Conservation properties of numerical integrators for highly oscillatory Hamiltonian systems

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Abstract

Modulated Fourier expansion is used to show long-time near-conservation of the total and oscillatory energies of numerical methods for Hamiltonian systems with highly oscillatory solutions. The numerical methods considered are an extension of the trigonometric methods. A brief discussion of conservation properties in the continuous problem and in the multi-frequency case is also given.

1 Introduction

We consider Hamiltonian systems

\begin{align*}
\dot{p} &= -\nabla_q H(p, q) \\
\dot{q} &= \nabla_p H(p, q),
\end{align*}

with the Hamiltonian function

\[ H(p, q) = K(p_1, q_1) + \frac{1}{2}p_2^T p_2 + \frac{\omega^2}{2} q_2^T q_2, \]

where the vectors \(p = (p_1, p_2)\) and \(q = (q_1, q_2)\) are partitioned according to the partition of the square matrix

\[ \Omega = \begin{pmatrix} 0 & 0 \\ 0 & \omega I \end{pmatrix} \]

with blocks of arbitrary dimension and where \(\omega\) is a large positive parameter.

We assume that the initial values satisfy

\[ \frac{1}{2}||p(0)||^2 + \frac{1}{2}||q(0)||^2 \leq E, \]

where \(E\) is independent of \(\omega\).

Our attention will go particularly to the near-conservation of the oscillatory energy

\[ I(p, q) = \frac{1}{2}(p_2^T p_2 + \omega^2 q_2^T q_2) \]
over long time intervals.

By taking the function $K$ in (1.2) to be $\frac{1}{2} p_1^T M(q)^{-1} p_1 + U(q)$, we get back the Hamiltonian function considered by Hairer and Lubich (2000) (see also (Hairer et al., 2002, Chap. XIII)). Our aim, in this article, is to extend the results of (Hairer & Lubich, 2000) to the more general Hamiltonian functions (1.2).

In particular, it is possible to consider coupling between the position $q$ and the momenta $p_1$, such as $K(p_1, q) = \frac{1}{2} p_1^T M(q)^{-1} p_1$, where $M(q)$ is a mass matrix. Simple examples described by such Hamiltonian are the stiff spring pendulum (Ascher & Reich, 1999a) or the diatomic molecule (Ascher & Reich, 1999b). More complicated examples can be found in physics, molecular dynamics or in astronomy (as we will see below).

**Example 1.1** As a concrete example, we consider the motion of a planar elastic dumbbell spacecraft acting under a central gravitational field. Such a satellite is composed by two equal masses $m$ connected by a stiff spring with stiffness constant $k >> 1$. As in (Sanyal et al., 2003), we place the origin at the center of the central body, the radial distance from the origin to the satellite is denoted by $r$, and the distance of each mass particle from the center of mass of the spacecraft is $q$. We denote by $\phi$ the angular position of the dumbbell and by $\theta$ the attitude angle. This is shown in Figure 1.

For this problem, the Lagrangian reads

$$L(\dot{r}, \phi, \dot{\phi}, \dot{\theta}, r, \phi, \theta, q) = m(\dot{r}^2 + \dot{q}^2 + q^2 \dot{\theta}^2 + 2q^2 \dot{\phi} \dot{\theta} + (r^2 + q^2) \dot{\phi}^2)$$

$$- V_g(r, \theta, q) - 2k(q - l)^2,$$  

(1.5)

where $l$ is half the unstretched length of the spring, and

$$V_g(r, \theta, q) = -\frac{\mu m}{r} \left( 2 - \frac{a^2}{r^2} (1 - 3 \cos^2(\theta)) \right)$$

Figure 1: Planar dumbbell spacecraft.
is the gravitational potential.

After a generalized coordinates change (for details see Appendix A and (Sanyal et al., n.d.)), we obtain the following Hamiltonian function

\[
H(p_\rho, p_\phi, p_\sigma, \rho, \phi, \theta, \sigma) = \frac{1}{2} \left( \frac{p_\rho^2}{\rho^2} + \frac{1}{\rho^2} (p_\phi - p_\theta)^2 + \frac{1}{(\sigma + \varepsilon)^2} p_\theta^2 + p_\sigma^2 - \frac{2}{\rho} \right) + \frac{(\sigma + \varepsilon)^2}{\rho^3} (1 - 3 \cos^2(\theta)) + \omega^2 \sigma^2, \tag{1.6}
\]

where the values for the parameters \(\varepsilon\) and \(\omega\) are taken from (Sanyal et al., n.d.) and are given by \(\varepsilon = 7.5 \cdot 10^{-5}\) and \(\omega = \sqrt{1800}\). This Hamiltonian function is of the type (1.2) with slow components (i.e. \(q_1\)) \((p, \phi, \theta)\) and fast component (i.e. \(q_2\)) \(\sigma\).

Let us use a very precise numerical method (namely DOP853, for a definition, see (Hairer et al., 1993)), and plot, see Figure 2, the different energies involved in this problem for the initial values taken from (Sanyal et al., n.d.):

- \(h(0) = 1\)
- \(\theta(0) = \pi/2\)
- \(\sigma(0) = 0.2\varepsilon\)
- \(p_\phi(0) = 0.999958 + (\sigma(0) + \varepsilon)^2(0.07 + 0.999958)\)
- \(p_\theta(0) = (\sigma(0) + \varepsilon)^2(0.07 + 0.999958)\)
- \(p_\rho(0) = 0\)

and zero for the remaining ones.

![Figure 2: Scaled total and oscillatory energies for Hamiltonian problem with (1.6), with a zoom of I.](image)

As mentioned above, the oscillatory energy is nearly preserved over long time intervals.

To explain this behaviour, we begin with presenting the modulated Fourier expansion of the exact solution (Section 2). Then, we discuss an extension of the numerical methods given in (Hairer & Lubich, 2000) (Section 3). In Section 4, we apply the approach of the modulated Fourier expansion to the numerical solution and explain its good behaviour. In the last section, we extend the class of studied problems by adding either a small perturbation in the function \(K\) of (1.2) or other frequencies as it was done in (Cohen et al., 2004).

### 2 Modulated Fourier expansion of the exact solution

To show the near-conservation of the oscillatory energy for Hamiltonian systems with the Hamiltonian function (1.2), we follow the lines of (Hairer et al., 2002, Sect. XIII.5). Here, we state the results omitting the proofs. A detailed version can be found in (Cohen, 2004, Chap. 5).
Fourier expansion of the exact solution.

Theorem 2.1. If the solution \( (p(t), q(t)) \) of Hamiltonian systems (1.1) with the Hamiltonian function (1.2) satisfies condition (1.3) and stays in a compact set for \( 0 \leq t \leq T \), then the solution admits an expansion

\[
\begin{align*}
    p(t) &= \sum_{|k| < N} e^{i k \omega t} \eta^k(t) + R_N(t), \\
    q(t) &= \sum_{|k| < N} e^{i k \omega t} \zeta^k(t) + S_N(t),
\end{align*}
\]

for arbitrary \( N \geq 2 \), where the remainder terms are bounded by

\[ R_N(t) = \mathcal{O}(\omega^{-N}), \quad S_N(t) = \mathcal{O}(\omega^{-N}), \quad \text{for} \quad 0 \leq t \leq T. \]

The real functions \( \eta = (\eta_1, \eta_2), \zeta = (\zeta_1, \zeta_2) \) and the complex functions \( \eta^k = (\eta_1^k, \eta_2^k), \zeta^k = (\zeta_1^k, \zeta_2^k) \) are bounded, together with all their derivatives, by

\[
\begin{align*}
    \zeta_1 &= \mathcal{O}(1), & \eta_1 &= \mathcal{O}(1), & \zeta_2 &= \mathcal{O}(\omega^{-2}), & \eta_2 &= \mathcal{O}(\omega^{-2}), \\
    \zeta_1^k &= \mathcal{O}(\omega^{-k}), & \eta_1^k &= \mathcal{O}(\omega^{-2}), & \zeta_2^k &= \mathcal{O}(\omega^{-1}), & \eta_2^k &= \mathcal{O}(\omega^{-1}),
\end{align*}
\]

for \( k = 2, \ldots, N - 1 \). Moreover, we have \( \eta^{-k} = \overline{\eta^k} \) and \( \zeta^{-k} = \overline{\zeta^k} \). These functions are unique up to terms of size \( \mathcal{O}(\omega^{-N}) \). The constants symbolized by the \( \mathcal{O} \)-notation are independent of \( \omega \) and \( t \) with \( 0 \leq t \leq T \) but depend on \( N, T \) and \( E \).

The modulation functions \( \eta^k \) and \( \zeta^k \) have almost-invariants that are related to the total energy \( H \) and to the oscillatory energy \( I \). To see this, let us define \( p = (p^{N+1}, \ldots, p^0, \ldots, p^{N-1}) \) with \( p^k = e^{i k \omega t} \eta^k \) (a similar notation is used for \( q \)). These modulation functions are determined to verify the following system (for \( k = 0, \ldots, N - 1 \))

\[
\begin{align*}
    p^k + \Omega^k q^k &= -\nabla_{q^{-k}} \mathcal{K}(p_1, q) + \mathcal{O}(\omega^{-N}) \quad \text{(2.3)} \\
    q^k &= \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix} p^k + \nabla_{p^{-k}} \mathcal{K}(p_1, q) + \mathcal{O}(\omega^{-N}), \quad \text{(2.4)}
\end{align*}
\]

with

\[
\mathcal{K}(p_1, q) = K(p_1^0, q^0) + \sum_{s(\alpha)+s(\beta)=0} \frac{1}{m! n!} D_1^m D_2^n K(p_1^0, q^0)(p_1^\alpha, q^\beta). \quad \text{(2.5)}
\]

Here, the sum is over all integers \( m \) and \( n \) greater or equal to zero and all multi-indices \( \alpha = (\alpha_1, \ldots, \alpha_m), \beta = (\beta_1, \ldots, \beta_n) \) with integers \( 0 < |\alpha_j|, |\beta_j| < N \) which have a given sum \( s(\alpha), \text{resp.} s(\beta) \).

Neglecting the \( \mathcal{O}(\omega^{-N}) \) terms, (2.3)–(2.4) is a Hamiltonian system with

\[
\mathcal{H}(p, q) = \frac{1}{2} \sum_{|k| < N} \left( q^{-kT} \Omega^k q^k + p^{-kT} \Omega^k p^k \right) + \mathcal{K}(p_1, q).
\]
Moreover, this formal invariant is close to the Hamiltonian (1.2). Beside this formal invariant, system (2.3)–(2.4) has another formal invariant

\[ I(p, q) = -i\omega \sum_{0 \leq |k| < N} kq^{-kT}p^k \]

which turns out to be close to the oscillatory energy (1.4).

This permits us to prove the main result of this section, which states that the oscillatory energy (1.4) is nearly conserved over long time intervals.

**Theorem 2.2** If the solution \((p(t), q(t))\) of the Hamiltonian problem (1.1) with the Hamiltonian function (1.2), with initial values satisfying (1.3), stays in a compact set for \(0 \leq t \leq \omega^N\), then

\[ I(p(t), q(t)) = I(p(0), q(0)) + O(\omega^{-1}) + O(t\omega^{-N}). \]

The constants symbolized by \(O\) are independent of \(\omega\) and \(t\), but depend on \(E\) and \(N\).

Benettin et al. (1987) studied almost similar Hamiltonian functions and showed, using other techniques, the near-conservation of the oscillatory energy over exponentially long time intervals.

To conclude this section, we want to mention that a finer analysis, similar to the one given in (Cohen et al., 2003) for the Hamiltonian function \(H(p, q) = \frac{1}{2}(p^T p + q^T\Omega^2 q) + U(q)\), should also show the near-conservation of the oscillatory energy over exponentially long time intervals.

# 3 Numerical methods

In this section, we adapt the trigonometric methods given in (Hairer & Lubich, 2000) to the case of the Hamiltonian function (1.2). Developing the Hamiltonian system for this Hamiltonian function, we obtain

\[ \begin{align*}
\dot{p}_1 &= -\nabla_{q_1} K(p, q) \\
\dot{p}_2 &= -\omega^2 q_2 - \nabla_{q_2} K(p, q) \\
\dot{q}_1 &= \nabla_{p_1} K(p, q) \\
\dot{q}_2 &= p_2.
\end{align*} \]

Treating the second components of \(p\) and \(q\) with a symmetric trigonometric method and the first components with the Störmer-Verlet method, one gets the
following numerical scheme
\[
\begin{align*}
p^{n+1/2} &= p^n - \frac{\hbar}{2} \hat{\Psi} q^n K(p_1^{n+1/2}, \Phi q^n) \\
qu_1^{n+1} &= q_1^n + \frac{\hbar}{2} (\nabla_{p_1} K(p_1^{n+1/2}, \Phi q^n) + \nabla_{p_1} K(p_1^{n+1/2}, \Phi q^{n+1})) \\
qu_2^{n+1} &= \cos(\hbar \omega) q_2^n + \hbar \sin(\hbar \omega) p_2^{n+1/2} \\
p_1^{n+1/2} &= p_1^{n+1/2} \\
p_2^{n+1/2} &= -\omega \sin(\hbar \omega) q_2^n + \cos(\hbar \omega) p_2^{n+1/2} \\
p^{n+1} &= \bar{p}^{n+1/2} - h \frac{\hbar}{2} \hat{\Psi} q^n K(p_1^{n+1/2}, \Phi q^{n+1}),
\end{align*}
\] (3.1)

where, here and in the following, \(\hat{\Psi} = \hat{\psi}(h \Omega)\), \(\Phi = \phi(h \Omega)\), \(\hat{\Psi}_2 = \hat{\psi}(h \omega)\), and \(\text{sinc}(\zeta) = \sin(\zeta)/\zeta\). The filter functions \(\psi, \phi\) are even real-valued functions with \(\hat{\psi}(0) = \phi(0) = 1\).

We remark that the method is explicit if the function \(K(p_1, q)\) takes the form \(K(p_1, q) = \frac{1}{2} p_1^T M(q_2) p_1 + U(q)\). This was not the case for the dumbbell problem of the first section, however, the special structure of the Hamiltonian (1.6) makes the numerical method explicit for this problem too.

As in (Hairer et al., 2002, Sect. XIII.2), we obtain the following condition for method (3.1) to be symplectic (for details see (Cohen, 2004, Chap. 5)).

**Proposition 3.1** If
\[
\hat{\psi}(\zeta) = \phi(\zeta)
\] (3.2)
holds, then method (3.1) is symplectic.

**Example 3.2** Let us come back to the dumbbell spacecraft. In Figure 3, we plot the total energy \(H\) and the oscillatory energy \(I\) obtained by numerical method (3.1). For the filter functions, we choose \(\hat{\psi}_2(\zeta) = \text{sinc}^2(\zeta/2)/\text{sinc}(\zeta)\) and \(\phi_2(\zeta) = \hat{\psi}_2(\zeta)\). With this choice, the numerical method is symmetric and symplectic.

We see that this numerical method also approximately conserves \(H\) and \(I\). This will be explained in the next section.
4 Modulated Fourier expansion of the numerical solution

In this section, we explain, with the help of the modulated Fourier expansion, the good behaviour of our numerical methods (3.1) applied to Hamiltonian problems (1.1) with the Hamiltonian function (1.2).

We are interested in the long-time conservation of the total energy $H$ and of the oscillatory energy $I$ along the numerical solution. We make the following assumptions:

- The initial values satisfy
  \[ \frac{1}{2} \| p^0 \|^2 + \frac{1}{2} \| \Omega q^0 \|^2 \leq E. \]  
  \[ (4.1) \]

- The numerical solution stays in a compact set.

- We impose a lower bound on the step size: $h/\omega \geq c_0 > 0$.

- We assume the numerical non-resonance condition
  \[ | \sin(\frac{1}{2}kh\omega) | \geq c\sqrt{h}, \text{ for } k = 1, \ldots, N, \text{ with } N \geq 2. \]  
  \[ (4.2) \]

For a given $h$ and $\omega$, this condition imposes a restriction on $N$. In the following, $N$ is a fixed integer such that (4.2) holds.

- For the filter functions, we require the following
  \[ | \hat{\psi}(h\omega) | \leq C_1 \text{sinc}^2(\frac{1}{2}h\omega), \]
  \[ | \hat{\psi}(h\omega) | \leq C_2 | \text{sinc}(h\omega) |. \]  
  \[ (4.3) \]

- Finally, for
  \[ \mu(\zeta) = \phi_2(\zeta)\hat{\psi}^{-1}(\zeta), \]  
  we require $\mu(h\omega) \geq c_1 > 0$.  

Now, we can state the main result of this section.
Theorem 4.1 Under the above assumptions, we have, for the numerical solution (3.1),

\[
H(p^n, q^n) = H(p^0, q^0) + O(h) \\
I(p^n, q^n) = I(p^0, q^0) + O(h),
\]

for \(0 \leq nh \leq h^{-N+1}\).

As in Section 2, we can prove that the numerical solution has on a small interval, say \(0 \leq t = nh \leq T\), an expansion

\[
p^n = \sum_{|k| < N} e^{ik\omega t} \eta_h(t) + O(th^{N-2}), \\
q^n = \sum_{|k| < N} e^{ik\omega t} \zeta_h(t) + O(th^{N-2}).
\]  

(4.5)

For the modulation functions, we have the following bounds

\[
\zeta_{h,1} = O(1), \quad \eta_{h,1} = O(1), \quad \zeta_{h,2} = O(\omega^{-2}), \quad \eta_{h,2} = O(\omega^{-1}), \\
\zeta_{h,1}^k = O(\omega^{-2}), \quad \eta_{h,1}^k = O(\omega^{-2}), \quad \zeta_{h,2}^k = O(\omega^{-1}), \quad \eta_{h,2}^k = O(\omega^{-1}), \\
\zeta_{h,1}^k = O(\omega^{-k-1}), \quad \eta_{h,1}^k = O(\omega^{-k-1}), \quad \zeta_{h,2}^k = O(\omega^{-k-2}), \quad \eta_{h,2}^k = O(\omega^{-k-1}), 
\]

(4.6)

for \(k = 2, \ldots, N - 1\). Moreover, we have \(\eta^{-k} = \overline{\eta^k}\) and \(\zeta^{-k} = \overline{\zeta^k}\).

To obtain these results, we use very similar ideas as in the proof of Theorem 5.2 of (Hairer et al., 2002, Sect. XIII.5.2). But, in this case, the proof becomes more complicated and more technical, and is therefore not given here. For details we refer to (Cohen, 2004, Sect. 5.5).

During the proof of these results, we show that the defect of the functions to the right of (4.5) inserted into the method (3.1) is small. This implies that the modulated functions verify the following system (this is to compare with (2.3)–(2.4))

\[
\hat{p}_h(t) - p_h(t - \frac{h}{2}) = -\frac{h}{2} \hat{\psi} q K(\hat{p}_{h,1}(t), \Phi q_h(t - \frac{h}{2})) \\
\hat{q}_{h,1}(t + \frac{h}{2}) - q_{h,1}(t - \frac{h}{2}) = \frac{h}{2} \left( \nabla_{p_1} K(\hat{p}_{h,1}(t), \Phi q_h(t - \frac{h}{2})) \right. \\
\left. + \nabla_{q_1} K(\hat{p}_{h,1}(t), \Phi q_h(t + \frac{h}{2})) \right) + O(h^N) \\
\hat{p}_{h,2}(t + \frac{h}{2}) + \omega \sin(h \omega) q_{h,2}(t - \frac{h}{2}) - \cos(h \omega) \hat{p}_{h,2}(t) = \\
-\frac{h}{2} \hat{\psi}_2(h \omega) \nabla_{q_2} K(\hat{p}_{h,1}(t), \Phi q_h(t + \frac{h}{2})) + O(h^N) \\
\hat{q}_{h,2}(t + \frac{h}{2}) - \cos(h \omega) q_{h,2}(t - \frac{h}{2}) = h \text{sinc}(h \omega) \hat{p}_{h,2} + O(h^N),
\]

(4.7)

where we define \(q_h(t) = \sum_{|k| < N} q^k_h(t), p_h(t) = \sum_{|k| < N} p^k_h(t)\) and \(\hat{p}_h(t) = \sum_{|k| < N} \hat{p}^k_h(t)\)

with \(q^k_h(t) = e^{ik\omega t} \eta^k_h(t), p^k_h(t) = e^{ik\omega t} \theta^k_h(t)\) and \(\hat{p}^k_h(t) = e^{ik\omega t} \zeta^k_h(t)\). Comparing the coefficient of \(e^{ik\omega t}\), we get, writing the resulting equations in terms of \(\hat{p}_h^k, p_h^k\)
and $q_h^k$,

$$
\begin{align*}
\hat{p}_h^k(t) & - p_h^k(t - \frac{h}{2}) = -\frac{h}{2} \hat{\varphi}_{-k} \nabla_{q^r} \mathcal{K}_h(\hat{p}_1(t), \mathbf{q}(t - \frac{h}{2})) \\
q_{h,1}^k(t + \frac{h}{2}) - q_{h,1}^k(t - \frac{h}{2}) & = \frac{h}{2} \left( \nabla_{p_i^r} \mathcal{K}_h(\hat{p}_1(t), \mathbf{q}(t - \frac{h}{2})) \right) + \mathcal{O}(h^N) \\
\n
\hat{p}_h^k(t + \frac{h}{2}) & - \hat{p}_h^k(t) = -\frac{h}{2} \nabla_{q_i} \mathcal{K}_h(\hat{p}_1(t), \mathbf{q}(t + \frac{h}{2})) + \mathcal{O}(h^N) \\
q_{h,2}^k(t + \frac{h}{2}) & - \hat{p}_h^k(t + \frac{h}{2}) = -\frac{h}{2} \psi_2(h \omega) \phi^{-1}_{q_2} \nabla_{q_2} \mathcal{K}_h(\hat{p}_1(t), \mathbf{q}(t + \frac{h}{2})) + \mathcal{O}(h^N) \\
q_{h,2}^k(t + \frac{h}{2}) & - \cos(h \omega) q_{h,2}^k(t - \frac{h}{2}) = h \sin(h \omega) \hat{p}_h^k(t) + \mathcal{O}(h^N),
\end{align*}
$$

where, similarly to (2.5), we define

$$
\mathcal{K}_h(\hat{p}_1, \mathbf{q}) = K(p_1^0, \Phi \mathbf{q}^0) + \sum_{s(\alpha)+s(\beta)=0} \frac{1}{m!n!} D^m_1 D^n_2 K(p_1^0, \Phi \mathbf{q}^0) (\hat{p}_1^\alpha, (\Phi \mathbf{q})^\beta),
$$

for a vector $\hat{p}_1 = (\hat{p}_{h,1}^N, \ldots, \hat{p}_{h,1}^1, \ldots, \hat{p}_{h,1}^0)$ and $\hat{p}_h^k = e^{i k \omega t} \xi_{h,1}^k(t)$, where $\xi_{h,1}^k(t)$ are the modulation functions of $\hat{p}_{h,1}(t)$. The same notation is used for $\mathbf{q}$. From here, we omit the index $h$ in the modulation functions.

As for the exact solution, the modulation functions $\eta = (\eta^{N+1}, \ldots, \eta^1)$ and $\zeta = (\zeta^{N+1}, \ldots, \zeta^1)$ have two formal invariants. We now give the result concerning the first one.

**Lemma 4.2** Under the assumptions of Theorem 4.1, the coefficient functions $\eta$ and $\zeta$ of the modulated Fourier expansion of the numerical solution satisfy

$$
\hat{\mathcal{H}}_h[\eta, \zeta](t) = \hat{\mathcal{H}}_h[\eta, \zeta](0) + \mathcal{O}(h^N),
$$

for $0 \leq t \leq T$. Moreover, we have

$$
\hat{\mathcal{H}}_h[\eta, \zeta](t) = 2 \omega^2 M(h \omega) (\xi_{-1}^{-1})^T \xi_2^{-1} + K(\eta_1, \Phi \zeta) + \mathcal{O}(h).
$$

**Proof.** The idea of the proof is to multiply the relations in (4.8) by a derivative of some coefficient functions, then we take the sum over all $k$ with $|k| < N$ and show that the resulting formula is in fact a total derivative of a function, say, $\hat{\mathcal{H}}_h[\eta, \zeta](t)$.

After multiplications and summations, we get from (4.8) that

$$
\begin{align*}
\sum_{|k| < N} \left\{ -\hat{q}_1^{-k}(t - \frac{h}{2})^T \Phi \hat{\varphi}_{-k} (\hat{p}_h^k(t) - p_h^k(t - \frac{h}{2})) + \hat{p}_h^k(t) \right\} \\
(\hat{q}_1^k(t + \frac{h}{2}) - q_h^k(t + \frac{h}{2})) - \hat{q}_1^{-k}(t + \frac{h}{2})^T (p_1^k(t + \frac{h}{2}) - p_1^k(t)) \\
- \hat{q}_2^{-k}(t + \frac{h}{2})^T \phi_2(h \omega) \hat{\psi}_2^{-1}(h \omega) (p_2^k(t + \frac{h}{2}) + \omega \sin(h \omega) q_2^k(t + \frac{h}{2})) \\
+ \omega \sin(h \omega) q_2^k(t - \frac{h}{2}) - \cos(h \omega) \hat{p}_h^k(t) \right\} \\
= \frac{h}{2} \hat{a}(t) \left\{ \mathcal{K}_h(\hat{p}_1(t), \mathbf{q}(t + \frac{h}{2}))+ \mathcal{K}_h(\hat{p}_1(t), \mathbf{q}(t - \frac{h}{2}) \right\} + \mathcal{O}(h^N).
\end{align*}
$$

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Expanding the functions $\zeta^k(t \pm \frac{h}{2})$ and $\eta^k(t \pm \frac{h}{2})$ around $t$ and replacing $\hat{\rho}^k(t)$ by the last formula of (4.8) shows that the left side of this equation is a total derivative. Moving the terms from the left to the right side of the equation, we get

$$\frac{d}{dt} \tilde{H}_h[\eta, \zeta](t) = \mathcal{O}(h^N),$$

and an integration yields statement (4.10) of the theorem.

This construction of $\tilde{H}_h[\eta, \zeta](t)$, the bounds of the modulation functions, hypothesis (4.3) on the filter functions and the fact that we have $\eta_2^1 = i\omega \zeta_2^1 + \mathcal{O}(h^2)$ yields (4.11) and concludes the proof. \hfill \Box

Concerning the second formal invariant, similarly to formula (6.16) in (Hairer et al., 2002, Sect. XIII.6), we have the following relation

$$\omega \sum_{0 < |k| < N} \frac{i}{k} \left\{ -q^{-k}(t - \frac{h}{2})^T \Phi \tilde{\Psi}^{-1}(\hat{\rho}^k(t) - p^k(t - \frac{h}{2})) + \hat{\rho}_1^{-k}(t)^T \right.$$

$$- (q_1^k(t + \frac{h}{2}) - q_1^k(t - \frac{h}{2})) - q_1^{-k}(t + \frac{h}{2})^T (p_1^k(t + \frac{h}{2}) - \hat{\rho}_1^k(t))$$

$$- q_2^{-k}(t + \frac{h}{2})^T \phi_2(h\omega) \tilde{\psi}_2^{-1}(h\omega) \left( p_2^k(t + \frac{h}{2}) + \omega \sin(h\omega) q_2^k(t - \frac{h}{2}) \right)$$

$$- \cos(h\omega) \hat{\rho}_2^k(t) \left. \right\} = \frac{h\omega}{2} \sum_{0 < |k| < N} \frac{i}{k} \left\{ \hat{\rho}^{-k}(t)^T \nabla_{\rho} K_h(\hat{p}_1(t), \mathbf{q}(t - \frac{h}{2})) \right.$$

$$+ q^k(t - \frac{h}{2})^T \nabla_{\eta} K_h(\hat{p}_1(t), \mathbf{q}(t - \frac{h}{2})) + \hat{\rho}^k(t)^T \nabla_{\rho} K_h(\hat{p}_1(t), \mathbf{q}(t + \frac{h}{2}))$$

$$+ q^k(t - \frac{h}{2})^T \nabla_{\eta} K_h(\hat{p}_1(t), \mathbf{q}(t + \frac{h}{2})) \right\} + \mathcal{O}(h^N).$$

The left side of this equation is again a total derivative. For the right side, we have, using (4.13), $0 + \mathcal{O}(h^N)$. Thus, we get

$$\frac{d}{dt} \tilde{I}_h[\eta, \zeta](t) = \mathcal{O}(h^N),$$

and an integration from 0 to $t$ yields the result (4.14). Like before, statement (4.15) follows from the bounds on the modulation functions. \hfill \Box
We now turn back to the proof of Theorem 4.1. We see that for symplectic numerical methods, we have \( h! = 1 \) and hence \( \tilde{F}_h[\eta, \zeta](nh) = I(p^n, q^n) + \mathcal{O}(h) \) and \( \tilde{F}_h[\eta, \zeta](nh) = H(p^n, q^n) + \mathcal{O}(h) \). This proves the theorem in the case of symplectic methods. The additional hypothesis on the function \( \mu \) (see (4.4)) and the arguments given in the proof of Theorem 7.1. in (Hairer et al., 2002, Sect. XIII.7) help us to show that the numerical method (3.1) nearly preserves the total energy \( H \) and the oscillatory energy \( I \) over long time intervals as stated in Theorem 4.1.

5 Further generalizations

In this section we apply similar techniques, like those given above, to two more general Hamiltonian problems. In the first generalization, we add a small perturbation in the function \( K \) of (1.2). In the second, we extend the single-frequency analysis to the multi-frequency case.

5.1 Adding some perturbation

The techniques of the previous sections can also be applied to the exact solution of Hamiltonian systems (1.1) with the Hamiltonian

\[
H(p, q) = K(p_1, \omega^{-1}p_2, q) + \frac{1}{2}p_2^T p_2 + \frac{\omega^2}{2} q_2^T q_2. \tag{5.1}
\]

Basically, the only thing that changes is the function \( K \), in this case we have

\[
K(p_1, \omega^{-1}p_2, q) = K(p_0, \omega^{-1}p_0, q) + \sum_{s(\alpha)+s(\beta)+s(\gamma)=0} \frac{1}{m!n!l!} D_1^m D_2^n D_3^l K(p_0^\alpha, \omega^{-1}p_0^\beta, q^\gamma)(p_1^\alpha, \omega^{-1}p_0^\beta, q^\gamma).
\]

This yields the following result.

**Theorem 5.1** If the initial values of the Hamiltonian problem (1.1) with the Hamiltonian (5.1) satisfy condition (1.3), then, as long as the exact solution of the system stays in a compact set for \( 0 \leq t \leq \omega^N \), we have

\[
I(p(t), q(t)) = I(p(0), q(0)) + \mathcal{O}(\omega^{-1}) \quad \text{for} \quad 0 \leq t \leq \omega^N, \tag{5.2}
\]

for the oscillatory energy \( I \) of (1.4).

**Numerical methods.** Concerning numerical methods to solve Hamiltonian problems with (5.1), we propose to rewrite this Hamiltonian as

\[
H(p, q) = K(p_1, q) + \frac{1}{2}p_2^T p_2 + \frac{\omega^2}{2} q_2^T q_2 + S(p, q), \tag{5.3}
\]

where \( S(p, q) \) is of size \( \mathcal{O}(\omega^{-1}) \). We then make a splitting and obtain the following numerical method

\[
\Phi_h = (\phi^{S}_{h/2})^* \circ \phi_h \circ \phi^{S}_{h/2}, \tag{5.4}
\]
where the $*$ denotes the adjoint method. For the numerical scheme $\phi_h$, we take the numerical method described in Section 3 and for $\phi^S_h/2$ we take either the explicit Euler method, the Störmer-Verlet scheme or the symplectic Euler method (all methods work as well).

The proofs given in the preceding section can be adapted to the numerical method (5.4). However, they become more technical and are therefore given in Appendix B.

**Example 5.2** The motion of a triatomic molecule can be modeled by a Hamiltonian system with the Hamiltonian function (5.3). To describe the motion of such a molecule, we use polar coordinates as shown in Figure 4.

![Triatomic molecule](image)

Figure 4: Triatomic molecule.

The third mass ($m_3$) is kept fixed, the angle between the other masses is stiff with stiffness constant $\omega_1 = \sqrt{2}$ and the two other springs have a stiffness constant $\omega$. The Hamiltonian reads

$$H(p_{r_1}, p_{r_2}, p_{\theta_1}, p_{\theta_2}, r_1, r_2, \theta_1, \theta_2) = \frac{1}{2}(p_{r_1}^2 + p_{r_2}^2 + (r_2 + 1)^{-2}(p_{\theta_2} - p_{\theta_1})^2$$

$$+ (r_1 + 1)^{-2} p_{\theta_1}^2) + \frac{\omega^2}{2}(r_1^2 + r_2^2 + \frac{\theta_1^2}{2}) + \frac{1}{2} \theta_2^2.$$ (5.5)

The last term is just an external potential to make the molecule moving. After suitable coordinates changes (see Appendix A), this Hamiltonian becomes

$$H(p_1, p_2, q_1, q_2, q_3) = \frac{1}{2}(p_1^2 + p_2^2 + p_{q_1}^2 + p_{q_2}^2 + p_{q_3}^2)$$

$$+ \frac{\omega_1^2}{2}(q_{q_1}^2 + q_{q_2}^2 + q_{q_3}^2) + \frac{1}{4}(q_1 - q_2, q_2 - q_3)^2 - \frac{1}{4}(q_1 - q_3, q_2 - q_2, q_3 - q_3)^2 

- \frac{1}{4} \frac{q_{q_1}^2 + q_{q_2}^2}{1 + q_{q_1}^2} (p_1 + p_{q_2})^2. \quad (5.6)$$

which is of the form (5.3) with

$$S(p, q) = \frac{1}{4} \frac{q_{q_2}^2 + q_{q_3}^2}{1 + q_{q_2}^2} (p_1 - p_{q_2}, q_2 - q_2, q_3 - q_3)^2 - \frac{1}{4} \frac{q_{q_1}^2 + q_{q_2}^2}{1 + q_{q_1}^2} (p_1 + p_{q_2})^2.$$

Let us apply our numerical method to this problem with $\omega = 50$ and initial conditions $p(0) = 1, q_1(0) = 0.4, q_{q_1}(0) = q_{q_2}(0) = 1/\omega, q_{q_3}(0) = 1/\sqrt{2}\omega$. In Figure 5, we plot the Hamiltonian $H$ and the oscillatory energy $I$ obtained by
5.2 Multi-frequency case

In this final section, we briefly discuss the multi-frequency case. We consider the Hamiltonian function (in accordance with the notations used in (Cohen et al., 2004))

\[ H(p, q) = K(p_1, \omega_2^{-1}p_2, \ldots, \omega_l^{-1}p_l, q) + \frac{1}{2} \sum_{j=2}^{l} (p_j^T p_j + \omega_j^2 q_j^T q_j), \]  

(5.7)

where \( q = (q_1, \ldots, q_l) \) with \( q_j \in \mathbb{R}^{d_j} \) (same notation is used for \( p \)), \( \omega_j = \lambda_j \frac{1}{\varepsilon} \) with \( \lambda_j \geq 1 \) real distinct numbers and \( \varepsilon \) a small positive parameter.

Concerning the exact solution of Hamiltonian systems with the Hamiltonian (5.7), in complete analogy to (Cohen et al., 2004, Theorem 6.1), we have the following result.

**Theorem 5.3** Let \( N \) be such that (weak non-resonance condition)

\[ |k \cdot \lambda| \geq C\sqrt{\varepsilon} \quad \text{for } k \in \mathbb{Z}^{l-1} \setminus \mathcal{M} \text{ with } |k| \leq N \]

where \( k \cdot \lambda = k_2 \lambda_2 + \ldots + k_l \lambda_l \), \( |k| = |k_2| + \ldots + |k_l| \) and \( \mathcal{M} = \{ k \in \mathbb{Z}^{l-1} : k_2 \lambda_2 + \ldots + k_l \lambda_l = 0 \} \). If the initial values satisfy (1.3), then, as long as the exact solution of the system stays in a compact set, we have

\[ I_j (p(t), q(t)) = I_j (p(0), q(0)) + O(\varepsilon) \quad \text{for } 0 \leq t \leq \varepsilon \cdot \min(\varepsilon^{-M+1}, \varepsilon^{-N}) \]

where

\[ I_j (p(t), q(t)) = \frac{1}{2} (p_j^T p_j + \omega_j^2 q_j^T q_j) \]  

(5.8)

for \( j = 2, \ldots, \ell \), and with \( M = \min\{|k| : 0 \neq k \in \mathcal{M}\} \).
The idea of the proof is still to write the solution as a modulated Fourier expansion and to construct a system that determine the modulation functions of this expansion. One gets a similar system as system (2.3)–(2.4) and finds almost-invariants related to (5.8).

Concerning the numerical solution, we extend method (5.4) to the multi-frequency case and obtain similar results concerning the near-conservation properties of the numerical solution as those given in (Cohen et al., 2004).

**Example 5.4** Taking different spring constants in Example 5.2, one can get a simple model of the water molecule. Following Izaguirre et al. (1999), we take for the bond length constant $\omega_2 = \sqrt{450}$ and for the harmonic bond angle constant $\omega_3 = \sqrt{55}$. For such a molecule, the Hamiltonian (5.6) now reads

$$H(p_1, p_{2,1}, p_{2,2}, p_3, q_1, q_{2,1}, q_{2,2}, q_3) = \frac{1}{2}(p_1^2 + p_{2,1}^2 + p_{2,2}^2 + p_3^2) + \frac{1}{2}(\omega_2^2 q_{2,1}^2 + \omega_2^2 q_{2,2}^2 + 2 \omega_3^2 q_3^2) + \frac{1}{4}(q_1 - q_3)^2 + \frac{1}{4}\left(\frac{1}{r_0} - \frac{1}{q_{2,2}}\right)^2 - 1 \tag{5.9}$$

where $r_0 = 0.9572$ is the unstretched length of the springs. For initial values $p(0) = 0.5, q_1(0) = \sqrt{2}, q_{2,1}(0) = 1/\omega_2, q_{2,2}(0) = 1/\omega_2, q_3(0) = 1/\omega_3,$ we plot, in Figure 6, the total and oscillatory energies and the the first component of $I$ along the numerical solution of Hamiltonian system with (5.7).

![Figure 6: Energies along the numerical solution of Hamiltonian problem (5.9) with $h = 0.01$ and using for $\phi_{h/2}^S$ the Störmer-Verlet method.](image)

As predicted, $I$ is nearly preserved. This is not the case for $I_2$, due to the fact that the frequencies $\omega_2$ and $\omega_3$ are not sufficiently large. Indeed, in Figure 7, we plot the same quantities as in Figure 6 but with a vector $\omega$ ten times larger.

This time all these quantities are nearly preserved.
Appendix A

Coordinates changes in Example 1.1. To obtain the Hamiltonian function (1.6), we first consider, as in (Sanyal et al., 2003), the Lagrangian

\[ L(\dot{\rho}, \dot{\phi}, \dot{\theta}, r, \phi, \theta, q) = m(\dot{r}^2 + \dot{\theta}^2 + 2q^2 \dot{\theta}^2 + 2q^2 \dot{\phi} + (r^2 + q^2) \dot{\phi}^2) - V_g(r, \theta, q) - 2k(q - l)^2 \]

and scale the variables: for \( R > 0 \), we define \( \tilde{\omega} = \sqrt{\frac{\mu}{R^3}} \) and \( \tau = \tilde{\omega}t \). We also define the new positions \( \rho = \frac{r}{R} \) and \( \sigma = \frac{q}{l} \). In the new variables, the Lagrangian function reads

\[ L(\dot{\rho}, \dot{\phi}, \dot{\theta}, \rho, \phi, \theta, \sigma) = \tilde{m}\tilde{\omega}^2 R^2 \left\{ \dot{\rho}^2 + \varepsilon^2 \dot{\sigma}^2 + \varepsilon^2 \sigma^2 \dot{\theta}^2 + 2\varepsilon^2 \sigma^2 \dot{\phi} \right\} + \left( \rho^2 + \varepsilon^2 \sigma^2 \right) \dot{\phi}^2 + \frac{1}{\rho} \left( 2 - \varepsilon^2 \sigma^2 \rho^2 (1 - 3 \cos^2(\theta)) \right) - 2\chi \varepsilon^2 (\rho - 1)^2 \right\}, \]

with \( \varepsilon = \frac{1}{R} \) and \( \chi = \frac{k}{\tilde{m}\tilde{\omega}^2} \). A last coordinate change, namely \( \sigma = \varepsilon(\sigma - 1) \), leads to

\[ L(\dot{\rho}, \dot{\phi}, \dot{\theta}, \rho, \phi, \theta, \sigma) = \frac{1}{2} \left\{ \dot{\rho}^2 + \rho^2 \dot{\phi}^2 + \sigma^2 + (\varepsilon + \sigma)^2 (\dot{\phi} + \theta)^2 + \frac{2}{\rho} \right\} - \frac{(\varepsilon + \sigma)^2}{\rho^4} (1 - 3 \cos^2(\theta)) - 2\chi \sigma^2 \left\}, \]

where we have chosen the constants such that we obtain a factor \( \frac{1}{2} \) in front of the Lagrangian. Finally, calculating the corresponding momenta, one gets the Hamiltonian function (1.6).

Coordinates changes in Example 5.2. To obtain the Hamiltonian (5.6), we rewrite (5.5) as

\[ H(p, q) = \frac{1}{2} p^T M p + \frac{1}{2} q^T A q + \ldots, \]

where the dots stand for small terms (i.e. terms containing \( r_1 \) or \( r_2 \)).
\((r_1, r_2, \theta_1, \theta_2)\) and
\[
M = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 2 & -1 \\
0 & 0 & -1 & 1
\end{pmatrix}
\quad \text{and} \quad
A = \begin{pmatrix}
\omega^2 & 0 & 0 & 0 \\
0 & \omega^2 & 0 & 0 \\
0 & 0 & \omega^2/2 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}.
\]

We make the symplectic change of coordinates \(\hat{\rho} = Cp, \hat{\varphi} = Dq\) with the following matrices
\[
C = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & \sqrt{2} & -\sqrt{2}/2 \\
0 & 0 & \sqrt{2}/2 & \sqrt{2}
\end{pmatrix}
\quad \text{and} \quad
D = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & \sqrt{2}/2 & 0 \\
0 & 0 & \sqrt{2}/2 & \sqrt{2}
\end{pmatrix}.
\]

The Hamiltonian function now reads
\[
H(\hat{\rho}, \hat{\varphi}) = \frac{1}{2} \hat{\rho}^T \hat{\rho} + \frac{1}{2} \hat{\varphi}^T \hat{\varphi} + \ldots
\]
with
\[
\hat{A} = \begin{pmatrix}
\omega^2 & 0 & 0 & 0 \\
0 & \omega^2 & 0 & 0 \\
0 & 0 & \omega^2 + 1/2 & -1/2 \\
0 & 0 & -1/2 & 1/2
\end{pmatrix},
\]
and it is of the desired form (5.1).

### Appendix B

**Numerical energy conservation for the method (5.4).** Here, we prove the analog of Theorem 4.1 for the numerical method (5.4) where for the choice of the method \(\phi^{S}_{h/2}\), we take the symplectic Euler method.

The proof of this conservation result follows the lines of the proof of the aforementioned theorem: we first recall the numerical method and then give the analog of the two lemmas 4.2 and 4.3. They permit to explain the near-conservation of the total and oscillatory energies for the numerical method (5.4) over long time intervals.

For our particular choice of \(\phi^{S}_{h/2}\), the numerical scheme (5.4) now reads
\[
\begin{align*}
\hat{p}^n &= p^n - \frac{h}{2} \nabla_q S(\hat{p}^n, q^n) \\
\hat{q}^n &= q^n + \frac{h}{2} \nabla_p S(\hat{p}^n, q^n) \\
\hat{p}^{n+1/2} &= \hat{p}^n - \frac{h}{2} \hat{\nabla}_q K(\hat{p}_1^{n+1/2}, \Phi \hat{q}^n) \\
\hat{q}_1^{n+1} &= \hat{q}_1^n + \frac{h}{2} \left( \nabla_p K(\hat{p}_1^{n+1/2}, \Phi \hat{q}_1^n) + \nabla_p K(\hat{p}_1^{n+1/2}, \Phi \hat{q}_1^{n+1}) \right) \\
\hat{q}_2^{n+1} &= \cos(h\omega)\hat{q}_2^n + h \text{ sinc}(h\omega)\hat{p}_2^{n+1/2} \\
\hat{p}_1^{n+1} &= \hat{p}_1^{n+1/2} - \frac{h}{2} \nabla_q K(\hat{p}_1^{n+1/2}, \Phi \hat{q}^{n+1}) \\
\hat{p}_2^{n+1} &= -\omega \sin(h\omega)\hat{q}_2^n + \cos(h\omega)\hat{p}_2^{n+1/2} - \frac{h}{2} \hat{\psi}_2(h\omega)\nabla_q K(\hat{p}_1^{n+1/2}, \Phi \hat{q}^{n+1}) \\
p^{n+1} &= \hat{p}^{n+1} - \frac{h}{2} \nabla_q S(\hat{p}^{n+1}, \hat{q}^{n+1}) \\
q^{n+1} &= \hat{q}^{n+1} + \frac{h}{2} \nabla_p S(\hat{p}^{n+1}, \hat{q}^{n+1}).
\end{align*}
\]

Like in (4.7), we have for the modulated Fourier expansions of the numerical scheme

\[
\begin{align*}
\hat{p}_h(t) &= p_h(t) - \frac{h}{2} \nabla_q S(\hat{p}_h(t), q_h(t)) \\
\hat{q}_h(t) &= q_h(t) + \frac{h}{2} \nabla_p S(\hat{p}_h(t), q_h(t)) \\
\hat{p}_h(t) - \hat{p}_h(t) - \frac{h}{2} = & - \frac{h}{2} \hat{\nabla}_q K(\hat{p}_h, t \Phi \hat{q}_h(t - \frac{h}{2})) \\
\hat{q}_h,1(t + \frac{h}{2}) - \hat{q}_h,1(t - \frac{h}{2}) = & \frac{h}{2} \left( \nabla_p K(\hat{p}_h, 1(t), \Phi \hat{q}_h(t - \frac{h}{2})) \\
& + \nabla_p K(\hat{p}_h, 1(t), \Phi \hat{q}_h(t + \frac{h}{2})) \right) \\
\hat{p}_h,1(t + \frac{h}{2}) - \hat{p}_h,1(t - \frac{h}{2}) = & - \frac{h}{2} \nabla_q K(\hat{p}_h, 1(t), \Phi \hat{q}_h(t + \frac{h}{2})) \\
\hat{p}_h,2(t + \frac{h}{2}) + \omega \sin(h\omega)\hat{q}_h,2(t - \frac{h}{2}) - \cos(h\omega)\hat{p}_h,2(t) = & - \frac{h}{2} \hat{\psi}_2(h\omega)\nabla_q K(\hat{p}_h, 1(t), \Phi \hat{q}_h(t + \frac{h}{2})) \\
\hat{q}_h,2(t + \frac{h}{2}) - \cos(h\omega)\hat{q}_h,2(t - \frac{h}{2}) = & h \text{ sinc}(h\omega)\hat{p}_h,2 \\
p_h(t) &= \hat{p}_h(t) - \frac{h}{2} \nabla_q S(\hat{p}_h(t), q_h(t)) + O(h^N) \\
q_h(t) &= \hat{q}_h(t) + \frac{h}{2} \nabla_p S(\hat{p}_h(t), q_h(t)) + O(h^N),
\end{align*}
\]

where we define \( q_h(t) = \sum_{|k|<N} q_h^k(t) \) and \( p_h(t) = \sum_{|k|<N} p_h^k(t) \) with \( q_h^k(t) = e^{ik\omega t} q_h^k(t) \), \( p_h^k(t) = e^{ik\omega t} p_h^k(t) \) (similar notations are used for \( \hat{p}_h(t), \hat{q}_h(t), \hat{p}_h(t), \hat{q}_h(t) \) and \( \hat{p}_h(t) \)). Comparing the coefficient of \( e^{ik\omega t} \), we get, writing the resulting
equations in terms of $p_h^k, q_h^k, \hat{p}_h^k, \hat{q}_h^k, \hat{p}_h^k$ and $\hat{q}_h^k$.

$$\hat{p}_h^k(t) = \hat{p}_h^k(t) - \frac{h}{2} \nabla_{q^k} S_h(\hat{p}(t), q(t))$$

$$\hat{q}_h^k(t) = \hat{q}_h^k(t) + \frac{h}{2} \nabla_{p^k} S_h(\hat{p}(t), q(t))$$

$$\hat{p}_h^k(t) - \hat{p}_h^k(t - \frac{h}{2}) = -\frac{h}{2} \Psi^{-1} \nabla_{q^k} K_h(\hat{p}_1(t), \hat{q}(t - \frac{h}{2}))$$

$$\hat{q}_h^k(t) + \frac{h}{2} - \hat{q}_h^k(1(t - \frac{h}{2})) = \frac{h}{2} (\nabla_{p^k} K_h(\hat{p}_1(t), \hat{q}(t - \frac{h}{2})) + \nabla_{p^k} K_h(\hat{p}_h^k(1(t), \hat{q}(t + \frac{h}{2})))$$

$$\hat{p}_h^k(t + \frac{h}{2}) - \hat{p}_h^k(t) = -\frac{h}{2} \Psi^{-1} \nabla_{q^k} K_h(\hat{p}_1(t), \hat{q}(t + \frac{h}{2}))$$

$$\hat{p}_h^k(t + \frac{h}{2}) + \omega \sin(h\omega) \hat{q}_h^k(t - \frac{h}{2}) - \cos(h\omega) \hat{p}_h^k(t) =$$

$$-\frac{h}{2} \Psi^{-1} \nabla_{q^k} K_h(\hat{p}_1(t), \hat{q}(t + \frac{h}{2}))$$

$$\hat{q}_h^k(t + \frac{h}{2}) - \cos(h\omega) \hat{q}_h^k(t - \frac{h}{2}) = h \sin(h\omega) \hat{p}_h^k(t)$$

$$\hat{p}_h^k(t) = \hat{p}_h^k(t) - \frac{h}{2} \nabla_{q^k} S_h(\hat{p}(t), q(t)) + \mathcal{O}(h^N)$$

$$\hat{q}_h^k(t) = \hat{q}_h^k(t) + \frac{h}{2} \nabla_{p^k} S_h(\hat{p}(t), q(t)) + \mathcal{O}(h^N),$$

where, similarly to (2.5), we define

$$K_h(\hat{p}_1, q) = K(\hat{p}_1^0, \Phi q^0) + \sum_{s(\alpha) + t(\beta) = 0} \frac{1}{m!n!} D_1^m D_2^n K(\hat{p}_1^0, \Phi q^0)(\hat{p}_1^+, (\Phi q)^\beta),$$

for a vector $\hat{p}_1 = (\hat{p}_{h,1}^{N+1}, \ldots, \hat{p}_{h,1}^0, \ldots, \hat{p}_{h,1}^{N-1})$ and $\hat{p}_h^k = e^{i\omega t} \xi_h^k(t)$, where $\xi_h^k(t)$ are the modulation functions of $\hat{p}_{h,1}(t)$. The same notation is used for $q$ and for the function $S_h(p, q)$. From here, we do not write the index $h$ in the modulation functions.

As before, the modulation functions $\eta = (\eta^{N+1}, \ldots, \eta^{N-1})$ and $\zeta = (\zeta^{N+1}, \ldots, \zeta^{N-1})$ have two formal invariants. We now give the result concerning the first one.

**Lemma B.1** Under the assumptions of Theorem 4.1, the coefficient functions $\eta$ and $\zeta$ of the modulated Fourier expansion of the numerical solution satisfy

$$\hat{H}_h[\eta, \zeta](t) = \hat{H}_h[\eta, \zeta](0) + \mathcal{O}(th^N),$$

for $0 \leq t \leq T$. Moreover, we have

$$\hat{H}_h[\eta, \zeta](t) = 2\omega^2 \mu(h\omega)(\zeta_2^{-1})^T \zeta_2^1 + K(\eta_1, \Phi \zeta) + \mathcal{O}(h).$$

**Proof.** To simplify the following proof, we consider the case $\mu(h\omega) = 1$ (that is, the numerical method $\phi_h$ in (5.4) is symplectic).

Multiplying the relations in (B.2) (except those that contain the function $S_h(p, q)$, they will be used after) by the same coefficient functions as in (4.12)
and summing up, we get
\[
\sum_{|k| < N} \left\{ \hat{q}^{-k}(t - \frac{h}{2})^T (\hat{p}^k(t) - \hat{p}^k(t - \frac{h}{2})) + \hat{p}^{-k}(t)^T (\hat{q}^k(t + \frac{h}{2}) - \hat{q}^k(t)) \right\}
\]
\[
= \frac{h}{2} \frac{d}{dt} \left\{ \mathcal{K}_h(\hat{p}(t), \hat{q}(t - \frac{h}{2})) + \mathcal{K}_h(\hat{p}(t), \hat{q}(t + \frac{h}{2})) \right\}.
\]

Expanding the functions \(\zeta^k(t \pm \frac{h}{2})\) and \(\eta^k(t \pm \frac{h}{2})\) around \(t\) shows that the left side of this equation is a total derivative. In contrast to the proof of Lemma 4.2, we have the following term
\[
\sum_{|k| < N} \left\{ \hat{q}^{-k}(t - \frac{h}{2})^T \hat{p}^k(t - \frac{h}{2}) - \hat{q}^{-k}(t + \frac{h}{2})^T \hat{p}^k(t + \frac{h}{2}) \right\}
\]
which depends on the numerical method \(\phi_h^{S/2}\). In order to show that this expression is also a total derivative, we insert the two first and two last formulas of (B.2) into it and get
\[
\sum_{|k| < N} \left\{ \hat{q}^{-k}(t - \frac{h}{2})^T \hat{p}^k(t - \frac{h}{2}) - \hat{q}^{-k}(t + \frac{h}{2})^T \hat{p}^k(t + \frac{h}{2}) \right\}
\]
\[
= \frac{h}{2} \frac{d}{dt} \left\{ \mathcal{K}_h(\hat{p}(t), \hat{q}(t - \frac{h}{2})) + \mathcal{K}_h(\hat{p}(t), \hat{q}(t + \frac{h}{2})) \right\} + O(h^N).
\]
The two first terms of this equation are in fact a total derivative. To show that
the remaining terms also are a total derivative, we add and remove \(\hat{p}^{-k}(t - \frac{h}{2})^T \nabla_{p^{-k}} \mathcal{S}_h(\hat{p}(t - \frac{h}{2}), \hat{q}(t - \frac{h}{2}))\)
and \(\hat{p}^{-k}(t + \frac{h}{2})^T \nabla_{p^{-k}} \mathcal{S}_h(\hat{p}(t + \frac{h}{2}), \hat{q}(t + \frac{h}{2}))\)
to make appear the total derivative of the functions \(\mathcal{S}_h(\hat{p}(t - \frac{h}{2}), \hat{q}(t - \frac{h}{2}))\) and of
the expressions \(p^k(t - \frac{h}{2})^T \nabla_{p^k} \mathcal{S}_h(\hat{p}(t - \frac{h}{2}), \hat{q}(t - \frac{h}{2}))\) and \(\nabla_{q^{-k}} \mathcal{S}_h(\hat{p}(t + \frac{h}{2}), \hat{q}(t + \frac{h}{2}))\) (and the corresponding one with argument \(t + \frac{h}{2}\)).
Moving the terms from the left to the right side of the equation, we get
\[
\frac{d}{dt} \mathcal{H}_h(\eta, \zeta)(t) = O(h^N),
\]
and an integration yields statement (B.4) of the theorem.

This construction of \( \hat{H}_h[\eta, \zeta](t) \), the bounds of the modulation functions, hypothesis (4.3) on the filter functions and the fact that we have \( \eta_k^2 = \omega_k \zeta_k^2 + \mathcal{O}(h^2) \) yields (B.5) and concludes the proof. \( \square \)

Concerning the second formal invariant, similarly to formula (6.16) in (Hairer et al., 2002, Sect. XIII.6), we have the following relation

\[
\omega \sum_{0 < |k| < N} ik \left( (\hat{p}^k)^T \nabla_{\hat{p}^k} K_h(\hat{p}_1, q) + (q^k)^T \nabla_{q^k} K_h(\hat{p}_1, q) \right) = 0, \tag{B.6}
\]

for \( K_h(\hat{p}_1(t), q(t)) \) of (B.3). This formula is also true for the function \( S_h(p(t), q(t)) \). The same tricks used in the proof of the latter lemma permit to prove the following lemma.

**Lemma B.5** Under the assumptions of Theorem 4.1, the coefficient functions of the modulated Fourier expansion of the numerical solution satisfy

\[
\dot{\tilde{I}}_h[\eta, \zeta](t) = \tilde{I}_h[\eta, \zeta](0) + \mathcal{O}(th^N), \tag{B.7}
\]

for \( 0 \leq t \leq T \). Moreover, we have

\[
\dot{\tilde{I}}_h[\eta, \zeta](t) = 2\omega^2 \mu(h\omega)(\zeta_i^{-1})^T \zeta_i^2 + \mathcal{O}(h^2). \tag{B.8}
\]

**Proof.** Again, for simplification, we only give the proof for \( \mu(h\omega) = 1 \). This time, we multiply and sum the equations in (B.2) in order to apply the identity (B.6). We get

\[
i\omega \sum_{0 < |k| < N} k \left\{ -\tilde{q}^{-k}(t - \frac{h}{2})^T (\hat{p}^k(t) - \hat{p}^k(t - \frac{h}{2})) + \hat{p}_1^{-k}(t)^T (\hat{q}_1(t) + \hat{q}_1(t - \frac{h}{2})) - \hat{p}_1^{-k}(t)^T (\hat{q}_1(t) + \hat{q}_1(t - \frac{h}{2})) \right\}
\]

\[
\left( \hat{q}_1(t + \frac{h}{2}) - \hat{q}_1(t - \frac{h}{2}) \right) - \hat{p}_1^{-k}(t)^T (\hat{p}_1(t + \frac{h}{2}) - \hat{p}_1(t)) \right) - \hat{q}_2^{-k}(t + \frac{h}{2})^T (\hat{p}_2(t + \frac{h}{2}) - \hat{p}_2(t)) + \omega \sin(h\omega) \hat{q}_2^{-k}(t - \frac{h}{2}) - \cos(h\omega) \hat{p}_2^{-k}(t) \right) \}
\]

\[
= \frac{h\omega}{2} \sum_{0 < |k| < N} ik \left\{ \hat{p}^{-k}(t)^T \nabla_{\hat{p}^k} K_h(\hat{p}_1(t), \hat{q}(t - \frac{h}{2})) \right.
\]

\[
+ \hat{q}^{-k}(t - \frac{h}{2})^T \nabla_{\hat{q}^k} K_h(\hat{p}_1(t), \hat{q}(t - \frac{h}{2})) + \hat{p}^{-k}(t)^T \nabla_{\hat{p}^k} K_h(\hat{p}_1(t), \hat{q}(t + \frac{h}{2}))
\]

\[
+ \hat{q}^{-k}(t + \frac{h}{2})^T \nabla_{\hat{q}^k} K_h(\hat{p}_1(t), \hat{q}(t + \frac{h}{2})) \right\}. 
\]

Inserting the definition of the modulation functions corresponding to the symplectic Euler scheme and its adjoint, adding and removing the following terms

\[
\hat{p}^{-k}(t - \frac{h}{2})^T \nabla_{\hat{p}^k} S_h(\hat{p}(t - \frac{h}{2}), q(t - \frac{h}{2}))
\]

and

\[
\hat{p}^{-k}(t + \frac{h}{2})^T \nabla_{\hat{p}^k} S_h(\hat{p}(t + \frac{h}{2}), q(t + \frac{h}{2}))
\]

we see that the left side of this equation is again a total derivative. Using (B.6), the right side is zero. Thus, we get

\[
\frac{d}{dt} \tilde{I}_h[\eta, \zeta](t) = \mathcal{O}(h^N),
\]

and an integration from 0 to \( t \) yields the result (B.7). Like before, statement (B.8) follows from the bounds on the modulation functions. \( \square \)
These two lemmas explain the long-time conservation of the total and of the oscillatory energies along the numerical solution of the scheme (5.4).

Finally, we would like to mention that the proofs given above can also be done for the composition

$$\Phi_h = \phi_{h/2}^S \circ \phi_h \circ \phi_{h/2}^S,$$

where $\phi_{h/2}^S$ is still the symplectic Euler method. This leads to conservation properties for a symplectic, non-symmetric numerical scheme.

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References


