

Convergence to equilibrium for many particle systems

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Abstract

The goal of this paper is to give a short review of recent results of the authors concerning classical Hamiltonian many particle systems. We hope that these results support the new possible formulation of Boltzmann's ergodicity hypothesis which sounds as follows. For almost all potentials, the minimal contact with external world, through only one particle of N , is sufficient for ergodicity. But only if this contact has no memory. Also new results for quantum case are presented.

Keywords: Markov processes, Boltzmann hypothesis, quantum controllability

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Part I

Introduction

The goal of this paper is to give a short review of recent results ([2])-([7]) of the authors. In these results classical Hamiltonian many particle systems were considered from new point of view: they have minimal contact with external world, for example only one particle of N can have this contact. Thus, we consider Hamiltonian systems with minimal possible randomness. In despite of this, ergodicity can be proved for almost all potentials of a wide natural class.

Also we present some new results concerning quantum situation and discuss common points and difference of our results with other research in mathematical physics and Markov chains theory, for example with [17, 18, 15, 14], [19, 20], [10, 12, 8, 11, 13, 9].

0.1 Intro to intro

To start with, we give very simple intuition. Let finite set X be given, and let $M(X)$ be the set of probability measures on X . Stochastic matrix P defines linear map $P : M(X) \rightarrow M(X)$, and discrete time Markov chain ξ_k depending on the initial distribution μ_0 of ξ_0 .

It is known that if the matrix P^k , for some k , has all elements positive, then there exists unique P -invariant measure π , and moreover for any initial measure μ_0 as $n \rightarrow \infty$

$$P^n \mu_0 \rightarrow \pi, \quad (1)$$

that is for any $A \subset X$ the sequence of real numbers $(P^n \mu_0)(A)$ converges to $\pi(A)$. We will call this property strong ergodicity. A weaker ergodicity property (we will call it Cesaro ergodicity)

$$\frac{1}{n} \sum_{k=1}^n P^k \mu \rightarrow \pi \quad (2)$$

follows. It can be formulated differently: for any real function $f(x)$ on X and for any initial state ξ_0 , time averages are approximately equal to space averages (this was Boltzmann's formulation of his famous hypothesis in statistical physics). Exact formulation for this could be:

$$\frac{1}{n} \sum_{k=1}^n f(\xi_k) \rightarrow \sum_{x \in X} f(x) \pi(x) \quad (3)$$

as $n \rightarrow \infty$, with L_1 -convergence, or in some other sense.

Deterministic map $U : X \rightarrow X$ is a particular case of Markov chains - when any element of matrix P is either 0 or 1. We will consider only one-to-one maps U . Then it is clear that

1. if $N = |X| > 1$ then strong convergence never holds because any U defines a partition $X = X_1 \cup \dots \cup X_m$ such that U is cyclic on any X_i ;
2. convergence of

$$\frac{1}{n} \sum_{k=1}^n f(U^k x)$$

holds for any U and any x (this is a trivial case of the famous Birkhoff-Khinchin ergodicity theorem) but Cesaro ergodicity (the limit is the unique invariant measure) holds iff there is only one cycle;

- note that there are N^N deterministic maps, among them $N!$ one-to-one maps, and among the latter only $(N-1)!$ maps with unique cycle. Thus, Cesaro ergodicity is also a rare event but not so rare as strong ergodicity.

If the set X is not finite, for example a smooth manifold, the situation becomes enormously more complicated. Ludwig Boltzmann did not give exact mathematical formulations. Later on, various formulations of the problem appeared. For some history of ergodicity theory we refer to [1] and references therein. What could be the ways to avoid extreme complexity? First of all, one must find wider and possibly alternative exact formulations of the problem.

0.2 Classical ergodicity

We will consider N -particle systems with arbitrary but finite N . Namely, N point particles in (coordinate) space R^d with coordinate vectors $q_i = (q_{i1}, \dots, q_{id})$, velocities $v_i = (v_{i1}, \dots, v_{id})$, momenta $p_i = m_i v_i$ and with the interaction defined by smooth symmetric potentials $V_{ij}(q_i, q_j)$. To avoid double indices we write further N instead of dN (thus the index i should be considered as a pair (particle number, coordinate number)). Then the dynamics in the phase space $R^{2N} = \{\psi = (q_1, \dots, q_N, p_1, \dots, p_N)\}$ is defined by the following system of Hamiltonian equations

$$\frac{dq_k}{dt} = \frac{\partial H}{\partial p_k} = v_k, \quad \frac{dp_k}{dt} = -\frac{\partial H}{\partial q_k}, \quad k = 1, \dots, N, \quad (4)$$

with the Hamiltonian

$$H = H(\psi) = \sum_{k=1}^N \frac{p_k^2}{2m_k} + Q, \quad Q = \sum_{1 \leq k < l \leq N} V_{kl}(q_k, q_l).$$

This dynamics defines a one parameter group of one-to-one transformations $U^t : R^{2N} \rightarrow R^{2N}$ of the phase space. We assume that $Q \rightarrow +\infty$ as $\max_k |q_k| \rightarrow \infty$, so that no particle could escape to infinity. This assumption is similar to assuming the system to be in some finite volume (system in the box) Λ with reflecting boundary $\partial\Lambda$. Then the energy surface $M_h = \{\psi : H(\psi) = h\} \subset R^{2N}$ is bounded for any h and (by the energy conservation law) is invariant with respect to this dynamics.

Liouville's theorem says that on any M_h there exists finite probability measure λ_h (Liouville's measure - normalized restriction of the Lebesgue measure λ on the phase space), invariant with respect to this dynamics.

We say that for a given H the system is ergodic if for any $\psi \in M_h$

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T f(U^t \psi) dt = \int_{M_h} f(\psi) d\lambda_h(\psi) \quad (5)$$

in some space of measurable functions. It can be L_2 , L_1 -convergence, or uniform convergence with respect to ψ .

Possible problems could be the following:

1. Give examples of V_{kl} or, better, classes of V_{kl} such that ergodicity holds for all sufficiently large N . We do not know any such example, but there are many counterexamples: linear (due to invariant tori) and non-linear integrable systems;

2. prove the contrary: for typical (or almost any) Q , from interesting classes of potentials, ergodicity does not hold. Of course, one should define what means <<almost all>>;

3. instead of problems 1 and 2 one could look for more natural problems. What are the reasons for this:

- a) the N -particle systems discussed above are closed systems, but it is not known whether closed systems exist in nature. More realistic is to assume that any system always has some contact with

external world. Then the first natural question is: how weak can be this contact for the system to be ergodic;

b) this does not contradict to the recent development of theoretical physics, where the notion of space point itself becomes an approximation. Namely, in quantum physics the dynamics is defined not as a transformation of the phase space, but of L_2 space of functions on the coordinate space. Moreover, in modern physics the notion of space itself is being reconsidered: discrete space, quantum space or no space at all.

0.3 Systems with minimal randomness

We consider three types of models with minimum randomness, or combinations of them.

1. Only one degree of freedom open to external influence Namely, we change only one equation (for $k = 1$) of the system (4)

$$\frac{dq_1}{dt} = \frac{\partial H}{\partial p_1} = p_1, \quad \frac{dp_1}{dt} = -\frac{\partial H}{\partial q_1} + F(x_1, p_1, t), \quad (6)$$

where we assume unit masses. All other equations (4) are left unchanged. This is used in part III.

2. Two deterministic evolutions with switching at random time moments Let $U_i^t, i = 1, 2, t \in [0, \infty)$, be two semigroups of deterministic transformations (of some set X). For example, when X is the phase space of N -particle system, and the equations are of the type (4). Consider the sequence

$$0 = t_0 < t_1 < t_2 < \dots \quad (7)$$

of time moments and denote $\tau_n = t_n - t_{n-1}$. For any integer $m \geq 1$ and non negative real $\tau_1, \tau_2, \dots, \tau_{2m+1} \geq 0$ consider the following transformations

$$J_0 = E, \quad J_1 = U_1^{\tau_1},$$

$$J_{2m}(\tau_1, \dots, \tau_{2m}) = U_2^{\tau_{2m}} U_1^{\tau_{2m-1}} \dots U_2^{\tau_2} U_1^{\tau_1}, \quad (8)$$

$$J_{2m+1}(\tau_1, \dots, \tau_{2m+1}) = U_1^{\tau_{2m+1}} J_{2m}(\tau_1, \dots, \tau_{2m}), \quad (9)$$

and define the evolution $W(t)$:

$$W(t) = U_1^{t-t_{2m}} J_{2m}(\tau_1, \dots, \tau_{2m}), t_{2m} \leq t < t_{2m+1}, \quad (10)$$

$$W(t) = U_2^{t-t_{2m+1}} J_{2m+1}(\tau_1, \dots, \tau_{2m+1}), t_{2m+1} \leq t < t_{2m+2}.$$

Define also the following sets of transformations

$$\mathcal{J}_n(U_1^t, U_2^t) = \{J_n(\tau_1, \dots, \tau_n) : \tau_1, \tau_2, \dots, \tau_n \geq 0\}.$$

We say that the triple (U_1^t, U_2^t, x) satisfies the covering (or contrallaility) condition if there exists n such that

$$\mathcal{J}_n(x) = \mathcal{J}_n^x(U_1^t, U_2^t) = \mathcal{J}_n(U_1^t, U_2^t)x = X, \quad (11)$$

that is, starting from x , n transformations cover all the set X . The triple satisfies strong covering (strong controllability) condition if n does not depend on x .

Below we always assume **Condition D**: τ_k are independent identically distributed positive random variables with $E\tau_1 < \infty$, having some density $p(s) = p_\tau(s)$ with respect to Lebesgue measure, positive for all $s \geq 0$. However, in some cases weaker assumptions are possible.

This model is used in section II.2.

3. One deterministic evolution with external deterministic intrusion at random time moments Let be given semigroup U_1^t and fixed transformation U_2 . We put $J(t) = U_2 U_1^t$ and for $t_n \leq t < t_{n+1}$ put

$$W(t) = U_1^{t-t_n} J(\tau_n) \dots J(\tau_1). \quad (12)$$

This model is used in section II.1. Note that in case 2 the trajectories are continuous, and here not.

Part II

Convergence and covering (controllability) property

1 Classical dynamics with random time velocity flips

On the phase space

$$L = L_{2N} = \mathbb{R}^{2N} = \{\psi = \begin{pmatrix} q \\ p \end{pmatrix}, q = (q_1, \dots, q_N)^T, p = (p_1, \dots, p_N)^T \in \mathbb{R}^N\} \quad (13)$$

(T denotes transposition, thus q, p, ψ are the column vectors) we consider quadratic Hamiltonian

$$H = H(\psi) = \frac{1}{2} \sum_{i=1}^N p_i^2 + \frac{1}{2} \sum_{i,j} V(i,j) q_i q_j = \frac{1}{2} \left(\begin{pmatrix} V & 0 \\ 0 & E \end{pmatrix} \psi, \psi \right)_2 \quad (14)$$

with (symmetric) positive definite matrix V , and the corresponding Hamiltonian system of linear ODE with $k = 1, \dots, N$

$$\dot{q}_k = p_k, \dot{p}_k = - \sum_{l=1}^N V_{kl} q_l. \quad (15)$$

Note that here the energy surface \mathcal{M}_h is a smooth manifold (ellipsoid) in L of codimension 1.

With $(2N \times 2N)$ -matrix

$$A = \begin{pmatrix} 0 & E \\ -V & 0 \end{pmatrix}$$

the system (15) can be rewritten as

$$\dot{\psi} = A\psi, \quad (16)$$

and the solution of (16) defines the transformation group

$$U_1^t = e^{tA}$$

Now define the transformation U_2 . Assume that at time moments (7) the following deterministic transformation $U_2 : L \rightarrow L$ occurs: all q_k, p_k are left unchanged, except for p_1 , the sign of which becomes inverted

$$p_1(t_m - 0) \rightarrow p_1(t_m) = -p_1(t_m - 0), m \geq 1.$$

One can say that U_2 is the velocity flip of the first coordinate of particle 1. Note that the Liouville measure π is invariant w.r.t. Hamiltonian dynamics and also w.r.t. velocity flips.

For any $t_n \leq t < t_{n+1}$ define linear transformations $L \rightarrow L$, putting as in (12)

$$W(t)\psi = e^{(t-t_n)A} U_2 e^{\tau_n A} \dots U_2 e^{\tau_1 A} \psi, \psi \in L.$$

Thus, we are in the situation of 0.3.3. It is clear that \mathcal{M}_h is invariant w.r.t. $W(t)$ for any $h > 0$ and $t \geq 0$.

What means “almost all” Define the mixing subspace

$$L_- = L_-(V) = \left\{ \begin{pmatrix} q \\ p \end{pmatrix} \in L : q, p \in l_V \right\}, \quad (17)$$

where $l_V = l_{V,1}$ is the subspace of \mathbb{R}^N , generated by the vectors $V^k e_1$, $k = 0, 1, 2, \dots$, where e_1, \dots, e_N is the standard basis in \mathbb{R}^N .

Let \mathbf{V} be the set of all positive-definite $(N \times N)$ -matrices, and let $\mathbf{V}^+ \subset \mathbf{V}$ be the subset of matrices for which

$$L_-(V) = L. \quad (18)$$

Note that \mathbf{V} can be considered as subset of $R^{\frac{N(N+1)}{2}}$, thus (the restriction of) Lebesgue measure is defined on it. Let $\omega_1^2, \dots, \omega_N^2$ be the eigenvalues of V , and let \mathbf{V}_{ind} be the set of $V \in \mathbf{V}$ such that the square roots $\omega_1, \dots, \omega_N$ of the eigenvalues are independent over the field of rational numbers.

Lemma 1 1) The set \mathbf{V}^+ is open and everywhere dense (assuming topology of $R^{\frac{N(N+1)}{2}}$) in \mathbf{V} ,
 2) The set $\mathbf{V}^+ \cap \mathbf{V}_{ind}$ is dense both in \mathbf{V}^+ and in \mathbf{V} , and the Lebesgue measures on $\mathbf{V}, \mathbf{V}^+, \mathbf{V} \cap \mathbf{V}_{ind}$ are all equal.

Covering theorem

Theorem 1 Assume that $V \in \mathbf{V}^+ \cap \mathbf{V}_{ind}$, then there exists $m \geq 1$ such that for any $\psi \in L$ we have

$$\mathcal{J}_m(\psi) = \mathcal{M}_h$$

Moreover, there is the following upper bound on m

$$m \leq \frac{2}{\min_k \beta_k^2} + 2$$

where $\beta_k = (v_k, e_1)$ and v_1, \dots, v_N are the eigenvectors of V . Moreover, from the properties of L_- it follows that all β_k are not zero.

Similar property was called pure state controllability in quantum case, see for example [16, 17, 15, 14].

Convergence theorem

Theorem 2 Assume that $V \in \mathbf{V}^+ \cap \mathbf{V}_{ind}$. Then, under condition D , for any initial $\psi(0)$ and any bounded measurable real function f on \mathcal{M}_h we have a.s.

$$M_f(T) \stackrel{def}{=} \frac{1}{T} \int_0^T f(\psi(t)) dt \rightarrow_{T \rightarrow \infty} \pi(f) \stackrel{def}{=} \int_{\mathcal{M}_h} f d\pi$$

If, for example, τ_i have exponential distribution with the density $\lambda \exp(-\lambda \tau)$, $\lambda > 0$, then it defines Markov process $\psi(t)$ with right continuous deterministic trajectories and random jumps. Such processes are often called piecewise deterministic Markov processes, see for example [11]. At the same time, this can be considered as an example from random perturbation theory, see [10] where the problem of invariant measures is studied.

2 Finite quantum dynamics with random time switching

Here we consider the situation of the section 0.3.2, and assume both groups U_i^t to be unitary evolutions in C^N . Examples could be quantum walks on finite lattices.

2.1 Definitions and Results

We consider $\mathcal{H} = C^N$, $N > 1$, as the Hilbert space with the scalar product (hermitian form)

$$(\psi, \psi') = \sum_{k=1}^N \psi_k \bar{\psi}'_k, \quad \psi, \psi' \in \mathcal{H}.$$

Let \mathcal{O} be the set of all hermitian (self adjoint) operators on \mathcal{H} . Lie algebra structure on \mathcal{O} is introduced as

$$\{A, B\} = i[A, B] = i(AB - BA) \in \mathcal{O}. \quad (19)$$

Let $U(N)$ be the group of unitary transformations of \mathcal{H} . Consider two its one-parametric subgroups $U_k^t = e^{-itH_k}$, $k = 1, 2$, $t \geq 0$, where $H_1, H_2 \in \mathcal{O}$. For any integer $m \geq 1$ and any real $s_1, s_2, \dots, s_{2m+1} \geq 0$ consider the transformations (8) and (9) and define the following sets of unitary matrices

$$\mathcal{J}_n(H_1, H_2) = \{J_n(s_1, \dots, s_n) : \tau_1, \tau_2, \dots, \tau_n \geq 0\}.$$

U-controllability We say that the pair (H_1, H_2) of hermitian operators satisfies the *U-controllability* condition, if there exists n such that

$$\mathcal{J}_n(H_1, H_2) = U(N).$$

Theorem 3 *For the pair of hermitian operators (H_1, H_2) the U-controllability condition holds iff the linear span $\mathcal{L} = \mathcal{L}(H_1, H_2)$ (over the field of real numbers) of the operators*

$$H_1, H_2, \{H_1, H_2\}, \{H_1, \{H_1, H_2\}\}, \{H_2, \{H_1, H_2\}\}, \dots \quad (20)$$

coincides with \mathcal{O} .

The proof of this assertion one can find in many sources: see [14], also theorem 3.2.1, p. 82 in the book [16], also many references in [15]. Then \mathcal{L} is a subalgebra of \mathcal{O} with respect to the operation (19), and $i\mathcal{L}$ is called the dynamical Lie algebra in [16].

Denote $\Sigma \subset \mathcal{O} \times \mathcal{O}$ the set of all pairs of hermitian operators (H_1, H_2) , for which the *U-controllability* property holds. For any $H_1 \in \mathcal{O}$ define the set $\Sigma(H_1)$ of all $H_2 \in \mathcal{O}$ such that the pair (H_1, H_2) is *U-controllable*. We shall say that the operator H_1 is **almost U-controllable**, if the set $\Sigma(H_1)$ is open and everywhere dense in \mathcal{O} .

Theorem 4 *[almost all theorem] The following assertions hold:*

- 1) Σ is open and everywhere dense in $\mathcal{O} \times \mathcal{O}$.
- 2) the set of almost *U-controllable* operators is open and everywhere dense in \mathcal{O} .

One can find the formulations of theorem 4 in the papers [14], [17] and [18]. We provide below formal rigorous proof. But first we want to give more constructive criteria. Let $\lambda_1, \dots, \lambda_N$ be the eigenvalues of H_2 and ψ_1, \dots, ψ_N be the corresponding eigenvectors.

Theorem 5 *Assume that the following two conditions hold:*

1. $(H_1\psi_k, \psi_j) \neq 0$ for all $k \neq j$;
2. $\lambda_k - \lambda_l \neq \lambda_{k'} - \lambda_{l'}$ for any ordered pairs $(k, l) \neq (k', l') \in \{1, \dots, N\}^2$.

Then for $\mathcal{L} = \mathcal{L}(H_1, H_2)$ the following assertions hold:

1. if $\text{Tr}(H_1) = \text{Tr}(H_2) = 0$, then \mathcal{L} coincides with the subalgebra of all hermitian operators with zero trace;

2. otherwise \mathcal{L} coincides with \mathcal{O} .

Corollary 1 *If the operator H has all eigenvalues different, then H is almost U -controllable.*

Note that for the second condition of this theorem to hold it is sufficient that $\lambda_1, \dots, \lambda_N$ were linearly independent over \mathbb{Z} . One could deduce theorem 5 from results of [19], but we will give below a direct and simpler proof.

Convergence to Haar measure Consider the sequence (7) of time moments. For $t \geq 0$ define the following continuous time random process with values in $U(N)$: if $t_{n-1} \leq t < t_n$ then

$$X(t) = J_n(\tau_1, \tau_2, \dots, \tau_{n-1}, t - t_{n-1}), \quad X(0) = E, \quad (21)$$

(that is $X(t) = W(t)$ from 10). Define also the discrete time <<embedded>> process

$$X_n = X(t_n) = J_n(\tau_1, \tau_2, \dots, \tau_{n-1}, \tau_n).$$

Note that X_n is a Markov chain with values in $U(N)$, but $X(t)$ in general is not Markov. For any Borel subset $A \subset U(N)$ let $P_n(A)$ be the probability distribution of the random variable X_n .

Denote π the normed Haar measure on $U(N)$.

Theorem 6 [*convergence to Haar measure*] *Assume Condition D and that the pair (H_1, H_2) satisfies the U -controllability condition. Then the following assertions hold:*

1. $P_n \rightarrow \pi$ in variation as $n \rightarrow \infty$ exponentially fast, that is for some positive constants $c > 0, q < 1$, all Borel subsets $A \subset U(N)$ and all $n \geq 1$

$$|P_n(A) - \pi(A)| \leq cq^n;$$

2. For any bounded measurable function f , defined on $U(N)$, a. s.

$$\frac{1}{T} \int_0^T f(X(t)) dt \xrightarrow{T \rightarrow \infty} \int_{U(N)} f(u) \pi(du).$$

Convergence for quantum states Consider the set \mathcal{S} of real valued linear functionals on the algebra \mathcal{O} , such that

$$F(E) = 1, \quad F(A^2) \geq 0,$$

for any $A \in \mathcal{O}$, where E is the identity operator. Remind that any functional $F \in \mathcal{S}$ can be written as

$$F(A) = \text{Tr}(\rho A)$$

for some non negative definite operator ρ such that $\text{Tr}(\rho) = 1$, that is

$$\rho = \rho^*, \quad (\rho\psi, \psi) \geq 0,$$

for all $\psi \in \mathcal{H}$.

Dynamics on the set \mathcal{S} is defined by the differential (Schrodinger) equation

$$\frac{d\rho(t)}{dt} = -i[H, \rho(t)], \quad (22)$$

having the solution

$$\rho(t) = U(t)\rho(0)U^*(t),$$

where $U(t) = e^{-iHt}$ is unitary and H is hermitian.

We will say that the function $\rho(t)$, $t \geq 0$, converges in Cesaro sense as $t \rightarrow \infty$ to $\rho \in \mathcal{S}$, if

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \text{Tr}(\rho(t)A) dt = \text{Tr}(\rho A)$$

for any $A \in \mathcal{O}$. We shall use the notation $\rho(t) \rightarrow^c \rho$.

Theorem 7 [pure state convergence]

Assume that all eigenvalues of the matrix H are different and $\rho(0) = P_\psi$ is the projector on the unit vector ψ , then

$$\rho(t) \xrightarrow{c} \sum_{k=1}^N |(\psi, \psi_k)|^2 P_{\psi_k}$$

as $t \rightarrow \infty$, where ψ_1, \dots, ψ_n -are the eigenvectors of H , which form the orthonormal basis on \mathcal{H} .

From this theorem it follows that Cesaro limit of $\rho(t)$ depends on $\rho(0)$ (thus there is no “ergodicity” in this case). Now consider the case when the Hamiltonian H is time dependent:

$$\frac{d\rho(t)}{dt} = -i[H(t), \rho(t)]. \quad (23)$$

Namely, for the time sequence (7) define $H(t)$ as follows

$$H(t) = \begin{cases} H_1, & t_{2k} \leq t < t_{2k+1} \\ H_2, & t_{2k+1} \leq t < t_{2k+2} \end{cases},$$

for $k = 0, 1, \dots$ and some pair of hermitian operators H_1, H_2 .

Then one can write down the solution of (23) in terms of the process $X(t)$ (see (21)):

$$\rho(t) = X(t)\rho(0)X^*(t). \quad (24)$$

Theorem 8 [mixed state convergence] Assume that the conditions of the theorem 6 hold. Then for any $\rho(0) \in \mathcal{S}$ with probability one we have

$$\rho(t) \xrightarrow{c} \frac{1}{N} E, t \rightarrow \infty.$$

Generalizations for a weaker controllability condition Let us say that the pair of hermitian operators (H_1, H_2) is pure states controllable (or controllable for short), if there exists n , such that for any $\psi \in \mathcal{H}$

$$\mathcal{J}_n^\psi(H_1, H_2) = \mathcal{H}.$$

It is obvious that this condition follows from the U -controllability condition. The inverse statement in general is not true. Moreover, in the book [16] there is a general criterion of when the pair (H_1, H_2) is controllable in terms of \mathcal{L} (theorem 3.4.7).

Define the random process $\psi(t) = X(t)\psi$ and the embedded chain $\psi_n = X_n\psi$ as $\psi \in \mathcal{H}$. Let $P_n(\psi, A)$ denote the probability that ψ_n belongs to Borel subset $A \subset \mathcal{H}$. Denote π^* the uniform measure on $S = \{\psi \in \mathcal{H} : (\psi, \psi) = 1\}$.

Theorem 9 [measure convergence for weaker controllability]

Assume condition D and that for the pair (H_1, H_2) the (pure state) controllability condition holds. Then:

1. $P_n(\psi, \cdot)$ converges to π^* in variation as $n \rightarrow \infty$ exponentially fast and uniformly in $\psi \in S$, that is for some positive constants $c > 0$ and $q < 1$, for any Borel subsets $A \subset \mathcal{H}$ and all $\psi \in S$

$$|P_n(\psi, A) - \pi(A)| \leq cq^n$$

for all $n \geq 1$.

2. For any bounded measurable function f on S and any initial $\psi(0) \in S$ a.s.

$$\frac{1}{T} \int_0^T f(\psi(t)) dt \xrightarrow{T \rightarrow \infty} \int_S f(\psi) d\pi^*(\psi).$$

The proof is exactly the same as the proof of theorem 6.

Theorem on mixed states convergence holds also under controllability condition.

Theorem 10 [mixed state convergence 2]

Assume that the conditions of theorem 9 hold. Then for any $\rho(0) \in \mathcal{S}$ as $t \rightarrow \infty$ a.s.

$$\rho(t) \xrightarrow{c} \frac{1}{N} E.$$

2.2 Proofs

2.2.1 Proof of Theorems 4 and 5

We prove first the Theorem 5.

Further on, all matrices are considered in the basis ψ_1, \dots, ψ_N . Note that the set

$$\mathcal{T} = \{H \in \mathcal{O} : (H\psi_k, \psi_k) = 0, \text{ for all } k = 1, \dots, N\}$$

is a linear real space of dimension $d = N(N-1)$.

Lemma 2 \mathcal{T} is a subset of \mathcal{L} .

Proof. Define the operator $T : \mathcal{O} \rightarrow \mathcal{O}$ by

$$T(H) = \{H_2, H\}.$$

To prove the lemma it is sufficient to show that the real linear space generated by the matrices

$$T(H_1), T^2(H_1), \dots, T^d(H_1), \dots \quad (25)$$

coincides with \mathcal{T} . For the (k, j) -th element of the matrix $T(H)$ we have

$$(T(H))_{k,j} = h_{k,j}(\lambda_k - \lambda_j)i,$$

where $H = (h_{k,j})$. It follows that

$$(T^n(H))_{k,j} = h_{k,j}((\lambda_k - \lambda_j)i)^n.$$

As all elements of the matrix H_1 are non zero, then, for all n , the linear dependence of $T(H_1), T^2(H_1), \dots, T^n(H_1)$ over \mathbb{C} is equivalent to the linear dependence of the matrices T_1, \dots, T_n over \mathbb{C} , where

$$(T_n)_{k,j} = ((\lambda_k - \lambda_j)i)^n.$$

But this is possible (due to the condition on the eigenvalues of H_2) only for $n > \frac{N(N-1)}{2} = \frac{d}{2}$. Lemma is proved.

We will need one more lemma. Denote $E_{k,j} \in \mathcal{O}$ the hermitian operator with the matrix

$$(E_{k,j}\psi_{k'}, \psi_{j'}) = \begin{cases} 1, & k' = j' = k, \\ -1, & k' = j' = j, \\ 0, & \text{otherwise.} \end{cases}$$

Lemma 3 For all $k \neq j = 1, \dots, N$

$$E_{k,j} \in \mathcal{L}.$$

Proof. By symmetry it is sufficient to prove that $E_{1,N} \in \mathcal{L}$. For this we shall define the operator $S \in \mathcal{T}$, such that $\{H_1, S\} = E_{1,N}$. Lemma will follow from this. For any $\psi \in \mathcal{H}$ and $S \in \mathcal{O}$ we have:

$$(\{H_1, S\}\psi, \psi) = i((S\psi, H_1\psi) - (H_1\psi, S\psi)) = 2\text{Im}((H_1\psi, S\psi)).$$

Denote $H_1 = (h_{k,j})$. Define now the operator $S \in \mathcal{T}$ as follows:

$$\begin{aligned} S\psi_1 &= b_1\psi_2, \\ S\psi_k &= a_k\psi_{k-1} + b_k\psi_{k+1}, \quad k = 2, \dots, N-1, \\ S\psi_N &= a_N\psi_{N-1}, \end{aligned}$$

where $b_k = \bar{a}_{k+1}$, $k = 1, \dots, N-1$ and

$$a_k = \frac{i}{2h_{k,k-1}}, \quad k = 2, \dots, N.$$

We have:

$$\begin{aligned} (\{H_1, S\}\psi_1, \psi_1) &= 2\text{Im}(h_{2,1}\bar{b}_1) = 1, \\ (\{H_1, S\}\psi_k, \psi_k) &= 2\text{Im}(h_{k-1,k}\bar{a}_k + h_{k+1,k}\bar{b}_k) = \text{Im}\left(-h_{k-1,k}\frac{i}{h_{k,k-1}} + h_{k+1,k}\frac{i}{h_{k+1,k}}\right) = 0, \\ (\{H_1, S\}\psi_N, \psi_N) &= 2\text{Im}(h_{N-1,N}\bar{a}_N) = -1, \end{aligned}$$

where $k = 2, \dots, N-1$. It follows that for some $T \in \mathcal{T}$ one can write $\{H_1, S\} = E_{1,N} + T \in \mathcal{L}$. This proves the Lemma.

Return now to the proof of the theorem. In the first case, $\text{Tr}(H_1) = \text{Tr}(H_2) = 0$, it follows from the definition of \mathcal{L} that the trace of any operator $H \in \mathcal{L}$ is zero. In other words, $i\mathcal{L} \subset su(N)$, where $su(N)$ is the Lie algebra of the group of special unitary matrices. The dimension of $su(N)$ is $N^2 - 1$. Moreover, as $E_{1,k} \in \mathcal{L}$, $k = 1, \dots, N-1$ are linearly independent and do not belong to \mathcal{T} , the dimension of \mathcal{L} also equals $N(N-1) + N-1 = N^2 - 1$. Thus, $i\mathcal{L} = su(N)$.

Consider now the second case of the Theorem, that is when for some $k = 1, 2$ the trace of H_k is not zero. Let D be the operator with diagonal matrix, having the (j, j) -th element equal to $(H_k)_{j,j}$. As $\mathcal{T} \subset \mathcal{L}$, then $D \in \mathcal{L}$. As the trace of D is not zero, then $D, E_{1,2}, \dots, E_{N-1,N}$ are linearly independent. Then, by the arguments similar to those in the first case above, we get the proof of the Theorem.

Now we will give the **proof of theorem 4**.

Proof of Theorem

Proof of assertion 1) To prove the first statement of the theorem it is sufficient to prove the following two assertions:

a) Σ is the complement to some algebraic set in $\mathcal{O} \times \mathcal{O}$, that is to the set of zeroes of some system of polynomial equations.

b) the set Σ is not empty. This follows from Theorem 5.

Let us prove the assertion a). Let \mathcal{P} be the countable set of all operators (20). That is the algebra \mathcal{L} is, by definition, the linear span of the vectors from \mathcal{P} . The set \mathcal{O} of all hermitian operators can be considered as N^2 -dimensional linear space over reals. Then for the set $S_1, \dots, S_{N^2} \in \mathcal{O}$ of such operators denote $F(S_1, \dots, S_{N^2})$ the determinant of the matrix, with rows of which are these vectors. Note that if $S_1, \dots, S_{N^2} \in \mathcal{P}$, then

$$G_{S_1, \dots, S_{N^2}}(H_1, H_2) = F(S_1, \dots, S_{N^2})$$

is the polynomial of the elements of the matrices H_1, H_2 . Let E be the complement to Σ in $\mathcal{O} \times \mathcal{O}$. It is clear that $(H_1, H_2) \in E$ iff for any $S_1, \dots, S_{N^2} \in \mathcal{P}$ will be

$$G_{S_1, \dots, S_{N^2}}(H_1, H_2) = 0. \quad (26)$$

But by Hilbert's Basis theorem there exists finite set of polynomials of the elements of the pair (H_1, H_2) , with the same set of zeroes as the set (26). Thus the first assertion is proved.

Proof of 2) We proved above that Σ is the complement to some algebraic set E , that is

$$E = \{(H_1, H_2) : F_1(H_1, H_2) = \dots = F_m(H_1, H_2) = 0\}$$

for some polynomials F_1, \dots, F_m of the coefficients of the matrices of operators H_1, H_2 in some fixed basis. Consider the following algebraic set in \mathcal{O} :

$$E(H_1) = \{H_2 : F_1(H_1, H_2) = \dots = F_m(H_1, H_2) = 0\}.$$

It is clear that for any $H_1 \in \mathcal{O}$ the set $\Sigma(H_1)$ is the complement to $E(H_1)$ in \mathcal{O} . Then $\Sigma(H_1)$ is either open and everywhere dense or empty. The latter possibility can occur iff for any $k = 1, \dots, N$ the polynomial (considered as the function of the matrix H_2) $f_k(H_2) = F_k(H_1, H_2)$ is identically zero.

Let us show first that the set of almost U -controllable H_1 , that is for which $\Sigma(H_1)$ is open and everywhere dense, is open. Let H_1 be almost U -controllable. Then there exists H_2 , such that $F_k(H_1, H_2) \neq 0$ for some $k = 1, \dots, m$. Then for all H in some neighborhood of H_1 the inequality $F_k(H, H_2) \neq 0$ holds. We get from this that $\Sigma(H) \neq \emptyset$, then H is also almost U -controllable. Now it is sufficient to prove that the set of almost U -controllable operators from \mathcal{O} is dense. Now take H_2 from theorem 5. It is clear that the set of all H_1 for which $H_2 \in \Sigma(H_1)$ is dense. Our statement follows from this.

Proof of the Corollary.

Let us prove that in some orthonormal basis all non-diagonal elements of the matrix of H are non zero. Let ψ_1, \dots, ψ_N be the eigenvectors of H . For $t \geq 0$ consider the orthonormal basis

$$\psi_k(t) = e^{itS} \psi_k, \quad k = 1, \dots, N,$$

where the hermitian operator S is such that $(S\psi_k, \psi_j) \neq 0$ for all $k, j = 1, \dots, N$. We have

$$(H\psi_k(t), \psi_j(t)) = (H(t)\psi_k, \psi_j), \quad H(t) = e^{-itS} H e^{itS},$$

and

$$\frac{dH(0)}{dt} = i[H, S].$$

It follows that

$$\left(\frac{dH(0)}{dt} \psi_k, \psi_j \right) = (S\psi_k, \psi_j) i(\lambda_j - \lambda_k),$$

where $\lambda_1, \dots, \lambda_N$ are the eigenvalues of H corresponding to ψ_1, \dots, ψ_N . Then for $t \rightarrow 0$

$$(H\psi_k(t), \psi_j(t)) = \lambda_k \delta_{k,j} + (S\psi_k, \psi_j) i(\lambda_j - \lambda_k) t + \bar{o}(t).$$

Using the assumptions on H and the choice of S we conclude that for some small t and all $k \neq j = 1, \dots, N$ the following inequality holds

$$(H\psi_k(t), \psi_j(t)) \neq 0.$$

Now take any hermitian operator H_2 , satisfying the conditions of Theorem 5 with eigenvectors $\psi_1(t), \dots, \psi_N(t)$. By this theorem (H_1, H_2) is U -controllable. In the proof of theorem 4 we got that there is the alternative: either $\Sigma(H_1)$ is open and everywhere dense or empty. The theorem is proved.

Note that the condition that all eigenvalues are different is important. Because one can show that there is no orthonormal basis in which the matrix elements of the operator

$$H = \begin{pmatrix} \lambda & 0 \\ 0 & E \end{pmatrix}, \quad \lambda \neq 1, \lambda > 0,$$

are non zero. Nevertheless, from this one cannot state that this H is not almost U -controllable.

2.2.2 Mixed states convergence: theorem 8

By equality (24) and Theorem 6 about convergence, we have (further on $u \in U(N)$)

$$\rho(t) \xrightarrow{c} \rho = \int_{U(N)} u\rho(0)u^* d\pi(u).$$

For any $g \in U(N)$ we have

$$g\rho g^* = \int_{U(N)} (gu)\rho(0)(gu)^* d\pi(u) = \int_{U(N)} u\rho(0)u^* d\pi(u).$$

The last equality follows from the invariance of Haar measure with respect to left and right multiplication. Then for any $g \in U(N)$

$$g\rho g^* = \rho.$$

It follows that

$$\rho = \frac{1}{N}E.$$

The proof is finished.

2.2.3 Theorem 10 for (pure state) controllability condition

One can write the initial state as follows

$$\rho(0) = \sum_{k=1}^N c_k P_{\psi_k}, \quad \sum_{k=1}^N c_k = 1, \quad c_k \geq 0, \quad k = 1, \dots, N,$$

where ψ_1, \dots, ψ_N is an orthonormal basis of \mathcal{H} . Then

$$\rho(t) = \sum_{k=1}^N c_k P_{\psi_k(t)},$$

where $\psi_k(t) = X(t)\psi_k$. By theorem 9 concerning convergence with probability 1 we have:

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \text{Tr}(P_{\psi_k(t)} A) dt = \int_S (A\psi, \psi) d\pi^*(\psi) = \text{Tr}(\rho A),$$

where we put

$$\rho = \int_S \psi\psi^* d\pi^*(\psi).$$

Thus, with probability 1

$$\rho(t) \xrightarrow{c} \rho.$$

As measure π^* is invariant with respect to unitary transformations, then for any unitary matrix $u \in U(N)$ we have:

$$u\rho u^* = \int_S (u\psi)(u\psi)^* d\pi^*(\psi) = \rho,$$

and it follows that

$$\rho = \frac{1}{N}E.$$

2.2.4 Theorem 7: pure state convergence

Use the expansion of vector ψ in the eigenvectors of H :

$$\psi = \sum_{k=1}^N a_k \psi_k, \quad a_k = (\psi, \psi_k).$$

Then

$$\rho(t) = P_{\psi(t)}, \quad \psi(t) = e^{-iHt}\psi.$$

Let $\lambda_1, \dots, \lambda_N$ be eigenvalues of H corresponding to eigenvectors ψ_1, \dots, ψ_N correspondingly. Then

$$\psi(t) = \sum_{k=1}^N a_k e^{-i\lambda_k t} \psi_k.$$

For any hermitian operator A we have:

$$\text{Tr}(\rho(t)A) = (A\psi(t), \psi(t)) = \sum_{k,j} a_k \bar{a}_j e^{it(\lambda_j - \lambda_k)} (A\psi_k, \psi_j).$$

As

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T e^{it(\lambda_j - \lambda_k)} dt = \begin{cases} 1, & k = j \\ 0, & k \neq j \end{cases},$$

the theorem is proved.

2.2.5 Theorem 6

Here it is convenient to denote $U(N) = \mathcal{M}$.

Convergence for embedded chain It is necessary to do some remarks concerning possible proofs. This assertion could be examined using the general theory of Markov chains with general state space, see for example [12, 9, 8], as it was done in simpler cases for random walks on groups (see for example [21] p. 83, theorem 3.2.6). However, our proof will be based on theorem 4.1 in [7].

Note that X_n is a Markov process, which is not time homogeneous. But $\xi_n = X_{2n}$ will already be time homogeneous Markov process. We shall study ergodic properties of ξ_n and will understand how they could be related to ergodic properties of X_n .

Otherwise speaking ξ_n on \mathcal{M} can be defined as follows:

$$\xi_n = U_2^{T_{2n}} U_1^{T_{2n-1}} \xi_{n-1} = X_{2n} g, \quad n = 1, \dots, \quad \xi_0 = g \in \mathcal{M}.$$

For $g \in \mathcal{M}$ and Borel subset $A \subset \mathcal{M}$ let $P(g, A)$ be the one step transition probability of the chain ξ_n . The probability $P_m(A)$, defined at the beginning of this section, and $P(g, A)$ are connected as follows:

$$P_{2m}(A) = P^m(e, A),$$

$$P_{2m+1}(A) = \int_{\mathcal{M}} P_1(du) P^m(u, A),$$

for all $m \geq 1$, where $e \in \mathcal{M}$ is the identity transformation, $P^m(\cdot, \cdot)$ — m -th degree of the kernel $P(\cdot, \cdot)$.

Using Theorem 11, we get:

$$|P_{2m}(A) - \pi(A)| = |P^m(e, A) - \pi(A)| \leq cq^m,$$

$$|P_{2m+1}(A) - \pi(A)| = \left| \int_{\mathcal{M}} P_1(du) P^m(u, A) - \pi(A) \right| \leq \int_{\mathcal{M}} P_1(du) |P^m(u, A) - \pi(A)| \leq cq^m.$$

Thus we have proved the first assertion of Theorem 6.

Theorem 11 *Assume that the conditions of Theorem 6 hold. Then $P^n(g, \cdot)$ converges to π in variation as $n \rightarrow \infty$ exponentially fast and uniformly in $g \in \mathcal{M}$, that is for some positive constants $c > 0, q < 1$, all Borel subsets $A \subset \mathcal{M}$ and all $g \in \mathcal{M}$:*

$$|P^n(g, A) - \pi(A)| \leq cq^n \quad (27)$$

for all $n \geq 1$.

To prove this theorem we shall use theorem 4.1 from [7]. Let us check the conditions of this theorem, namely that ξ_n is a weakly Feller process, and that for some $n \geq 1$ the measure $P^n(g, \cdot)$ is equivalent to Haar measure π for any $g \in \mathcal{M}$.

Lemma 4 *(Condition A2 from [7]) The kernel $P(\cdot, \cdot)$ is a weak Feller, that is for any open $O \subset \mathcal{M}$ the transition probability $P(g, O)$ is lower semicontinuous in $g \in \mathcal{M}$.*

For any g denote $\mathbf{1}_g(s_1, s_2)$ the indicator function on $R_+ \times R_+$, that is $\mathbf{1}_g(s_1, s_2) = 1$ if $J_2(s_1, s_2)g \in O$, and zero otherwise. Then we have

$$P(g, O) = \int_{R_+ \times R_+} \mathbf{1}_g(s_1, s_2) p(s_1) p(s_2) ds_1 ds_2.$$

Let $g_n \rightarrow g, g_n \in \mathcal{M}$ as $n \rightarrow \infty$. Fix $s_1, s_2 \geq 0$ and consider two cases:

1. $J_2(s_1, s_2)g \in O$, then starting from some n the inclusion $J_2(s_1, s_2)g_n \in O$ holds, as O is open. That is why

$$\lim_{n \rightarrow \infty} \mathbf{1}_{g_n}(s_1, s_2) = \mathbf{1}_g(s_1, s_2) = 1;$$

2. $J_2(s_1, s_2)g \notin O$. Then

$$\liminf_n \mathbf{1}_{g_n}(s_1, s_2) \geq \mathbf{1}_g(s_1, s_2) = 0.$$

Thus for any s_1, s_2

$$\liminf_n \mathbf{1}_{g_n}(s_1, s_2) \geq \mathbf{1}_g(s_1, s_2).$$

Then by Fatou lemma

$$\liminf_n P(g_n, O) \geq P(g, O).$$

So, the lemma is proved.

Lemma 5 *(Condition A1 from [7]) For some $m \geq 1$ the measures π and $P^m(g, \cdot)$ are equivalent for any g . Moreover, there is exist m -step transition density $p^m(g, u)$ measurable on $\mathcal{M} \times \mathcal{M}$ and positive almost everywhere, such that*

$$P^m(g, B) = \int_B p^m(g, u) d\pi(u)$$

for all $g \in \mathcal{M}$ and all Borel subset $B \subset \mathcal{M}$.

Let us remind that ξ_n can be presented as follows

$$\xi_n = J_{2n}(\tau_1, \tau_2, \dots, \tau_{2n})g,$$

where operator J_{2n} was defined above. Further on we assume that $m = 2n^2$, where n is as in the definition of U -controllability. Introduce the following set

$$\Omega_m = \{(s_1, \dots, s_m) : s_i \geq 0, i = 1, \dots, m\} \subset \mathbb{R}_{\geq 0}^m.$$

For any $g \in \mathcal{M}$ the function $J_m^g(s_1, \dots, s_m) = J_m(s_1, \dots, s_m)g$ acts from Ω_m to \mathcal{M} , then by definition of U -controllability:

$$J_m^g(\Omega_m) = \mathcal{M}.$$

Lemma 6 For any measurable $B \subset \mathcal{M}$ its Haar measure $\pi(B) = 0$ iff the Lebesgue measure λ of the set $(J_m^g)^{-1}(B)$ in Ω_m is zero.

1) Assume that for some $B \subset \mathcal{M}$ we have $\pi(B) = 0$. Let us show that $\lambda((J_m^g)^{-1}(B)) = 0$. Let A_{cr} be the set of critical points of the map J_m^g (that is points $\bar{\tau} = (\tau_1, \dots, \tau_m)$ where the rank of the Jacobian is not maximal) and let $E = J_m^g(A_{cr}) \subset \mathcal{M}$ be the set of critical values of J_m^g . By Sard's theorem $\pi(E) = 0$. But as $J_m^g(\Omega_m) = \mathcal{M}$, then there exists non-critical point $\bar{\tau} = (\tau_1, \dots, \tau_m) \in \Omega_m$, that is such that the rank of dJ_m^g at this point equals N^2 . As the map J_m^g is analytic in the variables τ_1, \dots, τ_m , the set of points A_{cr} , where the rank is less than N^2 , has Lebesgue measure zero. Then the equality $\lambda((J_m^g)^{-1}(B)) = 0$ follows from theorem 1 of [26].

2) Assume that for some $B \subset \mathcal{M}$ we have $\pi(B) > 0$, and let us show that $\lambda((J_m^g)^{-1}(B)) > 0$. By Lebesgue differentiation theorem there exists point $g' \in \mathcal{M} \setminus E$ and its neighborhood $O(g')$ such that $\pi(O(g') \cap B) > 0$. Then there is point $\bar{\tau} = \bar{\tau}(g') \in (J_m^g)^{-1}(g')$ and some its neighborhood $O(\bar{\tau}) \subset \Omega_m$, so that the restriction of J_m^g on $O(\bar{\tau})$ is a submersion. Then $\pi(O(g') \cap B) > 0$ implies $\lambda((J_m^g)^{-1}(B) \cap O(\bar{\tau})) > 0$. So, lemma 6 is proven.

Denote $p_{\bar{\tau}}^{(m)}$ the product of $2m$ densities p_{τ} , then as for any $B \subset \mathcal{M}$

$$P^m(g, B) = \int_{(J_m^g)^{-1}(B)} p_{\bar{\tau}}^{(m)}(\bar{\tau}) d\bar{\tau},$$

by lemma 6 we get that P^m and π are equivalent measures.

The proof of measurability of the transition density one can find in theorem 1, p. 180 of [9], and in Proposition 1.1, p.5, of [8].

So, lemma 5 is proven.

Let us continue the proof of the assertion of Theorem 11 concerning convergence of the embedded chain. Let us check that Haar measure is invariant with respect to ξ_n . For Borel subset $B \subset \mathcal{M}$ we have:

$$\begin{aligned} (\pi P)(B) &= \int_{\mathcal{M}} d\pi(u) P(u, B) = \int_{\mathcal{M}} d\pi(u) \int_{R_+ \times R_+} \mathbf{1}(U_2^{s_2} U_1^{s_1} u \in B) p(s_1) p(s_2) ds_1 ds_2 = \\ &= \int_{R_+ \times R_+} p(s_1) p(s_2) ds_1 ds_2 \int_{\mathcal{M}} d\pi(u) \mathbf{1}(U_2^{s_2} U_1^{s_1} u \in B) = \pi(B), \end{aligned}$$

where the last equality follows from the invariance of Haar measure with respect to multiplication.

Further we shall use Theorem 4.1 from [7]. In this paper there is no assertions concerning geometric rate convergence. However, during proof of the theorem 4.1 in [7] (see the end of the proof) the following inequality was proved:

$$S_{n+k}(A) - I_{n+k}(A) \leq (1 - \delta)(S_n(A) - I_n(A)), \text{ for all } n = 1, 2, \dots, \quad (28)$$

where $0 < \delta < 1$, $k > 1$, $A \subset \mathcal{M}$, and

$$I_n(A) = \inf_{g \in \mathcal{M}} P^n(g, A), \quad S_n(A) = \sup_{g \in \mathcal{M}} P^n(g, A).$$

But it is obvious that from (28) the assertion (27) holds. Thus, we have proved the first item of Theorem 6.

Cesaro convergence For any measurable bounded function f on \mathcal{M} and any $T > 0$ define the followings integrals

$$M_f(T) = \frac{1}{T} \int_0^T f(X(t)) dt, \quad \pi(f) = \int_{\mathcal{M}} f(u) d\pi(u).$$

Define the random time T_n as

$$T_n = \sum_{k=1}^{2n} \tau_k, \quad n = 1, 2, \dots$$

Lemma 7 For any measurable bounded function f on \mathcal{M} the following limit holds a.s.

$$\lim_{n \rightarrow \infty} M_f(T_n) = \pi(f).$$

Proof. Denote $Y_k = (\xi_k, \tau_{2k+1}, \tau_{2k+2})$, $k = 0, 1, \dots$, $\xi_0 = e$ the Markov chain with values in $\mathcal{Y} = \mathcal{M} \times \mathbb{R}_+ \times \mathbb{R}_+$. Then

$$\begin{aligned} \int_{T_k}^{T_{k+1}} f(X(s)) ds &= \int_{T_k}^{T_k + \tau_{2k+1}} f(U_1^{s-T_k} \xi_k) ds + \int_{T_k + \tau_{2k+1}}^{T_{k+1}} f(U_2^{s-(T_k + \tau_{2k+1})} U_1^{\tau_{2k+1}} \xi_k) ds = \\ &= \int_0^{\tau_{2k+1}} f(U_1^s \xi_k) ds + \int_0^{\tau_{2k+2}} f(U_2^s U_1^{\tau_{2k+1}} \xi_k) ds = F(Y_k), \end{aligned} \quad (29)$$

where

$$F(g, t_1, t_2) = \int_0^{t_1} f(U_1^s g) ds + \int_0^{t_2} f(U_2^s U_1^{t_1} g) ds, \quad (g, t_1, t_2) \in \mathcal{Y}.$$

Then

$$M_f(T_n) = \frac{1}{T_n} \sum_{k=0}^{n-1} \int_{T_k}^{T_{k+1}} f(X(s)) ds = \frac{1}{T_n} \sum_{k=0}^{n-1} F(Y_k). \quad (30)$$

It is easy to show that Y_k has invariant measure $\mu = \pi \times P_\tau$, $P_\tau = p_\tau(s_1) p_\tau(s_2) ds_1 ds_2$, satisfies the conditions of theorem 4.2 in [7] as ξ_k satisfies it. Then

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{k=0}^{n-1} F(Y_k) = \mu(F) = \int_{\mathcal{Y}} F(g, t_1, t_2) d\mu,$$

where

$$\begin{aligned} \mu(F) &= \int_{\mathbb{R}_+ \times \mathbb{R}_+} P_\tau(dt_1 dt_2) \int_{\mathcal{M}} d\pi(g) \left(\int_0^{t_1} f(U_1^s g) ds + \int_0^{t_2} f(U_2^s U_1^{t_1} g) ds \right) = \\ &= \int_{\mathbb{R}_+ \times \mathbb{R}_+} P_\tau(dt_1 dt_2) \left(\int_0^{t_1} ds \int_{\mathcal{M}} d\pi(g) f(U_1^s g) + \int_0^{t_2} ds \int_{\mathcal{M}} d\pi(g) f(U_2^s U_1^{t_1} g) \right) \\ &= \pi(f) \int_{\mathbb{R}_+ \times \mathbb{R}_+} P_\tau(dt_1 dt_2) \left(\int_0^{t_1} ds + \int_0^{t_2} ds \right) = 2\pi(f) E\tau_1. \end{aligned}$$

Moreover, by strong law of large numbers for independent random variables τ_k we have

$$\lim_{n \rightarrow \infty} \frac{T_n}{n} = 2E\tau_1.$$

Then by (30) we get the proof of the lemma.

To prove the second part of theorem 6 we have to estimate the difference between $M_f(T)$ and $M_f(T_n)$. Using the boundedness $|f(g)| \leq c$ we have

$$|M_f(T) - M_f(T_n)| \leq \left| \frac{1}{T} \int_{T_n}^T f(X(s)) ds \right| + \frac{|T - T_n|}{T} |M_f(T_n)| \leq \frac{|T - T_n|}{T} (c + |M_f(T_n)|). \quad (31)$$

For any $T > 0$ define the random index $n(t)$ so that

$$T_{n(t)} \leq T < T_{n(T)+1},$$

and note that

$$\frac{|T - T_{n(T)}|}{T} \leq \frac{\tau_{2n(T)+1} + \tau_{2n(T)+2}}{T_{n(T)}} = \frac{\tau_{2n(T)+1} + \tau_{2n(T)+2}}{\sum_{k=1}^{2n(T)} \tau_k}.$$

As $E\tau_1 < \infty$, the law of large numbers, as $n \rightarrow \infty$, gives a.s.

$$\frac{\tau_{2N+1} + \tau_{2N+2}}{\sum_{k=1}^{2N} \tau_k} \rightarrow 0.$$

But $n(T) \rightarrow \infty$ as $T \rightarrow \infty$. Then the right-hand side of (31) tends to 0 a.s. as $n = n(T)$ and $T \rightarrow \infty$. Thus, we complete the proof of theorem 6.

2.3 From unitary to symplectic

Here, on a general but very simple example, we show how convergence in situations with unitary transformations is related to the similar question for the symplectic transformations. More information one can find in physical literature, see [24, 23, 22]

We consider C^N as complex Hilbert space of dimension $N < \infty$ with the standard basis $e_n, n = 1, 2, \dots, N$. Then any vector $f \in C^N$ can be presented as

$$f = \sum_n \lambda_n e_n, \lambda_n = q_n + ip_n. \quad (32)$$

with real q_n, p_n . Now let $U^t = e^{it\hat{H}}$ be unitary group in C^N where \hat{H} is a selfadjoint operator in C^N with matrix

$$(a_{kl} + ib_{kl}), a_{kl} = a_{lk}, b_{kl} = -b_{lk}.$$

For the Hamiltonian \hat{H} the quantum dynamics $f(t) = e^{it\hat{H}} f(0)$ for any vector $f(0) \in C^N$ satisfies the Schrodinger equation

$$-i \frac{\partial f}{\partial t} = \hat{H} f, \quad (33)$$

or

$$-i \frac{d\lambda_k}{dt} = -i \left(\frac{dq_k}{dt} + i \frac{dp_k}{dt} \right) = \sum_l (a_{kl} + ib_{kl})(q_l + ip_l),$$

or

$$\frac{dp_k}{dt} = \sum_l (a_{kl} q_l - b_{kl} p_l), \quad \frac{dq_k}{dt} = \sum_l (-a_{kl} p_l - b_{kl} q_l). \quad (34)$$

If we introduce the quadratic Hamiltonian

$$H = -\frac{1}{2} \sum_{k,l=1}^N a_{kl} (q_k q_l - p_k p_l) + \sum_{k,l=1}^N b_{kl} q_k p_l, \quad (35)$$

then the equations (34) coincide with the classical Hamiltonian equations

$$\frac{dq_k}{dt} = \frac{\partial H}{\partial p_k}, \quad \frac{dp_k}{dt} = -\frac{\partial H}{\partial q_k}, \quad (36)$$

as

$$\frac{\partial(\sum_{k,l} b_{kl} q_k p_l)}{\partial p_k} = -\frac{\partial(\sum_{k,l} b_{lk} q_k p_l)}{\partial p_k} = -\frac{\partial(\sum_{l,k} b_{kl} p_l q_k)}{\partial p_k} = -\sum_{k,l} b_{kl} q_l.$$

Remark 1 *It is interesting that this class of classical Hamiltonian dynamics has nothing to do with the standard Hamiltonian dynamics considered in section II.1 and Part III. Possible convergence to Liouville and Gibbs measures of such (gyroscopic) dynamics we shall discuss elsewhere.*

Part III

Gibbs equilibrium and memory

Here we use the notation (13)-(16) from section II.1, and consider the system (15) with quadratic Hamiltonian (14). Then, the density of Gibbs measure μ_β with respect to Lebesgue measure λ on R^{2N} is given by

$$\frac{d\mu_\beta}{d\lambda} = Z_\beta^{-1} \exp(-\beta H) = Z_\beta^{-1} \exp\left(-\frac{1}{2}(C_{G,\beta}^{-1}\psi, \psi)_2\right). \quad (37)$$

So it is gaussian with covariance matrix

$$C_{G,\beta} = \frac{1}{\beta} \begin{pmatrix} V^{-1} & 0 \\ 0 & E \end{pmatrix}. \quad (38)$$

Although Gibbs distribution is invariant with respect to this dynamics, convergence (for closed system) to it is impossible due to the law of energy conservation. Thus we have to introduce some random influence, and we consider the dynamics defined by the system of $2N$ stochastic differential equations, as in (6),

$$\frac{dq_k}{dt} = p_k, \quad \frac{dp_k}{dt} = -\sum_{l=1}^N V(k,l)q_l + \delta_{k,1}(-\alpha p_k + f_t). \quad (39)$$

This means that only one degree of freedom, namely 1 (first coordinate of the particle 1) is subjected to damping (defined by the factor $\alpha > 0$) and to the external force f_t , which we assume to be a gaussian stationary stochastic process.

3 Large time behavior for fixed finite N

One can rewrite system (39) in the vector notation

$$\frac{d\psi}{dt} = A\psi + F_t, \quad (40)$$

where

$$A = \begin{pmatrix} 0 & E \\ -V & -\alpha D \end{pmatrix}, \quad (41)$$

E is the unit ($N \times N$)-matrix, D is the diagonal ($N \times N$)-matrix with all zeroes on the diagonal except $D_{11} = 1$, and F_t is the vector $(0, \dots, 0, f_t, 0, \dots, 0) \in R^{2N}$.

Covariance All our external forces f_t will be gaussian stationary processes with zero mean. Among them there is the white noise - the generalized stationary gaussian process having covariance $C_f(s) = \sigma^2 \delta(s)$, it is sometimes called process with independent values (without memory). All other stationary gaussian processes, which we consider here, are processes with memory. We will assume that they have continuous trajectories and integrable (short memory) covariance

$$C_f(s) = \langle f_t f_{t+s} \rangle = E(f_t f_{t+s}).$$

Then the solution of (40) with arbitrary initial vector $\psi(0)$ is unique and is equal to

$$\psi(t) = e^{tA} \left(\int_0^t e^{-sA} F_s ds + \psi(0) \right). \quad (42)$$

Our goal, in particular, is to show that even weak memory, in the generic situation, prevents the limiting invariant measure (which always exists and unique) from being Gibbs. To formulate more readable results we assume more: C_f belongs to the Schwartz space $S = S(\mathbb{R})$. Then also the spectral density

$$a(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-it\lambda} C_f(t) dt$$

belongs to the space S .

We shall say that some property (for given V) holds for almost all C_f from the space S if the set $S^{(+)} \subset S$ where this property holds is open and everywhere dense in S .

Invariant subspaces The subspace $L_- \subset L$ was introduced in (17). Now we describe important properties of this set.

Lemma 8 1. L_- and its orthogonal complement denoted by L_0 , are invariant with respect to the operator A .

2. The spectrum of the restriction A_- of A on the subspace L_- belongs to the left half-plane, and as $t \rightarrow \infty$

$$\|e^{tA_-}\|_2 \rightarrow 0$$

exponentially fast, Moreover, L_- can be defined as

$$L_- = \{\psi \in L : H(e^{tA}\psi) \rightarrow 0, t \rightarrow \infty\} \subset L$$

Role of the memory

Theorem 12 Let f_t be either white noise or has continuous trajectories and integrable C_f . Then for any Hamiltonian H with $L_0 = \{0\}$ the following holds:

1. there exists gaussian random $(2N)$ -vector $\psi(\infty)$ such that for any initial condition $\psi(0)$ the distribution of $\psi(t)$ converges, as $t \rightarrow \infty$, to that of $\psi(\infty)$;

2. for the process $\psi(t)$ we have $E\psi(t) \rightarrow 0$ and the covariance -

$$C_{\psi(\infty)}(s) = \lim_{t \rightarrow \infty} \langle \psi(t)\psi^T(t+s) \rangle = \lim_{t \rightarrow \infty} C_{\psi}(t, t+s) = W(s)C_{G,1} + C_{G,1}W(-s)^T, \quad (43)$$

where

$$W(s) = \int_0^{+\infty} e^{\tau A} C_f(\tau+s) d\tau; \quad (44)$$

3. For the white noise with variance σ^2 the vector $\psi(\infty)$ has Gibbs distribution (37) with the temperature

$$\beta^{-1} = \frac{\sigma^2}{2\alpha};$$

4. If $\alpha = 0, \sigma^2 > 0$, then for any i the mean energy EH_i , where

$$H_i = \frac{p_i^2}{2} + \sum_j V(i, j)q_i q_j,$$

of the particle i tends to infinity. If $\alpha > 0, \sigma^2 = 0$, then it tends to zero.

We will use here the shorter notation $C_{\psi(\infty)}(0) = C_\psi$.

Theorem 13 *Let $N \geq 2$, and the Hamiltonian H is such that $L_0 = L_0(H) = \{0\}$. Then the following assertions hold:*

1. *for any $C_f \in S$ the limiting distribution does not have correlations between coordinates and velocities;*
2. *for almost any $C_f \in S$ there are non zero correlations between velocities, that is for some $i \neq j$ $C_\psi(p_i, p_j) \neq 0$. It follows that the limiting distribution cannot be Gibbs.*

Classes of Hamiltonians Here we describe classes of potentials with $\dim L_0 = 0$.

Let $\Gamma = \Gamma_N$ be connected graph with N vertices $i = 1, \dots, N$, and not more than one edge per each (unordered) pair of vertices (i, j) . It is assumed that all loops (i, i) are the edges of Γ . Denote \mathbf{H}_Γ the set of (positive definite) V such that $V(i, j) = 0$ if (i, j) is not the edge of Γ . It is easy to see that the dimension of the set \mathbf{H}_Γ is equal to the number of edges of Γ .

Examples can be complete graph with N vertices, or we can consider the d -dimensional integer lattice Z^d and the graph $\Gamma = \Gamma(d, \Lambda)$, the set of vertices of which is the cube

$$\Lambda = \Lambda(d, M) = \{(x_1, \dots, x_d) \in Z^d : |x_i| \leq M, i = 1, \dots, d\} \subset Z^d$$

and the edges (i, j) , $|i - j| \leq 1$.

In general, V is called γ -local on Γ if $V(i, j) = 0$ for all pairs i, j having distance $r(i, j)$ between them greater than γ , where the distance $r(i, j)$ between two vertices i, j on a graph is the minimal length (number of edges) of paths between them.

We shall say that some property holds for almost any Hamiltonian from the set \mathbf{H}_Γ if the set $\mathbf{H}_\Gamma^{(+)}$, where the property holds, is open and everywhere dense. Moreover, the dimension of the set $\mathbf{H}_\Gamma^{(-)} = \mathbf{H}_\Gamma \setminus \mathbf{H}_\Gamma^{(+)}$ where it does not hold, is less than the dimension of \mathbf{H}_Γ itself.

Lemma 9 *For almost any $H \in \mathbf{H}_\Gamma$ we have $\dim L_0 = 0$.*

4 Thermodynamic limit

We have studied above the limit $t \rightarrow \infty$ for fixed N and fixed potential $V = V_N$. Here we discuss the limit

$$\lim_{N \rightarrow \infty} \lim_{t \rightarrow \infty} .$$

First of all, it is not clear that this limit exists, and even less how it can look like. The only immediate conclusion is that, if it exists, it will be gaussian, and will depend on the covariance C_f . One of the central question is of course: how the limiting distribution will look like far away from the place of external influence, that is far away from the particle 1. Will the effect of the memory disappear or not, that is will this limit have Gibbs covariance or not.

In the white noise case it is easy to prove that we will get anyway the Gibbs distribution. Consider now the case when f_t is not the white noise. We will prove that for large N the matrices C_ψ become close to the simpler matrix

$$C_V = \frac{\pi}{\alpha} \begin{pmatrix} a(\sqrt{V})V^{-1} & 0 \\ 0 & a(\sqrt{V}) \end{pmatrix},$$

where \sqrt{V} is the unique positive root of V . First of all note that: 1) C_V also defines an invariant measure with respect to pure (that is with $\alpha = 0, f_t = 0$) Hamiltonian dynamics; 2) for the white noise case C_V , corresponds to the Gibbs distribution.

We assume that some graph Γ is given with the set of vertices Λ , $|\Lambda| = N$. For any $V \in \mathbf{H}_\Gamma$ such that $L_0(V) = \{0\}$, the following representation of the limiting covariance matrix appears to be crucial

$$C_\psi = C_V + Y_V,$$

where Y_V is some remainder term.

The following theorem gives the estimates for Y_V . The norm $\|V\|_\infty$ of a matrix V we define by the formula

$$\|V\|_\infty = \max_i \sum_j |V(i, j)|.$$

Theorem 14 *Assume that V is γ -local and $\|V\|_\infty < B$ for some $B > 0$. Fix also some number $\eta = \eta(N) \geq \gamma$. Then the following assertions hold:*

1. *If $C_f \in S$ and has bounded support, that is $C_f(t) = 0$ if $|t| > b$ for some $b > 0$, then for any pair i, j far away from the particle 1, that is the distances $r(i, 1), r(j, 1) > \eta(N)$, there is the following estimate*

$$|Y_V(q_i, q_j)|, |Y_V(p_i, p_j)| < K_0 \left(\frac{K}{\eta} \right)^{\eta\gamma^{-1}}$$

for some constants $K_0 = K(C_f, B, b, \alpha, \gamma)$ and $K = K(C_f, B, b, \alpha, \gamma)$, not depending on N .

2. *For arbitrary $C_f \in S$ the estimate is*

$$|Y_V(q_i, q_j)|, |Y_V(p_i, p_j)| < C(k)\eta^{-k},$$

for any $k > 0$ and some constant $C(k) = C(C_f, k, B, \alpha, \gamma)$, not depending on N .

This theorem allows to do various conclusions concerning the thermodynamic limit. We give an example.

Fix some $C_f(t) \in S$ and some connected countable graph Γ_∞ with the set of vertices Λ_∞ and an increasing sequence of subsets $\Lambda_1 \subset \Lambda_2 \subset \dots \subset \Lambda_n \subset \dots$ such that $\Lambda = \cup \Lambda_n$. Let Γ_n be the subgraph of Γ_∞ with the set of vertices Λ_n , that is Γ_n inherits all edges between vertices of Λ_n from Γ . Here it will be convenient to assume that, for any fixed n , the specified particle (the only one having contact with external world) has number $N_n = |\Lambda_n|$. We assume also that for any $i \in \Lambda_\infty$ its distance $r_n(i, N_n)$ to the particle N_n tends to ∞ as $n \rightarrow \infty$.

Let $l^\infty(\Gamma_\infty)$ be the complex Banach space of bounded functions on the set of vertices of Γ_∞ :

$$l^\infty(\Gamma_\infty) = \{(x_i)_{i \in \Gamma_\infty} : \sup_{i \in \Gamma_\infty} |x_i| < \infty, x_i \in \mathbb{C}\}.$$

Fix some γ -local infinite matrix V on this space and such that $\|V\|_\infty \leq B$. It is clear that V defines a bounded linear operator on $l^\infty(\Gamma_\infty)$. Denote $\sigma(V)$ the spectrum of this operator. Let $V_n = (V(i, j))_{i, j \in \Lambda_n}$ be the restriction of V on Λ_n , it is a matrix of the order N_n . Assume that for all $n = 1, 2, \dots$ the matrices V_n are positive-definite. Note that the condition $L_-(V_n) = L$ may not hold for some n . However, one can choose a sequence of positive-definite matrices $V'_n \in \mathbf{H}_{\Lambda_n}$ such that $\|V_n - V'_n\|_\infty \rightarrow 0$ as $n \rightarrow \infty$ with $L_0(V'_n) = \{0\}$. Moreover, the convergence of V'_n to V_n can be chosen arbitrary fast. Denote $C_\psi^{(n)}$ the limiting covariance matrices corresponding to V'_n .

Corollary 2 *The following assertions hold:*

1. *for any $i, j \in \Lambda_\infty$ there exists the thermodynamic limit*

$$\lim_{n \rightarrow \infty} C_\psi^{(n)}(p_i, p_j) = C_\psi^{(\infty), p}(i, j),$$

that is for distribution of velocities;

2. if for any $i, j \in \Lambda_\infty$ there exists finite limits :

$$U(i, j) \doteq \lim_{n \rightarrow \infty} V_n^{-1}(i, j), \quad (45)$$

then for the coordinates we have

$$\lim_{n \rightarrow \infty} C_\psi^{(n)}(q_i, q_j) = C_\psi^{(\infty), q}(i, j);$$

3. assume that the spectral density $a(\sqrt{\lambda})$ is analytic on the open set containing the spectrum $\sigma(V)$. Then

$$C_\psi^{(\infty), p}(i, j) = a(\sqrt{V}),$$

where $a(\sqrt{V})$ is defined in terms of the operator calculus on $l^\infty(\Gamma_\infty)$ ([25], p. 568).

In ([5]) one can find all proofs in more general situation when more than one particle have contact with external world.

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