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The lack of continuity and the role of infinite and infinitesimal in numerical methods for ODEs: The case of symplecticity ☆

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ABSTRACT

When numerically integrating canonical Hamiltonian systems, the long-term conservation of some of its invariants, for example the Hamiltonian function itself, assumes a central role. The classical approach to this problem has led to the definition of symplectic methods, among which we mention Gauss–Legendre collocation formulae. Indeed, in the continuous setting, energy conservation is derived from symplecticity via an *infinite* number of *infinitesimal contact transformations*. However, this infinite process cannot be directly transferred to the discrete setting. By following a different approach, in this paper we describe a sequence of methods, sharing the same essential spectrum (and, then, the same essential properties), which are energy preserving starting from a certain element of the sequence on, i.e., after a finite number of steps.

1. Introduction

In order to make easier the following considerations, it is necessary to stress the differences between a continuous problem and a discrete problem obtained by applying to it a whatever numerical method. In the case of ODEs, the main difference between them, very often underrated by many authors, is the lack of continuity in time. The latter does not affect many aspects such as, e.g., the study of the qualitative behavior of solutions around asymptotically stable critical points (stability analysis). In fact, the respective theories, with minor changes, are very similar (see, e.g., [22]). As a consequence, many tools, already devised in the continuous analysis, can be transferred to the discrete analysis almost unchanged. This is the case, for example, of the linearization around asymptotically stable critical points, which has been extensively used in the numerical analysis of methods for differential problems (linear stability analysis). There are, however, other aspects for which continuity plays an essential role. For example, two solutions of the continuous problem need to stay away from each other while, in the discrete case, they may interlace (without having common points, of course). This fact has many mathematical and even physical implications (see, e.g., [20]). In this paper we shall deal with another case in which continuity plays an essential role. It regards the role of symplecticity which is central in discussing energy conservation in continuous Hamiltonian problems, while it is less crucial in the energy conservation of discrete problems. This depends on the interplay between infinitesimal contact transformations and the need of infinite processes (number of iterations) which cannot be operatively used in Numerical Analysis. This question has been already discussed in previous papers (see, e.g., [7]). Here, after a rapid introduction to the subject, we shall focus on a particular aspect, although very important, which concerns a property of the

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numerical methods, in the general class of collocation methods, which comes out by no more requiring symplecticity but still providing conservation of the Hamiltonian functions on a subset of points of the mesh. Clearly, this permits to avoid the drift of energy experienced when using many numerical methods proposed in the recent literature.

With this premise, the structure of the paper is the following: in Section 2 we recall the basic facts about canonical Hamiltonian problems and the approaches used for their numerical solution; one of them, resulting in the recently introduced class of *Hamiltonian Boundary Value Methods (HBVMs)*, is then sketched in Section 3; in Section 4 we state the main result of this paper, concerning the *isospectral property* of such methods; in Section 5 such property is further generalized to study the existing connections between HBVMs and Runge–Kutta collocation methods; a few concluding remarks are finally given in Section 6.

2. Canonical Hamiltonian problems

Canonical Hamiltonian problems are in the form

$$\dot{y} = J\nabla H(y), \quad y(t_0) = y_0 \in \mathbb{R}^{2m}, \tag{1}$$

where J is a skew-symmetric constant matrix, the Hamiltonian $H(y)$ is assumed to be sufficiently differentiable, and the state vector splits into two blocks, $y = (q^T, p^T)^T,\ q, p \in \mathbb{R}^m$ where, for mechanical systems, q denote the positions and p the (generalized) momenta. Such problems are of great interest in many fields of application, ranging from the macro-scale of celestial mechanics, to the micro-scale of molecular dynamics. They have been deeply studied, from the point of view of the mathematical analysis, since two centuries. Their numerical solution is a more recent field of investigation, where the main difficulty in dealing with them numerically stems from the fact that the meaningful isolated critical points of such systems are only marginally stable: neighboring solution curves do not eventually approach the equilibrium point either in future or in past times. This implies that the geometry around them critically depends on perturbations of the linear part. Consequently, the use of a linear test equation, which essentially captures the geometry of the linear part, whose utility has been enormous in settling the dissipative case, cannot be of any utility in the present case.

It is then natural to look for other properties of Hamiltonian systems that can be imposed on the discrete methods in order to make them effective. The first property which comes to mind is the symplecticity of the flow $\varphi_t := y_0 \mapsto y(t)$ associated with (1). This property can be described either in geometric form (invariance of areas, volumes, etc.) or in analytical form:

$$\left(\frac{\partial \varphi_t}{\partial y_0}\right)^T J \left(\frac{\partial \varphi_t}{\partial y_0}\right) = J.$$

In one way or the other, it essentially consists in moving *infinitesimally* on the trajectories representing the solutions. Infinitesimally means retaining only the linear part of the *infinitesimal time displacement* δt. It can be shown that this produces new values of the variables $q + \delta q, p + \delta p$ which leave unchanged the value of the Hamiltonian $H(q + \delta q, p + \delta p) = H(q, p)$ (*Infinitesimal Contact Transformation* (ICT), see [13, p. 386]). Consequently, since the composition of such *infinitesimal* transformations maintains the invariance, so does an *infinite number* of them.

It is not surprising that the first numerical attempts to design conservative methods have tried to transfer similar arguments to discrete methods, i.e. to design symplectic integrators [27,12] (see also the monographs [28,23,14] for more details on the subject; related approaches can be also found in [29,25]). A backward error analysis has shown that symplecticity seems somehow to improve the long-time behavior properties of the numerical solutions. Indeed, for a symplectic method of order r, implemented with a constant stepsize h, the following estimation reveals how the numerical solution y_n may depart from the manifold $H(y) = H(y_0)$ of the phase space, which contains the continuous solution itself:

$$H(y_n) - H(y_0) = O\left(nhe^{-\frac{h_0}{2h}}h^r\right), \tag{2}$$

where $h_0 > 0$ *is sufficiently small* and $h \leqslant h_0$. Relation (2) implies that a linear drift of the energy with respect to time $t = nh$ may arise. However, due to the presence of the exponential, such a drift will not appear as far as $nh \leqslant e^{\frac{h_0}{2h}}$: this circumstance is often referred to by stating that *symplectic methods conserve the energy function on exponentially long time intervals* (see, for example, [14,8.1, p. 367]). This is clearly a surrogate of the definition of stability in that the "good behaviour" of the numerical solution is not extended on *infinite* time intervals.

As matter of fact, since symplecticity requires an *infinite* sequence of *infinitesimal contact transformations* it cannot be transferred "*sic et simpliciter*" to the discrete methods, simply because infinite processes are not permitted in Numerical Analysis. A more efficient approach would require to design methods which avoid the necessity of using infinite processes while preserving the constant of motion, i.e., yielding a numerical solution belonging to the manifold $H(y) = H(y_0)$. In this paper we consider a recently introduced class of methods of any high order that provide energy conservation. More specifically, with any given order, one can associate an infinite sequences of methods, differing from each other for the number of internal mesh points that cover the same time window, say $[t_i, t_i + h]$: the more points we include, the better the conservation properties of the method. However, we show that, at least for polynomial Hamiltonian functions, such a process of increasing the number of internal points is not infinite. In fact we show that there exists a finite value of new added points starting from which the method become conservative, whatever is the stepsize h used.

The evolution of the approaches to the problem, i.e. to get efficient energy-conserving methods, has been slow. As a matter of fact, the first unsuccessful attempts to derive energy-preserving Runge–Kutta methods culminated in the wrong general feeling that such methods could not even exist [21]. One of the first successful attempts to solve the problem, outside the class of Runge–Kutta methods, is represented by *discrete gradient methods* (see [24] and references therein) which are second order accurate. Purely algebraic approaches have been also introduced (see, e.g., [11]), without presenting any energy preserving method. A further approach was considered in [26], where the *averaged vector field method* was proposed and shown to conserve the energy function, although it is only second order accurate. As was recently outlined in [10], approximating the integral appearing in such method by means of a quadrature formula (based upon polynomial interpolation) yields a family of second order Runge–Kutta methods. These latter methods represent an instance of energy-preserving Runge–Kutta methods for polynomial Hamiltonian problems: their first appearance may be found in [16], under the name of *s*-stage trapezoidal methods. Additional examples of fourth and sixth-order conservative Runge–Kutta methods (for polynomial Hamiltonians of suitable degree) were presented in [17,19]. All such energy-conserving methods have been derived by means of the new concept of *discrete line integral*.

The evolution of this idea eventually led to the definition of *Hamiltonian Boundary Value Methods (HBVMs)* [2–4], which is a wide class of methods able to preserve, for the discrete solution, polynomial Hamiltonians of arbitrarily high degree (and then, a *practical* conservation of any sufficiently differentiable Hamiltonian). In more details, in [3] HBVMs defined at Lobatto nodes have been analysed, whereas in [4] HBVMs defined at Gauss–Legendre abscissae have been considered. In the last reference, it has been actually shown that both formulae are essentially equivalent to each other, since the order and stability properties of the methods turn out to be independent of the abscissae distribution, and both methods are equivalent, when the number of the so called *silent stages* tends to *infinity*. In this paper this conclusion is further supported, since we prove that HBVMs, when cast as Runge–Kutta methods, are such that the corresponding matrix of the tableau has the nonzero eigenvalues coincident with those of the corresponding Gauss–Legendre formula (*isospectral property* of HBVMs). This property will be also used to further analyse the existing connections between HBVMs and Runge–Kutta collocation methods.

3. Hamiltonian Boundary Value Methods

The arguments in this section are worked out starting from those used in [3,4] to introduce and analyse HBVMs. Starting from the canonical Hamiltonian problems (1), the key formula which HBVMs rely on, is the *line integral* and the related property of conservative vector fields:

$$H(y_1) - H(y_0) = h\int_0^1 \dot\sigma(t_0+\tau h)^T \nabla H(\sigma(t_0+\tau h))\mathrm{d}\tau, \tag{3}$$

for any $y_1 \in \mathbb{R}^{2m}$, where σ is any smooth function such that

$$\sigma(t_0) = y_0, \quad \sigma(t_0+h) = y_1. \tag{4}$$

Here we consider the case where $\sigma(t)$ is a polynomial of degree s, yielding an approximation to the true solution $y(t)$ in the time interval $[t_0, t_0+h]$. The numerical approximation for the subsequent time-step, y_1, is then defined by (4). After introducing a set of s distinct abscissae,

$$0 < c_1, \ldots, c_s \leqslant 1, \tag{5}$$

we set

$$Y_i = \sigma(t_0 + c_i h), \quad i = 1, \ldots, s, \tag{6}$$

so that $\sigma(t)$ may be thought of as an interpolation polynomial, interpolating the *fundamental stages* Y_i, $i = 1,\ldots,s$, at the abscissae (5). We observe that, due to (4), $\sigma(t)$ also interpolates the initial condition y_0.

Remark 1. Sometimes, the interpolation at t_0 is explicitly required. In such a case, the extra abscissa $c_0 = 0$ is formally added to (5). This is the case, for example, of a Lobatto distribution of the abscissae [3].

Let us consider the following expansions of $\dot\sigma(t)$ and $\sigma(t)$ for $t \in [t_0, t_0+h]$:

$$\dot\sigma(t_0+\tau h) = \sum_{j=1}^{s} \gamma_j P_j(\tau), \quad \sigma(t_0+\tau h) = y_0 + h\sum_{j=1}^{s} \gamma_j \int_0^\tau P_j(x)\mathrm{d}x, \tag{7}$$

where $\{P_j(t)\}$ is a suitable basis of the vector space of polynomials of degree at most $s-1$ and the (vector) coefficients $\{\gamma_j\}$ are to be determined. We shall consider an orthonormal polynomial basis on the interval $[0,1]$ (though, in principle, different bases could be also considered [4,16,19,17]):

$$\int_0^1 P_i(t)P_j(t)\mathrm{d}t = \delta_{ij}, \quad i,j = 1,\ldots,s, \tag{8}$$

where δ_{ij} is the Kronecker symbol, and $P_i(t)$ has degree $i-1$. Such a basis can be readily obtained as

$$P_i(t) = \sqrt{2i-1}\,\widehat{P}_{i-1}(t), \quad i = 1,\ldots,s, \tag{9}$$

with $\widehat{P}_{i-1}(t)$ the shifted Legendre polynomial, of degree $i-1$, on the interval $[0,1]$ (see, e.g., [1]). We shall also assume that $H(y)$ is a polynomial, which implies that the integrand in (3) is also a polynomial so that the line integral can be exactly computed by means of a suitable quadrature formula. It is easy to observe that in general, due to the high degree of the integrand function, such quadrature formula cannot be solely based upon the available abscissae $\{c_i\}$: one needs to introduce an additional set of abscissae $\{\hat{c}_1,\dots,\hat{c}_r\}$, distinct from the nodes $\{c_i\}$, in order to make the quadrature formula exact:

$$\int_0^1 \dot{\sigma}(t_0+\tau h)^T\nabla H(\sigma(t_0+\tau h))\mathrm{d}\tau = \sum_{i=1}^{s}\beta_i\dot{\sigma}(t_0+c_ih)^T\nabla H(\sigma(t_0+c_ih)) + \sum_{i=1}^{r}\hat{\beta}_i\dot{\sigma}(t_0+\hat{c}_ih)^T\nabla H(\sigma(t_0+\hat{c}_ih)), \tag{10}$$

where β_i, $i=1,\dots,s$, and $\hat{\beta}_i$, $i=1,\dots,r$, denote the weights of the quadrature formula defined at the abscissae $\{c_i\}\cup\{\hat{c}_i\}$. Then, according to [3,4], we give the following definition.

Definition 1. The method defined by the polynomial $\sigma(t)$, determined by substituting the quantities in (7) into the right-hand side of (10), and by choosing the unknown coefficient $\{\gamma_j\}$ in order that the resulting expression vanishes, is called *Hamiltonian Boundary Value Method with k steps and degree s*, in short *HBVM*(k,s), where $k=s+r$.

According to [18], the right-hand side of (10) is called *discrete line integral* associated with the map defined by the HBVM(k,s) method, while the vectors

$$\widehat{Y}_i \equiv \sigma(t_0+\hat{c}_ih),\quad i=1,\dots,r, \tag{11}$$

are called *silent stages*: they just serve to increase, as much as one likes, the degree of precision of the quadrature formula, but they are not to be regarded as unknowns since, from (7) and (11), they can be expressed in terms of linear combinations of the fundamental stages (6).

Because of the equality (10), we can apply the procedure described in Definition 1 directly to the original line integral appearing in the left-hand side. With this premise, by considering the first expansion in (7), the conservation property reads

$$\sum_{j=1}^{s}\gamma_j^T\int_0^1 P_j(\tau)\nabla H(\sigma(t_0+\tau h))\mathrm{d}\tau = 0,$$

which, as is easily checked, is satisfied if we impose the following set of orthogonality conditions:

$$\gamma_j = \int_0^1 P_j(\tau)J\nabla H(\sigma(t_0+\tau h))\mathrm{d}\tau,\quad j=1,\dots,s. \tag{12}$$

Then, from the second relation of (7) we obtain, by introducing the operator

$$L(f;h)\sigma(t_0+ch) = \sigma(t_0) + h\sum_{j=1}^{s}\int_0^c P_j(x)\mathrm{d}x\int_0^1 P_j(\tau)f(\sigma(t_0+\tau h))\mathrm{d}\tau,\quad c\in[0,1], \tag{13}$$

that σ is the eigenfunction of $L(J\nabla H;h)$ relative to the eigenvalue $\lambda=1$:

$$\sigma = L(J\nabla H;h)\sigma. \tag{14}$$

According to [4], (14) is called the *Master Functional Equation* defining σ: it characterizes HBVM(k,s) methods, for all $k\geqslant s$. Indeed, such methods are uniquely defined by the polynomial σ, of degree s, the number of steps k being only required to obtain the exact quadrature formula (10).

To practically compute σ, we set (see (6) and (7))

$$Y_i = \sigma(t_0+c_ih) = y_0 + h\sum_{j=1}^{s}a_{ij}\gamma_j,\quad i=1,\dots,s, \tag{15}$$

where

$$a_{ij} = \int_0^{c_i} P_j(x)\mathrm{d}x,\quad i,j=1,\dots,s.$$

Inserting (12) into (15) yields the final formulae which define the HBVMs class based upon the orthonormal basis $\{P_j\}$:

$$Y_i = y_0 + h\sum_{j=1}^{s}a_{ij}\int_0^1 P_j(\tau)J\nabla H(\sigma(t_0+\tau h))\mathrm{d}\tau,\quad i=1,\dots,s. \tag{16}$$

For sake of completeness, we report the nonlinear system associated with the HBVM(k,s) method, in terms of the fundamental stages $\{Y_i\}$ and the silent stages $\{\widehat{Y}i\}$ (see (11)), by using the notation

$$f(y) = J\nabla H(y). \tag{17}$$

It represents the discrete counterpart of (16), which may be directly retrieved by evaluating, for example, the integrals in (16) by means of the (exact) quadrature formula introduced in (10):

$$Y_i = y_0 + h\sum_{j=1}^{s} a_{ij}\left(\sum_{l=1}^{s}\beta_l P_j(c_l) f(Y_l) + \sum_{l=1}^{r}\hat{\beta}_l P_j(\hat{c}_l) f(\hat{Y}_l)\right), \quad i = 1,\dots,s. \tag{18}$$

From the above discussion it is clear that, in the non-polynomial case, supposing to choose the abscissae $\{\hat{c}_i\}$ so that the sums in (18) converge to an integral as $r \equiv k - s$ tends to *infinity*, the resulting formula is (16), which has been named ∞-*HBVM of degree s* or *HBVM*(∞,*s*) in [4]. This implies that HBVMs may be as well applied in the non-polynomial case since, in finite precision arithmetic, HBVMs are undistinguishable from their limit formulae (16), when a sufficient number of silent stages is introduced, so that a *practical* energy conservation is obtained, for k large enough [3,4,16,19]. On the other hand, we emphasize that, in the non-polynomial case, (16) becomes an *operative method* only after that a suitable strategy to approximate the integrals appearing in it is taken into account. In the present case, if one discretizes the *Master Functional Equation* (13) and (14), HBVM(k,s) are then obtained, essentially by extending the discrete problem (18) also to the silent stages (11). In more details, by using (17) and introducing the following notation:

$$\{\tau_i\} = \{c_i\} \cup \{\hat{c}_i\}, \quad \{\omega_i\} = \{\beta_i\} \cup \{\hat{\beta}_i\},$$
$$y_i = \sigma(t_0 + \tau_i h), \quad f_i = f(\sigma(t_0 + \tau_i h)), \quad i = 1,\dots,k,$$

the discrete problem defining the HBVM(k,s) method becomes,

$$y_i = y_0 + h\sum_{j=1}^{s}\int_0^{\tau_i} P_j(x)\mathrm{d}x \sum_{\ell=1}^{k}\omega_\ell P_j(\tau_\ell) f_\ell, \quad i = 1,\dots,k. \tag{19}$$

By defining the vectors $\mathbf{y} = (y_1^T,\dots,y_k^T)^T$ and $e = (1,\dots,1)^T \in \mathbb{R}^k$, and the matrices

$$\Omega = \mathrm{diag}(\omega_1,\dots,\omega_k), \quad \mathcal{I}_s, \mathcal{P}_s \in \mathbb{R}^{k\times s}, \tag{20}$$

whose (i,j)th entry are given by

$$(\mathcal{I}_s)_{ij} = \int_0^{\tau_i} P_j(x)\mathrm{d}x, \quad (\mathcal{P}_s)_{ij} = P_j(\tau_i), \tag{21}$$

we can cast the set of Eq. (19) in vector form as

$$\mathbf{y} = e \otimes y_0 + h(\mathcal{I}_s\mathcal{P}_s^T\Omega) \otimes I_{2m} f(\mathbf{y}),$$

with an obvious meaning of $f(\mathbf{y})$. Consequently, the method can be regarded as a Runge–Kutta method with the following Butcher tableau:

$$\begin{array}{c|c} \tau_1 & \\ \vdots & \mathcal{I}_s\mathcal{P}_s^T\Omega \\ \tau_k & \\ \hline & \omega_1 \cdots \omega_k \end{array} \tag{22}$$

In particular, when a Gauss distribution of the abscissae $\{\tau_1,\dots,\tau_k\}$ is considered, it can be proved that the resulting HBVM(k,s) method [4] (see also [3,5]):

- has order $2s$ for all $k \geqslant s$;
- is symmetric and perfectly A-stable (i.e., its stability region coincides with the left-half complex plane, $\mathbb{C}^-$ [9]);
- reduces to the Gauss–Legendre method of order $2s$, when $k = s$;
- exactly preserves polynomial Hamiltonian functions of degree ν, provided that

$$k \geqslant \frac{\nu s}{2}. \tag{23}$$

4. The isospectral property

We are now going to prove a further additional result, related to the matrix appearing in the Butcher tableau (22), i.e., the matrix

$$A = \mathcal{I}_s\mathcal{P}_s^T\Omega \in \mathbb{R}^{k\times k}, \quad k \geqslant s, \tag{24}$$

whose rank is s. Consequently it has a $(k - s)$-fold zero eigenvalue. In this section, we are going to discuss its *essential spectrum*, i.e., the location of the remaining s nonzero eigenvalues of that matrix. Before that, we state a couple of preliminary results: their proofs follow, respectively, from [15, Theorem 5.6, p. 83] and from the properties of shifted Legendre polynomials (see, e.g., [1] or the Appendix in [3]).

Lemma 1. *The eigenvalues of the matrix*

$$X_s = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & -\xi_{s-1} \\ & & \xi_{s-1} & 0 \end{pmatrix}, \tag{25}$$

with

$$\xi_j = \frac{1}{2\sqrt{(2j+1)(2j-1)}}, \quad j \geqslant 1, \tag{26}$$

coincide with those of the matrix in the Butcher tableau of the Gauss–Legendre method of order 2s.

Lemma 2. *With reference to the matrices in (20) and (21), one has*

$$\mathcal{I}_s = \mathcal{P}_{s+1}\widehat{X}_s,$$

where

$$\hat{X}_s = \left(\begin{array}{cccc} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & -\xi_{s-1} \\ & & \xi_{s-1} & 0 \\ \hline & & & \xi_s \end{array}\right)$$

with the ξ_j defined by (26).

The following result then holds true.

Theorem 1 (*Isospectral property of HBVMs*). *For all $k \geqslant s$ and for any choice of the abscissae $\{\tau_i\}$ such that the quadrature defined by the weights $\{\omega_i\}$ is exact for polynomials of degree $2s-1$, the nonzero eigenvalues of the matrix A in (24) coincide with those of matrix (25), characterizing the Gauss–Legendre method of order 2s.*

Proof. For $k = s$, the abscissae $\{\tau_i\}$ have to be the s Gauss–Legendre nodes, so that HBVM(s,s) reduces to the Gauss Legendre method of order $2s$, as already outlined at the end of Section 3. When $k > s$, from the orthonormality of the basis, see (8), and considering that the quadrature with weights $\{\omega_i\}$ is exact for polynomials of degree (at least) $2s-1$, one obtains that (see (20) and (21)) for all $i = 1,\dots,s$ and $j = 1,\dots,s+1$,

$$\left(\mathcal{P}_s^T \Omega \mathcal{P}_{s+1}\right)_{ij} = \sum_{\ell=1}^{k} \omega_\ell P_i(\tau_\ell) P_j(\tau_\ell) = \int_0^1 P_i(t) P_j(t) \mathrm{d}t = \delta_{ij},$$

and, therefore,

$$\mathcal{P}_s^T \Omega \mathcal{P}_{s+1} = (I_s \ \mathbf{0}).$$

By taking into account the result of Lemma 2, one then obtains:

$$A\mathcal{P}_{s+1} = \mathcal{I}_s \mathcal{P}_s^T \Omega \mathcal{P}_{s+1} = \mathcal{I}_s (I_s \ \mathbf{0}) = \mathcal{P}_{s+1}\widehat{X}_s (I_s \ \mathbf{0}) = \mathcal{P}_{s+1}(\widehat{X}_s \ \mathbf{0}) = \mathcal{P}_{s+1} \left(\begin{array}{cccc|c} \frac{1}{2} & -\xi_1 & & & 0 \\ \xi_1 & 0 & \ddots & & \vdots \\ & \ddots & \ddots & -\xi_{s-1} & \vdots \\ & & \xi_{s-1} & 0 & 0 \\ \hline & & & \xi_s & 0 \end{array}\right) \equiv \mathcal{P}_{s+1}\widetilde{X}_s, \tag{27}$$

with the $\{\xi_j\}$ defined according to (26). Consequently, one obtains that the columns of $\mathcal{P}_{s+1}$ constitute a basis of an invariant (right) subspace of matrix A, so that the eigenvalues of $\widetilde{X}_s$ are eigenvalues of A. In more detail, the eigenvalues of $\widetilde{X}_s$ are those of X_s (see (25)) and the zero eigenvalue. Then, also in this case, the nonzero eigenvalues of A coincide with those of X_s, i.e., with the eigenvalues of the matrix defining the Gauss–Legendre method of order $2s$. □

It turns out that such methods, in the form here presented (i.e., having chosen the polynomial basis (9), can be regarded as a generalization of Gauss methods, in the sense that, they share the same nonzero spectrum, for all $k \geqslant s$. In the limit $k \to \infty$, the same essential spectrum is retained by the limit operator (see (14)). In the case of a polynomial Hamiltonian, such

sequence of methods starts to be energy-preserving for a finite value of k. Moreover, even though for a general Hamiltonian the method becomes energy-preserving in the limit $k \to \infty$, nevertheless, when using finite precision arithmetic, the limit is practically obtained for a finite value of k, namely as soon as full machine precision accuracy is achieved.

5. HBVMs and Runge–Kutta collocation methods

By using the previous results and notations, we now further elucidate the existing connections between HBVMs and Runge–Kutta collocation methods. Our starting point is a generic collocation method with k stages, defined by the tableau

$$\begin{array}{c|c} \tau_1 & \\ \vdots & \mathcal{A} \\ \tau_k & \\ \hline & \omega_1 \cdots \omega_k \end{array} \tag{28}$$

where, for $i, j = 1, \ldots, k$:

$$\mathcal{A} = (\alpha_{ij}) \equiv \left(\int_0^{\tau_i} \ell_j(x)\mathrm{d}x \right), \quad \omega_j = \int_0^1 \ell_j(x)\mathrm{d}x,$$

$\ell_j(\tau)$ being the jth Lagrange polynomial of degree $k-1$ defined on the set of abscissae $\{\tau_i\}$. Moreover, given a positive integer $s \leqslant k$, and considering the matrices defined in (20) and (21), we consider the matrix

$$\mathcal{P}_s \mathcal{P}_s^T \Omega \in \mathbb{R}^{k \times k}$$

with projects into the s-dimensional subspace spanned by the columns of $\mathcal{P}_s$. The class of Runge–Kutta methods we are interested in, is then defined by the tableau

$$\begin{array}{c|c} \tau_1 & \\ \vdots & A \equiv \mathcal{A}(\mathcal{P}_s \mathcal{P}_s^T \Omega) \\ \tau_k & \\ \hline & \omega_1 \cdots \omega_k \end{array} \tag{29}$$

We note that the Butcher array A has rank which cannot exceed s, because it is defined by *filtering* $\mathcal{A}$ by the rank s matrix $\mathcal{P}_s \mathcal{P}_s^T \Omega$. The following result then holds true, which clarifies the existing connections between classical Runge–Kutta collocation methods and HBVMs.

Theorem 2. *Provided that the quadrature formula defined by the weights $\{\omega_i\}$ is exact for polynomials at least $2s-1$ (i.e., the Runge–Kutta method defined by the tableau (29) satisfies the usual simplifying assumption B(2s)), then the tableau (29) defines a HBVM(k,s) method based at the abscissae $\{\tau_i\}$.*

Proof. Let us expand the basis $\{P_1(\tau), \ldots, P_s(\tau)\}$ along the Lagrange basis $\{\ell_j(\tau)\}$, $j = 1, \ldots, k$, defined over the nodes τ_i, $i = 1, \ldots, k$:

$$P_j(\tau) = \sum_{r=1}^{k} P_j(\tau_r)\ell_r(\tau), \quad j = 1, \ldots, s.$$

It follows that, for $i = 1, \ldots, k$ and $j = 1, \ldots, s$:

$$\int_0^{\tau_i} P_j(x)\mathrm{d}x = \sum_{r=1}^{k} P_j(\tau_r) \int_0^{\tau_i} \ell_r(x)\mathrm{d}x = \sum_{r=1}^{k} P_j(\tau_r)\alpha_{ir},$$

that is (see (20), (21), and (28)), $\mathcal{I}_s = \mathcal{A}\mathcal{P}_s$. Consequently,

$$\mathcal{A}\mathcal{P}_s \mathcal{P}_s^T \Omega = \mathcal{I}_s \mathcal{P}_s^T \Omega,$$

so that one retrieves the tableau (22) which defines the method HBVM(k,s). □

The resulting Runge–Kutta method (29) is then energy conserving if applied to polynomial Hamiltonian systems (1), when the degree of $H(y)$ is lower than or equal to a quantity, say ν, depending on k and s. As an example, when a Gaussian distribution of the nodes $\{\tau_i\}$ is considered, one obtains (23) and, moreover, HBVM(k,s) is also related to the Gauss–Legendre method of order $2k$, according to (29), whose Butcher array coincides with $\mathcal{A}$, with this choice of the nodes $\{\tau_i\}$.

Remark 2. It seems like the price paid to achieve such conservation property consists in the lowering of the order of the new method with respect to the original one (28). Actually this is not true, because a fair comparison would be to relate method

(22)–(29) to a collocation method constructed on s rather than on k stages, since the actual nonlinear system, deriving by the implementation of HBVM(k,s), turns out to have dimension s, as it has been shown in [3].

Further implications of the isospectral property of HBVMs, among which an alternative proof for their order of convergence, may be found in [6]. A further alternative proof can be found in [7,8].

6. Conclusions

In this paper, we have shown that the recently introduced class of energy-preserving methods {HBVM(k,s)}, when recast as Runge–Kutta methods, have the matrix of the corresponding Butcher tableau sharing the same nonzero eigenvalues which, in turn, coincides with those of the matrix of the Butcher tableau of the Gauss method of order $2s$, for all $k \geqslant s$ such that $B(2s)$ holds.

Moreover, HBVM(k,s) defined at the Gaussian nodes $\{\tau_1, \ldots, \tau_k\}$ on the interval $[0,1]$ are closely related to the Gauss method of order $2k$ which, although symplectic, is not in general energy-preserving.

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