Accuracy and efficiency of reduced stochastic models for chaotic Hamiltonian systems with time scale separation

Nilüfer Baba,[1,*] Wolfram Just,[2] Holger Kantz,[1] and Anja Riegert[1]

[1] *Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, D 01187 Dresden, Germany*
[2] *School of Mathematical Sciences, Queen Mary / University of London, Mile End Road London E1 4NS, UK*
(Dated: May 5, 2006)

The study of long time behaviour of systems with time scale separation is considerably facilitated if the fast degrees of freedom can be eliminated without affecting the slow dynamics. We investigate a technique in which the fluctuations due to a fast chaotic subsystem are replaced by a suitable stochastic process so that a Fokker-Planck equation for the slow variables results. The accuracy and efficiency of this technique is verified by the detailed numerical investigation of several coupled systems. The asymptotic behaviour as well as transients turn out to be well modelled by the reduced dynamics. We concentrate on low-dimensional problems and cover different types of coupling schemes as well as different chaotic subsystems. As a physical application we discuss the classical dynamics of a hydrogen atom in a strong magnetic field.

PACS numbers: 05.45.Ac, 02.50.Ey, 02.30.Mv
Keywords: time scale separation, fast chaos, stochastic modelling

INTRODUCTION

Many realistic complex systems are composed of subsystems which act on quite different time scales. From a numerical point of view, any integration routine must use temporal step widths which allow a proper resolution of the fastest time scale. On the other hand, the long time behaviour of a system is often determined solely by the slow degrees of freedom. Such long time behaviour is at the focus of scientific interest in many phenomena such as in the study of ecological evolution, molecular dynamics (e.g. conformation changes of large molecules), or climate changes. In the latter, the short time fluctuations of what is called weather exert essential impact on the long time evolution and cannot simply be ignored. The numerical simulation of the full system is usually a challenge even for modern supercomputers. A possible solution consists in reducing the model by elimination of the fast degrees of freedom without affecting the long time properties of the slow subsystem.

Problems related to dynamics on different time scales are known for long, e.g., in celestial mechanics. Time scale separation and the elimination of fast degrees of freedom play a central role as well for the investigation of instabilities in physical, chemical and biological systems [1]. Well established techniques for such reductions are known as adiabatic elimination [2–4] and averaging [5, 6]. While the first type of technique relies on the relaxation of the fast dynamics towards stable equilibrium states (the so called the centre manifold), the second class assumes a (quasi-)periodic evolution of the fast degrees of freedom. Averaging techniques can also be applied to obtain the lowest order approximation if the fast motion is stochastic or chaotic, although from the mathematical point of view the matter is quite subtle as one has to take carefully the feedback from the slow onto the fast subsystem into account [7]. In this paper we focus on the particular class of low-dimensional Hamiltonian systems with fast chaotic subsystems, for which adiabatic elimination cannot be applied and averaging gives unsatisfactory results.

More than 25 years ago Hasselmann [8] suggested in the framework of his stochastic climate model the replacement of fast chaotic variables by a suitable noise process, because both chaos and noise are aperiodic in time and share fast decay of correlations. Recent studies [9, 10] show in detail in which sense fast chaotic motion is indistinguishable from a suitable stochastic process. If the fast degrees are stochastic right from the outset, then a large body of work is available in the literature to eliminate fast degrees of freedom and to arrive at a reduced stochastic description [11]. On the other hand numerous concepts exist in the context of thermodynamics to model the influence of a deterministic thermodynamic heat bath by an effective stochastic force or noise. More importantly, one can show that certain low-dimensional chaotic Hamiltonian systems may act as a finite energy reservoir for slow subsystems, and that the slow motion can be modelled properly by a Fokker-Planck equation[12, 13]. In such a reduced description the eliminated chaotic degrees of freedom cause a viscous damping and a diffusion term. 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 bounded support. These features are captured by a proper fluctuation-dissipation relation. In view of the fact that even the averaging principle (which is included in [12, 13] as lowest order approximation) has not been proven in full generality, the validity of the formally derived Fokker-Planck model has to be checked for a representative class of systems. Moreover, there are further technical issues to be tested. For instance, since the law of large numbers does not apply in a system with a finite (small) number of degrees of freedom, it is essential to check numerically whether the fast chaotic dynamics can be described by a Gaussian statistics. More importantly, generic Hamiltonian chaos is characterized by a mixed phase space where regular and chaotic regions coexist. Thus a Markov approximation usually involved in the derivation of the reduced model needs to be justified a posteriori. Finally, the actual determination of the reduced equations of motion requires the evaluation of statistical averages for the drift and diffusion coefficients, where the choice of the sample is nontrivial. In particular, in numerical averages it is difficult to exclude fast initial conditions inside a regular island. For practical applicability of the method, it is also relevant to show that the computational effort required to determine the reduced model equations for a specific system is reasonable.

In this article we address on the basis of several examples the just mentioned aspects of practical relevance related to the stochastic modelling of Hamiltonian dynamics. The efficiency and accuracy of our elimination technique with regard to the quality by which expectation values of the slow dynamics are reproduced by the reduced model will be demonstrated by a detailed numerical analysis of systems with different time scale separation, coupling and chaotic subsystems, testing also short and long time properties of the reduced models.

EFFECTIVE FOKKER-PLANCK EQUATION

In this section we briefly recall the essential results for the stochastic modelling of fast chaotic fluctuations by a Fokker-Planck equation. We consider coupled Hamiltonian systems with two time scales. Of course real processes may require multiscale models which are much more difficult to study though basic ideas remain valid, since eventually there are only two classes of degrees of freedom: those which one likes to eliminate and those which should be modelled in detail. For simplicity, we assume here that the variables can be transformed in such a way that the phase space can be split into "fast" and "slow", so that the Hamiltonian we start from reads

$$\mathcal{H}(q,p,Q,P) = \mathcal{H}_s(Q,P) + \frac{1}{\epsilon}\mathcal{H}_f(q,p) + \mathcal{H}_c(q,Q) = \frac{E}{\epsilon}. \quad (1)$$

The first term $\mathcal{H}_s$ denotes the Hamiltonian of the slow subsystem with the variables (Q,P), the second one $\mathcal{H}_f$ that of the fast subsystem with chaotic variables (q,p) and the last term is the coupling between both systems. To keep the notation as simple as possible vector indices of the multidimensional variables P, Q, p and q are omitted. Furthermore, we assume that the time scale separation is given in terms of a small parameter $\epsilon \ll 1$. Most importantly, we assume that the dynamics of $\mathcal{H}_f(q,p)$ is chaotic for all energies and more specifically generates a fast decay of correlations. The total energy $E_{tot} = E/\epsilon$ is preserved. Although a scaling of the energy is not relevant for the perturbation expansion, we assume from the very beginning that the total energy E_{tot} grows like $1/\epsilon$ in the limit $\epsilon \to 0$, since otherwise the energy content in the fast subsystem would drop and its chaoticity could not be guaranteed without further conditions [15].

Starting from the Liouville equation for the time evolution of phase space densities of the full dynamics, one can derive an effective reduced description for the slow dynamics. With the help of the projection operator method [16] and a formal perturbation expansion in lowest nontrivial order of ϵ, involving a Markov approximation, a Fokker-Planck equation can be obtained [17]:

$$\begin{aligned}\frac{\partial}{\partial t}\bar{\rho}_t(Q,P) \;=\; &\left\{\frac{\partial}{\partial Q}\left(-\frac{\partial \mathcal{H}_s}{\partial P}\right) + \frac{\partial}{\partial P}\left(\frac{\partial \mathcal{H}_s}{\partial Q} + \left\langle \frac{\partial \mathcal{H}_c}{\partial Q}\right\rangle_{ad}\right)\right. \\ &\left. + \epsilon^2 \frac{\partial}{\partial P}\widetilde{\gamma}\frac{\partial \mathcal{H}_s}{\partial P} + \epsilon\frac{\partial^2}{\partial P^2}\widetilde{D}^{(2)}_{PP}\right\}\bar{\rho}_t \qquad (2)\end{aligned}$$

Here $\bar{\rho}_t(Q,P) = \int \rho_t(q,p,Q,P)dqdp$ denotes the density for the slow degrees of freedom. $\langle ... \rangle_{ad}$ indicates an average of the fast degrees of freedom with respect to the so called adiabatic density $\rho_{ad} := \delta(E - \epsilon\mathcal{H})/\int \delta(E - \epsilon\mathcal{H})dqdp$ which coincides with the microcanonical ensemble of $\mathcal{H}_f(q,p)/\epsilon + \mathcal{H}_c(q,Q)$ when the slow variable Q is considered as a fixed parameter. The coefficients of Eq.(2) can be summarized as drift and diffusion contributions

$$D^{(1)}_Q(Q,P) \;=\; \frac{\partial \mathcal{H}_s}{\partial P} \qquad (3a)$$

$$D^{(1)}_P(Q,P) \;=\; -\frac{\partial \mathcal{H}_s}{\partial Q} - \left\langle \frac{\partial \mathcal{H}_c}{\partial Q}\right\rangle_{ad} - \epsilon^2\widetilde{\gamma}\frac{\partial \mathcal{H}_s}{\partial P} \qquad (3b)$$

$$D^{(2)}_{PP}(Q,P) \;=\; \epsilon\widetilde{D}^{(2)}_{PP}\,. \qquad (3c)$$

In this reduced description the effects of the eliminated chaotic variables are accounted for by averaging of the slow vector field, i.e. by $\langle \mathcal{H}_c\rangle_{ad}$, by the damping term $\widetilde{\gamma}$, and by a diffusion process with coefficient $\widetilde{D}^{(2)}_{PP}$. Explicit expressions for the latter quantities read

$$\widetilde{D}^{(2)}_{PP}(Q,P) \;=\; \kappa^2\int_0^\infty \langle \delta_{ad}q\,\delta_{ad}q(t)\rangle_{ad}dt \qquad (4)$$

$$\widetilde{\gamma}(Q,P) \;=\; \frac{1}{Z(Q,P)}\frac{\partial}{\partial E}[\widetilde{D}^{(2)}_{PP}(Q,P)Z(Q,P)]\,. \qquad (5)$$

Here $Z(Q,P) = \int \delta(E - \epsilon\mathcal{H})dqdp$ abbreviates the partition function associated with the adiabatic density, $\delta_{ad}q = q - \langle q\rangle_{ad}$ the fast fluctuation field, and $\delta_{ad}q(t)$ denotes the time dependent solution of the Hamiltonian equations of motion of $\mathcal{H}_f(q,p) + \epsilon\mathcal{H}_c(q,Q)$ for fixed slow variables Q with $\delta_{ad}q(0) = \delta_{ad}q$. Since we are dealing with the Hamiltonian case, i.e. a unitary dynamics of $\delta_{ad}q(t)$, standard arguments of nonequilibrium statistical mechanics ensure that the correlation function

$\langle \delta_{ad} q \delta_{ad} q(t) \rangle_{ad}$ is an even function of time t and that the diffusion coefficient $\widetilde{D}^{(2)}_{PP}(Q,P)$ is non negative [14]. In writing down Eqs.(4) and (5) we have adopted for simplicity the harmonic choice $\mathcal{H}_c(q,Q) = -\kappa q Q$ for the coupling potential. As can be seen from Eq.(2) the damping term and the diffusion coefficients appear in different orders of ϵ. This is due to the mentioned rescaling of the total energy. While the diffusion is linear in ϵ, the damping is one order of ϵ smaller. Relation (5) ensures that the Fokker-Planck equation (2) obeys detailed balance and that the stationary solution is (up to a normalisation factor) given by $Z(Q,P)$ (cf. [16]). Thus our effective equation of motion is consistent with the underlying Hamiltonian dynamics and Eq.(5) may be called a proper fluctuation dissipation theorem.

Drift and diffusion coefficients still depend on the expansion parameter ϵ and may have an intricate dependence on the slow variables Q and P as well as on the energy E (cf. Eqs.(4) and (5)). It is in fact essential that the time evolution $\delta_{ad} q(t)$ which determines the correlation appearing in Eq.(4) matches with the adiabatic density that determines the average $\langle ... \rangle_{ad}$ in order to guarantee the decay of the correlation function. Any further approximation has to observe such a constraint. One may e.g. adopt an expansion in the parameter ϵ. But some care is needed since the energy of the slow system $\mathcal{H}_s(Q,P)$ takes large values and $\epsilon\mathcal{H}_s(Q,P)$ has to be treated as a quantity of order $\mathcal{O}(1)$. We thus choose the interaction $\epsilon\mathcal{H}_c(q,Q)$ to be a small quantity. To be consistent with the above mentioned fluctuation dissipation relation one has to discard the renormalisation of the drift by the interaction potential as well. Alternative approximation schemes exist, e.g. keeping $\epsilon\langle \mathcal{H}_c \rangle_{ad}$ and treating just the adiabatic fluctuation $\epsilon\delta_{ad}\mathcal{H}_c$ as a small quantity. But here we do not pursue such a scheme.

Within our approximation scheme it will turn out that drift and diffusion can be expressed solely in terms of quantities of the fast subsystem, namely its microcanonical partition function

$$Z^{(0)}(E) = \int \delta(E - \mathcal{H}_f)\; dq dp \tag{6}$$

and the integral of the autocorrelation function of the fast subsystem

$$d_0(E) := \int_0^\infty \langle \delta_f q \delta_f q(t) \rangle_f dt \; . \tag{7}$$

Here $\langle ... \rangle_f$ denotes the microcanonical average in the fast system, $\delta_f q = q - \langle q \rangle_f$ the fluctuation, and the dynamics $\delta_f q(t)$ is considered with respect to $\mathcal{H}_f(q,p)$ only. The right hand side of eq.(7) depends of course on the energy E of the microcanonical ensemble, as indicated by the argument of d_0. Now, if we neglect in lowest order the interaction $\epsilon\mathcal{H}_c$ then the adiabatic partition function is approximated by

$$Z(P,Q) \simeq Z^{(0)}(E - \epsilon\mathcal{H}_s) \tag{8}$$

while for the diffusion coefficient (4) we obtain by the same approach

$$\widetilde{D}^{(2)}_{PP}(Q,P) \simeq \kappa^2 d_0(E - \epsilon\mathcal{H}_s) \; . \tag{9}$$

Thus, both quantities inherit their dependence on the slow degrees of freedom because of conservation of energy. Finally, in view of Eq.(5) the damping term reads

$$\widetilde{\gamma} \simeq \kappa^2 \frac{\partial [Z^{(0)}(E - \epsilon\mathcal{H}_s) d_0(E - \epsilon\mathcal{H}_s)]/\partial E}{Z^{(0)}(E - \epsilon\mathcal{H}_s)} \; . \tag{10}$$

Further simplifications arise when we employ a simple analytical expression for the correlation integral (7). For our examples it will turn out that $d_0(E)$ to a good approximation is linear in the energy, $d_0(E) = \omega E, (E \geq 0)$ while the partition function shows a power law behaviour $Z^{(0)}(E) \sim E^\alpha$ with some exponent $\alpha > 0$. Then Eqs.(9) and (10) yield the explicit formulas

$$\begin{aligned} \widetilde{D}^{(2)}_{PP}(Q,P) &\simeq \kappa^2 \omega (E - \epsilon\mathcal{H}_s) && (11) \\ \widetilde{\gamma}(Q,P) &\simeq \kappa^2 \omega (1 + \alpha) \; . && (12) \end{aligned}$$

Eqs.(11) and (12) show explicitly that the diffusion tends to zero in those regions of the phase space where the slow system attains the total energy, while the damping remains finite in general. Thus, the reduced dynamics cannot leave the range of energies which is allowed by energy conservation of the original system. At this point we wish to emphasise the fact that for the computation of the Fokker-Planck coefficients in Eqs.(3) only the knowledge of the dynamics of the isolated fast chaotic subsystem for all values of the fast energy $E_f \leq E$ is needed.

NUMERICAL CONFIRMATION OF DRIFT AND DIFFUSION COEFFICIENTS

Estimation from time series

The Fokker-Planck equation (2) constitutes the reduced model which is supposed to properly generate the time evolution of the slow subsystem. In order to study the validity and the accuracy of this reduced model, two different approaches are possible. Either, one can assume that a Fokker Planck model is appropriate and just try to verify the drift and diffusion coefficients. Alternatively, and this will be done in the next section, one can compare the dynamics of the Fokker-Planck equation with the numerically calculated time evolution of the full system on the basis of computable dynamic observables like, for instance, the moments or the stationary density of the slow subspace. Even if the theory passed the first test, it might be that it fails the second, since neither the Markovianity nor the Gaussianity of the fluctuations have been proven.

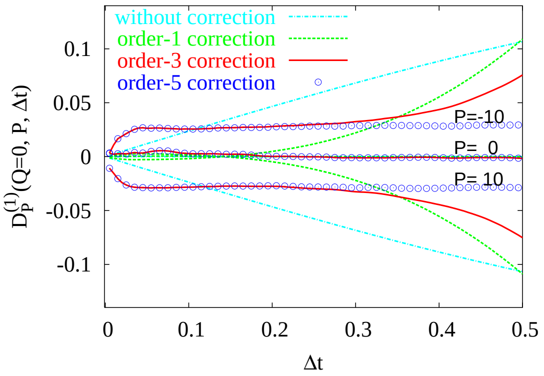

FIG. 1: (Color online) The evaluation of Eq.(15) for $D_P^{(1)}(0, P)$ including up to $O(\Delta t^5)$ corrections. Curves without and with 3rd order corrections are rescaled by factors of 1/100 and 1/10, respectively. Without corrections, the term $P\Delta t$ dominates the result and makes the estimate of the constant-in-Δt contribution impossible. Parameter are $\epsilon = 0.02$, $\kappa = 4$, $Q = 0$ and $E = 4$.

Assuming that the slow variables are governed by the Langevin dynamics corresponding to a Fokker-Planck equation, one can determine the drift and diffusion coefficients by mere data analysis. Estimates of these coefficients can be obtained from conditional time averages of a long trajectory of the full system [18] and read

$$\Delta t D_P^{(1)}(Q,P) + \mathcal{O}(\Delta t^2) = \langle \widetilde{P}(\Delta t)\rangle_{q,p} - P \tag{13a}$$
$$\Delta t D_{PP}^{(2)}(Q,P) + \mathcal{O}(\Delta t^2) = \left\langle (\widetilde{P}(\Delta t) - P)^2 \right\rangle_{q,p} \tag{13b}$$

Here, $\widetilde{P}(\Delta t) = \widetilde{P}(\Delta t; q, p, Q, P)$ is the solution of the equations of motion derived from Eq.(1) with initial condition $(Q, P, q, p)(0) = (Q, P, q, p)$ and $\langle ...\rangle_{q,p}$ denotes the conditional average over q and p on the energy shell $H(q, p, Q, P) = E/\epsilon$. Relations Eq.(13) are valid under the assumption that the system is Markovian for $\Delta t \gg \epsilon$.

A direct numerical estimate of $D_P^{(1)}$ through Eq.(13a), using trajectories of the full coupled system, is quite cumbersome due to the smallness of the damping term. In order to satisfy $\epsilon \ll \Delta t$, higher order corrections in Δt have to be taken into account to identify the small damping terms. Such corrections yield a more sophisticated estimator. In particular, if we assume for simplicity that the drift is a linear function of the phase space variables

$$\underline{D}^{(1)}(Q,P) = \underline{\underline{M}} \begin{pmatrix} Q \\ P \end{pmatrix} \tag{14}$$

where the constant matrix $\underline{\underline{M}}$ denotes the coefficients of the drift and if we neglect the phase space dependence of the diffusion constant then, by including higher order

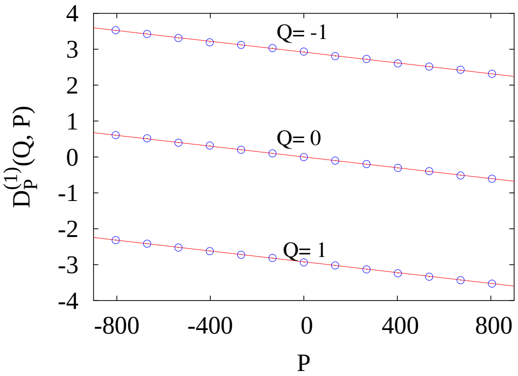

FIG. 2: (Color online) Viscous damping of the stochastic Kubo model: The drift terms derived from the analytical expression (lines; cf. Eq.(4)) and the numerical estimates using (15) and (14) (circles) for $Q = -1, 0$ and 1. Parameters are ϵ=0.02, κ=2, $E = 8000$.

corrections of Eq.(13a) we obtain the improved estimator

$$\underline{D}_{\rm est}^{(1)}(Q,P,\Delta t) = \underline{D}^{(1)}(Q,P) + \sum_{n=2}^{N} \frac{\Delta t^{n-1}}{n!} \underline{\underline{M}}^n \begin{pmatrix} Q \\ P \end{pmatrix} \tag{15}$$

An estimate of $\underline{\underline{M}}$ from Eq.(13a) can be used in a self-consistent way for successive corrections.

A good example where the small damping term can be observed with the help of the introduced estimator is a system of a slow harmonic oscillator $\mathcal{H}_s = \frac{1}{2}((1 + \kappa)Q^2 + P^2)$ which is coupled harmonically with a fast so-called Kubo oscillator. The Kubo oscillator is a harmonic oscillator driven by a multiplicative Gaussian white noise $\xi(t)$, $\langle \xi(t)\xi(t')\rangle = 2\delta(t - t')$ and $\langle \xi(t)\rangle = 0$, such that the energy is preserved [19]

$$\dot{q} = \frac{1}{\epsilon} p(1 + \sqrt{\epsilon}\xi(t)) \, , \quad \dot{p} = -\frac{1}{\epsilon} q(1 + \sqrt{\epsilon}\xi(t)) \quad . \tag{16}$$

Thus the fast dynamics fulfils ideally all the properties of a Markov process. In contrast to chaotic Hamiltonian systems this stochastic model allows a complete analytical treatment [13]. With the help of the elimination method one obtains analytically a viscous damping term $\kappa^2\epsilon^2 P/2$ and the diffusion coefficient $\kappa^2\epsilon(E - \epsilon\mathcal{H}_s)/2$. For an empirical estimation of the damping one can apply the mentioned estimator. Indeed, for reasonable parameter values $\kappa = 4$, $\epsilon = 0.02$, and $E = 4$, we had to take correction terms up to order Δt^5 into account to identify the damping term (see Fig. 1). As shown in Fig. 2, the damping is viscous. Such an empirical estimation of the drift coefficients of the slow subsystem from the trajectories of the full system yields perfect agreement with our theoretical predictions. Deviations of higher order ϵ are expected but are too small to be visible.

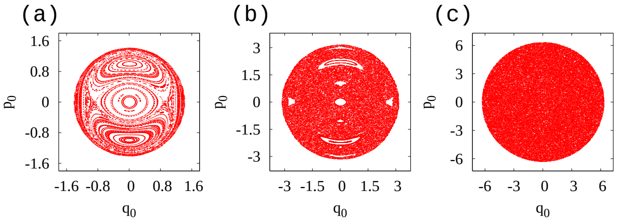

FIG. 3: (Color online) Poincare sections of the system (17) for the energy (a) $E = 1$, (b) $E = 5$ and (c) $E = 20$.

Lattice based estimator method

The straightforward estimation of the drift and diffusion coefficient according to Eq.(13) just needs one long trajectory which supplies the data. Due to multiple recurrences to a selected phase space point (Q, P) the required average over the fast degrees of freedom is possible, but time consuming. More importantly, the average over the fast variables is based on very large samples in those regions of the slow phase space where the reduced density is high and on very small samples where the reduced density is low.

Therefore we employ a more efficient method where the drift or diffusion coefficients are calculated for selected slow variables (Q, P) on a lattice. Every lattice point represents one initial condition for the slow subspace. The initial conditions for the fast variables are randomly drawn from the proper conditional distribution, which is the microcanonical distribution of $H_f(q,p)+\epsilon\mathcal{H}_c(q,Q)$ at the energy $E - \epsilon\mathcal{H}_s(Q,P)$ for the selected point (Q, P). The number of chosen initial conditions gives the sampling size. Each of these initial conditions requires only integration over the short time interval Δt. Apart from saving integration time the procedure enables us to use a faster integrator with less accuracy. We call this technique the *lattice based estimator method* for the calculation of drift and diffusion coefficients. It can only be used for Hamiltonian dynamics without transients, since otherwise the correct measure for the choice of (q, p) is unknown.

APPLICATION TO A CHAOTIC HAMILTONIAN SYSTEM

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

$$\mathcal{H}_f = \frac{1}{2}(p_0^2 + p_1^2 + q_0^2 + q_1^2 + q_0^2 q_1^2). \tag{17}$$

With increasing energy more and more regular islands vanish and larger regions of the phase space become chaotic (Fig. 3). Even for high energy when no islands are visible, it is not guaranteed that all regular areas are destroyed, i.e., there is no proof that this system is hyperbolic for sufficiently high energies.

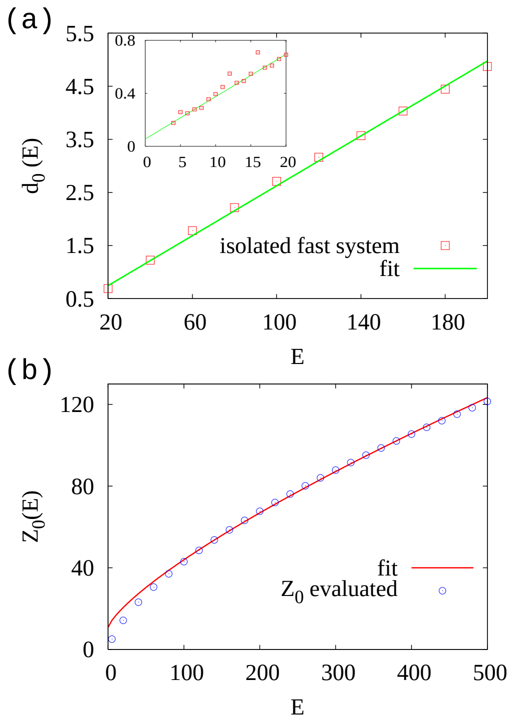

FIG. 4: (Color online) (a): Numerical evaluation of $d_0(E)$ (cf. Eq.(7) for the Hamiltonian (17) (symbols) and linear fit (line). (b) Partition function Eq.(18) (symbols) and fit according to a power law (line).

A slow harmonic oscillator, $\mathcal{H}_s = (1+\kappa)Q^2/2+P^2/2$, is coupled to these fast chaotic degrees of freedom through the variable q_1 and a harmonic potential, $\mathcal{H}_c(q, Q) = -\kappa q_1 Q$. An analytical computation of the fast autocorrelations and the required averages is not possible for this nonlinear fast subsystem, but one can evaluate Eqs.(9) and (10) numerically. For that purpose we calculate the fast autocorrelation function from ensembles of the numerical solutions of the fast system as a function of the fast energy. This gives rise to $d_0(E)$ in Eq.(7). As is shown in Fig. 4 (a), d_0 is essentially linear in E. The partition function can be reduced to an elliptic integral which can be evaluated numerically (see Fig. 4 (b)):

$$Z_0(E) \;=\; 2\pi \int_0^{\sqrt{2E}} \sqrt{\frac{2E - q_1^2}{1 + q_1^2}}\, dq_1 \approx E^{0.7}. \tag{18}$$

Inserting these results in Eqs.(9) and (10) yields Eqs.(11) and (12) with $\alpha \approx 0.7$ and $\omega \approx 0.0252$. Thus our theoretical results fully specify the reduced model. Since the diffusion coefficient is proportional to the energy in the fast subsystem, it vanishes when the slow energy exceeds the total energy E/ϵ, as expected.

The coefficients of this model are now to be checked by the estimation of the diffusion tensor from data of

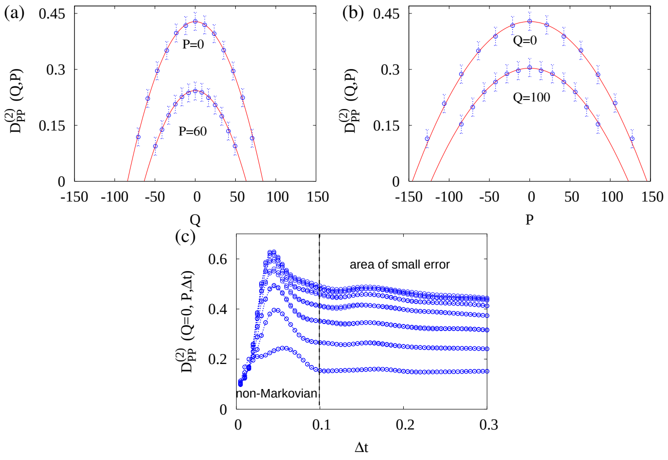

FIG. 5: (Color online) The diffusion terms derived from Eq.(9) (lines) and the numerical estimates using Eq.(13b) (circles) for different Q (chaotic fast subsystem, ϵ=0.02, κ=2, $E = 200$).

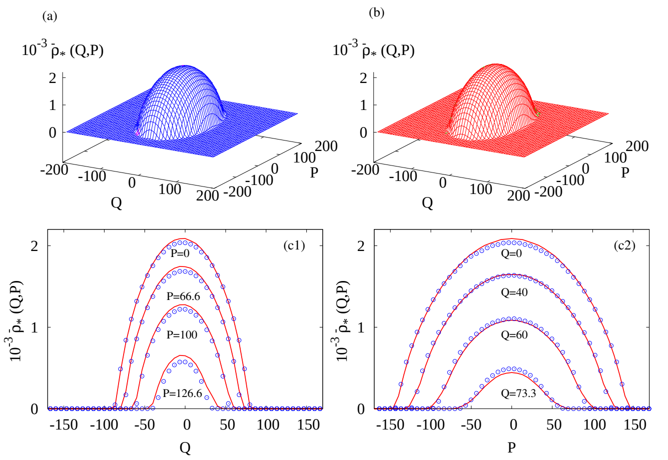

FIG. 6: (Color online) Stationary distribution of (a) the Hamiltonian system, (b) stochastic model. (c1)/(c2): comparison of the stationary density of the full system (circles) to the stationary density of the reduced model (lines; cf. Eq.(8)). Parameters are $\epsilon = 0.02$, $\kappa = 2$, and $E = 200$.

the full system. By the help of the lattice based estimation we obtain the diffusion tensor at lattice points in the slow phase space. As Fig.5 shows, the agreement is excellent. However, a more detailed consideration of these diffusion estimates reveals interesting additional insight (Fig.5c). The dependence of the estimated $D^{(2)}_{PP}$ on Δt (see Eq.(13b)) reveals some systematic deviations which reflect the non-Markovian range. Due to higher order Δt corrections one expects that smaller values for Δt yield smaller estimation errors. But the non-Markovian range of small Δt which extends here over the range $\Delta t < 0.1$ has to be identified and to be excluded. In this example, we determined the diffusion coefficients shown in Fig.5 a) and b) by averaging the corresponding values over the interval $0.1 \le \Delta t \le 0.3$. The estimation of the small damping term for this model from data is quite cumbersome since it is hidden by higher order Δt effects.

Although we were able to estimate diffusion coefficients in a concise way we still need to check whether a Fokker-Planck equation is an appropriate model for the slow dynamics. Hence, we will study in addition the dynamics of the reduced model and compare it to the dynamics of the slow variables of the full model.

First the stationary density of the Fokker-Planck equation will be compared with the density of the full coupled system which represents the asymptotic long time behaviour. The invariant density of the stochastic model is obtained by numerical integration of the corresponding Langevin equation while the density of the full system follows by integration of the Hamiltonian equations of motion in the full phase space. The agreement between both invariant densities is very good over the whole phase space (see Fig. 6). In particular, the support of the density of the reduced stochastic model is finite. Deviations between the exact density and those of the stochastic model are of the order of ϵ.

Time dependent moments are suitable quantities for the study of dynamics. In particular, they serve for the investigation of the time evolution of the slow subsystem in the short time as well as in the long time limit. Using the reduced equations of motion (2), the moments $\langle Q^2\rangle(t)$, $\langle P^2\rangle(t)$, and $\langle PQ\rangle(t)$ can be obtained analytically. One has to multiply the Fokker-Planck equation by Q^2, QP, or P^2, respectively, and to integrate over the slow subspace. This yields a set of coupled linear differential equations for the second moments of the reduced system

$$\frac{\partial}{\partial t}\langle Q^2\rangle(t) = 2\langle QP\rangle \tag{19a}$$

$$\frac{\partial}{\partial t}\langle QP\rangle(t) = -(1+\kappa)\langle Q^2\rangle - \epsilon^2\widetilde{\gamma}\langle QP\rangle + \langle P^2\rangle \tag{19b}$$

$$\frac{\partial}{\partial t}\langle P^2\rangle(t) = -\epsilon^2\Gamma\langle Q^2\rangle - 2(1+\kappa)\langle QP\rangle - \epsilon^2(2\widetilde{\gamma}+\Gamma)\langle P^2\rangle + 2\Gamma E \tag{19c}$$

with the decay rates $\widetilde{\gamma} = \omega(1+\alpha)\kappa^2 \approx 0.043\kappa^2$ and $\Gamma = \omega\kappa^2 \approx 0.0252\kappa^2$.

Due to the Markov approximation which has been employed for the derivation of Eq. (2), deviations between the slow part of the full dynamics and the slow stochastic model are expected on very short time scales. We hence compute the transient motion of the slow moment $\langle P^2\rangle(t)$ which corresponds to the averaged kinetic energy of the slow subsystem. Figure 7 shows the evolution of this moment starting from the initial condition $(Q(t=0), P(t=0)) = (0,0)$. The overall agreement between the Fokker-Planck equation (2) and the full system is very good. Approximation errors do only exist in

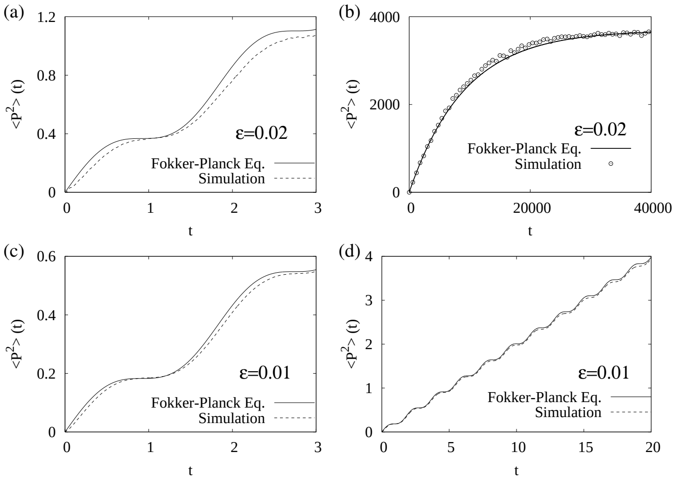

FIG. 7: A comparison of the averaged slow kinetic energy of numerical solutions (broken lines, circles) of the full system to the analytically predicted results (solid lines) of the effective dynamics. Short-time evolution: (a) $\epsilon = 0.02$, (c) $\epsilon = 0.01$ and (d). Long-time evolution: (b) $\epsilon = 0.02$. All panels: initial conditions $Q(0) = P(0) = 0$, $\kappa = 2$, $E = 200$.

the short time regime $t = \mathcal{O}(\epsilon)$, where the times are of the order of the decay time of the fast correlations (non-Markovian effects). For a more pronounced time scale separation the deviations are decreasing in accordance with the theory (Fig. 7 (c)). Deviations between the simulation and the theoretical results are of order $\mathcal{O}(\epsilon^2)$ which is on the other hand the accuracy of the damping and diffusion coefficients. The modulated linear increase of $\langle P^2\rangle(t)$ on the intermediate time scales corresponds to the free diffusion and reflects the smallness of the damping. Saturation on long time scales is expected to occur at $\langle P^2\rangle(\infty) \approx 3800$. As shown in Figure 7 (b) the predictions of the long time behavior are accurate on the basis of our elimination method.

CLASSICAL HYDROGEN ATOM IN A HOMOGENEOUS MAGNETIC FIELD

A system with time scale separation with a real physical meaning is a highly excited hydrogen atom (Rydberg atom) in a homogeneous magnetic field. Due to the high excitation, a classical treatment is appropriate. Chaos in the electronic degree of freedom is well established both for the classical and the quantum mechanical version [20]. The Hamiltonian is of the form

$$\mathcal{H} = \frac{1}{2m_e}\left(\underline{p}_e - \frac{e}{2}\underline{B}\times\underline{r}_e\right)^2 + \frac{1}{2M_p}\left(\underline{P}_p + \frac{e}{2}\underline{B}\times\underline{R}_p\right)^2 + V(\underline{r}_e - \underline{R}_p)\,, \tag{20}$$

where $\underline{r}_e$, $\underline{p}_e$ and $\underline{R}_p$, $\underline{P}_p$ denote the position vector and its canonically conjugated momentum of the electron and the nucleus, respectively. Here e and m_e are the charge and mass of the electron and M_p is the mass of the nucleus. $V(\underline{r}) = -e^2/|\underline{r}|$ denotes the Coulomb interaction potential. Due to the large mass ratio between the nucleus and the electron a pronounced time scale separation is generated between the center of mass motion and the internal relative motion. The dynamics of this system has been investigated theoretically as well as experimentally with high accuracy [20].

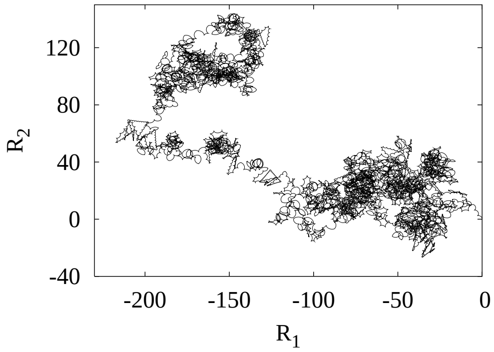

FIG. 8: Brownian like chaotic motion of the center of mass of a Rydberg atom in a homogeneous magnetic field (simulation time $T = 5\times10^9$, $B_z = 10^{-5}$, $E_t = -44.7\times10^{-6}$ atomic units.

Almost all investigations are focused on the relative motion of the electron with respect to the nucleus as such a feature is experimentally accessible through spectral analysis. The center of mass motion has been usually ignored because of the time scale separation. A notable exception is the numerical study by Schmelcher and Cederbaum [21] who showed that the center of mass motion is not negligible and can become chaotic, too. They observed a kind of *random walk* of the center of mass which spreads over increasingly larger parts of the position space when time increases (see Fig. 8). Through numerical scaling analysis of the end-to-end distances of such paths it was shown in [21] that indeed the centre of mass motion is a diffusion process in the long time limit.

The hydrogen atom in a homogeneous magnetic field fulfils all requirements for applying our elimination scheme to the fast chaotic relative motion. Thus we can derive a Fokker-Planck equation for the slow center of mass motion in a theoretically well justified way. As a starting-point for the application of the elimination procedure we choose the following splitting of the Hamiltonian

$$\widetilde{\mathcal{H}} = M\mathcal{H} = \widetilde{\mathcal{H}}_s + \frac{1}{\epsilon}\widetilde{\mathcal{H}}_f + \widetilde{\mathcal{H}}_c, \qquad \epsilon := \frac{\mu}{M} \tag{21a}$$

$$\widetilde{\mathcal{H}}_s = \frac{1}{2}\underline{P}^2 \tag{21b}$$

$$\widetilde{\mathcal{H}}_f = \frac{1}{2}\left\{ \left[\underline{p} - \frac{e\mu}{2\mu'}\underline{B}\times\underline{r}\right]^2 + \epsilon e^2(\underline{B}\times\underline{r})^2 -2\mu\frac{e^2}{|\underline{r}|}\right\} \tag{21c}$$

$$\widetilde{\mathcal{H}}_c = -e\underline{P}(\underline{B}\times\underline{r})\ , \tag{21d}$$

where $\mu = m_e M_p/(M_p + m_e)$ is the reduced mass, $\mu' = m_e M_p/(M_p - m_e)$ the modified reduced mass and $M = M_p + m_e$ the total mass. $\underline{r}$, $\underline{p}$ and $\underline{R}$, $\underline{P}$ denote the position vector and its canonically conjugated momentum of the relative motion and the center of mass. The corresponding equations of motions are given as follows

$$\dot{\underline{R}} = \underline{P} - e(\underline{B}\times\underline{r}) \tag{22a}$$

$$\dot{\underline{P}} = 0 \tag{22b}$$

$$\dot{\underline{r}} = \frac{1}{\epsilon}\left(\underline{p} - \frac{e\mu}{2\mu'}\underline{B}\times\underline{r}\right) \tag{22c}$$

$$\dot{\underline{p}} = -\frac{1}{\epsilon}\left[\epsilon e(\underline{B}\times\underline{P}) + \frac{e\mu}{2\mu'}(\underline{B}\times\underline{p}) -e^2\left(\frac{\mu^2}{4\mu'^2}+\epsilon\right)\underline{B}\times(\underline{B}\times\underline{r}) + e^2\mu\frac{\underline{r}}{|\underline{r}|^3}\right]. \tag{22d}$$

Following [21] we restrict ourselves to the case $\underline{P} = 0$ and $L_z = 0$. Taking the magnetic field to point in the z-direction, $\underline{B} = B_z\underline{e}_3$, the center of mass motion in configuration space is bound to a two-dimensional plane. By applying our elimination scheme for the chaotic internal relative motion one obtains the following effective diffusion equation for the center of mass

$$\frac{\partial}{\partial t}\bar{\rho}_t(\underline{R}) = \epsilon^2\left(\frac{\partial^2}{\partial R_1^2}\widetilde{D}^{(2)}_{22}\bar{\rho}_t - 2\frac{\partial^2}{\partial R_1\partial R_2}\widetilde{D}^{(2)}_{12}\bar{\rho}_t + \frac{\partial^2}{\partial R_2^2}\widetilde{D}^{(2)}_{11}\bar{\rho}_t\right)\ , \tag{23}$$

where the diffusion coefficients

$$\widetilde{D}^{(2)}_{ij} = (eB_z)^2\int_0^\infty \langle r_i(t)r_j(t+\tau)\rangle d\tau, \quad i,j = 1,2 \tag{24}$$

are defined by the time integral over the autocorrelation of the fast relative variables r_i. Since the coupling (21d) is a bilinear expression in the fast position $\underline{r}$ and the slow momentum $\underline{P}$ the resulting Fokker-Planck equation (23) contains a diffusion operator acting on the slow spatial coordinates. The question now is whether this stochastic model yields a reasonable description for the Brownian motion of the center of mass. For a detailed quantitative investigation of the quality of our predictions we evaluate the theoretical prediction of the diffusion coefficients

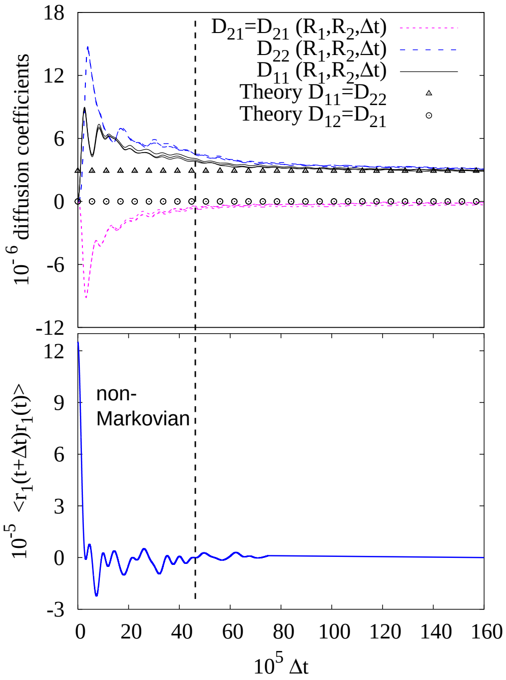

FIG. 9: (Color online) Top panel: A comparison of the evaluation of the "empirical" diffusion coefficient (13b) on numerical solutions of the full system (lines) to the analytically predicted results Eq.(4) (symbols) as a function of Δt, where deviations are due to violation of Markovianity on small time intervals. Note: Each coefficient is calculated for three different values of $\underline{R}$ to show $D^{(2)}_{ij}$ is independent of $\underline{R}$.
Bottom panel: Decay of the autocorrelation function of the relative motion. Parameters are $E_t = -49.2\times10^{-6}$ and $B_z = 10^{-5}$.

and compare them to the empirically estimated values. Figure 9 shows the results of this comparison for a total energy $E_t = -49.2\times10^{-6}$. As in the previous examples one clearly recognises the fast time scale on which the Markov property does not hold. On larger time scales, however, the Fokker-Planck description is well confirmed by the saturation of the moments for larger Δt. More importantly, the non-diagonal elements of the diffusion tensor vanish in almost perfect agreement with the theoretical predictions and the diagonal coefficients take the value $D^{(2)}_{11} = 2.6\times10^{-6}$. There are no cross correlations due to the symmetry of this problem.

Furthermore, we can verify for an extended energy interval in the chaotic regime the validity and accuracy of this stochastic modeling of the center of mass motion. As is shown in Figure 10 the predicted values of the diffusion coefficients $D^{(2)}_{11}$ are quite closed to the measured values for the energies $E_t \in [-22.4\times10^{-6}, -49.2\times10^{-6}]$. Deviations are negligible. Thus we conclude that the elimination method yields a good effective description for the slow center of mass motion.

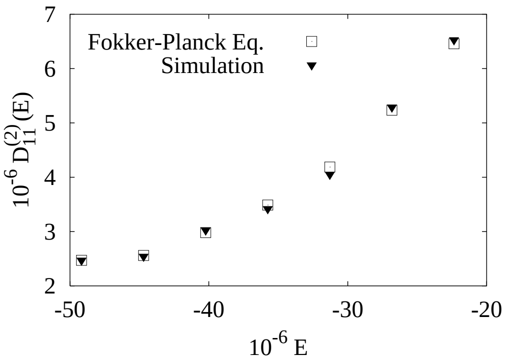

FIG. 10: Comparison of the "empirical" diffusion coefficient (13b) using the lattice based method in the full system (triangles) to the analytically predicted results (squares) for different energy values. Parameters: $B_z = 10^{-5}$.

CONCLUSION

Descriptions in terms of Fokker–Planck equations or Langevin equations are expected to be valid for Hamiltonian systems coupled to a heat bath, i.e. in situations where a large number of degrees of freedom is involved. Here we have shown by extensive numerical simulations that theoretical derivations of stochastic models are even valid for low-dimensional Hamiltonian chaos. Thus the thermodynamic limit is not necessary to justify either a Markov approximation or the Gaussian statistics of the residual forces. Both properties can be obtained from the time scale separation between fast and slow degrees of freedom.

We have been able to obtain explicit expressions for the drift as well as for the diffusion coefficient. The correct dependence of damping and diffusion on the expansion parameter and on the phase space coordinates ensures a fluctuation dissipation relation and guarantees the correct asymptotic dynamics on large time scales. It is worth noticing that the coefficients of the Fokker-Planck equation can be obtained with rather small numerical effort and that they are determined by properties of the fast dynamics solely.

We stress that our results are not rigorous from the mathematical point of view since our evidence relies on numerical simulations. In fact, performing proofs even for a simple setup seems to be quite a challenging task. Nevertheless, we believe that our results apply in quite general contexts. For instance, generic Hamiltonian chaos is dominated by a mixed phase space where regular islands are surrounded by a chaotic sea. Even in this case the stochastic model which is based on a Markov approximation yields predictions of the slow dynamics with rather high accuracy. Using recurrence time calculations of coupled symplectic maps we observed that the coupling of a system with mixed phase space to a slow dynamics speeds up the decay of correlations [22].

Finally we emphasise that similar elimination and modelling schemes apply to general, i.e. dissipative, dynamical systems as well (cf. [23]) and much effort has been spent on such cases (cf. e.g. [24]). Actually the literature on averaging procedures covers a rather broad range of topics, e.g. from an abstract and formal semigroup approach already developed several decades ago [25] to recent applications of multiple scaling techniques to the transport of passive scalars in fluids [26]. But one has to keep in mind that the case of general, i.e. non conservative, dynamical systems differs from the Hamiltonian case analysed here. Above all, fluctuation dissipation relations play a minor role for general dynamical systems as "dissipative" contributions are already appearing in the slow dynamics. In the Hamiltonian case dissipation is solely produced by the fast degrees of freedom and the corresponding fluctuation dissipation relation is crucial for the correct asymptotic behaviour. On the other hand the analysis of the Hamiltonian case is facilitated by the a priori knowledge of the invariant measure which is usually not known for general dynamical systems. Finally, transitions between coexisting states of the slow dynamics may cause long transient dynamics which seems to be difficult to be captured accurately by perturbation schemes, either for general dynamical systems or in the Hamiltonian case. Thus, the elimination of fast chaotic degrees of freedom and the modelling by suitable stochastic forces still poses considerable challenges for future research.

Acknowledgments

We acknowledge helpful discussions with Katrin Gelfert, Shmuel Fishman, and Rainer Klages.

---

* Electronic address: `baba@mpipks-dresden.mpg.de`

[1] M.C. Cross and P.C. Hohenberg, *Pattern-formation outside of equilibrium*, Rev. Mod. Phys. **65**, 851 (1993).
[2] H. Haken, *Synergetics* (Springer, Berlin, 1977).
[3] J. Guckenheimer and P. Holmes, *Nonlinear Oscillations, Dynamical Systems, and Bifurcations of Vector Fields* (Springer, New York, 1986).
[4] C. Jones, *Geometric singular perturbation theory*, in: *Dynamical Systems*, R. Johnson (ed.), (Springer, Berlin, 1995).
[5] N. Bogolubov and Y. Mitropolskii, *Asymptotic Methods in the Theory of Nonlinear Oscillations* (Gordon & Breach, New York, 1961).
[6] J. Sanders and F. Verhulst, *Averaging Methods in Nonlinear Dynamics* (Springer, Berlin, 1985).
[7] Y. Kifer, *Another proof of the averaging principle for fully coupled dynamical systems with hyperbolic fast motion*, Discr. Cont. Dyn. Syst. **13**, 1187 (2005).
[8] K. Hasselmann, *Stochastic climate models: part I theory*, Tellus **28**, 473 (1976).

[9] M. Cencini, M. Falcioni, H. Kantz, E. Olbrich and A. Vulpiani, *Chaos or noise – Difficulties of the distinction*, Phys. Rev. **E 62**, 427 (2000).

[10] H. Kantz, W. Just, N. Baba, K. Gelfert and A. Riegert, *Fast chaos versus white noise – entropy analysis and Fokker–Planck model for the slow dynamics*, Physica **D 187**, 200 (2004).

[11] D. Givon, R. Kupferman and A. Stuart, *Extracting macroscopic dynamics: model problems and algorithms*, Nonlinearity **17**, R55 (2004).

[12] C. Jarzynski, *Thermalization of a Brownian particle via coupling to low-dimensional chaos*, Phys. Rev. Lett. **74**, 2937 (1995).

[13] A. Riegert, N. Baba, K. Gelfert, H. Kantz and W. Just, *Hamiltonian Chaos Acts Like a Finite Energy Reservoir: Accuracy of the Fokker-Planck Approximation*, Phys. Rev. Lett. **94**, 054103 (2005).

[14] E. Fick and G. Sauermann *The Quantum Statistics of Dynamic Processes* (Springer, Berlin, 1990)

[15] A. Canergie and I.C. Percival, *Regular and chaotic motion in some quartic potentials*, J. Phys. **A 17**, 801 (1983).

[16] H. Mori, H. Fujisaka and H. Shigematsu, *A new expansion of the master equation*, Prog. Theor. Phys. **51**, 109 (1974).

[17] A detailed derivation will be published in A. Riegert, H. Kantz, W. Just and N. Baba, *Stochastic Modelling: Replacing fast chaotic degrees of freedom by Langevin forces* (in preparation)

[18] S. Siegert, R. Friedrich and J. Peinke, *Analysis of data sets of stochastic systems*, Phys. Lett. **A 243**, 275 (1998).

[19] H. Risken, *The Fokker–Planck Equation* (Springer, Heidelberg, 1989).

[20] H. Friedrich and D. Wintgen, *The hydrogen atom in a uniform magnetic field: An example of chaos*, Phys. Rep. **183**, 37 (1989).

[21] P. Schmelcher and L.S. Cederbaum, *Regularity and chaos of the center of mass motion of the hydrogen-atom in a magnetic field*, Z. Phys. **D 24**, 311 (1992).

[22] N. Baba, *Elimination schneller chaotischer Freiheitsgrade in Hamiltonischen Systemen*, thesis (2005).

[23] W. Just, K. Gelfert, N. Baba, A. Riegert and H. Kantz, *Elimination of fast chaotic degrees of freedom: On the accuracy of the Born approximation*, J. Stat. Phys. **112**, 277 (2003).

[24] A. Majda, I. Timofeyev, E. Vanden-Eijnden, *A priori tests of a stochastic mode reduction strategy*, Physica **D 170**, 206 (2002)

[25] T. G. Kurtz, *A limit theorem for perturbed operator semigroups with applications to random evolutions* J. Funct. Anal. **12**, 55 (1973).

[26] A. Mazzino, S. Muscacchio, and A. Vulpiani, *Multiple-scale analysis and renormalization for preasymptotic scalar transport*, Phys. Rev. **E 71**, 011113 (2005).