SIAM J. NUMER. ANAL.
Vol. 50, No. 6, pp. 2897–2916

ENERGY- AND QUADRATIC INVARIANTS–PRESERVING INTEGRATORS BASED UPON GAUSS COLLOCATION FORMULAE*

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Abstract. We introduce a new family of symplectic integrators for canonical Hamiltonian systems. Each method in the family depends on a real parameter α. When $\alpha = 0$ we obtain the classical Gauss collocation formula of order $2s$, where s denotes the number of the internal stages. For any given non-null α, the corresponding method remains symplectic and has order $2s-2$; hence it may be interpreted as an $O(h^{2s-2})$ (symplectic) perturbation of the Gauss method. Under suitable assumptions, we show that the parameter α may be properly tuned, at each step of the integration procedure, so as to guarantee energy conservation in the numerical solution, as well as to maintain the original order $2s$ as the generating Gauss formula.

Key words. Hamiltonian systems, collocation Runge–Kutta methods, symplectic integrators, energy-preserving methods

AMS subject classifications. 65P10, 65L05

DOI. 10.1137/110856617

1. Introduction.

We consider canonical Hamiltonian systems in the form

$$\begin{cases} \dot{y} = J\nabla H(y) \equiv f(y), \\ y(t_0) = y_0 \in \mathbb{R}^{2m}, \end{cases} \qquad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \in \mathbb{R}^{2m\times 2m} \tag{1.1}$$

(I is the identity matrix of dimension m). Concerning its numerical integration, two prominent lines of investigation are currently the definition and the study of symplectic methods and energy-conserving methods, respectively. This reflects the fact that symplecticity and energy conservation are the most relevant features characterizing a Hamiltonian system.

From the very beginning of this research activity, high-order symplectic formulae were already available within the class of Runge–Kutta methods, the Gauss collocation formulae being one noticeable example. One important implication of the symplecticity of the discrete flow is the conservation of quadratic invariants. This circumstance makes the symplecticity property of a method particularly appealing in the numerical simulation of isolated mechanical systems in the form (1.1), since it provides a precise conservation of the total angular momentum during the time evolution of the state vector. As a further positive consequence, a symplectic method also conserves quadratic Hamiltonian functions. (See the monographs [18, 25, 30] for a detailed analysis of symplectic methods.)

On the other hand, excluding the quadratic case, energy-conserving methods were initially not known. Among the first attempts to address this issue, we mention projection and symmetric projection techniques, which, coupled with classical nonconservative schemes, force the numerical solution to lie in a proper manifold rep-

*Received by the editors November 28, 2011; accepted for publication (in revised form) August 7, 2012; published electronically November 6, 2012. This work was developed within the project "Innovative Methods of Numerical Linear Algebra with Applications."
http://www.siam.org/journals/sinum/50-6/85661.html
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resenting a first integral of the original system (see [19, section VII.2], [1, 17], and [18, section V.4.1]).

A completely new approach is represented by *discrete gradient methods* which are based upon the definition of a discrete counterpart of the gradient operator so that energy conservation of the numerical solution is guaranteed at each step and for any choice of integration stepsize (see [15, 28]).

More recently, the conservation of energy issue has been approached by means of the definition of the *discrete line integral* in a series of papers (such as [22, 23]). This early study has led to the definition of *Hamiltonian boundary value methods* (HBVMs) (see, for example, [4, 5, 6, 7, 8]). These methods are able to preserve, in the discrete solution, Hamiltonian functions of polynomial type. In particular, HBVMs admit a Runge–Kutta formulation (see, for example, [6]) characterized by a rank-deficient Butcher matrix, where the rank, say, s, influences the order of the method, while the dimension, say, r, may be arbitrarily increased to ensure energy conservation of polynomial Hamiltonians of any high degree (and hence a *practical* conservation of any sufficiently differentiable Hamiltonian).[1] When $r = s$ the formula becomes a classical collocation method, while as $r \to \infty$ the formulae are linked with the *average vector field integrator* [29] and its extensions [5, 16], as well as to B-series methods [11, 12]. Further generalizations of HBVMs, aimed at preserving any number of invariants, have been also proposed [2].

Attempts to incorporate both symplecticity and energy conservation into the numerical method will clash with two nonexistence results. The first [14] refers to nonintegrable systems, that is, systems that do not admit other independent first integrals different from the Hamiltonian function itself. According to the authors,

> *If [the method] is symplectic, and conserved H exactly, then it is the time advance map for the exact Hamiltonian system up to a reparametrization of time.*

The second negative result [13] refers to B-series symplectic methods applied to general (not necessarily nonintegrable) Hamiltonian systems:

> *The only symplectic method (as B-series) that conserves the Hamiltonian for arbitrary $H(y)$ is the exact flow of the differential equation.*

The impossibility for a constant time stepping algorithm to be at the same time symplectic and energy conserving has led to research into methods which could inherit both features in a weaker sense. This delicate aspect has been thoroughly faced in [21], where the authors prove the existence of *symplectic-energy-momentum integrators* by using time-adaptive steps. Here the symplecticity property is interpreted in a space-time view with the aid of a discrete version of the variational principle for a nonautonomous Hamiltonian system, while time step adaption is used to impose energy conservation (see also [27]).

Second-order accurate *energy-momentum conserving algorithms* have been proposed in [32, 33]. In particular, in [33] the authors devise a one-parameter family of symplectic integrators suitable for separable Hamiltonian systems. Therefore, by construction, the time step takes place on the level set of constant angular momentum. They show that the parameter may be suitably tuned in such a way to enforce energy conservation.

Following this line of investigation, the aim of the present work is to devise methods of arbitrarily high order that conserve quadratic invariants and the energy associated with a general canonical Hamiltonian system.

[1] We refer the reader to [3] for complete documentation of HBVMs.

More precisely, we will begin with introducing a family of one-step methods

$$y_1(\alpha) = \Phi_h(y_0, \alpha) \tag{1.2}$$

(h is the stepsize of integration), depending on a real parameter α, with the following specifics:

1. For any fixed choice of $\alpha \neq 0$, the corresponding method is a symplectic Runge–Kutta method with s stages and of order $2s-2$.
2. For $\alpha = 0$ one gets the Gauss collocation method (of order $2s$).
3. For any choice of y_0 and in a given range of the stepsize h, there exists a value of the parameter, say, α^*, depending on y_0 and h, such that $H(y_1) = H(y_0)$ (energy conservation).

As the parameter α ranges in a small interval centered at zero, the value of the numerical Hamiltonian function $H(y_1)$ will match $H(y_0)$, thus leading to energy conservation. This result, which will be formally proved in section 3, is formalized as follows: *Under suitable assumptions, there exists a real sequence* $\{\alpha_k\}$ *such that the numerical solution defined by* $y_{k+1} = \Phi_h(y_k, \alpha_k)$*, with* y_0 *defined in* (1.1)*, satisfies* $H(y_k) = H(y_0)$*,* $k = 0, 1, \ldots$.

To clarify this statement and how it relates to the above nonexistence results, we emphasize that the energy conservation property only applies to the specific numerical orbit $\{y_k\}$ that the method generates, starting from the initial value y_0 and with stepsize h. For example, let us consider the very first step and assume the existence of a value $\alpha = \alpha_0$ that yields energy conservation between the two state vectors y_0 and y_1, as indicated in item 3 above. If α_0 is maintained constant, the map $y \mapsto \Phi_h(y, \alpha_0)$ is symplectic and, by definition, ensures the energy conservation condition $H(y_1) = H(y_0)$. However, it would fail to provide a conservation of the Hamiltonian function if we changed the initial condition y_0 or the stepsize h: in general, if $\hat{y}_0 \neq y_0$ or $\hat{h} \neq h$, we would obtain $H(\Phi_{\hat{h}}(\hat{y}_0, \alpha_0)) \neq H(y_0)$. Thus, the energy conservation property we are going to discuss is a weakened version of the standard energy conservation condition mentioned in the two nonexistence results above.

One of the most interesting features of symplectic Runge–Kutta methods is the fact that they are also able to preserve all quadratic invariants of the continuous dynamical system. Consequently, the methods described here are able to preserve both the energy and the quadratic invariants of the continuous dynamical system. This, in turn, provides better stability properties concerning the long-term simulation of, e.g., periodic orbits (see [10] for details). It is therefore this aspect which we would like to emphasize by naming such methods *energy and quadrating invariants preserving (EQUIP) methods*. In particular, here we shall not consider any kind of backward analysis in conjunction with the symplecticity of the discrete map.

The paper is organized as follows. In the next section we report the definition of the methods, which are derived from the Gauss collocation formulae. In section 3 we face the problem from a theoretical viewpoint and give some existence results that aim to explain the energy-preserving property of the new methods. In section 4 we report a few tests that give clear numerical evidence that a change in sign of the function $g(\alpha) = H(y_1(\alpha)) - H(y_0)$ does indeed occur along the integration procedure.

2. Definition of the methods. Let $c_1 < c_2 < \cdots < c_s$ and $b_1, \ldots, b_s$ be the abscissae and the weights of the Gauss–Legendre quadrature formula in the interval $[0, 1]$. We consider the Legendre polynomials $P_j(\tau)$, of degree $j-1$, for $j = 1, \ldots, s$,

shifted and normalized in the interval $[0,1]$, so that

$$\int_0^1 P_i(\tau)P_j(\tau)\mathrm{d}\tau = \delta_{ij}, \qquad i,j = 1,\dots,s \tag{2.1}$$

(δ_{ij} is the Kronecker symbol), and the matrix

$$\mathcal{P} = \begin{pmatrix} P_1(c_1) & P_2(c_1) & \cdots & P_s(c_1) \\ P_1(c_2) & P_2(c_2) & \cdots & P_s(c_2) \\ \vdots & \vdots & & \vdots \\ P_1(c_s) & P_2(c_s) & \cdots & P_s(c_s) \end{pmatrix}_{s\times s}. \tag{2.2}$$

Our starting point is the following decomposition of the Butcher array A of the Gauss method of order $2s$ (see [19, Theorem 5.6]):

$$A = \mathcal{P}X_s\mathcal{P}^{-1}, \tag{2.3}$$

where X_s is defined as

$$X_s = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & -\xi_{s-1} \\ & & \xi_{s-1} & 0 \end{pmatrix} \tag{2.4}$$

with

$$\xi_j = \frac{1}{2\sqrt{(2j+1)(2j-1)}}, \qquad j = 1,\dots,s-1. \tag{2.5}$$

We now consider the matrix $X_s(\alpha)$ obtained by perturbing (2.4) as follows:

$$X_s(\alpha) = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & -(\xi_{s-1}+\alpha) \\ & & \xi_{s-1}+\alpha & 0 \end{pmatrix} = X_s + \alpha W_s, \tag{2.6}$$

where α is a real parameter, and

$$W_s = \begin{pmatrix} 0 & 0 & & \\ 0 & 0 & \ddots & \\ & \ddots & \ddots & -1 \\ & & 1 & 0 \end{pmatrix}, \tag{2.7}$$

so that $X_s(\alpha)$ is a rank two perturbation of X_s.

The family of methods $y_1 = \Phi_h(y_0,\alpha)$ we are interested in is defined by the following tableau:

$$\begin{array}{c|c} c_1 & \\ \vdots & \mathcal{A}(\alpha) \equiv \mathcal{P}X_s(\alpha)\mathcal{P}^{-1} \\ c_s & \\ \hline & b_1 \ \dots\dots \ b_s \end{array}. \tag{2.8}$$

Therefore

$$\mathcal{A}(\alpha) = A + \alpha \mathcal{P} W_s \mathcal{P}^{-1}, \tag{2.9}$$

and hence $\mathcal{A}(0) = A$.

By exploiting Theorems 5.11 and 5.1 in [19, Chapter IV.5], we readily deduce that the symmetric method (2.8) has order $2s-2$ for any fixed $\alpha \neq 0$ and order $2s$ when $\alpha = 0$.[2]

We set

$$\omega = \begin{pmatrix} b_1 \\ \vdots \\ b_s \end{pmatrix}, \qquad \Omega = \begin{pmatrix} b_1 & & \\ & \ddots & \\ & & b_s \end{pmatrix}, \qquad e = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \in \mathbb{R}^s. \tag{2.10}$$

THEOREM 2.1. *For any value of α, the Runge–Kutta method defined by* (2.8) *is symplectic. Consequently, it preserves all quadratic invariants of the continuous dynamical system.*

Proof. On the basis of [18, Theorem 4.3, p. 192], we will prove the following sufficient condition for symplecticity:

$$\Omega \mathcal{A}(\alpha) + \mathcal{A}(\alpha)^T \Omega = \omega\, \omega^T.$$

Since the degree of the integrand functions in (2.1) does not exceed $2s-2$, such orthogonality conditions may be equivalently posed in discrete form as

$$\sum_{k=1}^{s} b_k P_i(c_k) P_j(c_k) = \delta_{ij}, \qquad i, j = 1, \ldots, s,$$

or in matrix notation as

$$\mathcal{P}^T \Omega P = I. \tag{2.11}$$

Considering that from (2.11) we get $\mathcal{P}^{-1} = \mathcal{P}^T \Omega$, from (2.9) we have that

$$\Omega \mathcal{A}(\alpha) + \mathcal{A}(\alpha)^T \Omega = \Omega A + A^T \Omega + \alpha \Omega \mathcal{P} (W_s + W_s^T) \mathcal{P}^T \Omega = \omega\, \omega^T \tag{2.12}$$

since the Gauss method is symplectic, and W_s is skew-symmetric so that $W_s + W_s^T = 0$. ∎

In the event that a value $\alpha^* \equiv \alpha^*(y_0, h)$ for the parameter α may be found such that the conservation condition $H(y_1(\alpha)) = H(y_0)$ is satisfied, we can extrapolate from the parametric method (2.8) a symplectic scheme

$$y \mapsto \Phi_h(y, \alpha^*) \tag{2.13}$$

that provides energy conservation if evaluated at y_0. The existence of such an α^* will be proved in section 3. One important implication of the symplectic nature of (2.13) is the conservation of all quadratic constants of motion associated with system (1.1). Consequently, the new formulae, when applied to the initial value system (1.1), are able to define a numerical approximation of any high order, along which

[2] Later on (see Theorem 3.3 and Remark 3.4), we shall see that a proper choice of the parameter α allows us to recover the order $2s$ of the method.

the Hamiltonian function and all quadratic first integrals of the system are precisely conserved.

Example 1. When $s = 2$, one obtains that the tableau (2.8)–(2.9) becomes

$$\begin{array}{c|cc} \frac{1}{2}-\frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4}-\frac{\sqrt{3}}{6}-\alpha \\ \frac{1}{2}+\frac{\sqrt{3}}{6} & \frac{1}{4}+\frac{\sqrt{3}}{6}+\alpha & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}. \tag{2.14}$$

Consequently, for $\alpha = 0$ one retrieves the two-stage Gauss method.

Example 2. When $s = 3$, one obtains that the tableau (2.8)–(2.9) becomes

$$\begin{array}{c|ccc} \frac{1}{2}-\frac{\sqrt{15}}{10} & \frac{5}{36} & \frac{2}{9}-\frac{\sqrt{15}}{15}-\alpha\frac{2}{3} & \frac{5}{36}-\frac{\sqrt{15}}{30}+\alpha\frac{2}{3} \\ \frac{1}{2} & \frac{5}{36}+\frac{\sqrt{15}}{24}+\alpha\frac{5}{12} & \frac{2}{9} & \frac{5}{36}-\frac{\sqrt{15}}{24}-\alpha\frac{5}{12} \\ \frac{1}{2}+\frac{\sqrt{15}}{10} & \frac{5}{36}+\frac{\sqrt{15}}{30}-\alpha\frac{2}{3} & \frac{2}{9}+\frac{\sqrt{15}}{15}+\alpha\frac{2}{3} & \frac{5}{36} \\ \hline & \frac{5}{18} & \frac{4}{9} & \frac{5}{18} \end{array}. \tag{2.15}$$

Consequently, for $\alpha = 0$ one retrieves the three-stage Gauss method.

2.1. Generalizations. The proof of Theorem 2.1 suggests how to extend the definition of the new formulae in order to get a family of methods depending on a set of parameters. Indeed, by looking at (2.12), one has that replacing matrix αW_s by any skew-symmetric matrix $\widetilde{W}_s$ still guarantees symplecticity.

THEOREM 2.2. *Consider any $s \times s$ skew-symmetric matrix $\widetilde{W}_s$. Then, the Runge–Kutta method defined by the Butcher tableau*

$$\begin{array}{c|c} c_1 & \\ \vdots & \mathcal{A}(\alpha) \equiv \mathcal{P}(X_s + \widetilde{W}_s)\mathcal{P}^{-1} \\ c_s & \\ \hline & b_1 \ \ldots\ldots \ b_s \end{array} \tag{2.16}$$

with $\widetilde{W}_s^T = -\widetilde{W}_s$ is symplectic.

For example, a natural choice for the matrix $\widetilde{W}_s$ is

$$\widetilde{W}_s = \begin{pmatrix} 0 & -\alpha_1 & & \\ \alpha_1 & 0 & \ddots & \\ & \ddots & \ddots & -\alpha_{s-1} \\ & & \alpha_{s-1} & 0 \end{pmatrix}, \tag{2.17}$$

leading to a multiparametric method depending on the $s-1$ parameters $\alpha_1, \ldots, \alpha_{s-1}$.[3]

2.2. Quasi-collocation conditions. Equation (2.9) shows the relation between the Butcher arrays associated with the new parametric method and the Gauss collocation method. To avoid loss of generality, in this subsection we solve the generic problem $\dot{y} = f(y)$.

[3]Also in this case, it can be shown that a proper choice of such parameters allows us to recover the order $2s$ of the original method (see Remark 3.4 and Theorem 3.5).

We wonder how the collocation conditions defining the Gauss methods are affected by the parameter α. This task is easily accomplished by expressing the coefficients of the perturbing matrix $\mathcal{P}W_s\mathcal{P}^{-1}$ in terms of linear combinations of the integrals $\int_0^{c_i} l_j(\tau)\mathrm{d}\tau$, where $l_j(\tau)$ is the jth Lagrange polynomial defined on the abscissae $c_1,\dots,c_s$. Let Γ be the solution of the matrix linear system $A\,\Gamma = \mathcal{P}W_s\mathcal{P}^{-1}$, which means that (see (2.3))

$$\Gamma \equiv (\gamma_{ij}) = \mathcal{P}X_s^{-1}W_s\mathcal{P}^{-1}. \tag{2.18}$$

The nonlinear system defining the block vector of the internal stages $\{Y_i\}$ is then given by

$$Y = e\otimes y_0 + h(A\otimes I)F(Y) + \alpha h(A\,\Gamma\otimes I)F(Y),$$

where e is the vector defined in (2.10), I is the identity matrix of dimension $2m$, and

$$Y = \begin{pmatrix} Y_1^T & \dots & Y_s^T \end{pmatrix}^T, \qquad F(Y) = \begin{pmatrix} f(Y_1)^T & \dots & f(Y_s)^T \end{pmatrix}^T.$$

Consequently, the polynomial $\sigma(t_0+\tau h)$, of degree s, that interpolates the stages Y_i at the abscissae c_i, $i=1,\dots,s$, and the initial condition y_0 at 0, is

$$\sigma(t_0+\tau h) = y_0 + h\sum_{j=1}^{s}\int_0^{\tau} l_j(x)\mathrm{d}x\, f(Y_j) + \alpha h\sum_{j=1}^{s}\left(\sum_{k=1}^{s}\gamma_{kj}\int_0^{\tau} l_k(x)\mathrm{d}x\right) f(Y_j). \tag{2.19}$$

Differentiating (2.19) with respect to τ gives

$$\dot\sigma(t_0+\tau h) = \sum_{j=1}^{s} l_j(\tau)\, f(\sigma(t_0+c_j h)) + \alpha\sum_{j=1}^{s}\left(\sum_{k=1}^{s}\gamma_{kj}l_k(\tau)\right) f(\sigma(t_0+c_j h)). \tag{2.20}$$

Finally, evaluating (2.19) at $\tau=0$ and (2.20) at $\tau=c_i$ yields

$$\begin{cases} \sigma(t_0) = y_0, \\ \dot\sigma(t_0+c_i h) = f(\sigma(t_0+c_i h)) + \alpha\displaystyle\sum_{j=1}^{s}\gamma_{ij}\, f(\sigma(t_0+c_j h)), \qquad i=1,\dots,s. \end{cases} \tag{2.21}$$

Clearly, for α small, we can regard (2.21) as *quasi-collocation conditions*, since for $\alpha=0$ we recover the classical collocation conditions defining the Gauss method.

3. Theoretical existence results. After defining the error function

$$g(\alpha) = H(y_1(\alpha)) - H(y_0),$$

the nonlinear system, in the unknowns $Y_1,\dots,Y_s$ and α, to be solved at each step for getting energy conservation, reads

$$\begin{cases} Y = e\otimes y_0 + h(\mathcal{A}(\alpha)\otimes I)F(Y), \\ g(\alpha) = 0, \end{cases} \tag{3.1}$$

and its solvability is equivalent to the existence of the energy-preserving method (2.13) we are looking for. After defining the vector function

$$G(h,y_1,\alpha) = \begin{pmatrix} y_1 - \Phi_h(y_0,\alpha) \\ H(y_1) - H(y_0) \end{pmatrix},$$

we see that system (3.1) is equivalent to $G(h, y_1, \alpha) = 0$. Of course $G(0, y_1, \alpha) = 0$ for any value of α and, in particular $G(0, y_1, 0) = 0$. The Jacobian of G with respect to the two variables y_1 and α reads

$$\frac{\partial G}{\partial(y_1, \alpha)}(h, y_1, \alpha) = \begin{pmatrix} I & \frac{\partial \Phi_h}{\partial \alpha}(y_0, \alpha) \\ \nabla^T H(y_1) & 0 \end{pmatrix}$$

with I the identity matrix of dimension $2m$. From (2.13) we see that $\frac{\partial \Phi_h}{\partial \alpha}(y_0, \alpha)$ coincides with $y_1'(\alpha)$ and hence with $\sigma_\alpha'(t_0+h)$. Due to the consistency of the method, it follows that, for $\alpha = 0$, $\sigma_\alpha'(t_0 + h) \to J\nabla H(y_0)$ as $h \to 0$. Therefore

$$\frac{\partial G}{\partial(y_1, \alpha)}(0, y_1, 0) = \begin{pmatrix} I & J\nabla H(y_0) \\ \nabla^T H(y_0) & 0 \end{pmatrix}. \tag{3.2}$$

Unfortunately, the Jacobian matrix (3.2) is always singular. Consequently, the implicit function theorem (in its classical formulation) does not help in retrieving existence results of the solution of (3.1) when h is small. However, the rank of the matrix (3.2) is $2m$ independently of the problem to be solved. This would suggest the use of the Lyapunov–Schmidt decomposition [31], which considers the restriction of the system to both the complement of the null space and the range of the Jacobian, to produce two systems to which the implicit function theorem applies.

In our case this approach is simplified in that the implicit function theorem ensures the existence of a solution $Y(\alpha)$ of the first system in (3.1) for all values of the parameter α ranging in a closed interval containing the origin and $|h| \le h_0$ with h_0 small enough. Then $y_1(\alpha) = y_0 + h(b^T \otimes I)Y(\alpha)$ is substituted into the second of (3.1) to produce the so-called bifurcation equation in the unknown α. When needed, we will explicitly write $g(\alpha, h)$ or $g(\alpha, h, y_0)$, in place of $g(\alpha)$, to emphasize the dependence of the function g upon the stepsize h, which has to be treated as a parameter, and the state vector y_0.

Let us fix a vector y_0 and look for solution curves of $g(\alpha, h) = 0$ in the (h, α) plane. Obviously $g(\alpha, 0) = 0$ for any α, which means that the axis $h = 0$ is a solution curve of the bifurcation equation; of course, we are interested in the existence of a different solution curve $\alpha^* = \alpha^*(h)$ passing through the origin. Since the gradient of g vanishes at $(0, 0)$, one has to compute the subsequent partial derivatives of g with respect to α and h. However, one verifies that $\frac{\partial^2 g}{\partial h^2} = \frac{\partial^2 g}{\partial \alpha^2} = \frac{\partial^2 g}{\partial \alpha \partial h}$ evaluated at $(0, 0)$ vanish as well, and this makes the computations even harder. For this reason, to address the question about the existence of a solution of (3.1), we make the following (mild and quite reasonable) assumptions:

- ($\mathcal{A}_1$) The function g is analytical in a rectangle $\mathcal{R} = [-\bar\alpha, \bar\alpha] \times [-\bar h, \bar h]$ centered at the origin.
- ($\mathcal{A}_2$) Let d be the order of the error in the Hamiltonian function associated with the Gauss method applied to the given Hamiltonian system (1.1) and the given state vector y_0, that is,

$$g(0, h) = H(y_1(0)) - H(y_0) = c_0 h^d + O(h^{d+1}) \tag{3.3}$$

with $c_0 \neq 0$. Then, we assume that for any fixed $(\alpha, h) \in \mathcal{R}$, $\alpha \neq 0$,

$$g(\alpha, h) = c(\alpha)h^{d-2} + O(h^{d-1})$$

with $c(\alpha) \neq 0$.

Remark 3.1. A couple of quick comments are in order before continuing. Excluding the case where the Hamiltonian $H(q,p)$ is quadratic (which would imply $g(\alpha,h)=0$ for all α), the error in the numerical Hamiltonian function associated with the Gauss method is expected to behave as $O(h^{2s+1})$. We cannot exclude a priori that special classes of problems or particular values for the state vector y_0 may occur, for which the order of convergence may be even higher. This is why we have introduced the integer d: such an integer will be at least $2s+1$. Moreover, we emphasize that the constant c_0 and the function $c(\alpha)$ will depend on y_0. In conclusion, what we are assuming is that for the method (2.8), when α is a given nonzero constant, the order of the error $H(y_1(\alpha))-H(y_0)$ is lowered by two units with respect to the underlying Gauss method of order $2s$, which is a quite natural requirement since such method has order $2s-2$.

THEOREM 3.2. *Under the assumptions* $(\mathcal{A}_1)$ *and* $(\mathcal{A}_2)$*, there exists a function* $\alpha^*=\alpha^*(h)$*, defined in a neighborhood of the origin* $(-h_0,h_0)$*, such that*

(i) $g(\alpha^*(h),h)=0$ *for all* $h\in(-h_0,h_0)$*,*

(ii) $\alpha^*(h)=\text{const}\cdot h^2+O(h^3)$*.*

Proof. From $(\mathcal{A}_1)$ and $(\mathcal{A}_2)$ we obtain that the expansion of g around $(0,0)$ is

$$g(\alpha,h)=\sum_{j=d}^{\infty}\frac{1}{j!}\frac{\partial^j g}{\partial h^j}(0,0)h^j+\sum_{i=1}^{\infty}\sum_{j=d-2}^{\infty}\frac{1}{i!j!}\frac{\partial^{i+j}g}{\partial\alpha^i\partial h^j}(0,0)h^j\alpha^i. \tag{3.4}$$

We are now in the right position to apply the implicit function theorem. We will look for a solution $\alpha^*=\alpha^*(h)$ in the form $\alpha^*(h)=\eta(h)h^2$, where $\eta(h)$ is a real-valued function of h. To this end, we consider the change of variable $\alpha=\eta h^2$ and insert it into (3.4), thus obtaining

$$\begin{aligned} g(\alpha,h)=&\frac{1}{d!}\frac{\partial^d g}{\partial h^d}(0,0)h^d+\frac{1}{(d-2)!}\frac{\partial^{d-1}g}{\partial\alpha\partial h^{d-2}}(0,0)h^d\eta\\ &+\frac{1}{(d-1)!}\frac{\partial^d g}{\partial\alpha\partial h^{d-1}}(0,0)h^{d+1}\eta+\text{higher-order terms}. \end{aligned} \tag{3.5}$$

Therefore, for $h\neq 0$, $g(\alpha,h)=0$ is equivalent to $\tilde g(\eta,h)=0$, where

$$\begin{aligned} \tilde g(\eta,h)=&\frac{1}{(d-1)d}\frac{\partial^d g}{\partial h^d}(0,0)+\frac{\partial^{d-1}g}{\partial\alpha\partial h^{d-2}}(0,0)\eta\\ &+\frac{1}{d-1}\frac{\partial^d g}{\partial\alpha\partial h^{d-1}}(0,0)h\eta+\text{higher-order terms}. \end{aligned} \tag{3.6}$$

By assumption $(\mathcal{A}_2)$, both $\frac{\partial^d g}{\partial h^d}(0,0)$ and $\frac{\partial^{d-1}g}{\partial\alpha\partial h^{d-2}}(0,0)$ are different from zero and hence the implicit function theorem ensures the existence of a function $\eta=\eta(h)$ such that $\tilde g(\eta(h),h)=0$. The solution of $g(\alpha,h)=0$ for the variable α takes the form

$$\alpha^*(h)=\eta(h)h^2=-\frac{1}{(d-1)d}\,\frac{\frac{\partial^d g}{\partial h^d}(0,0)}{\frac{\partial^{d-1}g}{\partial\alpha\partial h^{d-2}}(0,0)}\,h^2+O(h^3), \tag{3.7}$$

and this completes the proof. ∎

By exploiting [24, Theorem 6.1.2], we see that the function $\alpha^*(h)$ is analytic if the power series (3.4) is absolutely convergent for $|h|\le h_0$ and $|\alpha|\le\alpha_0$. In any event, the function $\alpha^*(h)$ is tangent to the h-axis at the origin, which means that a very small correction of the Gauss method is needed when the stepsize is small enough. As

a matter of fact, the needed correction is so small that the resulting method (2.13) has order $2s$ instead of $2s-2$, just as the Gauss method obtained by posing $\alpha = 0$. This is a consequence of the following result.

THEOREM 3.3. *Consider the parametric method* (2.8) *and suppose that the parameter* α *is actually a function of the stepsize* h*, in such a way that* $\alpha(h) = O(h^2)$*. Then, the resulting method has order* $2s$*.*

Proof. Let $y_1(\alpha, h)$ be the solution computed by method (2.8) at time $t_0 + h$, starting at $y_0 = y(t_0)$. The mean value theorem yields

$$y_1(\alpha, h) = y_1(0, h) + \left(\int_0^1 y'(t\alpha, h)\mathrm{d}t \right) \alpha.$$

We recall that $y_1(0, h)$ is the numerical solution provided after a single step of the Gauss method and hence it is $O(h^{2s+1})$ accurate, while for $\alpha \neq 0$, $y_1(\alpha, h)$ yields an approximation to the true solution of order $2s-1$. This implies that $\int_0^1 y'(t\alpha, h)\mathrm{d}t$ is $O(h^{2s-1})$. Consequently,

$$y_1(\alpha, h) - y(t_0+h) = y_1(0, h) - y(t_0+h) + \left(\int_0^1 y'(t\alpha, h)\mathrm{d}t \right) \alpha = O(h^{2s+1}) + \alpha O(h^{2s-1}),$$

which implies that the error at the left-hand side is $O(h^{2s+1})$ if and only if $\alpha = O(h^2)$. ∎

Remark 3.4. It is worth emphasizing that the result of Theorem 3.3 implies that the modified methods retain the order $2s$ of the generating Gauss formula.

Example 3. Figure 3.1 reports the level curves of the function $g(\alpha, h)$, in a neighborhood of the origin, for the Kepler problem described in subsection 4.1. (The

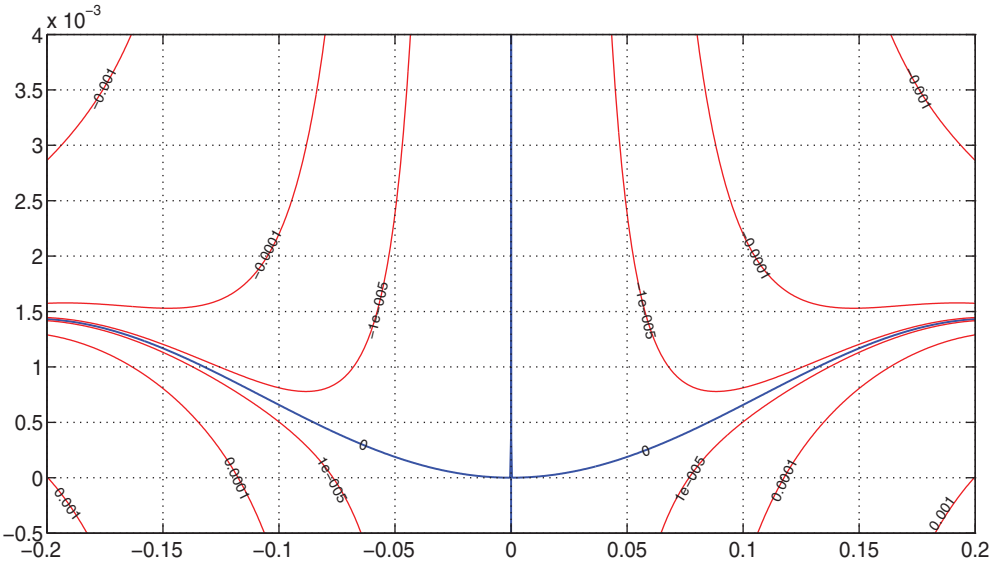

FIG. 3.1. *Level curves in the plane* (h, α) *of the function* $g(\alpha, h, y_0)$ *associated with the method* (2.8) *of order four for the Kepler problem (see subsection* 4.1*) in a neighborhood of the origin:* $h \in [-0.2, 0, 2]$*,* $\alpha \in [-0.5 \cdot 10^{-3}, 4 \cdot 10^{-3}]$*. Besides the* α*-axis, a zero level curve tangent to the* h*-axis at the origin is visible. Such a curve separates two regions around the origin where the function* g *has the opposite sign. We notice that just a small correction of the Gauss method suffices to recover the energy preservation even for relatively large stepsizes.*

vector y_0 is that given in (4.3).) The tick lines in the plot correspond to the points (α, h) in the plane where g vanishes. This zero level set consists of the vertical axis $h = 0$ and of the function $\alpha^*(h)$, which splits the region surrounding the origin into two adjacent subregions where the function g assumes opposite signs. Despite the local character of the above existence result, we see that the branches of the function $\alpha^*(h)$ extend far away from the origin. Similar bifurcation diagrams may be traced starting from different initial values y_0 for all the test problems we have considered; this suggests that, in the spirit of the long-time simulation of dynamical systems, a quite large stepsize may be used during the numerical integration performed by method (2.13).

We end this section by providing a straightforward generalization of Theorem 3.2 to the case where the parameter α is used to perturb a generic (not necessarily the last) element on the subdiagonal of the matrix X_s and its symmetric.

THEOREM 3.5. *Consider the method* (2.16) *with* $\widetilde{W}_s$ *as in* (2.17) *with* $\alpha_i = \delta_{ir}\alpha$ *for a given* $r \in \{1, \ldots, s-1\}$. *We assume that assumption* $(\mathcal{A}_1)$ *and the following assumption (replacing* $(\mathcal{A}_2)$*) hold true:*

$(\mathcal{A}_2^r)$ *let* d *be the order of the error in the Hamiltonian function associated with the Gauss method applied to the given Hamiltonian system* (1.1) *and the given state vector* y_0*, as indicated at* (3.3). *Then, we assume that for any fixed* $(\alpha, h) \in \mathcal{R}$, $\alpha \neq 0$,

$$g(\alpha, h) = c_r(\alpha) h^{d-2(s-r)} + O(h^{d-2(s-r)+1})$$

with $c_r(\alpha) \neq 0$.

Then, there exists a function $\alpha^* = \alpha^*(h)$ *defined in a neighborhood of the origin* $(-h_0, h_0)$ *and such that*

(i) $g(\alpha^*(h), h) = 0$ *for all* $h \in (-h_0, h_0)$,

(ii) $\alpha^*(h) = \text{const} \cdot h^{2(s-r)} + O(h^{2(s-r)+1})$.

Consequently, the symplectic energy conserving method resulting from this choice of the parameter has order $2s$.

Example 4. In the case $s = 3$, $\alpha_1 = \alpha$, and $\alpha_2 = 0$, (2.17) becomes

$$\widetilde{W}_s = \alpha \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{3.8}$$

and one obtains the following sixth-order EQUIP variant of the three-stage Gauss method (compare with (2.15)),

$$\begin{array}{c|ccc} \frac{1}{2} - \frac{\sqrt{15}}{10} & \frac{5}{36} & \frac{2}{9} - \frac{\sqrt{15}}{15} - 4\alpha\frac{\sqrt{5}}{15} & \frac{5}{36} - \frac{\sqrt{15}}{30} - \alpha\frac{\sqrt{5}}{3} \\ \frac{1}{2} & \frac{5}{36} + \frac{\sqrt{15}}{24} + \alpha\frac{\sqrt{5}}{6} & \frac{2}{9} & \frac{5}{36} - \frac{\sqrt{15}}{24} - \alpha\frac{\sqrt{5}}{6} \\ \frac{1}{2} + \frac{\sqrt{15}}{10} & \frac{5}{36} + \frac{\sqrt{15}}{30} + \alpha\frac{\sqrt{5}}{3} & \frac{2}{9} + \frac{\sqrt{15}}{15} + 4\alpha\frac{\sqrt{5}}{15} & \frac{5}{36} \\ \hline & \frac{5}{18} & \frac{4}{9} & \frac{5}{18} \end{array}, \tag{3.9}$$

due to the fact that, according to Theorem 3.5, $\alpha = O(h^4)$. Also in this case, for $\alpha = 0$ one retrieves the original three-stage Gauss method.

4. Numerical tests. In this section we present a few numerical tests showing the effectiveness of our approach. Method (2.13) and its generalizations are implemented by solving, at each step, system (3.1). The efficient solution of such a system will

be the subject of future investigations and will not be discussed here, though there is evidence that the computational cost of an EQUIP method is comparable with that of the corresponding Gauss method. In the present tests, we use a standard solver for Runge–Kutta methods coupled with either the secant/chord iteration or the bisection method for determining the parameter α^* that yields the energy conservation property.

The methods that we will consider in our experiments are

- method (2.13) with $s = 2$ (fourth-order, i.e., method (2.14));
- method (2.13) with $s = 3$ (sixth-order, i.e., method (2.15));
- the sixth-order variant of the EQUIP method given by (3.9), for which Theorem 3.5 applies with $s = 3$ and $r = 1$.

In order to distinguish between the two methods of order six, hereafter the latter will be referred to as "the order six method of the second type."

4.1. The Kepler problem. In this problem, two bodies subject to Newton's law of gravitation revolve around their center of mass, placed at the origin, in elliptic orbits in the (q_1, q_2)-plane. Assuming unitary masses and gravitational constant, the dynamics is described by the Hamiltonian function

$$H(q_1, q_2, p_1, p_2) = \frac{1}{2}\left(p_1^2 + p_2^2\right) - \frac{1}{\sqrt{q_1^2 + q_2^2}}. \tag{4.1}$$

Besides the total energy H, a relevant first integral for the system is represented by the angular momentum

$$L(q_1, q_2, p_1, p_2) = q_1 p_2 - q_2 p_1. \tag{4.2}$$

Due to its symplecticity, the quadratic first integral (4.2) will be automatically conserved by method (2.8) for any choice of the parameter α. On the other hand, we show that at each step of integration, the parameter α may be tuned in order to get energy conservation in the numerical solution.

As an initial condition we choose

$$q_1(0) = 1 - e, \quad q_2(0) = 0, \quad p_1(0) = 0, \quad p_2(0) = \sqrt{\frac{1+e}{1-e}}, \tag{4.3}$$

from which a periodic orbit of period 2π and eccentricity equal to e (in the (q_1, q_2)-plane) originates. Consequently, $H(q, p) = -0.5$ and $L(q, p) = \sqrt{1 - e^2}$. We set $e = 0.6$ since, in this experiment, we are going to use a constant stepsize (see [18, section I.2.3]). More precisely, we solve problem (4.1) in the interval $[t_0, T] = [0, 50]$ by the two-stage method (2.13) with the following set of stepsizes: $h_i = 2^{-i}$, $i = 1, \ldots, 7$. Figure 4.1 reports the errors in the Hamiltonian function H and in the angular momentum L for the numerical solution generated by the method implemented with the intermediate stepsize $h = 2^{-5}$. These plots, which remain almost the same whatever the stepsize considered in the given range, testify that the integration procedure performed by method (2.14) is indeed feasible and both energy and angular momentum preservation may be recovered in the discrete approximation of (1.1). For comparison purposes, we also report the same quantities for the Gauss method of order four (corresponding to the choice $\alpha = 0$ in (2.14)).

The second and third columns of Table 4.1 report the global error $e(h_i) = |y_N(h_i) - y(T)|$, $N = T/h_i$, at the end point of the integration interval and the corresponding numerical order. According to Theorem 3.3, we see that the maximum order

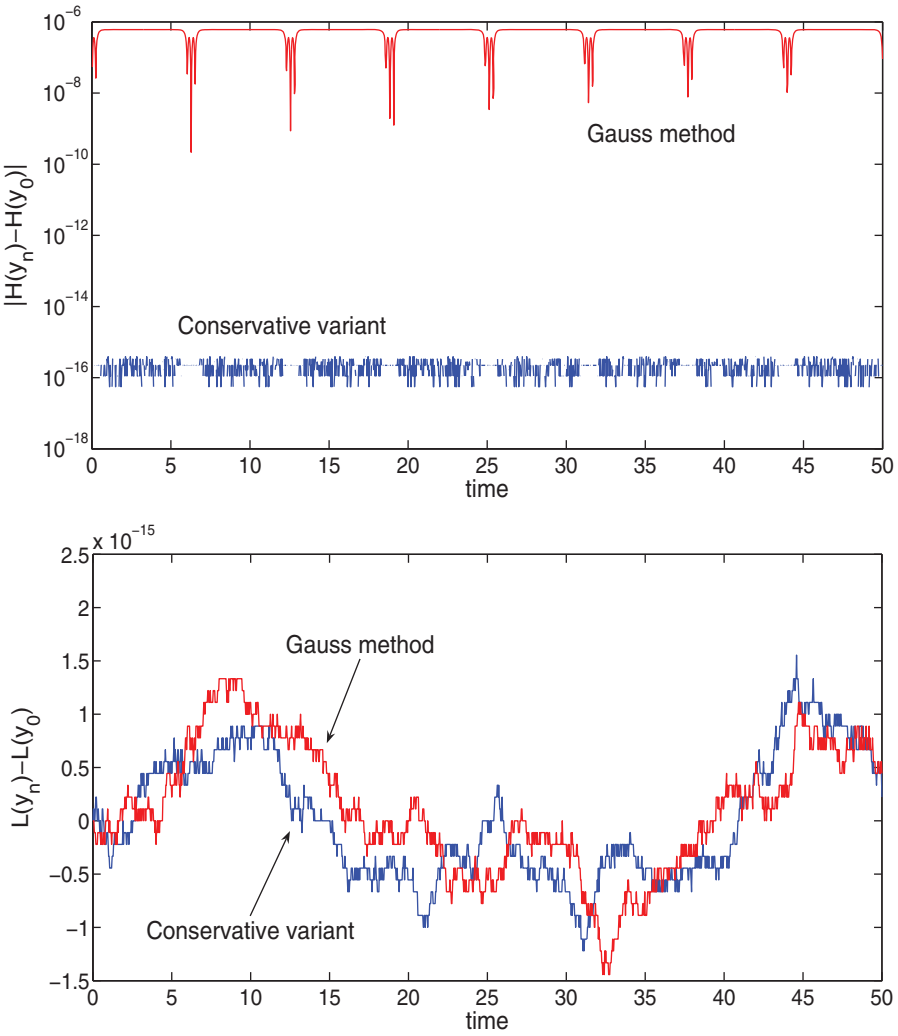

FIG. 4.1. *Top: errors in the Hamiltonian function of the Kepler problem evaluated along the numerical solution generated by the Gauss method of order four and that of its conservative variant* (2.14). *Bottom: error in the numerical angular momentum of the solution computed by the two methods. In both cases the stepsize used is* $h = 2^{-5}$.

(i.e., four) is preserved by method (2.14). Moreover, since the conservative variant of the Gauss method preserves *both* the angular momentum (4.2) and the energy (4.1), according to the analysis in [10], a more favorable error propagation with respect to the generating Gauss method is to be expected. This is indeed confirmed by the upper plot of Figure 4.2, where we see that the conservative variant exhibits a linear error growth, which is more than one order of magnitude smaller than that of the Gauss method.

In the lower plot of Figure 4.2 the sequence α_n^* is plotted for the case $h = 2^{-5}$. We consider $\delta(h) = \max_n(\alpha_n^*) - \min_n(\alpha_n^*)$ as a measure of the total variability of the values of the sequence $\{\alpha_n^*\}$. Such a quantity is reported in the fourth column of Table 4.1 for the values of the stepsize h_i used in this test. According to the result of Theorem 3.2, the last column in the table confirms that the dependence of $\delta(h)$ on the stepsize h is of the form $\delta = ch^2 + \text{h.o.t.}$ with $c \simeq 0.16$.

TABLE 4.1

Performance of the fourth-order method (2.14) *applied to the Kepler problem. The global error at* $T = 50$ *(second column) and the corresponding order obtained via the formula* $\log_2(e(h_i)/e(h_{i+1}))$ *indicate that the perturbations introduced in the Gauss collocation conditions (see* (2.21)*) are small enough that order four of the Gauss method with two stages is conserved by its energy-preserving variant. The last two columns give a measure of the perturbations and of the rate they tend to zero as* $h \to 0$*. The quantity* $\delta(h)$ *is the amplitude of the minimum interval that encloses all the values* α_n^* *for the given stepsize* h *and in the given integration interval. Hence, the last column confirms what was proved in Theorem* 3.2*, namely, that the perturbations are* $O(h^2)$*.*

h	$e(h)$	Order	$\delta(h)$	$\delta(h)/h^2$
2^{-1}	$2.62 \cdot 10^{0}$		$2.13 \cdot 10^{-2}$	$8.5374 \cdot 10^{-2}$
2^{-2}	$3.85 \cdot 10^{-1}$	2.763	$1.04 \cdot 10^{-2}$	$1.6700 \cdot 10^{-1}$
2^{-3}	$2.50 \cdot 10^{-2}$	3.945	$2.52 \cdot 10^{-3}$	$1.6185 \cdot 10^{-1}$
2^{-4}	$1.59 \cdot 10^{-3}$	3.970	$6.23 \cdot 10^{-4}$	$1.5951 \cdot 10^{-1}$
2^{-5}	$1.00 \cdot 10^{-4}$	3.991	$1.55 \cdot 10^{-4}$	$1.5878 \cdot 10^{-1}$
2^{-6}	$6.28 \cdot 10^{-6}$	3.997	$3.87 \cdot 10^{-5}$	$1.5862 \cdot 10^{-1}$
2^{-7}	$3.93 \cdot 10^{-7}$	3.999	$9.67 \cdot 10^{-6}$	$1.5856 \cdot 10^{-1}$

4.2. Test problem 2. We consider the problem defined by the following polynomial Hamiltonian function:

$$H(q_1, q_2, p_1, p_2) = \frac{1}{2}(p_1^2 + p_2^2) + (q_1^2 + q_2^2)^2. \tag{4.4}$$

This problem has been proposed in [26] as an example of a class of polynomial systems which, under suitable assumptions, admit an additional polynomial first integral F which is functionally independent of H. In this case, the additional (irreducible) first integral is

$$L(q_1, q_2, p_1, p_2) = q_1 p_2 - q_2 p_1. \tag{4.5}$$

The polynomial L being quadratic, we expect that our methods may preserve both H and L.[4]

We have solved problem (4.4) by means of two EQUIP methods of order six ($s = 3$): method (2.15) and the order six method of the second type described by (3.9).

Figure 4.3 reports the errors in the Hamiltonian function H and in the quadratic first integral L for the numerical solution generated by the latter method implemented with the intermediate stepsize $h = 2^{-3}$. (The former method provides very similar results.) For comparison purposes, we also report the same quantities for the Gauss method of order six.

Tables 4.2 and 4.3 are the analogues of Table 4.1 for these two EQUIP methods; we see that both methods achieve order six, but while in the former $\alpha^*(h) = O(h^2)$, in the latter $\alpha^*(h) = O(h^4)$ consistently with Theorems 3.2, 3.3, and 3.5.

4.3. The Hénon–Heiles problem. The Hénon–Heiles equation originates from a problem in celestial mechanics describing the motion of a star under the action of

[4] Of course, L may again be interpreted as the angular momentum of a mechanical system having (4.4) as the Hamiltonian function.

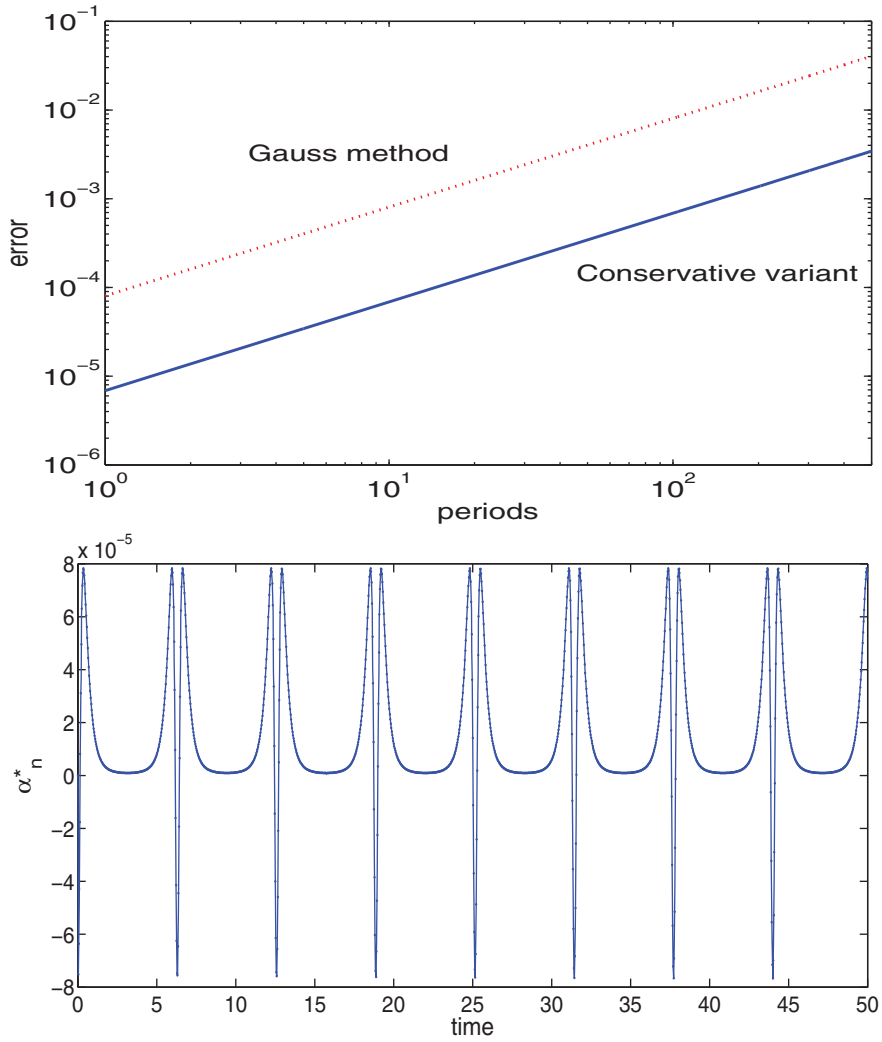

FIG. 4.2. *Top: linear error growth for the fourth-order Gauss method (dashed line) and its conservative variant* (2.14) *(solid line) when integrating the Kepler problem with stepsize* $h = 2\pi/200$. *Bottom: sequence of the values of the parameter* α^* *in the method* (2.14)*, with* $h = 2^{-5}$*, to obtain energy conservation.*

a gravitational potential of a galaxy which is assumed time-independent and with an axis of symmetry (the z-axis) (see [20] and references therein). The main question related to this model was to state the existence of a third first integral, beside the total energy and the angular momentum. By exploiting the symmetry of the system and the conservation of the angular momentum, Hénon and Heiles reduced the degrees of freedom from three (cylindrical coordinates) to two (planar coordinates), thus showing that the problem was equivalent to the study of the motion of a particle in a plane subject to an arbitrary potential $U(q_1, q_2)$:

$$H(q_1, q_2, p_1, p_2) = \frac{1}{2}(p_1^2 + p_2^2) + U(q_1, q_2). \tag{4.6}$$

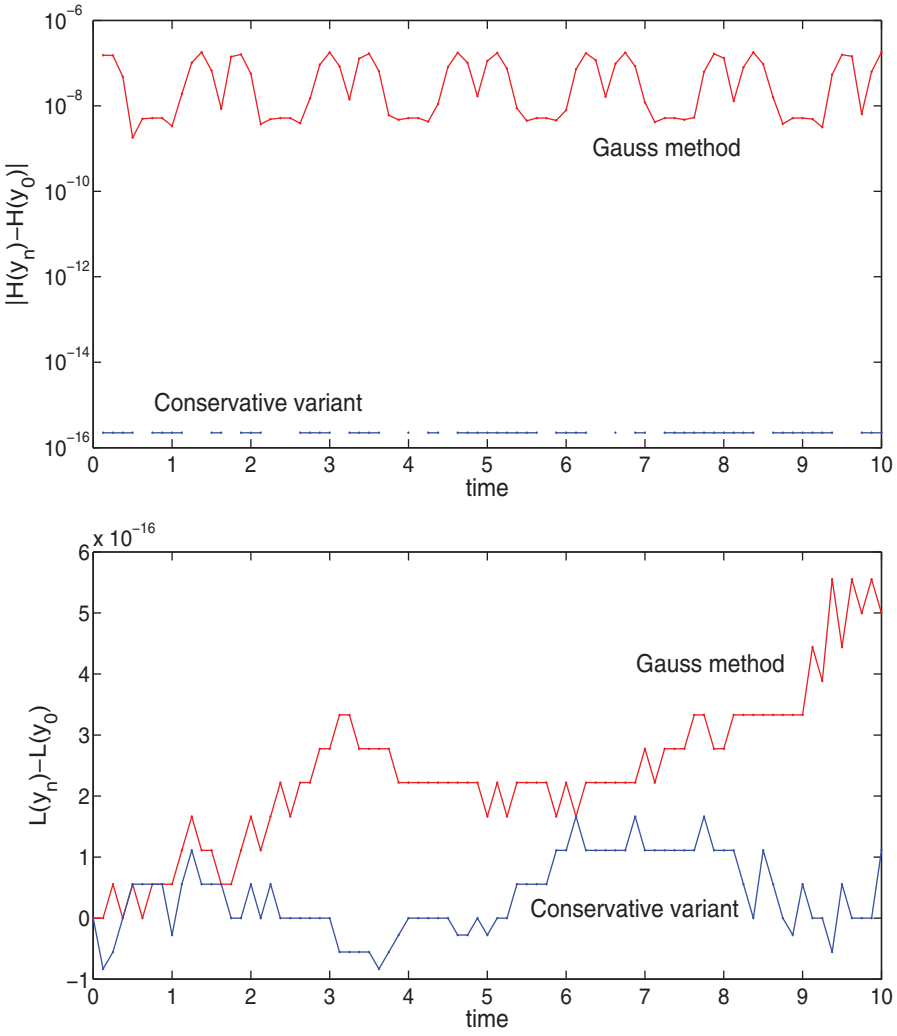

FIG. 4.3. *Top: errors in the Hamiltonian function of test problem* 2 *evaluated along the numerical solution generated by the Gauss method of order six and that of its conservative variant of the second type* (3.9). *Bottom: error in the quadratic first integral* (4.5) *for the solutions computed by the above two methods. In both cases the stepsize used is* $h = 2^{-3}$.

In particular, for their experiments they chose

$$U(q_1, q_2) = \frac{1}{2}(q_1^2 + q_2^2) + q_1^2 q_2 - \frac{1}{3}q_2^3, \tag{4.7}$$

which makes the Hamiltonian function a polynomial of degree three. When $U(q_1, q_2)$ approaches the value $\frac{1}{6}$, the level curves of U tend to an equilateral triangle, whose vertices are saddle points of U (see Figure 4.4). These vertices have coordinates $P_1 = (0, 1)$, $P_2 = (-\frac{\sqrt{3}}{2}, -\frac{1}{2})$, and $P_3 = (\frac{\sqrt{3}}{2}, -\frac{1}{2})$.

Since U in (4.6) has no symmetry in general, we can no longer consider the angular momentum as an invariant, so the only known first integral is the total energy represented by (4.6) itself, and the question is whether a second integral does exist. Hénon and Heiles conducted a series of tests with the aim of giving numerical evidence

TABLE 4.2
Performance of the EQUIP method (2.15) *of order six applied to problem* (4.4). *The reported quantities are the analogues of the ones presented in Table* 4.1.

h	$e(h)$	Order	$\delta(h)$	$\delta(h)/h^2$
2^{-1}	$2.17 \cdot 10^{-2}$		$1.59 \cdot 10^{-2}$	$6.37 \cdot 10^{-2}$
2^{-2}	$4.59 \cdot 10^{-4}$	5.562	$3.99 \cdot 10^{-3}$	$6.39 \cdot 10^{-2}$
2^{-3}	$7.77 \cdot 10^{-6}$	5.884	$9.99 \cdot 10^{-4}$	$6.40 \cdot 10^{-2}$
2^{-4}	$1.24 \cdot 10^{-7}$	5.970	$2.53 \cdot 10^{-4}$	$6.48 \cdot 10^{-2}$
2^{-5}	$1.94 \cdot 10^{-9}$	5.992	$6.33 \cdot 10^{-5}$	$6.49 \cdot 10^{-2}$
2^{-6}	$3.05 \cdot 10^{-11}$	5.994	$1.59 \cdot 10^{-5}$	$6.51 \cdot 10^{-2}$

TABLE 4.3
Performance of the sixth-order EQUIP method of the second type (3.9) *applied to problem* (4.4).

h	$e(h)$	Order	$\delta(h)$	$\delta(h)/h^4$
2^{-1}	$4.91 \cdot 10^{-2}$		$5.59 \cdot 10^{-2}$	0.895
2^{-2}	$1.46 \cdot 10^{-2}$	1.753	$1.51 \cdot 10^{-2}$	3.87
2^{-3}	$1.84 \cdot 10^{-4}$	6.304	$4.92 \cdot 10^{-4}$	2.01
2^{-4}	$3.23 \cdot 10^{-6}$	5.836	$4.07 \cdot 10^{-5}$	2.66
2^{-5}	$4.73 \cdot 10^{-8}$	6.091	$2.30 \cdot 10^{-6}$	2.41
2^{-6}	$7.03 \cdot 10^{-10}$	6.074	$1.50 \cdot 10^{-7}$	2.51

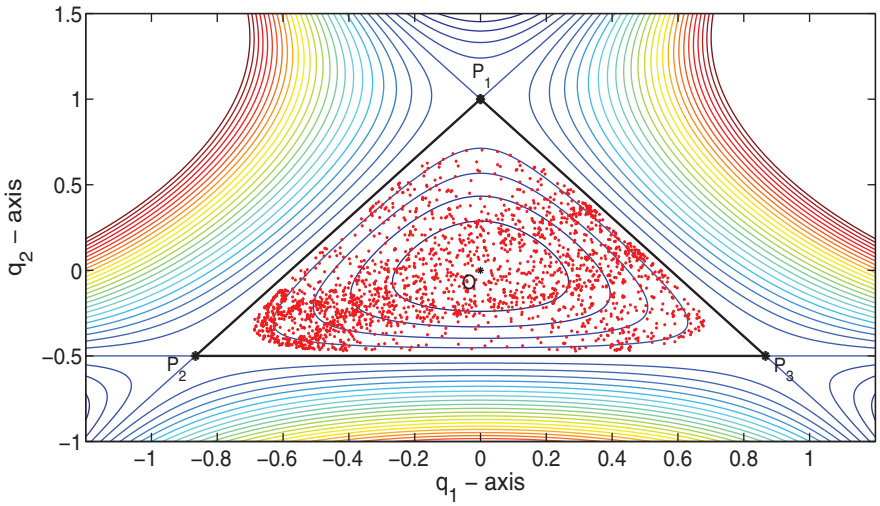

FIG. 4.4. *Level curves of the potential* $U(q_1, q_2)$ *of the Hénon–Heiles problem (see* (4.7)*). The origin* O *is a stable equilibrium point whose domain of stability contains the equilateral triangle having as vertices the saddle points* P_1, P_2, *and* P_3, *provided that the total energy does not exceed the value* $\frac{1}{6}$. *Inside the triangle, a numerical trajectory (small dots) computed by the sixth-order method of the second type* (3.9) *with stepsize* $h = 0.25$ *and in the time interval* $[0, 500]$ *is traced; its total energy is* 0.15.

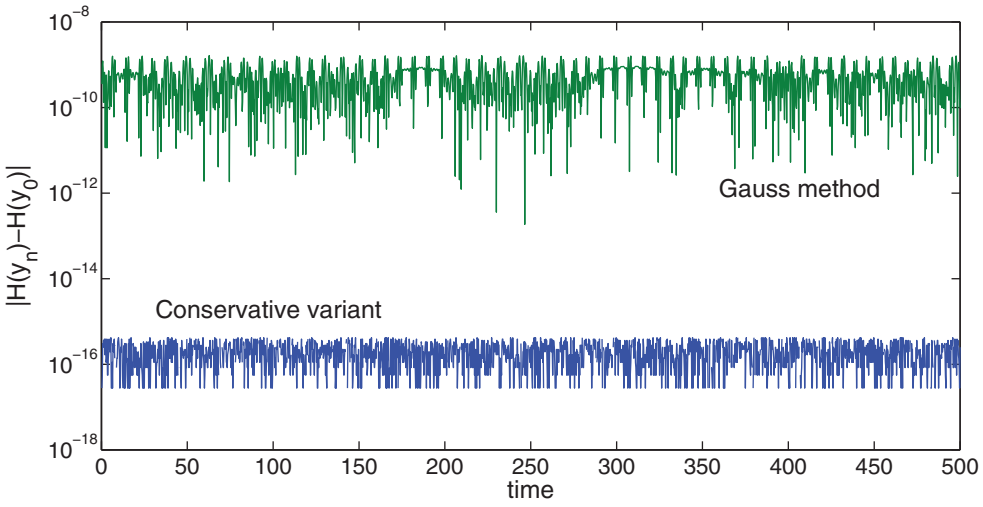

FIG. 4.5. *Errors in the Hamiltonian function* (4.6)–(4.7) *evaluated along the numerical solution generated by the Gauss method of order six and that of its conservative variant of the second type* (3.9). *Stepsize:* $h = 0.25$*; time interval:* $[0, 500]$*; initial condition* $(q_{10}, q_{20}, p_{10}, p_{20}) = (0, 0, \sqrt{\frac{3}{10}}, 0)$.

of the existence of such an integral for moderate values of the energy H and of the appearance of chaotic behavior when H becomes larger than a critical value; it is believed that for values of H in the interval $(\frac{1}{8}, \frac{1}{6})$ this second first integral does not exist (see also [18, section I3]).

We consider the initial point $y_0 = (q_{10}, q_{20}, p_{10}, p_{20}) = (0, 0, \sqrt{\frac{3}{10}}, 0)$, giving a total energy $H = 0.15 \in (\frac{1}{8}, \frac{1}{6})$. Therefore, the orbit originating from y_0 will never escape the triangle for any value of the time t. We have integrated problem (4.6) in the time interval $[0, 500]$ with stepsize $h = 0.25$ by using the Gauss method of order six and its conservative variant of the second type (3.9). Figure 4.5 shows the errors in the Hamiltonian function H for both methods.

5. Conclusions. We have defined a new class of symmetric and symplectic one-step methods of any high order that, under somewhat weak assumptions, are capable of computing a numerical solution along which the Hamiltonian function is precisely conserved. This feature has been achieved by first introducing a symplectic parametric perturbation of the Gauss method and then selecting the parameter, at each step of the integration procedure, in order to obtain energy conservation. A relevant implication of the symplectic nature of each formula is the conservation of all quadratic first integrals associated with the system. With the help of the implicit function theorem, we have shown that not only do these methods exist, but the correction required on the Gauss method is so small that the order of convergence of this latter method is preserved by its conservative variant(s). A few test problems have been reported to confirm the theoretical results presented and to show the effectiveness of the new formulae.

This approach opens a number of interesting routes of investigation. First, if preferred, the parameter could be selected to impose the conservation of other non-quadratic first integrals different from the Hamiltonian function itself. More generally, the multiparametric generalization introduced suggests the possibility of choosing the free parameters in order to impose the conservation of a number of functionally in-

dependent first integrals possessed by the continuous problem. Last but not least, the idea of considering symplectic corrections of the Gauss method could in principle be extended to other classes of symplectic methods known in the literature. The above described lines of investigation, as well as the efficient solution of the nonlinear systems arising from the conservation requirements, will be the subject of future research.

Acknowledgment. The authors are very grateful to an unknown referee for pointing out the pioneering work of J. E. Marsden and coworkers on energy-preserving and symplectic methods.

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