European Society of Computational Methods in Sciences and Engineering (ESCMSE)

Journal of Numerical Analysis, Industrial and Applied Mathematics (JNAIAM)
vol. ??, no. ??, 2009, pp. ??-??
ISSN 1790–8140

Energy drift in the numerical integration of Hamiltonian problems[1]

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Received February 7, 2008; accepted February 18, 2009.

Abstract: When approximating reversible Hamiltonian problems, the presence of a "drift" in the numerical values of the Hamiltonian is sometimes experienced, even when reversible methods of integration are used. In this paper we analyze the phenomenon by using a more precise definition of *time reversal symmetry* for both the continuous and the discrete problems. A few examples are also presented to support the analysis.

Keywords: Time reversal symmetry, Reversible Hamiltonian systems, Symmetric methods, Periodic orbits, Numerical drift.

Mathematics Subject Classification: 65L06, 65P10, 37J99.

1 Introduction

Many problems deriving from the mathematical modeling of mechanical systems, molecular dynamics, and so forth, are in Hamiltonian form, i.e.

$$y' \equiv \begin{pmatrix} q \\ p \end{pmatrix}' = \begin{pmatrix} \nabla_p H(q,p) \\ -\nabla_q H(q,p) \end{pmatrix} \equiv J \nabla_y H(q,p), \tag{1}$$

where, by setting I_m the identity matrix of dimension m,

$$q, p \in \mathbb{R}^m, \qquad J = J_{2m} \equiv \begin{pmatrix} & I_m \\ -I_m & \end{pmatrix}, \tag{2}$$

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and $H(q,p)$ is the Hamiltonian function. We shall use the notation $H(y)$, when this will be convenient for sake of brevity. Hereafter, we assume that the initial condition for (1) is given at

$$t_0 = 0, \qquad y(t_0) = y_0 \equiv \begin{pmatrix} q_0 \\ p_0 \end{pmatrix}. \tag{3}$$

When speaking about mechanical systems, the components of q and p are, respectively, the positions and the momenta while $H(q,p)$ often represents the total energy of the system.

Many mechanical systems are *reversible*. Usually this property is meant in the sense that if the time is reversed, the momenta are reversed as well, and the trajectory retraces backward in time. The numerical approximation of such systems has been recently studied by many authors (see, e.g. [3, 4] and the references therein). Nevertheless, in our opinion, the definition of *reversibility* is sometimes confused and, therefore, the main aim of this paper is to make this notion more precise in order to analyze the energy drift phenomenon sometimes observed in the numerical simulations (see, e.g., [2, 5]). With this premise, in the next section the notion of *time reversal symmetry* is discussed in detail for continuous problems; then, the subsequent section concerns its discrete counterpart; finally, the last two sections contain, respectively, some examples of application and a few concluding remarks.

2 Time reversal symmetry

Ce qui nous rend ces solutions périodiques si précieuses, c'est qu'elles sont, pour ainsi dire, la seule brèche par où nous puissions essayer de pénétrer dans une place jusqu'ici réputée inabordable.

H. Poincaré

Very often, especially when dealing with mechanical systems, the Hamiltonian satisfies the property

$$H(y) = H(Sy), \tag{4}$$

where S is a symmetric matrix which, usually, assumes the form

$$S = \begin{pmatrix} I_m & \\ & -I_m \end{pmatrix}, \tag{5}$$

even though any symmetric matrix satisfying (see (2))

$$SJS = -J. \tag{6}$$

is allowed, e.g.,

$$S = \begin{pmatrix} -I_m & \\ & I_m \end{pmatrix}. \tag{7}$$

As an example, both (5) and (7) are allowed in the case of the pendulum problem, which we shall consider later. Again, we emphasize that in the following we shall often consider the form (5), but all properties derived for it can be extended to any symmetric matrix S satisfying (6). This because, from the latter property, a corresponding property of the vector field associated with (1) derives. Indeed, by considering that

$$\nabla_y H(y) = \nabla_y H(Sy) = S^T \nabla_{(Sy)} H(Sy) = S \nabla_{(Sy)} H(Sy),$$

one has

$$Sy' = SJ\nabla_y H(y) = SJS\nabla_{Sy} H(Sy) = -J\nabla_{Sy} H(Sy). \tag{8}$$

That is, the vector $Sy(-t)$ satisfies the same equation as $y(t)$. Consequently, the following result holds true.

Theorem 1 *Let the Hamiltonian function of equation (1) satisfy (4)-(6) and assume that the initial condition (3) satisfies* $y_0 \in \ker(I - S)$. *Then,*

$$y(-t) \equiv Sy(t), \qquad t \geq 0. \tag{9}$$

Remark 1 *When* S *is defined according to (5), one immediately obtains that*

$$\ker(I - S) = \left\{ \begin{pmatrix} q \\ 0 \end{pmatrix} \; : \; q, 0 \in \mathbb{R}^m \right\}.$$

Remark 2 *The property that* $y(t)$ *and the time reversed vector* $Sy(t)$ *are both solution of (1), is often referred as* time reversal symmetry *(TRS, hereafter). We shall, however, according to some authors (see, e.g. [8, p. 234]), restrict such expression to the case where the two solutions have at least two distinct common points: the initial one,* y_0, *and, say,* $y^* \neq y_0$. *In other words, we restrict the TRS to periodic solutions (librations, in the astronomical terminology [7, p. 458]), according, as much as possible, to the intuitive definition (see, e.g. [6]) that a motion has TRS when it is impossible to distinguish whether its "movie" is played forward or backward in time. In this respect, it is obvious that when* $y(t)$ *has an open orbit, then at least one of its entries does not remain bounded for* $t > 0$, *and this will certainly characterize the time direction (i.e., the forward or backward playing of the "movie").*

According to Remark 2, we are interested in the case where the trajectory is (nontrivially) *periodic* of *period* $2T$, i.e. satisfying, for $y_0 \in \ker(I - S)$,

$$y(T) = y(-T), \qquad \text{i.e.} \qquad y(T) = Sy(T). \tag{10}$$

This implies that $y(T) \neq y_0$ and $y(T) \in \ker(I-S)$ as well. In such a case, the two trajectories $y(t)$ and $Sy(t)$ are on the *same orbit* for $t \in [0, +\infty)$. This means that each point on the orbit can be reached both *forward* and *backward* in time. This fact naturally leads to the following definition of TRS.

Definition 1 *An Hamiltonian problem (1)–(3) satisfying (4)-(6) has TRS if the initial condition* y_0 *satisfies* $y_0 = Sy_0$ *and both* $y(t)$ *and* $Sy(t)$ *are on the same orbit for* $t \in [0, +\infty)$.

In the next section, we shall consider a corresponding *discrete time reversal symmetry*, which is the exact counterpart of the continuous one just defined, to be fulfilled by the orbits of suitable discrete numerical methods approximating problem (1)–(3).

In the following we shall study in detail the simpler case where $m = 1$ and we shall consider, in more details, the matrix S in (5). In such a case, Theorem 1 can be rewritten as follows.

Theorem 2 *Let the Hamiltonian function of equation (1) satisfy (4) and assume that the initial condition (3) satisfies* $y_0 \in \ker(I - S)$, *where the matrix* S *is given by (5). Consequently,*

$$y_0 \equiv \begin{pmatrix} q_0 \\ 0 \end{pmatrix}, \qquad q_0 \in \mathbb{R}, \tag{11}$$

and

$$q(-t) \equiv q(t), \quad p(-t) = -p(t), \qquad t \geq 0. \tag{12}$$

Moreover, if there exists $T > 0$ *such that* $p(T) = 0$, *then the solution is periodic of period* $2T$ *and, therefore, the problem has the TRS property.*

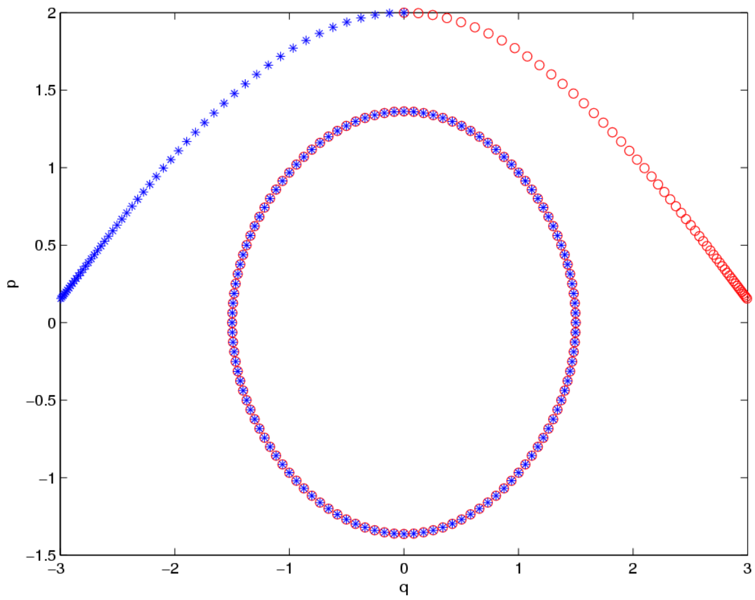

Figure 1: Pendulum problem. *Future solutions* (o) and *past solutions* (*).

Example 1 *The nonlinear pendulum is described by the equation*

$$\frac{d}{dt}\begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} p \\ -\sin(q) \end{pmatrix}, \tag{13}$$

with Hamiltonian

$$H(q,p) = \frac{1}{2}p^2 + 1 - \cos q. \tag{14}$$

This problem has both the symmetries (5) and (7). We shall here consider only the latter one. In the phase plane it has two types of orbits: the open ones and the closed ones around the critical point $(0,0)$ *(see Figure 1).*

The open orbits do not have a second point in $\ker(I-S)$*. On such orbits the variable* p *is periodic while the variable* q *is not, since it doesn't remain bounded. By looking only at the variable* p *it is impossible to distinguish if it corresponds to positive or negative values of time. On the contrary, the variable* q *gives us such a possibility: it is enough to establish that the "movie is played" forward if* q *is growing and backward if* q *is decreasing. As matter of fact, the open orbits do not satisfy Definition 1 since the two semi-orbits do not have common points except for the initial one. The same doesn't apply to the closed orbits, whose points are simultaneously on both future and past semi-orbits (see Figure 1).*

Example 2 *In the previous example, the variable* p *is the derivative of* q*. By reversing the sign of time, automatically it is reversed the velocity,* p*, of the variable* q*. However, in general, this is not always true: a sign change of* dq/dt *may not affect the sign of the second variable* p*. Consider, for example*[4]*, the problem defined by the following Hamiltonian [2, Eq. (4.1)],*

$$H(q,p) = T(p) + U(q) \equiv \frac{p^3}{3} - \frac{p}{2} + \frac{q^6}{30} + \frac{q^4}{4} - \frac{q^3}{3} + \frac{1}{6}, \tag{15}$$

[4] A more realistic example could be the equation describing the motion of an electron in a magnetic field.

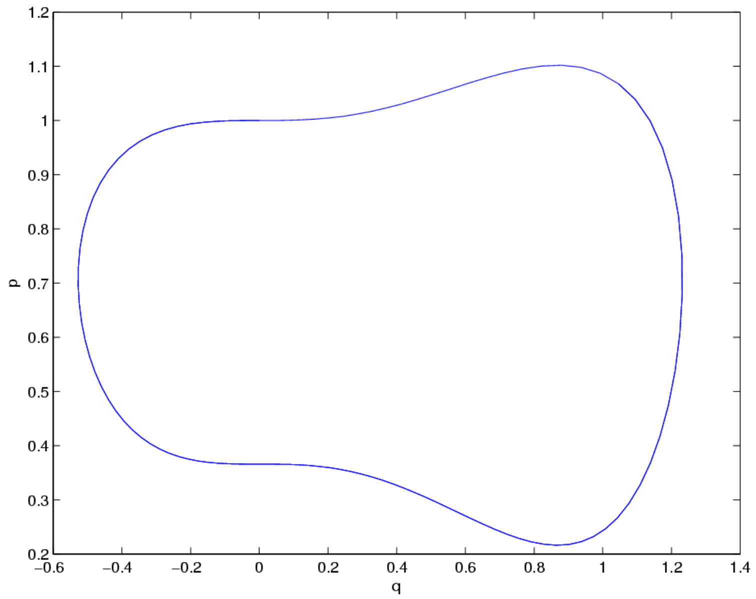

Figure 2: Solution of the problem defined by the Hamiltonian (15) and the initial condition (16).

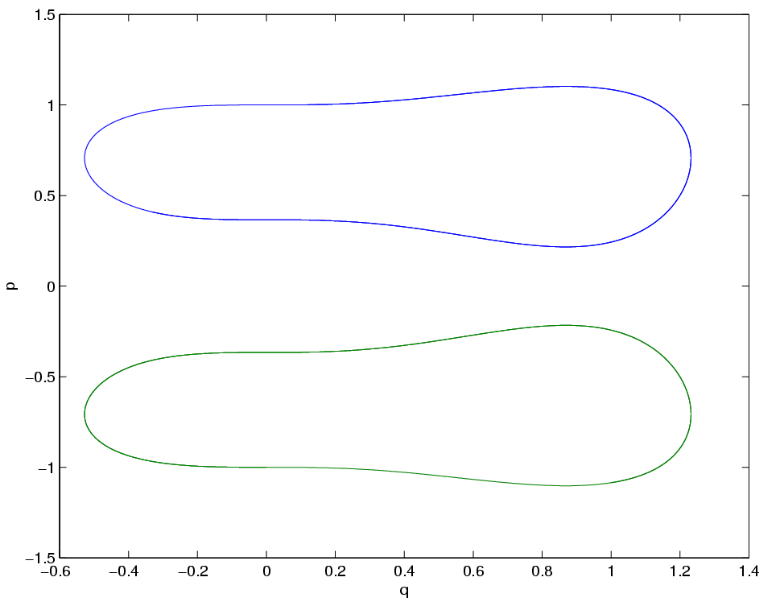

Figure 3: Problems defined by the Hamiltonian (17); trajectories with initial conditions (16) (upper plot) and (18) (lower plot).

with initial condition

$$q(0) = 0, \qquad p(0) = 1. \tag{16}$$

In such a case, even though the orbit is periodic (see Figure 2), the Hamiltonian doesn't satisfy (4), so that there is no TRS. However, the symmetry property (4), with S given by (5), is satisfied when considering the symmetrized *problem [2, Eq. (4.2)], with the Hamiltonian*

$$H(q,p) = (U(q) + T(p))(U(q) + T(-p)) \equiv U(q)^2 - T(p)^2, \tag{17}$$

and the same initial condition (16). In this case, even though the corresponding orbit is the same shown in Figure 2 and, moreover, (4) is obviously satisfied, the problem has no TRS, since the initial condition doesn't belong to $\ker(I-S)$ *(actually no points of the orbit belong to* $\ker(I-S)$*). To be more precise, in the case of the symmetrized problem (17), both variables q and p are periodic (they stay on a closed orbit). The transformation* $t \to -t$ *leaves unchanged the orbit. The transformation* $y \to Sy$*, however, does not, since, for all* $t \in [0, +\infty)$ *the two points* $y(t)$ *and* $Sy(t)$ *are on two separate orbits, even though both of them are solutions of the same equation. For example, in Figure 3 there are the plots of the orbit starting at (16) (upper plot) and that of the orbit starting at the symmetric point of (16) (see (5)), i.e.,*

$$q(0) = 0, \qquad p(0) = -1. \tag{18}$$

The paradox is explained by considering that they never can be the same solution, since there doesn't exist a nontrivial point of the form $(q,0)^T \in \ker(I-S)$*. Consequently, there is no TRS, according to our Definition 1.*

Remark 3 (Symmetry of the equations and TRS) *We have seen that the symmetry (4) of the Hamiltonian may imply the TRS. As already said, the two properties are often confused. Indeed, the first one regards the law of motion, i.e. the equations, while the second one regards the solutions, which, however, do depend also on the specified initial conditions. The fact that the symmetry of the equations and the TRS are often confused is testified by the following citation of J. C. Baez [9]:*

"Even people who claim to understand the distinction often slip ... I become infuriated when authors confuse symmetry of the laws with symmetry of the state."

The symmetry of the state is then a property of certain solutions but, in general, not of all of them.

3 Discrete approximation

In his work on dynamics Poincaré was led to focus attention primarily upon the periodic motions ... and it became a task of the first order of importance for him to determine what the actual distribution of the periodic motions was ....

G. D. Birkhoff

We are now concerned with the numerical integration of the trajectories of equation (1). We shall here consider (convergent) block methods which, at the first integration step (which is the one here considered for sake of simplicity), generate a discrete problem in the form

$$A \otimes I_{2m}\mathbf{y} - hB \otimes J_{2m}\nabla H(\mathbf{y}) = \mathbf{0}, \tag{19}$$

where h is the stepsize, the two matrices $A, B \in \mathbb{R}^{r\times r+1}$ (A with full rank) characterize the numerical method, and

$$\begin{aligned} \mathbf{y} &= ((q_0,p_0),(q_1,p_1),\dots(q_r,p_r))^T, \\ \nabla H(\mathbf{y}) &= (\nabla H(q_0,p_0),\nabla H(q_1,p_1),\dots\nabla H(q_r,p_r))^T. \end{aligned} \tag{20}$$

Moreover, the discrete solution is assumed to be uniquely determined once the initial condition $y_0 = (q_0,p_0)^T$ is fixed.

We observe that this is a quite general framework, which encompasses most of the available numerical methods. For example:

- Runge-Kutta methods,
- block Boundary Value Methods (block BVMs, see [1] for details),
- sequential applications of the above methods.

Remark 4 *We observe that the equations (19) are defined up to left multiplication by any nonsingular $r \times r$ matrix. Therefore, by also considering that the method is convergent, we may always assume that A satisfies the following* symmetry property*:*

$$P_r A P_{r+1} = -A, \qquad P_\ell = \begin{pmatrix} & & & 1 \\ & & \cdot & \\ & \cdot & & \\ 1 & & & \end{pmatrix}_{\ell\times\ell}, \quad \ell = r, r+1. \tag{21}$$

Example 3 *In the case of a Runge-Kutta method, one has that (19) holds true with*

$$A = \begin{pmatrix} -1 & 1 & & \\ \vdots & & \ddots & \\ -1 & & & 1 \end{pmatrix}_{r\times r+1}.$$

Then, left multiplication with the matrix

$$\begin{pmatrix} 1 & & & \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{pmatrix}_{r\times r},$$

results in the following "new" matrix A:

$$\begin{pmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{pmatrix}_{r\times r+1},$$

which fulfills (21).

We are now in the position of stating the following definition (see [1]).

Definition 2 *We say the the block method (19) is* symmetric *if, when it is rewritten so that (21) holds, it also satisfies*

$$P_r B P_{r+1} = B. \tag{22}$$

Remark 5 *According to this definition, symmetric Runge-Kutta methods are, for example, Gauss-Legendre and Lobatto IIIA methods. Further examples are provided by symmetric block BVMs [1].*

This definition of symmetry for a numerical method in the form (19) is exactly the same as the usual definition which requires the given method to coincide with its adjoint method (see, e.g., [3, 4]). In this setting, this is confirmed by the following result (see also [1]).

Theorem 3 *The method (19) provides the same discrete solution, either when started from (q_0, p_0) with stepsize h or when started from (q_r, p_r) with stepsize $-h$, if and only if it is symmetric (i.e. (21) and (22) hold true).*

Proof Indeed, by considering (21) and (22), one straightforwardly obtains that

$$\begin{aligned}\mathbf{0} &= P_r A P_{r+1} \otimes I_{2m} \left(P_{r+1} \otimes I_{2m}\right) \mathbf{y} - h P_r B P_{r+1} \otimes J_{2m} \left(P_{r+1} \otimes I_{2m}\right) \nabla H(\mathbf{y}) \\ &= -A \otimes I_{2m} \left(P_{r+1} \otimes I_{2m}\right) \mathbf{y} - B \otimes J_{2m} \nabla H\left(\left(P_{r+1} \otimes I_{2m}\right) \mathbf{y}\right).\end{aligned}$$

The first part of the thesis then follows by considering that left multiplication by $P_{r+1} \otimes I_{2m}$ reverses the order of the (block) entries of the vectors. The converse easily follows by reversing the above arguments. □

Concerning the time reversal symmetry for the discrete solutions, the following result is the discrete counterpart of Theorem 1.

Lemma 1 *Suppose that:*

i) the numerical method in the above form (19) is symmetric;

ii) the Hamiltonian function satisfies (4)-(6);

iii) $y_0 \in \ker(I - S)$.

Then, if $\{y_n\}$ is the solution for positive h, $\{Sy_n\}$ is the solution for negative h.

Proof By setting $\mathcal{S} = I_r \otimes S$ and $\mathcal{J} = I_r \otimes J$, we obtain

$$\begin{aligned}\mathbf{0} &= \mathcal{S}(A \otimes I_{2m})\mathcal{S}\,\mathcal{S}\mathbf{y} - h\left(\mathcal{S}(B \otimes I_{2m})\mathcal{S}\right)(\mathcal{S}\mathcal{J}\mathcal{S})\mathcal{S}\nabla H(\mathbf{y}) \\ &= (A \otimes I_{2m})\mathcal{S}\mathbf{y} + h(B \otimes I_{2m})\mathcal{J}\mathcal{S}\nabla H(\mathbf{y}) \;=\; (A \otimes I_{2m})\mathcal{S}\mathbf{y} + h(B \otimes J_{2m})\nabla H(\mathcal{S}\mathbf{y}),\end{aligned}$$

where the relation $\mathcal{S}\mathcal{J}\mathcal{S} = -\mathcal{J}$ has been used. In other words, if $\{y_0, y_1, \ldots, y_r\}$ is the discrete solution obtained with stepsize h, then $\{Sy_0, Sy_1, \ldots, Sy_r\}$ is the solution obtained with stepsize $-h$. □

On the contrary of what happens in the continuous case, in general it is not true that, when the method is applied to a continuous problem with TRS, there is another point of the discrete solution which belongs to $\ker(I - S)$. Said differently, not all the discrete trajectories are periodic. Nevertheless, it is sometimes possible, by using the continuous dependence of the discrete trajectories from the parameter h (in a suitable neighborhood of the origin), to force one or more components of the trajectories to enter $\ker(I - S)$. In the particular case $m = 1$, the following result, which provides the discrete extension of Theorem 2, holds true.

Theorem 4 *Suppose that:*

i) the continuous problem satisfies the hypotheses of Theorem 2;

ii) the continuous problem has periodic solutions passing by $y_0 \in \ker(I - S)$.

Then, by considering the application of the method (19):

- *if the method is symmetric, i.e., it satisfies both (21) and (22), there exist infinitely many discrete periodic orbits which accumulate as $h \to 0$;*
- *if a discrete periodic trajectory exists, then the method is symmetric.*

Proof Since the method is convergent and the continuous solution $y(t)$ is periodic, for h small enough there exist values of the stepsize such that, for any integer value of r greater than a suitable integer r_0, $y_r \in \ker(I - S)$ and $y_r \neq y_0$, where y_r denotes, as usual, the r-th point of the discrete trajectory obtained with the given stepsize h. That is, (see (5)), $0 \neq q_r \neq q_0$ and $p_r = 0$. Consequently, we have that $y_0, y_1, \ldots y_r$ are on the positive orbit and $Sy_0, Sy_1, \ldots Sy_r$ are on the negative orbit. Both orbits crosses at y_r, since $y_r = Sy_r$. The problem is now whether the points $\{y_i\}_{i>r}$ are new points or they coincide with $\{Sy_i\}_{i<r}$. If so, the solution is a periodic one. However, the result of Lemma 1 allows to conclude that a symmetric orbit of period $2r$ exists. In this case we have that $y_i = Sy_{2r-i}$, $i = 0, \ldots, 2r$.

Suppose now that a periodic trajectory exists. Then, from Lemma 1, also the backward trajectory is periodic and traces back the same points of the forward trajectory in reverse order. Consequently, from Theorem 3 the method coincides with its adjoint, i.e., it is symmetric. □

Remark 6 *In light of the above result, we have that only symmetric methods can generate discrete periodic orbits. Moreover, since these methods coincide with their respective adjoint ones, the points on the discrete orbit can be reached both in* forward *and in* reverse *(discrete) time. In analogy with the continuous case (see Definition 1), we say that* the discrete periodic orbit has the TRS property*.*

Remark 7 *In the above theorem, the assumption that h is small enough has been supposed for convenience. As matter of fact, some periodic orbits may occur for quite large values of h. For example, for the pendulum problem (13), periodic orbits of low period (say, 4), can be obtained for relatively large stepsizes ($h \simeq 2.09$).*

The importance of the existence of discrete periodic orbits is given by the following result.

Theorem 5 *Assume that, for a given stepsize h, a periodic orbit exists. Then, no drift of the Hamiltonian function can occur during the integration with that stepsize.*

Proof When the discrete trajectory is periodic, clearly at each period the Hamiltonian function assumes the same values on the discrete solution and, therefore, no drift can occur. □

A straightforward and useful generalization of the previous theorem is given by the following result.

Corollary 1 *The result of Theorem 5 continues to hold when the initial condition is not given by (3), but such point belongs to the orbit.*

Proof Indeed, let τ be the time when the trajectory passes from (3). From that point, all the above arguments continues to hold, by considering a time shift equal to τ. Similar arguments hold also true in the discrete case, provided that the method is symmetric, since there will exist infinitely many values of the stepsize h such that the discrete trajectory passes, for $r = r(h)$, from a point in the form $(\xi_h, 0)$. From that point, the result of Theorem 5 then applies. □

Remark 8 *From the above arguments, it follows that, when the continuous problem has the TRS property and the method is symmetric, periodic orbits accumulate as $h \to 0$. Consequently, for h suitably small, we are always "close" to a periodic orbit and, therefore, no drift is expected in the numerical Hamiltonian. Conversely, a drift may be observed when the discrete periodic orbits occur only in correspondence of isolated values of h. Nevertheless, if one is able to find one of such values, the drift will disappear.*

In addition to this, it is worth noting that, even in the case where there is no TRS and a drift is observed, such a drift is (for symmetric methods) in general less evident as the dimension r of the matrices in (19), defining the method, increases. As matter of fact, in the limit case of the trapezoidal rule, which actually covers any integration interval with exactly one block, no drift has been experienced so far (at least, for any reasonable value of the stepsize h).

All the above arguments will be confirmed by the numerical tests in the next section.

4 Examples

We now consider a couple of examples, in order to have evidence of the usefulness of the analysis made in the previous section. The first problem fulfills the condition in Remark 8, the second does not. In both cases, the symmetric method that we shall consider is the fourth order Lobatto IIIA method which, in the formulation (19)-(20), is symmetric with matrices

$$A = \begin{pmatrix} -1 & 1 & \\ & -1 & 1 \end{pmatrix}, \qquad B = \frac{1}{24}\begin{pmatrix} 5 & 8 & -1 \\ -1 & 8 & 5 \end{pmatrix}. \tag{23}$$

In all the examples, when not differently specified, the stepsize $h = 0.16$ is used, which is the same stepsize considered in [2] for integrating problem (15)-(16).

Pendulum problem

This is the problem described in Example 1. In this case, since the problem has both the symmetry (5) and (7), from the arguments in the previous section, we expect no drift in the numerical Hamiltonian, both when $y_0 \in \ker(I - S)$ and when $y_0 \notin \ker(I - S)$, provided that the continuous orbit is periodic (and, therefore, having the TRS property). Indeed, this is confirmed by the plots in Figure 4, showing the difference between the numerical Hamiltonian and its initial value, for two discrete trajectories of $2 \cdot 10^4$ steps, respectively starting at the following initial points:

$$q(0) = 0, \qquad p(0) = 1.1, \tag{24}$$

and

$$q(0) = 0.9, \qquad p(0) = \sqrt{1.1^2 - 2 + 2\cos(0.9)} \approx 0.6732, \tag{25}$$

which are on the same continuous orbit.

FHP problem

This is the problem described in Example 2, which is defined by the Hamiltonian (15). When considering the trajectory starting at (16), the plot of Figure 2 is obtained. Both the Hamiltonian and the orbit are unsymmetric, so the problem has no TRS. Consequently, when a generic stepsize h is used, a drift in the numerical Hamiltonian can be expected. This is confirmed by the plot in Figure 5, where such a drift is clearly seen, for a trajectory of $2 \cdot 10^4$ steps. In [2], the authors consider the symmetrized Hamiltonian (17), which satisfies (5). Nevertheless, as we have already pointed out in Example 2, in such a case the starting point (16) doesn't belong to $\ker(I - S)$ and, actually, the same continuous orbit of Figure 2 is obtained, when starting from it. When

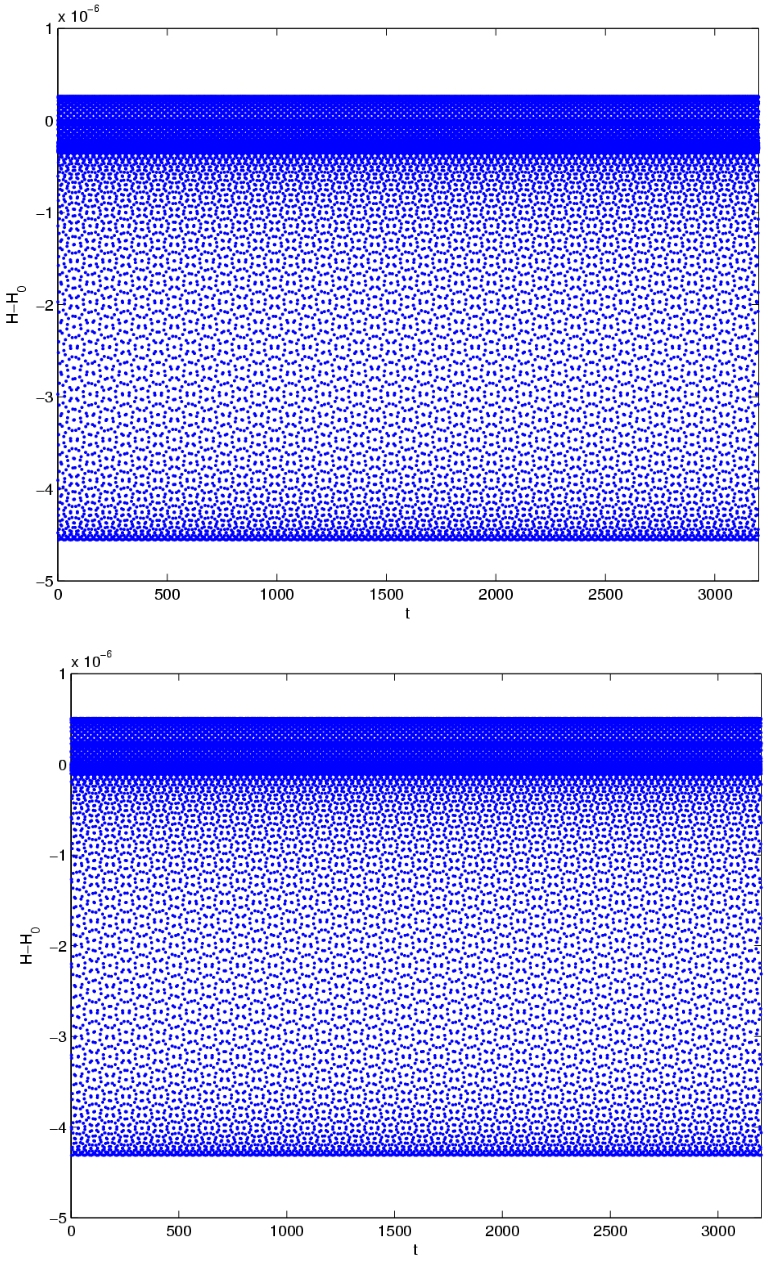

Figure 4: Numerical Hamiltonian for problem (13), initial point (24) (up) and (25) (down).

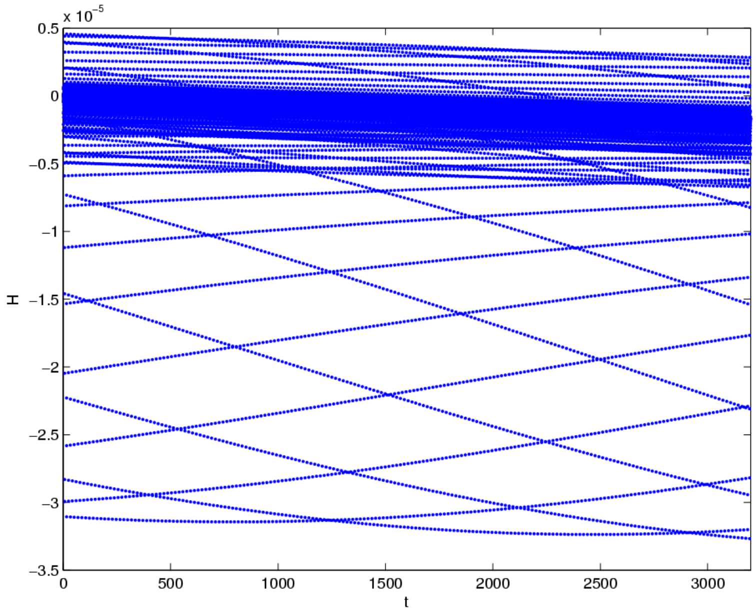

Figure 5: Numerical Hamiltonian (15) for the trajectory starting at (16).

starting from the symmetric initial point (18), the lower orbit in Figure 3 is obtained instead. We then conclude that, in this case as well, the problem has no TRS, despite the symmetry of the Hamiltonian function. Consequently, a drift in the numerical Hamiltonian can be expected also in this case. This fact was observed in [2] and it is confirmed by the plots in Figure 6, for a trajectory of $2 \cdot 10^4$ steps.

In order to make more evident the connection between the TRS property of the problem and a possible drift in the numerical Hamiltonian, we consider the problem (15) in which the function $T(p)$ is modified so that the symmetry (4)-(5) holds true:

$$H(q,p) = T(p) + U(q) \equiv \frac{p^4}{4} - \frac{p^2}{2} + \frac{q^6}{30} + \frac{q^4}{4} - \frac{q^3}{3} + \frac{1}{6}. \tag{26}$$

If we consider the trajectory starting at the following initial point, belonging to $\ker(I-S)$,

$$q(0) = 1, \qquad p(0) = 0, \tag{27}$$

then the upper plot in Figure 7 is obtained. Clearly, now the problem has the TRS property. Consequently, no drift in the numerical Hamiltonian is expected, according to the analysis in the previous section, when a symmetric method is used. This is confirmed by the lower plot in Figure 7, where, for a trajectory of 10^5 steps, the difference between the numerical Hamiltonian and its initial value is plotted. On the other hand, if we consider the problem defined by the same Hamiltonian (26) and by the initial value

$$q(0) = 1, \qquad p(0) = 1, \tag{28}$$

then the trajectory in the upper plot in Figure 8 is obtained. Clearly, in this case, even though the equations satisfy the symmetry (4)-(5), the problem has no TRS. Consequently, a drift in the numerical Hamiltonian could be expected. This is, indeed, confirmed by the lower plot in Figure 8, where the drift is clearly observable, for a trajectory of 10^5 steps.

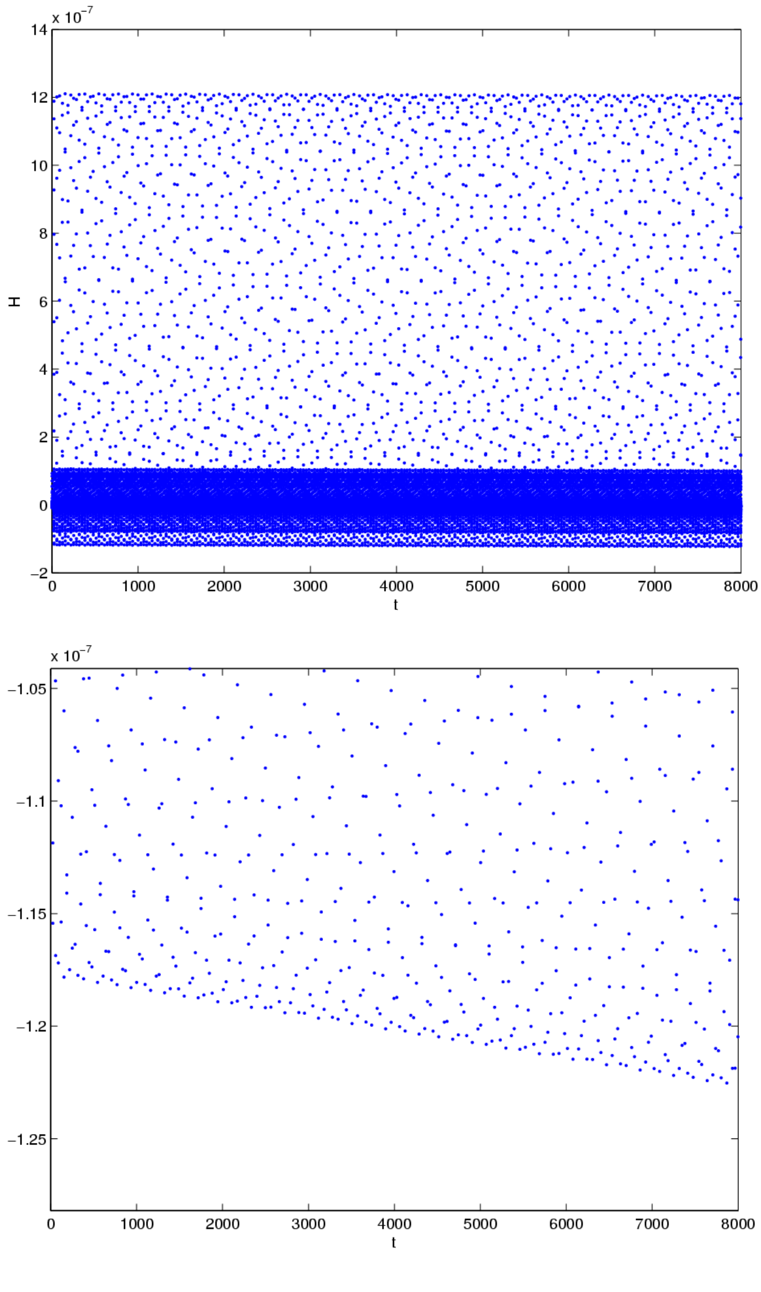

Figure 6: Numerical Hamiltonian (17), trajectory starting at (16) (up), with a detail of the "lower edge" (down).

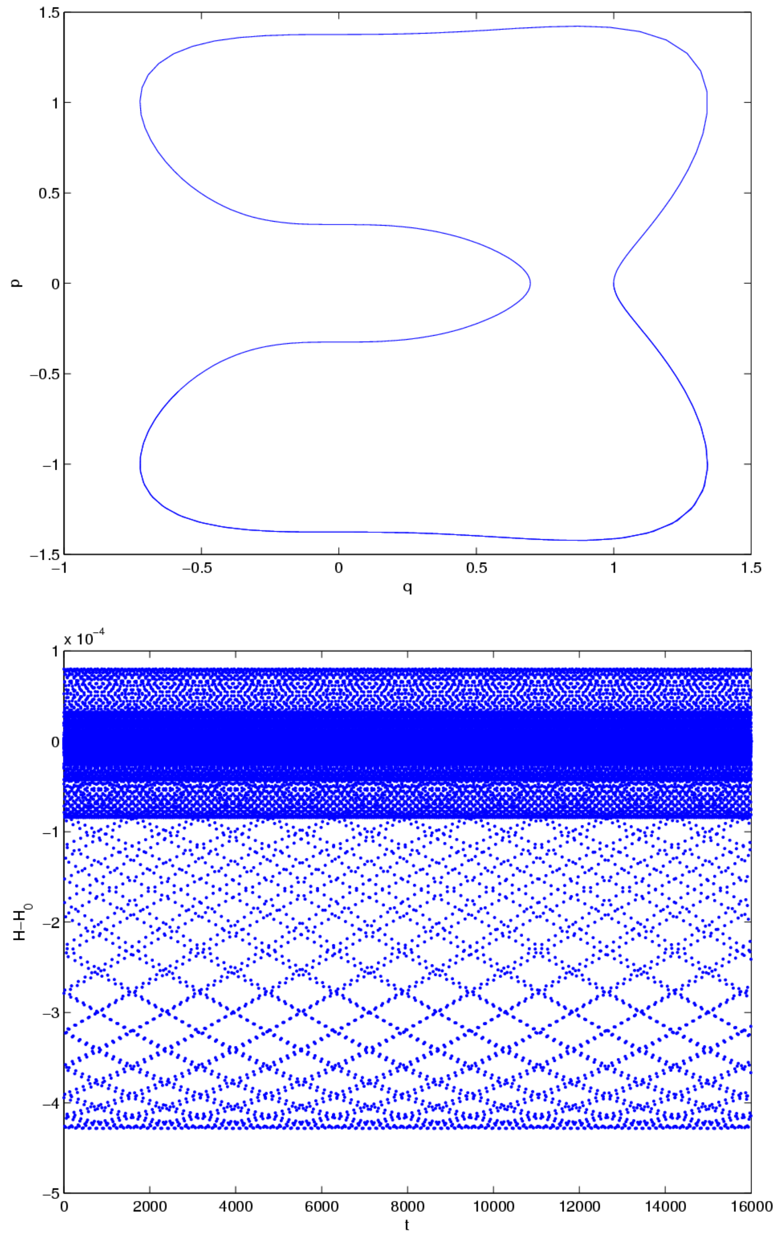

Figure 7: Orbit for the problem (26)-(27) (up) and corresponding numerical Hamiltonian (down).

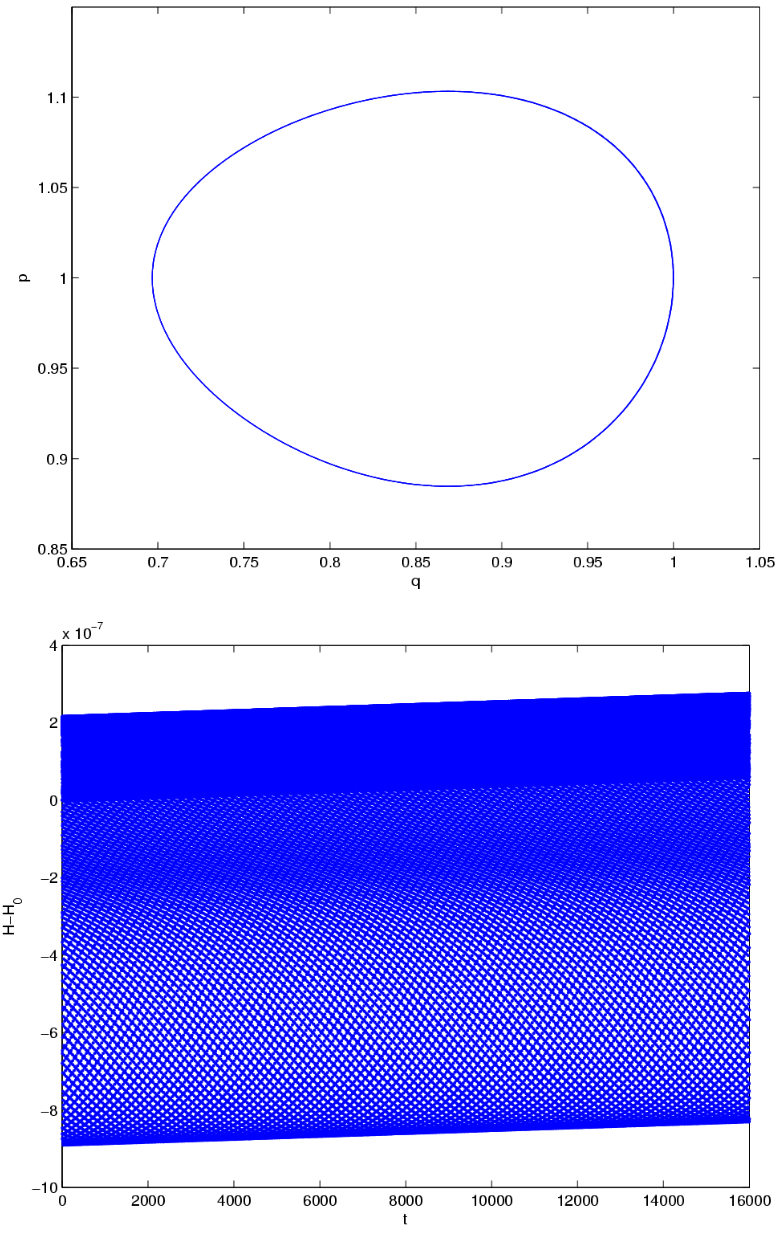

Figure 8: Orbit for the problem (26)-(28) (up) and corresponding numerical Hamiltonian (down).

Remark 9 *The arguments stated in the previous section allow to conclude that the TRS of the problem avoids the presence of a drift in the numerical Hamiltonian, when a symmetric numerical method is used. Nevertheless, we could have no drift even though the problem has no TRS: this is the case, for example, for the trapezoidal rule which, when applied to the problem (15)-(16), provides a discrete solution with no drift in the Hamiltonian (see Figure 10).*

On the other hand, even when using the method (23), a suitable mesh selection strategy could result in a discrete solution which approaches an asymptotically stable periodic solution (see Figure 9, where a periodic orbit of period 24 is approached). Clearly, in such a case, no drift in the numerical Hamiltonian can occur, as shown in the plot of Figure 11.

5 Conclusions

In this paper, the time reversal symmetry (TRS) of a problem has been investigated in some details. Such a property, which in general differs from the symmetry of the underlying equations, is able to prevent, at least in the plane, the occurrence of a drift in the numerical Hamiltonian, when a symmetric integration method is used. Indeed, symmetric methods are able to preserve, in the discrete setting, the TRS of the problem. Relevant numerical examples confirm the usefulness of this approach.

References

[1] L. Brugnano, D. Trigiante. *Solving Differential Problems by Multistep Initial and Boundary Value Methods*, Gordon and Breach Science Publ., 1998.

[2] E. Faou, E. Hairer, T. Pham. Energy conservation with non-symplectic methods: examples and counter-examples, *BIT* **44** (2004) 699–709.

[3] H. Hairer, C. Lubich, G. Wanner. *Geometric Numerical Integration*, Springer, 2004.

[4] B. Leimkuhler, S. Reich. *Simulating Hamiltonian Dynamics*, Cambridge, 2004.

[5] R. I. McLachlan, M. Perlmutter. Energy drift in reversible time integration, *J. Phys. A: Math. Gen.* **37** (2004) 593–598.

[6] J. S. W. Lamb, J. A. G. Roberts. Time-reversal symmetry in dynamical systems: a survey, *Physica D* **112** (1998) 1–39.

[7] H. Goldstein, C. Poole and J. Safko. *Classical Mechanics, 3rd Ed.*, Addison Wesley, 2000.

[8] T. L. Saaty, J. Bram. *Nonlinear Mathematics*, Dover, 1964.

[9] `http://math.ucr.edu/home/baez/time/`

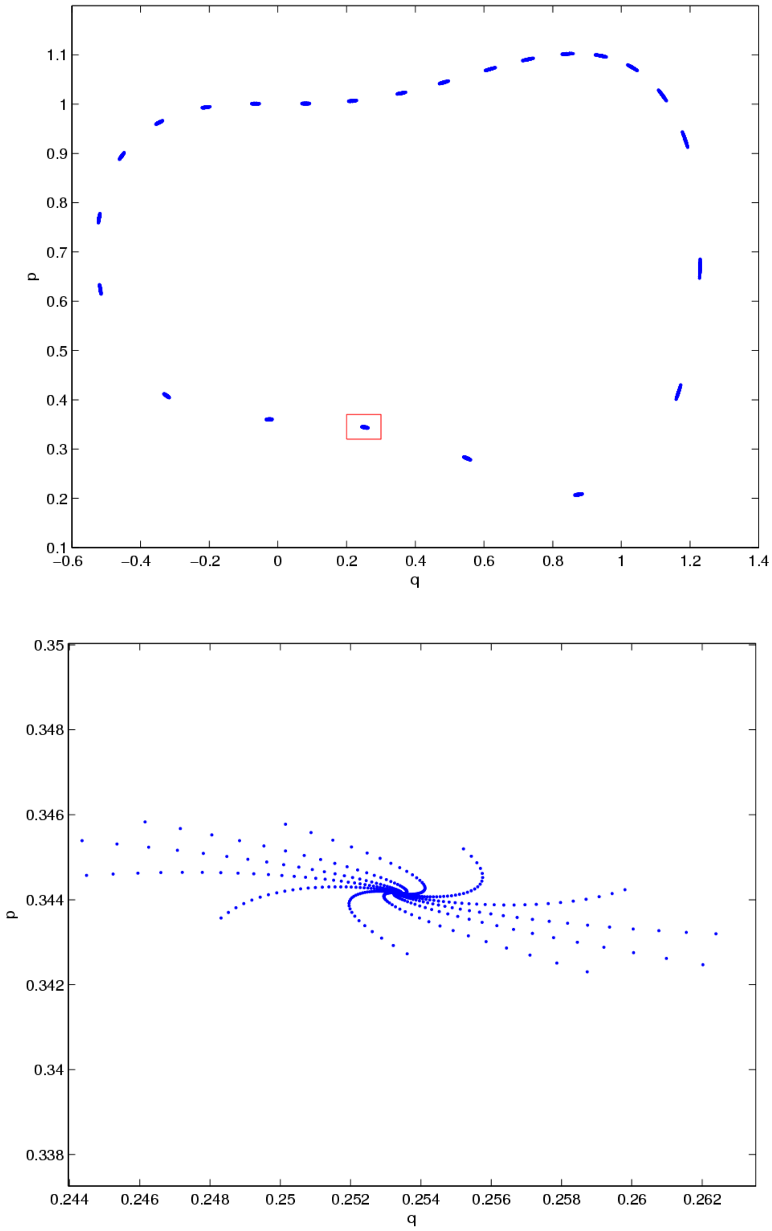

Figure 9: Asymptotically stable periodic orbit (up), problem (15)-(16), non constant stepsize, with detail of the square (down).

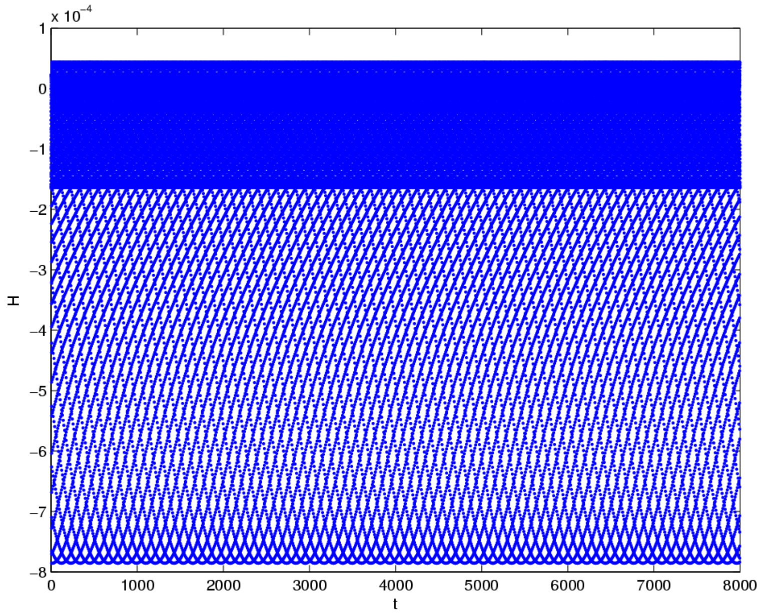

Figure 10: Numerical Hamiltonian (15), trajectory starting at (16), trapezoidal rule.

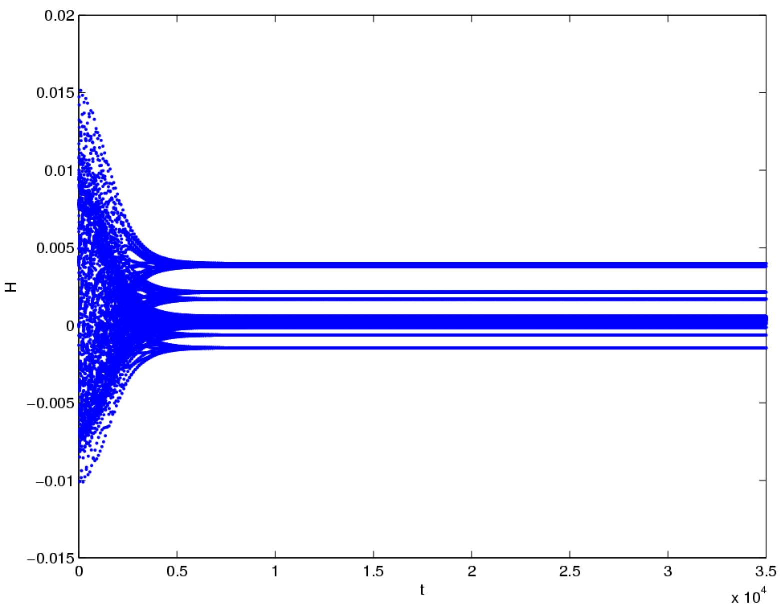

Figure 11: Numerical Hamiltonian (15) for the trajectory starting at (16), non constant stepsize.