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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 developed in [CCC⁺05]. Eventually, we demonstrate the efficiency of our approach on two test problems with one or several frequencies.

Keywords: highly-oscillatory, averaging, adiabatic invariance, filtering.

MSC numbers: 65L05, 65P10, 37M15

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 it 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, we are concerned more specifically with Hamiltonian systems whose solution is **highly-oscillatory**. A simple yet representative model of Hamiltonian system whose solutions have highly-oscillatory behaviour is given by the second-order differential system

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

where $x(t) = (x_1(t), x_2(t)) \in \mathbb{R}^m \times \mathbb{R}^d$ depends on time $t \geq 0$ and Ω is a positive semi-definite matrix with some *large* eigenvalues, while $g(x) = -\nabla U(x)$ derives from a potential function $U(x)$. The Hamiltonian associated with system (1.1) is

$$H(x, \dot{x}) = \frac{1}{2} \|\dot{x}\|^2 + \frac{1}{2} \|\Omega x\|^2 + U(x).$$

Note that the reason for the above splitting $x(t) = (x_1(t), x_2(t))$ becomes clear later in this text.

Dealing with *highly-oscillatory* systems leads to the following difficulties. Firstly, and even in the purely linear case ($g \equiv 0$), getting a bounded error propagation by means of a given explicit numerical method, requires the step size h be restricted according to

$$h\omega < C,$$

where C is a constant that depends on the numerical method, while ω is the largest eigenvalue of Ω . This constraint ceases to be numerically realistic whenever ω becomes large. On top of that, in applications to molecular dynamics for instance, *fast* forces are crudely modeled here by the harmonic term $-\Omega^2 x$ (short-range interactions), and they are much cheaper to evaluate than *slow* forces deriving from U (long-range interactions): in this case, it seems highly desirable to design numerical methods for which the number of evaluations of slow forces is not (too much) affected by the presence of fast forces, and the constraint $h\omega < C$ becomes even more prohibitive. Lastly, backward error analysis, which is the basic tool for obtaining large time error estimates in the present Hamiltonian situation, anyhow requires $h\omega \ll 1$. Again, as ω increases, this constraint cannot be fulfilled in practice, and one cannot draw any conclusion from the existence of a modified Hamiltonian system (see above), in terms of error bounds or so. In any circumstance, an alternative theory has to be proposed in the highly-oscillatory case.

Recently, Hairer and Lubich [HL00b] 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 particular case when Ω is block-diagonal with two blocks, the first block corresponding to the zero frequency and the other one being scaled by a large parameter, so that the original Hamiltonian system is assumed to split into

$$\frac{d^2}{dt^2} \begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix} + \frac{1}{\varepsilon^2} \begin{pmatrix} 0 & 0 \\ 0 & A \end{pmatrix} \begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix} = g(x_1(t), x_2(t)). \quad (1.2)$$

Here A is given and positive definite, $\varepsilon > 0$ is a small scaling parameter, and x_1 may be seen as the slow component while x_2 is the fast component in the original system. This setting will as well constitute our framework in the present paper. The work [HL00b] has been later extended by Cohen, Hairer and Lubich [CHL03, CHL05]. Their contribution explains the good behaviour of certain Gautschi type methods [Gau61, Deu79, GASSS99, HL99, HL00b], as far as preservation of the total energy H , and almost invariance of oscillatory energies (or *adiabatic invariants*) are concerned. Roughly speaking, the oscillatory energy in (1.2) is the energy

$$\|\dot{x}_2(t)\|^2 + \frac{1}{\varepsilon^2} \|A^{1/2} x_2(t)\|^2$$

of the harmonic oscillator attached with the fast component x_2 in system (1.2). It somehow is the fast oscillatory part of the total energy

$$H(x, \dot{x}) = \frac{1}{2} \|\dot{x}_1(t)\|^2 + \frac{1}{2} \|x_2(t)\|^2 + \frac{1}{2\varepsilon^2} \|A^{1/2}x_2(t)\|^2 + U(x_1(t), x_2(t)).$$

Even more, it turns out that rationally independent eigenvalues of $A^{1/2}$ actually give rise to independent oscillatory energies: they are obtained by decomposing x_2 onto the various eigenspaces of $A^{1/2}$, or, equivalently, by splitting the oscillatory signal $x_2(t)$ into components which oscillate at rationally independent frequencies. The name *adiabatic invariant* then stems from the fact that these oscillatory energies are either almost constant in time, or at least slowly varying functions of time when solving (1.2). As a last point of terminology, let us mention that in this context, *energy exchange* refers to the exchange of energy between the oscillatory energies, *i.e.* between the various components of $x_2(t)$ which oscillate at rationally independent frequencies.

Now, a careful study (see [HLW06] Chapter XIII.2.) shows that none of the above mentioned methods has perfect energy conservation: for values of the stepsize such that $h\omega$ is close to a multiple of π the errors become large. This is due to a resonance effect between the step-size and the natural eigenfrequencies of the system. Very recently, Grimm and Hochbruck have built up a new Gautschi type method which provably carries no resonant stepsize [GH06]. Yet the counterpart of this favorable feature is a loose reproduction of the energy exchange between oscillatory components.

In summary, an important challenge for a numerical method in this context is to approximate adequately both the adiabatic invariants and the energy exchange, while avoiding resonances.

In this paper, we introduce a new numerical method based on an averaged version of the original equations. It stems from a preconditioning of the Hamiltonian by the fast variables. This introduces an explicit representation of the highly oscillatory components, which can be averaged over a period (and somehow filtered out), by artificially decoupling the two time-scales in the problem. In Section 2, we justify the procedure and 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 as time increases. Besides, the solution of the averaged system is an $\mathcal{O}(\varepsilon)$ perturbation of the true solution on bounded time intervals, no matter how small the step size. But as usual in this context, the accuracy in terms of individual trajectories is not the point. 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, which is our main purpose. The method we propose involves the computation of a highly-oscillatory integral which constitutes the largest share of its cost and we address accordingly its numerical approximation. In Section 3, we consider the extension of this procedure to the case of multiple frequencies and show that all results carry on easily. Finally, in Section 4, we demonstrate on two simple test problems the validity of our theoretical results and hopefully the potential of our method, 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 literature (see for instance [HLW06]), a Hamiltonian system of the form

$$\begin{cases} \ddot{x}_1 &= g_1(x_1, x_2) = -\nabla_1 U(x_1, x_2), \\ \ddot{x}_2 + \frac{1}{\varepsilon^2} x_2 &= g_2(x_1, x_2) = -\nabla_2 U(x_1, x_2), \end{cases} \quad (2.1)$$

where $x_1 \in \mathbb{R}^m$ and $x_2 \in \mathbb{R}^d$, the function $U(x_1, x_2)$ is smooth¹ and real-valued, while $\varepsilon \in (0, \varepsilon_0)$ is a small parameter. To this system is associated the Hamiltonian²

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

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 have *bounded energy*, in that they satisfy the following condition, for some given positive ε_0 :

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

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

For the sake of conciseness, we will often work with the complex and rescaled variables

$$y_1 = x_1 + i\dot{x}_1, \quad y_2 = \frac{x_2}{\sqrt{\varepsilon}} + i\sqrt{\varepsilon}\dot{x}_2,$$

for which the equations (2.1) can be rewritten as

$$\begin{cases} \dot{y}_1 &= \Im(y_1) + ig_1(\Re(y_1), \mu\Re(y_2)), \\ \dot{y}_2 &= -\frac{i}{\varepsilon}y_2 + i\mu g_2(\Re(y_1), \mu\Re(y_2)), \end{cases} \quad (2.3)$$

where \Re (resp. \Im) denotes the real (resp. imaginary) part of a complex number, and where we have denoted for convenience

$$\mu = \sqrt{\varepsilon}.$$

To this system is associated³ the real-valued Hamiltonian with complex variables

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

and the bounded energy condition (2.2) reads

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

¹Here and below, we shall not provide details on the regularity required for U in each specific intermediate result, since our final and main result anyhow requires U possesses analytic regularity.

²Here 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 .

³Through 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 (in a similar spirit, see [BL07b, BL07a])

$$z_1 = y_1, \quad z_2 = e^{it/\varepsilon} y_2,$$

for which the system takes the simple form

$$\begin{cases} \dot{z}_1 &= \mathfrak{S}(z_1) + ig_1(\Re(z_1), \mu\Re(e^{-it/\varepsilon} z_2)), \\ \dot{z}_2 &= i\mu e^{it/\varepsilon} g_2(\Re(z_1), \mu\Re(e^{-it/\varepsilon} z_2)), \end{cases} \quad (2.6)$$

and the bounded energy condition (2.2) reads

$$\|\mathfrak{S}(z_1^0)\|^2 + \frac{\|z_2^0\|^2}{\varepsilon} \leq 2E.$$

Equations (2.6) are non-stiff (the term in $1/\varepsilon$ has disappeared), yet non-autonomous. They are associated with the time-dependent Hamiltonian

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

For brevity, we also write system (2.6) as

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

where $z = (z_1, z_2) \in \mathbb{R}^{m+d}$, and the periodic function⁴ $F(\tau, z) = (F_1(\tau, z), F_2(\tau, z))$ ($\tau \in \mathbb{T}$) is defined by

$$\begin{cases} F_1(\tau, z) &= \mathfrak{S}(z_1) + ig_1(\Re(z_1), \mu\Re(e^{-i\tau} z_2)), \\ F_2(\tau, z) &= i\mu e^{i\tau} g_2(\Re(z_1), \mu\Re(e^{-i\tau} z_2)). \end{cases} \quad (2.9)$$

The main ingredient in this paper is to replace the above system $\dot{z} = F(t/\varepsilon, z)$ by the averaged one

$$\dot{Z} = \langle F \rangle(Z), \quad (2.10)$$

where the average value $\langle F \rangle$ of F is defined by

$$\langle F \rangle(Z) := \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T F(\tau, Z) d\tau = \frac{1}{2\pi} \int_0^{2\pi} F(\tau, Z) d\tau.$$

System (2.10) is now a standard non-stiff system.

This replacement is relevant: it is indeed a well-known fact (which we actually prove below for the sake of completeness) that systems of the form $\dot{z} = F(t/\varepsilon, z)$ do converge towards $\dot{Z} = \langle F \rangle(Z)$ as $\varepsilon \rightarrow 0$, the order of convergence being of the order of $\mathcal{O}(\varepsilon)$ over any finite time interval, see e.g. [Arn89].

The surprising point is, in the next section we show that even if the solution of (2.10) approximates the solution of (2.6) over bounded time intervals only, it still has a **Hamiltonian structure**, it possesses the **same adiabatic invariants** as the exact solution of (2.6) over **unbounded time intervals**, and it **preserves the**

⁴In relation with the modulated Fourier expansion, let us note in passing that the function F we introduce here, obtained by conjugating the original function g through the oscillatory factor $e^{i\tau}$, is such that its Fourier coefficients - in τ - are roughly the coefficients of the \mathcal{U} in [HLW06].

initial energy (2.7) up to ε over long time as well, provided the potential function U satisfies some mild assumptions. System (2.10) thus is nicely approximated by its averaged version

$$\begin{cases} \dot{Z}_1 &= \Im(Z_1) + i\frac{1}{2\pi} \int_0^{2\pi} g_1(\Re(Z_1), \mu\Re(e^{-is}Z_2)) \, ds, \\ \dot{Z}_2 &= i\mu\frac{1}{2\pi} \int_0^{2\pi} e^{is} g_2(\Re(Z_1), \mu\Re(e^{-is}Z_2)) \, ds, \end{cases} \quad (2.11)$$

a Hamiltonian system with Hamiltonian

$$\langle K_C \rangle(Z_1, Z_2) = \|\Im(Z_1)\|^2 + \frac{1}{\pi} \int_0^{2\pi} U(\Re(Z_1), \mu\Re(e^{-is}Z_2)) \, ds. \quad (2.12)$$

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

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

where

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

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

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

with

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

2.1 Approximation over bounded time intervals

Lemma 2.2 *Let $F(\tau, z)$ be the complex function (2.9) of $\tau \in \mathbb{T}$ and $z \in \mathbb{C}^{m+d}$. Assume that the potential function U lies in $C^2(\mathbb{R}^d \times \mathbb{R}^d)$. Take a fixed vector $z^0 \in \mathbb{C}^{m+d}$.*

On the other hand, for any $\varepsilon \in (0, \varepsilon_0)$, let $z(t) = (z_1(t), z_2(t))$ be the solution of the oscillatory system (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)

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

Then, there exists a time $T^* > 0$ and a constant $C > 0$, independent of $\varepsilon \in (0, \varepsilon_0)$ and $\mu \in (0, \mu_0)$, such that the solutions $z(t)$ and $Z(t)$ exist until time $T^* > 0$ and satisfy for any $\varepsilon \in (0, \varepsilon_0)$ and $\mu \in (0, \mu_0)$, the relation

$$\forall t \in (0, T^*), \quad \|z(t)\| \leq C, \quad \text{and} \quad \|Z(t)\| \leq C.$$

Besides, there exists a constant C such that for any $\varepsilon \in (0, \varepsilon_0)$ and $\mu \in (0, \mu_0)$, we have

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

Remark 2.3 Note that the above statement does not use the bounded energy assumption (2.5), according to which $z_1^0 = y_1^0 = \mathcal{O}(1)$ and $z_2^0 = y_2^0 = \mathcal{O}(\sqrt{\varepsilon})$, and only requires the milder $z_1^0 = y_1^0 = \mathcal{O}(1)$, $z_2^0 = y_2^0 = \mathcal{O}(1)$.

Proof. The arguments being standard, we only sketch the proof.

Firstly, as U has C^2 regularity, it is clear that $g = -\nabla U$ belongs to C^1 , hence is locally Lipschitz. Examining the explicit value of $F(\tau, z)$ in terms of g (relation (2.9)), it appears that F is locally Lipschitz in z , independently of τ , of $\varepsilon \in (0, \varepsilon_0)$, and of $\mu \in (0, \mu_0)$, and so is $\langle F \rangle$. The first part of the statement follows.

Secondly, whenever $t \in (0, T^*)$, we may write

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

On top of that, 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} , which has at least C^1 smoothness in τ and z , such that for all $\tau \in \mathbb{T}$ and $z \in \mathbb{C}^{m+d}$,

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

(it suffices to take $J(\tau, z)$ as the antiderivative in τ of the left-hand-side), and using the explicit value of F again, we have the estimate $\|J_2(\tau, z(t))\| \leq C\mu$ whenever $t \in (0, T^*)$ for some constant C independent of ε , and μ , and similarly $\|\partial_z J_2(\tau, z(t))\| \leq C\mu$. Therefore, we may write

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

and for all $t \in (0, T^*)$, we recover

$$z(t) - Z(t) = \varepsilon J(t/\varepsilon, z(t)) - \varepsilon J(0, z^0) + \int_0^t \left(\langle F \rangle(z(s)) - \langle F \rangle(Z(s)) - \varepsilon \partial_z J(s/\varepsilon, z(s)) \cdot F(s/\varepsilon, z(s)) \right) ds.$$

This yields the result using the Gronwall Lemma, and the regularity at hand for F , $\langle F \rangle$, and J . \blacksquare

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

Corollary 2.4 Let $F(\tau, z)$ be the complex function (2.9) of $\tau \in \mathbb{T}$ and $z \in \mathbb{C}^{m+d}$. Assume that the potential function U lies in $C^2(\mathbb{R}^d \times \mathbb{R}^d)$. Take a fixed vector $y^0 \in \mathbb{C}^{m+d}$ and define $z^0 = y^0$. Define $y(t) = (y_1(t), y_2(t))$ as the solution to (2.3) with initial value y^0 , and $Z(t) = (Z_1(t), Z_2(t))$ as the solution to (2.11) with initial value z^0 (and $\mu = \sqrt{\varepsilon}$). Lastly, define the function

$$Y(t) = (Y_1(t), Y_2(t)) = (Z_1(t), e^{-it/\varepsilon} Z_2(t)).$$

Then, there exists a time $T^* > 0$ and a constant $C > 0$, independent of $\varepsilon \in (0, \varepsilon_0)$, such that the solutions $y(t)$ and $Y(t)$ exist until time $T^* > 0$ and satisfy for any $\varepsilon \in (0, \varepsilon_0)$, the relation

$$\forall t \in (0, T^*), \quad \|y(t)\| \leq C, \quad \text{and} \quad \|Y(t)\| \leq C.$$

Besides, there exists a constant C such that for any $\varepsilon \in (0, \varepsilon_0)$, we have

$$\forall t \in (0, T^*), \quad \|y_1(t) - Y_1(t)\| + \varepsilon^{-1/2} \|y_2(t) - Y_2(t)\| \leq C\varepsilon. \quad (2.16)$$

Remark 2.5 Again, the above statement does not use the bounded energy assumption (2.5), and only requires the milder $z_1^0 = y_1^0 = \mathcal{O}(1)$, $z_2^0 = y_2^0 = \mathcal{O}(1)$.

2.2 Hamiltonian and adiabatic invariants over long-time intervals

Quite remarkably, the adiabatic invariants of the original, oscillatory system (2.8) turn out to be preserved along the exact solution of the averaged system (2.11), on any time interval, as we now show.

Theorem 2.6 Under the assumptions of Lemma 2.2, let $Z(t) = (Z_1(t), Z_2(t))$ be the exact solution of the averaged Hamiltonian system (2.11). Then, the quantity

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

which can be interpreted as an adiabatic invariant, is preserved as long as the solution $Z(t)$ exists, i.e.

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

Remark 2.7 As claimed in the introduction, the quantity $\|Z_2(t)\|$ is the energy carried by the fast oscillating part $Z_2(t)$ of the full vector $Z(t)$.

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

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

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

$$\frac{d}{ds} (\Re(e^{-is} Z_2)) = \frac{1}{2} \frac{d}{ds} (e^{-is} Z_2 + e^{is} \overline{Z_2}) = -i \frac{1}{2} (e^{-is} z - e^{is} \overline{z}) = \Im(e^{-is} Z_2), \quad (2.17)$$

and using that $g_2 = -\nabla_2 U$ is real-valued, it is straightforward to obtain

$$\frac{d}{dt} \|Z_2\|^2 = \frac{1}{\pi} \int_0^{2\pi} \Im(\mu e^{-is} Z_2)^T \nabla_2 U(X, \mu \Re(e^{-is} Z_2)) ds = \frac{1}{\pi} \left[U(X, \mu \Re(e^{-is} Z_2)) \right]_{s=0}^{s=2\pi} = 0.$$

■

Based on the above Theorem, the following lemma now refines the bounds at hand on the exact solution of (2.11).

Lemma 2.8 *Under the assumptions of Lemma 2.2, let $E > 0$ be given, and assume the initial value $z^0 = (z_1^0, z_2^0)$ satisfies the bounded energy relation (2.5). Assume furthermore that the time $T \leq +\infty$, is such that the solution $Z(t) = (Z_1(t), Z_2(t))$ of (2.11) with initial value z^0 exists until time T , and remains in a given bounded set for any $t \in (0, T)$, independently of ε .*

Then we have the estimate

$$\forall \varepsilon \in (0, \varepsilon_0), \forall t \in (0, T), \quad \|Z_2(t)\|^2 = \|Z_2(0)\|^2 \leq 2\varepsilon E. \quad (2.18)$$

Moreover there exists a constant C such that

$$\forall \varepsilon \in (0, \varepsilon_0), \forall t \in (0, T), \quad |K_{\mathbb{C}}(t/\varepsilon; Z(t)) - K_{\mathbb{C}}(0; Z(0))| \leq C\varepsilon, \quad (2.19)$$

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

Remark 2.9 *In other words, and quite remarkably again, according to the second estimate, the solution of the averaged system preserves the time-dependent Hamiltonian of the oscillatory system over any time interval, up to an error of size ε .*

Remark 2.10 *The existence of a finite value of T such that the assumptions of the Lemma are met, is guaranteed by Lemma 2.2.*

Note that the situation $T = +\infty$ occurs when, say, g is globally Lipschitz, or when the potential function U is coercive ($U(x_1, x_2) \geq \|x_1\|^2 + \|x_2\|^2$ for large values of x), say.

Proof. Inequality (2.18) is a consequence of the previous theorem, combined with the bounded energy condition (2.5).

On the other hand, as $Z(t)$ is the exact solution of (2.11), the Hamiltonian function (2.12) is preserved:

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

Hence, we have

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

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 $t \geq 0$,

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

Using the boundedness of $Z(t)$ and estimate (2.18), according to which $Z_2(t)$ has size $\sqrt{2\varepsilon E}$, we easily obtain for all $t \geq 0$ and $s \in (0, 2\pi)$,

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

where C does not depend on ε nor on t . 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 2.11 Under the assumptions of Corollary 2.4, let $E > 0$ be given, and assume the initial value $y^0 = (y_1^0, y_2^0)$ satisfies the bounded energy relation (2.5). Define $Y(t)$ as in Corollary 2.4. Assume furthermore that the time $T \leq +\infty$ is such that $Y(t)$ exists until time T and remains in a given bounded set for any $t \in (0, T)$, independently of ε .

Then, we have for any $t \in (0, T)$ the upper-bounds

$$\|Y_2(t)\|^2 = \|Y_2(0)\|^2 \leq 2\varepsilon E, \quad (2.22)$$

and

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

where $H_{\mathbb{C}}$ denotes the Hamiltonian (2.4). and C does not depend on ε .

Remark 2.12 In other words, the reconstructed solution $Y(t)$ obtained from solving the averaged system preserves both the adiabatic invariant of the original system (first estimate) and its time-dependent Hamiltonian up to an error of size ε (second estimate).

Remark 2.13 One may have $T = +\infty$ under the assumptions of Remark 2.10.

Proof. Estimate (2.22) is an immediate consequence of Theorem 2.6. In order to show (2.23), we write, with the notation of Corollary 2.4,

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

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). It is to be hoped indeed that one may obtain in this way a method that preserves both the adiabatic invariant of the original, oscillatory system and its time-dependent Hamiltonian.

The first step towards this objective is the discretization of integrals contained in equations (2.11). Given 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

$$K_{\mathbb{C}}^N(Z_1, Z_2) = \|\mathfrak{S}(Z_1)\|^2 + \frac{2}{N} \sum_{n=0}^{N-1} U\left(\mathfrak{R}(Z_1), \mu \mathfrak{R}(e^{-i\frac{2n\pi}{N}} Z_2)\right), \quad (2.25)$$

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

$$\begin{cases} \dot{Z}_1^N &= \mathfrak{S}(Z_1^N) + i \frac{1}{N} \sum_{n=0}^{N-1} g_1\left(\mathfrak{R}(Z_1^N), \mu \mathfrak{R}(e^{-i\frac{2n\pi}{N}} Z_2^N)\right), \\ \dot{Z}_2^N &= i\mu \frac{1}{N} \sum_{n=0}^{N-1} e^{i\frac{2n\pi}{N}} g_2\left(\mathfrak{R}(Z_1^N), \mu \mathfrak{R}(e^{-i\frac{2n\pi}{N}} Z_2^N)\right). \end{cases} \quad (2.26)$$

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_0 , there exist constants K_0 and R_0 such that

$$\forall \alpha \in \mathbb{N}^{m+d}, \quad \forall x \in \mathbb{R}^{m+d} \quad \text{with} \quad \|x\| \leq B_0, \quad \left| \frac{\partial^{|\alpha|}}{\partial x^\alpha} U(x) \right| \leq \alpha! K_0 R_0^{-|\alpha|}, \quad (2.27)$$

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

We prove below that the exact solution of this semi-discrete set of equation enjoys similar properties than the true solution $Z(t)$ to the averaged system (conservation of energy and of the adiabatic invariant).

2.3.1 Approximation over bounded time intervals

We first estimate the difference on finite time intervals between the solutions $Z(t)$ of (2.11) and $Z^N(t)$ of (2.26). The difference $Z^N(t) - Z(t)$ turns out to have size μ^N over bounded time intervals.

Lemma 2.14 *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_2^0) , 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 $T \leq +\infty$. Suppose in addition that these solutions are uniformly bounded with respect to ε and N , in the following sense:*

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

for some constant $B \leq B_0$.

Then, for a sufficiently small ε_0 , and for any finite time $T^* < T$, there exists a constant C depending only on T^* and B such that

$$\forall 0 \leq t \leq T^*, \quad \|Z_1(t) - Z_1^N(t)\| + \mu^{-1} \|Z_2(t) - Z_2^N(t)\| \leq C\mu^N. \quad (2.29)$$

Remark 2.15 *As a consequence of the estimates below, the assumptions of the above Lemma are met whenever the initial data have norm estimated by $B/2$ (with $B \leq B_0$), say, and N is sufficiently large (or ε is sufficiently small).*

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

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

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

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

Since

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

the previous sum reduces to

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

On the other hand, for all $k \in \mathbb{Z}$, we have

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

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

$$\begin{aligned} \hat{h}_k(x_1, \mu z_2) = \\ -\frac{1}{2\pi} \sum_{n=0}^{k-1} \frac{\mu^n}{n!} \int_0^{2\pi} e^{-iks} \partial_1 \partial_2^n U(x_1, 0) (\Re(e^{-is} z_2), \dots, \Re(e^{-is} z_2)) ds + \frac{\mu^k}{k!} R_k(x_1, \xi z_2), \end{aligned} \quad (2.31)$$

where

$$R_k(x_1, \xi z_2) = \frac{1}{2\pi} \int_0^{2\pi} e^{-iks} \partial_1 \partial_2^k U(x_1, \xi \Re(e^{-is} z_2)) (\Re(e^{-is} z_2), \dots, \Re(e^{-is} z_2)) ds$$

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)

$$\left| \hat{h}_{jN}(\Re(Z_1^N), \mu Z_2^N) \right| = \frac{\mu^{jN}}{(jN)!} |R_{jN}(\Re(Z_1^N), \xi Z_2^N)| \leq K_0 \left(\frac{\mu B}{R_0} \right)^{jN}.$$

Plugging this estimate into the previous one, we conclude that for μ sufficiently small,

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

where C is independent of μ , 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 fashion. \blacksquare

Combining this result with Corollary 2.4 allows to pull back the above result in terms of the original y variables, as follows.

Theorem 2.16 *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 $T \leq +\infty$. 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, in that they satisfy (2.28) for some $B \leq B_0$, whenever $\varepsilon \in (0, \varepsilon_0)$. 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 , and for any finite time $T^ < T$, there exists a constant C , independent of ε and t , such that for all $\varepsilon \in (0, \varepsilon_0)$,*

$$\forall 0 \leq t \leq T^*, \quad \|y_1(t) - Y_1^N(t)\| + \varepsilon^{-1/2} \|y_2(t) - Y_2^N(t)\| \leq C\varepsilon. \quad (2.32)$$

Remark 2.17 *Again, the assumptions of the Theorem are met whenever the initial data have norm estimated by $B/2$ (with $B \leq B_0$), say, and N is sufficiently large (or ε is sufficiently small).*

2.3.2 Hamiltonian and adiabatic invariants over long-time intervals

Let us now turn our attention to the conservation of invariants by the semi-discrete solution $Z^N(t)$.

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. This result is of prior importance for our approach.

Theorem 2.18 *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 the bounded energy assumption (2.5). Suppose that the solutions $Z^N(t)$ exist until a time $T \leq +\infty$, and that there exists a constant $B \leq B_0$ independent of ε and $N \geq 3$, such that*

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

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

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

Remark 2.19 *As before, the assumptions of the Theorem are met, for some finite value of T at least, whenever the initial data have norm estimated by $B/2$ (with $B \leq B_0$), say, and N is sufficiently large (or ε is sufficiently small).*

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

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

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 $k \in \mathbb{Z}$. Hence, we get

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

and, using (2.30),

$$\frac{1}{2} \frac{d}{dt} \|Z_2^N\|^2 = 2 \sum_{j=1}^{\infty} (jN) \Im \left(\hat{f}_{jN}(X, \mu Z_2^N) \right). \quad (2.35)$$

Now, as in the proof of Lemma 2.14, estimates (2.33) and (2.27) imply

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

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)

$$\left| \frac{d}{dt} \|Z_2^N\|^2 \right| \leq CN \left(\frac{\mu \|Z_2^N\|}{R} \right)^N \quad (2.36)$$

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 $t \leq \frac{1}{2} (x_0^{r-1} (r-1)a)^{-1}$, we have $x(t) \leq 2x_0$. 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

$$\forall t \leq \min \left(\frac{c_0^N}{\mu^N \varepsilon^{N/2-2}}, T \right), \quad \|Z_2^N(t)\|^2 \leq 4E\varepsilon.$$

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

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

This completes the proof. \blacksquare

As before, it now becomes an easy task to pull back the above estimates in terms of the original y -variables.

Theorem 2.20 *Assume that U satisfies (2.27). For $N \geq 3$ 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 the bounded energy assumption (2.5). Assume that $Z^N(t)$ exists until a time $T \leq +\infty$, and satisfies (2.33) for some $B \leq B_0$. Define $Y^N(t) = (Z_1^N(t), e^{-it/\varepsilon} Z_2^N(t))$.*

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

$$\forall 0 \leq t \leq \min \left(\frac{c_0^N}{\mu^N \varepsilon^{N/2-2}}, T \right), \quad \left| \|Y_2^N(t)\|^2 - \|Y_2^N(0)\|^2 \right| \leq C\varepsilon^2, \quad (2.37)$$

and

$$\forall 0 \leq t \leq \min \left(\frac{c_0^N}{\mu^N \varepsilon^{N/2-2}}, T \right), \quad |H_{\mathbb{C}}(Y_1^N(t), Y_2^N(t)) - H_{\mathbb{C}}(y_1^0, y_2^0)| \leq C\varepsilon, \quad (2.38)$$

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

Remark 2.21 *In other words, the semi-discrete solution $Y^N(t)$ obtained through the solution of the averaged system (2.11) preserves both the energy and the adiabatic invariant of the original oscillatory system (2.3), up to error terms of size ε^2 resp. ε .*

Remark 2.22 *As usual, the assumptions of the Theorem are met, for some finite value of T , whenever the initial data have norm estimated by $B/2$ (with $B \leq B_0$), say, and N is sufficiently large (or ε is sufficiently small).*

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

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

where

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

According to the previous theorem, as long as $t \leq \min\left(\frac{c_0^N}{\mu^N \varepsilon^{N/2-2}}, T\right)$, the solution $Z^N(t)$ remains bounded and satisfies the estimates (2.33) and (2.34). Hence, as in the proof of Lemma 2.8, we can show that

$$\forall t \leq \min\left(\frac{c_0^N}{\mu^N \varepsilon^{N/2-2}}, T\right), \quad |(\Delta U)(t) - (\Delta U)(0)| \leq C\varepsilon$$

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

2.4 Fully-discrete solution

We now consider 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 (hence Φ_h^N represents one elementary step of the numerical integration). Finally, we define the numerical approximation as the sequence

$$Z^{N,0} = y^0 = (y_1^0, y_2^0) \in \mathbb{C}^{m+d}, \quad (2.39)$$

$$Z^{N,n} = \Phi_h^N(Z^{N,n-1}), \quad n \geq 1. \quad (2.40)$$

This entirely defines the numerical method we retain in this article (up to the choice of a symplectic numerical integrator Φ_h^N). Note that each computation of the vector field which defines Z^N , derived from the Hamiltonian $K_{\mathbb{C}}^N$ (see (2.25) and (2.26)), roughly has a cost of the order N . Note also that solving the semi-discrete problem by a standard, non-symplectic scheme would be pointless: energy would drift in that case.

Theorem 2.23 *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 the bounded energy condition (2.5). Assume that $Z^{N,n}$ is well-defined for all $n \geq 0$ such that $nh \leq T$, where $T \leq +\infty$ is some given time, and that $Z^{N,n}$ is bounded by a constant B independent of ε , h , $N \geq 3$ and n , in the sense that*

$$\forall nh \in (0, T), \quad \|Z^{N,n}\| \leq B. \quad (2.41)$$

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 $h \in (0, h_0)$,

$$\forall 0 \leq nh \leq \min\left(\frac{c_0^N}{\mu^N \varepsilon^{N/2-2}}, T\right), \quad \left| \|Z_2^{N,n}\|^2 - \|Z_2^{N,0}\|^2 \right| \leq C\varepsilon^2. \quad (2.42)$$

Remark 2.24 *In the particular case when the chosen symplectic integrator Φ_h^N is provided by the midpoint rule, the proof below establishes that the assumptions of the Theorem are met whenever the initial data have norm estimated by $B/2$ (with $B \leq B_0$), say, and N is sufficiently large (or ε is sufficiently small).*

In the general case when Φ_h^N may be any symplectic integrator, we simply mention that the methods developed in [HLW06], combined with our assumption that U has analytic smoothness (2.27), show that the assumptions of the Theorem are met under similar circumstances.

Note finally that one may again have $T = +\infty$ here, provided particular circumstances are met, such as a global Lipschitz bound on g , or some coercivity of U , see Remark 2.10.

Proof. For the sake of simplicity, 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].

Under these circumstances, sequence (2.40) becomes

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

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 2.18, from bound (2.41) we can derive the estimate

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

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

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

from which it follows, in combination with (2.43), that

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

Therefore, for $h \leq h_0$ sufficiently small, there exists a constant $\alpha > 0$ such that for any N we have $CN(1 + hc)^N/R^N \leq \alpha^N$, and we deduce

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

Finally we obtain

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

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

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

so that for

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

we have $\|Z_2^{N,n+1}\|^2 \leq 4E\varepsilon$ as well. 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),

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

■

On the other hand, and quite unsurprisingly, the numerical solution $Z^{N,n}$ obtained through a symplectic integrator clearly preserves the natural discretized Hamiltonian (2.25), $K_{\mathbb{C}}^N$, as shown by the following

Lemma 2.25 *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 $\varepsilon \in (0, \varepsilon_0)$, $N \geq 3$ and $h \in (0, h_0)$,*

$$\forall 0 \leq nh \leq \min(\exp(c/h), T), \quad |K_{\mathbb{C}}^N(Z^{N,n}) - K_{\mathbb{C}}^N(Z^{N,0})| \leq Ch^r$$

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). ■

Therefore, we are now in position to state that the numerical solution $Z^{N,n}$ preserves both the Hamiltonian and the adiabatic invariant of the original oscillatory system (up to small error terms).

To present the result cleanly, going back to the original variables, we first define the approximations $Y^{N,n}$ of $Y(t)$ (see above) by the formula

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

Combining previous results with Theorem 2.20, we immediately get the following

Theorem 2.26 *Assume that the hypotheses of Theorem 2.23 hold true for $\mu = \sqrt{\varepsilon}$ and define $Y^{N,n}$, $n \geq 0$ 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 $\varepsilon \in (0, \varepsilon_0)$, $N \geq 3$ and $h \in (0, h_0)$,*

$$\forall 0 \leq nh \leq \min\left(\frac{c_0^N}{\varepsilon^{N-2}}, T\right), \quad \left| \|Y_2^{N,n}\|^2 - \|Y_2^{N,0}\|^2 \right| \leq C\varepsilon^2, \quad (2.46)$$

and

$$\forall 0 \leq nh \leq \min\left(\frac{c_0^N}{\varepsilon^{N-2}}, \exp\left(\frac{c}{h}\right), T\right), \quad |H_{\mathbb{C}}(Y_2^{N,n}) - H_{\mathbb{C}}(Y_2^{N,0})| \leq C(\varepsilon + h^r) \quad (2.47)$$

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

Remark 2.27 *With the previous notation, it is clear that Theorem 2.16 (error estimate between the true solution and the approximate one, over bounded time intervals) extends straightforwardly to the fully discretized solution $Y^{N,n}$, the error in the equation (2.32) being then of order $\mathcal{O}(\varepsilon + h^r)$. More precisely, using the above notation, for sufficiently small ε_0 , and for any finite time $T^* < T$, there exists a constant C , independent of ε and n , such that for all $\varepsilon \in (0, \varepsilon_0)$, all $h \in (0, h_0)$,*

$$\forall 0 \leq nh \leq T^*, \quad \|y_1(nh) - Y_1^{N,n}\| + \varepsilon^{-1/2} \|y_2(nh) - Y_2^{N,n}\| \leq C(\varepsilon + h^r).$$

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 $\frac{1}{\varepsilon}A$:

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

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 $\omega_1, \dots, \omega_d$. Similarly to (2.2), we assume that the initial values depend on ε in such a way that the following energy is bounded

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

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

$$\begin{cases} \dot{y}_1 &= \mathfrak{S}(y_1) + ig_1(\Re(y_1), \mu A^{-1/2} \Re(y_2)), \\ \dot{y}_2 &= -i\frac{A}{\varepsilon} y_2 + i\mu A^{-1/2} g_2(\Re(y_1), \mu A^{-1/2} \Re(y_2)), \end{cases} \quad (3.2)$$

with Hamiltonian

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

The condition on the initial values now takes the form

$$\|\mathfrak{S}(y_1^0)\|^2 + \frac{\|A^{1/2} y_2^0\|^2}{\varepsilon} \leq 2E. \quad (3.4)$$

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

$$\begin{cases} \dot{z}_1 &= \mathfrak{S}(z_1) + ig_1(\Re(z_1), \mu A^{-1/2} \Re(e^{-i\frac{t}{\varepsilon} A} z_2)), \\ \dot{z}_2 &= i\mu e^{i\frac{t}{\varepsilon} A} A^{-1/2} g_2(\Re(z_1), \mu A^{-1/2} \Re(e^{-i\frac{t}{\varepsilon} A} z_2)), \end{cases} \quad (3.5)$$

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

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

As in the case $A = \text{Id}$, 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

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

The averaged system we consider can hence be written as

$$\begin{cases} \dot{Z}_1 &= \mathfrak{S}(Z_1) + i \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T g_1(\Re(Z_1), \mu A^{-1/2} \Re(e^{-isA} Z_2)) ds, \\ \dot{Z}_2 &= i\mu \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T e^{isA} A^{-1/2} g_2(\Re(Z_1), \mu A^{-1/2} \Re(e^{-isA} Z_2)) ds. \end{cases} \quad (3.8)$$

This is once again a Hamiltonian system associated with the Hamiltonian

$$\langle K_{\mathbb{C}} \rangle(Z_1, Z_2) = \|\mathfrak{S}(Z_1)\|^2 + 2 \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T U(\Re(Z_1), \mu \Re(e^{-isA} A^{-1/2} Z_2)) ds. \quad (3.9)$$

Some remarks about the numerical approximation of the above system are in order (the very discretization is discussed in detail in the next paragraphs). Firstly, as shown through the estimates (3.15) and (3.17) below, the discretization of the integrals involved in (3.9) will eventually have cost $\mathcal{O}(N)$ for some large N , for approximations of the integral that will have exponential accuracy. Secondly, note that after a possible change of unknowns and of function U , we can always assume that the matrix A is *diagonal*. From the point of view of the numerical cost, this means we readily consider the computation of the diagonal form of A as a pre-processing step, independent of our main task which is the filtering of the fast oscillations, so that we do not further investigate the very method that should be used to diagonalize A , nor its cost.

In the sequel, the eigenvalues of A are assumed to satisfy a non-resonance condition according to the following definition. Note that this condition is generically satisfied.

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

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

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

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

The orthogonal of the resonant module is defined by

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

Remark 3.2 The introduction of the resonant module \mathcal{M} is a way to select those component of the given frequency vector ω which are rationally independent. It generalizes more standard notions of 'non-resonance'. Let us give three simple examples.

The simplest case corresponds to $\omega = (\omega_1, \dots, \omega_d)$, where the ω_i 's are rationally independent. In that circumstance, the resonant module reduces to $\{0\}$, and the small-denominator estimate (3.10) is generically satisfied. This is the most standard notion of non-resonance: the vector ω is then said to be non-resonant.

The point is, our analysis can be carried out beyond this simple situation.

Indeed, in the case $\omega = (1, 1, \dots, 1)$, for instance, a highly resonant situation in the standard terminology, \mathcal{M} is the set of integer vectors α such that $\alpha_1 + \dots + \alpha_d = 0$, and the vector ω then is certainly non-resonant outside \mathcal{M} since $|\alpha \cdot \omega| \geq 1$ whenever $\alpha \notin \mathcal{M}$ in this case.

In the similar spirit, if $\omega = (1, 1, \sqrt{2})$, say, \mathcal{M} is the set of integer vectors $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ such that $\alpha_1 + \alpha_2 = 0$ and $\alpha_3 = 0$, and again ω is non-resonant outside \mathcal{M} as can be shown by using the fact

that $|k_1 + k_2\sqrt{2}| \geq \gamma(|k_1| + |k_2|)^{-\nu}$ (for some γ and ν) whenever $k_1 + k_2\sqrt{2} \neq 0$, and next setting $k_1 = \alpha_1 + \alpha_2$ and $k_2 = \alpha_3$.

These simple observations justify the fact that, generically, any vector ω is non-resonant outside the associated resonance module \mathcal{M} .

Remark 3.3 *The second reason for our introduction of the resonance module \mathcal{M} is the following. Not only does our assumption that ω is non-resonant outside \mathcal{M} allow to analyse the situation for any (generic) value of ω , including ω 's that are resonant in the standard sense, but the very value of \mathcal{M} also allows to read off the effective number of adiabatic invariants associated with the original ODE, as we show below, and to quantify the various energy exchanges. We refer to Remark 3.6 below.*

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 3.4 *Consider a function G of $\theta = (\theta_1, \dots, \theta_d) \in \mathbb{T}^d$ 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

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T G(\theta_0 + t\omega) dt = \sum_{\alpha \in \mathcal{M}} \widehat{G}(\alpha) e^{i\alpha \cdot \theta_0}. \quad (3.11)$$

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

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

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

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

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 $\|A^{1/2}Z_2(t)\|^2$ remains invariant along the exact solution of (3.8): Noticing that

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

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

$$\begin{aligned} \frac{d}{dt} \|A^{1/2} Z_2\|^2 &= 2 \Re(Z_2^* A \dot{Z}_2), \\ &= 2\mu \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \Re \left(i Z_2^* A^{1/2} e^{isA} g_2(X, \mu \Re(e^{-isA} A^{-1/2} Z_2)) ds \right), \\ &= 2 \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \Im(\mu e^{-isA} A^{1/2} Z_2) \nabla_2 U(X, \mu \Re(e^{-isA} A^{-1/2} Z_2)) ds, \\ &= 2 \lim_{T \rightarrow \infty} \frac{1}{T} \left[U(X, \mu \Re(e^{-isA} A^{-1/2} Z_2)) \right]_{s=0}^{s=T} = 0. \end{aligned}$$

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 3.5 *Assume that U is analytic (compare 2.27) and that ω is non-resonant outside \mathcal{M} .*

Then, for any $\beta = (\beta_1, \dots, \beta_d)$ 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).

Remark 3.6 *In other words, there are adiabatic invariants that are indexed by $\beta \in \mathcal{M}^\perp$. Due to the specific structure of the set \mathcal{M}^\perp , many of them coincide (up to a constant factor), and an appropriate choice of basis for the set \mathcal{M}^\perp is to be made, in order to count the effective number of independent adiabatic invariants we have exhibited here.*

Let us give but three examples.

In the case when $\omega = (\omega_1, \dots, \omega_d)$ and the ω_i 's are rationally independent, $\mathcal{M} = \{0\}$ and $\mathcal{M}^\perp = \mathbb{Z}^d$, a module that is generated by the d vectors $(1, 0, \dots, 0)$, \dots , $(0, \dots, 0, 1)$. The above Theorem asserts, in this case, the existence of d adiabatic invariants, namely $I_{1,0,\dots,0} = |Z_{2,1}(t)|^2$, \dots , $I_{0,\dots,0,1} = |Z_{2,d}(t)|^2$.

In the case when $\omega = (1, 1, \dots, 1)$, say, \mathcal{M} is the set of α 's such that $\alpha_1 + \alpha_2 + \dots + \alpha_d = 0$ so that \mathcal{M}^\perp is clearly the set of β 's such that $\beta_1 = \beta_2 = \dots = \beta_d$. Therefore, \mathcal{M}^\perp is generated by

the vector $(1, 1, \dots, 1)$ and the above theorem asserts the existence of one adiabatic invariant: $I_{1,1,\dots,1} = |Z_{2,1}(t)|^2 + |Z_{2,1}(t)|^2 + \dots + |Z_{2,d}(t)|^2 = \|Z_2(t)\|^2$.

In the case when $\omega = (1, 1, \sqrt{2})$, say, \mathcal{M} is the set of α 's such that $\alpha_1 + \alpha_2 = 0$, $\alpha_3 = 0$, so that \mathcal{M}^\perp is clearly the set of β 's such that $\beta_1 = \beta_2$. Therefore, \mathcal{M}^\perp is generated by the two vectors $(1, 1, 0)$ and $(0, 0, 1)$, and the above theorem asserts the existence of two adiabatic invariants: $I_{1,1,0} = |Z_{2,1}(t)|^2 + |Z_{2,1}(t)|^2$ and $I_{0,0,1} = |Z_{2,3}(t)|^2$.

In summary, one sees that the above Theorem asserts, in the general case, that the system possesses as many adiabatic invariants as ω has rationally independent components, and these invariants are indexed according to the independent components of ω .

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

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

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

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

We can then write

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

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 3.4 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 $j = 1, \dots, d$,

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

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,

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

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

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

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

Using the same procedure as in previous sections, we can show the following result (compare Theorem 2.20):

Theorem 3.7 *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 the bounded energy condition (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 until time $T \leq +\infty$, and is uniformly bounded with respect to $\varepsilon \in (0, \varepsilon_0)$ and $t \in (0, T)$ (the existence of such a T is guaranteed as in the one-frequency case). 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 $\varepsilon \in (0, \varepsilon_0)$,

$$\forall t \in (0, T), \quad \|A^{1/2} Y_2(t)\|^2 = \|A^{1/2} Y_2(0)\|^2 \leq 2\varepsilon E$$

and

$$\forall t \in (0, T), \quad |H_{\mathbb{C}}(Y_1(t), Y_2(t)) - H_{\mathbb{C}}(y_1^0, y_2^0)| \leq C\varepsilon,$$

where $H_{\mathbb{C}}$ denotes the Hamiltonian (3.3). Moreover, we have for any $\beta \in \mathcal{M}^\perp$,

$$\forall t \in (0, T), \quad I_\beta(Y_2(t)) = I_\beta(Y_2(0)).$$

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 3.4. Similarly to the proof of Lemma 2.14, 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 $j = 1, \dots, d$. For $\alpha \in \mathbb{Z}^d$, the Fourier coefficient

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

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 2.14, under the assumption (2.27), we have for bounded x_1 and z_2 , and for all $\alpha \in \mathbb{Z}^d$,

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

where $|\alpha| = |\alpha_1| + \dots + |\alpha_d|$ 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 $\xi : [0, 1] \rightarrow \mathbb{R}$ by $\xi(u) = e^{-\frac{1}{u(1-u)}}$ and $\varphi : [0, 1] \rightarrow \mathbb{R}$, the filter function, by $\varphi = \xi / \|\xi\|_{L_1(0,1)}$.

Lemma 3.8 *Assume that ω is non resonant outside \mathcal{M} , and that U satisfies (2.27). Assume that $B \leq B_0$ is a given constant.*

Then there exist positive constant $\varepsilon_0 > 0$, κ , ρ and C such that for all $T_0 > 0$, $\mu \in (0, \sqrt{\varepsilon_0})$ and any given vector $Z = (Z_1, Z_2)$ such that $\|Z\| \leq B$,

$$\left| \frac{1}{T_0} \int_0^{T_0} \varphi\left(\frac{s}{T_0}\right) K_{\mathbb{C}}(s, Z_1, Z_2) - \langle K_{\mathbb{C}} \rangle(Z_1, Z_2) \right| \leq C\mu \|Z_2\| \exp(-\kappa T_0^\rho), \quad (3.15)$$

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 $T_0 = N\delta$ in the above Lemma, where δ is a small parameter. We assume that ω is non-resonant outside \mathcal{M} and we require that δ obeys the following non-resonance condition

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

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 3.9 *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 $B \leq B_0$ 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 any given vector $Z = (Z_1, Z_2)$ such that $\|Z\| \leq B$*

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

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

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

for some δ satisfying 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 $Z^N(t)$ (i.e. a solution such that there exists a $B \leq B_0$ and a $T \leq +\infty$ such that $\|Z^N(t)\| \leq B$ for any $t \in (0, T)$), we have (using the fact that $\omega_j > 0$)

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

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

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

for some constant $C > 0$. Eventually,

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

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

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

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

Using these observations, we arrive at

Theorem 3.10 *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 the bounded energy condition (3.4). Eventually, assume that for some $T \leq +\infty$, solutions $Z^N(t)$ exist and satisfy $\|Z^N(t)\| \leq B$ for a constant $B \leq B_0$ independent of ε and N , whenever $t \in (0, T)$. 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 $N \geq 1$

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

and

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

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

$$\forall 0 \leq t \leq \min(\exp(\kappa N^\rho), T), \quad |I_\beta(Y_1^N(t), Y_2^N(t)) - I_\beta(y_1^0, y_2^0)| \leq C\varepsilon.$$

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). \blacksquare

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

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

Proceeding as in the proof of Theorem (2.23) and using similar arguments than before, we can show that under the assumptions of Theorem 3.10, we have for sufficiently small $h \leq h_0$ (compare (2.42))

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

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 3.11 *Under the hypotheses of Theorem 3.10, 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 $h \in (0, h_0)$,*

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

and

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

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 that

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

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:

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

- 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 predicted by Theorem 2.20.
- The exchange of oscillatory energies between the stiff springs is adequately reproduced, even for very large stepsizes. This is remarkably better than some other methods proposed in the literature (see the method of Garcia-Archilla et al. [GASSS99] for instance (method (C) page 481 of [HLW06]).
- There is no resonance 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 two 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

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

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

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

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 accurately reproduced.

5 Conclusion

Both theoretical and experimental results demonstrate that solving the averaged equations with a suitable one-step method makes sense. More precisely, we have exhibited here a numerical method which is accurate

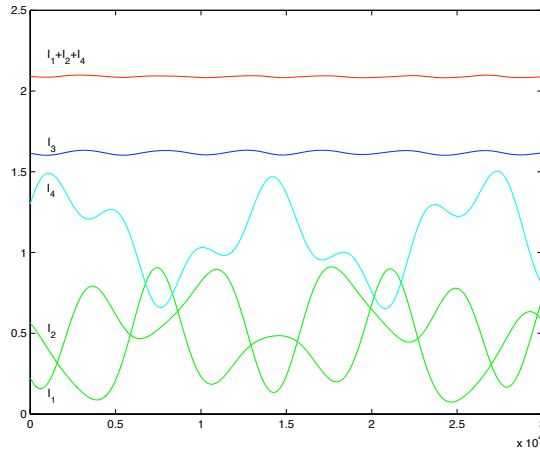


Figure 4: Oscillatory energies along the numerical solution of (4.1) for $T = 80$, $N = 120$ and $h = 10\epsilon$ (left) and $h = 1$ (right)

in terms of preservation of the natural adiabatic invariants over long time ; needless to recall, and as usual in the context of geometric numerical integration, the so-obtained trajectories roughly approximate the true trajectories to within $\mathcal{O}(\epsilon + h^r)$ only, for bounded values of time, where ϵ is the high-frequency parameter and h is the time step. 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. In the same spirit, note that other numerical schemes exist which do not suffer from resonances while almost-preserving the adiabatic invariants: considering indeed the first two terms of the modulated Fourier expansion (see eq. (3.3) on page 487 in [HLW06]), a standard scheme will solve this system without being affected by numerical resonances. However, such a scheme is difficult to write in the multi-frequency case, and besides, it requires the computation of the second derivatives of g . (Note yet that writing a basic first order approximation remains easy, since the second derivatives of g contain terms which are small and may be neglected in a first order approach).

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