An averaging technique for highly-oscillatory Hamiltonian problems

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Abstract

In this paper, we are concerned with the numerical solution of highly-oscillatory Hamiltonian systems with a stiff linear part. We construct an averaged system whose solution remains close to the exact one over bounded time intervals, possesses the same adiabatic and Hamiltonian invariants as the original system, and is non- stiff. We then investigate its numerical approximation through a method which combines a symplectic integration scheme and an acceleration technique for the evaluation of time-averages developped in [CCC + 05]. Eventually, we demonstrate the efficiency of our approach on two test problems with one or several frequencies.

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1 Introduction

There are many different systems in nature whose evolution is accurately described by Hamilton's equations. These are obtained from a variational principle and can be actually derived from a single scalar function, called the Hamiltonian, which is an invariant of the problem. Physically, it represents the (constant) energy of the system. Hamiltonian systems have the fundamental property that their exact flow is a symplectic transformation (see for instance [HLW06]) and often behave in a very remarkable way (as explained by the celebrated theory of Kolmogorov, Arnold and Moser [Arn63, Kol54, Mos62]). These features motivate, in accordance with the aims of *geometric* integration, the introduction of *symplectic* numerical flows that approximate the exact flow when, as occurs in practice, no closed expression of the solution can be found. Symplectic integration methods preserve the symplectic structure of the Hamiltonian system and it has been shown that they also preserve a *modified* Hamiltonian function over exponentially long intervals of time. The theory sustaining this remarkable result, known as *backward error analysis [HL00a, Rei99]*, is the key to many theoretical results describing the qualitative behaviour of numerical schemes applied to Hamiltonian systems.

In this paper however, we are concerned more specifically with Hamiltonian systems whose solution is **highly-oscillatory**. A simple yet representative model of Hamiltonian system whose solutions are highly-oscillatory in character is given by the second-order differential system

$$\ddot{x}(t) + \Omega^2 x(t) = g(x(t)), \tag{1.1}$$

where $x(t) \in \mathbb{R}^{m+d}$ is a function depending on time $t \geq 0$ and Ω is a positive semi-definite matrix with some *large* eigenvalues, and where $g(x) = -\nabla U(x)$ derives from a potential function $U(x)$. The corresponding Hamiltonian function is of the form $H(x, \dot{x}) = \frac{1}{2}\|\dot{x}\|^2 + \frac{1}{2}\|\Omega x\|^2 + U(x)$. In order to get a bounded error propagation for the purely linear case ($g \equiv 0$) with a given explicit numerical method, the step size h must be restricted according to

$$h\omega < C,$$

where C is a constant depending on the numerical method and ω is the largest frequency in Ω. In applications to molecular dynamics for instance, *fast* forces crudely modelized here by the term $-\Omega^2 x$ (short-range interactions) are much cheaper to evaluate than *slow* forces deriving from U (long-range interactions). In this case, it thus seems highly desirable to design numerical methods for which the number of evaluations of slow forces is not (at least not too much) affected by the presence of fast forces.

Another very undesirable consequence of the presence of large frequencies is the failure of backward error analysis for $h\omega >> 1$, for which all bounds of error terms involve the product $h\omega$. This prevents one from drawing any conclusion from the existence of a modified system and so an alternative theory has to be proposed. Very recently, Cohen, Hairer and Lubich [CHL03, CHL05] have introduced the so-called *modulated Fourier expansion*, which brings new light on the behaviour of highly-oscillatory Hamiltonian systems. In their approach they consider the situation of two blocks of frequencies in Ω, where the first block corresponds to the frequency zero and the other one is scaled by a large parameter (this will constitute our framework in this paper). Their contribution explains the good behaviour of certain Gautschi type methods [Gau61, Deu79, GASSS99, HL99, HL00b], as far as preservation of the total energy and almost invariance of oscillatory energies (*adiabatic invariants*) is concerned. However, a careful study (see [HLW06] Chapter XIII.2.) shows that none of these methods has perfect energy conservation: for values of the stepsize such that $h\omega$ is close to a mutiple of π the errors become large. Very recently, Grimm and Hochbruck have built up a new Gautschi type method which provably carries no resonnant stepsize [GH06]. The counterpart of this favorable feature is a loose reproduction of the energy exchange between oscillatory components.

Hence, the challenge for a numerical method is to approximate adequately both the adiabatic invariants and the energy exchange while avoiding resonnances. In this paper, we will introduce a new numerical method based on an averaged version of the original equations which stems from a preconditionning of the Hamiltonian by the fast variables. This introduces an explicit representation of the highly oscillatatory components which can averaged over a period (and somehow filtered out) by artificially decoupling the two time-scales present in the problem. In Section 2, we shall justify the procedure and try to give it a sound ground by comparing the exact solutions of the original system and the averaged one. As expected, the error on the solution itself grows unbounded rather quickly. In contrast and quite strikingly, the error on the Hamiltonian remains bounded over infinite time. Moreover, the adiabatic invariants of the original system become true quadratic invariants of the averaged one: this feature is the key to all further results since it allows for the construction of a numerical method that preserves adiabatic invariants. This method involves the computation of a highly-oscillatory integral which constitutes the largest share of its cost and we shall accordingly address its numerical approximation. In Section 3, we will consider the extension of this procedure to the case of multiple frequencies and show that all results carry on easily. Finally, we will demonstrate on two simple test problems the validity of our theoretical results and hopefully the potential of our method (Section 4), which preserves the total energy and the adiabatic invariants and does not suffer from any resonance.

2 A simplified model with one frequency

As a first step, we consider, as it has become common in the litterature (see for instance [HLW06]), a Hamiltonian system of the form

$$\left\{\begin{array}{rcl}\ddot{x}_1 & = & g_1(x_1,x_2) = -\nabla_1 U(x_1,x_2),\\ \ddot{x}_2 + \dfrac{1}{\varepsilon^2}x_2 & = & g_2(x_1,x_2) = -\nabla_2 U(x_1,x_2),\end{array}\right. \tag{2.1}$$

where $x_1 \in \mathbb{R}^m$ and $x_2 \in \mathbb{R}^d$, $U(x_1,x_2)$ is a real-valued function and $\varepsilon \in (0,\varepsilon_0)$ is a small parameter. To this system is associated the Hamiltonian[1]

$$H(x_1,x_2,\dot{x}_1,\dot{x}_2) = \frac{\|x_2\|^2}{2\varepsilon^2} + \frac{\|\dot{x}_1\|^2}{2} + \frac{\|\dot{x}_2\|^2}{2} + U(x_1,x_2).$$

In the whole paper, we will assume that the initial values x_1^0, $\dot{x}_1^0$, x_2^0, $\dot{x}_2^0$ satisfy the condition (of bounded energy) for a given positive ε_0

$$\forall\, \varepsilon \in (0,\varepsilon_0), \quad \frac{\|x_2^0\|^2}{2\varepsilon^2} + \frac{\|\dot{x}_1^0\|^2}{2} + \frac{\|\dot{x}_2^0\|^2}{2} \leq E, \tag{2.2}$$

where $E > 0$ is a fixed number, independent of ε.

For the sake of conciseness, we will often work with the complex (rescaled) variables $y_1 = x_1 + i\dot{x}_1$ and $y_2 = \dfrac{x_2}{\sqrt{\varepsilon}} + i\sqrt{\varepsilon}\dot{x}_2$, so that the equations can be rewritten as the system

$$\left\{\begin{array}{rcl}\dot{y_1} & = & \Im(y_1) + i g_1(\Re(y_1), \mu\Re(y_2)),\\ \dot{y_2} & = & -\dfrac{i}{\varepsilon}y_2 + i\mu g_2(\Re(y_1), \mu\Re(y_2)),\end{array}\right. \tag{2.3}$$

where $\Re$ denotes the real part of a complex number and where we have denoted for convenience $\mu = \sqrt{\varepsilon}$. To this system is associated[2] the real-valued Hamiltonian of complex variables

$$H_{\mathbb{C}}(y_1,y_2) = \|\Im(y_1)\|^2 + \frac{\|y_2\|^2}{\varepsilon} + 2U(\Re(y_1), \mu\Re(y_2)), \tag{2.4}$$

and condition (2.2) now reads correspondingly

$$\|\Im(y_1^0)\|^2 + \frac{\|y_2^0\|^2}{\varepsilon} \leq 2E. \tag{2.5}$$

[1] Here and in the sequel, the norm used is the Euclidean norm in the spaces $\mathbb{R}^m$ and $\mathbb{R}^d$ or $\mathbb{C}^m$ and $\mathbb{C}^d$.

[2] Through the equations $\dot{y}_j = -i\frac{\partial H_{\mathbb{C}}}{\partial \bar{y}_j}$, $j = 1,2$.

Note that under assumption (2.5) , the initial value y^0 satisfies $\|y_2^0\| = \mathcal{O}(\mu)$. Eventually, we will sometimes use the "pre-conditionned" variables (see [BL07]) $z_1 = y_1$ and $z_2 = e^{it/\varepsilon} y_2$, for which the system takes the simple form

$$\left\{ \begin{array}{rcl} \dot{z_1} & = & \Im(z_1) + i g_1(\Re(z_1), \mu \Re(e^{-it/\varepsilon} z_2)), \\ \dot{z_2} & = & i \mu e^{it/\varepsilon} g_2(\Re(z_1), \mu \Re(e^{-it/\varepsilon} z_2). \end{array} \right. \tag{2.6}$$

The bounded energy condition is the same as (2.5). Equations (2.6) are non-stiff (the term in $1/\varepsilon$ has disappeared), but non-autonomous and associated with the time-dependent Hamiltonian

$$K_{\mathbb{C}}(t/\varepsilon; z_1, z_2) = \|\Im(z_1)\|^2 + 2U(\Re(z_1), \mu \Re(e^{-it/\varepsilon} z_2))). \tag{2.7}$$

For brevity, we also write system (2.6) as

$$\dot{z} = F(t/\varepsilon, z) \tag{2.8}$$

with $z = (z_1, z_2) \in \mathbb{R}^{m+d}$ and where $F(\tau, z) = (F_1(\tau, z), F_2(\tau, z))$ defined by

$$\left\{ \begin{array}{rcl} F_1(\tau, z) & = & \Im(z_1) + i g_1(\Re(z_1), \mu \Re(e^{-i\tau} z_2)), \\ F_2(\tau, z) & = & i \mu e^{i\tau} g_2(\Re(z_1), \mu \Re(e^{-i\tau} z_2), \end{array} \right. \tag{2.9}$$

is periodic in $\tau \in \mathbb{T}$. The main ingredient of the approach developped in this paper is to replace system (2.8) by the averaged one

$$\dot{Z} = \lim_{T \to \infty} \frac{1}{T} \int_0^T F(\tau, Z) \, \mathrm{d}\tau = \frac{1}{2\pi} \int_0^{2\pi} F(\tau, Z) \, \mathrm{d}\tau \tag{2.10}$$

which is now a standard non-stiff system. In the next section we will show that even if the solution of (2.10) approximates the solution of (2.6) only over bounded time intervals, it still has a **Hamiltonian structure**, possesses the **adiabatic invariants** of the exact solution of (2.6) over unbounded time intervals, and **preserves the initial energy** (2.7) up to ε over long time under some mild assumptions on the potential function U . System (2.10) thus becomes

$$\left\{ \begin{array}{rcl} \dot{Z}_1 & = & \Im(Z_1) + i \dfrac{1}{2\pi} \displaystyle\int_0^{2\pi} g_1(\Re(Z_1), \mu \Re(e^{-is} Z_2)) \, \mathrm{d}s, \\ \dot{Z}_2 & = & i \mu \dfrac{1}{2\pi} \displaystyle\int_0^{2\pi} e^{is} g_2(\Re(Z_1), \mu \Re(e^{-is} Z_2) \, \mathrm{d}s. \end{array} \right. \tag{2.11}$$

As already mentionned, it is again Hamiltonian with Hamiltonian

$$\langle K_{\mathbb{C}} \rangle (Z_1, Z_2) = \|\Im(Z_1)\|^2 + \frac{1}{\pi} \int_0^{2\pi} U(\Re(Z_1), \mu \Re(e^{-is} Z_2)) \, \mathrm{d}s. \tag{2.12}$$

Example 2.1 *As an example, we consider the Fermi-Pasta-Ulam system, as described in [HLW06], i.e. with Hamiltonian*

$$H(q_1, q_2, p_1, p_2) \quad = \quad \frac{1}{2} p_1^T p_1 + \frac{1}{2} p_2^T p_2 + \frac{1}{2\varepsilon^2} q_2^T q_2 + U(q_1, q_2) \tag{2.13}$$

where

$$U(q_1,q_2) \quad = \quad \frac{1}{4}\left\{(q_{1,1}-q_{2,1})^4+\sum_{i=1}^{d-1}((q_{1,i+1}-q_{1,i})-(q_{2,i+1}+q_{2,i}))^4+(q_{1,d}+q_{2,d})^4\right\}.$$

Computing exactly the integrals in (2.11) and going back to the original variables leads to the following expression for the averaged Hamiltonian $\langle K\rangle$:

$$\langle K\rangle(q_1,q_2,p_1,p_2) \quad = \quad \frac{1}{2}p_1^Tp_1+V_\varepsilon(v_1,v_2), \tag{2.14}$$

with

$$V_\varepsilon(q_1,q_2)=\frac{1}{4}\big(q_{1,1}^4+\sum_{i=1}^{d-1}(q_{1,i+1}-q_{1,i})^4+q_{1,d}^4\big)+\frac{3}{4}q_{1,1}^2(q_{2,1}^2+\varepsilon^2p_{2,1}^2)+\frac{3}{4}(q_{1,d})^2(q_{2,d}^2+\varepsilon^2p_{2,d}^2)$$
$$+\frac{3}{4}\sum_{i=1}^{d-1}(q_{1,i+1}-q_{1,i})^2((q_{2,i+1}+q_{2,i})^2+\varepsilon^2(p_{2,i+1}+p_{2,i})^2)$$
$$+\frac{3}{32}(q_{2,1}^2+\varepsilon^2p_{2,1}^2)^2+\frac{3}{32}\varepsilon^2(p_{2,i+1}+p_{2,i})^2+(q_{2,d}^2+\varepsilon^2p_{2,d}^2)^2+\frac{3}{32}\sum_{i=1}^{d-1}(q_{2,i+1}+q_{2,i})^2.$$

2.1 Approximation on bounded time intervals

Lemma 2.2 *Let $F(\tau,z)$ be the complex function (2.9) of $\tau\in\mathbb{T}$ and $z\in\mathbb{C}^{m+d}$. For $z^0\in\mathbb{C}^{m+d}$ and $\varepsilon\in(0,\varepsilon_0)$, let $z(t)=(z_1(t),z_2(t))$ be the solution of (2.8)*

$$\dot z=F(t/\varepsilon,z),\quad z(0)=z^0\in\mathbb{C}^{m+d}$$

and let $Z=(Z_1(t),Z_2(t))$ be the solution of the average system (2.11)

$$\dot Z=\langle F\rangle(Z),\quad Z(0)=z^0\in\mathbb{C}^{m+d}.$$

Assume that for all ε_0, the solutions $z(t)$ and $Z(t)$ exist until a time $T>0$ and remain uniformly (w.r.t. ε) bounded. Then there exist a constant C depending on T, μ_0 and ε_0 such that

$$\forall\, t\in(0,T),\quad \|z_1(t)-Z_1(t)\|+\mu^{-1}\|z_2(t)-Z_2(t)\|\le C\varepsilon. \tag{2.15}$$

Proof. The arguments being standard, we only sketch he proof. We have

$$\begin{aligned}\dot z-\dot Z &= F(t/\varepsilon,z)-\langle F\rangle(Z)\\ &= \langle F\rangle(z)-\langle F\rangle(Z)+F(t/\varepsilon,z)-\langle F\rangle(z).\end{aligned}$$

Now there exists a function $J(\tau,z)=(J_1(\tau,z),J_2(\tau,z))$ from $\mathbb{T}\times\mathbb{C}^{m+d}$ to $\mathbb{C}^{m+d}$ such that for all $\tau\in\mathbb{T}$ and $z\in\mathbb{C}^{m+d}$,

$$F(\tau,z)-\langle F\rangle(z)=\partial_\tau J(\tau,z),$$

where, using (2.9), we have that $\|J_2(\tau,z)\|\le C\mu$ for a constant C depending on bounds on g_2 and on μ_0. It follows that

$$F(t/\varepsilon,z)-\langle F\rangle(z)=\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\big(J(t/\varepsilon,z)\big)-\varepsilon\partial_zJ(t/\varepsilon,z)\cdot F(t/\varepsilon,z),$$

and we find for all $t \in (0,T)$

$$z(t)-Z(t) = \varepsilon J(t/\varepsilon, z)-\varepsilon J(0,z^0)+\int_0^t \Big(\langle F\rangle(z(s))-\langle F\rangle(Z(s))-\varepsilon\partial_z J(s/\varepsilon,z(s))\cdot F(s/\varepsilon,z(s))\Big)\mathrm{d}s$$

and this yields the result using the Gronwall Lemma, owing to the fact that the function $Z\mapsto\langle F\rangle(Z)$ is uniformly Lipschitz with respect to ε. ■

Solving (2.11) thus provides us with an ε-close approximation of the solution of (2.3) over finite time. Going back to Y-variables, and as a straight consequence of Lemma 2.2, we obtain the following

Corollary 2.3 *For all $\varepsilon \in (0,\varepsilon_0)$, assume that the solutions $y(t) = (y_1(t), y_2(t))$ of (2.3) and $Z(t) = (Z_1(t), Z_2(t))$ of (2.11) with the same initial values $(y_1^0, y_2^0) \in \mathbb{C}^{m+d}$, exist until a time $T>0$. Define the function $Y(t) = (Y_1(t), Y_2(t)) = (Z_1(t), e^{-it/\varepsilon}Z_2(t))$. Then there exists a constant C depending on T and ε_0 such that for all time $t\in(0,T)$ and all $\varepsilon\in(0,\varepsilon_0)$,*

$$\|y_1(t)-Y_1(t)\| + \varepsilon^{-1/2}\|y_2(t)-Y_2(t)\| \le C\varepsilon. \tag{2.16}$$

Note that we do not require the assumption (2.5) of bounded energy to hold true to derive this result.

2.2 Hamiltonian and adiabatic invariants over long-time intervals

Quite remarkably, the adiabatic invariants of the original system are now exactly preserved along the exact solution of system (2.11).

Theorem 2.4 *Let $Z(t) = (Z_1(t), Z_2(t))$ be the exact solution of the averaged Hamiltonian system (2.11). Then, the quantity*

$$\|Z_2\|^2 = \sum_{i=1}^d |Z_{2,i}|^2,$$

which can be interpreted as an adiabatic invariant, is preserved as long as the solution exists, i.e.

$$\|Z_2(t)\| = \|Z_2(0)\|.$$

Proof. Let $X = \Re(Z_1)$. We have

$$\frac{d}{dt}\|Z_2\|^2 = 2\Re(Z_2^*\dot{Z}_2) = 2\mu\Re\Big(\frac{i}{2\pi}\int_0^{2\pi} e^{is}Z_2^* g_2(X,\mu\Re(e^{-is}Z_2))ds\Big),$$

where Z_2^* denotes the vector $(\overline{Z_2})^T$. Noticing that

$$\frac{\mathrm{d}}{\mathrm{d}s}\Re(e^{-is}Z_2)) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}s}(e^{-is}Z_2+e^{is}\bar{Z}_2) = -i\frac{1}{2}(e^{-is}z - e^{is}\bar{Z}_2) = \Im(e^{-is}Z_2), \tag{2.17}$$

it is straightforward to obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\|Z_2\|^2 = \frac{1}{\pi}\int_0^{2\pi}\sum_{j=1}^d \Im(\mu e^{-is}Z_{2,j})\frac{\partial U}{\partial x_{2,j}}(X,\mu\Re(e^{-is}Z_2))ds = \frac{1}{\pi}\Big[U(X,\mu\Re(e^{-is}Z_2))\Big]_{s=0}^{s=2\pi} = 0.$$

■

The following lemma considers the boundedness of the exact solution of (2.11), under the assumption that U is a Lyapunov function.

Lemma 2.5 *Let* $E > 0$ *be given, and for* $\varepsilon \in (0, \varepsilon_0)$, *let* (y_1^0, y_2^0) *be initial values in* $\mathbb{C}^{m+d}$ *satisfying* (2.5). *Assume that the solution* $Z = (Z_1(t), Z_2(t))$ *of* (2.11) *with initial values* $(Z_1(0), Z_2(0)) = (y_1^0, y_2^0)$ *exists until a time* $T > 0$, *possibly infinite, and remains bounded by a constant* B *:*

$$\forall \varepsilon \in (0, \varepsilon_0), \, \forall \, 0 \le t \le T, \, \|Z(t)\| \le B.$$

Then we have the estimate

$$\forall \varepsilon \in (0, \varepsilon_0), \, \forall \, 0 \le t \le T, \, \|Z_2(t)\|^2 = \|Z_2(0)\|^2 \le 2\varepsilon E. \tag{2.18}$$

Moreover there exists a constant C *such that*

$$\forall \varepsilon \in (0, \varepsilon_0), \, \forall t > 0, \, |K_{\mathbb{C}}(t/\varepsilon; Z(t)) - K_{\mathbb{C}}(0; Z(0))| \le C\varepsilon \tag{2.19}$$

where $K_{\mathbb{C}}(t/\varepsilon, Z)$ *is the Hamiltonian* (2.7) *associated with the non-averaged system* (2.6)

Proof. Inequality (2.18) is a consequence of the previous theorem and of the condition of bounded energy (2.5). As $Z(t)$ is the exact solution of (2.11), the Hamiltonian function (2.12) is preserved:

$$\forall t \ge 0, \, \langle K_{\mathbb{C}} \rangle (Z(t)) = \langle K_{\mathbb{C}} \rangle (Z(0)).$$

Hence, we have

$$K_{\mathbb{C}}(t/\varepsilon; Z(t)) - K_{\mathbb{C}}(0; Z(0)) = K_{\mathbb{C}}(t/\varepsilon; Z(t)) - \langle K_{\mathbb{C}} \rangle (Z(t)) - \big(K_{\mathbb{C}}(0; Z(0)) - \langle K_{\mathbb{C}} \rangle (Z(0))\big). \tag{2.20}$$

By definition of $K_{\mathbb{C}}$ (2.7) and of $\langle K_{\mathbb{C}} \rangle$ (2.12), we have for all $Y \in \mathbb{C}^{m+d}$ and all $t \ge 0$,

$$K_{\mathbb{C}}(t/\varepsilon; Y) \; - \; \langle K_{\mathbb{C}} \rangle (Y) \;\; = \;\; 2U(\Re(Y_1), \mu \Re(e^{-it/\varepsilon} Y_2)) \; - \; \frac{1}{\pi} \int_0^{2\pi} U(\Re(Y_1), \mu \Re(e^{-is} Y_2)) \, \mathrm{d}s \tag{2.21}$$

Using the boundedness of $Z(t)$ and estimate (2.18), we easily obtain for all $t \ge 0$ and $s \in (0, 2\pi)$,

$$|U(\Re(Z_1(t)), \mu \Re(e^{-it/\varepsilon} Z_2(t))) - U(\Re(Z_1(t)), \mu \Re(e^{-is} Z_2(t)))| \le 2M\mu \sqrt{2\varepsilon E},$$

where $M = \max \|\nabla_2 U\|$ over the compact set $\{Z \in \mathbb{C}^{m+d} \, | \, \|Z\| \le B\}$. Plugging this inequality into (2.21) and (2.20) then yields the result. ■

We can now pull the averaged solution $Z(t)$ back to the original variables. This leads to the following

Theorem 2.6 *For* $\varepsilon \in (0, \varepsilon_0)$, *let* $(y_1^0, y_2^0) \in \mathbb{C}^{m+d}$ *be such that condition* (2.5) *holds true independently of* ε. *Assume that the solution* $Z(t) = (Z_1(t), Z_2(t))$ *of* (2.11) *with initial values* (y_1^0, y_2^0) *exists until a time* $T > 0$, *possibly infinite, and is uniformly bounded with respect to* $\varepsilon \in (0, \varepsilon_0)$. *Consider* $Y(t) = (Y_1(t), Y_2(t)) = (Z_1(t), e^{-it/\varepsilon} Z_2(t))$ *: there exists a constant* $C > 0$ *such that for all time* t *and all* $\varepsilon \in (0, \varepsilon_0)$,

$$\|Y_2(t))\|^2 = \|Y_2(0))\|^2 \le 2\varepsilon E \tag{2.22}$$

and

$$|H_{\mathbb{C}}(Y_1(t), Y_2(t)) - H_{\mathbb{C}}(Y_1(0), Y_2(0))| \le C\varepsilon, \tag{2.23}$$

where $H_{\mathbb{C}}$ *denotes the Hamiltonian* (2.4).

Proof. Estimate (2.22) is an immediate consequence of Theorem 2.4. In oder to show (2.23), we write

$$H_{\mathbb{C}}(Y_1(t), Y_2(t)) = \frac{\|Z_2(t)\|}{\varepsilon} + K_{\mathbb{C}}(t/\varepsilon, Z_1(t), Z_2(t)) \tag{2.24}$$

so that (2.23) appears as a consequence of (2.19). ■

2.3 Semi-discrete solution

The results of the previous subsection motivate the search for a numerical approximation of the averaged equations (2.11) in place of the non-averaged ones (2.3). The first step towards this objective is the discretization of integrals contained in equations (2.11) . Given that the integrands are periodic functions, it is well-known that Riemann sums are particularly suited for that. We shall thus consider the sequence of problems associated with the Hamiltonians

$$K_{\mathbb{C}}^N(Z_1, Z_2) = \|\Im(Z_1)\|^2 + \frac{2}{N}\sum_{n=0}^{N-1} U\Big(\Re(Z_1), \mu\Re(e^{-i\frac{2n\pi}{N}} Z_2)\Big), \tag{2.25}$$

for $Z = (Z_1, Z_2) \in \mathbb{C}^{m+d}$, which are approximations of Hamiltonian $\langle K_{\mathbb{C}}\rangle(Z_1, Z_2)$, see (2.12). The corresponding system reads

$$\left\{\begin{array}{lcl} \dot{Z}_1^N & = & \Im(Z_1^N) + i\dfrac{1}{N}\displaystyle\sum_{n=0}^{N-1} g_1\Big(\Re(Z_1^N), \mu\Re(e^{-i\frac{2n\pi}{N}} Z_2^N)\Big), \\ \dot{Z}_2^N & = & i\mu\dfrac{1}{N}\displaystyle\sum_{n=0}^{N-1} e^{i\frac{2n\pi}{N}} g_2\Big(\Re(Z_1^N), \mu\Re(e^{-i\frac{2n\pi}{N}} Z_2^N)\Big). \end{array}\right. \tag{2.26}$$

In the sequel, we assume that the smooth function $U(x) = U(x_1, x_2)$ is analytic in the sense that, for a given constant B , there exist constants K and R such that

$$\forall\, \alpha \in \mathbb{N}^{m+d}, \quad \forall\, x \in \mathbb{R}^{m+d} \quad \text{with} \quad \|x\| \leq B, \qquad \left|\frac{\partial^{|\alpha|}}{\partial x^\alpha} U(x)\right| \leq \alpha!\, K\, R^{-|\alpha|}, \tag{2.27}$$

where $|\alpha| = \alpha_1 + \cdots + \alpha_{m+d}$ and $\alpha! = \alpha_1! \cdots \alpha_{m+d}!$ if $\alpha = (\alpha_1, \ldots, \alpha_{m+d})$.

2.3.1 Approximation over bounded time intervals

We estimate here the difference on finite time intervals between the solutions $Z(t)$ of (2.11) and $Z^N(t)$ of (2.26).

Lemma 2.7 *Assume that* U *satisfies* (2.27) *and let* $(y_1^0, y_2^0) \in \mathbb{C}^{m+d}$ *. Suppose that for all* $\varepsilon \in (0, \varepsilon_0)$ *, the solutions* $Z(t)$ *of* (2.11) *with initial values* (y_1^0, y_0^2) *, and* $Z^N(t) = (Z_1^N(t), Z_2^N(t))$ *,* $N \geq 1$ *, of* (2.26) *with the same initial values exist until a time* $T > 0$ *. Suppose in addition that these solutions are uniformly bounded with respect to* ε *and* N *, i.e.*

$$\forall\, \varepsilon \in (0, \varepsilon_0), \forall\, N \geq 1, \forall\, t \in (0, T), \quad \sup\big(\|Z^N(t)\|\,, \|Z(t)\|\,\big) \leq B, \tag{2.28}$$

for B *a constant (possibly depending only on* T *and on the initial values). Then, for a sufficiently small* ε_0 *, there exists a constant* C *depending only on* T *and* B *such that*

$$\|Z_1(t) - Z_1^N(t)\| + \mu^{-1}\|Z_2(t) - Z_2^N(t)\| \leq C\mu^N. \tag{2.29}$$

Proof. Let $F(\tau, Z)$ be defined by (2.9), and for all $n = 0, \ldots, N-1$, let $s_n = \frac{2\pi n}{N}$. We have

$$\dot{Z}_1 - \dot{Z}_1^N = \langle F_1 \rangle(Z) - \langle F_1 \rangle(Z^N) \\ + i\frac{1}{2\pi}\int_0^{2\pi} g_1(\Re(Z_1^N), \mu\Re(e^{-is}Z_2^N))\,\mathrm{d}s - i\frac{1}{N}\sum_{n=0}^{N-1} g_1(\Re(Z_1^N), \mu\Re(e^{-is_n}Z_2^N)).$$

For $x_1 \in \mathbb{R}^m$ and $z_2 \in \mathbb{C}^d$, the function $s \mapsto h(s, x_1, z_2) = g_1(x_1, \Re(e^{-is}z_2))$ is 2π -periodic and can be expanded as a Fourier series

$$h(s, x_1, z_2) = \sum_{k\in\mathbb{Z}} \hat{h}_k(x_1, z_2)e^{iks},$$

with smooth coefficients $\hat{h}_k(x_1, z_2)$. Noth that, as U is real-valued, we have $\hat{h}_{-k} = \overline{\hat{h}_k}$ for all $k \in \mathbb{Z}$. Now, we get

$$\frac{1}{N}\sum_{n=0}^{N-1} h(\Re(Z_1^N), \mu\Re(e^{-is_n}Z_2^N)) - \frac{1}{2\pi}\int_0^{2\pi} h(\Re(Z_1^N), \mu\Re(e^{-is}Z_2^N))\,\mathrm{d}s \\ = \sum_{k\in\mathbb{Z}\setminus\{0\}} \hat{h}_k(\Re(Z_1^N), \mu Z_2^N)\frac{1}{N}\sum_{n=0}^{N-1} e^{iks_n}.$$

Since

$$\frac{1}{N}\sum_{n=0}^{N-1} e^{iks_n} = \frac{1}{N}\sum_{n=0}^{N-1} e^{2i\pi nk/N} = \begin{cases} 0 & \text{if} \quad k/N \notin \mathbb{Z}, \\ 1 & \text{if} \quad k/N \in \mathbb{Z}, \end{cases} \tag{2.30}$$

the previous sum reduces to

$$2\sum_{j\in\mathbb{N}^*} \Re(\hat{h}_{jN}(\Re(Z_1^N), \mu Z_2^N)).$$

For all $k \in \mathbb{Z}$, we have

$$\hat{h}_k(x_1, \mu z_2) = -\frac{1}{2\pi}\int_0^{2\pi} e^{-iks}\partial_1 U\Big(x_1, \mu\Re(e^{-is}z_2)\Big)\mathrm{d}s.$$

Expanding the right hand side in $\mu \in (0, \sqrt{\varepsilon_0})$, we find for $k \geq 1$,

$$\hat{h}_k(x_1, \mu z_2) = \\ -\frac{1}{2\pi}\sum_{n=0}^{k-1}\frac{\mu^n}{n!}\int_0^{2\pi} e^{-iks}\partial_1\partial_2^n U(x_1, 0)\left(\Re(e^{-is}z_2), \cdots, \Re(e^{-is}z_2)\right)\mathrm{d}s + \frac{\mu^k}{k!}R_k(x_1, \xi z_2), \tag{2.31}$$

where

$$R_k(x_1, \xi z_2) = \frac{1}{2\pi}\int_0^{2\pi} e^{-iks}\partial_1\partial_2^k U(x_1, \xi\Re(e^{-is}z_2))\left(\Re(e^{-is}z_2), \cdots, \Re(e^{-is}z_2)\right)\mathrm{d}s$$

for some $0 < \xi < \mu$. In formula (2.31), the integrand is a homogeneous polynomial of degree $-(k-1) \leq n \leq k-1$ in e^{is} multiplied by e^{-iks}, and hence, its average over $[0, 2\pi]$ is equal to zero. For $k = jN$

with $j \geq 1$ we deduce using (2.28) and (2.27)

$$\left|\hat{h}_{jN}(\Re(Z_1^N), \mu Z_2^N)\right| = \frac{\mu^{jN}}{(jN)!}\left|R_{jN}(\Re(Z_1^N), \xi Z_2^N)\right| \leq K\left(\frac{\mu B}{R}\right)^{jN}$$

where K and R depend on T. Plugging this estimate into the previous one, we conclude that for μ sufficiently small,

$$\left|\frac{1}{N}\sum_{n=0}^{N-1} h(\Re(Z_1^N), \mu\Re(e^{-is_n} Z_2^N)) - \frac{1}{2\pi}\int_0^{2\pi} h(\Re(Z_1^N), \mu\Re(e^{-is} Z_2^N))\,\mathrm{d}s\right| \leq C\mu^N,$$

where C depends on N and T and hence

$$\|\dot{Z}_1 - \dot{Z}_1^N\| \leq \|\langle F_1\rangle(Z) - \langle F_1\rangle(Z^N)\| + C\mu^N.$$

Estimate (2.29) then follows from Gronwall Lemma. The counterpart for Z_2 can be obtained in a similar way. ■

Combining this result with Corollary 2.3 yields easily the following

Theorem 2.8 *Assume that U satisfies (2.27), and let $(y_1^0, y_2^0) \in \mathbb{C}^{m+d}$. For all $\varepsilon \in (0, \varepsilon_0)$, assume that the solution $y(t) = (y_1(t), y_2(t))$ of (2.3) with initial values (y_1^0, y_2^0) exists until a time $T > 0$. Assume moreover that the solution $Z^N(t) = (Z_1^N(t), Z_2^N(t))$ of (2.26) with $N \geq 2$ and with the same initial values, exists until time T. Eventually, suppose that these solutions are uniformly bounded, i.e. satisfy (2.28) for $\varepsilon \in (0, \varepsilon_0)$. Define the function $Y^N(t) = (Y_1^N(t), Y_2^N(t)) = (Z_1^N(t), e^{-it/\varepsilon} Z_2^N(t))$. Then for sufficiently small ε_0, there exists a constant C depending on T and ε_0 but independent on $N \geq 2$, such that for all time $t \in (0, T)$ and all $\varepsilon \in (0, \varepsilon_0)$,*

$$\|y_1(t) - Y_1^N(t)\| + \varepsilon^{-1/2}\|y_2(t) - Y_2^N(t)\| \leq C\varepsilon. \tag{2.32}$$

2.3.2 Hamiltonian and adiabatic invariants over long-time intervals

Strictly speaking, the adiabatic invariants of (2.11) are not any longer *exact* invariants of (2.26). However, we still are in the very favourable situation where the oscillatory energies remain almost constant over long intervals of time and it turns out that this result is of prior importance for our approach.

Theorem 2.9 *Assume that U satisfies (2.27). For all $\varepsilon \in (0, \varepsilon_0)$, let $Z^N(t) = (Z_1^N(t), Z_2^N(t))$ be the exact solution of (2.26) with initial values (y_1^0, y_2^0) satisfying (2.5). Suppose that the solutions $Z^N(t)$ exist until a time $T > 0$, possibly infinite, and that there exists a constant B independent of ε and $N \geq 3$, such that*

$$\forall\, 0 \leq t \leq T, \quad \|Z^N(t)\| \leq B. \tag{2.33}$$

Then there exist positive constants c_0 and C depending only on E and B such that for all $\varepsilon \in (0, \varepsilon_0)$, $N \geq 3$

$$\forall\, t \leq \min\left(\frac{c_0^N}{\mu^N \varepsilon^{N/2-2}}, T\right), \qquad \left|\|Z_2^N(t)\|^2 - \|Z_2^N(0)\|^2\right| \leq C\varepsilon^2. \tag{2.34}$$

Proof. Let $X(t) = \Re(Z_1^N(t))$ and for $0 \le n \le N-1$, let $s_n = \frac{2n\pi}{N}$. Using (2.17), we obtain for all time

$$\begin{aligned}
\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|Z_2^N\|^2 &= \Re(Z_2^{N*}\dot{Z}_2^N) \\
&= \mu\Re\Big(i\frac{1}{N}\sum_{n=0}^{N-1} e^{is_n}(Z_2^N)^* g_2(X, \mu\Re(e^{-is_n}Z_2^N))\Big), \\
&= \frac{1}{N}\sum_{n=0}^{N-1}\sum_{j=1}^{m} \Im(\mu e^{-is_n}Z_{2,j}^N)\frac{\partial U}{\partial x_{2,j}}(X, \mu\Re(e^{-is_n}Z_2^N)) \\
&= \frac{1}{N}\sum_{n=0}^{N-1} \frac{\mathrm{d}}{\mathrm{d}s}U(X, \mu\Re(e^{-is}Z_2^N))\Big|_{s=s_n}.
\end{aligned}$$

For fixed $x_1 \in \mathbb{R}^m$, $z_2 \in \mathbb{C}^d$, the function $s \mapsto f(s, x_1, z_2) = U(x_1, \Re(e^{-is}z_2))$ is 2π-periodic and can be expanded as a Fourier series

$$f(s, x_1, z_2) = \sum_{k\in\mathbb{Z}} \hat{f}_k(x_1, z_2)e^{iks},$$

with smooth coefficients $\hat{f}_k(x_1, z_2)$. As U is real valued, $\hat{f}_{-k} = \overline{\hat{f}_k}$ for all $k \in \mathbb{Z}$, $\hat{f}_{-k} = \overline{\hat{f}_k}$. Hence, we get

$$\frac{1}{N}\sum_{n=0}^{N-1}\frac{\mathrm{d}}{\mathrm{d}s}U(X, \mu\Re(e^{-is_n}Z_2^N)) = \sum_{k\in\mathbb{Z}}(ik)\hat{f}_k(X, \mu Z_2^N)\frac{1}{N}\sum_{n=0}^{N-1} e^{iks_n},$$

and, using (2.30),

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|Z_2^N\|^2 = 2\sum_{j=1}^{\infty}(jN)\Im\Big(\hat{f}_{jN}(X, \mu Z_2^N)\Big). \tag{2.35}$$

Now, as in the proof of Lemma 2.7, estimates (2.33) and (2.27) imply

$$\left|\hat{f}_{jN}(X, \mu Z_2^N)\right| = \frac{\mu^{jN}}{(jN)!}\left|R_{jN}(X, \xi Z_2^N)\right| \le K\left(\frac{\mu\|Z_2^N\|}{R}\right)^{jN}.$$

Owing to bound (2.33), we can assume that ε_0 is such that for all $\mu \in (0, \sqrt{\varepsilon_0})$,

$$\left(\frac{\mu\|Z_2^N\|}{R}\right)^N < \frac{1}{2},$$

and hence we get from (2.35)

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}\|Z_2^N\|^2\right| \le CN\left(\frac{\mu\|Z_2^N\|}{R}\right)^N \tag{2.36}$$

for some constant C depending on K. Now, for given numbers a and $r > 1$, the exact solution of the ODE $\dot{x} = ax^r$ is given by

$$x(t) = x_0(1 - x_0^{r-1}(r-1)at)^{-\frac{1}{r-1}},$$

so that for $t \le \frac{1}{2}(x_0^{r-1}(r-1)a)^{-1}$, we have $x(t) \le 2x_0$. Applying this estimate with $a = CN\mu^N R^{-N}$, $r = N/2 > 1$ and $x_0 = 2E\varepsilon$, we can show from (2.5) and (2.36) that there exists a constant c independent of ε and N such that

$$\forall\, t \le \min\big(\frac{c_0^N}{\mu^N \varepsilon^{N/2-2}}, T\big), \qquad \|Z_2^N(t)\|^2 \le 4E\varepsilon.$$

Plugging this estimate into (2.36), we obtain similarly the existence of constants c and C such that

$$\forall\, t \le \min\big(\frac{c_0^N}{\mu^N \varepsilon^{N/2-2}}, T\big), \qquad \big|\|Z_2^N(t)\|^2 - \|Z_2^N(0)\|^2\big| \le C\varepsilon^2.$$

This completes the proof. ■

Theorem 2.10 *Assume that* U *satisfies* (2.27)*. For* $N \ge 3$ *and* $\varepsilon \in (0, \varepsilon_0)$ *, let* $Z^N(t) = (Z_1^N(t), Z_2^N(t))$ *be the exact solution of* (2.26) *with initial values* (y_1^0, y_2^0) *satisfying* (2.5)*. Assume that* $Z^N(t)$ *exists until a time* $T > 0$ *, possibly infinite, and satisfies* (2.33) *for a constant* B *independent of* ε *and* N *. Define the functions* $Y^N(t) = (Z_1^N(t), e^{-it/\varepsilon} Z_2^N(t))$ *. Then there exist positive constants* c_0 *and* C *such that for all* $\varepsilon \in (0, \varepsilon_0)$ *and all* $N \ge 3$ *,*

$$\forall\, t \le \min\big(\frac{c_0^N}{\mu^N \varepsilon^{N/2-2}}, T\big), \qquad \big|\|Y_2^N(t)\|^2 - \|Y_2^N(0)\|^2\big| \le C\varepsilon^2, \tag{2.37}$$

and

$$\forall\, t \le \min\big(\frac{c_0^N}{\mu^N \varepsilon^{N/2-2}}, T\big), \qquad |H_{\mathbb{C}}(Y_1^N(t), Y_2^N(t)) - H_{\mathbb{C}}(y_1^0, y_2^0)| \le C\varepsilon, \tag{2.38}$$

where $H_{\mathbb{C}}$ *is the Hamiltonian* (2.4)*.*

Proof. The first inequality follows from previous theorem. Using (2.24) and the preservation of Hamiltonian (2.25), we obtain that

$$H_{\mathbb{C}}(Y_1^N(t), Y_2^N(t)) - H_{\mathbb{C}}(y_1^0, y_2^0) = 2(\Delta U)(t) - 2(\Delta U)(0) + \frac{\|Z_2^N(t)\|^2 - \|Z_2^N(0)\|^2}{\varepsilon},$$

where

$$\begin{aligned}\Delta U &= U\Big(\Re(Z_1^N), \mu\Re(e^{-it/\varepsilon} Z_2^N)\Big) - \frac{1}{N}\sum_{n=0}^{N-1} U\Big(\Re(w_1^N), \mu\Re(e^{-i\frac{2n\pi}{N}} Z_2^N)\Big),\\ &= \frac{1}{N}\sum_{n=0}^{N-1}\Big(U\Big(\Re(Z_1^N), \mu\Re(e^{-it/\varepsilon} Z_2^N)\Big) - U\Big(\Re(Z_1^N), \mu\Re(e^{-i\frac{2n\pi}{N}} Z_2^N)\Big)\Big).\end{aligned}$$

According to previous theorem, as long as $t \le \min\big(\frac{c_0^N}{\mu^N \varepsilon^{N/2-2}}, T\big)$, the solution $Z^N(t)$ remains bounded and satisfies the estimates (2.33) and (2.34). Hence, as in the proof of Lemma 2.5, we can show that

$$\forall\, t \le \min\big(\frac{c_0^N}{\mu^N \varepsilon^{N/2-2}}, T\big), \qquad |(\Delta U)(t) - (\Delta U)(0)| \le C\varepsilon$$

for a constant C independent of N and ε . We now get the result using (2.34). ■

2.4 Fully-discrete solution

We consider now the time discretization of (2.26) by a symplectic method. We denote by $F^N(Z) = (F_1^N(Z), F_2^N(Z))$ the right-hand side of (2.26) and, for a given step size $h > 0$, by $\Phi_h^N(\cdot)$ a symplectic integrator of order r applied to this system. Finally, we define the numerical approximation as the sequence

$$Z^{N,0} = y^0 = (y_1^0, y_2^0) \in \mathbb{C}^{m+d}, \tag{2.39}$$
$$Z^{N,n} = \Phi_h^N(Z^{N,n-1}), \quad n \geq 1. \tag{2.40}$$

Theorem 2.11 *Assume that U satisfies (2.27), and let $h_0 > 0$. For all $\varepsilon \in (0, \varepsilon_0)$ and $h \in (0, h_0)$, let $Z^{N,n} = (Z_1^{N,n}, Z_2^{N,n})$ be the numerical solution given by a symplectic integrator Φ_h^N applied to the system (2.26) with stepsize h and initial values (y_1^0, y_2^0) satisfying (2.5).*

Assume that $Z^{N,n}$ is well-defined for all $n \geq 0$ and is bounded by a constant B independent of ε, h, $N \geq 3$ and $n \geq 0$:

$$\forall\, n \geq 0, \quad \|Z^{N,n}\| \leq B. \tag{2.41}$$

Then for h_0 sufficiently small, there exist positive constants c_0 and C depending only on E and B such that for all $\varepsilon \in (0, \varepsilon_0)$, $N \geq 3$ and $h \in (0, h_0)$,

$$\forall\, nh \leq \frac{c_0^N}{\mu^N \varepsilon^{N/2-2}}, \qquad \left| \|Z_2^{N,n}\|^2 - \|Z_2^{N,0}\|^2 \right| \leq C\varepsilon^2. \tag{2.42}$$

Proof. For the sake of symplicity, we consider here the case of the midpoint rule. For a general symplectic method, we can adapt the proof along the lines of [HLW06, Thm. IV.2.2]. Sequence (2.40) thus becomes

$$Z^{N,n+1} = Z^{N,n} + hF^N\left(Z^{N,n+1/2}\right),$$

where for all n, $Z^{N,n+1/2} := (Z^{N,n+1} + Z^{N,n})/2$. Premultiplying the second component of by $(Z_2^{N,n+1/2})^*$ leads to

$$\|Z_2^{N,n+1}\|^2 = \|Z_2^{N,n}\|^2 + 2h(Z_2^{N,n+1/2})^* F_2^N(Z^{N,n+1/2}).$$

As in the proof of Theorem 2.9, from bound (2.41) we can derive the estimate

$$\forall n \geq 0, \left| \|Z_2^{N,n+1}\|^2 - \|Z_2^{N,n}\|^2 \right| \leq ChN \left(\frac{\mu \|Z_2^{N,n+1/2}\|}{R} \right)^N \tag{2.43}$$

valid for some constants R and C depending on U and B (compare with (2.36)). Using (2.33) again and the hypothesis on U, we easily see that there exists a constant c such that

$$\forall N \geq 3, \forall n \geq 0, \|Z_2^{N,n+1/2}\| \leq (1 + hc)\|Z_2^{N,n}\|.$$

As a consequence, for $h \leq h_0$ sufficiently small, there exists a constant $\alpha > 0$ such that

$$\forall n \geq 0, \|Z_2^{N,n+1}\|^2 \leq \|Z_2^{N,n}\|^2 \left(1 + h\mu^N \alpha^N \|Z_2^{N,n}\|^{N-2}\right),$$

and finally

$$\forall n \geq 0, \|Z_2^{N,n+1}\|^2 \leq \|Z_2^{N,0}\|^2 \exp\left(h\mu^N \alpha^N \sum_{p=0}^{n} \|Z_2^{N,n}\|^{N-2} \right).$$

Now, recall that $\|Z_2^{N,0}\|^2 \le 2E\varepsilon$ and assume that for $p = 0, \dots, n$, we have $\|Z_2^{N,p}\|^2 \le 4E\varepsilon$. Using last inequality, we thus have

$$\|Z_2^{N,n+1}\|^2 \le 2E\varepsilon \exp\Big(nh\mu^N\alpha^N(4E)^{N-2}\varepsilon^{N/2-1}\Big),$$

so that for

$$nh\,\mu^N\alpha^N(4E)^{N-2}\varepsilon^{N/2-1} \le \log 2 \tag{2.44}$$

we have $\|Z_2^{N,n+1}\|^2 \le 4E\varepsilon$. This proves by induction that for all n satisfying (2.44), $\|Z_2^{N,n+1}\| = \mathcal{O}(\mu)$. Eventually, plugging this bound into (2.43) shows that there exists a constant $\alpha > 0$ depending only on B, E, U and h_0 such that for all n satisfying (2.44),

$$\big|\|Z_2^{N,n+1}\|^2 - \|Z_2^{N,0}\|^2\big| \le nh\,\mu^N\alpha^N\varepsilon^{N/2}.$$

■

Lemma 2.12 *Under the hypotheses of the previous theorem, there exist positive constants h_0, c and C, depending only on E, B and U such that for all $\varepsilon \in (0, \varepsilon_0)$, $N \ge 3$ and $h \in (0, h_0)$,*

$$\forall\, nh \le \exp(c/h), \qquad \big|K_{\mathbb{C}}^N(Z^{N,n}) - K_{\mathbb{C}}^N(Z^{N,0})\big| \le Ch^r$$

where r is the order of the symplectic integrator, and where $K_{\mathbb{C}}^N(Z)$ is the discretized Hamiltonian (2.25).

Proof. Assumption (2.27) and definition (2.25) imply that $K_{\mathbb{C}}^N(Z)$ satisfies analytic estimates of the form (2.27) for some constants independent on N and ε. The statement thus follows from classical results in backward error analysis (see for instance [HLW06, Chap. IX] and references therein). ■

Going back to the original variables, we can define the approximations $Y^{N,n}$ by the formula

$$\forall\, n \ge 0, \quad Y_1^{N,n} = Z_1^{N,n} \quad \text{and} \quad Y_2^{N,n} = e^{-inh/\varepsilon} Z_2^{N,n}. \tag{2.45}$$

Combining previous results with Theorem 2.10, we then immediately get the following

Theorem 2.13 *Assume that the hypotheses of Theorem 2.11 hold true for $\mu = \sqrt{\varepsilon}$ and define $Y^{N,n}$, $n \ge 0$ by relation (2.45). Then, for h_0 sufficiently small, there exist positive constants c, c_0, C depending only on E and B such that for all $\varepsilon \in (0, \varepsilon_0)$, $N \ge 3$ and $h \in (0, h_0)$,*

$$\forall\, nh \le \frac{c_0^N}{\varepsilon^{N-2}}, \qquad \big|\|Y_2^{N,n}\|^2 - \|Y_2^{N,0}\|^2\big| \le C\varepsilon^2, \tag{2.46}$$

and

$$\forall\, nh \le \inf\big(\frac{c_0^N}{\varepsilon^{N-2}}, \exp(\frac{c}{h})\big), \qquad \big|H_{\mathbb{C}}(Y_2^{N,n}) - H_{\mathbb{C}}(Y_2^{N,0})\big| \le C(\varepsilon + h^r) \tag{2.47}$$

where r is the order of the symplectic integrator, and $H_{\mathbb{C}}$ the hamiltonian (2.4).

Remark 2.14 *With the previous notations, it is clear that Theorem 2.8 extends straightforwardly to the fully discretized solution $Y^{N,n}$, the error in the equation (2.32) being of order $\mathcal{O}(\varepsilon + h^r)$ over bounded time intervals.*

3 Extension to the multi-frequency case

In this section, we consider the extension of previous results to the case where different frequencies are present in the system. The equations are similar to (2.1), the only difference being that $\frac{1}{\varepsilon}$ is now replaced by a matrix $\frac{1}{\varepsilon}A$:

$$\begin{cases} \ddot{x}_1 & = & g_1(x_1,x_2) & = & -\nabla_1 U(x_1,x_2), \\ \ddot{x}_2 + \dfrac{1}{\varepsilon^2}A^2 x_2 & = & g_2(x_1,x_2) & = & -\nabla_2 U(x_1,x_2), \end{cases} \tag{3.1}$$

where $x_1 \in \mathbb{R}^m$ and $x_2 \in \mathbb{R}^d$, and where A is a $d \times d$ symmetric positive definite matrix with positive eigenvalues $\omega_1, \ldots, \omega_d$. Similarly to (2.2), we assume that the initial values depend on ε in such a way that

$$\forall\, \varepsilon \in (0,\varepsilon_0), \quad \frac{\|Ax_2^0\|^2}{\varepsilon^2} + \|\dot{x}_1^0\|^2 + \|\dot{x}_2^0\|^2 \le E.$$

Introducing variables $y_1 = x_1 + i\dot{x}_1$ and $y_2 = \dfrac{1}{\sqrt{\varepsilon}}A^{1/2}x_2 + i\sqrt{\varepsilon}A^{-1/2}\dot{x}_2$, system (3.1) can be rewritten as (compare (2.3))

$$\begin{cases} \dot{y}_1 & = & \Im(y_1) + i g_1(\Re(y_1), \mu A^{-1/2}\Re(y_2)), \\ \dot{y}_2 & = & -i\dfrac{A}{\varepsilon}y_2 + i\mu A^{-1/2} g_2(\Re(y_1), \mu A^{-1/2}\Re(y_2)), \end{cases} \tag{3.2}$$

with Hamiltonian

$$H_{\mathbb{C}}(y_1,y_2) = \|\Im(y_1)\|^2 + \frac{\|A^{1/2}y_2\|^2}{\varepsilon} + 2U(\Re(y_1), \mu A^{-1/2}\Re(y_2)). \tag{3.3}$$

The condition on the initial values now takes the form

$$\|\Im(y_1^0)\|^2 + \frac{\|A^{1/2}y_2^0\|^2}{\varepsilon} \le 2E. \tag{3.4}$$

The equations can be simplified further by introducing $z_1 = y_1$ and $z_2 = e^{i\frac{t}{\varepsilon}A}y_2$

$$\begin{cases} \dot{z}_1 & = & \Im(z_1) + i g_1(\Re(z_1), \mu A^{-1/2}\Re(e^{-i\frac{t}{\varepsilon}A}z_2)), \\ \dot{z}_2 & = & i\mu e^{i\frac{t}{\varepsilon}A}A^{-1/2} g_2(\Re(z_1), \mu A^{-1/2}\Re(e^{-i\frac{t}{\varepsilon}A}z_2)), \end{cases} \tag{3.5}$$

and are then associated to the non-autonomous (complex) Hamiltonian

$$K_{\mathbb{C}}(t/\varepsilon; z_1, z_2) = \|\Im(z_1)\|^2 + 2U(\Re(z_1), \sqrt{\varepsilon}A^{-1/2}\Re(e^{-it/\varepsilon}z_2))). \tag{3.6}$$

As in the case $A = \mathrm{Id}$, we can write (3.5) in the form (2.8) with a vector field $F(\tau, z)$ defined by (3.5) and consider the corresponding averaged system (2.11), where the averaging operator $\langle F\rangle$ is now defined by

$$\langle F\rangle(Z) = \lim_{T\to\infty}\frac{1}{T}\int_0^T F(\tau, Z)\,\mathrm{d}\tau. \tag{3.7}$$

The averaged system we consider can hence be written as

$$\begin{cases} \dot{Z}_1 & = & \Im(Z_1) + i \lim_{T\to\infty} \frac{1}{T}\int_0^T g_1(\Re(Z_1), \mu A^{-1/2}\Re(e^{-isA}Z_2))\mathrm{d}s, \\ \dot{Z}_2 & = & i\mu \lim_{T\to\infty} \frac{1}{T}\int_0^T e^{isA}A^{-1/2}g_2(\Re(Z_1), \mu A^{-1/2}\Re(e^{-isA}Z_2)\mathrm{d}s. \end{cases} \tag{3.8}$$

This is once again a Hamiltonian system associated with the Hamiltonian

$$\langle K_{\mathbb{C}}\rangle(Z_1,Z_2) = \|\Im(Z_1)\|^2 + 2\lim_{T\to\infty}\frac{1}{T}\int_0^T U(\Re(Z_1), \mu\Re(e^{-isA}A^{-1/2}Z_2))\,\mathrm{d}s. \tag{3.9}$$

Note that after a possible change of unknowns and of function U, we can assume that the matrix A is *diagonal*. In the sequel, the eigenvalues of A are assumed to satisfy a non-resonnance condition according to the following

Definition 3.1 *For a given set of frequencies $\omega = (\omega_1,\ldots,\omega_d) \in \mathbb{R}^d$, the resonance module $\mathcal{M}$ is defined as*

$$\mathcal{M} = \{\alpha \in \mathbb{Z}^d \,|\, \alpha_1\omega_1 + \ldots + \alpha_d\omega_d = 0\}.$$

The vector of frequencies ω is said to non-resonant outside $\mathcal{M}$ if

$$\exists\,\gamma,\nu > 0, \quad \forall\,\alpha \in \mathbb{Z}^d\backslash\mathcal{M}, \quad |\alpha\cdot\omega| > \gamma|\alpha|^{-\nu}. \tag{3.10}$$

The orthogonal of the resonant module is defined by

$$\mathcal{M}^\perp = \{\beta \in \mathbb{Z}^d \,|\, \forall\,\alpha \in \mathcal{M},\; \alpha_1\beta_1 + \cdots + \alpha_d\beta_d = 0\}.$$

If the eigenvalues of A satisfy such an assumption, then the limit (3.7) can be identified in terms of Fourier coefficients of the integrand with indices in $\mathcal{M}$:

Lemma 3.2 *Consider a function G of $\theta = (\theta_1,\ldots,\theta_d) \in \mathbb{T}^d$ and assume that it is analytic in a domain $\mathbb{T}^d + i[-\rho,\rho]^d$ where $\rho > 0$. Besides, assume that $\omega \in \mathbb{R}^d$ is non-resonant outside $\mathcal{M}$. Finally, for $\alpha \in \mathbb{Z}^d$, define $\widehat{G}(\alpha)$ as the α-Fourier coefficient of G. Then for all $\theta_0 \in \mathbb{T}^d$, we have*

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T G(\theta_0 + t\omega)\,\mathrm{d}t = \sum_{\alpha\in\mathcal{M}} \widehat{G}(\alpha)e^{i\alpha\cdot\theta_0}. \tag{3.11}$$

Proof. It is clear that for all time $t \geq 0$,

$$G(\theta_0 + t\omega) = \sum_{k\in\mathcal{M}} \widehat{G}(\alpha)e^{i\alpha\cdot\theta_0} + \sum_{k\in\mathbb{Z}^d\backslash\mathcal{M}} \widehat{G}(\alpha)e^{i\alpha\cdot(\theta_0+t\omega)}.$$

Integrating from $t = 0$ to $t = T$, and using (3.10), we immediatly get

$$\left|\frac{1}{T}\int_0^T G(\theta_0 + t\omega)\,\mathrm{d}t - \sum_{k\in\mathcal{M}} \widehat{G}(\alpha)e^{i\alpha\cdot\theta_0}\right| \leq \frac{2}{T\gamma}\sum_{\alpha\in\mathbb{Z}^d\backslash\mathcal{M}} |\alpha|^\nu|\widehat{G}(\alpha)|.$$

The analyticity of G guarantees that the $\widehat{G}(\alpha)$'s are exponentially decreasing with respect to $|\alpha|$, ensuring the convergence of the series in the right-hand side. This shows the result with a rate of convergence of $1/T$.
■

From a numerical point of view, the identification of the resonance module $\mathcal{M}$ is far from obvious in general. For this reason, we rely on (3.8) rather than a discretization in space.

In the following, we will not address the question of convergence of the exact solution over bounded time intervals for it is very similar to the single frequency case. We will rather focus on adiabatic invariance and discretization of the averaged system, since these aspects exhibit significant differences.

3.1 Hamiltonian and adiabatic invariants

A straightforward calculation shows that $\|A^{1/2}Z(t)_2\|^2$ remains invariant along the exact solution of (3.8): Noticing that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}s}\Re(e^{-isA}Z_2) &= \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}s}(e^{-isA}Z_2+e^{isA}\bar{Z}_2)\\ &= -i\frac{1}{2}A(e^{-isA}Z_2-e^{isA}\bar{Z}_2)\\ &= A\Im(e^{-isA}Z_2),\end{aligned}$$

we indeed obtain (with the notation $X=\Re(Z_1)$)

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\|A^{1/2}Z_2\|^2 &= 2\Re(Z_2^*A\dot{Z}_2),\\ &= 2\mu\lim_{T\to\infty}\frac{1}{T}\int_0^T\Re\Big(iZ_2^*A^{1/2}e^{isA}g_2(X,\mu\Re(e^{-isA}A^{-1/2}Z_2))\,\mathrm{d}s\Big),\\ &= 2\lim_{T\to\infty}\frac{1}{T}\int_0^T\Im(\mu e^{-isA}A^{1/2}Z_2)\nabla_2U(X,\mu\Re(e^{-isA}A^{-1/2}Z_2))\,\mathrm{d}s,\\ &= 2\lim_{T\to\infty}\frac{1}{T}\Big[U(X,\mu\Re(e^{-isA}A^{-1/2}Z_2))\Big]_{s=0}^{s=T}=0.\end{aligned}$$

However, there are additional structural properties in this situation: according to [BGG89], there exist further adiabatic invariants for (3.1) provided condition (3.10) holds. It turns out that, for (3.8), there exist corresponding invariants which are linear combination of the oscillatory energies $|Z_{2,j}|^2$.

Theorem 3.3 *Assume that U is analytic (compare 2.27) and that ω is non-resonant outside $\mathcal{M}$. Then, for any $\beta=(\beta_1,\ldots,\beta_d)$ in $\mathcal{M}^\perp$, the quantity*

$$I_\beta(Z_2)=\sum_{j=1}^d\beta_j|Z_{2,j}|^2$$

is invariant along the solution $Z(t)=(Z_1(t),Z_2(t))$ of (3.8).

Proof. System (3.8) is Hamiltonian with potential $\langle K_{\mathbb{C}}\rangle(Z)$ given by (3.9). The main ingredient of the proof is again a Fourier expansion of the integrand function

$$s\mapsto U(\Re(Z_1),\mu\Re(e^{-isA}A^{1/2}Z_2)),$$

for given (Z_1, Z_2). As before , we set $X = \Re(Z_1)$ and introduce the variables $(r, \phi) \in \mathbb{R}_+^d \times \mathbb{T}^d$ defined by

$$\forall\, j = 1, \dots, d, \quad \begin{cases} r_j &= \mu\, \omega_j^{-1/2} |Z_{2,j}|, \\ \phi_j &= \operatorname{Arg}(Z_{2,j}), \end{cases} \tag{3.12}$$

and the function $\Delta : \mathbb{R}_+^d \times \mathbb{T}^d \to \mathbb{R}^d$ defined by

$$\Delta(r, \theta) = \big(r_1 \cos\theta_1, \dots, r_d \cos\theta_d\big).$$

We can then write

$$U(X, \mu \Re(e^{-isA} A^{-1/2} Z_2)) = (U_X \circ \Delta)(r, \phi - s\omega) \tag{3.13}$$

where $U_X(Z_2) = U(X, Z_2)$. Using (2.27), it is easy to see that the function $\theta \mapsto (U_X \circ \Delta)(r, \theta)$ is analytic in a domain containing $\mathbb{T}^d \times [-\rho, \rho]^d$ for some $\rho > 0$. Lemma 3.2 hence allows to identify the time average of function (3.13), so that Hamiltonian (3.9) reads

$$\langle K_{\mathbb{C}} \rangle (Z_1, Z_2) = \|\Im(Z_1)\|^2 + 2 \sum_{\alpha \in \mathcal{M}} \widehat{U_X \circ \Delta}(r, \alpha) e^{i\alpha\cdot\phi}$$

where $\widehat{U_X \circ \Delta}(r, \alpha)$ denotes the α-Fourier coefficient of $(U_X \circ \Delta)(r, \theta)$. The differential equations for Z_2 are now of the form, for $j = 1, \dots, d$,

$$\begin{aligned} \dot{Z}_{2,j} &= -i \frac{\partial \langle K_{\mathbb{C}} \rangle}{\partial \bar{Z}_{2,j}} (Z_1, Z_2) \\ &= -2i \sum_{\alpha \in \mathcal{M}} \Big(\frac{\partial (\widehat{U_X \circ \Delta})}{\partial r_j} \frac{\partial r_j}{\partial \bar{Z}_{2,j}} + i\, \alpha_j\, (\widehat{U_X \circ \Delta}) \frac{\partial \phi_j}{\partial \bar{Z}_{2,j}} \Big) e^{i\alpha\cdot\phi} \\ &= -i \sum_{\alpha \in \mathcal{M}} \Big(\frac{\partial (\widehat{U_X \circ \Delta})}{\partial r_j} \frac{\mu \omega_j^{-1/2} Z_{2,j}}{|Z_{2,j}|} - \alpha_j\, (\widehat{U_X \circ \Delta}) \frac{Z_{2,j}}{|Z_{2,j}|^2} \Big) e^{i\alpha\cdot\phi}, \end{aligned}$$

where we have omitted the arguments (r, α) in the Fourier coefficients. As U is real-valued, we have for all $\alpha \in \mathbb{Z}^d$ and $r \in \mathbb{R}_+^d$,

$$\widehat{U_X \circ \Delta}(r, -\alpha) = \overline{\widehat{U_X \circ \Delta}}(r, \alpha).$$

Hence,

$$\Re(\dot{Z}_{2,j} \bar{Z}_{2,j}) = -2 \sum_{\alpha \in \mathcal{M}_+} \alpha_j\, \Im\Big(\widehat{U_X \circ \Delta})(r, \alpha) e^{i\alpha\cdot\phi} \Big)$$

where $(\mathcal{M}_+, \mathcal{M}_-)$ is a symmetric partition of $\mathcal{M}$ such that $\alpha \in \mathcal{M}_+$ if and only if $(-\alpha) \in \mathcal{M}_-$. Finally, we obtain

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} I_\beta(Z_2) &= \frac{1}{2} \sum_{j=1}^d \beta_j \Re(\dot{Z}_{2,j} \bar{Z}_{2,j}) \\ &= -\sum_{\alpha \in \mathcal{M}_+} \Big(\sum_{j=1}^d \beta_j \alpha_j \Big) \Im\Big(\widehat{U_X \circ \Delta}) e^{i\alpha\cdot\phi} \Big) = 0, \end{aligned}$$

as $\beta \in \mathcal{M}^\perp$. This shows the result. ∎

Using the same procedure as in previous sections, we can show the following result (compare Theorem 2.10):

Theorem 3.4 *Assume that* ω *is non-resonant outside* $\mathcal{M}$. *For* $\varepsilon \in (0, \varepsilon_0)$, *let* $(y_1^0, y_2^0) \in \mathbb{C}^{m+d}$ *satisfy conditions* (3.4) *with* $E > 0$ *independent of* ε. *Let* $Z(t) = (Z_1(t), Z_2(t))$ *be the exact solution of* (3.8) *with initial values* (y_1^0, y_2^0). *Assume that* $Z(t)$ *exists for all time, and is uniformly bounded with respect to* $\varepsilon \in (0, \varepsilon_0)$. *Define the function* $Y(t) = (Y_1(t), Y_2(t)) = (Z_1(t), e^{-it/\varepsilon} Z_2(t))$. *Then there exists a constant* $C > 0$ *such that for all time* t *and all* $\varepsilon \in (0, \varepsilon_0)$,

$$\|A^{1/2} Y_2(t))\|^2 = \|A^{1/2} Y_2(0))\|^2 \le 2\varepsilon E$$

and

$$|H_{\mathbb{C}}(Y_1(t), Y_2(t)) - H_{\mathbb{C}}(y_1^0, y_2^0)| \le C\varepsilon,$$

where $H_{\mathbb{C}}$ *denotes the Hamiltonian* (3.3). *Moreover , we have for all time* $t \ge 0$,

$$I_\beta(Y_2(t)) = I_\beta(Y_2(0)).$$

3.2 Semi-discrete solution

The specificity of the integrand in the definition of the Hamiltonian $K_{\mathbb{C}}(Z_1, Z_2)$ allows to refine Lemma 3.2. Similarly to the proof of Lemma 2.7, we set for $\theta \in \mathbb{T}^s$, $x_1 \in \mathbb{R}^m$ and $z_2 \in \mathbb{C}^d$,

$$h(\theta, x_1, z_2) = U(x_1, \mu \Re(e^{-i\theta} A^{-1/2} z_2))$$

where $e^{-i\theta} A^{-1/2} z_2$ is the vector with components, $e^{-i\theta_j} \omega_j^{-1/2} z_{2,j}$, for $j = 1, \ldots, d$. For $\alpha \in \mathbb{Z}^d$, the Fourier coefficient

$$\hat{h}(\alpha, x_1, z_2) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} e^{-i\alpha\cdot\theta} h(\theta, x_1, z_2)\, \mathrm{d}\theta$$

can be expanded with respect to $\mu \in (0, \sqrt{\varepsilon_0})$ as in (2.31). By using the same argument as in the proof of Lemma 2.7, under the assumption (2.27), we have for bounded x_1 and z_2, and for all $\alpha \in \mathbb{Z}^d$,

$$\left|\hat{h}(\alpha, x_1, z_2)\right| \le c(C\mu\|z_2\|)^{|\alpha|} \tag{3.14}$$

where $|\alpha| = |\alpha_1| + \cdots + |\alpha_d|$ and for some constants c and C depending on bounds on x_1 and z_2 and on U.

In the following, we define the function $\xi : [0,1] \to \mathbb{R}$ by $\xi(u) = e^{-\frac{1}{u(1-u)}}$ and $\varphi : [0,1] \to \mathbb{R}$, the filter function, by $\varphi = \xi / \|\xi\|_{L_1(0,1)}$.

Lemma 3.5 *Assume that* ω *is non resonant outside* $\mathcal{M}$, *and that* U *satisfies* (2.27). *Assume that* B *is a given constant. Then there exist positive constant* $\varepsilon_0 > 0$, κ, ρ *and* C *such that for all* $T > 0$, $\mu \in (0, \sqrt{\varepsilon_0})$ *and* $Z = (Z_1, Z_2)$ *such that* $\|Z\| \le B$,

$$\left| \frac{1}{T} \int_0^T \varphi\left(\frac{s}{T}\right) K_{\mathbb{C}}(s, Z_1, Z_2) - \langle K_{\mathbb{C}} \rangle (Z_1, Z_2) \right| \le C\mu \|Z_2\| \exp(-\kappa T^\rho), \tag{3.15}$$

where $K_{\mathbb{C}}(s, Z_1, Z_2)$ *is the time-dependent Hamiltonian* (3.6) *and* $\langle K_{\mathbb{C}} \rangle (Z_1, Z_2)$ *the averaged Hamiltonian* (3.9).

Proof. The proof of this result relies on a combination of techniques used in [CCC$^+$05] with estimate (3.14) on the Fourier coefficient of the integrand defining $\langle K_{\mathbb{C}}\rangle$. The fact that Z_2 is bounded ensures the convergence of the series, provided ε_0 is sufficiently small. ■

The next stage in the discretization of $\langle K_{\mathbb{C}}\rangle$ consists in approximating the integral (3.15). To this aim, we take $T = N\delta$, where δ is a small parameter. We assume that ω is non-resonant oustside $\mathcal{M}$ and we require that δ obeys the following non-resonnance condition

$$\exists\, \gamma_*, \nu^* > 0 \quad \forall\, \alpha \in \mathbb{Z}^d \backslash \mathcal{M}, \qquad \left| \frac{1 - e^{i\delta\alpha\cdot\omega}}{\delta} \right| \geq \gamma^* |\alpha|^{-\nu^*}. \tag{3.16}$$

Note that if ω is non-resonant outside $\mathcal{M}$, then for $\delta_0 > 0$, the set of $\delta < \delta_0$ satisfying this condition is open and dense in $(0, \delta_0)$. Its measure is of size δ_0^{a+1} for some $a > 0$ (see for instance [HLW06, Chap. X]).

Lemma 3.6 *Assume that ω is non-resonant outside $\mathcal{M}$, and let δ be such that (3.16) holds true. Assume that U satisfies (2.27) and let B be a given constant. Then there exist positive constants ε_0, κ_*, ρ_* and C_* such that for all $N \geq 3$, $\mu \in (0, \sqrt{\varepsilon_0})$ and $Z = (Z_1, Z_2)$ such that $\|Z\| \leq B$*

$$\left| \frac{1}{S_N} \sum_{n=0}^{N-1} \varphi\Big(\frac{n}{N}\Big) K_{\mathbb{C}}(n\delta, Z_1, Z_2) - \frac{1}{N\delta} \int_0^{N\delta} K_{\mathbb{C}}(s, Z_1, Z_2) ds \right| \quad \leq \quad C_* \mu \|Z_2\| \exp(-\kappa_* N^{\rho_*}), \tag{3.17}$$

where $S_N = \sum_{n=0}^{N-1} \varphi(n/N)$ and where $K_{\mathbb{C}}(s, Z_1, Z_2)$ is the time dependent Hamiltonian (3.6) and $\langle K_{\mathbb{C}}\rangle(Z_1, Z_2)$ the averaged Hamiltonian (3.9).

Proof. The proof is very similar to the proof of Theorem 2 in [CCC$^+$05] and is therefore omitted. Note that in estimate (3.17), the constants depend on δ, but are uniformly bounded in $\delta \in (0, \delta_0)$. ■

In the following, we consider the solution $Z^N(t) = (Z_1^N(t), Z_2^N(t))$ of the system associated with the discretized Hamiltonian

$$Kc^N(Z_1, Z_2) := \frac{1}{S_N} \sum_{n=0}^{N-1} \varphi\Big(\frac{n}{N}\Big) K_{\mathbb{C}}(n\delta, Z_1, Z_2), \tag{3.18}$$

for some δ satifying condition (3.16). Proceeding as in Subsection 3.1, and using similar calculations as in previous Lemma, we can prove that for a bounded solution $Z^N(t)$, we have (using the fact that $\omega_j > 0$)

$$\left| \frac{\mathrm{d}}{\mathrm{d}t} \|A^{1/2} Z_2^N(t)\|^2 \right| \leq C\mu \|A^{1/2} Z_2^N(t)\| \exp(-\kappa N^\rho)$$

for some constants ρ, C and κ, provided that ω is non-resonant outside $\mathcal{M}$, and that ε_0 is sufficiently small. From this equation and provided that $Z^N(0) = (y_1^0, y_2^0)$ satisfies (3.4), we obtain

$$\forall\, t \geq 0, \quad \|A^{1/2} Z_2^N(t)\| \leq C(\varepsilon^{1/2} + t\mu \exp(-\kappa N^\rho))$$

for some constant $C > 0$. Eventually,

$$\forall\, t \leq \exp(\kappa N^\rho), \quad \left| \|A^{1/2} Z_2^N(t)\|^2 - \|A^{1/2} Z_2^N(0)\|^2 \right| \leq C\varepsilon.$$

Under the same assumptions, and using this result, we also have that for all $\beta \in \mathcal{M}^\perp$

$$\forall\, t \leq \exp(\kappa N^\rho), \quad \Big| I_\beta(Z_2^N(t)) - I_\beta(Z_2^N(0)) \Big| \leq C\varepsilon,$$

with a possibly modified constant C (which now depends on β).

Theorem 3.7 *Assume ω is non-resonant outside $\mathcal{M}$, and let δ be such that (3.16) holds true. Suppose U satisfies (2.27) and let $N \geq 1$. For all $\varepsilon \in (0, \varepsilon_0)$, let $Z^N(t) = (Z_1^N(t), Z_2^N(t))$ be the exact solution of the Hamiltonian system associated with (3.18) with initial values (y_1^0, y_2^0) satisfying (3.4). Eventually, assume that solutions $Z^N(t)$ exist for all time and satisfy $\|Z^N(t)\| \leq B$ for a constant B independent of ε and N. Define the functions $Y^N(t) = (Z_1^N(t), e^{-it/\varepsilon} Z_2^N(t))$. Then there exist positive constants κ, ρ and C depending on δ, U, E and B such that for all $\varepsilon \in (0, \varepsilon_0)$ and $N \geq 1$*

$$\forall\, t \leq \exp(\kappa N^\rho),\ \big| \|A^{1/2} Y_2^N(t)\|^2 - \|A^{1/2} Y_2^N(0)\|^2 \big| \leq C\varepsilon,$$

and

$$\forall\, t \leq \exp(\kappa N^\rho),\ |H_{\mathbb{C}}(Y_1^N(t), Y_2^N(t)) - H_{\mathbb{C}}(Y_1^N(0), Y_2^N(0))| \leq C\varepsilon,$$

where $H_{\mathbb{C}}$ is the hamiltonian (3.3). Moreover, for all $\beta \in \mathcal{M}^\perp$, there exist constant κ, ρ and C such that $\forall\, t \leq \exp(\kappa N^\rho)$

$$|I_\beta(Y_1^N(t), Y_2^N(t)) - I_\beta(y_1^0, y_2^0)| \leq C\varepsilon.$$

Proof. The proof combines all previous arguments. The conservation of the Hamiltonian is a consequence of the conservation of $K_{\mathbb{C}}^N$ and of equations (3.15) and (3.17). ∎

3.3 Fully discrete solution

Finally, we consider the approximation of the solution $Z^N(t)$ of (3.18) by a symplectic integrator Φ_h^N. For $n \geq 1$, we define the numerical solution $Z^{N,n}$ as the sequence

$$\begin{aligned} Z^{N,0} &= y^0 \in \mathbb{C}^{m+d}, \\ Z^{N,n} &= \Phi_h^N(Z^{N,n-1}),\ n \geq 1. \end{aligned}$$

Proceeding as in the proof of Theorem (2.11) and using similar arguments than before, we can show that under the assumptions of Theorem 3.7, we have for sufficiently small $h \leq h_0$ (compare (2.42))

$$\forall\, nh \leq \exp(\kappa N^\rho), \qquad \big| \|A^{1/2} Z_2^{N,n}\|^2 - \|A^{1/2} Z_2^{N,0}\|^2 \big| \leq C\varepsilon$$

for some constants κ, ρ and C independent of N and h. Combining this estimate with the result given by the Backward error analysis, we can show the following

Theorem 3.8 *Under the hypotheses of Theorem 3.7, we define the approximation $Y^{N,n}$, $n \geq 0$ by the relation (2.45). Then, for h_0 sufficiently small, there exist positive constants κ, ρ, c and C such that for all $\varepsilon \in (0, \varepsilon_0)$, $N \geq 3$, and $h \in (0, h_0)$,*

$$\forall\, nh \leq \exp(\kappa N^\rho), \quad \big| \|A^{1/2} Y_2^{N,n}\|^2 - \|A^{1/2} Y_2^{N,0}\|^2 \big| \leq C\varepsilon,$$

and

$$\forall\, nh \leq \inf\left(\exp(\kappa N^{\rho}), \exp(\frac{c}{h})\right), \quad \left|H_{\mathbb{C}}(Y_2^{N,n}) - H_{\mathbb{C}}(Y_2^{N,0})\right| \leq C(\varepsilon + h^r)$$

where r *is the order of the symplectic integrator, and* $H_{\mathbb{C}}$ *Hamiltonian (2.4). Moreover, if* $\beta \in \mathcal{M}^{\perp}$ *, there exist positive constants* κ *,* ρ *and* C *such*

$$\forall nh \leq \exp(\kappa N^{\rho}),\ \left|I_{\beta}(Y_2^{N,n}) - I_{\beta}(Y_2^{N,0})\right| \leq C\varepsilon.$$

4 Numerical experiments

4.1 Single-frequency case: the FPU problem

We take over the Fermi-Pasta-Ulam problem (2.13) and solve it with the numerical scheme of section 2.4 (i.e. we solve equations (2.26) for $N = 4$ with the implicit midpoint rule). For comparison purposes, the parameter m and the initial conditions considered are taken from [HLW06], pp. 22. On Figures 1 and 2, we have plotted (from left to right and from top to bottom) the oscillatory energies I_j , $j = 1, 2, 3$ and the Hamiltonian (shifted by a constant value -0.8) along the numerical solution obtained for $h = \frac{\pi}{\omega}, \frac{2\pi}{\omega}, \frac{3\pi}{\omega}, \frac{4\pi}{\omega}$ with $\omega = 50$. Note that we have considered here the problem in its original formulation with Hamiltonian

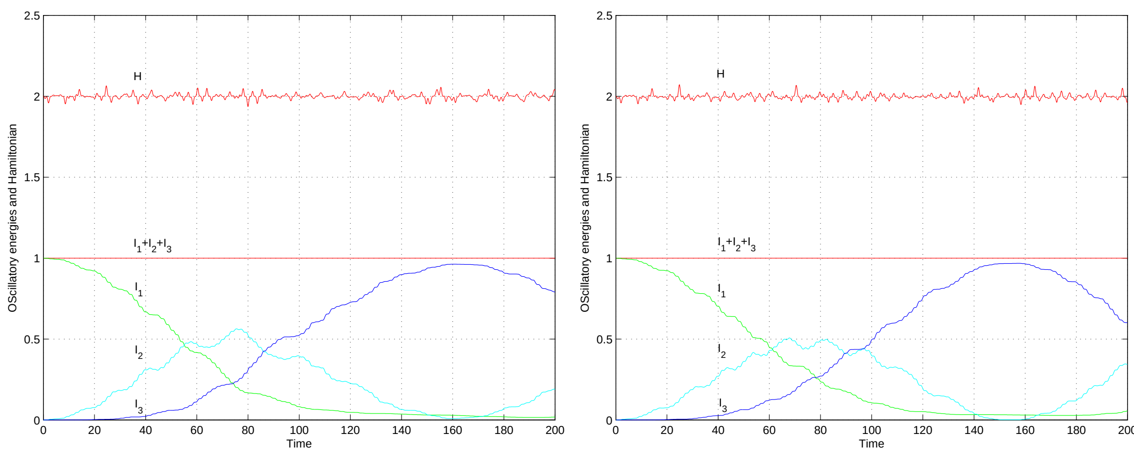

Figure 1: Numerical energies for the Fermi-Pasta-Ulam problem: $h = \frac{\pi}{50}$ (left) and $h = \frac{2\pi}{50}$ (right)

(2.13) and not the "averaged" equations with Hamiltonian (2.14). Several conclusions can be drawn from this experiment:

- The total oscillatory energy (in red with constant value 1) is almost perfectly conserved, in agreement with the theory which asserts that symplectic methods preserve quadratic invariants.
- The Hamiltonian of the problem is also very well preserved: it oscillates within a band of width ε , as predited by Theorem 2.10.
- The exchange of oscillatory energies between the stiff springs is adequatly reproduced, even for very large stepsizes. This is remarkably better than some other methods proposed in the litterature (see the method of Garcia-Archilla et al. [GASSS99] for instance (method (C) page 481 of [HLW06]).

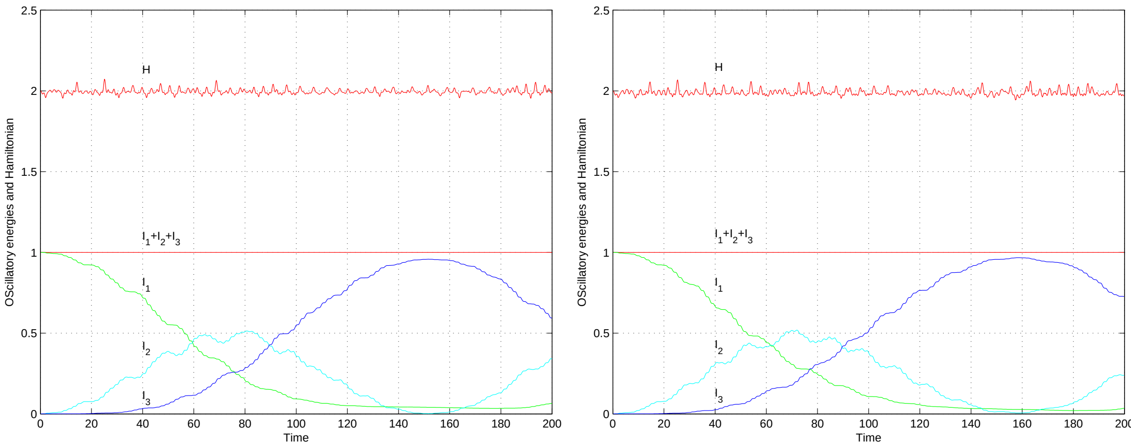

Figure 2: Numerical energies for the Fermi-Pasta-Ulam problem: $h = \frac{3\pi}{50}$ (left) and $h = \frac{4\pi}{50}$ (right)

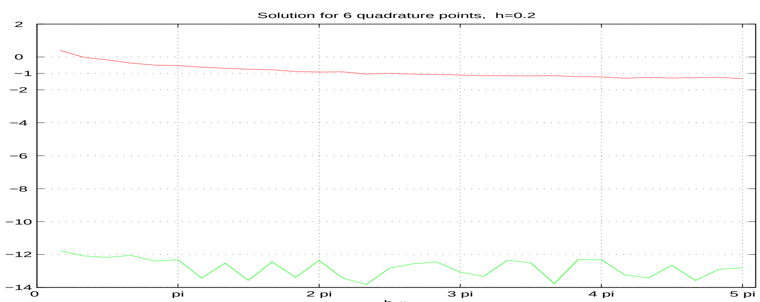

Figure 3: Deviation of the total oscillatory energy and error of the Hamiltonian for the FPU-problem

- There is no resonnance for the values of h considered. Figure 3 shows the errors on the Hamiltonian and the deviation of the total oscillatory energy versus $h\omega$ for a large spectrum of values (from 0 to 5π). Though these curves have been carefully computed with a significant number of points (h is kept constant equal to 0.2 and ω varies), no resonance occurs. This is also in contrast with most existing methods, where at least one of the too energies explodes for particular values of $h\pi$.

4.2 Multi-frequency case: a toy-problem from [HLW06]

We now consider a Hamiltonian of the form

$$H(x, \dot{x}) \quad = \quad \frac{1}{2}\left(\|\dot{x}_1\|^2 + \|\dot{x}_2\|^2 + \frac{1}{\varepsilon^2}\|Ax_2\|^2\right) + U(x_1, x_2), \tag{4.1}$$

where $A = \text{diag}(\lambda_1, \lambda_1, \lambda_2, \lambda_3) = \text{diag}(1, 1, \sqrt{2}, 2)$ and

$$U(x) \quad = \quad (c + x_{2,1} + x_{2,2} + x_{2,3} + \gamma x_{2,4})^4 + \frac{1}{8}x_1^2 x_{2,1}^2 + \frac{1}{2}x_1^2,$$

with $c = 0.05$ and $\gamma = 2.5$. Following [BGG89], one can show that the system has the following adiabatic invariants: the total oscillatory energy $I_T = I_1 + I_2 + I_3 + I_4$ and the energies $I_1 + I_2 + I_4$ and I_3 in accordance with the resonance module (see [HLW06]). On Fig. 4 we have reproduced the experiment of [HLW06] pp. 518-519 with $\varepsilon = 70^{-1}$ and $h = 10\varepsilon$, using the method described in previous section with $T = 80$ and $N = 120$. It can be observed that the qualitative behaviour of the exact solution is once again very well reproduced. For a larger stepsize $h = 1$, the oscillatory energies are still preserved, although the energy exchange is not as accuratly reproduced.

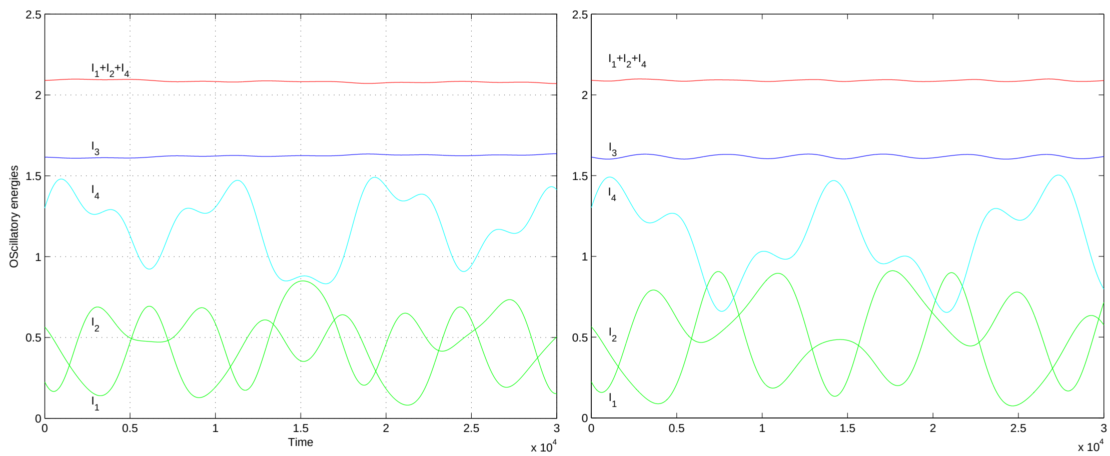

Figure 4: Oscillatory energies along the numerical solution of (4.1) for $T = 80$, $N = 120$ and $h = 10\epsilon$ (left) and $h = 1$ (right)

5 Conclusion

Both theoretical and experimental results demonstrate that solving the averaged equations with a suitable one-step method makes sense. The resulting numerical technique is both robust and qualitatively correct. However, one could argue that it is far from efficient: while a Gautschi-type method typically requires one evaluation of g per step, our method necessitates up to 100 more : this may seem unacceptable. Nevertheless, one should keep in mind that, on the one hand, these computations can be performed fully in *parallel* on a multi-processor machine, and on the other hand, that stepsizes up to 100 larger can be used.

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