Fast Hamiltonian chaos: Heat bath without thermodynamic limit

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Chaotic Hamiltonian systems with time scale separation display features known from nonequilibrium statistical physics even when no thermodynamic limit is involved. In particular, fast chaotic degrees of freedom can be modeled by suitable stochastic forces and a Fokker–Planck equation governing the slow parts of the motion can be derived. It turns out that the underlying Hamiltonian structure results in fluctuation–dissipation relations which link the parameters of the effective stochastic model. Such properties are crucial to ensure the correct stationary state of the stochastic description. Our results demonstrate that concepts from thermodynamics can be transferred to dynamical systems with few degrees of freedom.

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I. INTRODUCTION

The interpretation of many irrelevant degrees freedom as a heat bath and their respective elimination is a classical concept in the context of statistical mechanics. The corresponding scenario in this paper is the coupling of relevant degrees of freedom to a small irrelevant subsystem where consequently the statistical ensemble is the microcanonical one. Instead of resorting to the thermodynamic limit we require here a time scale separation between the relevant and the irrelevant subsystem together with chaotic properties of the latter. In this context, our issue is how to describe the relevant slow subsystem as an open system by kinetic equations which best reproduce the slow dynamics when being part of the full system. Evidently, one expects a fluctuation–dissipation theorem to hold which will be one of the results of our elimination procedure.

Pronounced time scale separation between different degrees of freedom naturally appears in many complex systems. For example, in climate modeling the characteristic time scales range from days for the dynamics in the atmosphere up to scales of the order of hundreds or thousands of years for changes in the deep ocean and ice shields [1]. As an other case one may consider classical multi–scale systems in astrophysics [2]. Typically the physically relevant observables are related to the slow variables while the details of the fast motion are of no interest. On the other hand, the implementation of numerical schemes requires a step size which can cope with the smallest time scale of the model. So the aim in analyzing such systems is to eliminate the fast degrees of freedom in such a way that one obtains an effective description for the slow variables which should possess the correct long time properties.

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The effective influence of the fast subsystem onto the slow variables strongly depends on the underlying dynamics. If the fast dynamics is purely contracting a centre manifold reduction can be performed [3] while in the case of a periodic fast system averaging procedures reduce the number of degrees of freedom [4]. In both well known cases the effective dynamics is governed by a purely deterministic vector field. But if the fast degrees of freedom are chaotic one expects that they can be modeled by noise, due to correlation decay. A classical realization of such a concept is, for instance, the eddy diffusivity in the hydrodynamic context (cf. e.g. [5] for a recent contribution). Within a general setup an effective description in terms of a Fokker–Planck equation can be derived where the drift and diffusion coefficient are determined by properties of the fast dynamics alone [6]. If the chaotic dynamics is fully hyperbolic methods from statistical averaging can be used [7]. In fact, the rigorous derivation of a Fokker-Planck equation for a particular chaotic dynamical system with few degrees of freedom has been performed in a certain scaling limit [8]. More general, the principal problem how to prove the validity of a kinetic equation for low-dimensional dynamical systems has been addressed as well, using projection operator techniques [9]. But here we do not dwell on rigorous projection operator approaches which are still a challenge for time continuous systems when unbounded generators have to be considered.

In this article, we focus on Hamiltonian systems with two characteristic time scales where the fast dynamics is chaotic. Like in dissipative systems the influence of the fast system leads to a diffusion contribution, so in order to fulfill energy conservation a damping should appear as well. Different formulations of the dissipative contribution have been proposed in [10–12]. We present a complete derivation of the Fokker–Planck equation as a description for the effective dynamics. We make use of a projection operator approach [13, 14] that allows for a perturbation expansion. A Markov approximation is justified by sufficiently fast decaying correlations of the fast chaotic subsystem. The eliminated degrees of freedom generally cause a viscous damping and a diffusion. A fluctuation–dissipation relation guarantees that the Fokker–Planck equation has the correct stationary solution and fulfills detailed balance. In some approximation, the dependence of damping and diffusion coefficient on the slow and fast dynamics can be decomposed where the part depending on the slow coordinates can be derived analytically from the equations of motion and the numerical values of the part stemming from the fast dynamics can be determined by numerically integrating the fast subsystem alone.

In section II we describe the general setup and introduce the notation. Section III briefly reviews the essentials of the projection operator approach and, in particular, introduces the appropriate projection operator which will be used for the time scale separation. A few remarks on the perturbation expansion are contained in section IV while the details of the computation are devoted to the appendix. The main result, i.e., the effective Fokker–Planck equation for the slow degrees of freedom is described in section V and the presentation is self-contained in the sense that a reader who is not interested in the formal derivation does not have to study the previous sections in detail. Finally, section VI comments on higher-dimensional slow subsystems as well.

II. HAMILTONIAN SYSTEM WITH TWO TIME SCALES

Our aim is to obtain a description for the effective dynamics of chaotic Hamiltonian systems with time scale separation. We consider N slow degrees of freedom with canonically conjugated variables V_i, X_i $(i = 1, \ldots, N)$ and n fast degrees of freedom p_α, q_α $(\alpha = 1, \ldots, n)$. For a general Hamiltonian system the equations of motion for a variable $z \in \{V_i, X_i, p_\alpha, q_\alpha\}$ are given by

$$\dot{z} = i\mathcal{L}z = \{\mathcal{H}, z\} \tag{1}$$

where the Poisson bracket is defined as

$$\begin{aligned} \{F, G\} &= \{F, G\}_s + \{F, G\}_f \\ &= \sum_{i=1}^{N} \left(\frac{\partial F}{\partial V_i} \frac{\partial G}{\partial X_i} - \frac{\partial G}{\partial V_i} \frac{\partial F}{\partial X_i} \right) \\ &\quad + \sum_{\alpha=1}^{n} \left(\frac{\partial F}{\partial p_\alpha} \frac{\partial G}{\partial q_\alpha} - \frac{\partial G}{\partial p_\alpha} \frac{\partial F}{\partial q_\alpha} \right) \quad . \end{aligned} \tag{2}$$

For the system with two different time scales the fast and slow subsystem are represented by $\mathcal{H}_f(\underline{p}, \underline{q})$ and $\mathcal{H}_s(V, X)$. In order to keep the notation simple we skip in what follows the labelling of different components of the slow system. The generalization to a higher–dimensional slow system is straightforward and will be given in section VI. The interaction $\mathcal{H}_c$ which couples both subsystems may depend on the fast variables $\underline{p}, \underline{q}$ and either on X or V. We will mainly focus on the case $\mathcal{H}_c(\underline{p}, \underline{q}, X)$. Systems coupled via $\mathcal{H}_c(\underline{p}, \underline{q}, V)$ show analogous results as discussed in section V. Due to the Hamiltonian structure there occurs a bidirectional coupling in the equations of motion (1). In order to obtain a dynamical system with time scale separation the Hamiltonian $\mathcal{H}$ is scaled in the following way:

$$\mathcal{H}(\underline{p}, \underline{q}, V, X) = \frac{1}{\varepsilon}\mathcal{H}_f(\underline{p}, \underline{q}) + \mathcal{H}_c(\underline{p}, \underline{q}, X) + \mathcal{H}_s(V, X) \tag{3}$$

Here the expansion parameter $\varepsilon \ll 1$ quantifies the time scale separation due to the parameters of the system. In classical cases like Brownian motion ε is usually given by a mass ratio [17], but in other physical contexts its identification might be a nontrivial task. The total energy of the system given by the Hamiltonian (3) is chosen to be E/ε with $E \sim \mathcal{O}(1)$. We assume that the fast subsystem possesses a chaotic region in phase space for all values of E.

According to (2) the corresponding Liouville operator $\mathcal{L}$ can be split with respect to its contributions that act either on fast or on slow variables:

$$\mathcal{L} = \frac{1}{\varepsilon}\mathcal{L}_0 + \mathcal{L}_1 \tag{4a}$$

with

$$i\mathcal{L}_0 z = \{\mathcal{H}_f + \varepsilon\mathcal{H}_c, z\}_f \tag{4b}$$

$$i\mathcal{L}_1 z = \{\mathcal{H}_s + \mathcal{H}_c, z\}_s \tag{4c}$$

So the equations of motion (1) can be written down in the following way:

$$\dot{V}(t) = i\mathcal{L}_1 V(t), \qquad \dot{X}(t) = i\mathcal{L}_1 X(t) \tag{5a}$$

$$\dot{\underline{p}}(t) = \frac{i}{\varepsilon}\mathcal{L}_0 \underline{p}(t), \qquad \dot{\underline{q}}(t) = \frac{i}{\varepsilon}\mathcal{L}_0 \underline{q}(t) \tag{5b}$$

An effective description for the dynamics of the slow degrees of freedom where the features of the fast system are only contained in the coefficients may be obtained in many different ways (e.g. [10–12]). Here we present a derivation based on a projection operator approach that is widely used in nonequilibrium statistical physics [13, 14]. For that purpose we assume that the Hamiltonian system does not admit any other first integral apart from the total energy and that the microcanonical distribution

$$\rho_E = \frac{\delta(\varepsilon\mathcal{H} - E)}{\mathrm{Tr}[\delta(\varepsilon\mathcal{H} - E)]} \tag{6}$$

is ergodic. Here, $\mathrm{Tr}[\ldots] = \int dp^n dq^n dV dX \ldots$ abbreviates the phase space integration. Furthermore, we assume that correlations decay sufficiently fast, although an exponential decay might not be required. Using a formal perturbation expansion we will derive a Fokker–Planck equation.

III. PROJECTION OPERATOR APPROACH

In order to apply projection operator techniques [13, 14] we turn from the equations of motion (5) to a description in terms of the phase space density $\rho_t(\underline{p},\underline{q},V,X)$ whose temporal evolution is given by the Liouville equation

$$\partial_t \rho_t = -i\mathcal{L}\rho_t \quad . \tag{7}$$

We are looking for the dynamics of the reduced density

$$\bar{\rho}_t = \int dp^n \, dq^n \rho_t =: \mathrm{Tr}_f[\rho_t] \quad . \tag{8}$$

Such a distribution can be obtained by a formal projection of the full density $\rho_t(\underline{p},\underline{q},V,X)$ onto a relevant density $\rho_t^{rel}(V,X;\underline{p},\underline{q})$. If one models the fast degrees of freedom by a distribution $\rho_{ad}(\underline{p},\underline{q}|V,X)$ which is parametrised by V, X the relevant density can be obtained by applying a projection operator $\mathcal{P}$:

$$\rho_t^{rel}(V,X;\underline{p},\underline{q}) = \mathcal{P}\rho_t = \rho_{ad}(\underline{p},\underline{q}|V,X)\mathrm{Tr}_f[\rho_t] \, . \tag{9}$$

The normalization of the density ρ_{ad} ensures that $\mathcal{P}$ is idempotent. Introducing the orthogonal projection by $\mathcal{Q} = \mathcal{I} - \mathcal{P}$ a formal integration of the equation of motion for the complementary irrelevant density $\rho_t^{irr} = \mathcal{Q}\rho_t$ yields an exact and closed equation of motion for the relevant density ρ_t^{rel} [13, 14]:

$$\frac{\partial \rho_t^{rel}}{\partial t} = -\mathcal{P}i\,\mathcal{L}\mathcal{P}\rho_t^{rel} + \int_0^t \mathcal{P}i\mathcal{L}\mathcal{Q}e^{-i\mathcal{Q}\mathcal{L}\mathcal{Q}t'}\mathcal{Q}i\mathcal{L}\mathcal{P}\rho_{t-t'}^{rel}dt' \tag{10}$$

provided the initial condition fulfills $\mathcal{Q}\rho_0 = 0$, i.e., the initial density is a relevant density. It is a long standing problem whether such a condition imposes a serious constraint on the validity of projection operator approaches, in particular, since $\mathcal{Q}\rho_0 = 0$ often implies the absence of correlations in the initial state. Recent formal results suggest [15] that such a condition does not impose a severe limitation as long as the fast dynamics is mixing. However, a rigorous proof would require a detailed examination of such a condition, in particular with regards to stability considerations. Above all, the usefulness of projection operator approaches and especially the quality of perturbation expansions depends crucially on the choice of ρ_{ad}.

It is in fact an essential property of the projection operator that it preserves the correct equilibrium state (6) since otherwise perturbation expansions may be corrupted. For the projection operator we thus require that

$$\mathcal{P}\rho_E = \rho_E \tag{11}$$

holds. Such a condition determines ρ_{ad} uniquely, when using Eqs. (6) and (9), and we obtain the result already proposed by Zwanzig several decades ago [18]:

$$\rho_{ad}(\underline{p},\underline{q}|V,X) = \frac{\delta\left(\varepsilon\mathcal{H} - E\right)}{\mathrm{Tr}_f\left[\delta\left(\varepsilon\mathcal{H} - E\right)\right]} \, . \tag{12}$$

Such a density can be viewed as a microcanonical distribution of the subsystem $\widetilde{\mathcal{H}}_f = \mathcal{H}_f + \varepsilon\mathcal{H}_c$ containing the energy $\widetilde{E} = E - \varepsilon\mathcal{H}_s(V,X)$ with the appropriate partition function

$$Z_E(V,X) = \mathrm{Tr}_f\left[\delta(E - \varepsilon\mathcal{H})\right] = \mathrm{Tr}_f\left[\delta(\widetilde{E} - \varepsilon\widetilde{\mathcal{H}}_f)\right] \tag{13}$$

for fixed values of X and V. The density (12) is an invariant density of the fast subsystem when the slow variables are considered to be constant. It can thus be viewed as an adiabatic density of the fast subsystem as well. Formally such a property is reflected by the condition

$$\mathcal{L}_0\rho_{ad}(\underline{p},\underline{q}|V,X) = 0 \tag{14}$$

which can be easily derived from Eqs. (4b) and (12). Actually, such an algebraic condition will be the key ingredient for a perturbation expansion of Eq. (10). Alternatively, one may consider the density ρ_{ad} as a ratio of two probability densities, namely the microcanonical density ρ_E, Eq. (6), and the reduced microcanonical density $\bar{\rho}_E = \mathrm{Tr}_f[\rho_E]$ since

$$\frac{\rho_E}{\bar{\rho}_E} = \frac{\delta(\varepsilon\mathcal{H} - E)}{\mathrm{Tr}\left[\delta(\varepsilon\mathcal{H} - E)\right]} \cdot \frac{\mathrm{Tr}\left[\delta(\varepsilon\mathcal{H} - E)\right]}{\mathrm{Tr}_f\left[\delta(\varepsilon\mathcal{H} - E)\right]} = \rho_{ad} \, . \tag{15}$$

Thus, the adiabatic density has as well the meaning of a conditional distribution. These two notions coincide for the Hamiltonian setup but differ in the context of dissipative dynamical systems [19].

With our choice for the relevant density (9), the following relations for the projection operator hold:

$$\mathcal{L}_0\mathcal{P} = 0 = \mathcal{P}\mathcal{L}_0 \tag{16}$$

The left hand condition follows directly from the definition of the adiabatic density (14) while the right hand identity takes into account that boundary contributions disappear. So, Eq. (10) leads to the exact dynamics of the reduced density:

$$\frac{\partial\bar\rho_t}{\partial t} = -\mathrm{Tr}_f[i\mathcal{L}_1\rho_{ad}]\bar\rho_t - \frac{\partial}{\partial V}\int_0^t \mathrm{Tr}_f\left[\frac{\partial\mathcal{H}_c}{\partial X}(\underline{p},\underline{q},X)\mathcal{Q}e^{-i\mathcal{QLQ}t'}\mathcal{Q}i\mathcal{L}_1\rho_{ad}\right]\bar\rho_{t-t'}dt' \ . \tag{17}$$

The first, local contribution which will be evaluated explicitly at the beginning of the next section reduces to the adiabatic average of the slow vector field. The second, nonlocal term still contains the full features of the fast system via the propagator $\exp(-i\mathcal{QLQ}t)$. So, in order to obtain a coefficient that is determined by integrating the fast dynamics alone, a lowest order approximation for the propagator has to be performed. Employing in addition a Markov approximation we will finally end up with a local contribution.

IV. PERTURBATION EXPANSION

The first contribution in (17) can easily be evaluated without any approximation:

$$-\mathrm{Tr}_f[i\mathcal{L}_1\rho_{ad}]\bar\rho_t = -i\mathcal{L}_s\bar\rho_t + \frac{\partial}{\partial V}\left\langle\frac{\partial\mathcal{H}_c}{\partial X}(\underline{p},\underline{q},X)\right\rangle_E\bar\rho_t \tag{18}$$

with the adiabatic average

$$\langle\ldots\rangle_E := \mathrm{Tr}_f[\ldots\rho_{ad}] \quad . \tag{19}$$

Eq. (18) contains the slow dynamics, $\mathcal{L}_s$, and a renormalization due to the interaction. If we denote the interaction force by

$$f_c(\underline{p},\underline{q},X) = -\frac{\partial\mathcal{H}_c}{\partial X}(\underline{p},\underline{q},X) \tag{20}$$

then the renormalization turns out to be a microcanonical version of a Born-Oppenheimer force acting on the slow degrees of freedom. In general, the local contribution (18) cannot be rewritten as a Poisson bracket. But it generates a differential equation which is determined by the adiabatically averaged vector field. We stress that the differential operator preserves the reduced microcanonical ensemble, i.e.

$$-i\langle\mathcal{L}_1\rangle_E\bar\rho_E = 0 \tag{21}$$

where $\langle\mathcal{L}_1\rangle_E$ abbreviates the operator contained in Eq. (18). It is straightforward to derive Eq. (21) by integrating the invariance condition of the microcanonical ensemble, $-i\mathcal{L}\rho_E = 0$, with respect to the fast degrees of freedom and using condition (15).

The second, nonlocal contribution to the exact dynamics of the reduced density seems to be rather complicated. But Eq. (17) is a good starting point for a perturbative approach. The formal perturbation expansion follows the usual idea of a Born approximation. To keep the presentation self-contained the details are summarised in the Appendix. The integral kernel is mainly determined by the autocorrelation of the chaotic fluctuations of the interaction force (20)

$$C_E(V,X;t) = \left\langle\delta f_c\left(\underline{p}_0(t),\underline{q}_0(t),V,X\right)\delta f_c\left(\underline{p},\underline{q},V,X\right)\right\rangle_E \tag{22}$$

where

$$\delta f_c = f_c - \langle f_c\rangle_E \tag{23}$$

denotes the static fluctuation and $\underline{p}_0(t) = \exp(i\mathcal{L}_0 t)\underline{p}$, $\underline{q}_0(t) = \exp(i\mathcal{L}_0 t)\underline{q}$ the time dependent solution of the fast equations of motion with fixed slow variable X and initial condition $\underline{q}(0) = \underline{q}$, $\underline{p}(0) = \underline{p}$. Since the autocorrelation function depends on the fast time scale t/ε a Markov approximation can be applied to obtain an equation local in time. Such an approximation requires a correlation which decays sufficiently fast, but an exponential decay is normally not necessary [20]. We just remark that any perturbation expansion, like the one described here, has to be consistent with the Markov approximation in the sense that the resulting expression for the correlation function becomes integrable.

V. FOKKER–PLANCK EQUATION

Collecting the local and nonlocal contributions calculated in the previous section and in the Appendix, the dynamics of the slow variables can be described effectively by the following Fokker–Planck equation:

$$\begin{aligned}\frac{\partial\bar\rho_t}{\partial t} =& -i\langle\mathcal{L}_1\rangle_E\bar\rho_t + \varepsilon^2\frac{\partial}{\partial V}\frac{\partial\mathcal{H}_s}{\partial V}\gamma_E(V,X)\bar\rho_t \\ &+ \varepsilon\frac{\partial^2}{\partial V^2}D_E(V,X)\bar\rho_t\end{aligned} \tag{24}$$

with

$$D_E(V,X) = \int_0^\infty dt\, C_E(V,X;t) \tag{25a}$$

$$\gamma_E(V,X) = \frac{1}{Z_E(V,X)}\frac{\partial}{\partial E}\left(Z_E(V,X)D_E(V,X)\right) \ . \tag{25b}$$

The first drift term of Eq. (24) contains the adiabatically averaged slow vector field already discussed in section IV. The second contribution contains the damping with coefficient γ_E given by (25b). The diffusion coefficient D_E defined in (25a) is determined by the integral over the autocorrelations of the fluctuations of the fast system with fixed slow variables. In the corresponding Langevin equation this is equivalent to a multiplicative noise. Since the dynamics is unitary in the Hamiltonian case standard arguments of nonequilibrium statistical mechanics ensure that the correlation function is an even function of t and that the diffusion coefficient D_E is non–negative [20]. Damping and diffusion both result from a lowest order perturbation expansion of the propagator (cf. (A5)) but due to the scaling of the energy the damping naturally appears in second order of ε, one order higher than the diffusion.

Eqs. (13) and (22) ensure that damping and diffusion depend on the phase space variables in a quite specific way, namely:

$$\begin{aligned} Z_E(V,X) &= \hat{Z}(E-\varepsilon\mathcal{H}_s, X) && (26a)\\ D_E(V,X) &= \hat{D}(E-\varepsilon\mathcal{H}_s, X) && (26b)\\ \gamma_E(V,X) &= \hat{\gamma}(E-\varepsilon\mathcal{H}_s, X)\,. && (26c)\end{aligned}$$

Thus the velocity dependence is entirely caused by conservation of energy while the additional coordinate dependence is due to the interaction potential and the interaction force (20). Relation (25b) together with the structure of the Fokker-Planck equation (24) ensures that the stationary solution is given by the reduced microcanonical density

$$\bar{\rho}_E = \mathrm{Tr}_f[\rho_E] = \frac{Z_E(V,X)}{\mathrm{Tr}\left[\delta(\varepsilon\mathcal{H}-E)\right]}\,. \tag{27}$$

When inserting (27) into Eq. (24), the systematic term vanishes as already stated by Eq. (21) while the contributions containing damping and diffusion cancel each other due to the identity

$$\frac{\partial}{\partial V}D_E\bar{\rho}_t + \varepsilon\frac{\partial\mathcal{H}_s}{\partial V}\frac{1}{Z_E}\frac{\partial}{\partial E}D_E Z_E\bar{\rho}_t = D_E\bar{\rho}_E\frac{\partial}{\partial V}\frac{\bar{\rho}_t}{\bar{\rho}_E}\,. \tag{28}$$

Thus, Eq. (25b) guarantees the stationarity of the correct equilibrium distribution. Hence, such a relation constitutes the microcanonical version of a fluctuation–dissipation theorem. Apart from the correct stationary behavior the positivity of the diffusion coefficient ensures relaxation towards equilibrium as well as the validity of a corresponding H–theorem [21]. Thus, our Fokker–Planck equation can be viewed as the best Fokker–Planck equation for our setup [22]. Any further improvement of the approximations will necessarily yield equations of motion which do not comply any longer with a Fokker–Planck structure [23].

So far our analysis has not involved any expansion with regard to the interaction Hamiltonian. Damping and diffusion have an intricate dependence on the slow phase space variables which is mainly caused by the interaction Hamiltonian. Thus, it is tempting to apply further approximations to evaluate such quantities. One has to keep in mind that detailed balance needs to be preserved. While the structure of the fluctuation–dissipation relation mainly ensures that approximations for the diffusion coefficient D_E and the partition function Z_E can be developed independently one has to observe that approximations for the latter have consequences for the treatment of the Born–Oppenheimer force. If, for instance, the interaction energy is neglected for computing the partition function, i.e. if the approximation

$$Z_E(V,X) = \mathrm{Tr}_f\delta[E-\mathcal{H}_f-\varepsilon\mathcal{H}_s] + \text{h.o.t.} \tag{29}$$

is employed, then the Born–Oppenheimer force has to be neglected as well

$$\langle\mathcal{L}_1\rangle_E = \mathcal{L}_s + \text{h.o.t.} \tag{30}$$

since otherwise Eq. (29) does not determine the stationary solution and detailed balance would be violated. For the diffusion coefficient D_E one can still use a completely independent approximation. However, if one applies the simplest approach, i.e. if one replaces the dynamics in the correlation function (22) by the dynamics of the fast subsystem, $\mathcal{H}_f$, one has to observe that the ensemble averages are evaluated with respect to the adiabatic density at lowest order

$$\rho_{ad} = \frac{\delta\left(E-\mathcal{H}_f-\varepsilon\mathcal{H}_s\right)}{\mathrm{Tr}_f\delta[E-\mathcal{H}_f-\varepsilon\mathcal{H}_s]} + \text{h.o.t.} \tag{31}$$

since otherwise consistency of the expressions would be violated and the correlations would not be stationary any longer. Within such a setup the diffusion coefficient evaluates as

$$\begin{aligned} D_E(V,X) = \int_0^\infty dt\,\mathrm{Tr}_f[\delta f_c(\underline{p}_f(t),\underline{q}_f(t),V,X)\\ \cdot\,\delta f_c(\underline{p},\underline{q},V,X)\rho_{ad}] + \text{h.o.t.} \quad (32)\end{aligned}$$

where the dynamics is entirely determined by the fast Hamiltonian, $\underline{p}_f(t) = \exp(i\mathcal{L}_f t)\underline{p}$, $\underline{q}_f(t) = \exp(i\mathcal{L}_f t)\underline{q}$. Finally, the damping constant is given in terms of the fluctuation–dissipation relation (25b). Thus all quantities can be numerically evaluated by integrating the fast subsystem alone [24, 25].

For the study of systems with an interaction that depends on the slow momentum V, i.e. $\mathcal{H}_c = \mathcal{H}_c(\underline{p},\underline{q},V)$, an approximate Fokker–Planck equation can be derived in a similar way. Such a result can be applied for example to the classical hydrogen atom [26] where the interaction is due to the Lorentz force: Our analysis verifies that the slow effective motion of the centre of mass is diffusive [25].

VI. HIGHER-DIMENSIONAL SLOW SUBSYSTEMS

For a slow system where the Hamiltonian consists of kinetic and potential energy, $\mathcal{H}_s = V^2/2 + U(X)$, the coefficient γ_E given by Eq. (25b) causes a viscous damping in the Langevin equation corresponding to (24). If more than one slow degree of freedom is considered the corresponding coefficient matrix $\underline{\underline{\gamma}}_E$ gives rise to additional effects for systems without time-reversal symmetry [12]. It is quite straightforward to generalize the previous derivation of the Fokker–Planck equation to cases when the slow subsystem explicitly contains N degrees of freedom. Replacing V, X by $\underline{V}, \underline{X}$ in the Hamiltonian (3), the higher–dimensional result reads

$$\frac{\partial \bar{\rho}_t}{\partial t} = -\, i\langle \mathcal{L}_1 \rangle_E \bar{\rho}_t + \varepsilon^2 \sum_{k,\ell=1}^{N} \frac{\partial}{\partial V_k} \gamma_{k\ell} \frac{\partial \mathcal{H}_s}{\partial V_\ell} \bar{\rho}_t + \varepsilon \sum_{k,\ell=1}^{N} \frac{\partial}{\partial V_k} \frac{\partial}{\partial V_\ell} D_{k\ell} \bar{\rho}_t \tag{33}$$

where

$$f_k(\underline{p}, \underline{q}, \underline{X}) = -\, \frac{\partial \mathcal{H}_c}{\partial X_k}(\underline{p}, \underline{q}, \underline{X}) \tag{34a}$$

$$-i\langle \mathcal{L}_1 \rangle_E = -\, i\mathcal{L}_s - \sum_{k=1}^{N} \frac{\partial}{\partial V_k} \langle f_k(\underline{p}, \underline{q}, \underline{X}) \rangle_E \tag{34b}$$

$$D_{k\ell}(\underline{V}, \underline{X}) = \int_0^\infty dt \Big\langle \delta f_k \left(\underline{p}_0(t), \underline{q}_0(t), \underline{V}, \underline{X} \right) \cdot \delta f_\ell \left(\underline{p}, \underline{q}, \underline{V}, \underline{X} \right) \Big\rangle_E \tag{34c}$$

$$\gamma_{k\ell}(\underline{V}, \underline{X}) = \frac{1}{Z_E} \frac{\partial Z_E D_{k\ell}}{\partial E} \ . \tag{34d}$$

As discussed in the previous section the velocity dependence is mainly caused by energy conservation (cf. Eq. (26)) while the interaction potential may result in an additional dependence on the coordinates.

The symmetric part of the matrix (34d) causes the damping while for systems without time–reversal symmetry an antisymmetric part appears as well

$$\gamma_{k\ell}^{(a)} = \frac{1}{2} \left(\gamma_{k\ell} - \gamma_{\ell k} \right) \tag{35}$$

which leads to a renormalization of the drift in the Fokker–Planck equation [20]. If we consider the motion of a single particle in the three dimensional configuration space, $N = 3$, or if we neglect the indirect interaction between different particles in a multi–particle setup then the corresponding contribution to the vector field can be written as a cross product

$$\sum_{\ell=1}^{3} \gamma_{k\ell}^{(a)} \frac{\partial \mathcal{H}_s}{\partial V_\ell} = -(\underline{V} \times \underline{B})_k \tag{36}$$

with the 'magnetic field' given by

$$\underline{B} = \frac{1}{2Z_E} \frac{\partial}{\partial E} \int_0^\infty \Big\langle \delta \underline{f} \left(\underline{p}_f(t), \underline{q}_f(t), \underline{V}, \underline{X} \right) \times \delta \underline{f}(\underline{p}, \underline{q}, \underline{V}, \underline{X}) \Big\rangle_E dt \ . \tag{37}$$

This magnetic field is the classical limit of the 2–form generating the quantum geometric phase. Thus our Fokker–Planck approximation derived with projection operator methods reproduces the result in [12].

VII. CONCLUSION

We have shown that Fokker–Planck equations modelling the effective slow dynamics of chaotic Hamiltonian systems can be derived perturbatively by projection operator methods where the expansion parameter is given by the ratio of different time scales. The approach does not require an expansion in terms of the interaction Hamiltonian. The decay of the correlations enables a Markov approximation. The effective equation contains a viscous damping and a diffusion coefficient which depends essentially on the slowly varying energy of the fast subsystem. A fluctuation–dissipation relation ensures detailed balance and the correct long term dynamics.

The analytically obtained expressions for damping and diffusion can be evaluated for Hamiltonian systems as the adiabatic density is explicitly known. If one compares the results with numerical studies [24, 25], not only the Fokker–Planck coefficients coincide, but also the dynamics of the effective description can be verified. In the short time regime, systematic deviations occur because the Markov property does not hold, while on all time scales larger $\mathcal{O}(\varepsilon)$ the agreement between the effective and the exact dynamics is rather perfect.

Our formal derivation of the Fokker–Planck equation was based on two essential assumptions, the ergodicity of the microcanonical distribution and a sufficiently fast decay of correlations in the fast subsystem. Whether an exponential decay of correlations is required, i.e. whether all Hamiltonian systems with mixed phase space have to be excluded from our discussion is difficult to judge a priori. At least general wisdom from Statistical Mechanics tells us that an algebraic decay of correlation functions does not prohibit the validity of kinetic equations in general, as long as the correlation functions are integrable. However, to explore the real limits of our approach one surely needs rigorous results.

APPENDIX A: EXPANSION OF THE MEMORY KERNEL

In this appendix we derive the approximate nonlocal contribution to the dynamics of the reduced density $\bar{\rho}_t$ given by (17) for a Hamiltonian two–scale system that is coupled via $\mathcal{H}_c = \mathcal{H}_c(\underline{p}, \underline{q}, X)$. The expansion of the memory kernel follows the standard procedure.

Using Eq. (4c) we obtain

$$\begin{aligned} \mathcal{Q} i\mathcal{L}_1(\rho_{ad}\bar{\rho}_{t-t'}) &= \mathcal{Q}\left(f_c(\underline{p}, \underline{q}, X)\frac{\partial}{\partial V} + i\mathcal{L}_s \right)(\rho_{ad}\bar{\rho}_{t-t'}) \\ &= \mathcal{Q} f_c \frac{\partial \rho_{ad}\bar{\rho}_{t-t'}}{\partial V} + \mathcal{Q}(i\mathcal{L}_s\rho_{ad})\bar{\rho}_{t-t'} \end{aligned} \tag{A1}$$

where we have used the property of the projection operator

$$\mathcal{Q}\rho_{ad} g = 0 \tag{A2}$$

which is valid for any function $g(V,X)$ depending solely on the slow variables. For the action of the slow Liouville operator straightforward computation yields

$$i\mathcal{L}_s\rho_{ad} = \frac{\varepsilon}{Z_E}\frac{\partial \mathcal{H}_s}{\partial V}\left(-\frac{\partial \mathcal{H}_c}{\partial X}\frac{\partial Z_E\rho_{ad}}{\partial E} + \rho_{ad}\frac{\partial}{\partial E}\mathrm{Tr}_f\left[\frac{\partial \mathcal{H}_c}{\partial X}\delta\left(\varepsilon\mathcal{H} - E\right)\right]\right) \tag{A3}$$

where the second term of Eq. (A3) does not contribute to Eq. (A1) because of the action of the projection operator (cf. Eq. (A2)).

So far we have not invoked any approximation. To evaluate the propagator of the memory kernel we resort to the property (16) of the projection operator resulting in

$$\mathcal{Q}i\mathcal{L}\mathcal{Q} = \frac{i}{\varepsilon}\mathcal{L}_0 + \mathcal{Q}i\mathcal{L}_1\mathcal{Q}\,. \tag{A4}$$

Approximation of the operator exponential by the leading order thus yields

$$e^{-i\mathcal{Q}\mathcal{L}\mathcal{Q}t} = e^{-i\mathcal{L}_0 t/\varepsilon} + \text{h.o.t.}\,. \tag{A5}$$

Combining Eqs. (A1), (A3), and (A5) we obtain for the kernel of Eq. (17) the expression

$$-\mathrm{Tr}_f\left[\frac{\partial \mathcal{H}_c}{\partial X}\mathcal{Q}e^{-i\mathcal{Q}\mathcal{L}\mathcal{Q}t'}\mathcal{Q}i\mathcal{L}_1\rho_{ad}\right]\bar\rho_{t-t'} = \mathrm{Tr}_f\left[e^{i\mathcal{L}_0 t'/\varepsilon}\delta f_c(\underline{p},\underline{q},V,X)\cdot f_c\left(\frac{\partial\rho_{ad}\bar\rho_{t-t'}}{\partial V} + \frac{\varepsilon}{Z_E}\frac{\partial \mathcal{H}_s}{\partial V}\frac{\partial Z_E\rho_{ad}}{\partial E}\right)\right] + \text{h.o.t.}\,. \tag{A6}$$

The action of the operator exponential can be readily expressed in terms of the solution $\underline{p}_0(t)$, $\underline{q}_0(t)$ of the fast equations of motion (5b) with fixed slow variables, and initial condition $\underline{p}(0) = \underline{p}$, $\underline{q}(0) = \underline{q}$

$$e^{i\mathcal{L}_0 t'/\varepsilon}\delta f_c(\underline{p},\underline{q},V,X) = \delta f_c(\underline{p}_0(t'/\varepsilon),\underline{q}_0(t'/\varepsilon),V,X)\,. \tag{A7}$$

The right hand side of Eq. (A6) can now be written in terms of the correlation function (22). Since the fluctuation of the force depends on the velocity just through ρ_{ad}, i.e. via the combination $\varepsilon\mathcal{H}_s - E$, we can rewrite derivatives with respect to the slow velocity in terms of derivatives with respect to energy as

$$\frac{\partial \delta f_c}{\partial V} = -\varepsilon\frac{\partial \mathcal{H}_s}{\partial V}\frac{\partial \delta f_c}{\partial E}\,. \tag{A8}$$

Then Eq. (A6) can be finally cast into the form

$$-\mathrm{Tr}_f\left[\frac{\partial \mathcal{H}_c}{\partial X}\mathcal{Q}e^{-i\mathcal{Q}\mathcal{L}\mathcal{Q}t'}\mathcal{Q}i\mathcal{L}_1\rho_{ad}\right]\bar\rho_{t-t'} = \frac{\partial}{\partial V}C_E(V,X;t'/\varepsilon)\bar\rho_{t-t'} + \frac{\varepsilon}{Z_E}\frac{\partial \mathcal{H}_s}{\partial V}\frac{\partial Z_E C_E(V,X;t'/\varepsilon)}{\partial E}\bar\rho_{t-t'} + \text{h.o.t.} \tag{A9}$$

when using the definition (22).

Eq. (17) with the approximation (A9) is still nonlocal in time. Since the autocorrelation function depends on the fast time scale t/ε a Markov approximation can be applied to obtain a time local expression to leading order in the expansion parameter:

$$\int_0^t dt' C_E(V,X;t'/\varepsilon)\bar\rho_{t-t'} = \int_0^{t/\varepsilon} dt''\varepsilon C_E(V,X;t'')\bar\rho_{t-\varepsilon t''} = \varepsilon\int_0^\infty dt'' C_E(V,X,t'')\bar\rho_t + \text{h.o.t.}\,.$$

Such an approximation requires a correlation which decays sufficiently fast, but an exponential decay is normally not necessary [20]. We just remark that any perturbation expansion, like the one presented here, has to be consistent with the Markov approximation in the sense that the resulting expression for the correlation function becomes integrable. With the Markov approximation (A10) we end up with the second and third contribution of the Fokker–Planck equation (24). These contributions appear in different orders of the formal expansion parameter since the identity (A1) contains different orders of ε caused by the trivial scaling of the total energy. The expansion is systematic with regards to the operator exponential (A5) and actually corresponds to an expansion with regards to the velocities of the slow subsystem (cf. [23]).

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