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Ergodic Properties of the Langevin Equation

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Abstract. We discuss the dissipative dynamics of a classical particle coupled to an infinite heat reservoir. We announce a number of results concerning the ergodic properties of this model. The novelty of our approach is that it extends beyond Markovian dynamics to the case where the Langevin equation is driven by colored noise.

In this Letter we discuss the dissipative dynamics of a classical particle interacting with a large reservoir. The reservoir is an infinite gas of free classical phonons at thermal equilibrium. We announce a number of results concerning the ergodic properties of the combined system *particle + reservoir*. In particular, it follows from our analysis that the dynamical system describing this model near thermal equilibrium is strongly mixing.

In a recent work ([JP]), we have investigated the problem of thermal relaxation for a finite dimensional Hamiltonian system $\mathcal{A}$ coupled to a heat reservoir $\mathcal{B}$. Our assumptions on the systems $\mathcal{A}$ and $\mathcal{B}$ are quite general and have simple physical interpretations. However the set of hypotheses that we need on the form of the coupling between the two systems is complicated. To avoid many of these technical details, we concentrate here on a simple model. This allows us to give a more transparent exposition of the results presented in [JP].

Using the statistical nature of the reservoir at thermal equilibrium, one can give a reduced probabilistic description of the particle based on a random integro-differential equation: The Langevin equation. The latter departs from the original Newton law by the addition of two terms: A random force describing the direct action of the reservoir on the particle, and a dissipative term arising from the reaction of the reservoir on the motion of the particle. We start by discussing our results in this well-known context (see [FK], [FKM], [LT], [N], [UO] and [W] for additional information on the Langevin equation).

Throughout this Letter, the small system $\mathcal{A}$ consists of a single particle of unit mass moving on the line under the influence of a confining C^∞ potential $V(q)$ †. The Hamiltonian function of the system $\mathcal{A}$ is

$$H_{\mathcal{A}}(q,p) \equiv \frac{p^2}{2} + V(q),$$

with $q, p \in \mathbf{R}$. The equation of motion of the isolated particle is

$$\begin{aligned} \dot{q}_t &= p_t, \\ \dot{p}_t &= -V'(q_t). \end{aligned} \tag{1}$$

Since V is smooth and confining, the initial value problem associated with Equation (1) has a global solution which defines a smooth flow on the phase space $\mathbf{R}^2$. The interaction of the particle with the reservoir is described in terms of a friction constant λ and a coupling function $\rho \in L^2(\mathbf{R})$, a normalized "charge density" ($\|\rho\| = 1$). Under the influence of the reservoir, which is assumed to be initially in thermal equilibrium at inverse temperature β, the equation of motion (1) is modified as follows:

$$\begin{aligned} \dot{q}_t &= p_t, \\ \dot{p}_t &= -V'_{\mathit{eff}}(q_t) + \lambda^2 \int_0^t D(t-s) q_s ds + \lambda \zeta_t. \end{aligned} \tag{2}$$

† The potential is confining in the sense that $\lim_{|q|\to\infty} V(q) = \infty$ and $\exp(-\beta V) \in L^1(\mathbf{R})$ for all $\beta > 0$.

Here ζ_t is a stationary Gaussian random process with mean zero and covariance

$$\langle \zeta_t \zeta_s \rangle_\beta = \beta^{-1} C(t-s) \equiv \beta^{-1} \int |\hat{\rho}(k)|^2 \cos(k(t-s)) \frac{dk}{2\pi},$$

and

$$D(t) = -\dot{C}(t) = \int k |\hat{\rho}(k)|^2 \sin(kt) \frac{dk}{2\pi}.$$

The effective potential is given by $V_{eff}(q) = V(q) + \lambda^2 q^2/2$, and $\hat{\rho}(k)$ is the Fourier transform of the function $\rho(x)$. From Equation (2) it is apparent that the reservoir plays a dual role: On one hand, its ability to absorb energy-momentum provides a physical mechanism for dissipation. On the other hand, its thermal fluctuations, encapsulated in ζ_t, prevent the particle from relaxing into some stationary state (see [KKS]). Equation (2) is known as the *Langevin equation*, and the resulting random process as the *Ornstein-Uhlenbeck process*. The derivation of the Langevin equation from "microscopic" considerations, i.e. from the Hamiltonian formalism describing the combined system $\mathcal{A} + \mathcal{B}$, is presented below.

The first question, of course, is whether the Langevin equation has a global solution. Our first result is

Theorem 1. *Suppose that*

$$\left\| \left(-\partial_x^2 + x^2\right)^s \rho \right\| < \infty,$$

for some $s > 1$. *Then for any* λ *and for almost all* ζ, *the initial value problem associated with Equation (2) has a global solution*

$$T_\zeta^t(q_0, p_0) = (q_t, p_t),$$

which defines a C^1*-flow on the phase space* $\mathbf{R}^2$.

Let $\mathcal{S}_\mathcal{A}$ be the set of probability measures on $\mathbf{R}^2$ which are absolutely continuous with respect to the Lebesgue measure. The elements of $\mathcal{S}_\mathcal{A}$ are initial states of the system $\mathcal{A}$. We say that the Ornstein-Uhlenbeck process has the property of *return to equilibrium* if for each measure $\mu \in \mathcal{S}_\mathcal{A}$ and for any observable $f \in L^\infty(\mathbf{R}^2)$ we have

$$\lim_{t\to\infty} \int \left\langle f \circ T_\zeta^t \right\rangle_\beta d\mu = \int f d\mu_\mathcal{A}^\beta, \tag{3}$$

where

$$d\mu_\mathcal{A}^\beta = \frac{1}{Z_\mathcal{A}^\beta} \mathrm{e}^{-\beta H_\mathcal{A}(q,p)} dq dp,$$

is the Gibbs canonical ensemble of the system $\mathcal{A}$ at the temperature of the reservoir. Clearly, return to equilibrium is equivalent to the mixing property of the Ornstein-Uhlenbeck process with respect to $\mu_{\mathcal{A}}^{\beta}$. Our main result is a set of necessary conditions which ensure that the OU process returns to equilibrium.

We note that, except in some special cases [TR], the question of return to equilibrium for the OU process was previously unsolved. The difficulties are related to the presence of memory in (2). A standard approach of these difficulties is based on an ad hoc limiting procedure (see e.g. [FK] or [TH], Example 3.1.9) which leads to the simplified equation

$$\begin{aligned} \dot{q}_t &= p_t, \\ \dot{p}_t &= -V'(q_t) - \frac{\eta^2}{2}\dot{q}_t + \eta\zeta_t. \end{aligned} \tag{4}$$

Here ζ_t is the white noise process,

$$\langle \zeta_t \zeta_s \rangle_\beta = \beta^{-1}\delta(t-s),$$

and η is the effective friction constant. The resulting OU process is Markovian and standard techniques based on Fokker-Planck equation apply. It is known that the process (4) is mixing with respect to the Gibbs measure $\mu_{\mathcal{A}}^{\beta}$ (see [TR]).

In [JP] we have proven a result which, specialized to the model (2), translates into the following statement:

Theorem 2. *Suppose that the conditions of Theorem 1 hold and that*

$$|\hat{\rho}(k)| \geq \frac{C}{(1+|k|)^\nu}, \tag{5}$$

for some positive constants C and ν and for all $k \in \mathbf{R}$. Then, for all non-zero λ, the Ornstein-Uhlenbeck process (2) has the property of return to equilibrium.

We now briefly summarize our program. Our first goal is to construct a differentiable dynamical system $(\mathcal{G}, \Xi_t, \mu^\beta)$ describing the combined system $\mathcal{A}+\mathcal{B}$ near thermal equilibrium. Here $\mathcal{G}$ is the phase space, Ξ_t is the Hamiltonian flow, and μ^β is the Gibbs canonical ensemble of the joint system at inverse temperature β. Admissible initial states which are "near" thermal equilibrium are probability measures on $\mathcal{G}$ which are absolutely continuous with respect to μ^β. We denote this class of states by $\mathcal{S}^\beta$. Observables of the system are elements of the algebra $L^\infty(\mathcal{G}, d\mu^\beta)$. The probabilistic description of the dynamics of the system $\mathcal{A}$ is obtained by "integrating out" the variables of the reservoir. If these variables are initially distributed according to the Gibbs canonical ensemble, then this reduced description should yield the

Langevin equation (2). The problem of return to equilibrium for the combined system can be formalized in the following way.

Definition 3. *We say that the combined system $\mathcal{A} + \mathcal{B}$ returns to equilibrium if the dynamical system $(\mathcal{G}, \Xi_t, \mu^\beta)$ satisfies*

$$\lim_{t\to\infty} \int F \circ \Xi_t \, d\mu = \int F \, d\mu^\beta,$$

for all $\mu \in \mathcal{S}^\beta$ and $F \in L^\infty(\mathcal{G}, d\mu^\beta)$.

The return to equilibrium for the Ornstein-Uhlenbeck process, Relation (3), is a special case of this definition. The second and main goal of our program is to find sufficient conditions to ensure that the system $\mathcal{A} + \mathcal{B}$ returns to equilibrium.

In the rest of this Letter we sketch how this program is carried out for the simple model of a particle coupled to an infinite harmonic string.

The heat reservoir – an infinitely extended gas of non-interacting classical phonons – is described by the classical field theory associated with the one-dimensional wave equation. In this Letter, $L^2(\mathbf{R})$ stands for the real Hilbert space of real-valued square integrable functions on $\mathbf{R}$. Let $H^1(\mathbf{R}) \subset L^2(\mathbf{R})$ be the usual Sobolev space. The phase space $\mathcal{H}_\mathcal{B}$ of finite energy configurations of the heat reservoir is the real Hilbert space obtained from the completion of $H^1(\mathbf{R}) \oplus L^2(\mathbf{R})$ with respect to the inner product

$$\left(\begin{pmatrix} \varphi \\ \pi \end{pmatrix}, \begin{pmatrix} \varphi \\ \pi \end{pmatrix} \right) \equiv \int \left(|\varphi'(x)|^2 + |\pi(x)|^2 \right) dx.$$

The Hamilton function of the free reservoir is

$$H_\mathcal{B}(\varphi, \pi) \equiv \frac{1}{2} \int \left(|\varphi'(x)|^2 + |\pi(x)|^2 \right) dx,$$

and the corresponding equation of motion is

$$\begin{aligned} \dot{\varphi}_t(x) &= \pi_t(x), \\ \dot{\pi}_t(x) &= \varphi''_t(x). \end{aligned} \tag{6}$$

The initial value problem associated to Equation (6) is solved by the strongly continuous unitary group $\exp(L_\mathcal{B} t)$, where

$$L_\mathcal{B} \equiv \begin{pmatrix} 0 & 1 \\ \partial_x^2 & 0 \end{pmatrix},$$

is a skew-adjoint operator on $\mathcal{H}_\mathcal{B}$.

The phase space of finite energy configurations of the combined system $\mathcal{A}+\mathcal{B}$ is given by $\mathbf{R}^2 \times \mathcal{H}_{\mathcal{B}}$, and its Hamilton function is

$$H(q,p,\varphi,\pi) \equiv H_{\mathcal{A}}(q,p) + \frac{\lambda^2}{2}q^2 + H_{\mathcal{B}}(\varphi,\pi) + \lambda q \int \rho(x)\varphi'(x)dx. \tag{7}$$

Here λ is a real coupling constant and ρ a normalized "charge density". These are the friction constant and coupling function figuring in (2). The choice of Hamiltonian (7) is motivated by the dipole approximation of classical electrodynamics.

To describe thermal equilibrium states of the system $\mathcal{A}+\mathcal{B}$, we have to extend the phase space $\mathcal{H}_{\mathcal{B}}$ to include infinite energy configurations. Let ϕ be the Gaussian random field indexed by the Hilbert space $\mathcal{H}_{\mathcal{B}}$, with covariance

$$\langle \phi(f)\phi(g)\rangle_\beta = \beta^{-1}(f,g),$$

for $f,g \in \mathcal{H}_{\mathcal{B}}$. Denote by $(\mathcal{G}_{\mathcal{B}}, \mathbb{G}_{\mathcal{B}}, \mu_{\mathcal{B}}^{\beta})$ the associated probability space. The phase space of the infinite heat reservoir at inverse temperature β is $\mathcal{G}_{\mathcal{B}}$, and $\mu_{\mathcal{B}}^{\beta}$ is its thermal equilibrium state. The construction of the space $\mathcal{G}_{\mathcal{B}}$ is discussed in detail in [JP], see also [GJ], [S]. We just mention here that there exists a space of "test functions" $\mathcal{N}$, continuously and densely embedded in $\mathcal{H}_{\mathcal{B}}$, and such that $\mathcal{G}_{\mathcal{B}}$ is the space of distributions on $\mathcal{N}$; more precisely,

$$\mathcal{N} \subset \mathcal{H}_{\mathcal{B}} \subset \mathcal{N}' = \mathcal{G}_{\mathcal{B}}.$$

For $\phi \in \mathcal{H}_{\mathcal{B}}$ the above duality reduces to the inner product, i.e.

$$\phi(f) = (\phi, f), \qquad f \in \mathcal{N}.$$

For notational purposes let us define the function $\alpha \in \mathcal{H}_{\mathcal{B}}$ by

$$\hat{\alpha}(k) \equiv \begin{pmatrix} (ik)^{-1}\hat{\rho}(k) \\ 0 \end{pmatrix}.$$

The Hamiltonian (7) then becomes

$$H(q,p,\phi) = H_{\mathcal{A}}(q,p) + \frac{\lambda^2}{2}q^2 + \frac{1}{2}\|\phi\|^2 + \lambda q \phi(\alpha).$$

The phase space of the system $\mathcal{A}+\mathcal{B}$ is $\mathcal{G} \equiv \mathbf{R}^2 \times \mathcal{G}_{\mathcal{B}}$, and its Gibbs canonical ensemble is the probability measure

$$d\mu^\beta = \mathrm{e}^{-\beta(\lambda q\phi(\alpha)+\lambda^2 q^2/2)} d\mu_{\mathcal{A}}^{\beta}(q,p)\, d\mu_{\mathcal{B}}^{\beta}(\phi).$$

The evolution equation for finite energy configurations are

$$\begin{aligned} \dot{q}_t &= p_t, \\ \dot{p}_t &= -V'_{\text{eff}}(q_t) - \lambda\phi_t(\alpha), \\ \dot{\phi}_t &= L_{\mathcal{B}}(\phi_t + \lambda q_t \alpha). \end{aligned} \tag{8}$$

The last equation is easily integrated to give

$$\phi_t(f) = \phi_0(\mathrm{e}^{-L_{\mathcal{B}}t}f) + \lambda\int_0^t (L_{\mathcal{B}}\alpha, \mathrm{e}^{-L_{\mathcal{B}}(t-s)}f)q_s ds,$$

and insertion into the second equation leads to

$$\dot{p}_t = -V'_{\text{eff}}(q_t) - \lambda^2\int_0^t (L_{\mathcal{B}}\alpha, \mathrm{e}^{-L_{\mathcal{B}}(t-s)}\alpha)q_s ds - \phi_0(\mathrm{e}^{-L_{\mathcal{B}}t}\alpha). \tag{9}$$

If the initial state of the reservoir is distributed according to $\mu_{\mathcal{B}}^{\beta}$, then

$$\zeta_t \equiv -\phi_0(\mathrm{e}^{-L_{\mathcal{B}}t}\alpha) \tag{10}$$

becomes a Gaussian random process, and Equation (9) is easily seen to be identical to the Langevin equation (2). The principal results of this Letter are:

Theorem 4. *Suppose that the conditions of Theorem 1 hold. Then for all λ, for all $(q_0, p_0) \in \mathbf{R}^2$, and for $\mu_{\mathcal{B}}^{\beta}$-almost all $\phi_0 \in \mathcal{G}_{\mathcal{B}}$, the initial value problem associated with Equation (8) has a global solution $(q_t, p_t, \phi_t) = \Xi_t(q_0, p_0, \phi_0)$ which defines a flow on the phase space $\mathcal{G}$. The measure μ^{β} is invariant under the Hamiltonian flow Ξ_t.*

Theorem 5. *Suppose that conditions of Theorem 2 hold. Then, for all non-zero λ, the system $\mathcal{A} + \mathcal{B}$ returns to equilibrium.*

Parenthetically, we remark that Theorems 1 and 2 are an immediate consequences of Theorems 4 and 5.

The proof of Theorem 4 is based on standard ideas and techniques and we will not discuss it here. The proof of Theorem 5 is difficult and requires some novel ideas. In the sequel we sketch the basic strategy of our argument on the heuristic level.

The Koopman space of the combined system $\mathcal{A} + \mathcal{B}$ is $L^2(\mathcal{G}, d\mu^{\beta})$ and the map

$$\mathfrak{U}^t: F \mapsto F \circ \Xi_t,$$

defines a strongly continuous unitary group on this space. Let $\mathcal{L}$ be the skew-adjoint generator of $\mathcal{U}^t$, and let $\mathfrak{F}_{sing} \subset L^2(\mathcal{G}, d\mu^\beta)$ be the spectral subspace associated to the singular spectrum of $\mathcal{L}$. We show that $\mathfrak{F}_{sing}$ consists only of constant functions. Theorem 5 is an immediate consequence of this fact (see e.g. [M] or [CFS]). Our argument splits into the following technically and conceptually distinct steps:

Change of variables. The map $(q, p, \phi) \mapsto (q, p, \psi) \equiv (q, p, \phi + \lambda q\alpha)$ transforms the Hamiltonian into $H_{\mathcal{A}}(q, p) + \|\psi\|^2/2$. In the new dynamical variables, the Koopman space factorizes as

$$L^2(\mathcal{G}, d\mu^\beta) \simeq L^2(\mathbf{R}^2, d\mu^\beta_{\mathcal{A}}) \otimes L^2(\mathcal{G}_{\mathcal{B}}, d\mu^\beta_{\mathcal{B}}).$$

This simple transformation is the critical first step of our argument.

Dynamical reduction. We exploit the particular (Lax-Phillips) structure of the reservoir, the time-reversal symmetry of the model, and the bound (5) to show that a vector $\Psi \in \mathfrak{F}_{sing}$ can depend only on q, p and finitely many field coordinates

$$\zeta_1 = \psi(e_1), \ldots, \zeta_N = \psi(e_N),$$

related to the value of the noise (10) and its derivatives at time zero. We obtain an explicit description of the subspace $\mathcal{H}_0 \subset \mathcal{H}_{\mathcal{B}}$ spanned by $e_1, \ldots, e_N$. The proof of this result involves inputs from the general theory of Gaussian random processes, Wiener prediction theory and harmonic analysis of Hardy classes.

Elimination of the reservoir. We show that the reservoir completely dominates the small time dynamics on the subspace of functions $\Psi(q, p, \zeta_1, \ldots, \zeta_N)$. Using the fact that the evolution of the free reservoir has no invariant subspaces in $\mathcal{H}_0$, we inductively eliminate the field variables ζ.

Kinematic reduction. The last step in the previous elimination process yields that $\mathfrak{F}_{sing}$ contains only functions of (q, p) which satisfy

$$\{H_{\mathcal{A}}, \Psi\} = 0, \qquad \{q, \Psi\} = 0, \tag{11}$$

where $\{\cdot, \cdot\}$ is the Poisson bracket on $\mathbf{R}^2$. It is easily shown that the constants are the only solutions of the system (11). This concludes the proof.

This strategy is effective in a more general setting. In fact, all what we require is that the system $\mathcal{A}$ is a Hamiltonian system whose configuration space is a finite-dimensional C^∞ manifold M. In particular, the system $\mathcal{A}$ could be a macroscopic gas of interacting particles in $\mathbf{R}^3$. The system $\mathcal{B}$ could be any linear dynamical system for which there is an outgoing subspace in the sense of Lax-Phillips theory. For the classical hyperbolic systems (wave equation, Maxwell's equations...) the existence of an outgoing subspace is a well-known fact. For our method to work, however, the coupling between the two systems has to be "simple", in the sense that it is a finite sum of terms of the form $u(\xi)\phi(\alpha)$, where $u(\xi) \in C^{\infty}(T^*M)$. Clearly, in this more general setting we require some additional hypotheses. First, we have to ensure that the combined system has a time-reversal symmetry. Second, we need a hypothesis ensuring kinematic completeness†. The latter has an intrinsic physical meaning: we require that the coupling could push the particle in any direction of its phase space. For additional information and proofs we refer the reader to [JP].

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References

[CFS] Cornfeld, I.P., S.V. Fomin and Ya. G. Sinai: *Ergodic Theory*, New York, Springer Verlag (1982).

[DM] Dym, H. and H.P. McKean: *Gaussian Processes, Function Theory, and the Inverse Spectral Problem*, New York, Academic Press (1976).

[FK] Ford, G.W. and M. Kac: On the Quantum Langevin Equation. J. Stat. Phys. **46**, 803 (1987).

[FKM] Ford, G.W., M. Kac and P. Mazur: Statistical mechanics of assemblies of coupled oscillators. J. Math. Phys. **6**, 504-515 (1965).

[GJ] Glimm, J. and A. Jaffe: *Quantum Physics*, New York, Springer Verlag (1987).

[JP] Jakšić, V. and C.-A. Pillet: Ergodic Properties of Classical Dissipative Systems. Preprint (1996).

[KKS] Komech, A., M. Kunze and H. Spohn: Radiative damping: Global convergence and exponential relaxation. Preprint (1995).

[LT] Lewis J.T. and L.C. Thomas: How to make a heat bath. In *Functional Integration and its Applications*, (Arthurs, A. M.). Oxford, Clarendon (1975).

† For the model discussed in this Letter this hypothesis is automatically satisfied.

[M] Mañé, R.: *Ergodic Theory and Differentiable Dynamics*, Berlin, Heidelberg, New York, Springer (1987).

[N] Nelson, E.: *Dynamical Theories of Brownian Motion*, Princeton, Princeton University Press (1976).

[RO] Robinson, D.W.: C*– algebras and quantum statistical mechanics. In *C*– Algebras and their Applications to Statistical Mechanics and Quantum Field Theory*, (Kastler, D.). Amsterdam, North-Holland (1976).

[RS] Reed, M. and B. Simon: *Methods of Modern Mathematical Physics III. Scattering Theory*, London, Academic Press (1978).

[S] Simon, B.: *The* $P(\phi)_2$ *Euclidean (Quantum) Field Theory*, Princeton, Princeton University Press (1974).

[TH] Thirring, W.: *Quantum Mechanics of Large Systems*, New York, Wien, Springer (1980).

[TR] Tropper, M.M.: Ergodic and quasi-deterministic properties of finite-dimensional stochastic systems. J. Stat. Phys. **17**, 491-509 (1977).

[UO] Uhlenbeck, G.E. and L.S. Ornstein: On the theory of Brownian motion. Phys. Rev. **36**, 823 (1930).

[W] Edited by Wax, N.: *Selected Papers on Noise and Stochastic Processes*, New York, Dover Publications (1954).