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Role of the Memory in Convergence to Invariant Gibbs Measure[1]

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Linear hamiltonian systems were always an interesting object to study (see, for example, [1, 2]), in particular in non-equilibrium statistical mechanics (see [3, 4] and references therein). For closed linear systems it is senseless to consider convergence to invariant Gibbs measure, as the invariant tori provide many invariant measures having nothing to do with the Gibbs measures. However, if even only one (of N) degree of freedom has direct contact with the external world (that is subjected to a random external force), the situation changes radically. The invariant subspaces and tori get intermixed by the dynamics and the convergence to the unique (invariant) measure becomes a generic property. This invariant measure is the Gibbs measure, if the external force is the white noise (having no time memory). If the external force has time correlations, then we will have the convergence to some invariant measure which typically will not be Gibbs. This assertion holds both for systems with finite number degrees of freedom and (in the thermodynamic limit) for degrees of freedom situated (infinitely) far away from the contacts with external world. Now we come to exact formularions.

Definitions. We consider the phase space with N degrees of freedom

$$L = L_{2N} = \mathbb{R}^{2N}$$

$$= \left\{ \psi = \begin{pmatrix} q \\ p \end{pmatrix} : q = (q_1, q_2, \ldots, q_N)^{\mathrm{T}}, \right.$$

$$\left. p = (p_1, p_2, \ldots, p_N)^{\mathrm{T}} \in \mathbb{R}^N \right\},$$

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(T denotes transposition, thus ψ is a column-vector) with the scalar product $(\psi, \psi')_2 = \sum_{i=1}^{N} (q_i q_i' + p_i p_i')$. It is the direct sum

$$L = l_N^{(q)} \oplus l_N^{(p)} \tag{1}$$

of orthogonal coordinate and momentum subspaces with the induced scalar products $(q, q')_2$ and $(p, p')_2$ correspondingly. We specify $1 \le m \le N$ degrees of freedom

$$\Lambda_m = \{N - m + 1, \ldots, N\} \subset \Lambda = (1, 2, \ldots, N),$$
$$m \ge 1,$$

and consider dynamics, defined by the system of $2N$ stochastic differential equations

$$\frac{dq_k}{dt} = p_k,$$
$$\frac{dp_k}{dt} = -\sum_{l=1}^{N} V(k, l) q_l - \alpha \delta_k^{(m)} p_k + F_{t, N+k}, \tag{2}$$

where $k = 1, \ldots, N$, $V = (V(k, l))$ is the positive definite $(N \times N)$-matrix, $\delta_k^{(m)} = 1$ for $k > N - m$ and $\delta_k^{(m)} = 0$ for $k \le N - m$. This means that only degrees of freedom from the specified subset $\Lambda^{(m)}$ (we call this set the boundary of Λ) is subjected to dissipation (defined by the factor $\alpha > 0$) and to the external forces. It is convenient to introduce the $2N$-vector F_t so that its components $F_{t,k} = 0$, $k \le \le 2N - m$, and for $k > 2N - m$ the processes $F_{t,k}$ are independent copies of some stationary gaussian process f_t.

If $\alpha = 0$, $f_t = 0$, then the system (2) becomes the linear hamiltonian system with the quadratic hamiltonian

$$H(\psi) = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + \frac{1}{2}\sum_{i,j} V(i,j) q_i q_j. \tag{3}$$

Note that the Gibbs distribution, corresponding to the hamiltonian (3),

$$Z^{-1}\exp(-\beta H) = Z^{-1}\exp\left(-\frac{1}{2}(C_{G,\beta}^{-1}\psi, \psi)_2\right) \tag{4}$$

is a gaussian vector, and its covariance in the (2×2)-block form, corresponding to the expansion (1), can be written as

$$C_{G,\beta} = \beta^{-1}\begin{pmatrix} V^{-1} & 0 \\ 0 & E \end{pmatrix}. \quad (5)$$

In the vector form the system (2) can be rewritten as

$$\frac{d\psi}{dt} = A\psi + F_t, \quad A = \begin{pmatrix} 0 & E \\ -V & -\alpha D \end{pmatrix}, \quad (6)$$

where E is the unit $(N \times N)$-matrix, D is the diagonal $(N \times N)$-matrix with $D_{k,k} = 1$, $k = N - m + 1, \ldots, N$ and $D_{kk} = 0$, $k \le N - m$.

Invariant subspaces Let us define the subset of the phase space L

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

Denote e_i the N-vectors-columns with all zero components, except the i-th component, equal to one.

Lemma 1. 1. *L_- is a linear subspace of L and* $L_- = \left\{\begin{pmatrix} q \\ p \end{pmatrix} \in L: q \in l_V, p \in l_V\right\}$, *where* l_V is the subspace of R^N, *generated by the vectors* $V^k e_i$, $i = N - m + 1, \ldots, N$; $k = 0, 1, \ldots$. *Moreover, L_- and its orthogonal complement L_0, are invariant with respect to the operator A.*

2. *The spectrum of the restriction A_- of the operator A onto the subspace L_- belongs to the left half-plane, and* $\|e^{tA_-}\|_2 \to 0$, *as* $t \to \infty$, *exponentially fast.*

Classes of hamiltonians For any N define the class $\mathbf{H}_N$ of all hamiltonians (3) with positive definite matrix V. The dimension of this set is $\dim \mathbf{H}_N = \frac{N(N+1)}{2}$, that coincides with the dimension of the set of all symmetric matrices V. In fact, take some positive definite matrix V, for example, a diagonal matrix. Then the matrix $V + V_1$, where V_1 is symmetric and has sufficiently small elements, will be positive definite.

More general, let $\Gamma = \Gamma_N$ be a connected (non-oriented) graph with N vertices $i = 1, \ldots, N$, where each pair (i, j) of vertices is connected by not more than one edge, and it is assumed that all pairs (i, i) are edges of Γ. Let $\mathbf{H}_\Gamma$ be the set of positive definite V such that $V(i, j) = 0$, if (i, j) is not the edge of Γ. The same argument shows that the dimension of the set $\mathbf{H}_\Gamma$ equals the number of edges of the graph Γ. Note that $\mathbf{H}_N = \mathbf{H}_\Gamma$ in the case of complete graph Γ with N vertices. In particular, one can consider the graph $\Gamma = \Gamma(d, \Lambda)$, the set of vertices of which is the cube of the d-dimensional lattice

$$\Lambda = \Lambda^{(M)} = \{(x_1, x_2, \ldots, x_d) \in Z^d: |x_i| \le M,$$
$$i = 1, 2, \ldots, d\} \subset Z^d,$$

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

We shall say that sone property holds for almost all 1 hamiltonians of $\mathbf{H}_\Gamma$, if the set $\mathbf{H}_\Gamma^{(+)}$, where this property holds, is open and everywhere dense.

Lemma 2. *For all* Γ, *defined above and almost all* $\mathbf{H} \in \mathbf{H}_\Gamma$ *we have* $\dim L_0 = 0$.

External forces The external force f_t is assumed to be a stationary gaussian process with zero mean. Among them we distinguish the process without memory, that is generalized gaussian process with independent values—the white noise with covariance $C_f(s) = \sigma^2\delta(s)$. Other processes, which we will consider here, processes with memory, are stationary gaussian processes with zero mean and covariance $C_f(s) = \langle f_t f_{t+s}\rangle$. We assume that these processes have continuous trajectories and integrable covariance. For all such processes it is known that the solution of the system (6), and any initial vector $\psi(0)$, exists for all t, is unique and equals

$$\psi(t) = e^{tA}\left(\int_0^t e^{-sA}F_s ds + \psi(0)\right). \quad (7)$$

To have more completed results we assume sometimes that C_f belongs to the Schwartz space S. The the spectral density

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

of the process also belongs to the space S.

We shall say that some property holds for almost any C_f from the class S, if the set $S^{(+)}$, where it holds, is open and everywhere dense subset of the Schwartz space.

Finite systems Taking (5) into account, put $C_G = C_{G,2\alpha}$, Fix some connected graph Γ with $N > 1$ vertices.

Theorem 1. *Let f_t is either-the white noise or has continuous trajectories and integrable covariance. Then for almost all hamiltonians $H \in \mathbf{H}_\Gamma$ the following holds*

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

2. *moreover, for the covariance of the process* $\psi(t)$ *we have*

$$C_{\psi(\infty)}(s) = \lim_{t \to \infty} C_\psi(t, t+s)$$
$$= \lim_{t \to \infty}\langle\psi(t)\psi^{\mathrm{T}}(t+s)\rangle = W(s)C_G + C_G W(-s)^{\mathrm{T}}, \quad (8)$$

where

$$W(s) = \int_0^{+\infty} e^{\tau A}C_f(\tau + s)d\tau. \quad (9)$$

Proposition 1. *If f_t is the white noise with variance* σ^2, *then the vector* $\psi(\infty)$ *has Gibbs distribution* (4) *with the temperature*

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

This result for $m = 1$ has been proved in [6]. From (8) it follows also another useful expression

$$C_\psi = -\int_{-\infty}^{+\infty} a(\lambda)(R_A(i\lambda)C_G + C_G R_A^{\mathrm{T}}(i\lambda))d\lambda$$

for $C_\psi = C_{\psi(\infty)}(0)$ in terms of the spectral density $a(\lambda)$ and the resolvent A

$$R_A(z) = (A - z)^{-1}.$$

Theorem 2. *Let $N \geq 2$, fix the graph Γ and some $H \in \mathbf{H}_\Gamma$ with $L_0 = \{0\}$. Then we have the following statements*:

2 1. *for any $C_f \in S$ in thye limiting distribution there are no correlations of the coordinate-velocity type, that is $C_\psi(q_i, p_j) = 0$ for any i, j;*

2. *for almost any $C_f \in S$ there are non-zero correlations between velocities, that is $C_\psi(p_i, p_j) \neq 0$ for some $i \neq j$. Thus, the limiting distribution is not Gibbs.*

Large N It is more interesting to prove that the convergence to Gibbs measure

is impossible even in the points infinitely far away from the boundary in the thermodynamic limit $N \to \infty$. The following results reduces (for large N) the calculation of the matrix C_ψ to the calculation of 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 square unique root of V. It is interesting to note that C_V is also an invariant measure with respect to the purely (that is for $\alpha = 0$, $F_t = 0$) hamiltonian dynamics, and corresponds to Gibbs measure in the white noise case.

Let be given some connected graph Γ with the set Λ, $|\Lambda| = N$ of vertices, and with the boundary $\Lambda^{(m)}$. The distance $r(i, j)$ between vertices i and j on the graph is defined as the minimal length (number of edges) of a path between them. Firther on we assume V to be γ-local on Γ, that is $V(i, j)$ is zero if $r(i, j) > \gamma$. Let $\eta \geq \ln m$.

Theorem 3. *Let V be is γ-local and $\|V\|_\infty =$*
3 *$\max_i \sum_j |V(i,j)| \leq B$ for some $B > 0$. for almot all $H \in \mathbf{H}_\Gamma$. Then the limiting covariance matrix has the decomposition*

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

where Y_V is the remainder term, which is small in the following sense. Then if $C_f(t)$ has bounded support, that is if $C_f(t) = 0$ for $|t| > b$, then for any pair i, j far from the boundary, that is on the distance $r(i, \Lambda^{(m)})$, $r(j, \Lambda^{(m)}) > \eta(N)$, the following estimate holds

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

for some constants $K_0 = K(b, B, \alpha, \gamma)$, $K = K(b, B, \alpha, \gamma)$, not depending on N. 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 all $k > 0$ and some constants $\|V^{-1}\|_\infty C(k) = C(k, b, B, \alpha, \gamma)$.

From this theorem one can extract various corollaries concerning thermodynamic limit. For example, let us fix $a(\lambda) \in S$, and also some connected graph Γ_∞ with the set Λ_∞ of vertices, and consider an increasing sequence $\Gamma_1 \subset \Gamma_2 \subset \ldots \subset \Gamma_n \subset \ldots$ of subgraphs such that $\Gamma = \cup\Gamma_n$. Let Λ_n be the set of vertices of Γ_n (we assume that the subgraph with the fixed set of vertices inherits all edges of the graph Γ, between these vertices), $N_n = |\Lambda_n|$ and assume that also the boundaries $\Lambda_n^{(m)}$ are given, so that $m = m(n) = o(N_n)$. Fix also so me γ-local positive definite V with $\|V\|_\infty \leq B$. Denote V_n the restriction of V onto Λ_n. Note that the condition $L_0(V_n) = \{0\}$ might be not valid.

However, there exists a sequence of positive definite operators V_n' such that for $L_0 = L_0(V_n') = \{0\}$ for n and $\|V_n - V_n'\|_\infty \to 0$ for $n \to \infty$ Denote $C_\psi^{(n)}$ the limiting covariance matrix for V_n'.

Theorem 4. *@@Если для всех $i, j \in \Gamma_\infty$ существует предел $\lim_{n\to\infty} V_n^{-1}(i,j) = V^{-1}(i, j)$ и $\|V^{-1}\|_\infty < \infty$, то @@ The thermodynamic limit $C_\psi^{(\infty)} = \lim_{n\to\infty} C_\psi^{(n)}$ exists, but is not Gibbs. More exactly, $C_\psi^{(\infty)}(p_i, p_j) \neq 0$ for any two vertices $i \neq j$* in Λ_∞ *such that $a(\sqrt{V})(i, j) \neq 0$ and such that, starting with some n, $r(i, \Lambda_n^{(m(n))})$, $r(j, \Lambda_n^{(m(n))}) \geq \ln m(n)$.*

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