Smoothed Langevin dynamics of highly oscillatory systems

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Abstract

We consider Hamiltonian systems containing a strong constraining potential. Such systems were first investigated by RUBIN & UNGAR who derived the corresponding reduced equations of motion for the slow degree of freedom. The purpose of this paper is twofold. (i) We transform the highly oscillatory degree of freedom to action-angle variables and use recent results on the truncation error of the corresponding normal form transformations to derive an estimate on the life-span of the underlying adiabatic invariant. (ii) We investigate thermally embedded Hamiltonian systems, i.e. Langevin dynamics, containing a strong constraining potential. Using again a transformation to action-angle variables and applying the principle of averaging, we derive reduced equations of motion for the slowly varying degrees of freedom. This includes in particular the derivation of a correcting force-term that stands for the coupling of the slow and fast degrees of motion. In case of strong thermal coupling, our reduced equations of motion suggest that the correcting force term can be approximated by the gradient of the FIXMAN potential as used in statistical mechanics. We also discuss smoothing in the context of constant temperature molecular dynamics and provide a numerical example.

Keywords: Hamiltonian systems, Langevin dynamics, highly oscillatory solutions, smoothed dynamics, averaging, correcting potential, constrained systems, molecular dynamics.

1 Introduction

Physical systems frequently exhibit fast oscillatory behavior coupled to slowly varying solution components. This is, for example, the case when the potential energy function $U(q)$ consists of a smooth contribution $V(q)$ and a strong constraining potential modeled through $[g(q)]^2/(2\epsilon^2)$ where $g(q)$ is a scalar-valued function and $\epsilon > 0$ is a small parameter, i.e.

$$U(q) \quad = \quad V(q) + \frac{1}{2\epsilon^2}[g(q)]^2 \,.$$

In the context of molecular dynamics [1], which provides the main motivation of this paper, the strong potential can, for example, stand for the bond stretching motion, i.e.

$$g(q) \quad = \quad r(q) - r_0 \,,$$

$r(q)$ the actual bond length and r_0 the equilibrium bond length, or for the bond angle bending motion, i.e.

$$g(q) \quad = \quad \phi(q) - \phi_0 \,,$$

$\phi(q)$ the actual bond angle and ϕ_0 the equilibrium bond angle. The parameter ϵ^2 is then the inverse of the corresponding force constant K, i.e., $\epsilon^2 = 1/K$. Assuming a positive definite mass matrix M, the Hamiltonian of the system is given by

$$H(q,p) \;=\; \frac{p^T M^{-1} p}{2} + U(q)\,,$$

$q, p \in R^{3N}$, and the corresponding equations of motion are

$$\frac{d}{dt}q \;=\; M^{-1}p\,, \tag{1}$$

$$\frac{d}{dt}p \;=\; -\nabla_q V(q) - \frac{1}{\epsilon^2} G(q)^T g(q)\,, \tag{2}$$

$G(q)$ the Jacobian of $g(q)$, i.e. $G(q) = g_q(q)$. We assume that the Jacobian $G(q)$ satisfies $||G(q)|| > d$ for all $q \in g^{-1}(0)$, $d > 0$ an appropriate constant. This implies that the set

$$\mathcal{M} := \{q \in R^{3N} : g(q) = 0\}$$

is a smooth sub-manifold of phase space of co-dimension one.

The system (1)-(2) exhibits rapid oscillations on a time-scale of order $O(\epsilon)$. The "interesting" dynamics happens however on time-scales of order $O(1)$. To capture this "essential" behavior of (1)-(2) one could, for example, send the solutions $(q(t), p(t))$ of (1)-(2) through a low-pass filter with cut-off frequency $\omega_c = O(1/\sqrt{\epsilon})$. Let us denote the corresponding time-functions by $(\langle q\rangle_{\sqrt{\epsilon}}(t), \langle p\rangle_{\sqrt{\epsilon}}(t))$, i.e., for example,

$$\langle q\rangle_{\sqrt{\epsilon}}(t) := \frac{1}{\sqrt{\epsilon}} \int_{-\infty}^{+\infty} \psi\left(\frac{t-t'}{\sqrt{\epsilon}}\right) q(t)\, dt' \tag{3}$$

with $\psi : R \to R$ an appropriate weight function [16]. The idea of *smoothed dynamics* [16],[4] is to find equations of motion with smooth solutions $(Q(t), P(t))$ that satisfy

$$Q(t) \;=\; \langle q\rangle_{\sqrt{\epsilon}}(t) \quad \text{and} \quad P(t) \;=\; \langle p\rangle_{\sqrt{\epsilon}}(t)$$

over time scales of order $1 = \epsilon^0$ as $\epsilon \to 0$. Such equations can indeed be defined and were first derived in [19] by RUBIN & UNGAR and recently discussed by BORNEMANN & SCHÜTTE [4] in the context of homogenization. One obtains the constrained Hamiltonian system

$$\frac{d}{dt}Q \;=\; M^{-1}P\,, \tag{4}$$

$$\frac{d}{dt}P \;=\; -\nabla_q V(Q) - J\,\nabla_q \sqrt{G(q)M^{-1}G(q)^T} - G(Q)^T\lambda\,, \tag{5}$$

$$0 \;=\; g(Q)\,, \tag{6}$$

$\lambda \in R$ a Langrange multiplier. Note the additional potential energy term

$$V_c(Q) \;=\; J\sqrt{G(Q)M^{-1}G(Q)^T}\,, \tag{7}$$

where $J > 0$ is a constant depending on the initial conditions $(q(0), p(0))$.

Starting from these results, the purpose of this paper is twofold:

(i) We show how the system (1)-(2) can be transformed into a system with the highly oscillatory degree of freedom formulated in terms of action-angle variables [2]. The reformulated system can then be analyzed using *normal form* theory [2]. In particular, a symplectic change of coordinates allows one to explicitly identify the slow and fast degrees of motions which, upon *averaging* over the fast phase variable, yields the same reduced equations (4)-(6) in the limit $\epsilon \to 0$. Thus the idea of *smoothed dynamics* is essentially equivalent to the classical principles of transformation to normal form and averaging. Furthermore, upon assuming that the Hamiltonian H is real-analytic and bounded in some complex neighborhood of a compact subset of phase space, it can be shown that the system (1)-(2) possesses an *adiabatic invariant* that is almost preserved over exponentially long periods of times as $\epsilon \to 0$. This implies that, upon neglecting small terms of order $\mathcal{O}(\epsilon)$, the reduced equations of motion (4)-(6) are, in fact, valid over long time intervals. The existence of an adiabatic invariants and its exponentially long life-span has been shown before by Benettin, Galgani & Giorgilli for the special case $V_c(Q) = \text{const.}$ [3]. See also Neishtadt [13] for exponential estimates for general system with a single high-frequency component.

(ii) We consider the limit $\epsilon \to 0$ for thermally embedded systems (Langevin dynamics)

$$\frac{d}{dt}q = M^{-1}p\,, \tag{8}$$

$$\frac{d}{dt}p = -\nabla_q U(q) - \gamma p + M^{1/2}\xi(t) \tag{9}$$

with $U(q)$ as before, γ a positive friction constant, and $\xi(t) \in R^{3N}$ a Gaussian white noise process with zero mean value and variance

$$\langle \xi_i(t)\,\xi_j(t+\tau)\rangle = 2\gamma k_B T \delta_{ij}\delta(\tau)\,, \qquad i,j = 1,\dots 3N\,,$$

k_B the Boltzmann constant, T the temperature of the heat bath, and $\langle . \rangle$ denotes the average over all realizations of the stochastic process $\xi(t)$ [1],[11]. Such a model is frequently used in molecular dynamics [1]. We derive reduced equations of motion by going to action-angle variables in the highly oscillatory degree of freedom and by applying the principle of averaging to the corresponding transformed stochastic differential equation.

Let us state item (ii) more precisely.

The equations (8)-(9) can be solved numerically by using the following generalization of the Verlet method [6, 8]:

$$p_{n+1/2} = p_n - \frac{\Delta t}{2}\left[\nabla_q U(q_n) + \gamma p_{n+1/2} - M^{1/2}\xi(t_n)\right]\,, \tag{10}$$

$$q_{n+1} = q_n + \Delta t M^{-1} p_{n+1/2}\,, \tag{11}$$

$$p_{n+1} = p_{n+1/2} - \frac{\Delta t}{2}\left[\nabla_q U(q_{n+1}) + \gamma p_{n+1/2} - M^{1/2}\xi(t_{n+1})\right] \tag{12}$$

with

$$\langle \xi_i(t_n)\xi_j(t_n)\rangle = 4\gamma k_B T \Delta t^{-1}\delta_{ij}\,.$$

The step-size Δt has to satisfy $\Delta t = \mathcal{O}(\epsilon)$ which implies a very small step-size compared to the slowly varying solution components. Thus we seek smoothed (averaged) Langevin equations of motion that possess solutions $(Q(t), P(t))$ such that the average $(\langle Q\rangle(t), \langle P\rangle(t))$ over all realizations of the stochastic process $\xi(t)$ satisfies

$$\langle Q\rangle(t) = \lim_{\epsilon\to 0} \langle\langle q\rangle_{\sqrt{\epsilon}}\rangle(t) \qquad \text{and} \qquad \langle P\rangle(t) = \lim_{\epsilon\to 0} \langle\langle p\rangle_{\sqrt{\epsilon}}\rangle(t)$$

over time scales of order, at least, $1 = \epsilon^0$.

As we will argue in §2.3, application of the principle of averaging to the stochastic differential equation (8)-(9) leads to the reduced equations of motion

$$
\begin{aligned}
\frac{d}{dt}Q &= M^{-1}P\,, && (13)\\
\frac{d}{dt}P &= -\nabla_Q V(Q) - J\,\nabla_Q\sqrt{G(Q)M^{-1}G(Q)^T} - \gamma P + \xi(t) - G(Q)^T\lambda\,, && (14)\\
0 &= g(Q)\,, && (15)\\
\frac{d}{dt}J &= -\gamma J + \frac{\Xi_x(t)\xi_x(t)}{\sqrt{G(Q)M^{-1}G(Q)^T}}, && (16)
\end{aligned}
$$

$\xi_x(t) = d\Xi_x(t)/dt$, $\xi_x(t)$ a Gaussian white noise process with zero mean and variance

$$\langle \xi_x(t)\xi(t+\tau)\rangle = 2\gamma k_B T\delta(\tau).$$

The correcting force term

$$F_{\rm c}(Q,J(t)) \;\;=\;\; -J\,\nabla_Q\sqrt{G(Q)M^{-1}G(Q)^T} \qquad (17)$$

depends on the variable J which satisfies the stochastic differential equation (16).

As we will discuss in §2.3, the expectation value of the energy in the highly oscillatory degree of freedom satisfies $\langle E\rangle \approx k_B T$ provided γ is large enough. This suggests that the correcting force term $F_{\rm c}$ can be approximated by a potential force term due to FIXMAN [7, 15, 1], i.e., $F_{\rm c}(Q) = -\nabla_Q V_{\rm c}(Q)$,

$$V_{\rm c}(Q) \;\;=\;\; k_B T \ln\sqrt{G(Q)M^{-1}G(Q)^T}\,. \qquad (18)$$

This result seem particularly interesting in the context of molecular dynamics and extends the analysis of HELFAND [9] on the FIXMAN potential and its application to molecular dynamics.

Note that the equations (13)-(15) can be solved numerically by the SHAKE/RATTLE variant of (10)-(12) [1, 12, 8].

2 A Simplified Model Problem

2.1 The Model and Transformation to Action-Angle Variables

To limit the technical aspects of our analysis, we restrict ourselves to a simplified version of (8)-(9). Namely, we assume that M is the identity matrix and that $q, p \in R^2$. The general case (8)-(9) will be discussed in §3.

The behavior of our model system becomes more apparent when going to (local) coordinates $x := g(q)$ and $y := b(q)$. Here $b : R^2 \to R$ is an appropriate function such that $G(q)B(q)^T = 0$, $B(q)$ the Jacobian of $b(q)$, for all q in the domain of the coordinate transformation. The corresponding conjugate momenta p_x and p_y are implicitly defined by the relation

$$p \;\;=\;\; p_x G(q)^T + p_y B(q)^T\,.$$

We introduce

$$m_x(x,y) := G(q)G(q)^T \quad \text{and} \quad m_y(x,y) := B(q)B(q)^T$$

and assume, for simplicity, that $m_x(x,y)$ and $m_y(x,y)$ do not depend on x. Thus we end up with the transformed system

$$\begin{aligned}
\frac{d}{dt}x &= m_x(y)p_x\,,\\
\frac{d}{dt}p_x &= -\epsilon^{-2}x - \nabla_x V(x,y) - \gamma p_x + [m_x(y)]^{-1/2}\xi_x(t)\,,\\
\frac{d}{dt}y &= m_y(y)p_y\,,\\
\frac{d}{dt}p_y &= -\nabla_y V(x,y) - \frac{1}{2}\nabla_y\left[m_x(y)p_x^2 + m_y(y)p_y^2\right] - \gamma p_2 + [m_y(y)]^{-1/2}\xi_y(t)\,.
\end{aligned}$$

Here $\xi_x(t)$ and $\xi_y(t)$ are independent Gaussian white noise processes with zero mean value and variance

$$\langle \xi_x(t)\,\xi_x(t+\tau)\rangle = 2\gamma k_B T\delta(\tau)$$

and

$$\langle \xi_y(t)\,\xi_y(t+\tau)\rangle = 2\gamma k_B T\delta(\tau)\,.$$

For $\gamma = 0$, the equations of motion are conservative with Hamiltonian

$$H(x,y,p_x,p_y;\epsilon) := \frac{m_x(y)}{2}p_x^2 + \frac{m_y(y)}{2}p_y^2 + V(x,y) + \frac{\epsilon^{-2}}{2}x^2$$

which is a first integral of motion. For $\gamma > 0$, γ bounded, the energy

$$H(t;\epsilon) = H(x(t),y(t),p_x(t),p_y(t);\epsilon)$$

is no longer constant. But over a time-interval of order one, the variations in $H(t;\epsilon)$ will remain bounded. Thus, if the initial conditions are chosen such that the corresponding initial energy $H(t=0;\epsilon)$ remains bounded as $\epsilon \to 0$, then $H(t;\epsilon) = \mathcal{O}(1)$ over time-intervals of order $1 = \epsilon^0$. From this we can conclude that $x(t) = \mathcal{O}(\epsilon)$ and we re-scale x by ϵ, i.e., we replace $\epsilon^{-1}x$ by $\tilde{x}$. This yields the system

$$\begin{aligned}
\frac{d}{dt}\tilde{x} &= \epsilon^{-1}m_x(y)p_x\,,\\
\frac{d}{dt}p_x &= -\epsilon^{-1}\tilde{x} - \nabla_x V(\epsilon\tilde{x},y) - \gamma p_x + [m_x(y)]^{-1/2}\xi_x(t)\,,\\
\frac{d}{dt}y &= m_y(y)p_y\,,\\
\frac{d}{dt}p_y &= -\nabla_y V(\epsilon\tilde{x},y) - \frac{1}{2}\nabla_y\left[m_x(y)p_x^2 + m_y(y)p_y^2\right] - \gamma p_y + [m_y(y)]^{-1/2}\xi_y(t)\,.
\end{aligned}$$

This system is Hamiltonian for $\gamma = 0$ with

$$H(\tilde{x},y,p_x,p_y;\epsilon) = \frac{m_x(y)}{2}p_x^2 + \frac{m_y(y)}{2}p_y^2 + V(\epsilon\tilde{x},y) + \frac{1}{2}\tilde{x}^2$$

and modified structure matrix[1]

$$\mathcal{J} = \begin{bmatrix} 0 & \epsilon^{-1} & 0 & 0 \\ -\epsilon^{-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix}. \tag{19}$$

[1] The equations of motion are given by $\dot{z} = \mathcal{J}\nabla_z H(z)$, $z = (\tilde{x},p_x,y,p_y)^T$.

We also introduce functions h and f by

$$V(\epsilon\tilde{x}, y) = h(y) + \epsilon f(\tilde{x}, y; \epsilon) \qquad \text{with} \qquad h(y) = V(0, y)\,.$$

The motion in $(\tilde{x}, p_x)$ is highly oscillatory. To make this more transparent, we introduce action-angle variables $(J, \phi) \in R \times S$ and new "slow" variables $(z, p_z) \in R^2$ via the generating function

$$W \;=\; z p_y + \epsilon \frac{\omega(z)}{2} (p_x)^2 \cot\phi\,,$$

$\omega(z) = \sqrt{m_x(z)}$. The corresponding canonical change of coordinates is given by

$$\begin{aligned}
\tilde{x} &= \epsilon^{-1}\frac{\partial W}{\partial p_x} \;=\; \omega(z)\, p_x \cot\phi\,, \\
J &= \epsilon^{-1}\frac{\partial W}{\partial \phi} \;=\; \frac{\omega(z)}{2}(p_x)^2 \sin^{-2}\phi\,, \\
y &= \frac{\partial W}{\partial p_y} \;=\; z\,, \\
p_z &= \frac{\partial W}{\partial z} \;=\; p_y + \epsilon \nabla_z \frac{\omega(z)}{2}(p_x)^2 \cot\phi\,.
\end{aligned}$$

This is equivalent to

$$\begin{aligned}
\tilde{x} &:= \sqrt{2\omega(z) J}\cos\phi\,, \\
p_x &:= \sqrt{\frac{2J}{\omega(z)}}\sin\phi\,, \\
J &:= \frac{1}{2\omega(z)}\left[\omega(z)^2 p_x^2 + \tilde{x}^2\right]\,, && (20) \\
\phi &:= \arctan\left(\frac{\tilde{x}}{\omega(z) p_x}\right)\,, && (21)
\end{aligned}$$

and $z = y$, $p_z = p_y + \mathcal{O}(\epsilon)$. The corresponding transformed Hamiltonian is

$$\mathcal{H}(\phi, J, z, p_z; \epsilon) \;=\; \omega(z) J + \frac{m_y(z)}{2} p_z^2 + h(z) + \epsilon F(\phi, J, z, p_z; \epsilon) \qquad (22)$$

which, for $\gamma = 0$, is a first integral of motion. The term $\epsilon F(\phi, J, z, p_z; \epsilon)$ represents $\epsilon f(\tilde{x}, y; \epsilon)$ and all other terms of order $\mathcal{O}(\epsilon)$ and higher. The equations of motion are now given by

$$\begin{aligned}
\frac{d}{dt}\phi &= \epsilon^{-1}\omega(z) - \nabla_J F(\phi, J, z, p_z; \epsilon) + \gamma\cos\phi\,\sin\phi + \frac{1}{\sqrt{2\omega(z)J}}\cos\phi\;\xi_x(t)\,, && (23) \\
\frac{d}{dt}J &= -\nabla_\phi F(\phi, J, z, p_z; \epsilon) - 2\gamma J \sin^2\phi + \sqrt{\frac{2J}{\omega(z)}}\sin\phi\;\xi_x(t)\,, && (24) \\
\frac{d}{dt}z &= m_y(z) p_z + \epsilon \nabla_{p_z} F(\phi, J, z, p_z; \epsilon)\,, && (25) \\
\frac{d}{dt}p_z &= -\nabla_z h(z) - \frac{p_z^2}{2}\nabla_z m_y(z) - \nabla_z\omega(z) J - \gamma p_z + \frac{\xi_y(t)}{\sqrt{m_y(z)}} - \epsilon\nabla_z F(\phi, J, z, p_z; \epsilon)\,. && (26)
\end{aligned}$$

2.2 The Energy Conserving Case

We first investigate the case $\gamma = 0$ in more detail. The corresponding Hamiltonian system is characterized by the Hamiltonian (22) and the modified structure matrix (19). Let us assume that the Hamiltonian $\mathcal{H}$ is smooth. Then we can apply a symplectic transformation to normal form as described, for example, in [13, 2].[2] Let us denote the transformed variables by $(\bar{\phi}, \bar{J}, \bar{z}, \bar{p}_z)$. Then the transformed Hamiltonian is of the general form

$$\bar{\mathcal{H}}(\bar{\phi}, \bar{J}, \bar{z}, \bar{p}_z; \epsilon) = \omega(\bar{z})\bar{J} + \frac{m_y(\bar{z})}{2}\bar{p}_z^2 + h(\bar{z}) + \epsilon \bar{F}(\bar{J}, \bar{z}, \bar{p}_z; \epsilon) + \epsilon^k R(\bar{\phi}, \bar{J}, \bar{z}, \bar{p}_z; \epsilon)$$

where one can make the integer $k \geq 2$ arbitrarily large.

We like to mention that the principle of averaging implies that

$$\bar{F}(\bar{J}, \bar{z}, \bar{p}_z; 0) = \frac{1}{2\pi}\int_0^{2\pi} F(\phi, J, z, p_z; 0) d\phi, \qquad (\bar{J}, \bar{z}, \bar{p}_z) = (J, z, p_z).$$

This fact will be needed in the following subsection.

Let us assume that the Hamiltonian $\mathcal{H}$ is analytic and bounded on a complex neighborhood of some compact subset $\mathcal{K} \subset S \times R^+ \times R^2$ of phase space and that $\mathcal{K}$ covers the whole circle S. Let us also assume that $\omega(\bar{z})$ is bounded from below on $\mathcal{K}$. Then the non-normalized term $\epsilon^k R(\bar{\phi}, \bar{J}, \bar{z}, \bar{p}_z; \epsilon)$ can be made exponentially small in ϵ as $\epsilon \to 0$. See [13, 2, 17] for details. This implies in particular that the variable J is almost constant along solutions of our model system over exponentially long periods of time, i.e.

$$|J(t) - J(0)| \leq c_1 \epsilon \quad \text{for} \quad |t| \leq c_2 e^{c_3/\epsilon},$$

$c_1, c_2, c_3 > 0$ appropriate constants, provided the solution under consideration stays in the compact subset $\mathcal{K}$. Thus, upon neglecting perturbations of size $\mathcal{O}(\epsilon)$, the reduced system (4)-(6) is, in fact, justified over much longer periods of time than $|t| = \mathcal{O}(\epsilon^0)$.

We mention that the case of constant $\omega(z) = \omega_0$ has been treated before by Benettin, Galgani & Giorgilli who also proved the preservation of an action variable[3] over exponentially long periods of time [3]. Compared to the approach used here and by Neishtadt [13], a significantly altered perturbative scheme is used in [3] which, however, could be adjusted to also cover the non-constant frequency case.

2.3 The Non-Conservative Case

In the previous subsection we applied normal form theory to the model system (23)-(26) with $\gamma = 0$. We consider now the case $\gamma > 0$. In a first step we treat the random forcing term in (24). We use the identity

$$F_f(t) = \sqrt{\frac{2J}{\omega(z)}} \sin\phi \; \xi_x(t) = p_x(t)\, \xi_x(t)$$

and write

$$p_x(t)\,\xi_x(t) = \int_{t-\tau}^{t} dt' \,\frac{d}{dt'} p_x(t')\xi_x(t) + p_x(t-\tau)\,\xi_x(t)$$

which, in the limit $\tau \to 0$, reduces to

$$p_x(t)\,\xi_x(t) = \lim_{\tau \to 0}\left[\int_{t-\tau}^{t} dt' \,\frac{\xi_x(t')}{\omega(z(t))}\xi_x(t) + p_x(t-\tau)\,\xi_x(t)\right].$$

Taking note of the independence of $p_x(t-\tau)$ and $\xi_x(t)$, this can be simplified to

$$p_x(t)\,\xi_x(t) = \frac{\Xi_x(t)\,\xi_x(t)}{\omega(z(t))}\,, \qquad \xi_x(t) = \frac{d}{dt}\Xi_x(t)\,,$$

[2] Because of the non-canonical structure matrix (19), one has to modify the normal form recursion slightly to make sure that the corresponding normal form transformation is symplectic under (19). See [17] for details.

[3] The action variable is, in this case, the energy in the highly oscillatory degree of freedom.

without effecting the expectation value of $p_x(t)\xi_x(t)$. Thus the equation (24) in (23)-(26) can be replaced by

$$\frac{d}{dt}J = -\nabla_\phi F(\phi, J, z, p_z; \epsilon) - 2\gamma J \sin^2\phi + \frac{\Xi_x(t)\xi_x(t)}{\omega(z(t))}. \tag{27}$$

We now apply the principle of averaging to the equations (23), (27), and (25)-(26). In particular, there is a change of coordinates ϵ-close to the identity such that the transformed equations of motion in the new variables $(\bar{J}, \bar{z}, \bar{p}_z)$ are equivalent to the equations obtained by averaging over the rapidly rotating phase ϕ (up to terms of size $\mathcal{O}(\epsilon)$). To obtain these averaged equations of motions, we first average over the angle ϕ in (22) and drop all terms of order $\mathcal{O}(\epsilon^2)$ or higher. This yields (using the notations from the previous subsection)

$$\widetilde{\mathcal{H}}(J, z, p_z) = \omega(z)J + \frac{m_y(z)}{2}p_z^2 + h(z) + \epsilon\bar{F}(J, z, p_z; 0).$$

Next we average over the phase ϕ in the dissipative force term

$$F_d = -2\gamma J \sin^2\phi$$

in equation (27). This results in

$$-2\gamma J \frac{1}{2\pi}\int_0^{2\pi} d\phi\, \sin^2\phi = -\gamma J.$$

Thus we obtain the averaged equations of motion

$$\begin{aligned} \frac{d}{dt}\bar{J} &= -\gamma\bar{J} + \frac{\Xi_x(t)\,\xi_x(t)}{\omega(z)}, & (28)\\ \frac{d}{dt}\bar{z} &= m_y(\bar{z})\bar{p}_z, & (29)\\ \frac{d}{dt}\bar{p}_z &= -\nabla_{\bar{z}}h(\bar{z}) - \frac{\bar{p}_z^2}{2}\nabla_{\bar{z}}m_y(\bar{z}) - J\nabla_{\bar{z}}\omega(\bar{z}) - \gamma\bar{p}_z + [m_y(\bar{z})]^{-1/2}\xi_y(t), & (30) \end{aligned}$$

where we dropped all terms of order $\mathcal{O}(\epsilon)$ or higher. Note that

$$J - \bar{J} = \mathcal{O}(\epsilon), \quad z - \bar{z} = \mathcal{O}(\epsilon), \quad p_z - \bar{p}_z = \mathcal{O}(\epsilon),$$

and, in the limit $\epsilon \to 0$, we can identify the variables $(\bar{J}, \bar{z}, \bar{p}_z)$ with (J, z, p_z).

In terms of the Cartesian coordinates $(q, p) \in R^4$, the equations (28)-(30) are equivalent to the constraint system

$$\begin{aligned} \frac{d}{dt}J &= -\gamma J + \frac{\Xi_x(t)\xi_x(t)}{\sqrt{G(Q)G(Q)^T}}, \\ \frac{d}{dt}Q &= P, \\ \frac{d}{dt}P &= -\nabla_Q V(Q) - J\nabla_Q\sqrt{G(Q)G(Q)^T} - \gamma P + \xi(t) - G(Q)^T\lambda, \\ 0 &= g(Q) \end{aligned}$$

on the manifold

$$\mathcal{N} = \{(Q, P, J) \in R^5 : g(Q) = 0, G(Q)P = 0\}.$$

Note that (z, p_z, J) are local coordinates on $\mathcal{N}$. Capital $(Q, P) \in R^4$ was used to indicate that these are the averaged equations of motion.

If we formally set $\gamma = 0$, then the system (4)-(6) is recovered. Another interesting case is that of $\gamma > 0$ relatively large compared to the changes in $\omega(z(t))$. This leads formally to a system with three different time-scales. The fastest motion is due to the strong constraining force, the "medium" time-scale is due to friction, and the slowest time-scale occurs in the variables (Q, P). We have already dealt with the fastest time-scale. The effect of strong friction is now discussed by making the parameter $\gamma > 0$ sufficiently large. To find out about the impact of strong damping on the dynamics of the variable J, we first introducing the energy

$$E := \omega(z)\, J,$$

and rewrite eq. (28) as

$$\frac{d}{dt}E = -\left(\gamma - \frac{d}{dt}\ln\left[\omega(z(t))\right]\right) E + \Xi_x(t)\xi_x(t). \tag{31}$$

If

$$\left|\frac{d}{dt}\ln\left[\omega(z(t))\right]\right| \ll \gamma$$

(strong thermal coupling), then $\langle E\rangle(t)$ follows its equilibrium value (after an initial transient depending on the initial value $E(0)$)

$$\langle E\rangle(t) \approx k_B T. \tag{32}$$

This suggest that the equations of motion can be simplified to

$$\begin{aligned}
\frac{d}{dt}Q &= P\,, && (33)\\
\frac{d}{dt}P &= -\nabla_Q V(Q) - k_B T \nabla_Q \ln\sqrt{G(Q)G(Q)^T} - \gamma P + \xi(t) - G(Q)^T\lambda\,, && (34)\\
0 &= g(Q)\,. && (35)
\end{aligned}$$

Now the correcting force term is equivalent to the one suggested by Fixman [7]. This concludes the formal analysis of our simplified model problem. In §3, we relate this analysis back to our original problem formulation (8)-(9).

2.4 Harmonic Oscillator

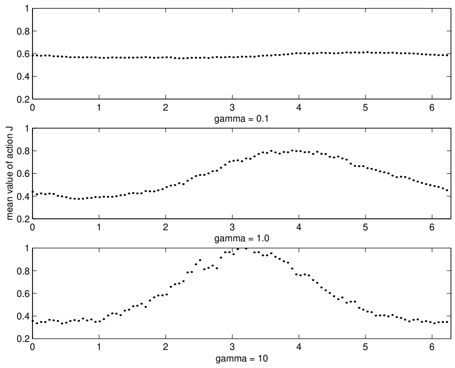
To "validate" the formal analysis on averaging of stochasticly forced rapidly oscillating systems, as provided in the previous subsection, we consider Langevin dynamics of a "stiff" harmonic oscillator

$$\begin{aligned}
\frac{d}{dt}x &= \omega(z)^2 p_x\,, && (36)\\
\frac{d}{dt}p_x &= -\epsilon^{-2}x - \gamma p_x + [\omega(z)]^{-1}\xi_x(t)\,, && (37)\\
\frac{d}{dt}z &= 1 && (38)
\end{aligned}$$

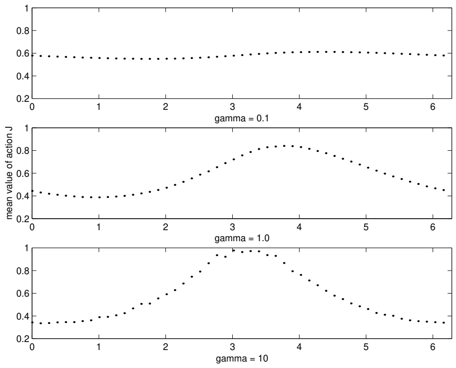
with

$$\omega(z) := 2 + \cos(z)\,.$$

This system can be viewed as a special case of our model system, written in (x, p_x, y, p_y) coordinates, with $V(x, y) = 0$, $dy/dt = 1$, and $dp_y/dt = 0$.



(a) free dynamics



(b) averaged dynamics

Figure 1: The mean value of the action J as a function of the angle $\phi = z \bmod 2\pi$ for different values of the friction constant γ. The figure on the left gives the results for the free dynamics (36)-(38) and the figure on the right for the averaged system (39)-(40).

We studied this system numerically for initial data $q = 0$, $p = 1$, and parameter values $\epsilon = 0.01$, $\gamma = 0.1$, $\gamma = 1.0$, and $\gamma = 10$. The results were compared to those obtained for the averaged system

$$\frac{d}{dt}J = -\gamma J + \frac{\Xi_x(t)\xi_x(t)}{\omega(z)}\,, \tag{39}$$

$$\frac{d}{dt}z = 1\,. \tag{40}$$

In both cases, the equations were integrated over a time interval $[0, 500]$ using a step-size $\Delta t = 0.0001$. Since the fast system is 2π-periodic in z, we computed the average value of the action

$$J(z) = \frac{1}{2\omega(z)}\left((\omega(z)p_x)^2 + (\epsilon^{-1}x)^2\right)$$

as a function of $\phi := z \bmod 2\pi$, i.e.

$$\langle J\rangle(\phi) = \frac{1}{N}\sum_{i=1}^{N} J(z(t_i)) \quad \text{with} \quad z(t_i) \bmod 2\pi = \phi\,.$$

The results can be found in Fig. 1 and show good agreement for the free and the averaged dynamics.

3 General highly oscillatory systems

We have made several assumptions on our model problem from §2 that we now like to re-examine. First, the mass matrix M was assumed to be the identity matrix. This is certainly not crucial for the derivation of the averaged equations of motion. Thus, we define

$$\omega(q) = \sqrt{G(q)M^{-1}G(q)^T}$$

for the general system (8)-(9). Furthermore, the assumption that there is only one slow degree of freedom can easily be dropped[4]. Finally, since $x = \mathcal{O}(\epsilon)$, the simplifying assumption that m_x and

[4] The fact that there is only a single fast degree of motion is, however, crucial.

m_y do not depend on x is not essential[5] in the limit $\epsilon \to 0$. This yields the constrained equations of motion

$$\begin{aligned}
\frac{d}{dt}J &= -\gamma J + \frac{\Xi_x(t)\xi_x(t)}{\sqrt{G(Q)G(Q)^T}}\,, \\
\frac{d}{dt}Q &= M^{-1}P\,, \\
\frac{d}{dt}P &= -\nabla_Q V(Q) - J\nabla_Q\sqrt{G(Q)M^{-1}G(Q)^T} - \gamma P + \xi(t) - G(Q)^T\lambda\,, \\
0 &= g(Q)
\end{aligned}$$

which describe the averaged motion on the manifold

$$\mathcal{N} := \{(Q,P,J) \in R^{6N+1} : g(Q) = 0,\, G(Q)M^{-1}P = 0\}\,.$$

In case of no friction ($\gamma = 0$), we obtain $J =$ const. and the averaged equations of motion are equivalent to the ones given by RUBIN & UNGAR in [19]. In the strong thermal coupling limit (32), we formally obtain, according to (33)-(35), the equations

$$\begin{aligned}
\frac{d}{dt}Q &= M^{-1}P\,, \\
\frac{d}{dt}P &= -\nabla_Q V(Q) - k_BT\,\nabla_Q \ln\sqrt{G(Q)M^{-1}G(Q)^T} - \gamma P + \xi(t) - G(Q)^T\lambda\,, \\
0 &= g(Q)
\end{aligned}$$

and the additional temperature-dependent potential energy term is equivalent to the FIXMAN potential [7, 16]. For intermediate values of γ (weak thermal coupling), the equations (13)-(16) have to be solved.

If $g(q)$ becomes vector-valued, i.e., we consider more than one fast degree of motion, then averaging becomes more delicate and depends on the special structure of the (now) matrix-valued function $G(q)M^{-1}G(q)^T$. See [20, 5, 18] for first results[6] on the special case $\gamma = 0$.

4 Application to constant temperature molecular dynamics

An interesting application of the ideas developed in this paper is related to constant temperature molecular dynamics [14, 10]. In the Hoover formulation, the equations of motion are

$$\frac{d}{dt}q = M^{-1}p\,, \tag{41}$$

$$\frac{d}{dt}p = -\nabla_q U(q) - \gamma p\,, \tag{42}$$

$$\frac{d}{dt}\gamma = \left[p^T M^{-1}p - Xk_BT\right]/D\,, \tag{43}$$

where γ is now a time-dependent friction constant, D a parameter, and X the total number of degrees of freedom. As shown in [10], the macro-canonical distribution function is a steady equilibrium solution of these equations for the variables (q,p). If

$$U(q) = V(q) + \frac{1}{2\epsilon^2}[g(q)]^2\,,$$

[5]Any term of the form $g(\epsilon\tilde{x}, y)$ can be written as $g(0,y) + \mathcal{O}(\epsilon)$ and the corresponding small contribution of order ϵ to the Hamiltonian $\mathcal{H}$ is added to the function F in (22).

[6]In [16], we investigated such systems under the assumption that the fast degrees satisfy thermodynamic equipartitioning of energy and the Fixman potential was derived as a correcting potential. This equipartitioning assumption does not, in general, hold for short term simulations. But it might lead to the "correct" long term equilibrium statistics.

then one can, in the limit $\epsilon \to 0$, again average over the fast degree of motion to obtain smoothed equations of motion. Following the same arguments as presented in §2, it can be shown that these equations are

$$\frac{d}{dt}Q = M^{-1}P\,, \tag{44}$$

$$\frac{d}{dt}P = -\nabla_Q V(Q) - J\,\nabla_Q\sqrt{G(Q)M^{-1}G(Q)^T} - \gamma P - G(Q)^T\lambda\,, \tag{45}$$

$$0 = g(Q)\,, \tag{46}$$

$$\frac{d}{dt}J = -\gamma\,J\,, \tag{47}$$

$$\frac{d}{dt}\gamma = \left[E_{\mathrm{N}} + P^T M^{-1}P - Xk_BT\right]/D \tag{48}$$

with

$$E_{\mathrm{N}} = J\sqrt{G(Q)M^{-1}G(Q)^T}$$

the energy in the fast degree of motion.

If one is only interested in the configurational part of the macro-canonical distribution function and neglects fluctuations in the kinetic energy, then one can use the formulation

$$\frac{d}{dt}Q = M^{-1}P\,, \tag{49}$$

$$\frac{d}{dt}P = -\nabla_Q V(Q) - J\,\nabla_Q\sqrt{G(Q)M^{-1}G(Q)^T} - \gamma P - G(Q)^T\lambda\,, \tag{50}$$

$$0 = g(Q)\,, \tag{51}$$

$$\frac{d}{dt}J = -\gamma\,J\,, \tag{52}$$

$$0 = E_{\mathrm{N}} + P^T M^{-1}P - Xk_BT \tag{53}$$

which is obtained by formally setting $D \to 0$ [14]. Thus the parameter γ takes now the role of a Langrange multiplier that forces the time-evolution of (Q,P) to satisfy the constraint (53).

Furthermore, taking into account that, for the macro-canonical distribution function, we have $\langle E_{\mathrm{N}}\rangle = k_BT$, this simplifies to

$$\begin{aligned}
\frac{d}{dt}Q &= M^{-1}P\,,\\
\frac{d}{dt}P &= -\nabla_Q V(Q) - k_BT\nabla_Q \ln\sqrt{G(Q)M^{-1}G(Q)^T} - \gamma P - G(Q)^T\lambda\,,\\
0 &= g(Q)\,,\\
0 &= P^T M^{-1}P - (X-1)k_BT\,.
\end{aligned}$$

and the correcting force-term is the FIXMAN potential.

5 A nonlinear test example

Let us define the function $g(q)$ in (1)-(2) by

$$g(q) = \sqrt{aq_1^2 + bq_2^2} - 1\,.$$

For $a = b = 1$, we obtain $g(q) = r(q) - 1$ which yields the potential energy function of a stiff spring. The potential energy function V was set equal to zero. Thus the equations of motion are

$$\frac{d}{dt}q_1 = p_1 \,, \tag{54}$$

$$\frac{d}{dt}q_2 = p_2 \,, \tag{55}$$

$$\frac{d}{dt}p_1 = -\epsilon^{-2} a \frac{\sqrt{aq_1^2 + bq_2^2} - 1}{\sqrt{aq_1^2 + bq_2^2}} q_1 - \gamma p_1 + \xi_1(t) \,, \tag{56}$$

$$\frac{d}{dt}p_2 = -\epsilon^{-2} b \frac{\sqrt{aq_1^2 + bq_2^2} - 1}{\sqrt{aq_1^2 + bq_2^2}} q_2 - \gamma p_2 + \xi_2(t) \,. \tag{57}$$

Next we have to find an expression for the adiabatic invariant J. Using the general expression (20), this requires the energy $E_{\rm N}$ in the fast x-degree of freedom:

$$E_{\rm N} = \omega(y)^2 \frac{p_x^2}{2} + \frac{\epsilon^{-2}}{2} x^2.$$

Here we have used that $x = g(q)$, $p_x = [G(q)G(q)^T]^{-1} G(q)p$, and that the frequency ω is defined by

$$\omega = \sqrt{a^2 q_1^2 + b^2 q_2^2} \,.$$

Thus $J = E_{\rm N}/\omega$.

The averaged equations of motion are

$$\frac{d}{dt}q_1 = p_1 \,, \tag{58}$$

$$\frac{d}{dt}q_2 = p_2 \,, \tag{59}$$

$$\frac{d}{dt}p_1 = -\frac{J a^2 q_1}{\sqrt{a^2 q_1^2 + bq_2^2}} - \gamma p_1 + \xi_1(t) - a q_1 \lambda \,, \tag{60}$$

$$\frac{d}{dt}p_2 = -\frac{J b^2 q_2}{\sqrt{a^2 q_1^2 + b^2 q_2^2}} - \gamma p_2 + \xi_2(t) - b q_2 \lambda \,, \tag{61}$$

$$0 = \sqrt{aq_1^2 + bq_2^2} - 1 \,, \tag{62}$$

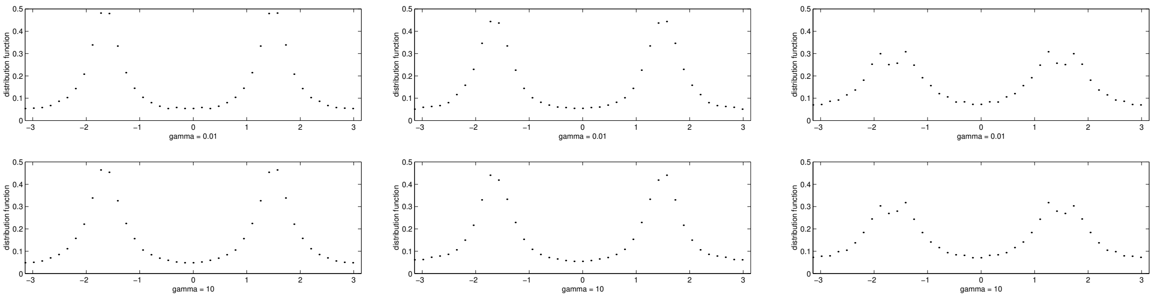
$$\frac{d}{dt}J = -\gamma J + \frac{\Xi_x(t)\xi_x(t)}{\sqrt{a^2 q_1^2 + b^2 q_2^2}} \,. \tag{63}$$

The constraint manifold

$$\mathcal{M} = \{q \in R^2 : \sqrt{aq_1^2 + bq_2^2} = 1\}$$

can be parameterized (in polar coordinates) by the angle ϕ, i.e., $\mathcal{M}$ is diffeomorph to the unit circle. We are interested in the equilibrium distribution of the angle ϕ. The corresponding distribution function is denoted by $\rho(\phi)$.

For the numerical experiments we chose $a = 9$, $b = 1$, $k_B T = 2.0$, $\epsilon = 0.01$ and different values for the friction constant γ. The initial conditions were $q = (0, 1)$ and $p = (2, 2)$. The corresponding equations of motion for the free dynamics, the averaged system, and the constrained system with no correcting force term, i.e. $J(t) = 0$, were integrated over a time-interval $[0, 2000]$ using a step-size of $\Delta t = 0.001$. In Fig. 2, the distribution functions $\rho(\phi)$ are shown for $\gamma = 0.01$ and $\gamma = 10$. Intermediate values of $\gamma \in [0.1, 10]$ gave similar results. Again the free dynamics and the



(a) free dynamics (b) averaged dynamics (c) constrained dynamics

Figure 2: The equilibrium distribution $\rho(\phi)$ for two different values of the friction constant γ. The figure on the left gives the results for the free dynamics (54)-(57), the figure in the middle for the averaged system (58)-(63), and the figure on the right for the constrained system with $J(t) = 0$ (no correcting force term).

averaged dynamics are in good agreement. The constrained system without a correcting force term gives qualitatively wrong results.

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