Mathematical physics. — *On the notion of ergodicity for finite quantum systems*, by
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ABSTRACT. — We show that the orginal definition of ergodicity of Boltzmann can be directly applied to finite quantum systems, such as those arising from the quantization of classical systems on a compact phase space. It yields a notion of quantum ergodicity strictly stronger than the notion due to von Neumann. As an example, we remark that the quantized hyperbolic symplectomorphisms (a particular case is the quantized Arnold cat) are ergodic in this sense.

1. INTRODUCTION

The first notion of quantum ergodicity goes back to the 1932 treatise of von Neumann [vN]. Consider for the sake of simplicity a discrete dynamics defined by the iterations U^k, $k \in \mathbb{Z}$, of a unitary operator U with discrete spectrum acting in a separable Hilbert space $\mathcal{H}$. Let e_ℓ, $\ell = 0, 1, \ldots$, be the orthonormal basis in $\mathcal{H}$ consisting of the eigenvectors of U. Let A be a quantum observable, expressed by a bounded self-adjoint operator in $\mathcal{H}$. Then the discrete dynamics is ergodic in the sense of von Neumann iff

$$(1.1) \qquad \overline{f} := \lim_{m \to \infty} \frac{1}{m} \sum_{k=0}^{m-1} \langle f, U^k A U^{-k} f \rangle = \sum_{\ell=0}^{\infty} |a_\ell|^2 \langle e_\ell, A e_\ell \rangle.$$

Here $f = \sum_{\ell=0}^{\infty} a_\ell e_\ell$ is the initial state in $\mathcal{H}$.

Unlike in classical ergodic theory, the existence of the time average $\overline{f}$ is trivial; a straightforward computation yields

$$\overline{f} = \sum_{\ell=0}^{\infty} |a_\ell|^2 \langle e_\ell, A e_\ell \rangle + \sum_{\ell \neq m} a_\ell \overline{a}_m \langle e_\ell, A e_m \rangle.$$

The second term is the contribution coming from the eigenvectors corresponding to degenerate eigenvalues; $\lambda_\ell = \lambda_m$, $\ell \neq m$.

On the other hand, assuming that the phases of the coefficients a_ℓ are randomly distributed, the space average $A_f^* := \langle f, A f \rangle$ of the observable A has the value

$$A_f^* = \sum_{\ell=0}^{\infty} |a_\ell|^2 \langle e_\ell, A e_\ell \rangle.$$

Therefore the ergodicity property (time average = space average) holds whenever the spectrum of U is simple, or all matrix elements $\langle e_\ell, A e_m \rangle$ for eigenvectors corresponding to the same degenerate eigenvalue vanish. This notion of ergodicity is however considerably weaker than the classical one, because the time average still depends on the weights $|a_\ell|^2$, i.e. on the initial condition f. It follows that the time average is not a microcanonical average, because the weights are arbitrary within the normalization condition $\sum_{\ell=0}^{\infty} |a_\ell|^2 = 1$. Ergodicity in the usual sense is recovered if, for instance, all matrix elements $\langle e_\ell, A e_\ell \rangle$ are equal. This property cannot hold in general; however, it has been explicitly verified, but only in the classical limit, in many instances in which the quantum system is the quantization of a classical ergodic one (see e.g. [CdV], [HMR], [DEGI], [Sc], [Ze]). The existence of the classical limit of the matrix elements $\langle e_\ell, A e_\ell \rangle$ for almost every sequence of eigenfunctions and its coincidence with the classical ergodic average has therefore been proposed in the mathematical literature as a definition of quantum ergodicity more satisfactory than the one due to von Neumann (see e.g. [Sa]). Referring the reader to the introduction of [DEGI] and [GM] for a discussion of this point, here we limit ourselves to remarking that even this last definition of ergodicity is rather weak: for example, it holds even when the quantum evolution is localized while the corresponding classical one is delocalized as $t \to \infty$ (see [GL]).

The purpose of this paper is to point out that, at least for quantum systems with a finite number of states, such as those arising from the quantization of classical systems admitting a compact phase space, the original Boltzmann definition of ergodicity can be transferred to quantum mechanics essentially word for word. It yields a notion of quantum ergodicity strictly stronger and more satisfactory than the one due to von Neumann as far as the dependence on the initial condition is concerned; moreover, it reduces to the classical notion when the Schnirelman theorem holds. Moreover, the quantized hyperbolic symplectic maps of the 2-torus represent examples which are ergodic in the sense of this definition, which is to be described in the next section. In Section 3 we discuss its application to finite quantum systems, and in Section 4 we review some examples.

2. THE ORIGINAL NOTION OF BOLTZMANN ERGODICITY AND QUANTUM SYSTEMS WITH A FINITE NUMBER OF STATES

Following Gallavotti ([Ga, §1.3]) we recall the original definition of ergodicity given by Boltzmann.

Let Σ be a compact phase space, for example, a compact constant energy surface of a Hamiltonian system. Let μ be a measure on Σ (Lebesgue measure in typical examples), and T be a measure-preserving transformation of Σ onto itself (for example, T is a unit time Hamiltonian evolution preserving the measure μ). We can assume $\mu(\Sigma) = 1$.

Then we say with Boltzmann that the dynamical system (Σ, T, μ) is *ergodic* if for any $N \in \mathbb{N}$ there exists a partition $\mathcal{V}$ of Σ into N disjoint cells $\mathcal{C}_1, \ldots, \mathcal{C}_N$ of

measure $h = 1/N$ such that the finite dynamics defined by the finite sequence T^k, $k = 0, \dots, N-1$, $T^0 = I$, represents a one-cycle permutation of the cells of $\mathcal{V}$:

$$(2.1) \qquad T^k \mathcal{C}_\ell = \mathcal{C}_{\ell+k}, \qquad T^N \equiv T.$$

Here of course the cells have been numbered according to the order of visits. Typically one should think of each cell as a square of area $\Delta p \Delta q \sim h$. For a thorough discussion of this purely classical limitation the reader is referred again to [Ga, §1.2].

Let now $f : \Sigma \to \mathbb{R}$ be any smooth observable. Assume that f takes a constant value on each cell, and for $x \in \mathcal{C}_\ell$, ℓ arbitrary, form the average of the time evolution:

$$(2.2) \qquad \overline{f}_N(x) = \frac{1}{N} \sum_{k=0}^{N-1} f(T^k x).$$

Then $\overline{f}_N(x)$ is clearly independent of x, i.e. of the particular cell $\mathcal{C}_\ell$; moreover,

$$(2.3) \qquad \overline{f}_N(x) = \int_\Sigma f(x)\, d\mu =: f_N^*.$$

Thus under the above assumptions the time and space averages coincide, and this is the standard definition of ergodicity. For general observables f, the time average on the r.h.s. of (2.2) is also a Riemann sum of the space average f^*. Thus as $N \to \infty$, or equivalently, as $h \to 0$, the standard definition of ergodicity is recovered:

$$(2.4) \qquad \overline{f}(x) := \lim_{N \to \infty} \frac{1}{N} \sum_{k=0}^{N-1} f(T^k x) = \int_\Sigma f(x)\, d\mu, \qquad \mu\text{-a.e.},$$

or, replacing the discrete dynamics by the limiting continuous one S_t, $t \in \mathbb{R}$,

$$(2.5) \qquad \overline{f}(x) := \lim_{T \to \infty} \frac{1}{T} \int_0^\infty f(S_t x) = \int_\Sigma f(x)\, d\mu, \qquad \mu\text{-a.e.}$$

Note that the above notion is just an approximation of the standard one; moreover, *it explicitly depends on the cell decomposition*. Of course, for an ergodic system in the standard sense of (2.4) or (2.5) any non-ergodic cell decomposition becomes ergodic as $h \to 0$; however, as long as h is kept different from zero, in general there might be no decomposition satisfying (2.1). Consider for example the simplest chaotic systems, namely the hyperbolic symplectomorphisms of the 2-torus $\mathbb{T}^2$. Here T is the map defined by the 2×2 matrix with integer elements

$$(2.6) \qquad T = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

with $|a + d| > 1$ and $ad - bc = 1$. The Arnold cat map corresponds to $a = 2$, $b = c = d = 1$. In this case the only cell decomposition for $h > 0$ which keeps its

form under the evolution is the Markov partition (see e.g. [Si]), but even this is not ergodic.

As explained in [Ga], the phase space decomposition into finite cells is introduced just to apply a discrete probability argument, because continuous probability theory was still to come at the time; there was however no doubt in Boltzmann's mind that the limit $h \to 0$ should always be taken. However, since (see [LL, §48]) to each quantum state there corresponds in the classical limit a cell in phase space of area h, the idea of a direct application of this notion in quantum mechanics arises spontaneously, on account also of the fact that there exist many interesting examples of quantum systems admitting a finite number of states.

We therefore consider a quantum system with a finite number of states; i.e., the corresponding Hilbert space $\mathcal{H}_N$ has dimension N, and is thus isomorphic to $\mathbb{C}^N$. Systems of this type arise, for example, from the quantization of classical systems admitting a compact phase space, which we can always take of unit measure. As recalled above, the physical intuition behind this fact is that each quantum state occupies a cell of area h in phase space. Hence if the total area is 1 there can be at most $N = 1/h$ states. In the case of the quantization of the torus this result has been first obtained by Hannay–Berry [HB], and later put on the rigorous basis of the discrete Weyl quantization in [DE].

We can always assume that there exists a one-to-one correspondence between the N quantum states and an orthonormal basis in $\mathcal{H}_N$. Given a unitary operator U in $\mathcal{H}_N$, we further assume:

(i) The iterations $U^k, k = 0, 1, \ldots, U^0 = I$, define a discrete dynamics of period N, i.e. $U^N = I$.

(ii) The discrete dynamics generates a one-cycle permutation of the basis vectors, i.e. there are $\alpha_{\ell,k} \in \mathbb{R}$, $\ell, k = 1, \ldots, N$, such that

$$(2.7) \qquad U^k \psi_\ell = e^{i\alpha_{\ell,k}} \psi_{\ell+k}, \qquad \psi_{k+N} = \psi_k, \qquad \alpha_{\ell,N} = 0 \ (\mathrm{mod}\ 2\pi).$$

Then we say that the discrete dynamics generated by U acts ergodically on the basis $\psi_k, k = 0, \ldots, N-1$.

DEFINITION 1. *A discrete evolution U of a finite quantum system will be called ergodic if there is an orthonormal basis $\psi_0, \ldots, \psi_{N-1}$ on which U acts ergodically.*

Let indeed A be any observable, i.e. any self-adjoint operator in $\mathcal{H}_N$. The corresponding Heisenberg observable with respect to the discrete dynamics generated by U is $U^k A U^{-k}, k = 1, \ldots, N$. Define the time average of the Heisenberg observable on any basis vector ψ_ℓ:

$$(2.8) \qquad \overline{A}_l = \frac{1}{N} \sum_{k=0}^{N-1} \langle \psi_\ell, U^k A U^{-k} \psi_\ell \rangle.$$

Then we have

$$\overline{A_l} = \frac{1}{N} \sum_{k=0}^{N-1} \langle \psi_\ell, U^k A U^{-k} \psi_\ell \rangle = \frac{1}{N} \sum_{k=0}^{N-1} \langle U^{-k} \psi_\ell, A U^{-k} \psi_\ell \rangle$$

$$= \frac{1}{N} \sum_{k=0}^{N-1} \langle e^{-i\alpha_{\ell,k}} \psi_{\ell+k}, A e^{-i\alpha_{\ell,k}} \psi_{\ell+k} \rangle = \frac{1}{N} \sum_{k=0}^{N-1} \langle \psi_{k+\ell}, A \psi_{k+\ell} \rangle.$$

It is now natural to define the *space average* of the observable A on the basis $\psi_1, \ldots, \psi_N$ to be the quantity

$$(2.9) \qquad\qquad A^* = \frac{1}{N} \sum_{k=0}^{N-1} \langle \psi_k, A \psi_k \rangle.$$

Therefore the above formula can be rewritten as

$$(2.10) \qquad\qquad \overline{A_l} = A^*.$$

In words: On the basis $\psi_1, \ldots, \psi_N$, the time average $\overline{A_l}$ is equal to the space average A^* and is thus *independent* of ℓ, i.e. of the initial condition, in complete analogy with the classical notion. This notion of quantum ergodicity, being simply the transposition in quantum mechanics of the original notion of Boltzmann, depends on the basis, exactly as the classical notion depends on the cell decomposition.

Let us now examine the relation between the above notion of ergodicity and the one due to von Neumann.

PROPOSITION 1. *A discrete evolution U ergodic in the sense of Definition* 1 *is also ergodic in the sense of von Neumann, i.e.*

$$(2.11) \qquad\qquad \frac{1}{N} \sum_{k=0}^{N-1} \langle u, U^k A U^{-k} u \rangle = \sum_{\ell=0}^{N-1} |c_\ell|^2 \langle e_\ell, A e_\ell \rangle.$$

Here $u \in \mathcal{H}_N$ is arbitrary, with expansion $u = \sum_{\ell=0}^{N-1} c_\ell e_\ell$ with respect to the orthonormal basis $e_1, \ldots, e_N$ corresponding to the eigenvalues $\lambda_0, \ldots, \lambda_{N-1}$ (counted with multiplicity) of U.

PROOF. First we remark that if U is ergodic then it admits a cyclic vector; actually, each vector of the basis $\psi_0, \ldots, \psi_{N-1}$ is cyclic. Therefore the spectrum of U is simple. Since, moreover, $U^{N-1} = I$, each eigenvalue λ_ℓ, $\ell = 0, \ldots, N-1$, must be an N-th root of unity:

$$\lambda_\ell = e^{i 2\pi \ell / N}.$$

Hence we can compute the time average on the l.h.s. of (2.11):

$$\frac{1}{N}\sum_{k=0}^{N-1}\langle u, U^k A U^{-k} u\rangle = \frac{1}{N}\sum_{k=0}^{N}\sum_{\ell,m=0}^{N-1} c_\ell \bar{c}_m \langle e_\ell, U^k A U^{-k} e_m\rangle$$

$$= \frac{1}{N}\sum_{k=0}^{N-1}\sum_{\ell,m=0}^{N-1} c_\ell \bar{c}_m \langle e_\ell, U^k A U^{-k} e_m\rangle$$

$$= \sum_{\ell,m=0}^{N-1} c_\ell \bar{c}_m \langle e_\ell, A e_m\rangle \frac{1}{N}\sum_{k=1}^{N} e^{ik(\lambda_\ell - \lambda_m)}$$

$$= \sum_{\ell,m=0}^{N-1} c_\ell \bar{c}_m \langle e_\ell, A e_m\rangle \delta_{\ell,m} = \sum_{\ell=0}^{N-1} |c_\ell|^2 \langle e_\ell, A e_\ell\rangle$$

on account of the fact that

$$\frac{1}{N}\sum_{k=0}^{N-1} e^{ik(\lambda_\ell - \lambda_m)} = \delta_{\ell,m}$$

because by the simplicity of the spectrum $\lambda_\ell - \lambda_m = 2\pi i(\ell - m)/N$. This proves the proposition.

REMARKS. 1. The converse statement is not true. Even though the simplicity of the spectrum entails that U admits a cyclic vector, denoted ϕ, the vectors $U^k \phi$, $k = 0, \ldots, N-1$, which span $\mathcal{H}_N$ are not necessarily orthogonal. The orthogonality of the basis on which the dynamics acts as a one-cycle permutation is clearly the quantum analog of the pairwise disjointness of the cells in the decomposition $\mathcal{V}$.

2. In a classical ergodic system the time average of an observable, being equal to the space average, is independent of (μ almost any) initial datum. We have already remarked that, by (2.10), the time average of a quantum system ergodic according to Definition 1 does not depend on the initial state chosen within the orthonormal basis $\psi_1, \ldots, \psi_N$; this fact cannot be true for the von Neumann notion unless the matrix elements $\langle e_\ell, A e_\ell\rangle$ are all equal.

3. In the classical limit, the notion of quantum ergodicity (or the stronger one of quantum unique ergodicity) based on the validity of the Schnirelman theorem is clearly recovered.

3. AN EXAMPLE: THE QUANTIZED HYPERBOLIC SYMPLECTOMORPHISMS OF THE TORUS

To describe the example, we recall the main results of [DEGI] (see also [Hu]). Consider the symplectic hyperbolic maps of the torus $\mathbb{T}^2$ defined by the 2×2 matrix (2.6). On the smooth observables $f : \mathbb{T}^2 \to \mathbb{C}$ defined by the double Fourier series

$$(3.1) \qquad f(\phi) = \sum_{n \in \mathbb{Z}^2} f_n e^{i\langle n, \phi\rangle}, \qquad n = (n_1, n_2), \phi = (\phi_1, \phi_2),$$

the map T acts as follows:

$$(3.2) \qquad f(T\phi) = \sum_{n \in \mathbb{Z}^2} f_n e^{i\langle T^t n, \phi \rangle} = \sum_{n \in \mathbb{Z}^2} f_{(T^t)^{-1} n} e^{i\langle n, \phi \rangle},$$

where T^t is the matrix transposed to T.

The basis observables $U(n) := e^{i\langle n, \phi \rangle}$ and the action (3.2) can be canonically quantized looking for the unitary Hilbert space representations of the discrete Weyl–Heisenberg algebra:

$$(3.3) \qquad \widehat{X}(n)\widehat{X}(m) = e^{i\pi\hbar\omega(m,n)} \widehat{X}(m+n)$$

where $\omega(m,n) = m_1 n_2 - m_2 n_1$ is the discrete symplectic 2-form. The result is the following (see [DE]).

1. The discrete Weyl–Heisenberg algebra admits infinitely many inequivalent representations of dimension $N = 1/h$, indexed by $\theta \in \mathbb{T}^2$. Explicitly: the Hilbert space can be identified with $\mathbb{C}^N$; denoting by e_ℓ, $\ell = 1, \ldots, N$, the vectors of the canonical basis, the action of $\widehat{X}(n)$ in the representation labeled by θ is specified as follows:

$$(3.4) \qquad \widehat{X}(n; \theta) = e^{\pi i n_1 n_2 / N} t_2^{n_2} t_1^{n_1},$$

$$(3.5) \qquad t_1 e_\ell = e^{2\pi i (\theta_1 + \ell)/N} e_\ell, \qquad t_1^N = e^{2\pi i \theta_1} I,$$

$$(3.6) \qquad t_2 e_\ell = e^{2\pi i \theta_2 / N} e_{\ell+1}, \qquad t_2^N = e^{2\pi i \theta_2} I.$$

2. For all $\theta \in \mathbb{T}^2$, $\widehat{X}(T^t n; \theta)$ is still an irreducible representation of (3.3), and there exists a unitary operator $V_T(\theta)$ such that

$$(3.7) \qquad \widehat{X}(A^t n, \theta) = V_T(\theta)^{-1} \widehat{X}(n, \varphi(\theta)) V_T(\theta)$$

where

$$\varphi_T(\theta) = T\theta + \frac{1}{2}\begin{pmatrix} abN \\ cdN \end{pmatrix}.$$

$V_T(\theta)$ is called the *propagator* quantizing the map T. In fact, by (3.1, 3.2, 3.4, 3.7) and the linearity of the quantization procedure, the quantum operator corresponding to the classical observable f in the representation θ is

$$\hat{f}(\theta) := \sum_{n \in \mathbb{Z}^2} \widehat{X}(n; \theta).$$

and the Heisenberg operator corresponding to $f(T\phi)$ is

$$V_T(\theta)^{-1} \hat{f}(\theta) V_T(\theta) = V_T(\theta)^{-1} \sum_{n \in \mathbb{Z}^2} f_n \widehat{X}(n, \varphi(\theta)) V_T(\theta).$$

3. Consider for simplicity the case of N prime, and

$$a = 2g, \quad b = 1, \quad c = 4g^2 - 1, d = 2g, \quad g \in \mathbb{N},$$

i.e.

$$(3.8) \qquad T = \begin{pmatrix} 2g & 1 \\ 4g^2 - 1 & 2g \end{pmatrix}$$

Then we can choose $\theta = (0, 0)$. In this case the elements of the $N \times N$ matrix representing $V_T(0, 0) := V_T$ in the canonical basis have the expression

$$(3.9) \qquad V_T(m, n) = \frac{C_N}{\sqrt{N}} \exp\left[\frac{2\pi i}{N}(gm^2 - mn + gn^2)\right].$$

Assume now that $4g^2 - 1$ is a quadratic residue of N, i.e, there is $x \in \mathbb{Z}_N := \mathbb{Z} \pmod{N}$ such that $4g^2 - 1 = x^2 \pmod{N}$. We remark that, since N is a prime, $\mathbb{Z}_N$ is a field, i.e. each $x \in \mathbb{Z}_N$ has a unique inverse $x^{-1} \in \mathbb{Z}_n$. Equivalently: the equation $xy = 1 \pmod{N}$ has a unique solution $y := x^{-1}$. If T is considered as a linear map from $\mathbb{Z}_N$ into itself, this amounts to requiring that its eigenvalues, denoted λ and λ^{-1} (note that $\lambda^{-1} = N - \lambda$), belong to $\mathbb{Z}_N$ and are given by

$$\lambda = (2g + 2p)^{-1} \pmod{N}, \qquad p := \frac{1}{2}\sqrt{4g^2 - 1}.$$

Set now

$$(3.10) \qquad \Psi_{p,\ell}(q) = \exp\left[\frac{2\pi i}{N}(pq^2 + \ell q)\right], \qquad \ell \in \mathbb{Z}_N.$$

One has

$$\langle \Psi_{p,\ell}(q), \Psi_{p,\ell'}(q) \rangle = \delta_{\ell,\ell'},$$

i.e., the vectors $\Psi_{p,\ell}$, $\ell = 0, \ldots, N - 1$, represent an orthornormal basis in $\mathbb{C}_N$.

Let now N be such that $V^{N-1} = I$. In that case the orbit of λ in $\mathbb{Z}_N$, i.e. the set λ^s, $s = 0, \ldots, N - 1 \pmod{N}$, coincides with $\mathbb{Z}_N$. Then the basic result for our purposes is the following one:

PROPOSITION 2.

$$(3.11) \qquad V_T\Psi_{p,\ell} = \left(\frac{\lambda}{N}\right)\exp\left[-\frac{2\pi i}{N}(\lambda\ell)^2(g + p)\right]\Psi_{p,\lambda\ell},$$

Here

$$\left(\frac{\lambda}{N}\right) := \begin{cases} 1 & \text{if } \lambda = x^2 \pmod{N}, \\ -1 & \text{if } \lambda \neq x^2 \pmod{N}, \end{cases}$$

is the Legendre symbol.

In fact, Proposition 2 immediately entails

$$V_T^k\Psi_{p,\ell} = e^{i\alpha_{k,\ell}}\Psi_{p,\lambda^k\ell}, \qquad k = 0, \ldots, N - 1,$$

$$\alpha_{k,\ell} := \left(\frac{\lambda}{N}\right)^k \exp\left[-\frac{2\pi i}{N}\sum_{s=0}^{k}(\lambda^s\ell)^2(g + p)\right],$$

which is formula (2.7) with $U := V_T$. We remark that, even though the numerical evidence supports the conjecture that primes N enjoying the above property are actually generic [PV], the actual existence of such primes N is far from being trivial; it follows from the validity of the Artin conjecture, in turn equivalent to the generalized Riemann hypothesis (see e.g. [Mu]).

4. Discussion

We have seen that the original definition of ergodicity given by Boltzmann can be applied in a natural way to finite quantum systems; the notion of quantum ergodicity thus obtained is stronger than von Neumann's. Furthermore, unlike the quantum ergodicity notion based on the convergence of the matrix elements to the classical ergodic average in the classical lmit, it holds for any value of the Planck constant. We have also seen that finite quantum systems which come from the quantization of the simplest classically chaotic ones are actually ergodic according to this notion. Two natural questions arising in this context are: first, the possibility of verifying the ergodicity in this sense for finite quantum systems such as the quantization of classically chaotic but discontinuous maps, for example, the quantized baker's map [DBDEG]. The construction of [DEGI] leading to the ergodic action (2.7) does not seem to apply in this case, so that different arguments are required. A second and more important question is the generality of this notion, i.e. the possibility of applying it to more realistic quantum systems, let alone the verification. The most significant example from a physical point of view, namely the quantization of a classically ergodic flow on a compact, constant energy surface, requires the preliminary understanding of no smaller difficulty, namely, the quantization of the classical symplectic reduction on a constant energy surface when the flow on it is ergodic. Since, as above, each quantum state occupies a volume in phase space proportional to $\hbar$, the resulting quantum systems, if any, should have a finite number of states, and the above definition should be applicable.

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