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Convergence of the Quantum Boltzmann Map

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Abstract. We consider a non-linear map on the space of density matrices, which we call the Boltzmann map τ. It is the composition of a doubly stochastic map T on the space of n-body states, and the conditional expectation onto the one-body space. When T is ergodic, then the iterates of τ take any initial state to the uniform distribution. If the energy levels are equally spaced, and T conserves energy and is ergodic on each energy shell, then iterates of τ take any initial state of finite energy to a canonical distribution.

1. Introduction

(1.1) This paper is the quantum version of [1]. Let $\mathscr{H}$ be a Hilbert space with $\dim \mathscr{H} = N \leqq \infty$. A (normal) state ϱ is then a positive operator with unit trace. We denote the set of trace-class operators by $\mathscr{B}(\mathscr{H})_1$ and the normal[1] states by $\sigma(\mathscr{H})$. A stochastic map is a linear map T from $\mathscr{B}(\mathscr{H})$ to $\mathscr{B}(\mathscr{H})$ mapping $\sigma(\mathscr{H})$ to itself and preserving the trace: $\mathrm{Tr}(T\varrho) = \mathrm{Tr}\,\varrho$, $\varrho \in \mathscr{B}(\mathscr{H})_1$. A doubly stochastic map is a stochastic map T such that $T1_N = 1_N$, where 1_N is the identity on $\mathscr{H}$ [4].

A unitary or anti-unitary conjugation $\varrho \mapsto T\varrho = U\varrho U^{-1}$ is doubly stochastic, as is any convex combination of such maps.

(1.2) Let $\mathscr{K}$ be a Hilbert space, the one-particle space, and

(1.3) let $\mathscr{H} = \mathscr{K} \otimes \ldots \otimes \mathscr{K}$ (n factors) be the n-particle space.

We shall be interested in a doubly stochastic map $T: \mathscr{B}(\mathscr{H}) \to \mathscr{B}(\mathscr{H})$ that preserves the symmetry under permutations of the factors $\mathscr{K}$. To such a T we define the corresponding *Boltzmann map* τ to be the composition of maps:

(1.4) $$\varrho \mapsto \varrho \otimes \ldots \otimes \varrho \mapsto T(\varrho \otimes \ldots \otimes \varrho) \mapsto \mathrm{Tr}_{2\ldots n} T(\varrho \otimes \ldots \otimes \varrho) = \tau(\varrho).$$

Here, $\mathrm{Tr}_{2\ldots n}$ means the trace over the second, third, ..., n^{th} factors $\mathscr{K}$. Obviously, (1.4) defines a non-linear map $\tau : \sigma(\mathscr{K}) \to \sigma(\mathscr{K})$.

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1 Normal in the sense [2] of linear functionals on the W^*-algebra $\mathscr{B}(\mathscr{H})$, not in the sense of [3]

(1.5) Alicki and Messer [5] have suggested a similar map for continuous time, where the analogue of T is completely positive. Our choice is motivated by the following result:

(1.6) **Theorem.** *Let $\varrho \in \sigma(\mathscr{H})$ have finite entropy: $S(\varrho) = -\mathrm{Tr}\,\varrho \log \varrho < \infty$. Then*

$$S(\tau\varrho) \geqq S(\varrho). \tag{1.7}$$

Proof.

$$nS(\tau\varrho) = \sum_j S(\mathrm{Tr}_{1\ldots\hat{j}\ldots n} T(\varrho \otimes \ldots \otimes \varrho))$$

by symmetry, where $\hat{j}$ means j is omitted

$$\geqq S(T(\varrho \otimes \ldots \otimes \varrho))$$

by [6, Proposition 2.5.6]

$$\geqq S(\varrho \otimes \ldots \otimes \varrho)$$

by [4, Lemma 2-5, Corollary]

$$= nS(\varrho). \quad \square$$

(1.8) To show that $\tau^m \varrho$ converges to the uniform distribution if $N < \infty$, we must postulate some ergodic properties. Now, T is a linear operator on the Hilbert space of Hilbert-Schmidt operators on $\mathscr{H}$. Let us say T is *ergodic* if 1_N is the only fixed-point of T in $\mathscr{B}(\mathscr{H})$. Let us say that T has a spectral gap Δ, $0 < \Delta < 1$ if it is ergodic and the spectrum of T^*T is contained in $[0, 1-\Delta] \cup \{1\}$.

2. Entropy Gain Under a Doubly Stochastic Map

We give a sharp estimate which will imply the convergence of $\tau^m \varrho$ when T is ergodic.

(2.1) **Lemma.** *Let $\mathscr{H}$ be a Hilbert space with $\dim \mathscr{H} = N < \infty$, and denote by $\mathscr{B}(\mathscr{H})_2$ the Hilbert space of operators on $\mathscr{H}$ with scalar product $\langle A, B \rangle = \mathrm{Tr}(A^*B)$. Let $T: \mathscr{B}(\mathscr{H})_2 \to \mathscr{B}(\mathscr{H})_2$ be a doubly stochastic map, ergodic with spectral gap Δ. Let $A \in \sigma(\mathscr{H})$ and let $B = TA$. Then*

$$S(B) - S(A) \geqq \frac{\Delta}{2} \|A - N^{-1} 1_N\|_2^2. \tag{2.2}$$

Proof. Let $\{\varphi_i, a_i\}$ and $\{\psi_i, b_j\}$ be the orthonormal eigenvectors and eigenvalues of A and B, respectively. Then $0 \leqq a_i, b_j \leqq 1$. Let $f(x) = x \log x$, $c_{ij} = \langle \varphi_i, \psi_j \rangle_{\mathscr{H}}$. Then, as in [6, 2.5.2] we have

$$\begin{aligned} &\langle \varphi_i, \{f(A) - f(B) - (A-B)f'(B) - \tfrac{1}{2}(A-B)^2\}\varphi_i \rangle_{\mathscr{H}} \\ &= \sum_{i,j} |c_{ij}|^2 \{f(a_i) - f(b_j) - (a_i - b_j)f'(b_j) - \tfrac{1}{2}(a_i - b_j)^2\}. \end{aligned}$$

Now, in the range of a_i, b_j we have

$$f(x) - f(y) - (x-y)f'(y) = \tfrac{1}{2}(x-y)^2 f''(\xi),$$

where $0 \leqq \xi \leqq 1$ and $f''(\xi) = \frac{1}{\xi} \geqq 1$. Thus

$$f(a_i) - f(b_j) - (a_i - b_j) f'(b_j) - \tfrac{1}{2}(a_i - b_j)^2 \geqq 0.$$

Summing over i gives the following sharper form of [6, Proposition 2.5.3]:

$$\mathrm{Tr}\{A \log A - B \log B - (A-B)(\log B + 1) - \tfrac{1}{2}(A-B)^2\} \geqq 0,$$

i.e.

$$\text{(2.3)} \qquad \mathrm{Tr}\{A(\log A - \log B)\} \geqq \tfrac{1}{2}\mathrm{Tr}(A-B)^2.$$

By [4, Theorem 2-2], there exist unitaries U_α and non-negative numbers w_α with $\sum_\alpha w_\alpha = 1$ and $B = TA = \sum_\alpha w_\alpha A_\alpha$, $A_\alpha = U_\alpha A U_\alpha^{-1}$. Then for each α, $\mathrm{Tr} A_\alpha(\log A_\alpha - \log B) \geqq \frac{1}{2}\mathrm{Tr}(A_\alpha - B)^2$, so multiplying by w_α and summing, and noting that $\mathrm{Tr} A_\alpha \log A_\alpha = \mathrm{Tr} A \log A$ and $\sum_\alpha w_\alpha = 1$:

$$\mathrm{Tr}(A \log A - B \log B) \geqq \tfrac{1}{2}\sum_\alpha w_\alpha \mathrm{Tr}(A_\alpha - B)^2$$

i.e.

$$\begin{aligned} S(B) - S(A) &\geqq \tfrac{1}{2}\sum_\alpha w_\alpha\{\langle A_\alpha, A_\alpha\rangle - \langle A_\alpha, B\rangle - \langle B, A_\alpha\rangle + \langle B, B\rangle\} \\ &= \tfrac{1}{2}\{\langle A, A\rangle - \langle B, B\rangle\} = \tfrac{1}{2}\{\langle A, A\rangle - \langle A, T^*TA\rangle\}. \end{aligned}$$

Now 1_N is a simple eigenvalue of T^*T, and we may write the orthogonal decomposition $A = \frac{1}{N} 1_N \oplus \left(A - \frac{1}{N} 1_N\right)$. Hence

$$\begin{aligned} S(B) - S(A) &\geqq \tfrac{1}{2}\langle A, (1_N - T^*T)A\rangle \\ &= 2^{-1}\langle A - N^{-1}1_N, (1_N - T^*T)(A - N^{-1}1_N)\rangle \\ &\geqq \frac{\Delta}{2}\left\| A - \frac{1}{N} 1_N \right\|_2^2 \end{aligned}$$

since Δ is the smallest eigenvalue of $1 - T^*T$ apart from 0. □

(2.4) **Corollary.** *Let* $A = \varrho_{12}$ *on* $H_1 \otimes H_2$, *and* $B = \varrho_1 \otimes \varrho_2$, *where* $\varrho_1 = \mathrm{Tr}_2 \varrho_{12}$, *etc. Then* $-\mathrm{Tr} A \log A = S_{12}$, $-\mathrm{Tr} A \log B = S_1 + S_2$ *in the sub-additive entropy inequality* [4, *Proposition 2.5.6*] *gives a quantitative estimate*

$$S_1 + S_2 - S_{12} \geqq \tfrac{1}{2}\|\varrho_{12} - \varrho_1 \otimes \varrho_2\|_2^2.$$

(2.5) **Theorem.** *The microcanonical limit. Let* $\dim K = k < \infty$, *and* T *a symmetry-preserving ergodic doubly stochastic map on* $K \otimes \ldots \otimes K$. *Then for any* $\varrho \in \sigma(K)$, $\tau^m \varrho \to k^{-1} 1_K$ *as* $m \to \infty$.

Proof. The entropy $S(\tau^m \varrho)$ is increasing and bounded above, and so converges. Hence the increment $S(\tau^{m+1}\varrho) - S(\tau^m \varrho)$ converges to 0. In finite dimensions $\Delta > 0$, so (2.2) implies that

$$\left\| \tau^m \varrho \otimes \ldots \otimes \tau^m \varrho - \bigotimes_1^n k^{-1} 1_{\mathscr{K}} \right\|_2 \to 0,$$

and so $\tau^m \varrho \to k^{-1} 1_{\mathscr{K}}$, as $m \to \infty$.

3. Energy Conservation

(3.0) In order to discuss the canonical Gibbs state, we must introduce an energy operator H on $\mathscr{K}$ ($\mathscr{K}$ can be ∞-dimensional in what follows). Thus let H have spectrum $0, 1, 2, \ldots$ and suppose that the multiplicity $m(j)$ of the energy-level j is finite and that for some $\kappa > 0$ and integer r,

$$m(j) \leq \kappa j^r, \quad j = 1, 2, \ldots . \tag{3.1}$$

These conditions ensure that $e^{-\beta H}$, $\beta > 0$, is of trace class. The equal spacing of the energy levels limits the theory to a rather special class; but it does allow thorough mixing to take place by scattering that conserves energy. This would not be possible if, for example, the energy levels were not commensurate.

(3.2) Let $H = \sum_1^\infty j(E_j - E_{j-1})$ be the spectral resolution of H, and let $H_M = \sum_1^M j(E_j - E_{j-1})$. Then $H_M \in \mathscr{B}(\mathscr{K})$. We say that a state ϱ on $\mathscr{B}(\mathscr{K})$, not necessarily normal, has finite mean energy $\mathscr{E}$ if

$$\lim_{M \to \infty} \mathrm{Tr}(\varrho H_M) = \mathscr{E} < \infty .$$

(3.3) We again consider a doubly stochastic map T on $\bigotimes^n \mathscr{K} = \mathscr{H}$. We require T to mix up states in $\mathscr{H}$ of the same energy, but not to mix up states of differing energy. Thus let $\mathfrak{h}$ be the generator of $\bigotimes^n e^{iHt}$; then $\mathfrak{h}$ is an operator on $\mathscr{H}$ with spectrum $0, 1, 2, \ldots$ and having finite multiplicity. Let $\mathscr{H}_\eta$, $\eta = 0, 1, \ldots$ be the subspace with energy η. $\mathscr{B}(\mathscr{H}_\eta)$, called the "energy-shell η" is a finite-dimensional space that can be identified with the subspace of $\mathscr{B}(\mathscr{H})_2$ consisting of operators mapping $\mathscr{H}_\eta$ to $\mathscr{H}_\eta$ and being zero on $\mathscr{H}_\eta^\perp$. In the scalar product of (2.1), we may write $\mathscr{B}(\mathscr{H})_2$ as a direct sum of orthogonal subspaces

$$\mathscr{B}(\mathscr{H})_2 = \bigotimes_{\eta=0}^{\infty} \mathscr{B}(\mathscr{H}_\eta) \bigotimes \mathscr{L} ,$$

where $\mathscr{L}$ is orthogonal to all energy shells. We consider doubly stochastic maps T that mix up each energy shell $\mathscr{B}(\mathscr{H}_\eta)$:

(3.4) T maps $\mathscr{B}(\mathscr{H}_\eta)$ to itself, $\eta = 0, 1, 2, \ldots$ and maps $\mathscr{L}$ to itself. Restricted to $\mathscr{B}(\mathscr{H}_\eta)$, T is ergodic. T commutes with permutations of the n factors $\mathscr{B}(\mathscr{K})$.

This class of doubly stochastic maps is the quantum analogue of the classical version [1]. Our assumption (3.4) leads to the conservation of mean energy under τ (but not the mean of functions of energy, such as its variance):

(3.5) **Theorem.** *Let T map each $\mathscr{B}(\mathscr{H}_\eta)$ and $\mathscr{L}$ into itself, and commute with permutations. Then the mean energy is invariant under τ.*

Proof. Let $\varrho \in \mathscr{B}(\mathscr{K})_1$ be such that

$$\mathrm{Tr}(\varrho H) = \lim_{M \to \infty} \mathrm{Tr}(\varrho H_M) = \mathscr{E} < \infty .$$

We note that

$$\mathfrak{h}_M = H_M \otimes 1 \ldots \otimes 1 + \ldots + 1 \otimes \ldots \otimes 1 \otimes H_M .$$

Then by the symmetry of T

$$\mathrm{Tr}(H_M \tau \varrho) = n^{-1}\,\mathrm{Tr}_{1\ldots n}\{\mathfrak{h}_M T(\varrho \otimes \ldots \otimes \varrho)\}.$$

This is a finite-dimensional trace and it can be evaluated in any basis, e.g. in a basis of eigenvectors of $\mathfrak{h}_M$. Then it involves only the block diagonal terms of $\varrho \otimes \ldots \otimes \varrho$, which are in $\mathscr{B}(\mathscr{H}_\eta)$, $\eta = 0, \ldots, nM$. On each of these subspaces, $\mathfrak{h}_M$ is $\eta \cdot 1_{\mathscr{H}_\eta}$, and so commutes with T. Hence

$$\mathrm{Tr}(H_M \tau \varrho) = n^{-1}\,\mathrm{Tr}_{1\ldots n}(T(\mathfrak{h}_M \varrho \otimes \ldots \otimes \varrho)) = n^{-1}\,\mathrm{Tr}_{1\ldots n}(\mathfrak{h}_M \varrho \otimes \ldots \otimes \varrho)$$

as T is trace-preserving

$$= \mathrm{Tr}(H_M \varrho).$$

Hence $\lim\limits_{M\to\infty} \mathrm{Tr}(H_M \tau \varrho) = \mathscr{E}$, so $\tau\varrho$ has finite mean energy, $\mathscr{E}$ the same value as ϱ.

(3.6) *Remark.* It has been pointed out by the referee that it is not enough to suppose that T commutes with the time-evolution $A \mapsto e^{i\mathfrak{h}t} A e^{-i\mathfrak{h}t}$ of density matrices $A \in \mathscr{B}(\mathscr{H})_1$: the mean energy fails to be conserved in general unless T maps $\mathscr{B}(\mathscr{H}_\eta)$ and $\mathscr{L}$ to themselves. As a counterexample in two dimensions, let $\mathfrak{h} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ and $T\begin{pmatrix} a & b \\ b^* & c \end{pmatrix} = \begin{pmatrix} c & 0 \\ 0 & a \end{pmatrix}$. Then T commutes with $[\,\cdot\,, \mathfrak{h}]$, but does not leave the diagonal blocks invariant. Average energy is not invariant under T. Physically, such transformations T are "too stochastic" and do not lead to the canonical ensemble.

4. Weak * Convergence

(4.1) The set of all states of $\mathscr{B}(\mathscr{H})$, not necessarily normal ones, is w^*-compact. The sequence $\{\tau^m \varrho\}_{m=0,1,\ldots}$ therefore has a w^*-convergent subnet $\{\varrho_\alpha\}_{\alpha \in I}$. If ϱ has mean energy $\mathscr{E}$, then by (3.5)

(4.2) $$\mathrm{Tr}(\varrho_\alpha H) = \mathscr{E} \quad \text{for} \quad \alpha \in I.$$

(4.3) The entropy of a state $\varrho \in \mathscr{B}(\mathscr{H})_1$ of finite mean energy is finite and $\leqq$ the entropy of the Gibbs state of the same energy. Since the entropy is non-decreasing under τ, $S(\tau^m \varrho)$ converges as $m \to \infty$, and $S(\varrho_\alpha)$ converges to the same limit as $\alpha \to \infty$.

(4.4) **Lemma.** *Let* $\varrho_\infty = w^* \lim\limits_{\alpha\to\infty} \varrho_\alpha$. *Let* $P_j = \varrho_\infty(E_j)$, $j = 0, 1, 2, \ldots$. *Then* $\lim\limits_{j\to\infty} P_j = 1$.

(4.5) *Remark.* This is tantamount to showing that ϱ_∞ is normal.

(4.6) *Proof.* Let $p_j = P_j - P_{j-1}$, $j = 0, 1, 2, \ldots$ and $p_j^\alpha = \mathrm{Tr}\,\varrho_\alpha(E_j - E_{j-1})$. Then $\mathscr{E} = \mathrm{Tr}(\varrho_\alpha H) = \sum\limits_j j p_j^\alpha$, and $p_j = \lim\limits_\alpha p_j^\alpha$. Hence p_j obeys the conditions of [1, (3.15)], and so $\sum\limits_0^\infty p_j = \lim\limits_{j\to\infty} P_j = 1$.

(4.7) It does not seem easy to prove that $\sum j p_j = \mathscr{E}$ unless, of course, $k = \dim \mathscr{H} < \infty$. This might indicate that, for certain initial states, energy can escape up the energy ladder, say, by "heat solitons". But since for any M, $\sum\limits_1^M j p_j^\alpha \leqq \mathscr{E}$, we have $\sum\limits_1^M j p_j \leqq \mathscr{E}$. Hence $\lim\limits_{M\to\infty} \varrho_\infty(H_M) = \sum\limits^\infty j p_j \leqq \mathscr{E}$ and the limit state ϱ_∞ has finite mean energy $\leqq \mathscr{E}$.

(4.8) We now give an estimate for the entropy in the tail of a state.

(4.9) **Lemma.** *Let H be as in* (3.1), *and ϱ be a positive operator of trace class such that* $\operatorname{Tr}\varrho = q$ *and* $\operatorname{Tr}(\varrho H) \leqq \mathscr{E}$. *Then* $-\operatorname{Tr}(\varrho \log \varrho) = O(q \log q)$ *as* $q \to 0$.

(4.10) *Proof.* The largest value of $-\operatorname{Tr}\varrho \log \varrho$, subject to the conditions $\operatorname{Tr}(\varrho H) \leqq \mathscr{E}$, $\operatorname{Tr}\varrho = q$ is achieved at the Gibbs-like operator ϱ, diagonal in a basis provided by the eigenvectors of H. Then the problem reduces to the classical case: maximize

$$s = -\sum_0 m(j) p_j \log p_j$$

among sequences of non-negative numbers $\{p_j\}$ obeying the constraints

(4.11) $$\sum_0 m(j) p_j = q\,, \qquad \sum_1 m(j) j p_j \leqq \mathscr{E}\,.$$

When the multiplicity $m(j)$ is 1 for all j, then Lemma 3.19 of [1] shows that

$$s \leqq -2q \log q + q(1 + \log \mathscr{E}) = O(q \log q)\,.$$

The same method also works when $m(j) \leqq \kappa$. So we have proved the lemma when the index r of (3.1) is zero. We proceed by induction on r. Suppose the lemma is true for all sequences $\{p_j\}$ obeying (3.3) with $m(j) \leqq \kappa j^{r-1}$, $j = 1, 2, \ldots$. Now let $\{p_j\}$ satisfy (4.11) with $m(j) \leqq \kappa j^r$. Write $\{p_j\}$ together with repetitions for multiplicity as the union of sequences $\{p_j^{(\alpha)}\}$, $\alpha = 1, 2, \ldots$ defined by

(4.12) $$p_j^{(\alpha)} = \begin{cases} p_j & \text{if } j \geqq \alpha\,, \\ 0 & \text{otherwise}\,. \end{cases}$$

In the sequence $\{p_j^{(\alpha)}\}_{j=0,1,\ldots}$ we repeat $p_j^{(\alpha)}$ with multiplicity $m(\alpha, j)$ which might be 0 or as large as $m(j)/j \leqq \kappa j^{r-1}$. It is possible to do this so that $m(j) = \sum_\alpha m(\alpha, j)$. Define

$$q^{(\alpha)} = \sum_j m(\alpha, j) p_j^{(\alpha)}\,,$$
$$\mathscr{E}^{(\alpha)} = \sum_j m(\alpha, j) j p_j^{(\alpha)} \leqq \mathscr{E}\,,$$
$$s^{(\alpha)} = -\sum_j m(\alpha, j) p_j^{(\alpha)} \log p_j^{(\alpha)}\,.$$

Then $\sum_\alpha q^{(\alpha)} = q$, $\sum_\alpha \mathscr{E}^{(\alpha)} \leqq \mathscr{E}$, $\sum_\alpha s^{(\alpha)} = s$.

Now, the induction hypothesis implies that $s^{(\alpha)} = O(-q^{(\alpha)} \log q^{(\alpha)})$ uniformly in α. Also, the condition (4.12) implies $\sum \alpha q^{(\alpha)} \leqq \mathscr{E}$:

$$\begin{aligned} \sum \alpha q^{(\alpha)} &= \sum_\alpha \sum_i \alpha m(\alpha, j) p_j^{(\alpha)} \leqq \sum_\alpha \sum_j j m(\alpha, j) p_j^{(\alpha)} \\ &\leqq \sum_j j \sum_\alpha m(\alpha, j) p_j^{(\alpha)} \leqq \sum_j j m(j) p_j = \mathscr{E}\,. \end{aligned}$$

Thus $\{q^{(\alpha)}\}$ itself obeys the conditions of [1, Lemma 3.19], namely $\sum_\alpha q^{(\alpha)} = q$, $\sum \alpha q^{(\alpha)} \leqq \mathscr{E}$. So by [1, (3.19)]:

$$-\operatorname{Tr}\varrho \log \varrho \leqq s = 0\Big(\sum_\alpha -q^{(\alpha)} \log q^{(\alpha)}\Big) = O(-q \log q)\,. \quad \square$$

The main point is that $s \to 0$ as $q \to 0$. This result gives an extension of the classical theory [1] to the case with multiplicity $m(j)$ as in (3.1).

5. Convergence to a Gibbs State

(5.1) Suppose now that T maps $\mathscr{L}$ to itself and each $\mathscr{B}(\mathscr{H}_\eta)$ to itself, and is ergodic on each $\mathscr{B}(\mathscr{H}_\eta)$. Let $\sigma_m = \tau^m \varrho \otimes \ldots \otimes \tau^m \varrho$ and let $\sigma_m(\eta)$ be the diagonal block matrix obtained from σ_m by restricting to $\mathscr{H}_\eta$. Then, as in Theorem (2.5), we see that the component of $\sigma_m(\eta)$ orthogonal [in the sense of $\mathscr{B}(\mathscr{H})_2$] to multiples of the identity $1_{\mathscr{H}_\eta}$, converges to 0 as $m \to \infty$. In particular, the off-diagonal elements converge to 0. This does not (yet) show that $\sigma_m(\eta)$ converges, as we have not controlled the trace. But along the convergent subnet ϱ_α we also get convergence of σ_α and of $\sigma_\alpha(\eta)$: this must converge to a multiple of $1_{\mathscr{H}_\eta}$. To see clearly why this implies that ϱ_∞ is diagonal in the energy basis, first take $n=2$. Write, in Dirac notation

$$\varrho = \sum \varrho_{ij}^{\mu\nu} |\mu i\rangle \langle \nu j|,$$

where i,j are energy labels and $1 \leqq \mu \leqq m(i)$, $1 \leqq \nu \leqq m(j)$; μ, ν label the multiple states of energy i,j, respectively. Then $\sigma = \varrho \otimes \varrho$ has the off-diagonal terms

$$\varrho_{ij}^{\mu\nu} \varrho_{i'j'}^{\mu'\nu'} |\mu i\rangle |\mu' i'\rangle \langle \nu j| \langle \nu' j'|,$$

including the case $i \neq j$ or $\mu \neq \nu$ where $i'=j$, $i=j'$, $\mu'=\nu$, $\mu=\nu'$. Thus the coefficient $\varrho_{ij}^{\mu\nu} \varrho_{ji}^{\nu\mu} = |\varrho_{ij}^{\mu\nu}|^2$ converges to 0 as $m \to \infty$. This is the general off-diagonal element of ϱ. Thus ϱ_∞ is diagonal in the energy basis.

If $n > 2$ we note at least one diagonal element $\varrho_{kk}^{\mu\mu}$ does not converge to zero, by (4.4). Then if $(n-2)k + i + j = \eta$, the off-diagonal element of $\sigma(\eta)$,

$$\varrho_{kk}^{\mu\mu} \ldots \varrho_{kk}^{\mu\mu} \varrho_{ij}^{\lambda\nu} \varrho_{ji}^{\nu\lambda} = |\varrho_{kk}^{\mu\mu}|^{n-2} |\varrho_{ij}^{\lambda\nu}|^2,$$

converges to zero for any i, $\lambda \neq j$, ν; then $\varrho_{ij}^{\lambda\nu} \to 0$. Thus ϱ_∞ is diagonal in the energy basis. The argument now reduces to the classical case [1]: in order for $\sigma_\infty = \varrho_\infty \otimes \ldots \otimes \varrho_\infty$ to be a multiple of the identity on each H_η, ϱ_∞ being diagonal, we obtain the result: ϱ_∞ is a Gibbs state, ϱ_β. From (4.7), its energy is $\leqq \mathscr{E}$. To be precise, we have shown that ϱ_∞ coincides with ϱ_β as a state on $\bigcup_j \mathscr{B}(E_j \mathscr{K})$. Recalling that $\{E_j\}$ is the spectral resolution of H, we have for any j and $A \in \mathscr{B}(\mathscr{K})$,

$$\varrho_\infty(A) = \varrho_\infty(E_j A E_j) + \varrho_\infty((1-E_j) A E_j) + \varrho_\infty(E_j A (1-E_j)) + \varrho_\infty((1-E_j) A (1-E_j)).$$

By Schwarz' inequality for states,

$$|\varrho_\infty(1-E_j) A E_j| \leqq [\varrho_\infty(1-E_j)]^{1/2} [\varrho_\infty(E_j A^* A E_j)]^{1/2},$$

and by (4.4), $\varrho_\infty(1-E_j) \to 0$ as $j \to \infty$, the other factor being bounded. Similarly, the other terms converge to 0 as $j \to \infty$. But $\varrho_\infty(E_j A E_j) = \varrho_\beta(E_j A E_j)$, and this converges to $\varrho_\beta(A)$ as $j \to \infty$, as ϱ_β is normal. Hence $\varrho_\infty(A) = \varrho_\beta(A)$ for all $A \in \mathscr{B}(\mathscr{K})$.

(5.2) The same argument shows that any other w^* convergent subnet $\{\varrho_\beta\}_{\beta \in J}$ of $\{\tau^m \varrho\}$ converges to a Gibbs state of energy $\leqq \mathscr{E}$, but (so far), it could be different from ϱ_∞. We show they are the same by showing they have the same entropy, namely $\lim_m S(\tau^m \varrho)$.

(5.3) **Theorem.** *Under the above conditions,* $S(\varrho_\alpha)\to S(\varrho_\infty)$, $\alpha\to\infty$.

Proof. Choose $\varepsilon>0$. Write $\varrho_\alpha=E_j\varrho_\alpha E_j+A$, $A=\varrho_\alpha-E_j\varrho_\alpha E_j\geqq 0$ and

(5.4) $$q=\operatorname{Tr}A=\sum_{k=j}^{\infty}\operatorname{Tr}(E_{k+1}-E_k)\varrho_\alpha\leqq j^{-1}\sum_{k=j}^{\infty}\operatorname{Tr}k(E_{k+1}-E_k)\varrho_\alpha$$
$$=j^{-1}\operatorname{Tr}(H\varrho_\alpha)=j^{-1}\mathscr{E}.$$

Choose j_0 large enough so that q is small enough so that, by (4.9), $S(A)<\varepsilon$ for all α and all $j\geqq j_0$. Then, by the subadditivity of the entropy [7],

(5.5) $$S(\varrho_\alpha)\leqq S(E_j\varrho_\alpha E_j)+S(A)\leqq S(E_j\varrho_\alpha E_j)+\varepsilon$$

for all α and all $j\geqq j_0$. Since $E_j\varrho_\alpha E_j$ (j fixed) has finite rank, S is continuous on this subspace. Taking limits of (5.5) gives for $j\geqq j_0$:

(5.6) $$s=\lim_\alpha S(\varrho_\alpha)\leqq\lim_\alpha S(E_j\varrho_\alpha E_j)+\varepsilon=S(E_j\varrho_\infty E_j)+\varepsilon.$$

Taking the limit $j\to\infty$ gives [8, Appendix] $s\leqq S(\varrho_\infty)+\varepsilon$. Since this is true for every $\varepsilon>0$, we get $s\leqq S(\varrho_\infty)$. Now let j be so large that

$$S(\varrho_\infty)\leqq S(E_j\varrho_\infty E_j)+\frac{\varepsilon}{2}.$$

This is possible [8, Appendix].

For this j choose α_0 so large that for all larger α,

$$S(E_j\varrho_\alpha E_j)\geqq S(E_j\varrho_\infty E_j)-\frac{\varepsilon}{2}.$$

Then

$$S(\varrho_\infty)\leqq S(E_j\varrho_\infty E_j)+\frac{\varepsilon}{2}\leqq S(E_j\varrho_\alpha E_j)+\varepsilon\leqq S(\varrho_\alpha)+\varepsilon$$

for all larger α,

$$\leqq s+\varepsilon.$$

Since this is true for every $\varepsilon>0$, we have $S(\varrho_\infty)\leqq s$. This gives $S(\varrho_\infty)=s$. □

(5.8) We can now put together the results.

Theorem. *Let H be a self-adjoint operator on $\mathscr{K}$ with spectrum* $0,1,2,\ldots$, *and the finite multiplicity $m(j)$ of eigenvalue j obeys $m(j)\leqq\kappa j^r$, $j=1,2,\ldots$. Let $\mathscr{H}=\mathscr{K}\otimes\ldots\otimes\mathscr{K}$, and let T be a symmetry-preserving doubly stochastic map on $\mathscr{B}(\mathscr{H})_1$, T mapping $\mathscr{L}$ and each $\mathscr{B}(\mathscr{H}_\eta)$ to itself and ergodic on each energy shell. Let τ be the corresponding Boltzmann map. Let ϱ be any density matrix on $\mathscr{K}$ with finite mean energy $\mathscr{E}$.*

Then $\tau^m\varrho$ converges as $m\to\infty$ in trace norm to a Gibbs state $\varrho_\infty=e^{-\beta H}/\operatorname{Tr}e^{-\beta H}$ of energy $\leqq\mathscr{E}$, as $m\to\infty$.

Proof. Any convergent subnet of $\{\tau^m\varrho\}$ converges w^* to a Gibbs state (Sect. 5.1). All such limit states have the same entropy (Sect. 5.3) and are therefore the same.

Therefore, $\{\tau^m \varrho\}$ converges in the w^* topology to a Gibbs state. Its energy is $\leqq \mathscr{E}$, by Sect. 4.7. The convergence in trace-norm follows from

$$\|\tau^m \varrho - \varrho_\infty\|_1 \leqq \|\tau^m \varrho - E_j \tau^m \varrho E_j\|_1 + \|E_j \varrho_\infty E_j - E_j \tau^m \varrho E_j\|_1 + \|\varrho_\infty - E_j \varrho_\infty E_j\|_1$$

and (5.4), using that $\tau^m \varrho \to \varrho_\infty$ when restricted to the finite-dimensional space $E_j \mathscr{H}$.

(5.9) If T is not ergodic on the energy shells, but is ergodic when restricted to a smaller slice conserving two numbers (e.g. energy and particle number), we prove convergence to a grand canonical ensemble in a similar way.

(5.10) If $\dim \mathscr{H} < \infty$, then $\mathrm{Tr}(H\varrho)$ is continuous, and so ϱ_∞ has mean energy $\mathscr{E}$. Then $\lim \tau^m \varrho$ is the same state for all ϱ with mean energy $\mathscr{E}$.

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