Linear Hamiltonian Systems under Microscopic Random Influence

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Abstract

It is known that a linear hamiltonian system has too many invariant measures, thus the problem of convergence to Gibbs measure has no sense. We consider linear hamiltonian systems of arbitrary finite dimension and prove that, under the condition that one distinguished coordinate is subjected to dissipation and white noise, then, for almost any hamiltonians and almost any initial conditions, there exists the unique limiting distribution. Moreover, this distribution is Gibbsian with the temperature depending on the dissipation and of the variance of the white noise.

1 Main Results

Consider the phase space

$$L = L_{2N} = \mathbb{R}^{2N} = \{ \psi = (q, p) : q = (q_1, \dots, q_N), p = (p_1, \dots, p_N) \in \mathbb{R}^N \}$$

with the scalar product

$$(\psi, \psi')_1 = \sum_{i=1}^N (q_i q'_i + p_i p'_i).$$

The space L is the direct sum $L = l_N^{(q)} \oplus l_N^{(p)}$ of orthogonal coordinate space and momentum space with the induced scalar products $(q, q')_1$ and $(p, p')_1$ correspondingly. We are most interested in the case of large N, but we do not use it in the present paper.

We shall study the following system of 2N stochastic differential equations (k = 1, ..., N)

$$dq_{k} = p_{k} dt,$$

$$dp_{k} = \sum_{l=1}^{N} \left((-V(k,l)q_{l} - D(k,l)p_{l}) dt + B(k,l) dw_{t,l} \right),$$
(1)

where V = (V(i, j)) is a positive definite $(N \times N)$ -matrix, D = (D(i, j)) is the non-negative definite symmetric $(N \times N)$ -matrix, B = (B(k, l)) is an arbitrary real matrix, $w_{t,l}$, $l = 1, \ldots, N$, are the standard brownian processes, independent in l.

If D = B = 0, then the system is a linear hamiltonian system with the quadratic hamiltonian

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

We will consider systems where the matrices B and D are as follows (for some n = 1, ..., N)

$$D = \alpha \Delta_n, \quad B = \sigma \Delta_n,$$

where $\Delta_n = (\delta_{i,j}\delta_{i,n})$ is the matrix with one diagonal element equal to 1 and other elements are all zero. Note that in this case the system will be subjected to only one white noise $dw_{t,n}$. We assume that the index n is fixed, and write for shortness $dw_t = dw_{t,n}$. Further on, unless otherwise stated, we assume that $\alpha > 0, \sigma > 0$.

System (1) can be rewritten in the matrix form

$$d\psi = A\psi \, dt + \sigma g_n \, dw_t,\tag{3}$$

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where

$$A = \left(\begin{array}{cc} 0 & E \\ -V & -D \end{array} \right),$$

E is the unit $(N \times N)$ -matrix, $g_n = (0, e_n) \in l_N^{(p)}$, and $e_n = (0, \ldots, 0, 1, 0, \ldots, 0) \in \mathbb{R}^N$ is *n*-th standard basis vector. The solution of the latter equation with arbitrary initial vector $\psi(0)$ is uniquely defined and can be written as (for example, see section 12.4 of [8])

$$\psi(t) = e^{tA} \left(\sigma \int_0^t e^{-sA} g_n \, dw_s + \psi(0) \right).$$

Introduce the set

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

We will need the following results.

Lemma 1. The set L_{-} is a linear subspace of the space L, and moreover $L_{-} = \{(q, p) \in L : q \in l_V, p \in l_V\}$ where l_V -is the subspace of \mathbb{R}^N , generated by the vectors $V^k e_n$, k = 0, 1, ..., in particular $g_n \in L_{-}$. Moreover, L_{-} and its orthogonal complement, denoted further by L_0 , are invariant with respect to the operator A.

All assertions of this lemma have been proven in [4].

By this lemma any initial vector $\psi(0)$ can be uniquely decomposed as

$$\psi(0) = \psi_0 + \psi_-, \qquad \psi_0 \in L_0, \quad \psi_- \in L_-$$

Then the solution $\psi(t)$ of the stochastic equation (3) with initial vector $\psi(0)$ for any $t \ge 0$ can be decomposed as

$$\psi(t) = \psi^{(0)}(t) + \psi^{(-)}(t), \tag{4}$$

where $\psi^{(0)}(t)$, $\psi^{(-)}(t)$ satisfy the equations

$$\dot{\psi}^{(0)}(t) = A\psi^{(0)}(t), \quad d\psi^{(-)}(t) = A\psi^{(-)} dt + \sigma g_n dw_t$$

with the initial conditions $\psi^{(0)}(0) = \psi_0$, $\psi^{(-)}(0) = \psi_-$ correspondingly. In fact, the sum of these equations give the equation (3).

By Lemma 1, the function $\psi^{(0)}(t) \in L_0, t \in [0, \infty)$, is deterministic and can be written as

$$\psi^{(0)}(t) = e^{At}\psi^{(0)}(0),\tag{5}$$

and $\psi^{(-)}(t)$ is a gaussian random process with values in L_{-} (as $g_n \in L_{-}$).

Theorem 1. For any $\psi(0)$ the convergence in distribution

$$\psi^{(-)}(t) \underset{t \to \infty}{\longrightarrow} \xi$$

takes place, where $\xi \in L_{-}$, and its distribution is absolutely continuous with respect to Lebesgue measure on L_{-} (defined by the euclidean structure), and has the following density with respect to this measure

$$p_{\xi}(\psi) = \frac{1}{Z} \exp\left(-\frac{2\alpha}{\sigma^2} H(\psi)\right), \qquad \psi \in L_{-}.$$
(6)

The limit of the mean energy is:

$$\lim_{t \to +\infty} \mathbf{E} H(\psi^{(-)}(t)) = \frac{\sigma^2}{4\alpha} \dim L_-$$

Thus, the action of the random force and dissipation on one particle only garanties convergnce to the invariant Gibbs measure with the temperature depending on α and σ .

The first assertion of the next theorem shows that convergence to Gibbs distribution is a typical property of linear hamiltonian systems with dissipation and random force. The second assertion shows that the dissipative term is necessary for this convergence.

For given N denote \mathbf{H}_N the smooth manifold of all possible hamiltonians H as in (2), that is the smooth manifold of all positive definite $(N \times N)$ -matrices V. Let μ be an arbitrary absolutely continuous probability measure on \mathbf{H}_N , and let $\mathbf{H}_N^{(+)}$ be the set of all hamiltonians of \mathbf{H}_N , for which the dimension of L_0 is greater than zero.

Theorem 2. 1. The measure μ of the subset $\mathbf{H}_N^{(+)}$ is zero. 2. If $\alpha = 0$, then for any initial condition $\psi(0)$ we have

$$\mathbf{E} H(\psi(t)) = \frac{\sigma^2}{2} t + O(1).$$

Note that for more restricted (physical) classes of hamiltonians the property dim $L_0 = 0$ is not typical (see [4] in this respect).

In this short note we restrict ourselves to the most interesting case of one distinguished particle, which shows that even the minimal introducing of stochasticity to the system garanties the convergence to the physical equilibrium. Note however, that most results can be generalized to arbitrary matrices D and B. Similar systems, mainly one-dimensional (one of the goal was to justify the Fourier law of heat conduction) were considered in the 1960-70 in the series of papers by J. Lebowitz and colleagues (see [1], [2] and references therein).

2 Proofs

Proof of theorem 1. Assume first that dim $L_0 = 0$. In this case the spectrum of the matrix A belongs to the left half-plane.

Let us prove the convergence first. By the latter assumption, we can consider only the process $\psi^{(-)}(t)$, admitting the following decomposition

$$\psi^{(-)}(t) = \psi^{(g)}(t) + \psi^{(d)}(t),$$

$$\psi^{(g)}(t) = \sigma e^{tA} \int_0^t e^{-sA} g_n \, dw_s, \quad \psi^{(d)}(t) = e^{tA} \psi^{(-)}(0).$$

By definition of L_{-} the function $\psi^{(d)}(t)$ tends to zero if $t \to +\infty$. That is why it is sufficient to prove the convergence of $\psi^{(g)}(t)$. Denote $C(t) = (\mathbf{E} \{\psi_i^{(g)}(t)\psi_i^{(g)}(t)\})$ the covariance matrix. Then

$$C(t) = \mathbf{E} \{ \psi^{(g)}(t)(\psi^{(g)})^T(t) \} = \sigma^2 e^{tA} \mathbf{E} \left\{ \int_0^t e^{-sA} g_n \ dw_s \int_0^t g_n^T e^{-sA^T} \ dw_s \right\} e^{tA^T},$$

where T denotes transposition. Using the Ito isometry [7], we get

$$C(t) = \sigma^2 e^{tA} \int_0^t e^{-sA} g_n g_n^T e^{-sA^T} \, ds \, e^{tA^T}.$$
(7)

Let us calculate the integral in the last formula by finding the matrix U, not depending on time and such that

$$\int_{0}^{t} e^{-sA} g_n g_n^T e^{-sA^T} \, ds = e^{-tA} U e^{-tA^T} - U. \tag{8}$$

Differentiation (8) in t shows that the exponents cancel and we get

$$AU + UA^T = -g_n g_n^T.$$

This equation with respect to U has the unique solution, as the spectrum of A lies in the left half-plane, see section 4.4 of [5]. It is easy to check that the solution is the following matrix

$$U = \frac{1}{2\alpha} \begin{pmatrix} V^{-1} & 0\\ 0 & E \end{pmatrix}.$$
 (9)

Thus, from (7) and (8) we get $C(t) = \sigma^2 (U - e^{tA} U e^{tA^T})$. As the spectrum of A lies in the left half-plane, then $\lim_{t \to +\infty} C(t) = \sigma^2 U$. That is why the following limit in distribution

$$\xi = \lim_{t \to \infty} \psi^{(g)}(t) = \lim_{t \to \infty} \psi^{(-)}(t),$$

exists and is the gaussian vector with zero mean and covariance matrix $\sigma^2 U$.

Now prove the last assertion of theorem 1. From (9) and from positive definiteness of V, it follows that U is non-degenerate. Thus the distribution of ξ has the density $p_{\xi}(\psi)$ with respect to the standard Lebesgue measure $dq_1 \cdots dp_N$ on L. As the matrix $(2\alpha U)^{-1}$ defines the quadratic form H, then

$$p_{\xi}(\psi) = \frac{1}{Z} \exp\left(-\frac{2\alpha}{\sigma^2}H(\psi)\right).$$

Remind that $H(\psi) = (Q\psi, \psi)_1/2$, where the $(2N \times 2N)$ -matrix $Q = (q_{i,j})$ is defined by the equality of the vectors Q(q, p) = (Vq, p). Then for the mean energy we get

$$\lim_{t \to +\infty} \mathbf{E} H(\psi^{(-)}(t)) = \mathbf{E} H(\xi) = \frac{1}{2} \sum_{i,j=1}^{2N} q_{i,j} c_{i,j} = \frac{\sigma^2}{2} \operatorname{tr} (QU) = \frac{\sigma^2}{4\alpha} \dim L$$

Thus for the case $L_0 = \{0\}$ theorem 1 is proved.

Consider now the case $L_0 \neq \{0\}$. Let v_1, \ldots, v_d be an arbitrary orthonormal basis of the subspace l_V with the only restriction that $v_1 = e_n$. Using it, define the orthonormal basis in L_- as follows

$$h_k^{(q)} = (v_k, 0), \quad h_k^{(p)} = (0, v_k), \qquad k = 1, \dots, d.$$

The coordinates on L_{-} in this basis we denote $\psi' = (\psi'_1, \ldots, \psi'_{2d})$. In these coordinates our equation on L_{-} can be written as

$$d\psi' = A'\psi'\,dt + g_1'\,dw_t,$$

where $A' = \begin{pmatrix} 0 & E \\ -V' & -D' \end{pmatrix}$, *E* is the unit matrix of the order *d*, *V'*, *D'* and *g'*₁ are the matrices of the operators *V*, *D* and the distinguished vector, in the new coordinates, correspondingly.

The latter equation looks like the main equation (3). The operator A' is the restriction of the operator A onto the subspace L_- ; let $L_- = L'_0 \oplus L'_-$ be the corresponding decomposition of L_- in A'. Then $L'_0 = 0$ and we can apply the assertions proven for the case $L_0 = 0$. Note that the quadratic form H' on L_- , generated by V', coincides with the restriction of the quadratic form H on the subspace L_- . This proves Theorem 1 completely.

Proof of theorem 2. If $\alpha = 0$, then the energy conservation law gives $L_{-} = 0$. Decompose the solution $\psi(t)$ as

$$\psi(t) = \psi_h(t) + \psi_I(t),$$

where $\psi_h(t)$ -is the solution of the homogeneous equation with initial condition $\psi(0)$, and $\psi_I(t)$ is the solution of the inhomogeneous equation with zero initial conditions. As $H(\psi(t))$ has the norm properties, then

$$|H(\psi(t)) - H(\psi_I(t))| \leq H(\psi_h(t)) = H(\psi(0)).$$

The latter equality holds as $\alpha = 0$, and thus the energy is conserved. Let us find $\mathbf{E} H(\psi_I(t))$. Denote $\psi_I(t) = (q^{(I)}(t), p^{(I)}(t))$. The solution with zero initial conditions is similar to the known (see for example [6]) formula for ordinary differential equations

$$q(t) = \sigma (\sqrt{V})^{-1} \int_0^t \sin(\sqrt{V}(t-s)) e_n \, dw_s$$
$$p(t) = \sigma \int_0^t \cos(\sqrt{V}(t-s)) e_n \, dw_s.$$

Using again the Ito isometry we get

$$\begin{split} \mathbf{E} \, T &=& \frac{\sigma^2}{2} \, \mathbf{E} \, (p(t), p(t))_1 = \frac{\sigma^2}{2} \, \mathbf{E} \, \{ p^T p \} = \frac{\sigma^2}{2} \int_0^t e_n^T \cos^2 \left(\sqrt{V} (t-s) \right) e_n \, ds, \\ \mathbf{E} \, U &=& \frac{\sigma^2}{2} \, \mathbf{E} \, (Vq(t), q(t))_1 = \frac{\sigma^2}{2} \, \mathbf{E} \{ q^T V q \} = \frac{\sigma^2}{2} \int_0^t e_n^T \sin^2 \left(\sqrt{V} (t-s) \right) e_n \, ds \\ \mathbf{E} \, H(\psi_I(t)) &=& \mathbf{E} \, \{ T+U \} = \frac{\sigma^2}{2} \int_0^t e_n^T e_n \, ds = \frac{\sigma^2}{2} \, t. \end{split}$$

We have thus proved the second assertion of theorem 2.

Note that \mathbf{H}_N is a smooth manifold. Define the matrix $\Sigma(V)$ so that its k-th column is equal to the vector $V^k e_n$. Then

$$\mathbf{H}_{N}^{(+)} = \{V: \dim l_{V} < N\} = \{V: \det(\Sigma(V)) = 0\}.$$

Note that $\det(\Sigma(V)) \neq 0$ for matrices $V \in \mathbf{H}_N$ with simple spectrum and eigenvalue basis v_1, \ldots, v_N , with the property that $(v_k, e_n)_1 \neq 0$ for all $k = 1, \ldots, N$, see [4]. That is why the function $\det(\Sigma(V))$ is not identically zero on the manifold \mathbf{H}_N . Thus, $\mathbf{H}_N^{(+)}$ is the set of zeros of the polynomial on \mathbf{H}_N . It follows that its dimension is less than the dimension of all \mathbf{H}_N , and its measure μ equals zero.

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