\|$ $n=0,1,2,\dots$

and therefore a Frechet space. Since T^{-1} is a nuclear operator $\mathcal{D}[t]$ is a nuclear space.

ii) Every operator $A \in \mathcal{L}^+(\mathcal{D})$ is a closed operator of $\mathcal{D}$ into $\mathcal{D}$ with respect to the norm $\|.\|_o$. Thus A is also closed as an operator of $\mathcal{D}[t]$ into $\mathcal{D}[t]$. Since $\mathcal{D}[t]$ is a Frechet space, A is continuous.

Especially, we get that $\|A\phi\| \leq C\|\phi\|_r = C\|T^r\phi\|$ for certain $C, r > 0$, $\phi \in \mathcal{D}$. Thus $\|AT^{-r}\phi\| \leq C\|\phi\|$, i.e. AT^{-r} is bounded. From the relation $(A^+T^{-s}) = T^{-s}A$ we get that also $T^{-s}A$ is bounded for a certain s. $\vdash\!\dashv$

Lemma 2

$\mathfrak{S}_1(\mathcal{D})$ is the set of all bounded operators ρ with $\rho\mathcal{H} \subset \mathcal{D}$ and $\rho^*\mathcal{H} \subset \mathcal{D}$.

Proof: For the proof we can restrict ourselves to symmetric $\rho^* = \rho$. Let us suppose that $\rho\mathcal{H} \subset \mathcal{D}$. It follows from the closed graph theorem that ρ is continuous from $\mathcal{H}$ into $\mathcal{D}[t]$. Let $s > 0$ be arbitrary, then $\|\rho\phi\|_{2s} = \|T^{2s}\rho\phi\| \leq c\|\phi\|$ with a certain $c > 0$. Further, from $(T^{2s}\rho)^* = \rho T^{2s}$ we get

$$\|\rho T^{2s}\phi\| \leq c\|\phi\|, \text{ i.e. } \|\rho\phi\| \leq c\|T^{-2s}\phi\| = c\|\phi\|_{-2s}$$

Thus ρ is continuous from $\mathcal{H}_o$ into $\mathcal{H}_{2s}$ and also from $\mathcal{H}_{-2s}$ into $\mathcal{H}_o$. By the interpolation theorem /3/ we get that ρ is also continuous from $\mathcal{H}_{-s}$ into $\mathcal{H}_s$. Thus $\|\rho\phi\|_s \leq c\|\phi\|_{-s}$ i.e. $\|T^s\rho T^s\psi\| \leq c\|\psi\|$ for all $\psi \in \mathcal{D}$. Hence $T^s\rho T^s$ is a bounded operator. Since T^{-1} is nuclear, from $T^s\rho T^s = T^{-1}(T^{s+1}\rho T^{s+1})T^{-1}$ we get that $T^s\rho T^s$ is nuclear for all s. Now let $A, B \in \mathcal{L}^+(\mathcal{D})$ then

$$A\rho B = (AT^{-r})(T^r\rho T^r)(T^{-r}B).$$

Since $T^r\rho T^r$ is nuclear and AT^{-r}, $T^{-r}B$ are bounded for sufficiently large r (Lemma 1), $A\rho B$ is nuclear. Thus $\rho \in \mathfrak{S}_1(\mathcal{D})$. The opposite direction of the Lemma was proved in /5/.

Proof of Theorem 1: First we prove that $\mathfrak{S}_1(\mathcal{D})$ is a Frechet space (complete) with respect to the topology $\mathfrak{f}$ defined by the seminorms $\|\rho\|_k = \|T^k\rho T^k\|$, $k=0,1,2,3,\ldots$. Let ρ_α be a

Cauchy set in $\mathfrak{S}_1(\mathcal{D})$ with respect to $\mathfrak{f}$. Without lost of the generality we may suppose $\rho_\alpha = \rho_\alpha^*$. Then, for $\phi \in \mathcal{H}$ $\rho_\alpha\phi$ is a Cauchy set in $\mathcal{D}[t]$ and therefore $\rho_\alpha\phi$ converges in $\mathcal{D}[t]$. Hence, $\rho\phi = \lim \rho_\alpha\phi$ defines a symmetric operator on $\mathcal{H}$ mapping $\mathcal{H}$ into $\mathcal{D}$. By Lemma 2 we get $\rho \in \mathfrak{S}_1(\mathcal{D})$.

We have yet to prove $\rho_\alpha \longrightarrow \rho$ with respect to the topology $\mathfrak{f}$. Let $\phi \in \mathcal{H}$, $\|\phi\| \leq 1$, an arbitrary vector of the unit sphere in $\mathcal{H}$. Then

$$\|T^k(\rho - \rho_\alpha)T^k\phi\| \leq \|T^k(\rho_\beta - \rho_\alpha)T^k\| + \|T^k(\rho - \rho_\beta)T^k\phi\|.$$

Now the first part on the right-hand side is less than $\varepsilon/2$ for $\beta > \alpha > \alpha_o(\varepsilon)$ and the second part becomes also less than $\varepsilon/2$ for large β. Thus $\|T^k(\rho - \rho_\alpha)T^k\phi\| < \varepsilon$ for $\alpha > \alpha_o$, $\|\phi\| \leq 1$, i.e. $\|\rho - \rho_\alpha\|_k < \varepsilon$ for $\alpha > \alpha_o$, i.e. $\rho_\alpha \longrightarrow \rho$ with respect to $\mathfrak{f}$. Since the topology $\mathfrak{f}$ is given by a countable system of norms, $\mathfrak{S}_1(\mathcal{D})[\mathfrak{f}]$ is a Frechet space.

Now we have yet to show $\beta^* = \mathfrak{f}$. Then the theorem is completely proved.

Let $A \in \mathcal{L}^+(\mathcal{D})$, then $F_A(\rho) = \operatorname{tr}\rho A$ is a continuous linear functional on $\mathfrak{S}_1(\mathcal{D})[\mathfrak{f}]$. In fact, we have for sufficiently large k

$$|F_A(\rho)| = |\operatorname{tr}(T^k\rho T^k)(T^{-k}A)T^{-k}| \leq \|T^{-k}A\| \, \|T^{-k}\|_{tr} \, \|\rho\|_k ,$$

where $\|T^{-k}\|_{tr}$ is the trace norm of T^{-k}. Since $\mathfrak{S}_1(\mathcal{D})[\mathfrak{f}]$ is a Frechet space, any weakly bounded set $\mathfrak{A} \in \mathcal{L}^+(\mathcal{D})$ is equicontinuous with respect to the dual pair $(\mathfrak{S}_1(\mathcal{D}), \mathcal{L}^+(\mathcal{D}))$ and therefore $q_{\mathfrak{A}}(\rho) = \sup_{A \in \mathfrak{A}} |\rho(A)|$ is continuous with respect to $\mathfrak{f}$, i.e. β^* is weaker than $\mathfrak{f}$. To do this, we show that for a certain bounded set $\mathfrak{A}$ the seminorm $q_{\mathfrak{A}}(\rho)$ is equal to $\|T^k\rho T^k\|$. In fact, if we denote by $P_{\phi,\psi}$ the operator $P_{\phi,\psi}\Omega = \langle\phi,\Omega\rangle\psi$ and by $\mathfrak{A}$ the set of all operators $A = T^kP_{\psi,\phi}T^k$, $\phi, \psi \in \mathcal{K} = \{\phi \in \mathcal{D}, \|\phi\| \leq 1\}$ then we get

$$\begin{aligned} q_{\mathfrak{A}}(\rho) &= \sup_{\phi,\psi \in K} |\operatorname{tr}\rho T^kP_{\phi,\psi}T^k| = \sup_{\phi,\psi \in K} |\operatorname{tr}(T^k\rho T^k)P_{\phi,\psi}| \\ &= \sup_{\phi,\psi \in K} |\langle\phi, T^k\rho T^k\psi\rangle| = \|T^k\rho T^k\| = \|\rho\|_k. \end{aligned}$$

Now the theorem is completely proved.

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