On the periodic solutions of discrete Hamiltonian systems [1]

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Abstract. Almost all numerical methods for solving conservative problems cannot avoid a more or less perceptible drift phenomenon. Considering that the drift would be absent on a periodic or quasi-periodic solution, one way to eliminate such unpleasant phenomenon is to look for discrete periodic or quasi-periodic solutions. It is quite easy to show that only symmetric methods are able to provide solutions having such behavior. The open problem is to find the suitable stepsize and to be sure that the obtained periodic solution is stable. In the preliminary results here presented we show that this problem is strongly connected with a classical problem of evolution of planar polygons already discussed by Schoenberg in [5, 6] and more recently treated in [2].

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When an Hamiltonian system is numerically integrated, the presence of a drift can be experienced in the values of the Hamiltonian function. Obviously, if the discrete solution is periodic or quasi-periodic, such phenomenon disappears. Generally, it is not true that when a numerical method is applied to a continuous problem having periodic or quasi-periodic solutions, the discrete solution share such property with the continuous one. As it was proved in [1, 4], in order to have discrete periodic trajectories the applied method needs to be symmetric. For this reason, from now on we focus our attention only on symmetric methods. Nevertheless, the existence of discrete periodic orbits can also depend from other factors such as, for example, the stepsize, some parameters characterizing the used method (the number of stage for a Runge-Kutta scheme, the blocksize for a block Boundary Value Method) and, certainly, from the nonlinearity of the problem we are dealing with. It is quite easy to prove that the solutions of systems having quadratic Hamiltonian are periodic (or quasi-periodic) independently of the choice of the stepsize of integration. Concerning the trapezoidal rule this can be verified by means of the computations we are going to do. To fix the ideas, let us consider the linear pendulum described by

$$\frac{d}{dt}\begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} q \\ p \end{pmatrix} \equiv J\begin{pmatrix} q \\ p \end{pmatrix}. \tag{1}$$

By introducing on the interval of integration the uniform mesh $t_n = nh, n = 0,1,\dots,N$, with h denoting the stepsize, the generated discrete problem provided by the trapezoidal rule assumes the following form

$$y_{n+1} - y_n = \frac{h}{2}J\left(y_{n+1} + y_n\right), \tag{2}$$

where $y_n \equiv (q_n, p_n)^T, q_n \approx q(t_n), p_n \approx p(t_n)$. By setting I the identity matrix of dimension 2, the previous relation can be written as

$$\left(I - \frac{h}{2}J\right)y_{n+1} = \left(I + \frac{h}{2}J\right)y_n,$$

from which, posing $R(h) = \left(I - \frac{h}{2}J\right)^{-1}\left(I + \frac{h}{2}J\right)$,

$$y_n = (R(h))^n\, y_0. \tag{3}$$

Considering that

$$\left(I - \frac{h}{2}J\right)^{-1} = \frac{1}{1+\frac{h^2}{4}}\left(I + \frac{h}{2}J\right),$$

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the matrix $R(h)$ can be written in the equivalent form

$$R(h)=\frac{1}{1+\frac{h^2}{4}}\left(\left(1-\frac{h^2}{4}\right)I+hJ\right).$$

By defining

$$\sin\vartheta=\frac{h}{1+\frac{h^2}{4}},\tag{4}$$

we may state that $R(h)$ is a rotation matrix. Therefore, if $N\vartheta=2\pi$, the corresponding solution is periodic. In fact, in this case $(R(h))^N=I$. Therefore, the relation (3) immediately implies that $y_N=y_0$. Moreover, by taking into account that

$$\sin\left(2\frac{\pi}{N}\right)=\frac{2\tan\left(\frac{\pi}{N}\right)}{1+\tan^2\left(\frac{\pi}{N}\right)},$$

from (4) we get

$$h=2\tan\left(\frac{\pi}{N}\right).\tag{5}$$

Consequently, the discrete linear pendulum has periodic solutions for every values of N to which there correspond values of h which accumulate as $N\to+\infty$. In particular, period two would exist only for $h=+\infty$ and period four is obtained in correspondence of $h=2$.
Moreover, since a nonlinear problem can be sometimes considered as a perturbation of its linearization, by using the same parameter h which provides a periodic solution in the linear case, a quasi-periodic trajectory can be derived in the nonlinear one. In order to put into evidence this fact, we consider a couple of examples which are described by the equations

$$\begin{aligned}\frac{d}{dt}\begin{pmatrix}q\\p\end{pmatrix}&=\begin{pmatrix}p\\-\sin(q)\end{pmatrix}=J\begin{pmatrix}q\\p\end{pmatrix}+\begin{pmatrix}0\\-\sin(q)+q\end{pmatrix},&(6)\\ \frac{d}{dt}\begin{pmatrix}q\\p\end{pmatrix}&=\begin{pmatrix}p\\1-\exp(q)\end{pmatrix}=J\begin{pmatrix}q\\p\end{pmatrix}+\begin{pmatrix}0\\1-\exp(q)+q\end{pmatrix},&(7)\end{aligned}$$

respectively. In both cases, the corresponding discrete problem is obtained by applying the trapezoidal method with stepsize $h=2\tan\left(\frac{\pi}{8}\right)$ and initial point $(q(0),p(0))=(1,0)$. The corresponding orbits are drawn in the phase plane in the plots on the left of Figure 1. As one can see, both of them are quasi-periodic. Moreover, on the same plots, the orbit provided by the same scheme used for discretizing the linear problem (1) is reported. As expected from the previous analysis, it has period eight. In addition, in the plot on the right of the same figure, the difference between the numerical Hamiltonian H and its initial value H_0 for the corresponding trajectories of $3\cdot10^4$ steps is shown. It is evident that no drift occurs.

As already stressed, our goal is to find a device for determining discrete periodic solutions along with the corresponding stepsize. At this aim, an obvious way is to consider a discrete boundary value problem having periodic boundary conditions. For sake of simplicity, we shall again refer to the trapezoidal method, even if other schemes could be applied as well. In this case the discrete linear problem assumes the following form:

$$\left(\hat{A}\otimes I-h\hat{B}\otimes J\right)\mathbf{y}=\mathbf{0},\tag{8}$$

where $\mathbf{y}=((q_0,p_0),(q_1,p_1),\dots,(q_N,p_N))^T=(y_0,y_1,\dots,y_N)^T$, and the two matrices $\hat{A},\hat{B}\in\mathbb{R}^{N\times(N+1)}$ are

$$\hat{A}\equiv[a|A]=\left(\begin{array}{c|ccccc}-1&1&&&&\\&-1&1&&&\\&&\ddots&\ddots&&\\&&&&-1&1\end{array}\right),\qquad \hat{B}\equiv[b|B]=\frac{1}{2}\left(\begin{array}{c|ccccc}1&1&&&&\\&1&1&&&\\&&\ddots&\ddots&&\\&&&&1&1\end{array}\right).$$

Then, by imposing $y_N=y_0$, (8) can be equivalently written as

$$(A_c\otimes I-hB_c\otimes J)\,\mathbf{y}=\mathbf{0},$$

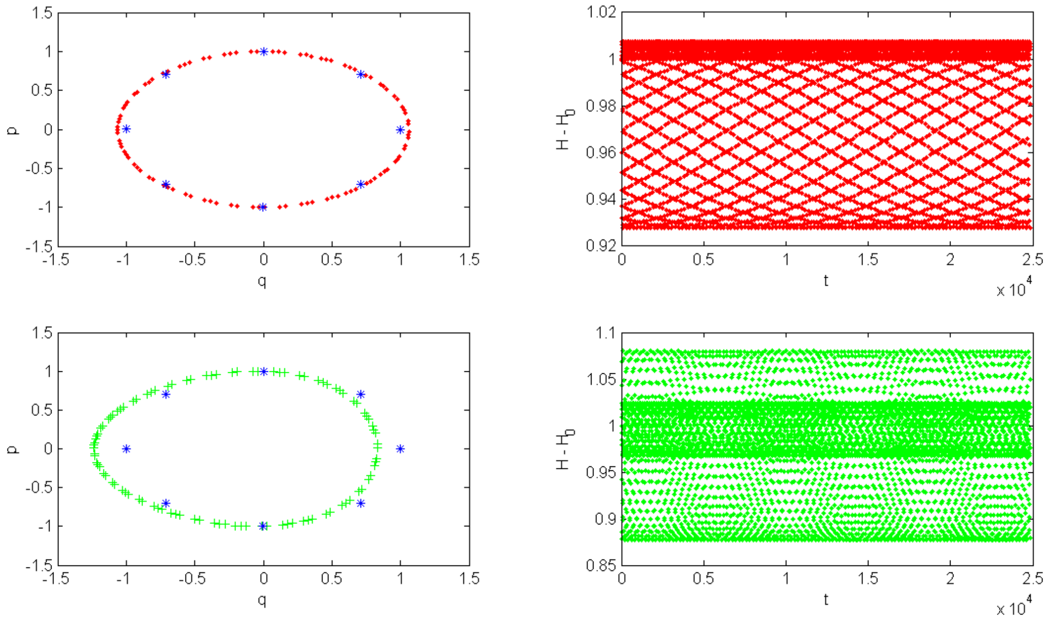

FIGURE 1. On the left: orbits for the problem in (6) (.) and for the problem in (7) (+) both of them together with the orbit of the linear problem (1) ($*$) having period eight. On the right: corresponding numerical Hamiltonian.

where $A_c \equiv (A + a\mathbf{e}_N^T)$ and $B_c \equiv (B + b\mathbf{e}_N^T)$, being $\mathbf{e}_N$ the Nth vector of the canonical basis in $\mathbb{R}^N$. Both the matrices A_c and B_c are circulant and A_c is singular. Denoting, as usual, by A_c^+ the pseudoinverse of A_c, and setting $C \equiv A_c^+ B_c \otimes J$, from the previous relation we get the iterative method

$$\mathbf{y}^{(n)} = hC\mathbf{y}^{(n-1)}, \qquad n \geq 1. \tag{9}$$

Assuming that each entry of vector $\mathbf{y}^{(0)}$, i.e., $(q_j, p_j), j = 1, 2, \ldots, N$, is a vertex of a planar polygon which may be non-convex and self-intersecting, relation (9) describes its linear evolution. The parameter h is to be determined in order to have the sequence $\{\mathbf{y}^{(n)}\}$ bounded and not vanishing. This requires to choose $h = \rho(C)^{-1}$, where $\rho(C)$ is the spectral radius of C. Considering that C is a circulant matrix, by using the FFT it is an easy matter both to evaluate the spectrum of C and to perform the iteration (9). It turns out that h assumes the same value (5). The only difference being that this time N is fixed. This shows that there is a strict relation between N and h on the periodic solutions. It is worth to note that in this case, as $n \to +\infty$, the polygon converges to an ellipse independently of the choice of $\mathbf{y}^{(0)}$. The problem to get polygons by using linear transformations like (9) in the complex plane is already known in the literature, see [2, 5, 6].

It would be very interesting to extend the previous approach to nonlinear problems. The corresponding iterative method is

$$\mathbf{y}^{(n)} = hCf(\mathbf{y}^{(n-1)}), \qquad n \geq 1, \tag{10}$$

with f a suitable nonlinear function. Therefore, the question is to establish under what conditions of the function f the equation (10) is able to retain the above mentioned properties of the linearized problem.

Moreover, once a periodic or quasi-periodic solution has been located, it is important to understand if it is stable or not. In fact, it may happen that the system evolves from an unstable periodic solution to a stable one having different period, if any. In order to show such behavior, we consider as example the Lotka-Volterra problem in logarithmic scale given by

$$\frac{d}{dt}\begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} 8\,(1 - \mathrm{e}^p) \\ (\mathrm{e}^q - 1) \end{pmatrix}, \tag{11}$$

with $t \in [0, 40000]$ and initial value $(q(0), p(0)) = (\log 4, 0)$. We discretize it by applying the 3-step ETR, used as block BVM with minimal blocksize (see [4] for the details on the method), with $h = 2\tan(\pi/47)$. In Figure 2 there is the

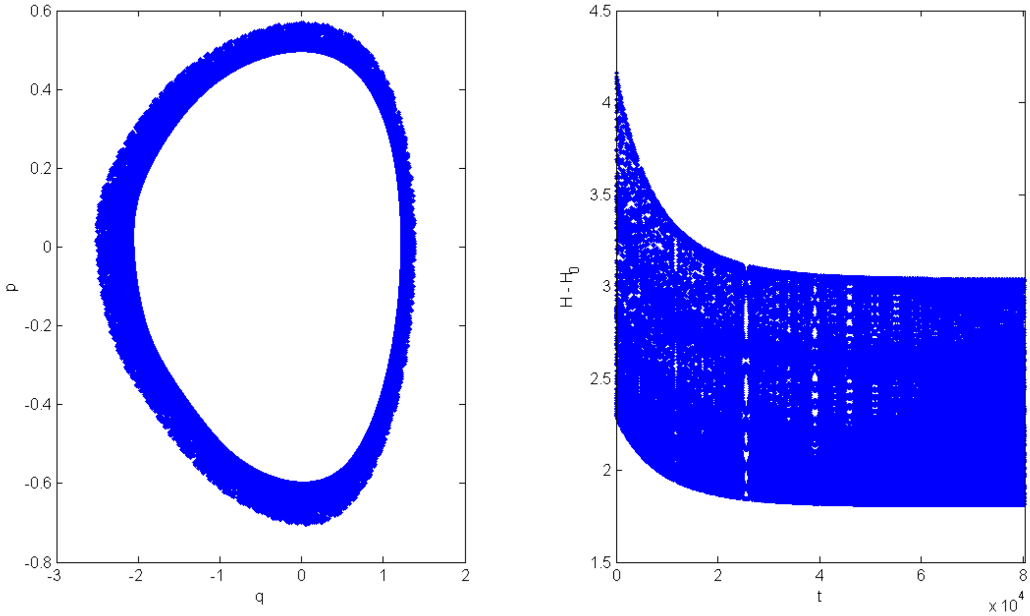

FIGURE 2. On the left: orbit for the problem (11) in the phase plane. On the right: corresponding numerical Hamiltonian.

plot of the orbit for the discrete problem (11) in the phase plane (on the left) and the difference between the numerical Hamiltonian and its initial value for the corresponding trajectories of $2 \cdot 10^5$ steps (on the right). In particular, the last picture shows that, starting from an unstable periodic solution, the system evolves towards a stable quasi-periodic solution near period six.

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