Chapter 4

Isospectral Property of HBVMs and their connections with Runge-Kutta collocation methods

When applied to initial value problems, HBVMs may be viewed as a special subclass of Runge-Kutta (RK) methods of collocation type. In Chapter 1 (see also [6, 7]) the RK formulation turned out useful in stating results pertaining to the order of the new formulae. Here, the RK notation will be exploited to derive the isospectral property of HBVMs and elucidate the existing connections between HBVMs and RK collocation methods [9]. In doing this, our aim is twofold:

1. to better elucidate the close link between the new formulae and the classical collocation Runge-Kutta methods;

2. to make the handling of the new formulae more comfortable to the scientific community working in the context of RK methods.

In fact, we think that HBVMs (and consequently their RK formulation) may be of interest beyond their application to Hamiltonian systems. Each HBVM(k,s) becomes a classical collocation method when $k = s$, while, for $k > s$, it conserves all the features of the generating collocation formula, including the order (which may be even improved, reaching eventually order $p = 2s$) and the dimension of the associated nonlinear system.

Let us then consider the matrix appearing in the Butcher tableau (1.27), corresponding to HBVM(k, s), i.e., the matrix

$$A = \mathcal{I}_s \mathcal{P}_s^T \Omega \in \mathbb{R}^{k\times k}, \qquad k \geq s, \tag{4.1}$$

whose rank is s (see (1.24)–(1.25)). Consequently it has a $(k-s)$-fold zero eigenvalue. To begin with, we are going to discuss the location of the remaining s eigenvalues of that matrix.

Before that, we state the following preliminary result, whose proof can be found in [23, Theorem 5.6 on page 83].

Lemma 1. *The eigenvalues of the matrix*

$$X_s = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & -\xi_{s-1} \\ & & \xi_{s-1} & 0 \end{pmatrix}, \tag{4.2}$$

with

$$\xi_j = \frac{1}{2\sqrt{(2j+1)(2j-1)}}, \qquad j = 1, \dots, s-1, \tag{4.3}$$

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

We also need the following preliminary result, whose proof derives from the properties of shifted-Legendre polynomials (see, e.g., [1] or the Appendix in [6]).

Lemma 2. *With reference to the matrices in (1.24)–(1.25), one has*

$$\mathcal{I}_s = \mathcal{P}_{s+1} \hat{X}_s, \tag{4.4}$$

where

$$\hat{X}_s = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & -\xi_{s-1} \\ & & \xi_{s-1} & 0 \\ \hline & & & \xi_s \end{pmatrix}, \tag{4.5}$$

with the ξ_j *defined by (4.3).*

The following result then holds true [8].

Theorem 4 (Isospectral Property of HBVMs). *For all* $k \geq s$ *and for any choice of the abscissae* $\{\tau_i\}$ *such that* $B(2s)$ *holds true, the nonzero eigenvalues of the matrix* A *in (4.1) coincide with those of the matrix of the Gauss-Legendre method of order* $2s$.

Proof For $k = s$, the abscissae $\{\tau_i\}$ have to be the s Gauss-Legendre nodes on $[0, 1]$, so that HBVM(s, s) reduces to the Gauss Legendre method of order $2s$, as already observed in Example 2.

When $k > s$, from the orthonormality of the basis, see (1.7), and considering that the quadrature with weights $\{\omega_i\}$ is exact for polynomials of degree (at least) $2s-1$, one easily obtains that

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

since, for all $i = 1,\dots,s$, and $j = 1,\dots,s+1$:

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

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

$$\begin{aligned} A\mathcal{P}_{s+1} &= \mathcal{I}_s \mathcal{P}_s^T \Omega \mathcal{P}_{s+1} = \mathcal{I}_s\,(I_s\,\mathbf{0}) = \mathcal{P}_{s+1}\hat{X}_s\,(I_s\,\mathbf{0}) = \mathcal{P}_{s+1}\left(\hat{X}_s\,\mathbf{0}\right) \\ &= \mathcal{P}_{s+1} \left(\begin{array}{cccc|c} \frac{1}{2} & -\xi_1 & & & 0 \\ \xi_1 & 0 & \ddots & & \vdots \\ & \ddots & \ddots & -\xi_{s-1} & \vdots \\ & & \xi_{s-1} & 0 & 0 \\ \hline & & & \xi_s & 0 \end{array}\right) \equiv \mathcal{P}_{s+1}\widetilde{X}_s, \end{aligned} \tag{4.6}$$

with the $\{\xi_j\}$ defined according to (4.3). 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 (4.2)) 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 $2s$. □

4.1 HBVMs and collocation methods

By using the previous result and notations, now we go to elucidate the existing connections between HBVMs and RK collocation methods. We shall continue to use an orthonormal basis $\{P_j\}$, along which the underlying *extended collocation* polynomial $\sigma(t)$ is expanded, even though the arguments could be generalized to more general bases, as sketched below. On the other hand, the distribution of the internal abscissae can be arbitrary.

Our starting point is a generic collocation method with k stages, defined by the tableau

$$\begin{array}{c|c} \tau_1 & \\ \vdots & \mathcal{A} \\ \tau_k & \\ \hline & \omega_1\,\dots\,\omega_k \end{array} \tag{4.7}$$

where, for $i, j = 1, \dots, k$, $\mathcal{A} = (\alpha_{ij}) \equiv \left(\int_0^{\tau_i} \ell_j(\tau)\mathrm{d}\tau\right)$ and $\omega_j = \int_0^1 \ell_j(\tau)\mathrm{d}\tau$, $\ell_j(t)$ being the jth Lagrange polynomial of degree $k-1$ defined on the set of abscissae $\{\tau_i\}$.

Given a positive integer $s \le k$, we can consider a basis $\{p_1(\tau), \dots, p_s(\tau)\}$ of the vector space of polynomials of degree at most $s-1$, and we set

$$\hat{\mathcal{P}}_s = \begin{pmatrix} p_1(\tau_1) & p_2(\tau_1) & \cdots & p_s(\tau_1) \\ p_1(\tau_2) & p_2(\tau_2) & \cdots & p_s(\tau_2) \\ \vdots & \vdots & & \vdots \\ p_1(\tau_k) & p_2(\tau_k) & \cdots & p_s(\tau_k) \end{pmatrix}_{k\times s} \tag{4.8}$$

(note that $\hat{\mathcal{P}}_s$ is full rank since the nodes are distinct). The class of RK methods we are interested in is defined by the tableau

$$\begin{array}{c|c} \tau_1 & \\ \vdots & A \equiv \mathcal{A}\hat{\mathcal{P}}_s\Lambda_s\hat{\mathcal{P}}_s^T\Omega \\ \tau_k & \\ \hline & \omega_1 \;\ldots\ldots\; \omega_k \end{array} \tag{4.9}$$

where $\Omega = \mathrm{diag}(\omega_1, \dots, \omega_k)$ and $\Lambda_s = \mathrm{diag}(\eta_1, \dots, \eta_s)$; the coefficients η_j, $j = 1, \dots, s$, have to be selected by imposing suitable consistency conditions on the stages $\{Y_i\}$ [7]. In particular, when the basis is orthonormal, as we shall assume hereafter, then matrix $\hat{\mathcal{P}}_s$ reduces to matrix $\mathcal{P}_s$ in (1.24)–(1.25), $\Lambda_s = I_s$, and consequently (4.9) becomes

$$\begin{array}{c|c} \tau_1 & \\ \vdots & A \equiv \mathcal{A}\mathcal{P}_s\mathcal{P}_s^T\Omega \\ \tau_k & \\ \hline & \omega_1 \;\ldots\ldots\; \omega_k \end{array} \tag{4.10}$$

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 RK collocation methods and HBVMs.

Theorem 5. *Provided that the quadrature formula defined by the weights $\{\omega_i\}$ is exact for polynomials at least $2s-1$ (i.e., the RK method defined by the tableau (4.10) satisfies the usual simplifying assumption $B(2s)$), then the tableau (4.10) defines a HBVM(k, s) method based at the abscissae $\{\tau_i\}$.*

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

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

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 (1.24)–(1.25) and (4.7)),

$$\mathcal{I}_s = \mathcal{A}\mathcal{P}_s. \tag{4.11}$$

By substituting (4.11) into (4.10), one retrieves that tableau (1.27), which defines the method HBVM(k, s). This completes the proof. □

The resulting Runge-Kutta method (4.10) is then energy conserving if applied to polynomial Hamiltonian systems (1.1) 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 (1.29).

Remark 9 (About Simplecticity). *The choice of the abscissae* $\{\tau_1, \ldots, \tau_k\}$ *at the Gaussian points in* $[0, 1]$ *has also another important consequence, since, in such a case, the collocation method (4.7) is the Gauss method of order* $2k$ *which, as is well known, is a* symplectic method*. The result of Theorem 5 then states that, for any* $s \leq k$*, the HBVM*(k, s) *method is related to the Gauss method of order* $2k$ *by the relation:*

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

where the filtering matrix $(\mathcal{P}_s\mathcal{P}_s^T\Omega)$ *essentially makes the Gauss method of order* $2k$ *"work" in a suitable subspace.*

It seems like the price paid to achieve such conservation properties consists in the lowering of the order of the new method with respect to the original one (4.7). Actually this is not true, because a fair comparison would be to relate method (1.27)–(4.10) to a collocation method constructed on s rather than on k stages. This fact will be fully elucidated in Chapter 5.

4.1.1 An alternative proof for the order of HBVMs

We conclude this chapter by observing that the order $2s$ of an HBVM(k, s) method, under the hypothesis that (4.7) satisfies the usual simplifying assumption $B(2s)$, i.e., the quadrature defined by the weights $\{\omega_i\}$ is exact for polynomials of degree at least $2s-1$, may be stated by using an alternative, though equivalent, procedure to that used in the proof of Theorem 1.

Let us then define the $k \times k$ matrix $\mathcal{P} \equiv \mathcal{P}_k$ (see (1.24)–(1.25)) obtained by "enlarging" the matrix $\mathcal{P}_s$ with $k-s$ columns defined by the normalized shifted Legendre polynomials $P_j(\tau)$, $j = s+1, \ldots, k$, evaluated at $\{\tau_i\}$, i.e.,

$$\mathcal{P} = \begin{pmatrix} P_1(\tau_1) & \ldots & P_k(\tau_1) \\ \vdots & & \vdots \\ P_1(\tau_k) & \ldots & P_k(\tau_k) \end{pmatrix}.$$

By virtue of property $B(2s)$ for the quadrature formula defined by the weights $\{\omega_i\}$, it satisfies

$$\mathcal{P}^T \Omega \mathcal{P} = \begin{pmatrix} I_s & O \\ O & R \end{pmatrix}, \qquad R \in \mathbb{R}^{k-s \times k-s}.$$

This implies that $\mathcal{P}$ satisfies the property $T(s,s)$ in [23, Definition 5.10 on page 86], for the quadrature formula $(\omega_i, \tau_i)_{i=1}^k$. Therefore, for the matrix A appearing in (4.10) (i.e., (1.27), by virtue of Theorem 5), one obtains:

$$\mathcal{P}^{-1} A \mathcal{P} = \mathcal{P}^{-1} \mathcal{A} \mathcal{P} \begin{pmatrix} I_s & \\ & O \end{pmatrix} = \begin{pmatrix} \widetilde{X}_s & \\ & O \end{pmatrix}, \tag{4.12}$$

where $\widetilde{X}_s$ is the matrix defined in (4.6). Relation (4.12) and [23, Theorem 5.11 on page 86] prove that method (4.10) (i.e., HBVM(k,s)) satisfies $C(s)$ and $D(s-1)$ and, hence, its order is $2s$.

Remark 10 (Invariance of the order). *From the previous result we deduce the invariance of the superconvergence property of HBVM(k,s) with respect to the distribution of the abscissae* τ_i, $i = 1, \ldots, k$, *the only assumption to get the order* $2s$ *being that the underlying quadrature formula has degree of precision* $2s-1$. *Such exceptional circumstance is likely to have interesting applications beyond the purposes here presented.*