Hamiltonian chaos acts like a finite energy reservoir: Accuracy of the Fokker–Planck approximation

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The Hamiltonian dynamics of slow variables coupled to fast degrees of freedom is modelled by an effective stochastic differential equation. Formal perturbation expansions, involving a Markov approximation, yield a Fokker–Planck equation in the slow subspace which respects conservation of energy. A detailed numerical and analytical analysis of suitable model systems demonstrates the feasibility of obtaining the system specific drift and diffusion terms and the accuracy of the stochastic approximation on all time scales. Non–Markovian and non–Gaussian features of the fast variables are negligible.

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Introduction – While fluctuations and damping in thermodynamic systems, i.e. in many–particle systems close to equilibrium, are fairly well understood the corresponding features in low–dimensional Hamiltonian dynamics are still under debate. Although it might be conjectured that, on the basis of general arguments, fast chaotic Hamiltonian degrees of freedom can be modelled by suitable stochastic forces the question is far from being settled. In fact, the just mentioned problem has several facets. Firstly, it is relevant for principal aspects of physics like damping and fluctuations on atomic scales (cf. e.g. [1]) or in nuclear physics. Secondly, modelling of systems with different time scales as they appear e.g. in such diverse fields like molecular dynamics and climate research [2] is important from the practical point of view as the implementation of numerical schemes requires step sizes which can cope with the smallest time scale of the effective dynamical model. Here we address the problem how to deal with Hamiltonian dynamics where two kinds of degrees of freedom enter, fast chaotic and slow variables. We will demonstrate that suitable stochastic models are capable to describe the motion of the slow degrees of freedom accurately.

As pointed out in [3] few chaotic Hamiltonian degrees of freedom, either classical or quantum mechanical, may act as a thermodynamic heat bath introducing damping and fluctuations. The underlying structure, in particular the formal derivation of an effective Fokker–Planck equation for the slow motion was further elucidated in [4]. This analysis was mainly motivated by an investigation of corrections to the adiabatic theorem [5, 6]. But so far it is still an open issue whether such a formal treatment can be cast into a systematic perturbation scheme and whether higher order contributions beyond the Born approximation are really negligible. Such types of question are of course of utmost importance when one wants to cope with the asymptotic dynamics on long time scales.

This letter is intended to fundamentally clarify all issues of practical relevance related to the stochastic modelling of Hamiltonian dynamics. We will trace explicitly the time scale separation through an expansion parameter ϵ. For consistency, the total energy of the system has to scale like $1/\epsilon$, which affects the Einstein–like relation between the viscous damping and diffusion term of the effective stochastic model. We find a damping which is one order ϵ smaller than the diffusion. The energy conservation of the full system translates into a multiplicative noise term which guarantees that the invariant density of the Fokker–Planck equation has a bounded support. Being intimately linked to the Hamiltonian structure of the full system, these features are captured by a proper fluctuation–dissipation relation. Finally, we demonstrate by suitable examples that the system specific damping and diffusion terms of the stochastic model can be obtained with reasonable effort by a (numerical) analysis of the fast dynamics alone, and that the stochastic model yields very good approximations of the full dynamics on all time scales beyond $t \sim \mathcal{O}(\epsilon)$.

Reduced equation – To set up the notation we consider a Hamiltonian of the form

$$H(q,p,Q,P) = \frac{1}{\epsilon} H_f(q,p) + H_s(Q,P) + V_c(q,Q) \ . \quad (1)$$

We assume an *a priori* separation of slow variables Q, P and fast variables q, p, mediated by the small parameter $\epsilon \ll 1$. The variables may be vector valued, but to keep the notation simple we refrain from labelling the different components. We intend to approximate the Hamiltonian equations of motion of the slow variables by a suitable stochastic model. Whereas the effective equation of motion for Q is identical to the exact equation, the time evolution of P will be governed by a suitable stochastic equation. To determine the parameters of the latter on a merely empirical level, one has to compute [7] the first two moments

$$\tau D_P^{(1)}(Q,P)+\mathcal{O}(\tau^2) = \langle\widetilde{P}(\tau)\rangle_{q,p} - P \qquad (2a)$$

$$\tau D_{PP}^{(2)}(Q,P)+\mathcal{O}(\tau^2) = \left\langle (\widetilde{P}(\tau)-P)^2\right\rangle_{q,p} \ . \qquad (2b)$$

Here, $\widetilde{P}(\tau) = \widetilde{P}(\tau; q, p, Q, P)$ is the solution of the initial value problem $(Q, P, q, p)(0) = (Q, P, q, p)$ of the equations of motion derived from eq. (1). $\langle\ldots\rangle_{q,p}$ denotes the average over q and p on the energy shell $H(q, p, Q, P) = E/\epsilon$ where the scaling of the total energy with $1/\epsilon$ is suggested by the time scale separation of the Hamiltonian (1). If a stochastic description is appropriate and if higher order moments are neglected then, following the spirit of the Kramers–Moyal expansion [8], the stochastic differential equation

$$dP = D_P^{(1)}(Q,P)dt + \sqrt{D_{PP}^{(2)}(Q,P)}dW \qquad (3)$$

yields an approximation of the statistical properties of the slow degrees of freedom. Here, dW denotes as usual the differential of the Wiener process, i.e. a Gaussian white noise. This approximation becomes meaningful if $\epsilon \ll \tau$. It guarantees that on the time scale τ the correlations of the fast motion decay by assumption and a description in terms of a Langevin equation or the corresponding Fokker–Planck equation becomes feasible.

Until here we have not proven that a stochastic model (3) is justified, nor does the above method supply an analytical determination of the drift and diffusion terms. Such a theoretical derivation may be obtained by applying a formal second order perturbation expansion with respect to the time scale separation parameter ϵ to the Liouville equation governing the dynamics of the full phase space density $\rho_t(q, p, Q, P)$. Under suitable projection we obtain the following effective Fokker–Planck equation for the reduced density $\bar{\rho}_t(Q, P) = \int \rho_t \, dp \, dq$ describing the properties of the slow degrees of freedom in a probabilistic way [9] (see also e.g. [10] for related concepts in the context of dissipative dynamical systems)

$$\partial_t\bar{\rho}_t = -i\langle\mathcal{L}\rangle_{ad}\bar{\rho}_t + \epsilon^2\partial_P\frac{\partial H_s}{\partial P}\gamma\bar{\rho}_t + \epsilon\partial_P^2\hat{D}_{PP}^{(2)}\bar{\rho}_t \qquad (4)$$

where

$$\hat{D}_{PP}^{(2)}(Q,P) = \kappa^2\int_0^\infty \langle\delta_{ad}q\;\delta_{ad}q_f(t)\rangle_{ad}dt \qquad (5a)$$

$$\gamma(Q,P) = \frac{1}{Z(Q,P)}\partial_E\left(\hat{D}_{PP}^{(2)}(Q,P)Z(Q,P)\right) \ . \qquad (5b)$$

Here $\langle\ldots\rangle_{ad}$ abbreviates the average over the adiabatic density $\rho_{ad}^\epsilon = \delta(\epsilon H - E)/Z$ with $Z(Q, P) = \int \delta(\epsilon H - E)dq\,dp$, $\delta_{ad}q = q - \langle q\rangle_{ad}$ and $q_f(t)$ denotes the time dependent solution of the Hamiltonian equations of motion for fixed slow variables with $q_f(0) = q$. For simplicity, we have considered a harmonic coupling $V_c(q, Q) = -\kappa q Q$. We want to stress that eq. (4) and the expressions (5) are based solely on the smallness of the parameter ϵ and on the assumption of an exponential decay of the fast autocorrelations due to chaos. In particular, no assumptions on the size of the coupling V_c are needed.

As the coefficients (5) depend on the slow variables it is useful to consider also the expanded expressions

$$\hat{D}_{PP}^{(2)}(Q,P) = (1-\epsilon H_s\partial_E)d_0 + \mathcal{O}(\epsilon^2) \qquad (6a)$$

$$\gamma = Z_0^{-1}\partial_E\left(d_0 Z_0\right) + \mathcal{O}(\epsilon) \qquad (6b)$$

where Z_0 respectively d_0 denote the numerical values of Z and $\hat{D}_{PP}^{(2)}$ at $\epsilon = 0$. Since Z_0 and d_0 do not depend on P and Q, their numerical values can be determined by integrating the fast subsystem alone.

In eq. (4) the first term contains the adiabatically averaged Liouvillian $\mathcal{L}$. The second contribution yields a viscous damping term of order ϵ^2 if $H_s(Q, P) = P^2/2 + U(Q)$, since in lowest order the damping coefficient (6b) does not depend on the slow variables. The diffusion coefficient (5a) is determined by the autocorrelation function of the fluctuations of the fast chaotic variables and hence tends to zero when the slow subsystem contains the total energy. Eq. (5b) linking the damping constant with the diffusion coefficient expresses a fluctuation–dissipation relation for our system.

By the help of examples we will now explore the accuracy of the effective model eq. (4) in two ways: we check the drift and diffusion terms using eq.(2) assuming the validity of a stochastic model, and we verify the ability of our Fokker–Planck equation to reproduce the dynamics of the full system. For ease of the numerics and to furnish the proof of nontrivial effects of the fast dynamics we study a slow harmonic oscillator coupled linearly to fast degrees of freedom, i.e.

$$\dot{Q} = P, \quad \dot{P} = -(1+\kappa)Q + \kappa q \ . \qquad (7)$$

Since for chaotic Hamiltonian systems analytical treatments are not feasible, for the sake of simplicity we first focus on a system where the exponential decay of the fast auto-correlations is caused by noise instead of chaos.

Analytical considerations – We hence choose as fast subsystem the so called Kubo oscillator [8], which is a conservative harmonic oscillator with an energy conserving multiplicative Gaussian white noise $\xi(t)$:

$$\dot{q} = \frac{1}{\epsilon}p(1+\sqrt{\epsilon}\xi(t)) \ , \quad \dot{p} = -\frac{1}{\epsilon}(q-\epsilon\kappa Q)(1+\sqrt{\epsilon}\xi(t)) \ . \quad (8)$$

The full coupled four dimensional stochastic system eqs. (7) and (8) has all features which are essential for our elimination scheme. In particular the energy $E/\epsilon = (p^2 + q^2)/(2\epsilon) + (P^2 + (1 + \kappa)Q^2)/2 - \kappa q Q$ is conserved. Due to the simplicity of the system we can evaluate analytically the coefficients of the reduced two–dimensional Fokker–Planck equation using eqs. (6) (and, for comparison, also by the Kramers–Moyal expansion (2)) [11]. As a result, (4) contains a viscous damping term $-\epsilon^2 P\kappa^2/2$, and the diffusion coefficient $\epsilon\kappa^2\left(E-\epsilon H_s\right)/2$ decreases to zero on the closed curve $H_s(Q,P)=E/\epsilon$, reflecting energy conservation of the full system. The invariant density $\bar{\rho}_*(Q,P)$, i.e. the stationary solution of the Fokker–Planck equation, is constant for $H_s(Q,P)<E/\epsilon$ and zero otherwise. Stationary quantities such as $\bar{\rho}_*(Q,P)$ as well as dynamical quantities like the correlation function $\langle Q\,Q(t)\rangle$ coincide with the exact analytical expressions of the full system in lowest nontrivial order of ϵ. Let us stress that in the stochastic model (4) damping and diffusion appear at different orders of the perturbation expansion, in contrast to the approaches mentioned in the introduction. Hence, a direct numerical estimate of the order ϵ^2 damping in $D_P^{(1)}$ through eq. (2a) using trajectories of the coupled system is nontrivial, since one has to fulfill the constraint $\tau\gg\epsilon$. For obtaining meaningful results higher order–τ corrections have to be taken into account. In fact, for reasonable parameter values $\kappa=2$ and $\epsilon=0.02$ (E=4), we had to take correction terms up to order τ^5 into account to identify the damping term $\epsilon^2\gamma=8\cdot10^{-4}$. Nonetheless, such an empirical estimation of the drift and diffusion terms of the reduced equation from trajectories of the full system yields perfect agreement with our theoretical predictions.

Fast Hamiltonian chaos – As a nontrivial example, we study fast chaotic degrees of freedom which are governed by the Hamiltonian

$$H_f(q_1,q_2,p_1,p_2)=\frac{1}{2}(p_1^2+p_2^2+q_1^2+q_2^2+q_1^2q_2^2)\,. \quad (9)$$

Coupling to the slow dynamics (7) is mediated by the variable q=q_1. Here, an analytic treatment is impossible. But we can easily evaluate our analytical expressions (6) numerically. For that purpose we compute the fast autocorrelations in (6a) from ensembles of numerical solutions of the fast system (9) and the partition sum Z_0 by, e.g., a Monte–Carlo–sampling of the fast phase space. While d_0 is essentially linear in E (cf. Fig.1), we obtain an approximate power law $Z_0\approx E^{0.7}$ for the partition integral (not shown). Hence, the diffusion coefficient is proportional to the energy in the fast subsystem and vanishes when the slow energy exceeds the total energy E/ϵ. A comparison of our theoretical prediction eq. (6a) for the diffusion coefficient with the evaluation of eq. (2b) on numerical solutions of the full system shows a perfect agreement between numerical data and theory, Fig.2. For the viscous damping constant (6b) we obtain $\gamma\approx1.7d_0$ according to eq. (6b). Due to the smallness of γ such a relation cannot be verified directly by a numerical evaluation of the Kramers–Moyal expansion (2a). Of course, the numerical value of γ is available through the integral of the correlation function, d_0.

In order to check the accuracy of the effective model eq. (4) we compare its stationary state to the one of the full Hamiltonian equations of motion (cf. Fig.3). The

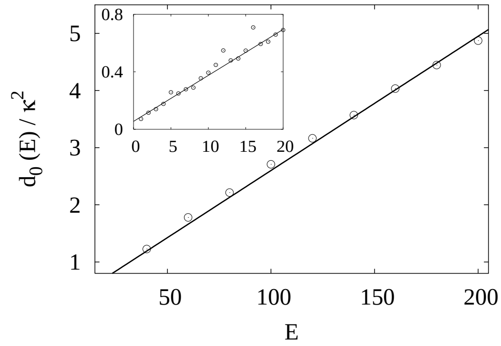

FIG. 1: Numerically computed integral of the fast autocorrelations d_0/κ^2 as a function of energy (symbols) for the model eq.(9). Inset: enlargement of the small energy range. Lines: linear fit.

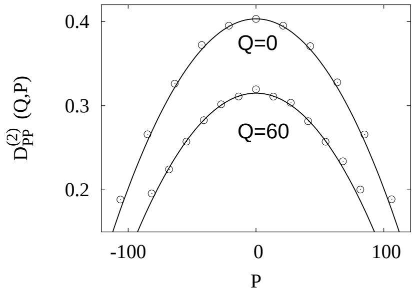

FIG. 2: The diffusion term derived from (6a) (lines) and the numerical estimates (symbols) using (2b) (chaotic fast subsystem (9), ϵ=0.02, κ=2, $E=200$).

invariant density eq. (4) is obtained by a numerical integration of the corresponding Langevin equation. Just as in the previous example the support of the two densities, as given by $H_s(Q,P)\le E/\epsilon$, is identical up to order ϵ. It is worth emphasising that we obtain a very good quantitative agreement between both densities everywhere in the slow phase space.

So far the differences between the full Hamiltonian dynamics and the effective stochastic description are hardly visible. However, deviations are expected to occur in the short time regime. For an illustration of the limit of the approach we consider the transient motion of the kinetic energy. Fig.4 shows averages $\langle P^2/2\rangle(t)$ starting from initial conditions with $(Q,P)(0)=(0,0)$ and $E=200$. Systematic deviations are visible in the short time regime $t\simeq\mathcal{O}(\epsilon)$, where correlations of the fast dynamics cause oscillations (non–Markovian effects). Beyond this time scale, the agreement is of order ϵ, which is the accuracy of our damping and diffusion coefficients. The modulated linear increase on intermediate time scales (inset) corresponds to free diffusion and reflects the smallness of the damping, which is followed by a saturation at $\langle P^2/2\rangle\approx1900$ in the long time limit (not shown).

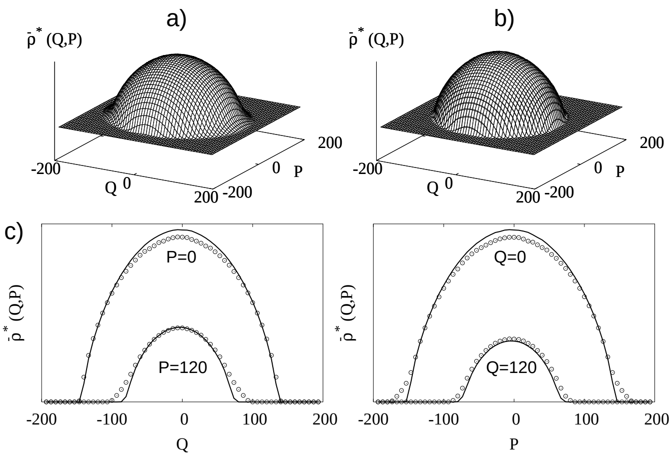

FIG. 3: a) Numerically determined invariant slow density $\bar{\rho}_*(Q,P)$ of the full system eq. (9) in comparison with b) the invariant density of the Langevin equation containing the drift and diffusion terms proposed by our projection operator technique. c) Sections through these two densities. Symbols: Full system, lines: Fokker–Planck model. Parameters as in Fig.2

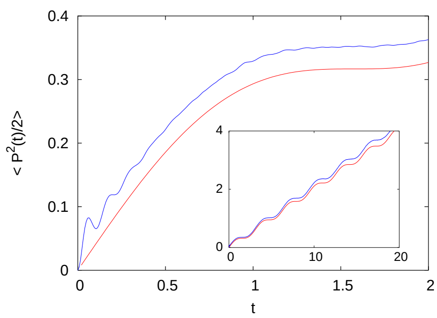

FIG. 4: Time evolution of ensemble averages of the slow kinetic energy $\langle P^2/2\rangle(t)$. Simulation of the full microscopic equations of motion, eqs.(7) and (9) with an ensemble representing $\rho(Q,P,q,p,t=0) \propto \delta(Q)\delta(P)\delta(H_f - E)$ (continuous curves), and result of the corresponding stochastic model, eqs.(4) and (6) (dashed lines). Parameters as in fig. 2.

In the fast chaotic subsystem, one generally has to face the problem of stable islands (KAM tori), at least when its energy is small. Although a trajectory of the full system with initial conditions in a chaotic region cannot enter these islands and hence remains chaotic for all times, so called cantori may surround the islands and create intermittent fast dynamics with potential power law tails in the autocorrelations [12]. In such a case evaluation of the damping and diffusion constants may become tedious.

Conclusion – We have demonstrated that the action of fast Hamiltonian chaotic degrees of freedom is captured by an effective description in terms of a Fokker–Planck or Langevin equation. In order to cope with the essential time scale separation we have assumed from the very beginning that the underlying microscopic Hamiltonian contains an expansion parameter which distinguishes between slow and fast degrees of freedom. While in classical cases like Brownian motion such an expansion parameter is usually a mass ratio [1] its identification in other physical contexts might be a nontrivial task. Above all, the introduction of the time separation parameter ϵ requires that the total energy scales as $1/\epsilon$.

Explicit formulas for the damping and diffusion constants of the effective Fokker–Planck equation can be obtained e.g. by a projection operator technique. For their evaluation only the solution of the fast subsystem is needed. Consistency of the perturbation expansion requires the damping to be of higher order, since the total energy becomes large in the limit $\epsilon \ll 1$.

Comparing the results of the effective dynamics with the exact one, the approximation by a Fokker–Planck equation works surprisingly well on all time scales larger $\mathcal{O}(\epsilon)$. Non–Gaussian and non–Markovian features of the fast chaotic motion are negligible, but the correct form of the diffusion and the size of the damping are crucial for respecting the conservation of energy. Thus fast chaos acts like a reservoir with a finite heat capacity, generating a stochastic slow motion with a finite support. Altogether this opens the possibility of efficient long time simulations with high accuracy.

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