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Long-time averaging for integrable Hamiltonian dynamics

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Summary Given a Hamiltonian dynamical system, we address the question of computing the space-average of an observable through the limit of its time-average. For a completely integrable system, it is known that ergodicity can be characterized by a diophantine condition on its frequencies and that the two averages then coincide. In this paper, we show that we can improve the rate of convergence upon using a filter function in the time-averages. We then show that this convergence persists when a symplectic numerical scheme is applied to the system, up to the order of the integrator.

Key words integrable Hamitonian systems – averaging – filter functions – Riemann sums – symplectic solvers – invariant tori

1 Introduction

Consider a Hamiltonian dynamical equation in $\mathbb{R}^d \times \mathbb{R}^d$

$$\begin{cases} \dot{p}(t) = -\nabla_q H(p(t), q(t)),\ p(0) = p_0, \\ \dot{q}(t) = \quad \nabla_p H(p(t), q(t)),\ q(0) = q_0. \end{cases} \tag{1}$$

Let $M(p_0, q_0)$ be the manifold $\{(p,q) \in \mathbb{R}^{2d} \,|\, H(p,q) = H(p_0,q_0)\}$. The solution of (1) is a dynamical system on $M(p_0, q_0)$ with the invariant measure

$$d\rho(p,q) = \frac{d\sigma(p,q)}{\|\nabla H(p,q)\|_2},$$

where $d\sigma(p,q)$ is the measure induced on $M(p_0,q_0)$ by the Euclidean metric of $\mathbb{R}^{2d}$ (see for instance [4]), and $\|\cdot\|_2$ the Euclidean norm in $\mathbb{R}^{2d}$.

It is a common problem to estimate the *space* average of an observable[1] A over the manifold $M(p_0,q_0)$

$$\frac{\int_{M(p_0,q_0)} A(p,q)d\rho(q,p)}{\int_{M(p_0,q_0)} d\rho(q,p)}, \tag{2}$$

through the limit of the *time* average

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T A(p(t),q(t))dt, \tag{3}$$

where $(p(t),q(t))$ is the solution of (1). Our wish is here to give a sound ground to (and in some cases improve [3]) the numerical simulations of (3) commonly used in the field of molecular dynamics.

The conditions under which the two quantities (2) and (3) coincide can not be stated *in general.* In contrast, a dynamical system is known to have an ergodic behavior in two clearly identified -and somewhat opposite- situations:

- in the case of a differential equation with an hyperbolic structure, giving rise to mixing, the convergence of (3) toward (2) for T going to infinity is insured at a typical rate of $1/\sqrt{T}$. It is the belief of the authors that not much can be gained in this situation due to the presence of chaos;
- in the case of an *integrable* system, a well-known result of Bohl, Sierpinski and Weyl (see [2] and references therein) states that, under a *non-resonant* condition on the frequency vector associated with the initial condition, the space average of a continuous function on the manifold

$$\begin{aligned} S(p_0,q_0) = \{(p,q) \in \mathbb{R}^d \times \mathbb{R}^d \ ; \\ I_1(p,q) = I_1(p_0,q_0), \ldots, I_d(p,q) = I_d(p_0,q_0)\}, \end{aligned} \tag{4}$$

[1] Properties of a physical system at thermodynamical equilibrium such as *radial distributions, free energies, transport coefficients* can be computed as averages of some observables over the phase space of a representative microscopic system. In most applications of interest, this microscopic system is composed of a high number of particles, making the computation of averages a challenging issue.

where $I_1, \ldots, I_d$ are the d invariants of the problem (1), coincide with the long-time average of this function. Moreover, if the frequencies satisfy a *diophantine* condition, the convergence is of order T^{-1}. Being more analytically tractable, this case allows for the design of more elaborated averaging methods than the straightforward numerical simulation of (3).

In realistic situations, Hamiltonian systems belong nor to the first category, neither to the second one: they typically exhibit different behaviors for different energy levels. Nevertheless, the acceleration techniques presented in this paper are relevant to actual computations for the following two reasons:

- their efficiency shows off also in situations where integrability assumptions are not satisfied (see the companion paper [3]).
- their induced computational overhead is only marginal and thus not penalizing when integrability assumptions are violated. Meanwhile, when the explored energy level is such that the system can be (locally) considered as integrable, a significant acceleration is observed.

Integrable systems under some diophantine condition will thus constitute a natural framework for this work. Besides, all the results presented here could be extended with only minor modifications to the case of near-integrable systems.

In the following, we consider a completely integrable Hamiltonian system (1) in the sense of the Arnold-Liouville theorem [2,5]: There exist d invariants $I_1 = H, I_2, \ldots, I_d$ in involution (i.e. their Poisson Bracket $\{I_i, I_j\} = 0$) such that their gradient are everywhere independent, and the trajectories of the system remain bounded. Under these conditions, there exist action-angles variables (a, θ) in a neighborhood U of $S(p_0, q_0)$. We have $(p, q) = \psi(a, \theta)$, where ψ is a symplectic transformation

$$\psi : D \times \mathbb{T}^d \ni (a, \theta) \mapsto (p, q) \in U,$$

with $\mathbb{T}^d = (\mathbb{R}/2\pi\mathbb{Z})^d$ the standard d-dimensional flat torus, and D a neighborhood in $\mathbb{R}^d$ of the point a_0 such that $(a_0, \theta_0) = \psi^{-1}(p_0, q_0)$. By definition of action-angle variables, the Hamiltonian $H(p, q)$ of (1) is writen $H(p, q) = K(a)$ in the coordinates (a, θ), and thus the dynamics reads

$$\begin{cases} \dot{a}(t) = 0, \\ \dot{\theta}(t) = \omega(a(t)), \end{cases} \tag{5}$$

where $\omega = \partial K/\partial a$ is the frequency vector associated with the problem. The solution of this system for initial data (a_0, θ_0) is simply writen $a(t) = a_0$ and $\theta(t) = \omega(a_0)t + \theta_0$.

For fixed $(a_0, \theta_0) = \psi(p_0, q_0)$, the image of $S(p_0, q_0)$ under ψ^{-1} is the torus $\{a_0\} \times \mathbb{T}^d$. On this torus, the measure $d\theta$ is invariant by the flow of (5). Considering the pull-back of this measure by the transformation ψ, we thus get a measure $d\mu(p, q)$ on $S(p_0, q_0)$ which is invariant by the flow of (1). For any function $A(p, q)$ defined on $S(p_0, q_0)$ we define the *space* average:

$$\langle A \rangle := \frac{\int_{S(p_0,q_0)} A(p,q) d\mu(p,q)}{\int_{S(p_0,q_0)} d\mu(p,q)} = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} A \circ \psi(a_0, \theta) d\theta. \qquad (6)$$

For a fixed time T, the *time* average is defined as

$$\langle A \rangle(T) := \frac{1}{T} \int_0^T A(p(t), q(t)) dt. \qquad (7)$$

In a first step, we will investigate the extent to which the convergence of the time average (7) toward the space average (6) can be accelerated through the use of weighted integrals of the form

$$\langle A \rangle_\varphi(T) := \frac{\int_0^T \varphi\big(\frac{t}{T}\big) A(p(t), q(t)) dt}{\int_0^T \varphi\big(\frac{t}{T}\big) dt}, \qquad (8)$$

where φ is a positive smooth function with compact support in $[0, 1]$ (later on, we will refer to φ as the *filter* function; it is sometimes refereed as a *window* function in the context of signal processing [10]). In a second step, we will consider the time-discretization of (8), i.e. the discretization of both the integral through Riemann sums and the trajectory with symplectic integrators. In particular, we will derive estimates of the convergence with respect to T and the size h of the time-grid, which are in perfect agreement with the numerical experiments conducted in [3].

2 The complete analysis of the *d*-dimensional harmonic oscillator

In this section, we illustrate the main ideas of the paper in the rather simple situation of the d-dimensional harmonic oscillator, where most of the analysis can be conducted in an explicit way. Hereafter, $H(p, q)$ is thus the Hamiltonian function from $\mathbb{R}^d \times \mathbb{R}^d$ to $\mathbb{R}$ defined as

$$H(p, q) = \frac{1}{2} \sum_{k=1}^{d} (\omega_k^2 q_k^2 + p_k^2), \qquad (9)$$

and the corresponding dynamics is governed by the equations

$$\begin{cases} \dot{p}_k = -\omega_k^2 q_k \\ \dot{q}_k = \qquad p_k \end{cases}, \quad k = 1, \ldots, d.$$

The exact trajectory lies on the d-dimensional manifold $S(p_0, q_0)$ defined by (4) where the $I_k(p,q) = \frac{1}{2}\left(\omega_k^2 q_k^2 + p_k^2\right)$ are the conserved energies of the d oscillators. Hence, denoting $r_k^0 = \sqrt{2I_k(p_0, q_0)}$, $k = 1, \ldots, d$ and $z = (\omega_1 q_1 + ip_1, \ldots, \omega_d q_d + ip_d)$ the aggregated vector of rescaled positions and momenta, the exact solution is of the form

$$z(t) = \left(r_1^0 e^{i(\omega_1 t + \phi_1)}, \ldots, r_d^0 e^{i(\omega_d t + \phi_d)}\right), \tag{10}$$

where $\phi = (\phi_1, \ldots, \phi_d)$ depends on the initial conditions (p_0, q_0). As a consequence, the space average (6) we wish to approximate may be written here as:

$$\langle A \rangle = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} (A \circ \Delta)(r^0, \theta) d\theta,$$

where $\Delta(r^0, \theta) = (\frac{r_1^0}{\omega_1}\cos(\theta_1), r_1^0 \sin(\theta_1), \ldots, \frac{r_d^0}{\omega_d}\cos(\theta_d), r_d^0 \sin(\theta_d))$. As for the time-average (7), it reads:

$$\langle A \rangle(T) = \frac{1}{T} \int_0^T (A \circ \Delta)(r^0, \omega t + \phi) dt.$$

In order to estimate the rate of convergence of (7) toward (6), we expand $A \circ \Delta$ in a Fourier series (the conditions under which this expansion is valid will be detailed in the following sections):

$$(A \circ \Delta)(r^0, \theta) = \sum_{\alpha \in \mathbb{Z}^d} \widehat{A \circ \Delta}(r^0, \alpha) e^{i\alpha \cdot \theta},$$

where $\alpha \cdot \theta = \alpha_1 \theta_1 + \ldots + \alpha_d \theta_d$ and with:

$$\widehat{A \circ \Delta}(r^0, \alpha) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} (A \circ \Delta)(r^0, \theta) e^{-i\alpha \cdot \theta} d\theta.$$

In particular, $\widehat{A \circ \Delta}(r^0, 0) = \langle A \rangle$. Hence, we have:

$$|\langle A \rangle - \langle A \rangle(T)| \leq \frac{1}{T} \sum_{\alpha \in \mathbb{Z}^d, \, \alpha \neq 0} \frac{2|\widehat{A \circ \Delta}(r^0, \alpha)|}{|\alpha \cdot \omega|}. \tag{11}$$

This infinite sum can then be bounded if we assume, on one hand, that the vector of frequencies $\omega = (\omega_1, \ldots, \omega_d)$ satisfies *Siegel's diophantine condition*

$$\exists\, \gamma, \nu > 0, \quad \forall\, \alpha \in \mathbb{Z}^d, \quad |\alpha \cdot \omega| > \gamma |\alpha|^{-\nu}, \tag{12}$$

and on the other hand, that the Fourier coefficients decay sufficiently rapidly. This relatively poor rate of convergence $(1/T)$ may now be considerably improved by considering *iterated* averages of the form:

$$\langle A \rangle_k(T) := \frac{1}{T^k} \int_0^T \ldots \int_0^T (A \circ \Delta)(r^0, (t_1 + \ldots + t_k)\, \omega + \phi) dt_1 \ldots dt_k. \tag{13}$$

Using Fourier expansions as in (11), we indeed obtain in a very similar way the following error estimate for (13):

$$|\langle A \rangle - \langle A \rangle_k(T)| \leq \frac{1}{T^k} \sum_{\alpha \in \mathbb{Z}^d,\, \alpha \neq 0} \frac{2 |\widehat{A \circ \Delta}(r^0, \alpha)|}{|\alpha \cdot \omega|^k}, \tag{14}$$

and under slightly more stringent bounds on the $|\widehat{A \circ \Delta}(r^0, \alpha)|$, (14) leads to a rate of convergence of $1/T^k$. Inspired by these computations, and noticing that (13) is a special case of (8) (more precisely $\langle A \rangle_k(T/k) = \langle A \rangle_\varphi(T)$ with $\varphi \equiv \chi^{*k}_{[0,1/k]}$, the k^{th}-convolution of the characteristic function of $[0, 1/k]$), we will consider in the sequel more general *filter* functions and demonstrate that the rate of convergence can be further improved.

Now, a natural question that arises is whether the techniques explained above are amenable to numerical computations, when both the trajectory $z(t)$ and the integrals (7) or (13) are approximated using numerical schemes. In the case of the harmonic oscillator, it turns out that the numerical trajectory $z^h(t_n)$ (i.e. the approximation at time $t_n = nh$ of $z(t_n)$), when the underlying scheme is a symplectic (or symmetric) Runge-Kutta method, may be interpreted as the exact solution of a harmonic oscillator with *modified* frequencies $\omega_k^h = \omega_k \Theta(h\omega_k)$. In particular, the numerical trajectory lies on the same manifold $S(q_0, p_0)$ as the exact one. For the velocity-Verlet scheme (and partitioned methods), the same interpretation is possible, though the numerical trajectory would lie on an invariant torus $\mathcal{O}(h^2)$-close to $S(q_0, p_0)$: this situation is more typical of what happens for general integrable Hamiltonian systems.

In our situation, we have:

$$z^h(t_n) = \left(r_1^0 e^{i(\omega_1 \Theta(h\omega_1) t_n + \phi_1)}, \ldots, r_d^0 e^{i(\omega_d \Theta(h\omega_d) t_n + \phi_d)} \right),$$

where Θ is a smooth function defined by

$$\Theta(y) = \frac{1}{y} \arctan\left(\frac{R(iy) - R(-iy)}{i(R(iy) + R(-iy))}\right),$$

$R(z)$ being the *stability function* of the method (in fact, Θ is real analytic as soon as R has no pole on the imaginary axis and satisfies $\Theta(y) = 1 + \mathcal{O}(y^r)$ where r denotes the order of convergence of the Runge-Kutta method). As a consequence, the Riemann sum associated with (13) (note that (15) with $k = 1$ corresponds to (7)) reads, for $T = nh$, $n \in \mathbb{N}$,

$$\langle A \rangle_k^{\mathrm{Rie}}(T) := \frac{1}{n^k} \sum_{j_1=0}^{n-1} \ldots \sum_{j_k=0}^{n-1} (A \circ \Delta)(r^0, (j_1 + \ldots + j_k)h\,\omega\,\Theta(\omega h) + \phi), \tag{15}$$

where $\omega\Theta(\omega h) = (\omega_1\Theta(\omega_1 h), \ldots, \omega_d\Theta(\omega_d h))$, so that using once again Fourier expansions, we get straightforwardly:

$$|\langle A \rangle - \langle A \rangle_k^{\mathrm{Rie}}(T)| \leq \frac{1}{n^k} \sum_{\alpha \in \mathbb{Z}^d,\, \alpha \neq 0} |\widehat{A \circ \Delta}(r^0, \alpha)| \left|\frac{e^{inh\alpha\cdot(\omega\Theta(\omega h))} - 1}{e^{ih\alpha\cdot(\omega\Theta(\omega h))} - 1}\right|^k. \tag{16}$$

Bounding the above infinite sum now requires to bound the term $|e^{inx} - 1|/|e^{ix} - 1|$ for x of the form $x = h\alpha \cdot (\omega\Theta(\omega h))$. To this aim, we use the following two inequalities

$$\exists\, C_0, x_0 > 0,\ \forall n \in \mathbb{N},\ \forall |x| \leq x_0,\ \left|\frac{e^{inx} - 1}{e^{ix} - 1}\right| \leq C_0 \frac{1}{|x|}, \tag{17}$$

$$\forall n \in \mathbb{N},\ \forall x \in \mathbb{R},\ \left|\frac{e^{inx} - 1}{e^{ix} - 1}\right| \leq n, \tag{18}$$

according to whether $|x|$ is small (17) or not (18). The bound we are looking for is now based on the following lemma:

Lemma 1 *Assume that the vector of frequencies ω satisfies the diophantine condition* (12) *and the Runge-Kutta method is of order r. Then, there exist strictly positive constants c and h_0 such that*

$$\forall\, h \leq h_0 \quad \forall\, \alpha \in \mathbb{Z}^d, \quad |\alpha \cdot (\omega\,\Theta(\omega h))| \leq \frac{\gamma}{2}\,|\alpha|^{-\nu} \Longrightarrow |\alpha| \geq c\,h^{-\frac{r}{\nu+1}}.$$

Proof. Assume that there exists $\alpha \in \mathbb{Z}^d$ such that

$$|\alpha \cdot (\omega\,\Theta(\omega h))| \leq \frac{\gamma}{2}\,|\alpha|^{-\nu}.$$

Then, from $\Theta(h\omega_k) = 1 + \mathcal{O}(|h\,\omega_k|^r)$, we obtain for h sufficiently small:

$$\begin{aligned}\frac{\gamma}{2}\,|\alpha|^{-\nu} &\geq |\omega\cdot\alpha| - C|\alpha|\,|h\,\omega|^r,\\ &\geq \gamma|\alpha|^{-\nu} - C|\alpha|\,|h\,\omega|^r,\end{aligned}$$

where C is the strictly positive constant contained in the term $\mathcal{O}$ (note that if $\Theta \equiv 1$, although the constant C is zero, there is no α violating condition (12) and the lemma remains valid). Hence,

$$|\alpha| \geq \left(\frac{\gamma}{2C|\omega|^r}\,h^{-r}\right)^{\frac{1}{\nu+1}}.$$

■

But for $|\alpha| \leq ch^{-r/(\nu+1)}$ we have $|h\alpha\cdot\omega\Theta(\omega h)| \leq \tilde{c}h^{1-r/(\nu+1)}$ for a constant $\tilde{c}$ independent of h. Hence if $\nu > r-1$, then for small enough h we have $|h\alpha\cdot\omega\Theta(\omega h)| \leq x_0$ defined in (17). Now we can split the sum in (16) into

$$\sum_{1\leq|\alpha|\leq ch^{-\frac{r}{\nu+1}}} |\widehat{A\circ\Delta}(r^0,\alpha)|\,\frac{C_0^k}{n^k h^k|\alpha\cdot(\omega\,\Theta(\omega h))|^k} + \sum_{|\alpha|\geq ch^{-\frac{r}{\nu+1}}} |\widehat{A\circ\Delta}(r^0,\alpha)|. \tag{19}$$

Using Lemma 1 for the first term and assuming that the Fourier coefficients $|\widehat{A\circ\Delta}(r^0,\alpha)|$ decay exponentially with $|\alpha|$, an estimate of the form

$$|\langle A\rangle - \langle A\rangle_k^{\mathrm{Rie}}(T)| = \mathcal{O}\left(\frac{1}{T^k} + \exp\Big(-ch^{-s}\Big)\right),$$

with $s = r/(\nu+1)$. Whenever a symplectic partitioned method is used, the quadratic invariants I_k might be preserved only up to the order of the scheme, and an additional term h^r then comes into play which becomes dominant: for general Runge-Kutta methods, the best possible estimate is thus of the form

$$|\langle A\rangle - \langle A\rangle_k^{\mathrm{Rie}}(T)| = \mathcal{O}\left(\frac{1}{T^k} + h^r\right). \tag{20}$$

The term $1/T^k$ is the intrinsic error component of the *iterated*-average, whereas the term h^r reflects the use of a numerical scheme of order r. It is worth noticing that there is **no secular component** in h^r (neither in the bound $e^{-\frac{c}{h^s}}$): symplectic schemes (partitioned or not) preserve quadratic invariants for *all times* (either exactly or up to the order of the method). Our aim in next sections is to prove that (20) remains true over *exponentially long times* for averages with general filter functions and for general integrable Hamiltonian systems with bounded trajectories.

3 Approximation of the average: The continuous case

The function φ considered in Formula (8) is somewhat arbitrary. The most commonly used function in practice is $\varphi \equiv 1$, which corresponds to the usual time-average as defined in (7), for which convergence when T tends to infinity is rather slow (with rate $1/T$). For the harmonic oscillator, we have seen that the use of iterated-averages (which can be seen as a special case of filtered-averages) allows for a significant acceleration of the convergence. Theorem 1 below shows that with increasingly smooth functions φ satisfying appropriate zero boundary conditions, it is possible to improve the rate of convergence to $1/T^k$ for any integer $k > 1$, not only for the harmonic oscillator, but for a general integrable Hamiltonian system. It is then natural to investigate what happens in the limit when k tends to infinity. To this aim, we shall consider, as an example of infinitely differentiable functions φ with compact support $[0,1]$ that satisfy $\varphi^{(k)}(0) = \varphi^{(k)}(1) = 0$ for any $k \in \mathbb{N}$, the function ξ defined below:

$$\begin{aligned} \xi : [0,1] &\longrightarrow [0,+\infty[\\ x &\longmapsto \exp\left(-\frac{1}{x(1-x)}\right). \end{aligned} \tag{21}$$

In the sequel, we shall assume that the estimates

$$\|\xi^{(k)}\|_{\mathrm{L}^1} := \int_0^1 |\xi^{(k)}(x)|dx \le \mu\beta^k k^{\delta k}, \tag{22}$$

$$\|\xi^{(k)}\|_{\mathrm{L}^\infty} := \sup_{x\in[0,1]} |\xi^{(k)}(x)| \le \mu\beta^k k^{\delta k}, \tag{23}$$

hold for some strictly positive constants μ, β and δ. The existence of such constants will be shown in appendix (Lemma 3).

Theorem 1 *Consider the completely integrable system* (1)*, and assume that the diophantine condition* (12) *is satisfied for* $\omega(a_0)$ *defined in* (5) *by the initial condition* (q_0, p_0)*, with* $(q_0, p_0) = \psi(a_0, \theta_0)$*. Consider a function* A *real analytic on* $\mathbb{R}^d \times \mathbb{R}^d$ *(the observable). Recall that to this function we associate the space-average* $\langle A\rangle$*, the time-average* $\langle A\rangle(T)$ *and the filtered time-average* $\langle A\rangle_\varphi(T)$ *respectively defined in* (6)*,* (7) *and* (8)*, where* $\varphi \in C^0(0,1)$ *(the filter function)* *is assumed to be positive. Then we have the following convergence estimates:*

1. *There exists a constant c depending on A, d, ν and γ such that*

$$|\langle A\rangle(T) - \langle A\rangle| \le \frac{c}{T}.$$

2. *Let $k \ge 1$. If φ is $C^{k+1}(0,1)$ with $\varphi^{(j)}(0) = \varphi^{(j)}(1) = 0$ for all $j = 0, \dots, k-1$, then there exist positive constants c_0 and R depending on A, φ, d, ν and γ, such that (here $\nu \in \mathbb{N}$, though a similar formula holds for general ν using the Γ function)*

$$|\langle A\rangle(T) - \langle A\rangle| \le \frac{c(k,\varphi)}{T^{k+1}},$$

where

$$c(k,\varphi) = c_0 R^{k+1}(\nu(k+1)+1)! \\ \times \frac{1}{\|\varphi\|_{\mathrm{L}^1}}\Big(|\varphi^{(k)}(0)| + |\varphi^{(k)}(1)| + \|\varphi^{(k+1)}\|_{\mathrm{L}^1}\Big)$$

3. *If ξ defined in (21) is taken as the filter function, then there exist strictly positive constants c_1, κ and ρ depending on A, d, ν and γ, such that*

$$|\langle A\rangle_\xi(T) - \langle A\rangle| \le c_1 e^{-\kappa T^{1/\rho}}.$$

Proof. Statement 1. is proved in Arnold [2]. It may also be obtained as a special case of 2. with $\varphi \equiv 1$. Now, if A is real analytic on $\mathbb{R}^d \times \mathbb{R}^d$, then so is $A \circ \psi$ on the d-dimensional torus $\mathbb{T}^d$ and we can expand it as a Fourier series

$$(A \circ \psi)(a_0, \alpha) = \sum_{\alpha \in \mathbb{Z}^d} \widehat{A \circ \psi}(a_0, \alpha) e^{i\alpha\cdot\theta},$$

with exponentially decaying coefficients:

$$\forall\, \alpha \in \mathbb{Z}^d,\ |\widehat{A \circ \psi}(a_0, \alpha)| \le C e^{-\frac{|\alpha|}{C}},$$

where C is a strictly positive real constant. The integral over $\mathbb{T}^d$ of the first coefficient of the series ($\alpha = 0$) is straightforwardly identified as the space-average

$$\widehat{A \circ \psi}(a_0, 0) = \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d} (A \circ \psi)(a_0, \theta) d\theta.$$

Writing $\int_0^T \varphi\big(\frac{t}{T}\big)dt = T\|\varphi\|_{\mathrm{L}^1} := \chi^{-1}$, the error can be computed as follows:

$$\begin{aligned}\langle A\rangle_\varphi(T) - \langle A\rangle &= \chi \sum_{\alpha\in\mathbb{Z}^d,\ \alpha\neq 0} \widehat{A\circ\psi}(a_0,\alpha)\int_0^T \varphi\Big(\frac{t}{T}\Big)e^{i\alpha\cdot(\theta_0+t\omega(a_0))}dt \\ &= \chi \sum_{\alpha\in\mathbb{Z}^d,\ \alpha\neq 0} \widehat{A\circ\psi}(a_0,\alpha)e^{i(\alpha\cdot\theta_0)}\int_0^T \varphi\Big(\frac{t}{T}\Big)e^{it(\alpha\cdot\omega(a_0))}dt. \quad (24)\end{aligned}$$

Now, the integral in each term of the series can be integrated by parts

$$\begin{aligned}\int_0^T \varphi\Big(\frac{t}{T}\Big)e^{it(\alpha\cdot\omega(a_0))}dt &= \left[\frac{\varphi\big(\frac{t}{T}\big)e^{it(\alpha\cdot\omega(a_0))}}{i(\alpha\cdot\omega(a_0))}\right]_0^T \\ &\quad -\frac{1}{Ti(\alpha\cdot\omega(a_0))}\int_0^T \varphi'\Big(\frac{t}{T}\Big)e^{it(\alpha\cdot\omega(a_0))}dt.\end{aligned}$$

Integrating repeatedly by parts, this last term can be written as

$$\begin{aligned}&\frac{e^{iT(\alpha\cdot\omega(a_0))}\varphi(1)-\varphi(0)}{i(\alpha\cdot\omega(a_0))} - \frac{1}{Ti(\alpha\cdot\omega(a_0))}\int_0^T \varphi'\Big(\frac{t}{T}\Big)e^{it(\alpha\cdot\omega(a_0))}dt \\ &\qquad = \ldots = \frac{(-1)^k}{(Ti(\alpha\cdot\omega(a_0)))^k}\int_0^T \varphi^{(k)}\Big(\frac{t}{T}\Big)e^{it(\alpha\cdot\omega(a_0))}dt,\end{aligned}$$

and eventually,

$$\begin{aligned}\int_0^T \varphi\Big(\frac{t}{T}\Big)e^{it(\alpha\cdot\omega(a_0))}dt &= \frac{(-1)^k}{(Ti(\alpha\cdot\omega(a_0)))^{k+1}}T\left[\varphi^{(k)}\Big(\frac{t}{T}\Big)e^{it(\alpha\cdot\omega(a_0))}\right]_0^T \\ &\quad - \frac{(-1)^k}{(Ti(\alpha\cdot\omega(a_0)))^{k+1}}\int_0^T \varphi^{(k+1)}\Big(\frac{t}{T}\Big)e^{it(\alpha\cdot\omega(a_0))}dt.\end{aligned}$$

Inserting this expression in equation (24) and taking the moduli of both sides, we finally get the bound

$$\begin{aligned}|\langle A\rangle_\varphi(T) - \langle A\rangle| &\le \frac{(|\varphi^{(k)}(0)| + |\varphi^{(k)}(1)| + \|\varphi^{(k+1)}\|_{\mathrm{L}^1})}{T^{k+1}\|\varphi\|_{\mathrm{L}^1}} \\ &\quad \times \sum_{\alpha\in\mathbb{Z}^d,\ \alpha\neq 0} \frac{|\widehat{A\circ\psi}(a_0,\alpha)|}{|\alpha\cdot\omega(a_0)|^{k+1}}\end{aligned}$$

It remains to justify the convergence of the series considered above (and to bound its limit). This is a consequence of the diophantine condition $|\alpha \cdot \omega(a_0)| \leq \frac{\gamma}{|\alpha|^\nu}$, which gives here

$$\sum_{\alpha \in \mathbb{Z}^d,\ \alpha \neq 0} \frac{|\widehat{A \circ \psi}(a_0, \alpha)|}{|\alpha \cdot \omega(a_0)|^{k+1}} \leq \sum_{\alpha \in \mathbb{Z}^d,\ \alpha \neq 0} C e^{-\frac{|\alpha|}{C}} \left(\frac{|\alpha|}{\gamma^{1/\nu}} \right)^{\nu(k+1)},$$

$$\leq C \eta^{\nu(k+1)} \sum_{\alpha \in \mathbb{Z}^d,\ \alpha \neq 0} e^{-\frac{|\alpha|}{C}} \left(\frac{|\alpha|}{\eta \gamma^{1/\nu}} \right)^{\nu(k+1)}.$$

We now take $\eta = \frac{2C}{\gamma^{1/\nu}}$ so that $1/(\gamma^{1/\nu}\eta) = 1/(2C)$ and we obtain:

$$\sum_{\alpha \in \mathbb{Z}^d,\ \alpha \neq 0} \frac{|\widehat{A \circ \psi}(a_0, \alpha)|}{|\alpha \cdot \omega(a_0))|^{k+1}} \leq C \eta^{\nu(k+1)} (\nu(k+1)+1)! \sum_{\alpha \in \mathbb{Z}^d} e^{-\frac{|\alpha|}{2C}},$$

$$\leq \frac{C(2C)^{\nu(k+1)}(8C)^d}{\gamma^{k+1}} (\nu(k+1)+1)!,$$

where we have used $x^n \leq e^x (n+1)!$. Statement 3. is a consequence of Statement 2. with a suitably chosen k: since $\xi^{(k)}(0) = \xi^{(k)}(1) = 0$ for any $k \in \mathbb{N}$, we have indeed that for all $k \geq 0$:

$$|\langle A \rangle_\xi(T) - \langle A \rangle| \leq c_1 \left(\frac{r_1}{T} \right)^{k+1} (k+1)^{\delta(k+1)} (\nu(k+1)+1)!,$$

with $c_1 = c_0 \mu$ and $r_1 = R\beta$, μ and β being the constants of (22). Now let $\tilde{\nu}$ be the nearest integer to ν toward infinity. This gives:

$$|\langle A \rangle_\xi(T) - \langle A \rangle| \leq c_1 \left(\frac{r_1 \tilde{\nu}^{\tilde{\nu}}}{T} \right)^{k+1} (k+1)^{(\delta+\tilde{\nu})(k+1)},$$

$$\leq c_1 e^{f(k+1)},$$

where $f(\ell) = \ell[\log(r_1 \tilde{\nu}^{\tilde{\nu}}/T) + (\delta + \tilde{\nu}) \log(\ell)]$. The minimum of f for positive ℓ is attained for $\ell = \frac{1}{e} \left(\frac{T}{r_1 \tilde{\nu}^{\tilde{\nu}}} \right)^{1/(\tilde{\nu}+\delta)}$ and is

$$f_{min} = -\frac{(\delta + \tilde{\nu})}{e} \left(\frac{T}{r_1 \tilde{\nu}^{\tilde{\nu}}} \right)^{\frac{1}{(\delta+\tilde{\nu})}}.$$

■

Remark 1 In the proof of Theorem 1, one gets $c_0 = C(8C)^d$, $R = (2C)^\nu/\gamma$, $c_1 = \mu c_0$, $\kappa = (\delta + \tilde{\nu}) e^{-1} \tilde{\nu}^{-\frac{\tilde{\nu}}{\tilde{\nu}+\delta}}$ and $\rho = (\delta + \tilde{\nu})$, where $\tilde{\nu} = \nu + 1$. The values of these constants rely heavily on the sharpness of estimates (22) and it is likely that they might be improved. Nevertheless, the convergence behavior would be essentially the same for large dimensions: even if ξ were analytic, one would get $\rho = 1 + \tilde{\nu}$. More noticeably, since almost all frequencies $\omega(a_0)$ satisfy the diophantine condition for some γ as soon as $\nu > d - 1$, we may think of $\tilde{\nu}$ as being d and thus δ as being approximately $1 + d$. The rate of convergence thus directly depends on the dimension of the phase-space.

4 Semi-discrete averages

We now wish to investigate whether the estimates of Theorem 1 persist when one replaces the integrals by Riemann sums. It turns out, quite remarkably, that its proof can be almost readily adapted.

Theorem 2 *Assume that the conditions of Theorem* 1 *are satisfied and let* $T = nh > 0$ *for a given integer* $n \geq 2$*. Let us further define the Riemann sums corresponding to the* continuous *time-average*

$$\langle A \rangle^{\mathrm{Rie}}(T) := \frac{1}{n} \sum_{j=0}^{n-1} A(p(jh), q(jh)),$$

and the filtered time-average

$$\langle A \rangle_{\varphi}^{\mathrm{Rie}}(T) := \frac{\sum_{j=0}^{n-1} \varphi(\frac{j}{n}) A(p(jh), q(jh))}{\sum_{j=0}^{n-1} \varphi(\frac{j}{n})},$$

where $\varphi \in C^0(0,1)$ *is the filter function. Then we have the following convergence estimates:*

1. *There exist constants* c *and* c^* *depending on* A, d, ν, γ *and* $\omega = \omega(a_0)$ *such that*

$$\left| \langle A \rangle^{\mathrm{Rie}}(T) - \langle A \rangle \right| \leq \frac{c}{T} + c^* \exp\left(-\frac{1}{c^* h} \right).$$

2. *Let* $k \geq 1$*. If* φ *is* $C^{k+1}(0,1)$ *with* $\varphi^{(j)}(0) = \varphi^{(j)}(1) = 0$ *for all* $j = 0, \ldots, k-1$*, then there exist strictly positive constants* c^*, c_0 *and* R *depending on* A, φ, d, ν, γ *and* ω *such that*

$$\left| \langle A \rangle^{\mathrm{Rie}}(T) - \langle A \rangle \right| \leq \frac{c(k,\varphi)}{T^{k+1}} + c^* \exp\left(-\frac{1}{c^* h} \right),$$

   where

$$c(k,\varphi) = c_0 R^{k+1} k^k (\nu(k+1)+1)! \times \frac{1}{\|\varphi\|_{\mathrm{L}^1}} \left(|\varphi^{(k)}(0)| + |\varphi^{(k)}(1)| + \|\varphi^{(k+1)}\|_{\mathrm{L}^\infty} \right).$$

3. *If ξ is taken as the filter function, then there exist strictly positive constants c^*, c_1, κ and ρ depending on A, d, ν, γ and ω, such that*

$$\left|\langle A\rangle_{\xi}^{\mathrm{Rie}}(T) - \langle A\rangle\right| \leq c_1 e^{-\kappa T^{1/\rho}} + c^* \exp\left(-\frac{1}{c^* h}\right).$$

Remark 2 In the proof of Theorem 2, one gets $\rho = (\delta + 1 + \tilde{\nu})$ and $\kappa = (\delta + 1 + \tilde{\nu}) e^{-1} (\tilde{\nu})^{-\frac{\tilde{\nu}}{\tilde{\nu}+\delta+1}}$, where $\tilde{\nu} = \nu + 1$.

Proof. Statement 1. is a special case of Statement 2. with $\varphi \equiv 1$, so that we focus on the error estimate for the filtered average. Expanding $(A \circ \psi)$ in Fourier series as in Theorem 1 and denoting $S_n = \sum_{j=0}^{n-1} (1/n)\varphi(j/n)$, we have:

$$\langle A\rangle_{\varphi}^{\mathrm{Rie}}(T) - \langle A\rangle = \frac{1}{nS_n} \sum_{\alpha \in \mathbb{Z}^d,\ \alpha \neq 0} \widehat{A \circ \psi}(a_0, \alpha) e^{i(\alpha \cdot \theta_0)} \times \sum_{j=0}^{n-1} \varphi\left(\frac{j}{n}\right) e^{i\alpha \cdot jh\omega},$$

where $\omega = \omega(a_0)$. We use the following result, whose proof is given in Appendix:

Lemma 2 *For a given filter-function φ in $C^{k+1}(0,1)$ with $\varphi^{(j)}(0) = \varphi^{(j)}(1) = 0$ for all $j = 0, \ldots, k-1$, and a given integer $n \geq k+2$, let φ_j be the real numbers defined by $\varphi_j = \varphi(j/n)$ for $j = 0, \ldots, n$. If $b \neq 1$ is a complex number of modulus 1, then we have the estimate*

$$\left| \sum_{0 \leq j \leq n-1} \varphi_j b^j \right| \leq \frac{2e^2 k^k}{n^k |1-b|^{k+1}} \left(|\varphi^{(k)}(0)| + |\varphi^{(k)}(1)| + \|\varphi^{(k+1)}\|_{\mathrm{L}^\infty} \right).$$

Now, we can bound the previous sum by using the following splitting

$$|\langle A\rangle_{\varphi}^{\mathrm{Rie}}(T) - \langle A\rangle| \leq \frac{C(k,\varphi)}{n^{k+1} S_n} \sum_{\alpha \in \mathbb{Z}^d,\ 0<|\alpha| \leq (h|\omega|)^{-1}} \frac{|\widehat{A \circ \psi}(a_0, \alpha)|}{|1 - e^{i\alpha \cdot h\omega}|^{k+1}} + \sum_{\alpha \in \mathbb{Z}^d,\ |\alpha| > (h|\omega|)^{-1}} |\widehat{A \circ \psi}(a_0, \alpha)|. \quad (25)$$

where we have denoted

$$C(k,\varphi) = 2e^2 k^k \left(|\varphi^{(k)}(0)| + |\varphi^{(k)}(1)| + \|\varphi^{(k+1)}\|_{\mathrm{L}^\infty} \right).$$

Note that, since $0 < |\alpha| \leq (h|\omega|)^{-1}$ in the first term, we have $0 < |h\alpha \cdot \omega| \leq 1$, so that $b = e^{ih\alpha\cdot\omega} \neq 1$.

The second term in the right-hand side can be straightforwardly bounded by $c^* \exp(-\frac{1}{c^* h})$. Using (12), we have for all $|\alpha| \le (h|\omega|)^{-1}$:

$$\frac{1}{|1-e^{i\alpha\cdot h\omega}|} \le C_0 \frac{1}{h|\alpha\cdot\omega|}.$$

The first term in the right-hand side can be estimated as

$$\frac{C(k,\varphi)C_0^{k+1}}{T^{k+1}S_n} \sum_{\alpha\in\mathbb{Z}^d,\ 0<|\alpha|\le(h|\omega|)^{-1}} \frac{|\widehat{A\circ\psi}(a_0,\alpha)|}{|\alpha\cdot\omega|^{k+1}}$$

and we can conclude as in the proof of Theorem 1. ■

5 Fully discrete averages

We consider the numerical trajectory (p_n, q_n) for $n \ge 0$ obtained by a symplectic r^{th}-order numerical scheme Φ_h from the initial point $(p_0, q_0) = \psi^{-1}(a_0, \theta_0)$.

For $T = nh$ and $n \in \mathbb{N}$, the corresponding Riemann sum reads

$$\langle A\rangle^{\mathrm{Rie}}_{\varphi,h}(T) := \frac{\sum_{j=0}^{n-1}\varphi(\frac{j}{n})A(p_j,q_j)}{\sum_{j=0}^{n-1}\varphi(\frac{j}{n})}. \tag{26}$$

Theorem 4.4 and 4.7 of Chapter X in [5], which strongly rely on the theory developed by Kolmogorov, Arnold and Moser [1,6–9] and on results from the backward analysis (see [5] pp. 288 and references therein), yield the following result:

Theorem 3 (Hairer, Lubich, Wanner [5]) *Let $a^* \in \mathbb{T}^d$ such that $\omega(a^*)$ satisfies the diophantine condition* (12) *with constants γ and ν, and suppose that $H(p,q)$ is analytic on a neighborhood of the torus $\{(p,q) = \psi(a^*,\theta)\,|\,\theta\in\mathbb{T}^d\}$. Then there exists positive constants ρ, c_0, c, C_0 and h_0 such that for all $h \le h_0$ and $\mu \le \min(r,\alpha)$ where $\alpha = \nu + d + 1$, the following holds: There exists a symplectic change of coordinates $\psi_h : (a,\theta) \mapsto (b,\chi)$ analytic for*

$$\|a-a^*\| \le c_0 h^{2\mu} \quad \textit{and} \quad \theta \in U_\rho = \{\theta\in\mathbb{T}^d + i\mathbb{R}^d\,|\,|\mathrm{Im}\theta| < \rho\}$$

and h^r-close to the identity in the sense that

$$\|(a,\theta)-\psi_h(a,\theta)\| \le C_0 h^r \quad \textit{for} \quad \|a-a^*\| \le c_0 h^{2\mu} \quad \textit{and} \quad \theta\in U_{\rho/2},$$

such that in coordinates (b,χ), the numerical trajectory $(b_n,\chi_n) = \psi_h^{-1}\circ\psi^{-1}(p_n,q_n)$ satisfies

$$\begin{aligned} b_n &= b_0 + \mathcal{O}(\exp(-ch^{-\mu/\alpha})),\\ \chi_n &= nh\omega_h(b_0) + \mathcal{O}(h^{-2\mu/\alpha}\exp(-ch^{-\mu/\alpha})), \end{aligned} \tag{27}$$

for $nh \leq \exp(ch^{-\mu/\alpha})$*, where* $\omega_h(b) = \omega(b) + \mathcal{O}(h^r)$ *uniformly in* b*.*

Using this result, we get the following Theorem:

Theorem 4 *Under the conditions and notations of Theorem 3, if the numerical trajectory starts with*

$$\|a_0 - a^*\| \leq c_0 h^{2\mu} \tag{28}$$

where $(a_0, \theta_0) = \psi^{-1}(p_0, q_0)$*, then we have:*

1. *If* φ *is* C^{k+1} *with* $\varphi^{(j)}(0) = \varphi^{(j)}(1) = 0$ *for all* $j = 0, \dots, k-1$ *and if* A *is real analytic on* $\mathbb{R}^d$*, then there exist constants* c_1 *and* C *depending on* A*,* γ*,* ν*,* d*,* k*,* φ*, such that*

$$\forall h \leq h_0 \quad \forall T = nh \leq \exp(c_1 h^{-\mu/\alpha}),$$
$$|\langle A \rangle^{\mathrm{Rie}}_{\varphi,h}(T) - \langle A \rangle| \leq C \left(\frac{1}{T^{k+1}} + h^r \right). \tag{29}$$

2. *If* ξ *is taken as the filter function, if* A *is real analytic, then there exist constants* c_1 *and* C*, depending on* A*,* γ*,* ν *and* d *such that*

$$\forall h \leq h_0 \quad \forall T = nh \leq \exp(c_1 h^{-\mu/\alpha}),$$
$$|\langle A \rangle^{\mathrm{Rie}}_{\xi,h}(T) - \langle A \rangle| \leq C \left(e^{-\kappa T^{1/\rho}} + h^r \right). \tag{30}$$

Proof. With the notation $S_n = \sum_{j=0}^{n-1} (1/n)\varphi(j/n)$, we have using Theorem 3 that

$$\langle A \rangle^{\mathrm{Rie}}_{\varphi,h}(T) := \frac{1}{nS_n} \sum_{j=0}^{n-1} \varphi(\frac{j}{n}) A \circ \psi \circ \psi_h(b_j, \chi_j).$$

Using the Fourier expansion of $A \circ \psi \circ \psi_h$ and (27), we obtain

$$\langle A \rangle^{\mathrm{Rie}}_{\varphi,h}(T) := \frac{1}{nS_n} \sum_{\alpha \in \mathbb{Z}^d} A \widehat{\circ \psi \circ} \psi_h(b_0, \alpha) e^{i\alpha\cdot\varphi_0} \sum_{j=0}^{n-1} \varphi\left(\frac{j}{n}\right) e^{i\alpha\cdot jh\omega_h}$$
$$+ \mathcal{O}(\exp(-ch^{-\mu/\alpha})) \tag{31}$$

for $nh \leq \mathcal{O}(\exp(ch^{-\mu/\alpha}))$ (we write c for a generic constant in the exponential), where $\omega_h = \omega_h(b)$.
As ψ_h is an analytic function $\mathcal{O}(h^r)$-close to the identity, we have

$$A \widehat{\circ \psi \circ} \psi_h(b_0, 0) = \langle A \rangle + \mathcal{O}(h^r),$$

and the Fourier coefficients $A \widehat{\circ \psi \circ} \psi_h(b_0, \alpha)$ decay exponentially with respect to α, uniformly with respect to h. Now similarly to Lemma 1 we get that

$$\forall\, h \leq h_0 \quad \forall\, \alpha \in \mathbb{Z}^d, \quad |\alpha \cdot (h\omega_h))| \leq \frac{\gamma}{2} |\alpha|^{-\nu} \Longrightarrow |\alpha| \geq c\, h^{-\frac{r}{\nu+1}}.$$

And we conclude as in the proof of Theorem 2 using Lemma 2 and a splitting similar to (25). ∎

6 Remarks on the implementation and numerical experiments

Though optimal with respect to the rate of convergence, the filter function ξ does not seem to allow for the derivation of an error estimate: Given that the values of the constant C in (30) is out of reach, the value of n for which

$$R_n^\varphi := \frac{\sum_{j=0}^n \varphi(j/n) A_j}{n\|\varphi\|_{\mathrm{L}^1}}$$

becomes sufficiently close (up to user's tolerance) to its limit as n goes to infinity can not be determined in advance. An update formula for R_n^φ from n to $n+1$ thus appears of much use and this should guide the choice of φ. In order to get such a formula, we study the dependence on T of

$$a(T) = \int_0^T \varphi\Big(\frac{t}{T}\Big) A(p(t), q(t)) dt.$$

Differentiating with respect to T leads to

$$\frac{da(T)}{dT} = \varphi(1) A(p(T), q(T)) - \frac{1}{T}\int_0^T \frac{t}{T}\varphi'\Big(\frac{t}{T}\Big) A(p(t), q(t)) dt. \tag{32}$$

To be of practical use, it is thus necessary that $x\varphi'(x)$ is of the form $\alpha\varphi(x)$ (where α is an arbitrary constant) so that (32) becomes an ordinary differential equation for $a(T)$. The only admissible solutions are thus monomials in x. We thus consider the following polynomial filter functions

$$\varphi_p(x) = x^p (1-x)^p, \ p \in \mathbb{N}. \tag{33}$$

Denoting for p and n in $\mathbb{N}$ the *elementary* Riemann sums

$$S_n^p = \sum_{j=0}^n \Big(\frac{j}{n}\Big)^p A_j,$$

it is easy to get the desired update formula

$$S_0^p = 0 \text{ and } S_n^p = A_n + (1-1/n)^p S_{n-1}^p, n \geq 1.$$

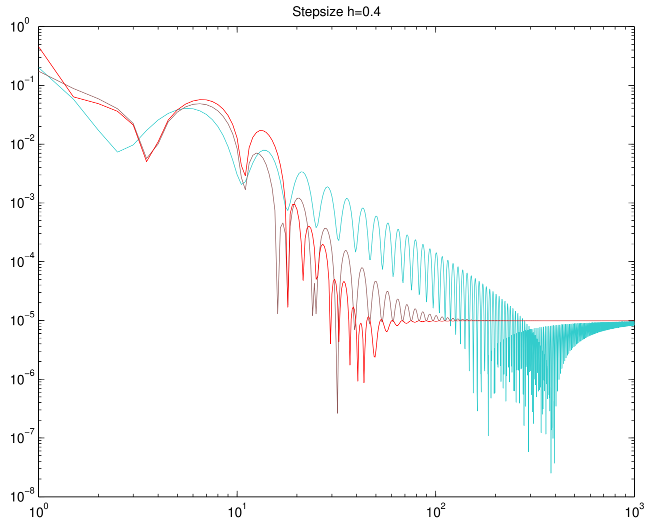

Fig. 1. Error in the averages for $p = 1, 3, 5$ and $h = 0.4$ (2D-Kepler problem).

Now, since

$$\varphi_p(x) = \sum_{k=0}^{p} (-1)^k \binom{p}{k} x^{p+k} \text{ and } \|\varphi_p\|_{\mathrm{L}^1} = \frac{(p!)^2}{(2p+1)!}$$

the approximation we seek for can be obtained as the linear combination

$$R_n^{\varphi_p} = \frac{(2p+1)!}{n(p!)^2} \sum_{k=0}^{p} (-1)^k \binom{p}{k} S_n^{p+k}.$$

We now consider the application of our method to the modified 2-dimensional Kepler problem with Hamiltonian

$$H(p,q) = p_1^2 + p_2^2 - \frac{1}{\sqrt{q_1^2 + q_2^2}} - \frac{\mu}{(\sqrt{q_1^2 + q_2^2})^3}.$$

Besides the Hamiltonian, this system has one other invariant, the angular momentum

$$L = q_2 p_1 - q_1 p_2.$$

Our goal is here to estimate the average over the manifold

$$S = \{(p,q) \in \mathbb{R}^4;\ L(p,q) = L(p_0,q_0),\ H(p,q) = H(p_0,q_0)\}$$

For $\mu = 0.2$, $p_0 = (0, 1.1)^T$ and $q_0 = (1, 0)^T$ this leads to $\langle r \rangle = 1.021466044527120$.

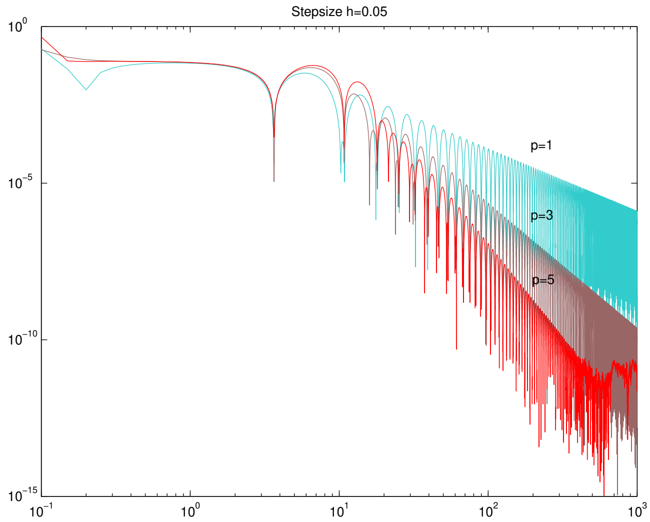

Fig. 2. Error in the averages for $p = 1, 3, 5$ and $h = 0.05$ (2D-Kepler problem).

To this aim, we consider the Verlet method as the basic step and use the 8^{th}-order 15-stage composition of [13]. In Figure 2 are represented the errors $|\langle r\rangle_{\varphi_p}(T) - \langle r\rangle|$ in logarithmic scale for two different step-sizes. On the left of the figure, the three curves all reach a plateau corresponding to the h^r-error term. Refining the step-size removes this plateau (or at least shifts it to the right, see the right graphics). In both cases, the predicted rate of convergence in $1/T^{p+1}$ is clearly observed (it corresponds to a slope of $p + 1$ for φ_p).

Appendix: some technical results

In this appendix section, we collect a few technical results used in the paper.

Lemma 3 *Let ξ be the function defined on $[0, 1]$ by $\xi(x) = e^{-\frac{1}{x(1-x)}}$. There exist strictly positive constants $\mu \leq 1$, $\beta \leq (2\sqrt{3} + 6)/e^2$ and $\delta \leq 3$ such that the following estimates hold for all $k \in \mathbb{N}^*$:*

$$\|\xi^{(k)}\|_{\mathrm{L}^1} := \int_0^1 |\xi^{(k)}(x)|dx \leq \mu\beta^k k^{\delta k},$$
$$\|\xi^{(k)}\|_{\mathrm{L}^\infty} = \sup_{x\in[0,1]} |\xi^{(k)}(x)| \leq \mu\beta^k k^{\delta k}.$$

Proof. Looking for an expression of $\xi^{(k)}(x)$ of the form

$$\xi^{(k)}(x) = \frac{P_k(x)}{[\Pi(x)]^{2k}} e^{-\frac{1}{x(1-x)}},$$

where $\Pi(x) = x(1-x)$ and where P_k is a polynomial, we easily find the recurrence relation:

$$P_0 \equiv 1 \text{ and } P_{k+1} = \Pi' \,(1 - 2k\Pi)\, P_k + P_k' \,\Pi^2, \; k \geq 0, \tag{34}$$

We now look for bounds on balls B_r of radius $r > 0$ and center $z = 1/2 + 0\,i \in \mathbb{C}$. The bounds for Π and Π' read

$$\sup_{z \in B_r} |\Pi(z)| \leq (r^2 + 1/4), \; \sup_{z \in B_r} |\Pi'(z)| \leq r,$$

and the Cauchy integral representation of P_k' leads to

$$\forall\, \varepsilon > 0, \; \sup_{z \in B_r} |P_k'(z)| \leq \frac{r+\varepsilon}{\varepsilon} \sup_{z \in B_{r+\varepsilon}} |P_k(z)|.$$

Inserting these bounds in (34) we get:

$$\begin{aligned}
\sup_{z \in B_r} |P_{k+1}(z)| \leq r[k(2r^2 - 1/2) + 1] \sup_{z \in B_r} |P_k(z)| \\
+ (r^2 + 1/4)^2 \frac{r+\varepsilon}{\varepsilon} \sup_{z \in B_{r+\varepsilon}} |P_k(z)|, \\
\leq \left(r[k(2r^2 - 1/2) + 1] + \frac{r+\varepsilon}{\varepsilon}(r^2 + 1/4)^2 \right) \sup_{z \in B_{r+\varepsilon}} |P_k(z)|.
\end{aligned}$$

Denoting $C(r,k,\varepsilon) := r[k(2r^2 - 1/2) + 1] + \frac{r+\varepsilon}{\varepsilon}(r^2 + 1/4)^2$, we finally get

$$\begin{aligned}
\sup_{z \in B_r} |P_{k+1}(z)| &\leq C(r,k,\varepsilon) \sup_{z \in B_{r+\varepsilon}} |P_k(z)|, \\
&\leq C(r,k,\varepsilon) C(r+\varepsilon, k-1, \varepsilon) \sup_{z \in B_{r+2\varepsilon}} |P_{k-1}(z)|, \\
&\leq \left(\prod_{i=0}^{k} C(r + i\varepsilon, k-i, \varepsilon) \right) \sup_{z \in B_{r+(k+1)\varepsilon}} |P_0(z)|.
\end{aligned}$$

A bound can then be obtained as follows: let $\varepsilon_0 = \frac{-1+\sqrt{3}}{2}$, $\varepsilon = \frac{\varepsilon_0}{k}$ and $r = 1/2$. Then it is easy to check that for all $0 \leq i \leq k$, we have

$$\begin{aligned}
C(\frac{1}{2} + i\frac{\varepsilon_0}{k}, k-i, \frac{\varepsilon_0}{k}) &\leq \frac{\sqrt{3}}{2}[k - i + 1] + \frac{1}{\sqrt{3}-1} k + i + 1, \\
&\leq \frac{\sqrt{3}+3}{2}(k+1),
\end{aligned}$$

and hence,

$$\left(\prod_{i=0}^{k} C(r+i\varepsilon, k-i, \varepsilon)\right) \le [\frac{\sqrt{3}+3}{2}(k+1)]^{k+1}.$$

Taking into account that $P_0 \equiv 1$, we obtain

$$\forall k \in \mathbb{N}^*, \sup_{z\in B_{1/2}} |P_k(z)| \le [\frac{\sqrt{3}+3}{2}k]^k.$$

It remains to bound $\frac{1}{[\Pi(x)]^{2k}}e^{-\frac{1}{x(1-x)}}$. Denoting $Y = \frac{1}{x(1-x)}$, we have:

$$\begin{aligned}\sup_{x\in[0,1]} \frac{1}{[\Pi(x)]^{2k}}e^{-\frac{1}{x(1-x)}} &= \sup_{Y\ge 4} e^{-Y}Y^{2k}\\ &\le e^{-2k}(2k)!\\ &\le \left(\frac{4}{e^2}\right)^k k^{2k}.\end{aligned}$$

■

Proof of lemma 2. Let us denote by ∇ the operator of *backward divided differences* defined by:

$$\forall j \in \{0,\dots,n\},\ \nabla^0\varphi_j = \varphi_j,$$
$$\forall j \in \{m+1,\dots,n\},\ \nabla^{m+1}\varphi_j = \nabla^m\varphi_j - \nabla^m\varphi_{j-1}.$$

The sum in the statement can then be written as

$$\begin{aligned}\sum_{j=0}^{n-1}\varphi_j b^j &= \sum_{j=1}^{n-1} b^j \sum_{i=1}^{j}\nabla\varphi_i + \sum_{j=0}^{n-1}\varphi_0 b^j,\\ &= \frac{1-b^n}{1-b}\varphi_0 + \sum_{i=1}^{n-1}\nabla\varphi_i\frac{b^i-b^n}{1-b},\\ &= \frac{\varphi_0 - b^n\varphi_{n-1}}{1-b} + \frac{1}{1-b}\sum_{j=1}^{n-1}(\nabla\varphi_j)b^j = \dots,\\ &= \sum_{m=0}^{k}\frac{b^m\nabla^m\varphi_m - b^n\nabla^m\varphi_{n-1}}{(1-b)^{m+1}} + \frac{1}{(1-b)^{k+1}}\sum_{j=k+1}^{n-1}(\nabla^{k+1}\varphi_j)b^j.\end{aligned}$$

Denoting $h = 1/n$, it is well-known that, for all $n-1 \le j \ge k+1$, there exists $\zeta_{j,k+1} \in [(j-k-1)h, jh] \subset [0,1]$ such that we have:

$$\nabla^{k+1}\varphi_j = \varphi^{(k+1)}(\zeta_{j,k+1})h^{k+1}$$

Hence, we can bound the second term in (35) as follows:

$$\left| \sum_{j=k+1}^{n-1} (\nabla^{k+1}\varphi_j) b^j \right| \leq \|\varphi^{(k+1)}\|_{\mathrm{L}^\infty} h^{k+1}(n-k-2).$$

In order to estimate the first sum, we notice that, for $0 \leq m \leq k \leq n-2$,

$$\nabla^m \varphi_m = \varphi^{(m)}(\zeta_{m,m}) h^m$$

for some $\zeta_{m,m} \in [0, mh]$ and a Taylor-Lagrange expansion of $\varphi^{(m)}(\zeta_{m,m})$ at order $k+1-m$ gives

$$\nabla^m \varphi_m = \frac{\zeta_{m,m}^k h^k}{(k-m)!} \varphi^{(k)}(0) + \frac{\zeta_{m,m}^{k+1} h^{k+1}}{(k+1-m)!} \varphi^{(k+1)}(\eta_m)$$

for some $\eta_m \in [0, mh] \subset [0,1]$. Hence, we have:

$$\begin{aligned} \left| \sum_{m=0}^{k} \frac{b^m}{(1-b)^m} \nabla^m \varphi_m \right| &\leq |\varphi^{(k)}(0)| \frac{k^k h^k}{|1-b|^{k+1}} \sum_{m=0}^{k} \frac{|1-b|^m}{(m)!} \\ &\quad + \|\varphi^{(k+1)}\|_{\mathrm{L}^\infty} \frac{k^k h^{k+1}}{|1-b|} \sum_{m=0}^{k} \frac{|1-b|^m}{(m+1)!}, \\ &\leq \frac{e^2 k^k h^k}{|1-b|^{k+1}} \left(|\varphi^{(k)}(0)| + h \|\varphi^{(k+1)}\|_{\mathrm{L}^\infty} \right). \end{aligned}$$

Similarly we have:

$$\nabla^m \varphi_{n-1} = \varphi^{(m)}(\zeta_{n-1,m}) h^m$$

for some $\zeta_{n-1,m} \in [1-(m+1)h, 1-h] \subset [0,1]$, so that

$$\left| \sum_{m=0}^{k} \frac{b^n}{(1-b)^m} \nabla^m \varphi_{n-1} \right| \leq \frac{2e^2 k^k h^k}{|1-b|^{k+1}} \left(|\varphi^{(k)}(1)| + h \|\varphi^{(k+1)}\|_{L^\infty} \right).$$

Gathering the contributions of all terms then gives the result. ■

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